Asymmetric Retro-Claisen Reaction by Chiral Primary Amine Catalysis

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Supporting Information

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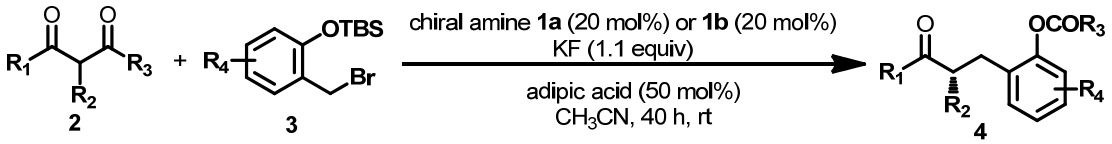
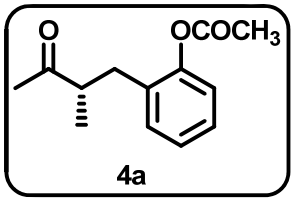
General information: Commercial reagents were purified prior to use following the guidelines of Perrin and Armarego.[1] All solvents were purified according to the method of Grubbs.[2] Nuclear magnetic resonance (NMR) spectra were recorded using Bruker AV-400 and AV-500 spectrometers. ^{1}H and ^{13}CNMR spectra were measured on a NMR instrument (400 and 500 MHz for ^{1}H NMR, 100 and 125 MHz for ^{13}C NMR). Tetramethylsilane (TMS) served as the internal standard for ^{1}H NMR, and $CDCl_3$ and CD_3OD served as the internal standard for ^{13}C NMR. The enantiomeric excesses were determined by HPLC analysis on Chiral Daicel Chiralpak AD-H, OD-H, AS-H, OJ-H columns. Optical rotation were measured on a commercial polarimeter and reported as follows: $[\alpha]_D^{22}$ (c = g/100 mL, solvent). HRMS was recorded on a commercial instrument (ESI and APCI Source).

Materials: The corresponding ortho-quinone methide precursors **3** were prepared following known procedures [3, 4]. **2b** and **2c** was prepared according to literature precedent.[5] **2a**, **2d-i** and **2m** were prepared by alkylation of the corresponding α-unsubstituted β-diketons with alkyl iodide or alkyl bromine.[6] **2j** was prepared according to literature procedure.[7] **2k** was prepared according to literature procedure.[8] **2l** was prepared according to literature procedure.[9] Cyclic β-diketons **2n-p** were prepared according to literature precedent.[10]

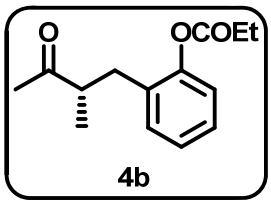
General Procedure of the catalytic reactions



General procedure: To a mixture of 1,3-diketons **2** (0.1 mmol), chiral amine **1** (20 mol%), adipic acid (50 mol%) and KF (0.11 mmol) in a standard glass tube were added the corresponding bromide **3** (0.11 mmol), followed by 0.7 mL dry MeCN via syringe. The resultant mixture was stirred at room temperature until completion as indicated by TLC (<40 h). Solvent was removed and purification by silica gel column to give the desired product.

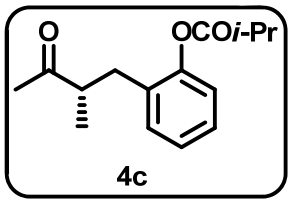


4a: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 86% yield, 95% *ee*. $[\alpha]_D^{22}$ = +22.4 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 2% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 14.26 min (major), 19.48 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.13 (m, 3H), 7.04 (d, J = 8.0 Hz, 1H), 2.94 (dd, J = 13.7, 6.7 Hz, 1H), 2.86 – 2.73 (m, 1H), 2.48 (dd, J = 13.7, 7.6 Hz, 1H), 2.33 (s, 3H), 2.09 (s, 3H), 1.09 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.9, 169.5, 149.2, 131.7, 131.1, 127.7, 126.2, 122.7, 47.5, 33.3, 29.0, 21.1, 16.6. IR (thin film, cm^{-1}) 2967, 2934, 1766, 1713, 1489, 1454, 1370, 1208, 1173, 1115, 1012, 916, 802, 749. HRMS (ESI) calcd for $C_{13}H_{16}O_3Na^+$: 243.0992, found 243.0993.



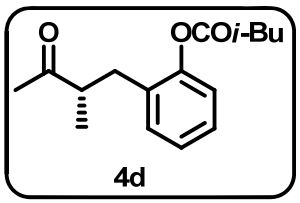
4b: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 74%

yield, 95% *ee*. $[\alpha]_D^{22}$ = +25.6 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 7.58 min (major), 9.16 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.12 (m, 3H), 7.05 – 7.01 (m, 1H), 2.92 (dd, J = 13.6, 6.7 Hz, 1H), 2.85 – 2.74 (m, 1H), 2.62 (q, J = 7.6 Hz, 2H), 2.47 (dd, J = 13.6, 7.6 Hz, 1H), 2.08 (s, 3H), 1.29 (t, J = 7.6 Hz, 3H), 1.08 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.9, 173.0, 149.3, 131.7, 131.1, 127.7, 126.1, 122.7, 47.5, 33.4, 29.0, 27.9, 16.6, 9.3. IR (thin film, cm^{-1}) 2974, 2935, 1760, 1713, 1490, 1453, 1358, 1263, 1218, 1172, 1143, 1115, 803, 752. HRMS (ESI) calcd for $C_{14}H_{18}O_3Na^+$: 257.1148, found 257.1147.



4c

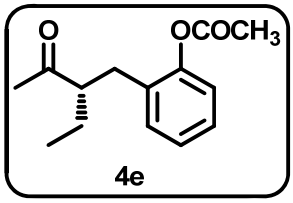
4c: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (25% Et_2O/petroleum ether). 55% yield, 96% *ee*. $[\alpha]_D^{22}$ = 21.2 (c = +1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 8.94 min (major), 9.89 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.12 (m, 3H), 7.00 (d, J = 7.9 Hz, 1H), 2.93 – 2.77 (m, 3H), 2.49 (dd, J = 13.5, 7.5 Hz, 1H), 2.07 (s, 3H), 1.34 (d, J = 7.0 Hz, 6H), 1.08 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.0, 175.6, 149.3, 131.8, 131.2, 127.7, 126.0, 122.6, 47.4, 34.4, 33.3, 29.1, 19.2, 16.6. IR (thin film, cm^{-1}) 2976, 2937, 1755, 1715, 1489, 1456, 1363, 1218, 1172, 1116, 1096, 1047, 802, 752. HRMS (ESI) calcd for $C_{15}H_{20}O_3Na^+$: 271.1305, found 271.1305.



4d

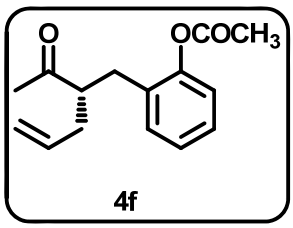
4d: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 70% yield, 95% *ee*. $[\alpha]_D^{22}$ = +20.2 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak

AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 5.57 min (major), 6.13 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.13 (m, 3H), 7.02 (d, J = 7.8 Hz, 1H), 2.92 (dd, J = 13.6, 6.8 Hz, 1H), 2.86 – 2.75 (m, 1H), 2.52 – 2.46 (m, 3H), 2.26 (dd, J = 13.6, 6.8 Hz, 1H), 2.08 (s, 3H), 1.08 (d, J = 6.6 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.9, 171.6, 149.3, 131.7, 131.2, 127.7, 126.1, 122.7, 47.4, 43.4, 33.4, 29.0, 25.9, 22.6, 16.6. IR (thin film, cm^{-1}) 2963, 2933, 2876, 1758, 1715, 1490, 1454, 1362, 1292, 1218, 1172, 1152, 1114, 1101, 802, 750. HRMS (ESI) calcd for $C_{16}H_{22}O_3Na^+$: 285.1461, found 285.1463.



4e

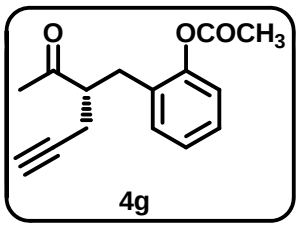
4e: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (15% Et_2O/petroleum ether). 79% yield, 97% *ee*. $[\alpha]_D^{22}$ = +29.6 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 7.56 min (major), 8.54 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.12 (m, 3H), 7.03 (dd, J = 8.0, 0.8 Hz, 1H), 2.81 (dd, J = 13.2, 8.1 Hz, 1H), 2.75 – 2.69 (m, 1H), 2.60 (dd, J = 13.2, 5.7 Hz, 1H), 2.33 (s, 3H), 2.01 (s, 3H), 1.70 – 1.58 (m, 1H), 1.56 – 1.44 (m, 1H), 0.90 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.1, 169.6, 149.1, 131.9, 131.1, 127.7, 126.3, 122.7, 54.7, 31.8, 30.4, 24.9, 21.1, 11.8. IR (thin film, cm^{-1}) 2964, 2934, 1766, 1712, 1489, 1454, 1369, 1210, 1172, 1117, 1103, 1012, 916, 800, 752. HRMS (ESI) calcd for $C_{14}H_{18}O_3Na^+$: 257.1148, found 257.1148.



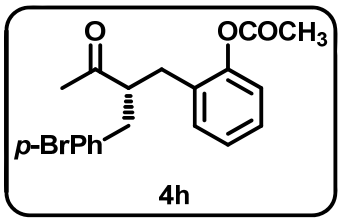
4f

4f: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 84% yield, 96% *ee*. $[\alpha]_D^{22}$ = +12.0 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak

AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 7.75 min (major), 8.47 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.11 (m, 3H), 7.03 (d, J = 7.9 Hz, 1H), 5.78 – 5.67 (m, 1H), 5.13 – 5.02 (m, 2H), 2.90 – 2.77 (m, 2H), 2.68 – 2.60 (m, 1H), 2.41 – 2.30 (m, 4H), 2.23 – 2.12 (m, 1H), 1.99 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.3, 169.5, 149.1, 135.2, 131.6, 131.2, 127.8, 126.3, 122.7, 117.6, 52.8, 36.1, 31.8, 30.7, 21.1. IR (thin film, cm^{-1}) 2962, 2926, 1766, 1713, 1489, 1369, 1209, 1173, 1098, 1012, 915, 800, 750. HRMS (ESI) calcd for $C_{15}H_{18}O_3Na^+$: 269.1148, found 269.1150.

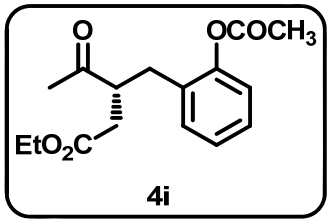


4g: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (15% Et_2O/petroleum ether). 80% yield, 95% *ee*. $[\alpha]_D^{22}$ = -9.1 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 12.75 min (major), 14.67 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 1H), 7.23 – 7.14 (m, 2H), 7.05 (dd, J = 8.0, 0.8 Hz, 1H), 3.00 – 2.90 (m, 1H), 2.83 (dd, J = 7.3, 1.8 Hz, 2H), 2.38 (td, J = 6.7, 2.6 Hz, 2H), 2.34 (s, 3H), 2.06 (s, 3H), 2.03 (t, J = 2.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 169.6, 149.2, 131.2, 130.9, 128.1, 126.4, 122.9, 81.5, 70.5, 51.6, 31.6, 30.7, 21.1, 20.6. IR (thin film, cm^{-1}) 3286, 2962, 2929, 1761, 1714, 1490, 1452, 1428, 1369, 1208, 1174, 1101, 1012, 914, 797, 751, 661. HRMS (ESI) calcd for $C_{15}H_{16}O_3Na^+$: 267.0992, found 2467.0993.



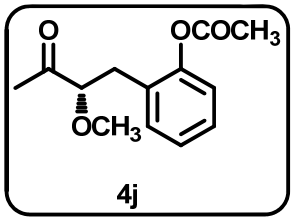
4h: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (25% Et_2O/petroleum ether). 40%

yield, 97% *ee*. $[\alpha]_D^{22}$ = -5.6 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 20% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 16.97 min (major), 13.05 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.3 Hz, 2H), 7.25 – 7.21 (m, 1H), 7.18 – 7.13 (m, 2H), 7.02 (d, J = 8.3 Hz, 3H), 3.08 – 3.01 (m, 1H), 2.89 – 2.79 (m, 2H), 2.64 – 2.58 (m, 2H), 2.19 (s, 3H), 1.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.6, 169.6, 149.1, 138.4, 131.8, 131.2, 131.2, 130.9, 128.0, 126.4, 122.8, 120.5, 54.8, 37.6, 32.5, 31.7, 20.9. IR (thin film, cm^{-1}) 2962, 2926, 1764, 1713, 1488, 1449, 1368, 1261, 1208, 1172, 1096, 1071, 1011, 915, 798, 753. HRMS (ESI) calcd for $C_{19}H_{19}O_3BrNa^+$: 397.0410, found 397.0409.



4i

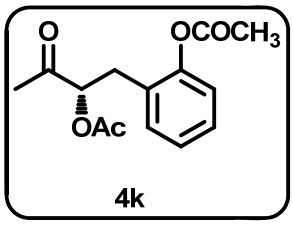
4i: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (30% Et_2O/petroleum ether). 68% yield, 92% *ee*. $[\alpha]_D^{22}$ = +69.7 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak OD-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 16.68 min (major), 14.04 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 1H), 7.22 – 7.15 (m, 2H), 7.07 (d, J = 8.0 Hz, 1H), 4.07 (q, J = 7.1 Hz, 2H), 3.31 – 3.17 (m, 1H), 2.83 (dd, J = 13.7, 7.2 Hz, 1H), 2.73 (dd, J = 17.1, 9.5 Hz, 1H), 2.55 (dd, J = 13.7, 8.0 Hz, 1H), 2.36 (s, 3H), 2.31 (dd, J = 17.7, 13.0 Hz, 1H), 2.11 (s, 3H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.6, 172.2, 169.5, 149.2, 131.1, 130.4, 128.2, 126.4, 122.9, 60.8, 48.2, 35.6, 32.4, 30.5, 21.1, 14.2. IR (thin film, cm^{-1}) 2968, 2929, 1766, 1732, 1716, 1491, 1370, 1207, 1173, 1100, 1014, 916, 800, 753. HRMS (ESI) calcd for $C_{16}H_{20}O_5Na^+$: 315.1203, found 315.1203.



4j

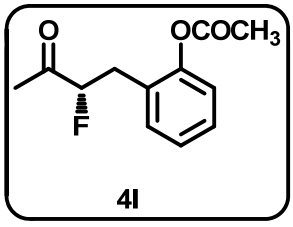
4j: Prepared according to the general procedure and obtained as colorless oil

after purification by flash chromatography (20% Et_2O/petroleum ether). 60% yield, 96% *ee*. $[\alpha]_D^{22}$ = -36.0 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H*2, 3% *iso*-propanol/hexane, flow rate = 0.6 mL/min, λ = 207 nm, retention time: 33.80 min (major), 35.04 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (td, J = 7.4, 1.6 Hz, 2H), 7.18 (td, J = 7.5, 1.1 Hz, 1H), 7.09 – 7.04 (m, 1H), 3.74 (dd, J = 8.3, 4.5 Hz, 1H), 3.27 (s, 3H), 2.89 (dd, J = 14.1, 4.4 Hz, 1H), 2.80 (dd, J = 14.1, 8.3 Hz, 1H), 2.34 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.9, 169.6, 149.3, 131.7, 129.7, 128.1, 126.2, 122.7, 87.4, 58.8, 33.1, 25.8, 21.1. IR (thin film, cm^{-1}) 2970, 2932, 1766, 1715, 1490, 1455, 1369, 1260, 1208, 1174, 1104, 1041, 1012, 916, 801, 752. HRMS (ESI) calcd for $C_{13}H_{16}O_4Na^+$: 259.0941, found 259.0941.



4k

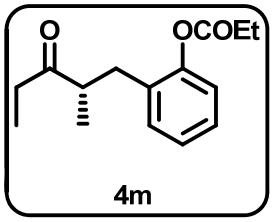
4k: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (50% Et_2O/petroleum ether). 98% yield, 94% *ee*. $[\alpha]_D^{22}$ = +4.0 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 20% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 206 nm, retention time: 12.79 min (major), 14.71 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.25 (m, 2H), 7.22 – 7.15 (m, 1H), 7.08 (d, J = 8.0 Hz, 1H), 5.18 (dd, J = 8.3, 5.1 Hz, 1H), 3.05 (dd, J = 14.3, 5.1 Hz, 1H), 2.94 (dd, J = 14.3, 8.3 Hz, 1H), 2.35 (s, 3H), 2.10 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 170.5, 169.4, 149.4, 131.4, 128.5, 128.1, 126.3, 122.8, 78.2, 31.3, 26.9, 21.1, 20.7. IR (thin film, cm^{-1}) 2968, 2929, 1766, 1744, 1731, 1490, 1455, 1372, 1239, 1206, 1172, 1105, 1074, 1045, 1012, 914, 799, 752. HRMS (ESI) calcd for $C_{14}H_{16}O_5Na^+$: 287.0890, found 287.0891.



4l

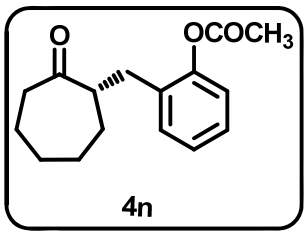
4l: Prepared according to the general procedure and obtained as colorless oil

after purification by flash chromatography (20% Et_2O/petroleum ether). 42% yield, 60% *ee*. $[\alpha]_D^{22}$ = -36.0 (c = 0.3, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 10.17 min (major), 9.27 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.31 (m, 2H), 7.24 – 7.16 (m, 1H), 7.09 (d, J = 8.1 Hz, 1H), 4.89 (ddd, J = 49.9, 8.0, 3.6 Hz, 1H), 3.17 (ddd, J = 29.9, 14.9, 3.6 Hz, 1H), 2.95 (ddd, J = 23.1, 14.9, 8.0 Hz, 1H), 2.34 (s, 3H), 2.19 (d, J = 4.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.3, 207.7, 169.5, 149.3, 131.7, 128.6, 127.8, 126.3, 122.9, 96.2, 94.4, 32.9, 32.7, 26.4, 21.1. IR (thin film, cm^{-1}) 2965, 2923, 1760, 1723, 1491, 1369, 1260, 1207, 1172, 1103, 1077, 1015, 915, 800, 750. HRMS (ESI) calcd for $C_{12}H_{13}O_3FNa^+$: 247.0741, found 247.0742.

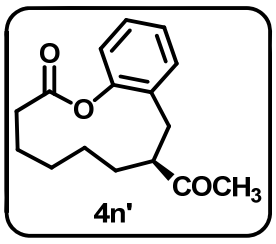


4m

4m: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 30% yield, 96% *ee*. $[\alpha]_D^{22}$ = +33.9 (c = 0.66, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 5.43 min (major), 6.34 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.11 (m, 3H), 7.02 (d, J = 8.0 Hz, 1H), 2.89 (dd, J = 13.3, 7.1 Hz, 1H), 2.81 (dd, J = 13.9, 7.0 Hz, 1H), 2.62 (q, J = 7.5 Hz, 2H), 2.54 – 2.36 (m, 2H), 2.29 – 2.20 (m, 1H), 1.30 (t, J = 7.6 Hz, 3H), 1.07 (d, J = 6.8 Hz, 3H), 0.97 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 214.7, 173.0, 149.3, 131.9, 131.2, 127.7, 126.1, 122.7, 46.5, 35.4, 33.8, 27.9, 17.0, 9.4, 7.7. IR (thin film, cm^{-1}) 2970, 2935, 1760, 1714, 1489, 1455, 1383, 1358, 1262, 1218, 1172, 1142, 1109, 1076, 983, 803, 753. HRMS (ESI) calcd for $C_{15}H_{20}O_3Na^+$: 271.1305, found 271.1305.

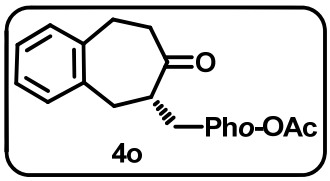


4n: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (15% Et_2O/petroleum ether). 45% yield, 95% *ee*. $[\alpha]_D^{22}$ = +48.0 (c = 0.6, $CHCl_3$). HPLC analysis: Daicel Chiralpak OD-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 206 nm, retention time: 9.11 min (major), 8.37 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.13 (m, 3H), 7.05 – 7.00 (m, 1H), 3.02 (dd, J = 14.0, 5.6 Hz, 1H), 2.79 – 2.77 (m, 1H), 2.53 – 2.43 (m, 3H), 2.33 (s, 3H), 1.90 – 1.71 (m, 4H), 1.68 – 1.61 (m, 1H), 1.41 – 1.28 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 215.3, 169.7, 149.4, 132.1, 131.3, 127.6, 126.1, 122.6, 52.4, 43.2, 32.3, 30.6, 29.5, 28.7, 24.4, 21.1. IR (thin film, cm^{-1}) 2928, 2854, 1764, 1699, 1489, 1453, 1369, 1261, 1209, 1172, 1129, 1092, 1040, 1012, 917, 802, 754. HRMS (ESI) calcd for $C_{16}H_{20}O_3Na^+$: 283.1305, found 283.1307.



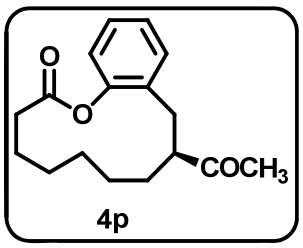
4n': Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 46% yield, 98% *ee*. $[\alpha]_D^{22}$ = +49.6 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 11.04 min (major), 10.18 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.18 (m, 2H), 7.18 – 7.07 (m, 2H), 2.96 (dd, J = 13.8, 7.7 Hz, 1H), 2.85 (dd, J = 13.8, 2.6 Hz, 1H), 2.80 –2.72 (m, 1H), 2.66 (dt, J = 14.2, 5.1 Hz, 1H), 2.60 – 2.50 (m, 1H), 2.14 – 2.00 (m, 4H), 1.88 – 1.74 (m, 2H), 1.70 – 1.44 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.8, 171.7, 148.7, 133.6, 131.5, 127.5, 126.1, 122.7, 52.6, 32.7, 29.6, 29.3, 28.3, 24.3, 22.8, 21.5. IR (thin film, cm^{-1}) 2942, 2873, 1751, 1710, 1487, 1451, 1351, 1217, 1171, 1157, 1128, 1104, 1074, 1019, 802, 750. HRMS (ESI) calcd for $C_{16}H_{20}O_3Na^+$:

283.1305, found 283.1306.



4o

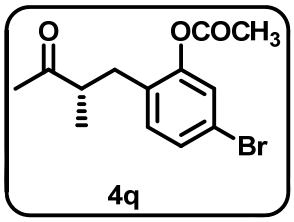
4o: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (30% Et_2O/petroleum ether). 85% yield, 96% *ee*. $[\alpha]_D^{22}$ = +21.8 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 20% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 207 nm, retention time: 9.47 min (major), 11.13 min (minor). ^{1}H NMR (500 MHz, CD_3OD) δ 7.29 – 7.13 (m, 6H), 7.07 – 7.01 (m, 2H), 2.99 – 2.81 (m, 5H), 2.77 – 2.64 (m, 2H), 2.59 – 2.46 (m, 2H), 2.23 (s, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 214.3, 171.1, 150.8, 141.8, 140.1, 132.9, 131.9, 130.9, 130.1, 128.6, 128.3, 128.1, 127.1, 123.7, 54.6, 44.5, 37.1, 31.9, 31.8, 20.8. IR (thin film, cm^{-1}) 2956, 2929, 1760, 1703, 1489, 1455, 1369, 1208, 1172, 1093, 1011, 919, 800, 751. HRMS (ESI) calcd for $C_{20}H_{20}O_3Na^+$: 331.1305, found 331.1304.



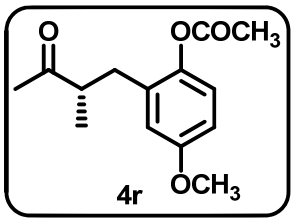
4p

4p: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 24% yield, 98% *ee*. $[\alpha]_D^{22}$ = +16.0 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OD-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 205 nm, retention time: 7.12 min (major), 7.10 min (minor). ^{1}H NMR (500 MHz, CD_3OD) δ 7.26 – 7.19 (m, 1H), 7.17 (dd, J = 7.6, 1.7 Hz, 1H), 7.11 (td, J = 7.5, 1.2 Hz, 1H), 7.02 (dd, J = 8.1, 1.0 Hz, 1H), 2.95 (dd, J = 13.3, 2.6 Hz, 1H), 2.87 – 2.74 (m, 2H), 2.68 (dd, J = 13.2, 10.1 Hz, 1H), 2.48 (ddd, J = 14.7, 10.4, 2.3 Hz, 1H), 2.15 – 2.03 (m, 1H), 1.97 (s, 3H), 1.94 – 1.82 (m, 1H), 1.76 – 1.67 (m, 2H), 1.60 – 1.42 (m, 6H). ^{13}C NMR (125 MHz, CD_3OD) δ 213.8, 174.9, 150.7, 134.1, 132.6, 128.6, 126.9, 124.0, 53.0, 36.0, 31.2,

30.1, 29.8, 29.2, 25.9, 24.3, 23.4. IR (thin film, cm^{-1}) 2934, 2870, 2859, 1750, 1712, 1489, 1448, 1351, 1260, 1215, 1171, 1128, 1104, 803, 752. HRMS (ESI) calcd for $C_{17}H_{22}O_3Na^+$: 297.1461, found 297.1461.

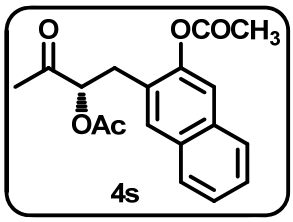


4q: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 50% yield, 94% *ee*. $[\alpha]_D^{22}$ = +15.8 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 204 nm, retention time: 12.20 min (major), 18.28 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (dd, J = 8.2, 1.9 Hz, 1H), 7.23 (d, J = 1.9 Hz, 1H), 7.08 (d, J = 8.2 Hz, 1H), 2.89 (dd, J = 13.8, 6.8 Hz, 1H), 2.83 – 2.71 (m, 1H), 2.43 (dd, J = 13.8, 7.3 Hz, 1H), 2.33 (s, 3H), 2.10 (s, 3H), 1.09 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.5, 169.1, 149.6, 132.2, 131.0, 129.4, 126.0, 120.2, 47.3, 32.8, 29.0, 21.0, 16.7. IR (thin film, cm^{-1}) 2970, 2934, 1770, 1713, 1482, 1369, 1263, 1199, 1174, 1123, 1075, 1012, 925, 800. HRMS (ESI) calcd for $C_{13}H_{15}O_3BrNa^+$: 321.0097, found 321.0099.

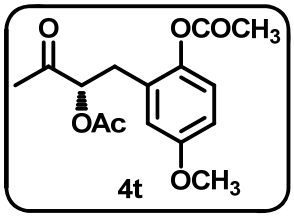


4r: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (25% Et_2O/petroleum ether). 79% yield, 96% *ee*. $[\alpha]_D^{22}$ = +15.7 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H*2, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 203 nm, retention time: 36.89 min (major), 39.20 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, J = 8.8 Hz, 1H), 6.80 – 6.69 (m, 2H), 3.78 (s, 3H), 2.89 (dd, J = 13.6, 6.6 Hz, 1H), 2.85 – 2.74 (m, 1H), 2.43 (dd, J = 13.6, 7.5 Hz, 1H), 2.31 (s, 3H), 2.10 (s, 3H), 1.09 (d, J = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.8, 170.0, 157.3, 142.7,

132.8, 123.3, 116.2, 112.6, 55.6, 47.4, 33.5, 29.0, 21.0, 16.6. IR (thin film, cm^{-1}) 2965, 2934, 1759, 1713, 1498, 1369, 1213,1195, 1180, 1033, 825, 803. HRMS (ESI) calcd for $C_{14}H_{18}O_4Na^+$: 273.1097, found 273.1099.

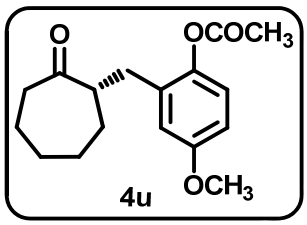


4s: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (50% Et_2O/petroleum ether). 99% yield, 92% *ee*. $[\alpha]_D^{22}$ = +33.8 (c = 1.55, $CHCl_3$). HPLC analysis: Daicel Chiralpak AD-H, 2% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 225 nm, retention time: 32.15 min (major), 34.79 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (dd, J = 9.2, 6.0 Hz, 2H), 7.72 (s, 1H), 7.57 (s, 1H), 7.50 – 7.41 (m, 2H), 5.29 (dd, J = 8.4, 5.0 Hz, 1H), 3.22 (dd, J = 14.4, 5.0 Hz, 1H), 3.08 (dd, J = 14.4, 8.4 Hz, 1H), 2.41 (s, 3H), 2.11 (s, 3H), 2.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 205.4, 170.5, 169.5, 147.3, 133.1, 131.6, 130.6, 127.5, 127.5, 127.4, 126.6, 126.2, 120.0, 78.2, 31.9, 27.0, 21.2, 20.7. IR (thin film, cm^{-1}) 2959, 2932, 1760, 1744, 1731, 1507, 1434, 1371, 1233, 1200, 1146, 1090, 1045, 1011, 923, 904, 750. HRMS (ESI) calcd for $C_{18}H_{18}O_5Na^+$: 337.1046, found 337.1045.

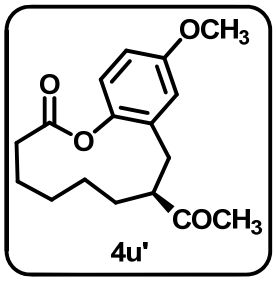


4t: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (40% Et_2O/petroleum ether). 72% yield, 92% *ee*. $[\alpha]_D^{22}$ = +4.4 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak AD-H, 10% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 204 nm, retention time: 11.03 min (major), 10.35 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.99 (d, J = 8.8 Hz, 1H), 6.81 (dd, J = 8.8, 3.0 Hz, 1H), 6.78 (d, J = 3.0 Hz, 1H), 5.17 (dd, J = 8.4, 5.0 Hz, 1H), 3.78 (s, 3H), 3.00 (dd, J = 14.3, 5.0 Hz, 1H), 2.89 (dd, J = 14.3, 8.4

Hz, 1H), 2.33 (s, 3H), 2.11 (s, 3H), 2.09 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 205.2, 170.5, 169.8, 157.4, 142.9, 129.0, 123.5, 116.4, 113.5, 78.2, 55.7, 31.5, 26.9, 21.0, 20.7. IR (thin film, cm^{-1}) 2968, 2943, 1763, 1744, 1731, 1500, 1429, 1372, 1238, 1196, 1179, 1046, 1036, 1011, 897, 817. HRMS (ESI) calcd for $C_{15}H_{18}O_6Na^+$: 317.0996, found 317.0995.

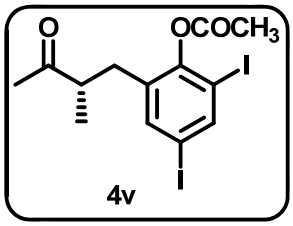


4u: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 51% yield, 95% *ee.* $[\alpha]_D^{22}$ = +35.3 (c = 0.56, $CHCl_3$). HPLC analysis: Daicel Chiralpak AD-H*2, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 203 nm, retention time: 37.28 min (major), 38.91 min (minor). ^{1}H NMR (400 MHz, CD_3OD) δ 6.95 – 6.89 (m, 1H), 6.80 – 6.74 (m, 2H), 3.77 (s, 3H), 2.95 – 2.77 (m, 2H), 2.52 – 2.38 (m, 3H), 2.28 (s, 3H), 1.91 – 1.74 (m, 4H), 1.69 – 1.58 (m, 1H), 1.38 – 1.35 (m, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 217.7, 171.7, 158.8, 144.2, 134.3, 124.3, 117.1, 113.4, 56.0, 53.5, 43.9, 33.4, 31.6, 30.4, 29.6, 25.4, 20.8. IR (thin film, cm^{-1}) 2965, 2927, 2854, 1759, 1698, 1608, 1591, 1496, 1455, 1369, 1260, 1217, 1195, 1179, 1099, 1039, 1016, 800. HRMS (ESI) calcd for $C_{17}H_{22}O_4Na^+$: 313.1410, found 313.1411.



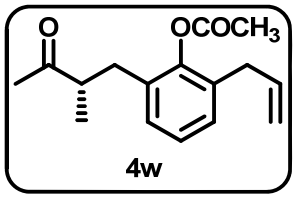
4u': Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (25% Et_2O/petroleum ether). 42% yield, 98% *ee.* $[\alpha]_D^{22}$ = +12.3 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 5% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 204 nm, retention time: 24.84 min (major), 16.72 min (minor). ^{1}H NMR (400 MHz, CD_3OD) δ 7.03 (d, J = 8.8 Hz, 1H), 6.77 (dd, J = 8.8, 3.0 Hz, 1H), 6.71 (d, J = 3.0 Hz, 1H), 3.74 (s,

3H), 2.85 – 2.81 (m, 2H), 2.77 – 2.58 (m, 3H), 2.07 (s, 3H), 2.05 – 1.96 (m, 1H), 1.86 – 1.73 (m, 2H), 1.70 – 1.44 (m, 5H). ^{13}C NMR (100 MHz, CD_3OD) δ 213.0, 173.7, 158.6, 143.5, 135.6, 124.5, 117.3, 113.2, 56.0, 53.7, 33.3, 30.3, 29.6, 29.1, 25.4, 23.6, 22.4. IR (thin film, cm^{-1}) 2934, 2970, 1749, 1710, 1608, 1591, 1493, 1466, 1358, 1178, 1158, 1130, 1038, 803. HRMS (ESI) calcd for $C_{17}H_{22}O_4Na^+$: 313.1410, found 313.1412.



4v

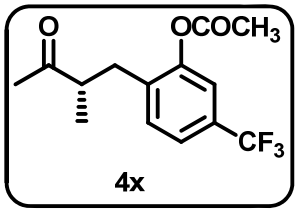
4v: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 44% yield, 95% *ee*. $[\alpha]_D^{22}$ = +8.8 (c = 1.0, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 10% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 225 nm, retention time: 17.97 min (major), 13.35 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 2.0 Hz, 1H), 7.50 (d, *J* = 2.0 Hz, 1H), 2.91 (dd, *J* = 14.0, 6.6 Hz, 1H), 2.81 – 2.71 (m, 1H), 2.38 (s, 3H), 2.12 (s, 3H), 1.10 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 210.9, 168.2, 150.1, 145.4, 140.0, 136.2, 93.4, 91.3, 47.0, 33.6, 28.9, 21.3, 16.9. IR (thin film, cm^{-1}) 2962, 2923, 1767, 1712, 1544, 1435, 1367, 1190, 1135, 1010, 900, 864, 797. HRMS (APCI) calcd for $C_{13}H_{14}O_3I_2Na^+$: 494.8925, found 494.8926.



4w

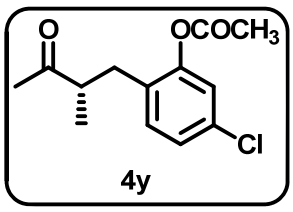
4w: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 73% yield, 94% *ee*. $[\alpha]_D^{22}$ = +19.4 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 203 nm, retention time: 7.38 min (major), 9.00 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 – 7.10 (m, 2H), 7.09 – 7.05 (m, 1H), 5.95 – 5.81 (m, 1H), 5.11 – 5.03 (m, 2H), 3.25 (d, *J* = 6.7 Hz, 2H), 2.90 (dd, *J* = 13.8, 6.7 Hz, 1H), 2.86 – 2.76 (m, 1H), 2.42 (dd, *J* = 13.8,

7.5 Hz, 1H), 2.33 (s, 3H), 2.09 (s, 3H), 1.09 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 212.0, 169.3, 147.7, 135.9, 132.7, 132.3, 129.1, 128.7, 126.3, 116.5, 47.3, 35.0, 33.7, 29.0, 20.8, 16.7. IR (thin film, cm^{-1}) 2967, 2929, 1760, 1713, 1457, 1370, 1209, 1161, 1011, 915, 797. HRMS (APCI) calcd for $C_{16}H_{20}O_3Na^+$: 283.1305, found 283.1307.



4x

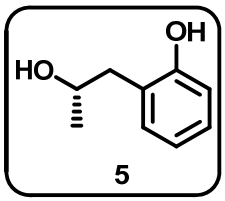
4x: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 50% yield, 97% *ee*. $[\alpha]_D^{22}$ = +3.6 (c = 1.01, $CHCl_3$). HPLC analysis: Daicel Chiralpak AS-H, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 204 nm, retention time: 8.51 min (major), 11.83 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, J = 8.0 Hz, 1H), 7.33 (d, J = 8.3 Hz, 2H), 3.00 (dd, J = 13.9, 6.9 Hz, 1H), 2.81 (dd, J = 14.2, 7.1 Hz, 1H), 2.52 (dd, J = 13.9, 7.3 Hz, 1H), 2.36 (s, 3H), 2.11 (s, 3H), 1.12 (d, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) ^{13}C NMR (125 MHz, $CDCl_3$) δ 211.17, 169.09, 149.18, 136.23, 131.69, 130.55, 130.29, 130.03, 129.76, 126.90, 124.73, 123.00, 122.97, 122.94, 122.91, 122.57, 120.41, 120.13, 120.10, 120.07, 47.23, 32.98, 28.93, 21.01, 16.80. IR (thin film, cm^{-1}) 2970, 2931, 1171, 1715, 1422, 1371, 1330, 1202, 1180, 1124, 1071, 1013, 939. HRMS (APCI) calcd for $C_{14}H_{15}O_3F_3Na^+$: 311.0866, found 311.0865.



4y

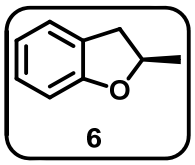
4y: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (20% Et_2O/petroleum ether). 51% yield, 98% *ee*. $[\alpha]_D^{22}$ = +2.4 (c = 0.98, $CHCl_3$). HPLC analysis: Daicel Chiralpak OJ-H, 3% *iso*-propanol/hexane, flow rate = 1.0 mL/min, λ = 203 nm, retention time: 15.79 min (major), 16.87 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.11 (m, 2H), 7.08 (s, 1H), 2.91 (dd, J = 13.8, 6.8 Hz, 1H), 2.77 (dd, J = 14.1, 7.0 Hz,

1H), 2.46 (d, J = 7.3 Hz, 1H), 2.33 (s, 3H), 2.09 (s, 3H), 1.09 (d, J = 7.0 Hz, 3H). IR (thin film, cm^{-1}) 2970, 2929, 1768, 1714, 1487, 1369, 1261, 1200, 1175, 1081, 1013, 932, 799. ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.5, 169.1, 149.5, 132.7 131.9, 130.5, 126.4, 123.2, 47.4, 32.8, 29.0, 21.0, 16.7. HRMS (APCI) calcd for $C_{13}H_{15}O_3ClNa^+$: 277.0602, found 277.0604.



5

5: Prepared according to the literature report obtained as colorless oil after purification by flash chromatography (50% Et_2O/petroleum ether).[11] 92% yield. $[\alpha]_D^{22}$ = +5.2 (c = 1.3, EtOH). The (***S***)-absolute configuration for the product **4a** was determined by comparison of the optical rotation of **5** with the literature known product.[12] ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.19 – 7.10 (m, 1H), 7.02 (dd, J = 7.4, 1.2 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.84 (td, J = 7.4, 1.0 Hz, 1H), 4.28 – 4.20 (m, J = 8.9, 4.5 Hz, 1H), 2.86 (dd, J = 14.6, 2.5 Hz, 1H), 2.77 (dd, J = 14.6, 7.4 Hz, 1H), 2.46 (s, 1H), 1.27 (d, J = 6.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 131.8, 128.5, 125.3, 120.5, 117.3, 70.6, 40.7, 23.4.

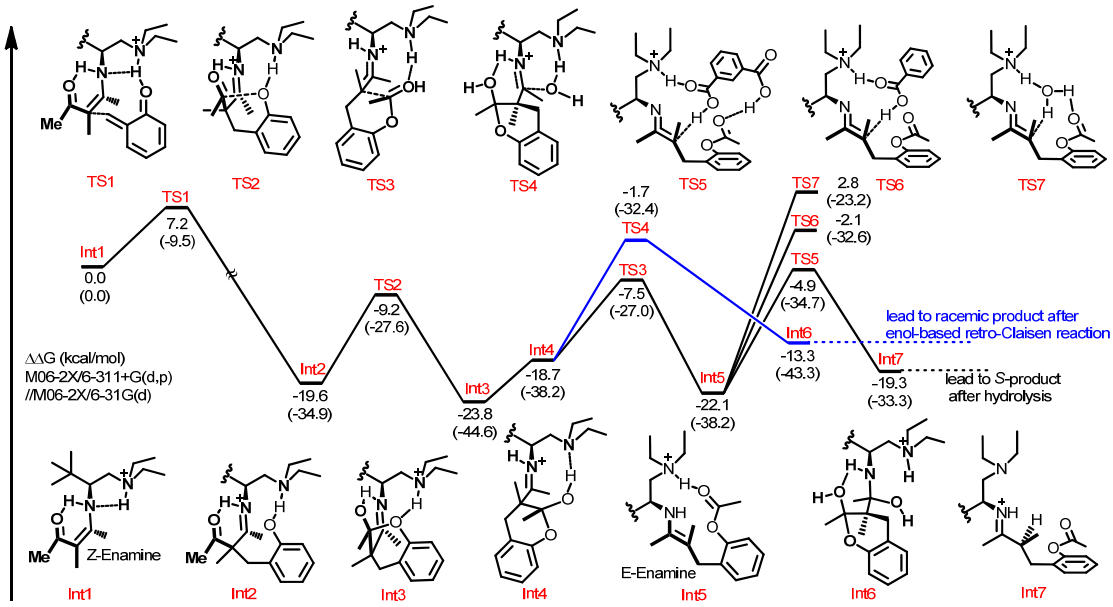


6

6: Prepared according to the literature report obtained as colorless oil after purification by flash chromatography (5% Et_2O/petroleum ether).[13] 60% yield, 94% *ee*. HPLC analysis: Daicel Chiralpak OJ-H, 1% *iso*-propanol/hexane, flow rate = 0.5 mL/min, λ = 202 nm, retention time: 12.32 min (major), 11.32 min (minor). ^1H NMR (500 MHz, $CDCl_3$) δ 7.15 (d, J = 7.3 Hz, 1H), 7.10 (t, J = 7.7 Hz, 1H), 6.82 (td, J = 7.4, 0.8 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 5.01 – 4.84 (m, 1H), 3.31 (dd, J = 15.4, 8.8 Hz, 1H), 2.82 (dd, J = 15.4, 7.7 Hz, 1H), 1.47 (d, J = 6.3 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 128.1, 127.2, 125.1, 120.3, 109.5, 79.6, 37.3, 21.9.

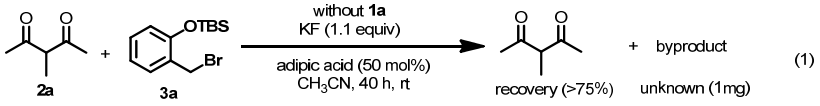
Mechanistic studies

Scheme 1S. The Reaction Energy Profile by DFT

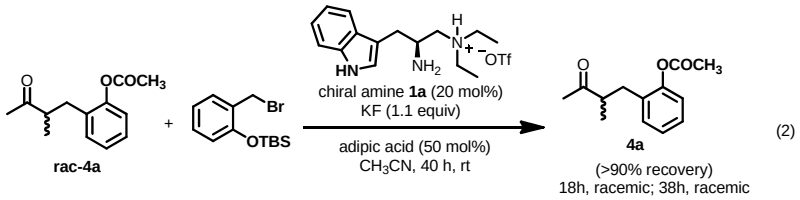


Control experiments

a) **Reaction in the absence of aminocatalyst 1a**: To a mixture of 1,3-diketons **2a** (0.1 mmol), adipic acid (50 mol%) and KF (0.11 mmol) in a standard glass tube were added the corresponding bromide **3a** (0.11 mmol), followed by 0.7 mL dry MeCN via syringe. The resultant mixture was stirred at room temperature for 40h. Solvent was removed and NMR of the crude mixture indicated a trace byproduct. **2a (8.5 mg)** was recovered by column chromatograph.



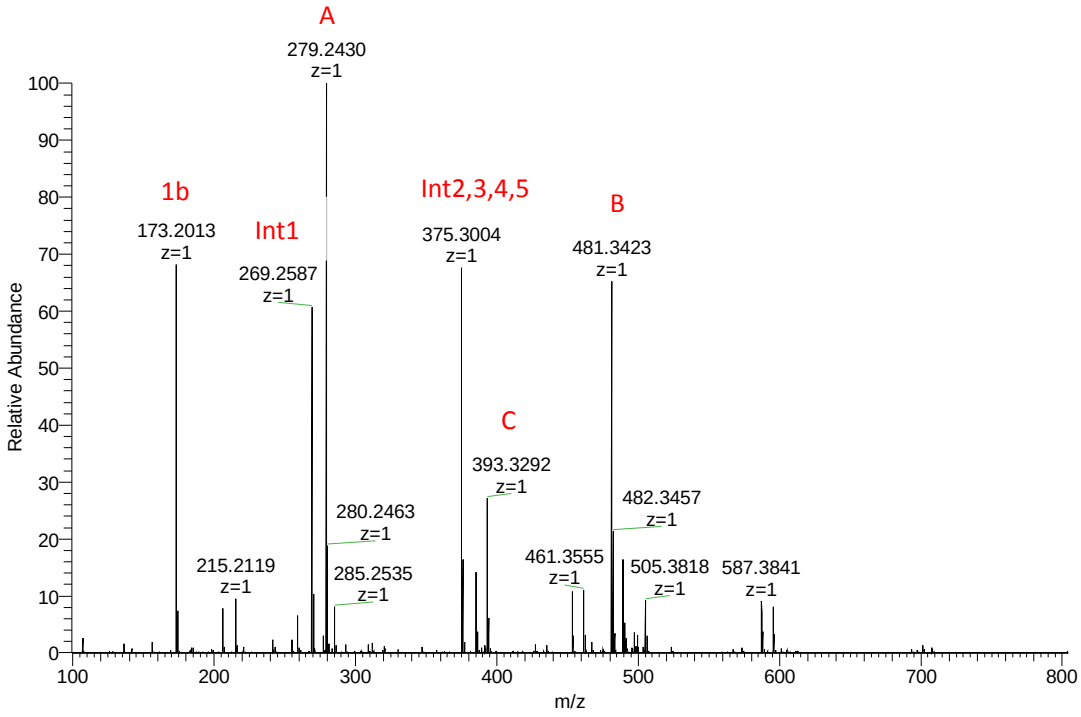
b) Treatment of product 4a under catalytic conditions. To a mixture of the product rac-**4a** or (*S*)-**4a** (0.1 mmol), chiral amine **1a** (20 mol%), adipic acid (50 mol%) and KF (0.11 mmol) in a standard glass tube were added the corresponding bromide **3a** (0.11 mmol), followed by 0.7 mL dry MeCN via syringe. The resultant mixture was stirred at room temperature for 18-38 h. Solvent was removed and purification by silica gel column to recover **4a** (>90% yield).



(2)

In-*situ* ESI- HRMS analysis of reaction mixture

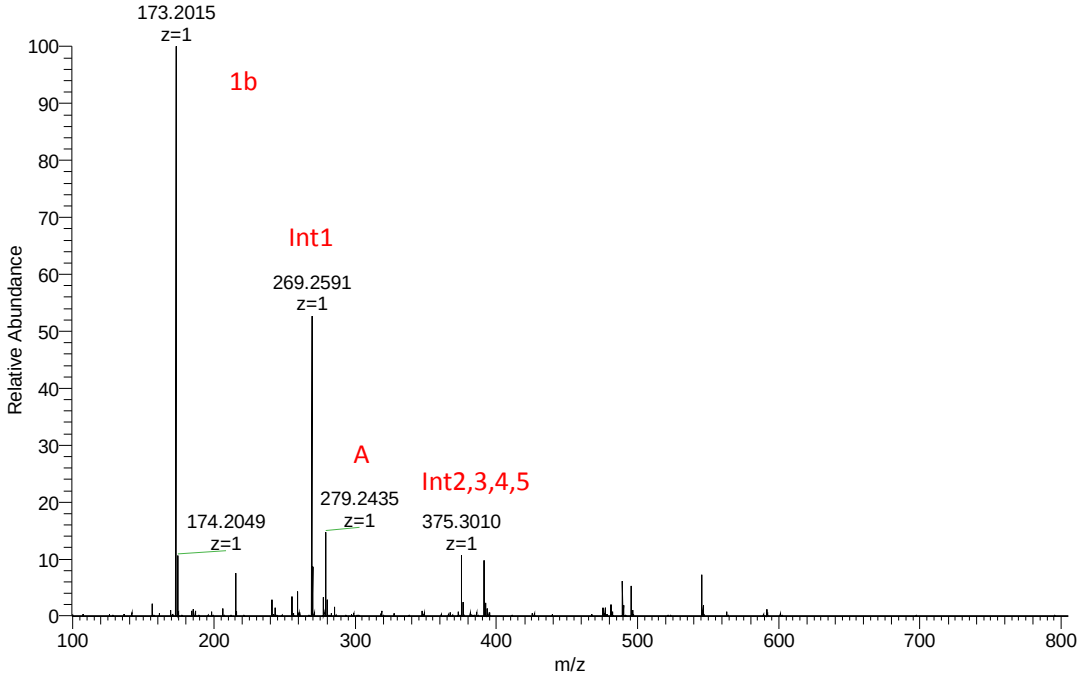
a) **Without *m*-phthalic acid**: To a mixture of 1,3-diketons **2a** (0.1 mmol), chiral amine **1b** (20 mol%), and KF (0.11 mmol) in a standard glass tube were added the corresponding bromide **3a** (0.11 mmol), followed by 0.7 mL dry MeCN via syringe. After 2h, 50 uL of the reaction solution was taken, diluted with 1.0 mL of CH_3CN, and injected to the mass spectrometer. Positive mode was used. ESI-HRMS conditions: flow rate: 0.2 mL/min, solvent: CH_3CN.



Peak	Mass	Expected Formula	Calculated Mass	Difference
1b	173.2013	$C_{10}H_{25}N_2^+$	173.2012	0.0001
Int1 (Scheme 1)	269.2587	$C_{16}H_{33}N_2O^+$	269.2587	0.0000

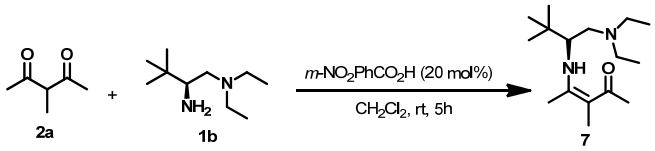
A	279.2430	$C_{17}H_{31}N_2O^+$	279.2431	0.0001
Int2,3,4,5 (Scheme 1)	375.3004	$C_{23}H_{39}N_2O_2^+$	375.3006	0.0002
C	393.3292	$C_{23}H_{45}N_2OSi^+$	393.3296	0.0004
B	481.3423	$C_{30}H_{45}N_2O_3^+$	481.3425	0.0002

b) **With *m*-phthalic acid**: To a mixture of 1,3-diketons **2a** (0.1 mmol), chiral amine **1b** (20 mol%), *m*-phthalic acid (50 mol%) and KF (0.11 mmol) in a standard glass tube were added the corresponding bromide **3a** (0.11 mmol), followed by 0.7 mL dry MeCN via syringe. After 2h, 50 uL of the reaction solution was taken, diluted with 1.0 mL of CH_3CN, and injected to the mass spectrometer. Positive mode was used. ESI-HRMS conditions: flow rate: 0.2 mL/min, solvent: CH_3CN.



In-situ analysis of the reaction mixture by ESI-HRMS in the absence of m-phthalic acid revealed several by-products (**A** and **C**) arisen from the poison of aminocatalyst. A notable peak @481.3423, could also be identified to be a double benzylated adduct **B**, arisen from further benzylation with the enamine intermediate **int5**. This observation suggests that enamine protonation would be disfavored in the absence of weak acid, to note that no formation of **B** was detected in the presence of phthalic acid. Thus, one role of weak acid is to provide a favorable acid-base buffer system to suppress the side pathways.

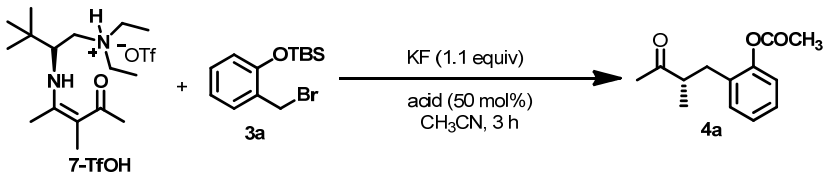
Stoichiometric Reactions



Synthesis of enamine intermediate 7: To β-diketone **2a** (1 mmol), chiral primary amine **1b** (1 mmol) in CH_2Cl_2 (0.5 mL), was added *m*-nitrobenzoic acid (0.2 equiv). The reaction was stirred at room temperature for 5h and directly purified by basic alumina column with 20% Et_2O/petroleum ether to give the enamine **7** as colorless oil. **7**: ^1H NMR (500 MHz, $CDCl_3$) δ 12.57 (d, J = 9.4 Hz, 1H), 3.26 (t, J = 9.5 Hz, 1H), 2.63 (d, J = 13.4 Hz, 1H), 2.53-2.46 (m, 2H), 2.41-2.32 (m, 3H), 2.13 (s, 3H), 2.00 (s, 3H), 1.85 (s, 3H), 0.96 (s, 9H), 0.93 (t, J = 7.1 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.24, 163.79, 97.08, 62.57, 56.25, 48.17, 34.47, 28.52, 26.88, 15.89, 15.18, 12.35.

Stoichiometric Reactions: To a solution of enamine **7** in dry CH_2Cl_2 was added TfOH (1.0 equiv) dropwise with vigorous stirring under N_2 at 0 ^oC. After 10 min, the solvent was removed under reduced pressure to give **7-TfOH** as a white solid.

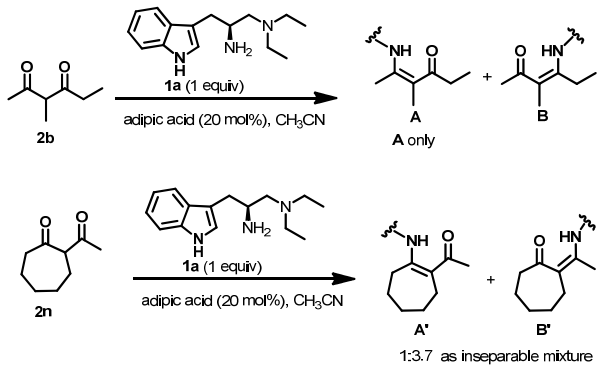
To a mixture of freshly prepared **7-TfOH** (20 mol%), acid (50 mol% or none) and KF (0.11 mmol), followed by 0.3 mL CH_3CN in a standard glass tube, were added the corresponding bromide **3a** (0.11 mmol) at 0 ^oC. The reaction was stirred for 3h and then quenched by aqueous acetonitrile solution (5 uL H_2O dissolved in 0.3 mL acetonitrile) via syringe pump for 5h or by aqueous NH_4Cl solution (10 uL) directly. The solvent was removed and purified by silica gel column with 20% Et_2O/petroleum ether to give the desired product.

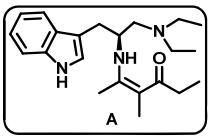


entry	Variations of conditions	acid	yield(%)	*ee*(%)
1	syringe pump addition of water	*m*-phthalic acid	76	76
2	sat.NH_4Cl (one portion addition)	*m*-phthalic acid	82	72
3	syringe pump addition of water	$PhCO_2H$	71	26
4	sat.NH_4Cl (one portion addition)	$PhCO_2H$	76	23
5	syringe pump addition of water	no	20	9
6	Syringe pump addition of 7/TfOH (0.3 mL CH_3CN) for 3-20 hrs, quenched by H_2O (one portion)	*m*-phthalic acid	70-76	80-84

Synthesis of enamine with diketone 2b and 2n.

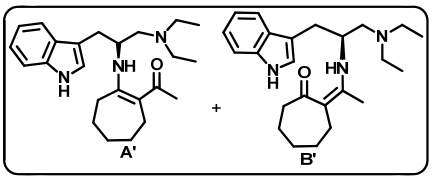
To a standard glass tube containing 1,3-diketons **2b** or **2n** (0.2 mmol) in 0.5 mL CH_3CN was added chiral primary amine **1** (0.2 mmol, 1.0 equiv) and adipic acid (20 mol%). The reaction was stirred at room temperature for 3h and directly purified by basic alumina column (Et_2O/petroleum ether) to give the desired enamine.





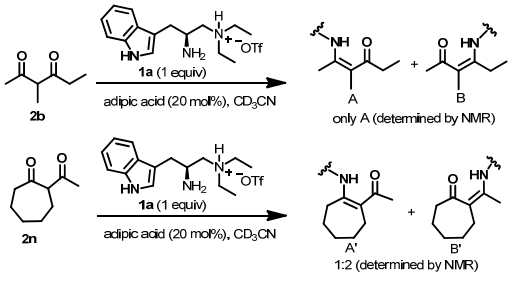
A: Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (Et_2O/petroleum ether = 4/1). 15% yield. ^1H NMR (500 MHz, CD_3CN) δ 12.14 (d, J = 8.5 Hz, 1H), 9.09 (s, 1H), 7.54 (d, J = 7.7 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.14 – 7.07 (m, 1H), 7.04 – 6.98 (m, 2H),

3.97 – 3.87 (m, 1H), 3.16 – 3.08 (m, 1H), 2.74 (dd, J = 14.6, 8.1 Hz, 1H), 2.55 – 2.43 (m, 6H), 2.35 (q, J = 7.4 Hz, 2H), 1.74 (s, 3H), 1.72 (s, 3H), 1.00 (t, J = 7.4 Hz, 3H), 0.95 (t, J = 7.1 Hz, 6H). ^{13}C NMR (125 MHz, CD_3CN) δ 197.5, 162.8, 137.4, 128.7, 124.4, 122.4, 119.8, 119.58, 113.0, 112.3, 97.7, 60.1, 54.7, 48.5, 33.4, 31.1, 15.8, 14.3, 12.4, 9.9.

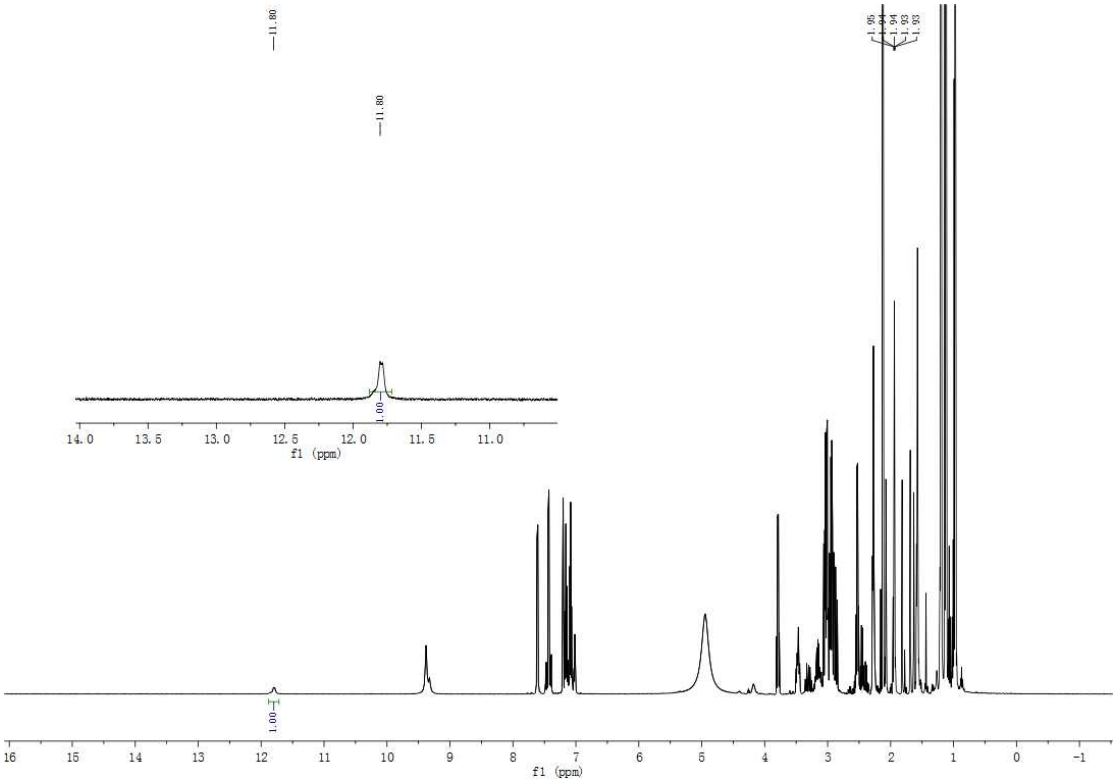


A'/ B'(inseparable mixture): Prepared according to the general procedure and obtained as colorless oil after purification by flash chromatography (Et_2O). 72% yield. ^{1}H NMR (500 MHz, CD_3CN) δ 12.32 (d, J = 8.5 Hz, 1H), 11.99 (d, J = 9.0 Hz, 1H), 9.35 (s, 1H), 7.53 (d, J = 7.9 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.14 – 7.07 (m, 1H), 7.05 – 6.97 (m, 2H), 4.01 – 3.84 (m, 1H), 3.18 – 3.06 (m, 1H), 2.73 (dt, J = 14.5, 7.2 Hz, 1H), 2.58 – 2.42 (m, 8H), 2.35 – 2.32 (m, 1H), 2.28 – 2.23 (m, 2H), 2.05 (s, 1H), 1.73 – 1.64 (m, 4H), 1.62 – 1.57 (m, 2H), 1.50 – 1.32 (m, 2H), 0.97-0.94 (m, 6H). ^{13}C NMR (125 MHz, CD_3CN) δ 200.4, 193.2, 170.3, 162.4, 137.4, 137.4, 128.8, 128.7, 124.6, 124.5, 122.3, 119.8, 119.8, 119.6, 119.5, 112.8, 112.7, 112.3, 106.2, 105.5, 60.01, 59.95, 54.8, 54.6, 48.6, 48.5, 44.6, 32.3, 31.9, 31.3, 31.2, 30.7, 29.5, 29.1, 29.1, 28.6, 28.4, 26.2, 26.1, 15.4, 12.5, 12.4.

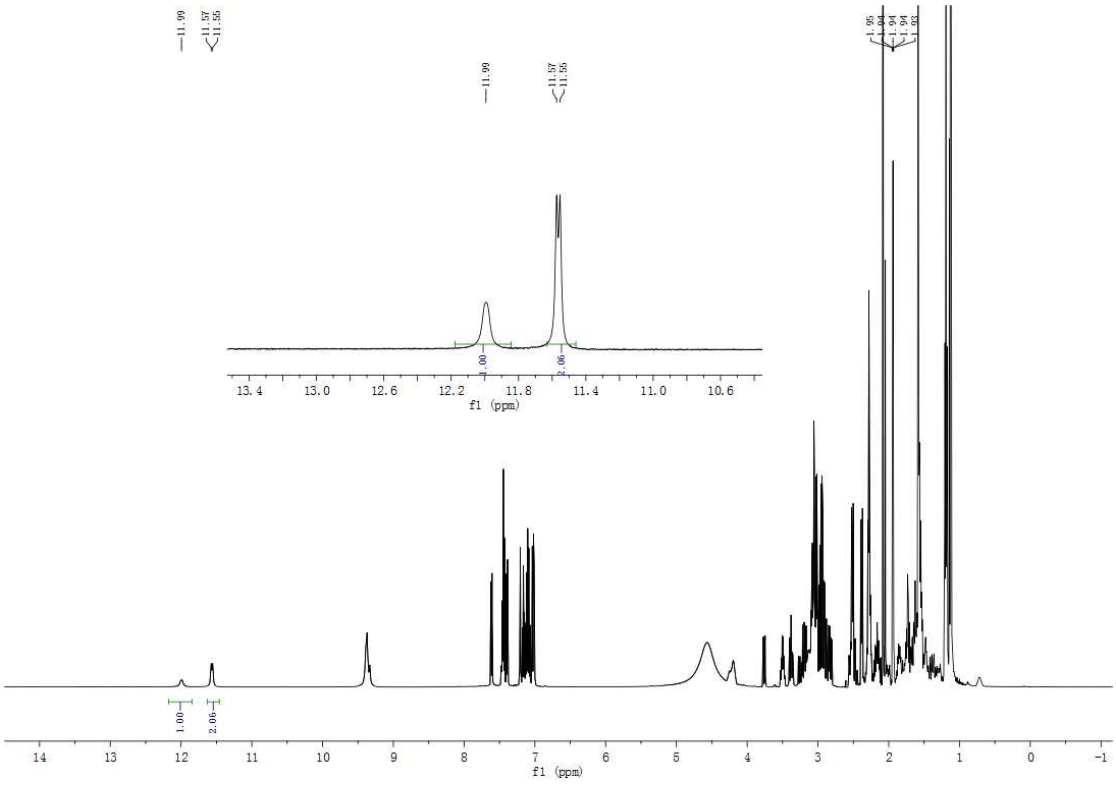
***In-situ* NMR characterization of enamine intermediate of 2b and 2n:** To a standard glass tube containing 1,3-diketons **2b** or **2n** (0.1 mmol) in 0.5 mL CD_3CN was added chiral primary amine **1a/TfOH** (0.1 mmol, 1.0 equiv) and adipic acid (20 mol%). The reaction was stirred at room temperature for 6h and directly characterized by *in-situ* ^{1}HNMR.



In-situ [1]HNMR of the reaction of **1a**/TfOH with **2b**



In-situ [1]HNMR of the reaction **1a**/TfOH with **2n**

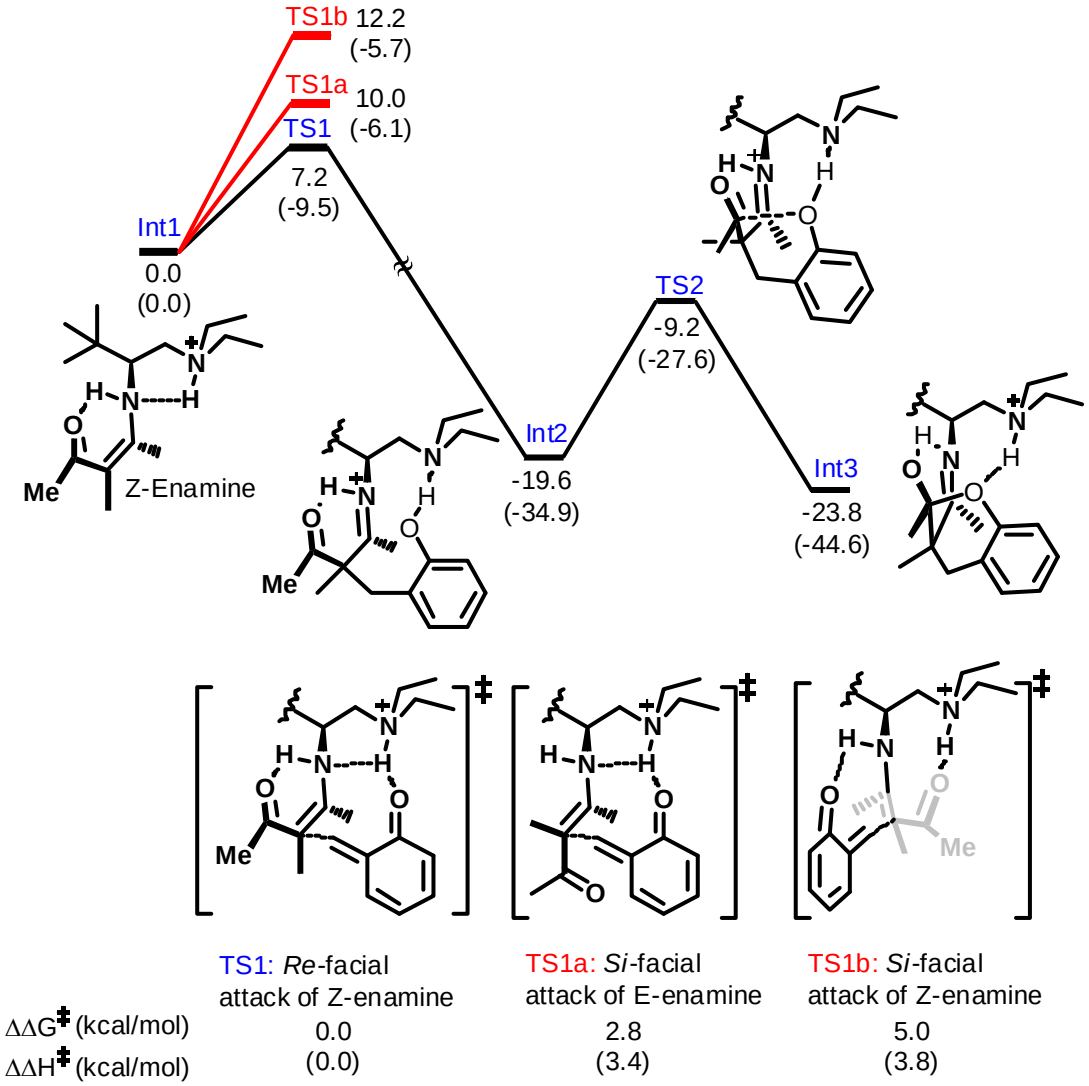


Computational Studies

DFT calculations were performed with the Gaussian 09 program package.[14] The recently developed M06-2X functional[15] together with the 6-31G(d) basis set were used for the geometry optimizations and vibrational calculations. Each geometry was confirmed as a minimum (no imaginary frequency) or a transition state (one imaginary frequency) by calculation of harmonic vibrational frequencies. The SMD continuum solvation model[16] with acetonitrile as the solvent were used in single point energy calculations and these calculations were performed at the M06-2x/6-311+G(d,p) level with gas phase optimized structures.

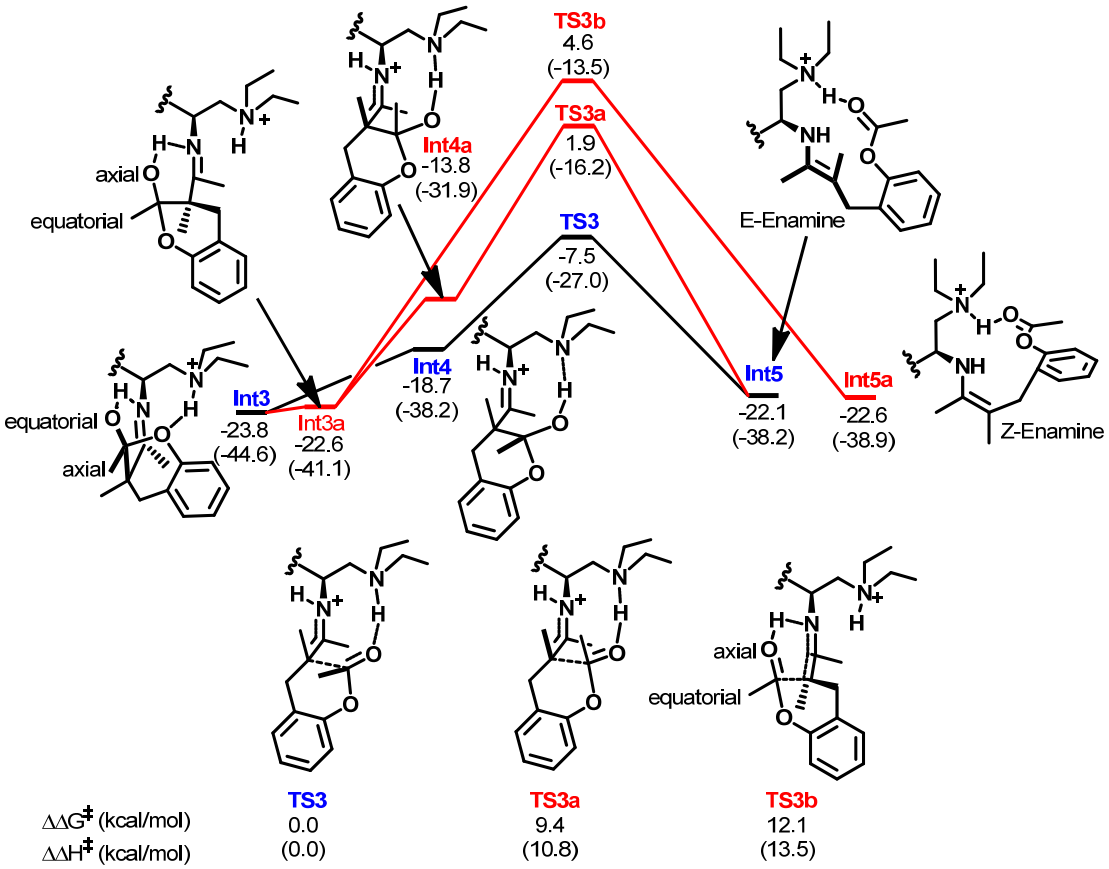
1. The Michael addition of enamine to *o*-QM and the following ketalization

We have clarified that the *Z*-enamine was mainly formed in the reaction mixture by X-ray, NMR as well as DFT calculations,[17] the Michael addition of *Z*-enamine to quinone methide via *Re*-facial attack was promoted by protonated tertiary amine assisted hydrogen-bond activation, which was found to have the lowest barrier. Both of the *Si*-facial attacking of *Z*- and *E*-enamines were higher in energy. The following ketalization was very facial and a much stable ketal intermediate was formed.



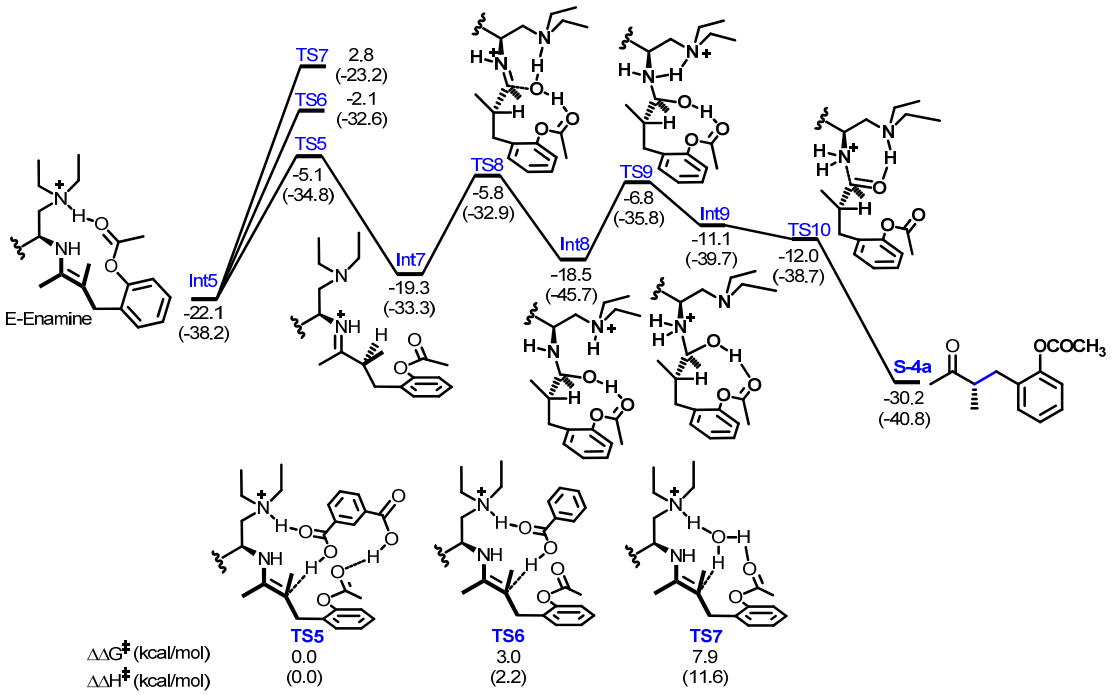
2. The retro-Claisen process

Unlike the classical retro-Claisen process, the C-C bond cleavage of **int3** via six-membered ring transition state (direct proton transfer from O-H to imine) could not be found. Instead, a C-C bond rotation was occurred first to form the less stable ketal **int4**, then the C-C bond cleavage proceeded via a crown-like nine-membered ring TS where the tertiary amine assisted the proton abstraction of ketal O-H, *E*-enamine was formed following this process. The **int3a** could also be formed via a conformation change of **int3**, however, both of the direct retro claisen step via six-membered ring **TS3b** and the tertiary amine assisted retro-Claisen step via nine-membered ring **TS3a** were much higher in energy than **TS3**.



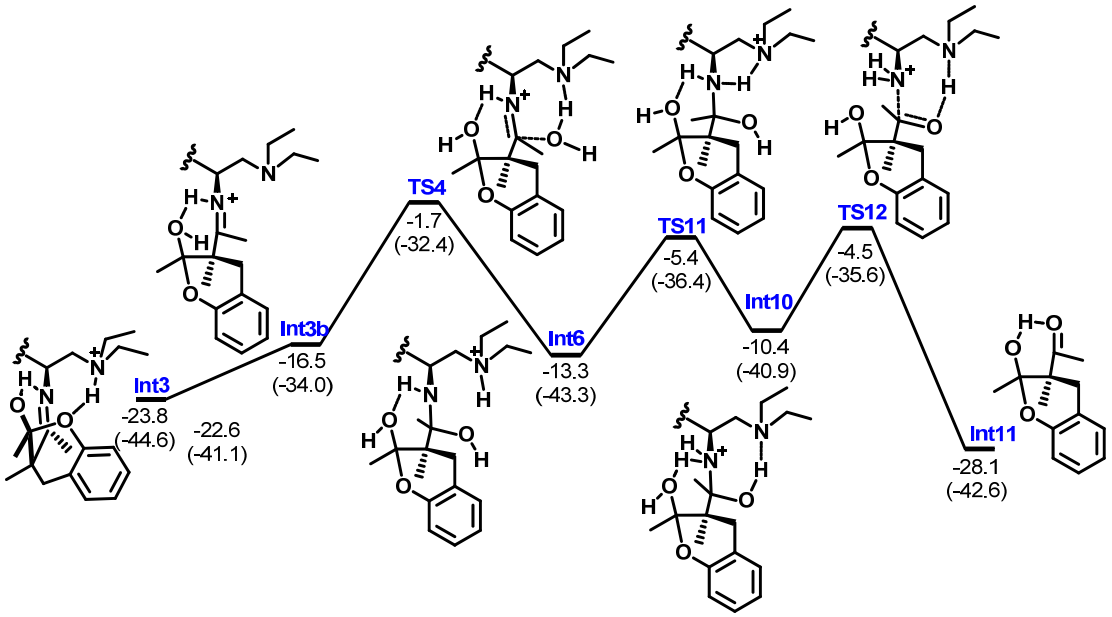
3. The protonation and product hydrolysis process

With *E*-enamine **int5**, the following protonation step was completed with the aid of a proton shuttle. Both water and weak acid could act as a proton shuttle, and the dicarboxylic acid shutlle gave the lowest activation energy. All of these TSs produced a stereocenter with *S*-configuration, and the *S*-product was finally formed after rapid hydrolysis process along with the release of primary amine catalyst.



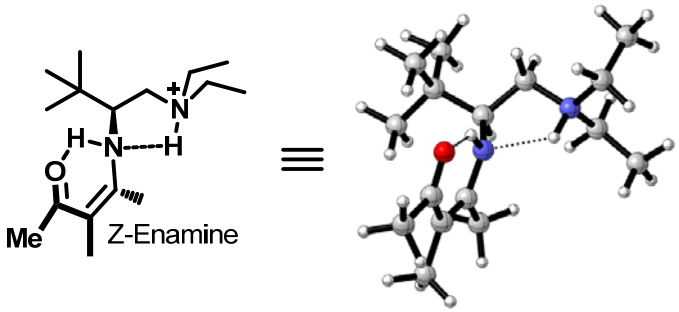
4. The hydrolysis of ketal int3

Besides the retro-Claisen process, the hydrolysis of **int3** could also occur with the activation energy of 16.2 kcal/mol, after the release of catalyst, the residue would undergo enol-based retro-Claisen reaction to give the racemic product.



5. The structure, energies and coordinates of intermediates and transition states.

(1) Int1



E_{sol} = -814.0312336

Zero-point correction=	0.485646 (Hartree/Particle)
Thermal correction to Energy=	0.509309
Thermal correction to Enthalpy=	0.510253
Thermal correction to Gibbs Free Energy=	0.432794
Sum of electronic and zero-point Energies=	-813.221465
Sum of electronic and thermal Energies=	-813.197802
Sum of electronic and thermal Enthalpies=	-813.196857
Sum of electronic and thermal Free Energies=	-813.274316

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	319.596	88.705	163.026
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.671
Rotational	0.889	2.981	33.922
Vibrational	317.819	82.743	86.433

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.004854	2.418100	0.165835
2	6	0	-1.101889	3.434279	0.481722
3	1	0	-1.518458	3.278852	1.484694
4	1	0	-0.693520	4.448453	0.449009
5	1	0	-1.920489	3.395341	-0.245637
6	6	0	1.197674	2.679644	1.093100
7	1	0	0.901464	2.623343	2.147370
8	1	0	2.011008	1.967827	0.916649

9	1	0	1.593625	3.684099	0.915385
10	6	0	0.459790	2.583027	-1.289287
11	1	0	1.292549	1.918209	-1.539855
12	1	0	-0.348372	2.408458	-2.008724
13	1	0	0.802475	3.610428	-1.445024
14	6	0	-0.526415	0.982275	0.447364
15	1	0	-0.687853	0.909281	1.529536
16	6	0	-1.871906	0.718553	-0.262733
17	1	0	-1.802077	0.977815	-1.322920
18	1	0	-2.693566	1.279840	0.184334
19	7	0	0.374965	-0.093915	0.036147
20	1	0	-1.239758	-1.168636	-0.166111
21	7	0	-2.194767	-0.746199	-0.186619
22	6	0	-2.900973	-1.266849	-1.410160
23	1	0	-2.267481	-0.989675	-2.256364
24	1	0	-2.899620	-2.356194	-1.337223
25	6	0	-2.870022	-1.097105	1.109304
26	1	0	-2.251862	-0.659948	1.897412
27	1	0	-3.833750	-0.582775	1.116915
28	6	0	-3.017730	-2.595119	1.305863
29	1	0	-3.741811	-3.035507	0.616518
30	1	0	-2.058336	-3.110150	1.191506
31	1	0	-3.375889	-2.782274	2.320648
32	6	0	-4.307160	-0.716839	-1.562389
33	1	0	-4.319555	0.376617	-1.583486
34	1	0	-4.715779	-1.069050	-2.512153
35	1	0	-4.976035	-1.064713	-0.770900
36	1	0	0.703893	-0.009782	-0.935366
37	6	0	1.420658	-0.560299	0.838766
38	6	0	2.610936	-0.966838	0.305458
39	6	0	1.114466	-0.657328	2.312171
40	1	0	0.056500	-0.889398	2.469229
41	1	0	1.691759	-1.448632	2.787322
42	1	0	1.331825	0.281241	2.834657
43	6	0	3.725083	-1.506245	1.175817
44	1	0	3.641721	-1.172356	2.210128
45	1	0	3.760088	-2.602532	1.176307
46	1	0	4.696942	-1.155439	0.821778
47	6	0	2.854366	-0.900202	-1.154289
48	8	0	2.014467	-0.487669	-1.958068
49	6	0	4.191686	-1.361483	-1.685481
50	1	0	4.985821	-0.675432	-1.371028
51	1	0	4.452563	-2.355085	-1.309223
52	1	0	4.144355	-1.375488	-2.773901

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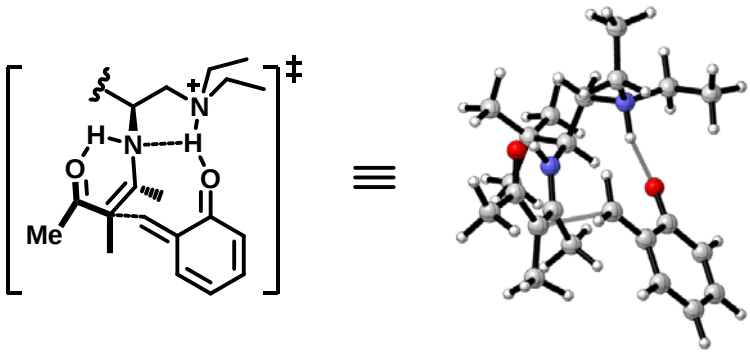
(2) TS1



E_{sol} = -1159.537356

Zero-point correction=	0.598537 (Hartree/Particle)
Thermal correction to Energy=	0.628112
Thermal correction to Enthalpy=	0.629057
Thermal correction to Gibbs Free Energy=	0.540407
Sum of electronic and zero-point Energies=	-1158.525421
Sum of electronic and thermal Energies=	-1158.495845
Sum of electronic and thermal Enthalpies=	-1158.494901
Sum of electronic and thermal Free Energies=	-1158.583551

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	394.146	115.472	186.579
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.453
Vibrational	392.369	109.510	107.466

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.027860	-0.957534	-1.575458
2	6	0	-3.909902	0.001634	-2.387434
3	1	0	-3.307828	0.636491	-3.048182
4	1	0	-4.594000	-0.573879	-3.018061
5	1	0	-4.528403	0.645964	-1.754952
6	6	0	-2.394269	-1.964998	-2.541612
7	1	0	-1.805669	-1.465041	-3.318420
8	1	0	-1.753346	-2.681409	-2.017574
9	1	0	-3.183454	-2.533674	-3.042245
10	6	0	-3.882314	-1.720861	-0.555476

11	1	0	-3.270201	-2.371489	0.079648
12	1	0	-4.463963	-1.051820	0.087578
13	1	0	-4.599442	-2.358097	-1.081561
14	6	0	-1.900314	-0.148491	-0.865242
15	1	0	-1.337646	0.419495	-1.616241
16	6	0	-2.472879	0.840794	0.157812
17	1	0	-2.936071	0.295023	0.984200
18	1	0	-3.235645	1.475322	-0.295133
19	7	0	-0.965326	-0.984294	-0.123891
20	1	0	-0.473819	1.424346	0.331541
21	7	0	-1.404406	1.728078	0.735610
22	6	0	-1.295171	1.603738	2.229967
23	1	0	-1.183526	0.533597	2.435567
24	1	0	-0.361310	2.094570	2.515767
25	6	0	-1.553141	3.142961	0.242784
26	1	0	-1.504165	3.066710	-0.846747
27	1	0	-2.551978	3.485361	0.526631
28	6	0	-0.465185	4.065172	0.760499
29	1	0	-0.551652	4.249215	1.834480
30	1	0	0.523205	3.657253	0.535083
31	1	0	-0.557754	5.028874	0.254235
32	6	0	-2.480779	2.199424	2.968450
33	1	0	-3.431191	1.773422	2.633336
34	1	0	-2.378993	1.978488	4.033193
35	1	0	-2.528614	3.285887	2.858392
36	1	0	-1.223384	-1.247918	0.834061
37	6	0	0.224407	-1.474117	-0.485572
38	6	0	1.032493	-2.170123	0.449714
39	6	0	0.744301	-1.294026	-1.876969
40	1	0	0.145148	-0.612338	-2.475431
41	1	0	1.769617	-0.909526	-1.839975
42	1	0	0.785948	-2.267125	-2.379450
43	6	0	2.255493	-2.892300	-0.065774
44	1	0	1.999407	-3.701354	-0.760053
45	1	0	2.933374	-2.210469	-0.592535
46	1	0	2.827977	-3.336026	0.749705
47	6	0	0.511368	-2.472403	1.788028
48	8	0	-0.500017	-1.919466	2.246089
49	6	0	4.204277	1.737535	-1.793628
50	6	0	4.875231	0.845328	-0.898051
51	6	0	4.159338	0.215216	0.070408
52	6	0	2.744167	0.438447	0.214253
53	6	0	2.051735	1.329404	-0.719857
54	6	0	2.862913	1.978592	-1.714302

55	1	0	4.786082	2.236607	-2.563841
56	1	0	5.942822	0.686954	-0.997103
57	1	0	4.643322	-0.459607	0.772781
58	1	0	2.361201	2.649092	-2.403939
59	8	0	0.800765	1.502074	-0.686996
60	6	0	2.023233	-0.186941	1.209829
61	1	0	2.551927	-0.753174	1.973387
62	1	0	1.014883	0.129675	1.460883
63	6	0	1.251300	-3.450584	2.672297
64	1	0	1.349001	-4.425935	2.186081
65	1	0	2.263753	-3.097827	2.898646
66	1	0	0.695873	-3.558205	3.603470

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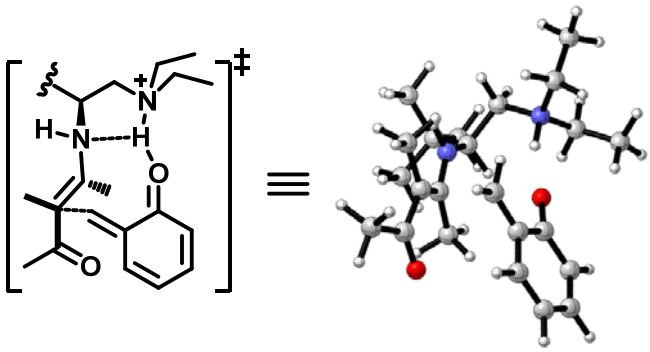
(3) TS1a



E_{sol} = -1159.531346

Zero-point correction=	0.597635 (Hartree/Particle)
Thermal correction to Energy=	0.627491
Thermal correction to Enthalpy=	0.628435
Thermal correction to Gibbs Free Energy=	0.538739
Sum of electronic and zero-point Energies=	-1158.509057
Sum of electronic and thermal Energies=	-1158.479202
Sum of electronic and thermal Enthalpies=	-1158.478258
Sum of electronic and thermal Free Energies=	-1158.567954

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	393.756	116.342	188.782
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.545
Vibrational	391.979	110.380	109.576

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-2.727811	-1.966753	-1.170705
2	6	0	-3.763319	-1.364279	-2.130293
3	1	0	-3.284040	-0.721004	-2.877519
4	1	0	-4.276196	-2.167123	-2.668017
5	1	0	-4.536581	-0.782804	-1.617884
6	6	0	-1.804385	-2.888838	-1.975134
7	1	0	-1.324859	-2.358342	-2.803925
8	1	0	-1.024349	-3.330429	-1.347009
9	1	0	-2.389867	-3.707904	-2.403315
10	6	0	-3.436195	-2.791408	-0.088267
11	1	0	-2.724648	-3.233967	0.619534
12	1	0	-4.168818	-2.202253	0.475371
13	1	0	-3.980400	-3.619360	-0.552047
14	6	0	-1.891242	-0.818500	-0.530664
15	1	0	-1.499820	-0.179211	-1.328850
16	6	0	-2.735094	0.054837	0.409111
17	1	0	-2.848478	-0.438770	1.379352
18	1	0	-3.736281	0.225294	0.010036
19	7	0	-0.751990	-1.286856	0.251558
20	1	0	-1.064661	1.319588	0.409280
21	7	0	-2.097977	1.392626	0.641981
22	6	0	-2.188450	1.839779	2.070660
23	1	0	-1.746568	1.031646	2.661756
24	1	0	-1.538015	2.711836	2.166699
25	6	0	-2.619745	2.403557	-0.347616
26	1	0	-2.380601	1.990569	-1.331162
27	1	0	-3.707145	2.431711	-0.236973
28	6	0	-1.998776	3.778782	-0.183643
29	1	0	-2.316902	4.271255	0.739084
30	1	0	-0.909265	3.710968	-0.213917
31	1	0	-2.326023	4.404314	-1.017617
32	6	0	-3.607148	2.143314	2.518187
33	1	0	-4.274730	1.288446	2.373820
34	1	0	-3.600015	2.381158	3.584124
35	1	0	-4.024198	3.005236	1.991051
36	1	0	-0.998362	-1.686754	1.148321
37	6	0	0.553565	-1.397645	-0.102548
38	6	0	1.465156	-1.778416	0.894295
39	6	0	0.968008	-1.119574	-1.511820
40	1	0	0.145313	-0.773725	-2.132498
41	1	0	1.779167	-0.389652	-1.536199
42	1	0	1.391923	-2.032847	-1.941212
43	6	0	0.927874	-2.192456	2.245825

44	1	0	0.297995	-1.408805	2.691084
45	1	0	0.326521	-3.111156	2.193670
46	1	0	1.728408	-2.378911	2.961518
47	6	0	2.866883	-2.124305	0.532340
48	8	0	3.376469	-1.755959	-0.511622
49	6	0	3.411422	2.721362	-1.742053
50	6	0	4.336398	2.055038	-0.880630
51	6	0	3.861269	1.288007	0.136399
52	6	0	2.448097	1.158013	0.363920
53	6	0	1.500305	1.797573	-0.547653
54	6	0	2.057496	2.609415	-1.590835
55	1	0	3.802807	3.331277	-2.551983
56	1	0	5.401310	2.162677	-1.049586
57	1	0	4.538394	0.764635	0.806424
58	1	0	1.365449	3.102089	-2.265875
59	8	0	0.249729	1.618842	-0.452645
60	6	0	1.950730	0.426170	1.419646
61	1	0	2.621439	0.052278	2.189816
62	1	0	0.902741	0.521418	1.691713
63	6	0	3.691492	-2.917118	1.530002
64	1	0	3.905514	-2.322238	2.426304
65	1	0	3.179188	-3.828044	1.853586
66	1	0	4.635665	-3.175881	1.051266

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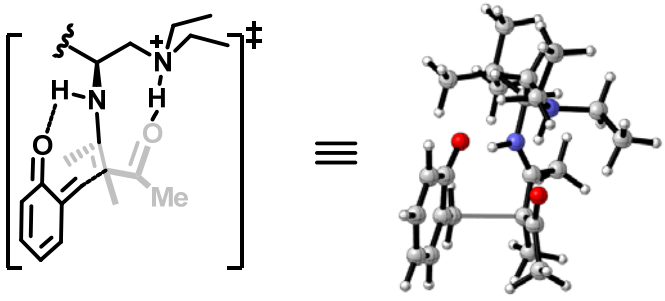
(4) TS1b



E_{sol} = -1159.530717

Zero-point correction=	0.598243 (Hartree/Particle)
Thermal correction to Energy=	0.627647
Thermal correction to Enthalpy=	0.628591
Thermal correction to Gibbs Free Energy=	0.541613
Sum of electronic and zero-point Energies=	-1158.519347
Sum of electronic and thermal Energies=	-1158.489943
Sum of electronic and thermal Enthalpies=	-1158.488999
Sum of electronic and thermal Free Energies=	-1158.575977

E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	393.855	115.359	183.062
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.286
Vibrational	392.077	109.397	104.115

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.988064	-0.935428	-1.446944
2	6	0	4.312228	-0.183258	-1.638883
3	1	0	4.925751	-0.204931	-0.729884
4	1	0	4.889725	-0.656805	-2.437946
5	1	0	4.156279	0.860547	-1.929984
6	6	0	3.289800	-2.425956	-1.261810
7	1	0	3.958759	-2.603480	-0.411571
8	1	0	2.371992	-3.005962	-1.117299
9	1	0	3.784421	-2.814786	-2.156783
10	6	0	2.107697	-0.768100	-2.691306
11	1	0	1.174941	-1.334041	-2.605814
12	1	0	1.840502	0.271932	-2.898082
13	1	0	2.649973	-1.148758	-3.562403
14	6	0	2.286318	-0.398891	-0.161348
15	1	0	2.905925	-0.673623	0.699600
16	6	0	2.139800	1.136998	-0.215447
17	1	0	1.749949	1.436307	-1.189408
18	1	0	3.107476	1.612233	-0.045841
19	7	0	0.940479	-0.939980	0.022691
20	1	0	0.316346	1.085094	0.794413
21	7	0	1.178770	1.681380	0.795218
22	6	0	0.687782	3.050294	0.406872
23	1	0	0.266528	2.916919	-0.592198
24	1	0	-0.136852	3.279394	1.084682
25	6	0	1.723051	1.583030	2.190586
26	1	0	1.865320	0.513728	2.374556
27	1	0	2.705572	2.063658	2.193592
28	6	0	0.795243	2.178038	3.236870
29	1	0	0.748688	3.267790	3.172347
30	1	0	-0.213030	1.767314	3.139603
31	1	0	1.179583	1.923493	4.227379
32	6	0	1.766703	4.116560	0.446491
33	1	0	2.582909	3.905867	-0.250033

34	1	0	1.323840	5.069816	0.148453
35	1	0	2.184126	4.249128	1.448783
36	1	0	0.226754	-0.400153	-0.544083
37	6	0	0.499498	-1.888417	0.827498
38	6	0	-0.906711	-1.995156	1.084810
39	6	0	1.445982	-2.865128	1.465729
40	1	0	2.489548	-2.563812	1.383584
41	1	0	1.189535	-3.009257	2.518194
42	1	0	1.348234	-3.840567	0.974778
43	6	0	-1.414170	-3.335031	1.580508
44	1	0	-1.001678	-4.155551	0.985627
45	1	0	-1.165883	-3.532999	2.631490
46	1	0	-2.500782	-3.398514	1.491776
47	6	0	-1.586669	-0.783937	1.534838
48	8	0	-1.142726	0.362682	1.388212
49	6	0	-2.926977	-0.943276	2.213418
50	1	0	-3.639789	-1.436100	1.543818
51	1	0	-2.845866	-1.557059	3.116110
52	1	0	-3.305915	0.045682	2.469424
53	6	0	-3.860335	1.878108	-1.735815
54	6	0	-4.610703	0.722978	-1.354049
55	6	0	-3.952306	-0.436653	-1.084557
56	6	0	-2.522141	-0.521281	-1.184880
57	6	0	-1.751052	0.679585	-1.488098
58	6	0	-2.497952	1.862488	-1.815482
59	1	0	-4.396128	2.794278	-1.968631
60	1	0	-5.692453	0.774453	-1.309369
61	1	0	-4.503444	-1.340988	-0.835363
62	1	0	-1.936053	2.744557	-2.105715
63	8	0	-0.481964	0.693040	-1.452058
64	6	0	-1.866628	-1.733442	-1.012148
65	1	0	-2.451140	-2.641278	-0.881079
66	1	0	-0.870025	-1.863870	-1.422440

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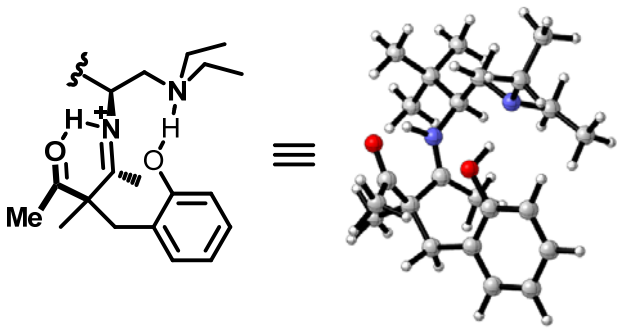
(5) Int2



E_{sol} = -1159.578363

Zero-point correction=	0.598645 (Hartree/Particle)
Thermal correction to Energy=	0.628732
Thermal correction to Enthalpy=	0.629676
Thermal correction to Gibbs Free Energy=	0.538643
Sum of electronic and zero-point Energies=	-1158.565851
Sum of electronic and thermal Energies=	-1158.535764
Sum of electronic and thermal Enthalpies=	-1158.534820
Sum of electronic and thermal Free Energies=	-1158.625853

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	394.535	116.247	191.595
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.352
Vibrational	392.758	110.285	112.582

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.674751	-0.725129	-0.455124
2	6	0	-4.752363	0.237702	-0.973073
3	1	0	-4.488485	0.644653	-1.956141
4	1	0	-5.699044	-0.299653	-1.080710
5	1	0	-4.931327	1.071653	-0.288990
6	6	0	-3.621954	-1.945234	-1.384708
7	1	0	-3.339736	-1.656677	-2.404581
8	1	0	-2.911867	-2.700102	-1.030724
9	1	0	-4.606419	-2.418860	-1.435011
10	6	0	-4.028701	-1.174759	0.968708
11	1	0	-3.291598	-1.867543	1.393573
12	1	0	-4.138224	-0.326643	1.651888
13	1	0	-4.986232	-1.704011	0.953908
14	6	0	-2.295734	-0.012787	-0.509252
15	1	0	-2.134564	0.301996	-1.541075
16	6	0	-2.156248	1.193212	0.433601
17	1	0	-2.174727	0.830703	1.468145
18	1	0	-3.035825	1.837700	0.295961
19	7	0	-1.237635	-0.968702	-0.147827
20	7	0	-0.912399	1.955555	0.248123
21	6	0	-0.649520	2.806722	1.435998
22	1	0	-0.614534	2.133666	2.299327

23	1	0	0.359442	3.215711	1.327200
24	6	0	-0.951091	2.730366	-1.007985
25	1	0	-1.088191	2.021339	-1.830845
26	1	0	-1.829361	3.394024	-1.018403
27	6	0	0.317686	3.528458	-1.268680
28	1	0	0.438979	4.355412	-0.563741
29	1	0	1.205107	2.888733	-1.208275
30	1	0	0.276663	3.958381	-2.272447
31	6	0	-1.642205	3.938915	1.683305
32	1	0	-2.663296	3.569708	1.816854
33	1	0	-1.363746	4.469846	2.597078
34	1	0	-1.642806	4.667665	0.867317
35	1	0	-1.331494	-1.400455	0.789064
36	6	0	-0.113079	-1.229622	-0.720279
37	6	0	0.858319	-2.194740	-0.047235
38	6	0	0.233584	-0.689312	-2.069171
39	1	0	0.985382	0.101681	-1.953977
40	1	0	0.689201	-1.477598	-2.673800
41	1	0	-0.627517	-0.296170	-2.606127
42	6	0	0.413693	-3.622314	-0.467956
43	1	0	-0.584317	-3.846708	-0.082907
44	1	0	0.408952	-3.724924	-1.557673
45	1	0	1.114925	-4.359720	-0.065887
46	6	0	0.733629	-2.162068	1.498359
47	8	0	-0.368141	-2.123963	2.016998
48	6	0	4.347549	1.830965	-0.253268
49	6	0	4.923553	0.748196	-0.915869
50	6	0	4.240553	-0.459067	-0.979130
51	6	0	2.977418	-0.621103	-0.397595
52	6	0	2.414471	0.477278	0.264489
53	6	0	3.100728	1.691404	0.341665
54	1	0	4.874040	2.777538	-0.188330
55	1	0	5.900379	0.844262	-1.377209
56	1	0	4.691470	-1.303842	-1.495363
57	1	0	2.647533	2.510777	0.892758
58	8	0	1.192145	0.328623	0.866304
59	6	0	2.309862	-1.981420	-0.531531
60	1	0	2.364357	-2.284926	-1.583802
61	1	0	2.921591	-2.724666	-0.006944
62	6	0	1.969435	-2.312033	2.339155
63	1	0	2.708706	-1.544774	2.093330
64	1	0	1.680492	-2.236867	3.387004
65	1	0	2.428997	-3.291944	2.164422
66	1	0	0.516309	1.003608	0.550100

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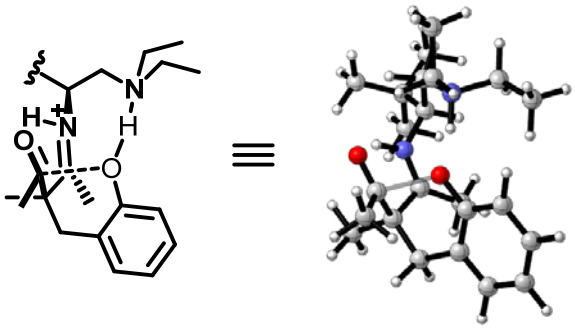
(6) TS2



E_{sol} = -1159.565403

Zero-point correction=	0.598617 (Hartree/Particle)
Thermal correction to Energy=	0.627281
Thermal correction to Enthalpy=	0.628226
Thermal correction to Gibbs Free Energy=	0.542271
Sum of electronic and zero-point Energies=	-1158.548321
Sum of electronic and thermal Energies=	-1158.519657
Sum of electronic and thermal Enthalpies=	-1158.518712
Sum of electronic and thermal Free Energies=	-1158.604667

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	393.625	113.458	180.906
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.263
Vibrational	391.848	107.496	101.982

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.640444	-0.867865	-0.726211
2	6	0	-4.632901	0.073750	-1.420304
3	1	0	-4.234469	0.448608	-2.370624
4	1	0	-5.556348	-0.468485	-1.642636
5	1	0	-4.908057	0.930046	-0.796772
6	6	0	-3.460454	-2.121987	-1.590596
7	1	0	-3.094587	-1.867056	-2.592625
8	1	0	-2.763841	-2.833295	-1.134397
9	1	0	-4.421156	-2.630619	-1.710874
10	6	0	-4.170144	-1.265987	0.656287
11	1	0	-3.474086	-1.924377	1.188733

12	1	0	-4.376835	-0.394849	1.286987
13	1	0	-5.111432	-1.811694	0.543174
14	6	0	-2.262831	-0.164167	-0.618746
15	1	0	-1.944774	0.103024	-1.631530
16	6	0	-2.265082	1.084737	0.275508
17	1	0	-2.391905	0.789024	1.320983
18	1	0	-3.084226	1.754815	0.004980
19	7	0	-1.257452	-1.041925	-0.018009
20	7	0	-0.986523	1.862123	0.183019
21	6	0	-0.673103	2.574979	1.476904
22	1	0	-0.608810	1.776972	2.222697
23	1	0	0.334752	2.977005	1.359246
24	6	0	-1.014988	2.759183	-1.018863
25	1	0	-1.325487	2.137201	-1.863020
26	1	0	-1.801415	3.500145	-0.850628
27	6	0	0.322093	3.409680	-1.315842
28	1	0	0.629944	4.100690	-0.526865
29	1	0	1.105583	2.659942	-1.455195
30	1	0	0.232049	3.984886	-2.240456
31	6	0	-1.678227	3.647950	1.849780
32	1	0	-2.696291	3.255543	1.930359
33	1	0	-1.406908	4.047778	2.829664
34	1	0	-1.676962	4.485001	1.146284
35	1	0	-1.224337	-1.026769	1.046966
36	6	0	-0.125404	-1.451247	-0.490821
37	6	0	0.850724	-2.009929	0.532048
38	6	0	0.204182	-1.431646	-1.941680
39	1	0	1.088223	-0.803443	-2.103150
40	1	0	0.480313	-2.447032	-2.247276
41	1	0	-0.622085	-1.100188	-2.568561
42	6	0	0.347683	-3.395250	0.990139
43	1	0	-0.643396	-3.328408	1.447124
44	1	0	0.303686	-4.091873	0.146265
45	1	0	1.038112	-3.810341	1.729887
46	6	0	0.825597	-1.041980	1.760913
47	8	0	-0.280169	-0.741465	2.259163
48	6	0	4.401436	1.487038	-0.999342
49	6	0	4.909619	0.250809	-1.394295
50	6	0	4.191604	-0.901912	-1.097525
51	6	0	2.961735	-0.847503	-0.438949
52	6	0	2.425599	0.408100	-0.080402
53	6	0	3.180407	1.563417	-0.341916
54	1	0	4.964603	2.394835	-1.193071
55	1	0	5.862671	0.183902	-1.907349

56	1	0	4.596749	-1.874105	-1.371869
57	1	0	2.796402	2.517342	0.008042
58	8	0	1.231594	0.484945	0.525843
59	6	0	2.269262	-2.139581	-0.050168
60	1	0	2.247553	-2.830241	-0.903176
61	1	0	2.872345	-2.653937	0.709232
62	6	0	2.043267	-0.976897	2.645832
63	1	0	2.970340	-0.784941	2.106779
64	1	0	1.873123	-0.195357	3.387027
65	1	0	2.133584	-1.934491	3.173428
66	1	0	-0.123980	1.213352	0.116595

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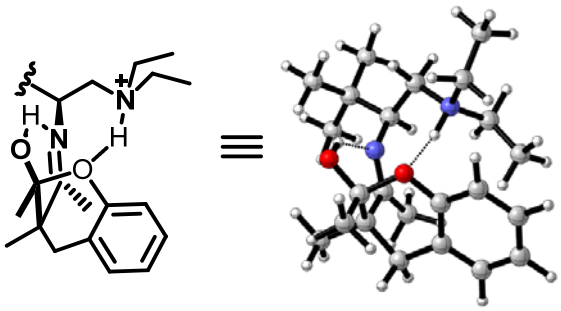
(7) Int3



E_{sol} = -1159.596873

Zero-point correction=	0.604277 (Hartree/Particle)
Thermal correction to Energy=	0.631697
Thermal correction to Enthalpy=	0.632641
Thermal correction to Gibbs Free Energy=	0.550529
Sum of electronic and zero-point Energies=	-1158.577240
Sum of electronic and thermal Energies=	-1158.549820
Sum of electronic and thermal Enthalpies=	-1158.548875
Sum of electronic and thermal Free Energies=	-1158.630988

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	396.396	111.759	172.820
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.145
Vibrational	394.618	105.797	94.015

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.725940	-0.287775	-0.271855

2	6	0	-4.757159	0.815341	-0.538045
3	1	0	-4.603438	1.283418	-1.517972
4	1	0	-5.765090	0.390296	-0.530206
5	1	0	-4.731106	1.596494	0.229816
6	6	0	-3.944965	-1.436990	-1.263654
7	1	0	-3.896350	-1.083812	-2.300670
8	1	0	-3.197550	-2.226982	-1.128393
9	1	0	-4.931932	-1.883505	-1.110742
10	6	0	-3.888369	-0.822874	1.155603
11	1	0	-3.214774	-1.662603	1.351119
12	1	0	-3.715094	-0.054926	1.917529
13	1	0	-4.913152	-1.181606	1.292031
14	6	0	-2.297344	0.272706	-0.526366
15	1	0	-2.243440	0.505370	-1.599316
16	6	0	-2.004996	1.552079	0.273461
17	1	0	-2.193311	1.380905	1.336471
18	1	0	-2.600616	2.399454	-0.071663
19	7	0	-1.288485	-0.663073	-0.083367
20	7	0	-0.553885	1.937547	0.149742
21	6	0	-0.079321	2.775304	1.311463
22	1	0	-0.152602	2.119433	2.183337
23	1	0	0.979982	2.966397	1.132102
24	6	0	-0.277669	2.549587	-1.199787
25	1	0	-0.793423	1.922084	-1.929777
26	1	0	-0.767251	3.526458	-1.198700
27	6	0	1.196064	2.646189	-1.546185
28	1	0	1.752185	3.297075	-0.868383
29	1	0	1.674615	1.661528	-1.552356
30	1	0	1.278968	3.069558	-2.550554
31	6	0	-0.858342	4.063682	1.500912
32	1	0	-1.916320	3.882407	1.705901
33	1	0	-0.443615	4.586229	2.366171
34	1	0	-0.771337	4.737260	0.644426
35	1	0	-0.984798	-1.263812	1.632971
36	6	0	-0.435450	-1.260651	-0.821054
37	6	0	0.595692	-2.156640	-0.111849
38	6	0	-0.388299	-1.197597	-2.330351
39	1	0	0.451891	-0.571385	-2.655748
40	1	0	-0.220378	-2.195749	-2.744075
41	1	0	-1.310705	-0.810712	-2.762732
42	6	0	0.030506	-3.585463	-0.131793
43	1	0	-0.873429	-3.643635	0.479899
44	1	0	-0.213415	-3.897949	-1.152425
45	1	0	0.761138	-4.296680	0.261804

46	6	0	0.835373	-1.684764	1.363148
47	8	0	-0.292187	-1.726823	2.146779
48	6	0	4.120344	1.542607	0.020803
49	6	0	4.428345	0.809516	-1.124946
50	6	0	3.710134	-0.346684	-1.414546
51	6	0	2.661188	-0.779305	-0.598131
52	6	0	2.331403	0.004817	0.516159
53	6	0	3.074669	1.140198	0.843024
54	1	0	4.702725	2.420899	0.280598
55	1	0	5.241958	1.119598	-1.771576
56	1	0	3.974703	-0.943296	-2.284395
57	1	0	2.835273	1.670475	1.759999
58	8	0	1.246584	-0.278916	1.307714
59	6	0	1.952610	-2.092300	-0.836468
60	1	0	1.843372	-2.283881	-1.908069
61	1	0	2.578174	-2.910300	-0.457912
62	6	0	1.913916	-2.458865	2.105470
63	1	0	2.902028	-2.331957	1.659594
64	1	0	1.936433	-2.074432	3.126918
65	1	0	1.663381	-3.520675	2.144573
66	1	0	-0.016621	1.054447	0.239756

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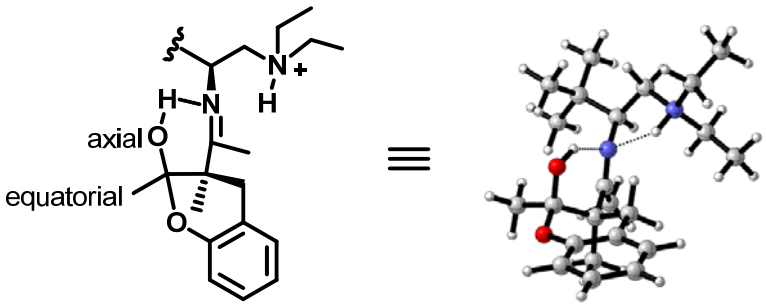
(8) Int3a



E_{sol} = -1159.591199

Zero-point correction= 0.603171 (Hartree/Particle)
Thermal correction to Energy= 0.631698
Thermal correction to Enthalpy= 0.632642
Thermal correction to Gibbs Free Energy= 0.546635
Sum of electronic and zero-point Energies= -1158.558725
Sum of electronic and thermal Energies= -1158.530198
Sum of electronic and thermal Enthalpies= -1158.529254
Sum of electronic and thermal Free Energies= -1158.615261

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	396.397	114.154	181.018

Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.609
Vibrational	394.619	108.192	101.749

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.174454	-1.746436	-0.496809
2	6	0	4.681493	-1.519067	-0.682532
3	1	0	5.168786	-1.255795	0.264131
4	1	0	5.149198	-2.437310	-1.049199
5	1	0	4.898622	-0.735399	-1.416674
6	6	0	2.974385	-2.982455	0.385850
7	1	0	3.474383	-2.871172	1.354835
8	1	0	1.914011	-3.187722	0.562405
9	1	0	3.399046	-3.861386	-0.108099
10	6	0	2.511073	-1.997557	-1.856671
11	1	0	1.444713	-2.222176	-1.757255
12	1	0	2.615969	-1.152667	-2.546790
13	1	0	2.988203	-2.857615	-2.336203
14	6	0	2.557766	-0.507487	0.224576
15	1	0	2.962601	-0.494749	1.246319
16	6	0	2.984852	0.798553	-0.480196
17	1	0	2.943112	0.677581	-1.565496
18	1	0	3.992261	1.104825	-0.193594
19	7	0	1.104796	-0.516421	0.197498
20	1	0	1.110878	1.472696	-0.222198
21	7	0	2.041616	1.920282	-0.151322
22	6	0	2.087080	3.038214	-1.161540
23	1	0	1.924496	2.567025	-2.133633
24	1	0	1.229335	3.681022	-0.955415
25	6	0	2.181614	2.371648	1.277241
26	1	0	2.009703	1.480473	1.886584
27	1	0	3.219822	2.684372	1.413879
28	6	0	1.198636	3.469829	1.643814
29	1	0	1.436721	4.420684	1.161494
30	1	0	0.171508	3.189376	1.387483
31	1	0	1.239539	3.629300	2.723603
32	6	0	3.389870	3.815855	-1.129752
33	1	0	4.254634	3.181162	-1.339817
34	1	0	3.351247	4.584305	-1.905198
35	1	0	3.543414	4.322836	-0.173443

36	1	0	-0.095859	-0.773865	-1.295864
37	6	0	0.344913	-0.944329	1.139686
38	6	0	-1.169983	-0.832375	0.902064
39	6	0	0.818730	-1.533909	2.442467
40	1	0	1.899611	-1.493206	2.567458
41	1	0	0.339468	-1.026673	3.284061
42	1	0	0.515145	-2.585154	2.498681
43	6	0	-1.994697	-1.336586	2.094054
44	1	0	-1.750460	-2.365885	2.366592
45	1	0	-1.840265	-0.704639	2.974047
46	1	0	-3.057657	-1.304076	1.850401
47	6	0	-1.576041	-1.628292	-0.397925
48	8	0	-1.002043	-1.041089	-1.535430
49	6	0	-5.530821	0.984561	-0.936176
50	6	0	-4.928265	2.091667	-0.337197
51	6	0	-3.643214	1.974671	0.175179
52	6	0	-2.938959	0.772048	0.095798
53	6	0	-3.559072	-0.322253	-0.509241
54	6	0	-4.851362	-0.222291	-1.020742
55	1	0	-6.535836	1.062431	-1.337844
56	1	0	-5.460465	3.034051	-0.265683
57	1	0	-3.170062	2.828945	0.655571
58	1	0	-5.296756	-1.099778	-1.476851
59	8	0	-2.969607	-1.559492	-0.565834
60	6	0	-1.534844	0.642688	0.623203
61	1	0	-0.843879	1.044773	-0.130274
62	1	0	-1.415939	1.231567	1.543094
63	6	0	-1.253788	-3.112709	-0.333802
64	1	0	-1.568959	-3.563608	-1.276940
65	1	0	-0.175289	-3.264735	-0.221614
66	1	0	-1.779611	-3.606113	0.486237

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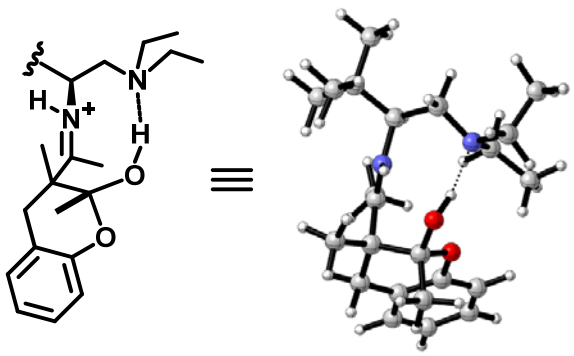
(9) Int4



E_{sol} = -1159.586123

Zero-point correction= 0.602907 (Hartree/Particle)

Thermal correction to Energy=	0.631130
Thermal correction to Enthalpy=	0.632074
Thermal correction to Gibbs Free Energy=	0.547756
Sum of electronic and zero-point Energies=	-1158.573145
Sum of electronic and thermal Energies=	-1158.544922
Sum of electronic and thermal Enthalpies=	-1158.543978
Sum of electronic and thermal Free Energies=	-1158.628296

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	396.040	113.563	177.462
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.348
Vibrational	394.262	107.601	98.454

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.322097	-1.703218	-0.707358
2	6	0	-4.555802	-1.190576	-1.461316
3	1	0	-4.284771	-0.774450	-2.438686
4	1	0	-5.248789	-2.019026	-1.634595
5	1	0	-5.095714	-0.424665	-0.896726
6	6	0	-2.743146	-2.906715	-1.461434
7	1	0	-2.503555	-2.649764	-2.499954
8	1	0	-1.839298	-3.297740	-0.978482
9	1	0	-3.474598	-3.719727	-1.484927
10	6	0	-3.723141	-2.147765	0.705543
11	1	0	-2.881879	-2.593157	1.250125
12	1	0	-4.136511	-1.330518	1.305388
13	1	0	-4.498448	-2.916197	0.634509
14	6	0	-2.250591	-0.578563	-0.673313
15	1	0	-1.865277	-0.434933	-1.685583
16	6	0	-2.754013	0.772245	-0.132615
17	1	0	-3.301667	0.605785	0.803224
18	1	0	-3.470946	1.168621	-0.865427
19	7	0	-1.119469	-0.975363	0.184618
20	7	0	-1.682271	1.731843	0.146586
21	6	0	-2.188737	2.848073	0.976134
22	1	0	-2.582252	2.400013	1.895566
23	1	0	-1.326077	3.447947	1.276175
24	6	0	-1.014372	2.164674	-1.095686

25	1	0	-0.474289	1.294811	-1.490984
26	1	0	-1.761434	2.449749	-1.854912
27	6	0	-0.015305	3.295327	-0.889971
28	1	0	-0.508192	4.248695	-0.684245
29	1	0	0.666138	3.061337	-0.067802
30	1	0	0.575479	3.420857	-1.801419
31	6	0	-3.249544	3.732647	0.325466
32	1	0	-4.165382	3.179330	0.097060
33	1	0	-3.519274	4.542170	1.008542
34	1	0	-2.886540	4.189340	-0.600618
35	1	0	-1.290495	-0.826107	1.181426
36	6	0	0.100758	-1.282452	-0.112481
37	6	0	1.063980	-1.389479	1.062214
38	6	0	0.519271	-1.451820	-1.535474
39	1	0	1.028503	-0.538469	-1.867425
40	1	0	1.246529	-2.260567	-1.623840
41	1	0	-0.323443	-1.660565	-2.192659
42	6	0	0.481056	-2.317611	2.141508
43	1	0	-0.373030	-1.869454	2.658386
44	1	0	0.174673	-3.276338	1.711040
45	1	0	1.241530	-2.522108	2.898068
46	6	0	1.214911	0.091721	1.613992
47	8	0	-0.001362	0.603762	2.030489
48	6	0	4.525967	1.124169	-1.681966
49	6	0	4.983113	-0.193849	-1.689114
50	6	0	4.318536	-1.155247	-0.938480
51	6	0	3.198795	-0.827565	-0.169825
52	6	0	2.766618	0.501642	-0.168958
53	6	0	3.418583	1.476027	-0.921182
54	1	0	5.038340	1.883106	-2.263942
55	1	0	5.851554	-0.468662	-2.277518
56	1	0	4.666262	-2.185595	-0.944865
57	1	0	3.050865	2.496309	-0.887650
58	8	0	1.637869	0.900977	0.516868
59	6	0	2.457870	-1.869486	0.633521
60	1	0	2.390737	-2.814373	0.081479
61	1	0	3.018698	-2.108194	1.544361
62	6	0	2.195573	0.198440	2.771022
63	1	0	3.204555	-0.108597	2.489934
64	1	0	2.217236	1.248064	3.070258
65	1	0	1.852594	-0.393672	3.622143
66	1	0	-0.461406	1.079768	1.275913

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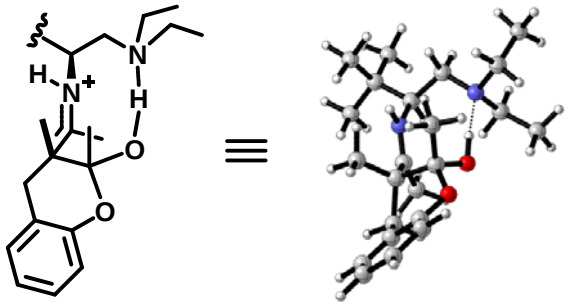
(10) Int4a



E_{sol} = -1159.575432

Zero-point correction=	0.601950 (Hartree/Particle)
Thermal correction to Energy=	0.630527
Thermal correction to Enthalpy=	0.631471
Thermal correction to Gibbs Free Energy=	0.545012
Sum of electronic and zero-point Energies=	-1158.554519
Sum of electronic and thermal Energies=	-1158.525942
Sum of electronic and thermal Enthalpies=	-1158.524998
Sum of electronic and thermal Free Energies=	-1158.611457

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	395.662	114.155	181.968
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.632
Vibrational	393.884	108.194	102.676

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.199336	-2.271670	-0.319801
2	6	0	4.721826	-2.138431	-0.185634
3	1	0	5.008172	-1.800885	0.817216
4	1	0	5.189121	-3.112978	-0.353267
5	1	0	5.140750	-1.442730	-0.918405
6	6	0	2.718273	-3.424506	0.570821
7	1	0	3.017355	-3.271520	1.614348
8	1	0	1.628943	-3.542757	0.533882
9	1	0	3.159966	-4.367213	0.234999
10	6	0	2.833968	-2.574191	-1.779579
11	1	0	1.766249	-2.795053	-1.903559
12	1	0	3.109325	-1.761414	-2.460173
13	1	0	3.375499	-3.465100	-2.110389
14	6	0	2.533653	-0.963227	0.183816

15	1	0	2.695004	-0.898851	1.260742
16	6	0	3.026277	0.335754	-0.477878
17	1	0	2.898271	0.254902	-1.565248
18	1	0	4.105097	0.422514	-0.285228
19	7	0	1.078354	-1.016110	-0.050422
20	1	0	0.493070	1.511169	0.291384
21	7	0	2.300811	1.526863	-0.022907
22	6	0	2.441104	2.636176	-0.992239
23	1	0	2.077628	2.260395	-1.955701
24	1	0	1.745809	3.424341	-0.688346
25	6	0	2.715788	1.898540	1.347686
26	1	0	2.429013	1.071948	2.009347
27	1	0	3.812957	1.982318	1.404882
28	6	0	2.064739	3.175496	1.864967
29	1	0	2.431017	4.063652	1.343774
30	1	0	0.975539	3.137063	1.770444
31	1	0	2.309326	3.295522	2.923211
32	6	0	3.848440	3.204649	-1.154165
33	1	0	4.559556	2.446829	-1.497830
34	1	0	3.836304	4.004878	-1.898559
35	1	0	4.225893	3.629572	-0.219493
36	1	0	0.841115	-0.964225	-1.040262
37	6	0	0.075704	-0.960709	0.763877
38	6	0	-1.299697	-0.731718	0.148083
39	6	0	0.261057	-1.051035	2.237124
40	1	0	1.266888	-1.344229	2.531981
41	1	0	0.015437	-0.068556	2.656691
42	1	0	-0.450401	-1.771864	2.648031
43	6	0	-1.514642	-1.662306	-1.059327
44	1	0	-0.806971	-1.505734	-1.879713
45	1	0	-1.446958	-2.709446	-0.745805
46	1	0	-2.512742	-1.502646	-1.472956
47	6	0	-1.284232	0.831543	-0.215330
48	8	0	-0.421282	1.473000	0.679164
49	6	0	-5.963534	0.465790	-0.770596
50	6	0	-6.015600	-0.790209	-0.169414
51	6	0	-4.891520	-1.303064	0.475986
52	6	0	-3.722513	-0.552627	0.532974
53	6	0	-3.685232	0.693206	-0.087204
54	6	0	-4.790376	1.217708	-0.742158
55	1	0	-6.840479	0.863528	-1.270739
56	1	0	-6.931408	-1.370420	-0.201272
57	1	0	-4.926962	-2.282105	0.946916
58	1	0	-4.723116	2.197911	-1.201849

59	8	0	-2.535341	1.440027	0.019671
60	6	0	-2.431792	-0.970144	1.172728
61	1	0	-2.252518	-0.352678	2.061224
62	1	0	-2.464532	-2.021090	1.480751
63	6	0	-0.897751	1.134851	-1.660105
64	1	0	-0.887872	2.222637	-1.764308
65	1	0	0.099741	0.761066	-1.923461
66	1	0	-1.629916	0.722518	-2.358420

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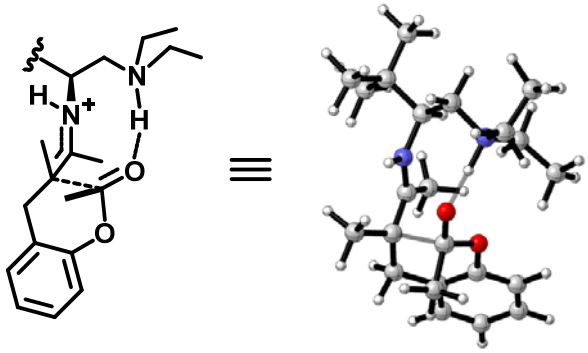
(11) TS_3



E_{sol} = -1159.565358

Zero-point correction=	0.600008 (Hartree/Particle)
Thermal correction to Energy=	0.628193
Thermal correction to Enthalpy=	0.629137
Thermal correction to Gibbs Free Energy=	0.544983
Sum of electronic and zero-point Energies=	-1158.554813
Sum of electronic and thermal Energies=	-1158.526628
Sum of electronic and thermal Enthalpies=	-1158.525683
Sum of electronic and thermal Free Energies=	-1158.609838

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	394.197	113.248	177.118
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.387
Vibrational	392.420	107.287	98.071

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.325567	-1.789365	-0.687928
2	6	0	-4.498007	-1.273546	-1.532998
3	1	0	-4.152218	-0.847255	-2.482651

4	1	0	-5.171876	-2.101651	-1.770865
5	1	0	-5.090076	-0.517848	-1.006627
6	6	0	-2.706457	-3.004831	-1.388113
7	1	0	-2.403081	-2.760957	-2.413174
8	1	0	-1.834652	-3.382325	-0.842792
9	1	0	-3.438090	-3.816001	-1.446359
10	6	0	-3.831801	-2.215895	0.695727
11	1	0	-3.032744	-2.654418	1.303863
12	1	0	-4.287318	-1.390505	1.254075
13	1	0	-4.602879	-2.983159	0.579124
14	6	0	-2.229286	-0.688245	-0.580929
15	1	0	-1.816214	-0.540612	-1.582418
16	6	0	-2.782765	0.653599	-0.076811
17	1	0	-3.263709	0.515549	0.897185
18	1	0	-3.532542	1.031691	-0.775369
19	7	0	-1.140944	-1.102713	0.301098
20	7	0	-1.743178	1.705820	0.106505
21	6	0	-2.255695	2.827865	0.961441
22	1	0	-2.576665	2.362490	1.897246
23	1	0	-1.392627	3.450995	1.200713
24	6	0	-1.150634	2.152647	-1.193125
25	1	0	-0.622766	1.284921	-1.595533
26	1	0	-1.971872	2.399965	-1.874353
27	6	0	-0.176125	3.308988	-1.037417
28	1	0	-0.680582	4.248929	-0.801617
29	1	0	0.565615	3.086350	-0.265975
30	1	0	0.351555	3.446145	-1.984527
31	6	0	-3.375204	3.635098	0.326550
32	1	0	-4.267165	3.031832	0.136604
33	1	0	-3.663398	4.435432	1.012204
34	1	0	-3.063785	4.103448	-0.611560
35	1	0	-1.354421	-1.065550	1.293228
36	6	0	0.138431	-1.357403	0.006722
37	6	0	1.050718	-1.488953	1.075721
38	6	0	0.552080	-1.373835	-1.436332
39	1	0	0.795568	-0.361777	-1.782693
40	1	0	1.449260	-1.977678	-1.571572
41	1	0	-0.235029	-1.788386	-2.068490
42	6	0	0.487719	-2.034549	2.382757
43	1	0	-0.127823	-1.292892	2.907770
44	1	0	-0.119486	-2.932816	2.215496
45	1	0	1.297953	-2.312604	3.060171
46	6	0	1.169166	0.477217	1.492028
47	8	0	0.000784	0.876983	1.778098

48	6	0	4.719272	0.963339	-1.663846
49	6	0	5.158233	-0.351280	-1.511203
50	6	0	4.420327	-1.233960	-0.734833
51	6	0	3.241248	-0.846620	-0.087468
52	6	0	2.830216	0.481167	-0.248729
53	6	0	3.556213	1.377291	-1.031908
54	1	0	5.284592	1.664824	-2.268358
55	1	0	6.069185	-0.685539	-1.995939
56	1	0	4.757286	-2.261759	-0.620765
57	1	0	3.191130	2.395466	-1.122778
58	8	0	1.650436	0.981244	0.277722
59	6	0	2.483954	-1.868833	0.738877
60	1	0	2.526484	-2.839219	0.224530
61	1	0	3.020677	-2.025672	1.681830
62	6	0	2.191454	0.497561	2.615147
63	1	0	3.155875	0.070425	2.343498
64	1	0	2.340499	1.554142	2.860201
65	1	0	1.787699	-0.000697	3.496226
66	1	0	-0.918207	1.284417	0.720695

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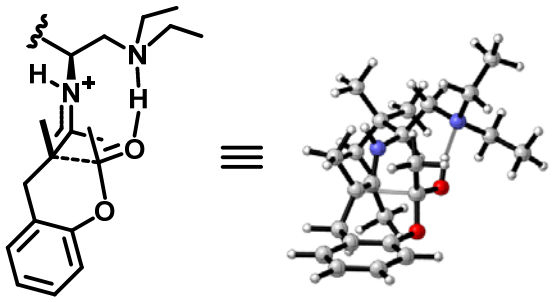
(12) TS3a



E_{sol} = -1159.546747

Zero-point correction=	0.598202 (Hartree/Particle)
Thermal correction to Energy=	0.626816
Thermal correction to Enthalpy=	0.627760
Thermal correction to Gibbs Free Energy=	0.541331
Sum of electronic and zero-point Energies=	-1158.539586
Sum of electronic and thermal Energies=	-1158.510972
Sum of electronic and thermal Enthalpies=	-1158.510028
Sum of electronic and thermal Free Energies=	-1158.596457

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	393.333	113.626	181.905
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660

Rotational	0.889	2.981	35.613
Vibrational	391.555	107.664	102.632

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.469973	-1.997378	-0.018912
2	6	0	-4.802654	-1.596086	-0.666722
3	1	0	-4.654516	-1.225635	-1.688219
4	1	0	-5.459393	-2.469105	-0.724735
5	1	0	-5.337393	-0.830533	-0.097120
6	6	0	-2.918511	-3.218387	-0.764695
7	1	0	-2.774906	-3.002000	-1.830094
8	1	0	-1.963880	-3.553208	-0.346249
9	1	0	-3.624540	-4.050701	-0.690063
10	6	0	-3.694913	-2.356939	1.454252
11	1	0	-2.764925	-2.669396	1.944414
12	1	0	-4.128691	-1.525360	2.020611
13	1	0	-4.392077	-3.196999	1.528839
14	6	0	-2.454916	-0.830864	-0.162035
15	1	0	-2.364038	-0.606947	-1.227249
16	6	0	-2.867484	0.455342	0.570300
17	1	0	-2.706611	0.318522	1.646909
18	1	0	-3.939336	0.639022	0.431020
19	7	0	-1.122322	-1.194318	0.331406
20	1	0	-0.677245	1.301589	-0.357211
21	7	0	-2.089449	1.634306	0.134786
22	6	0	-1.988542	2.647781	1.213181
23	1	0	-1.559722	2.137693	2.083253
24	1	0	-1.255802	3.395457	0.893676
25	6	0	-2.671779	2.188892	-1.116489
26	1	0	-2.613056	1.398173	-1.871962
27	1	0	-3.737756	2.404759	-0.959796
28	6	0	-1.947844	3.424791	-1.631694
29	1	0	-2.095419	4.289843	-0.979649
30	1	0	-0.875524	3.240204	-1.740339
31	1	0	-2.345703	3.685177	-2.615339
32	6	0	-3.299355	3.319875	1.607059
33	1	0	-4.050071	2.589691	1.924471
34	1	0	-3.123146	3.998454	2.445307
35	1	0	-3.718105	3.910088	0.787369
36	1	0	-1.047273	-1.192414	1.342671
37	6	0	0.025449	-1.393858	-0.329990

38	6	0	1.244142	-1.291676	0.357653
39	6	0	0.001061	-1.594953	-1.815513
40	1	0	-0.956270	-1.347427	-2.268253
41	1	0	0.771753	-0.984600	-2.290977
42	1	0	0.211210	-2.648765	-2.031274
43	6	0	1.262076	-1.378940	1.871588
44	1	0	0.579215	-0.690905	2.380442
45	1	0	1.014541	-2.397128	2.199861
46	1	0	2.266172	-1.158035	2.246265
47	6	0	1.276619	0.820941	-0.275441
48	8	0	0.198625	1.129417	-0.942111
49	6	0	5.795923	0.919976	0.089849
50	6	0	5.957201	-0.380761	0.559603
51	6	0	4.909593	-1.296962	0.470408
52	6	0	3.689652	-0.924809	-0.088634
53	6	0	3.558456	0.387148	-0.531699
54	6	0	4.578653	1.318765	-0.461048
55	1	0	6.614583	1.628806	0.152813
56	1	0	6.903913	-0.687169	0.991817
57	1	0	5.042757	-2.315006	0.826831
58	1	0	4.419280	2.323507	-0.838396
59	8	0	2.332749	0.750954	-1.105008
60	6	0	2.514355	-1.854850	-0.266416
61	1	0	2.382941	-2.047274	-1.334644
62	1	0	2.745571	-2.822136	0.198033
63	6	0	1.461996	1.473890	1.069117
64	1	0	1.619513	2.541886	0.875203
65	1	0	0.553239	1.364200	1.663240
66	1	0	2.316878	1.085151	1.619798

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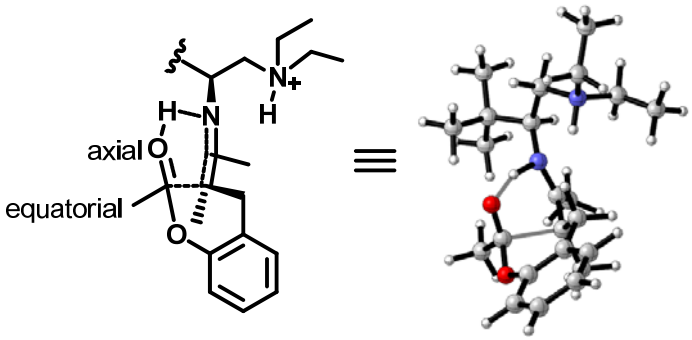
(13) TS3b



E_{sol} = -1159.541174

Zero-point correction= 0.596876 (Hartree/Particle)

Thermal correction to Energy= 0.625665

Thermal correction to Enthalpy= 0.626609

Thermal correction to Gibbs Free Energy= 0.540013
Sum of electronic and zero-point Energies= -1158.517019
Sum of electronic and thermal Energies= -1158.488230
Sum of electronic and thermal Enthalpies= -1158.487286
Sum of electronic and thermal Free Energies= -1158.573881

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	392.611	113.932	182.256
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.592
Vibrational	390.833	107.970	103.004

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.938108	-1.840463	-0.710345
2	6	0	4.430448	-1.653178	-1.025659
3	1	0	5.006912	-1.399771	-0.127260
4	1	0	4.838291	-2.586495	-1.424113
5	1	0	4.605169	-0.881158	-1.782912
6	6	0	2.792989	-3.080366	0.177008
7	1	0	3.406380	-2.999229	1.082335
8	1	0	1.755524	-3.245026	0.479427
9	1	0	3.121994	-3.969331	-0.369243
10	6	0	2.157845	-2.053529	-2.012738
11	1	0	1.096218	-2.247734	-1.835488
12	1	0	2.229738	-1.196497	-2.692785
13	1	0	2.576319	-2.913720	-2.544384
14	6	0	2.421184	-0.598919	0.076833
15	1	0	2.897928	-0.628755	1.064763
16	6	0	2.862224	0.708673	-0.622677
17	1	0	2.645848	0.657684	-1.693527
18	1	0	3.925595	0.907514	-0.482764
19	7	0	0.975973	-0.502912	0.240010
20	1	0	1.132437	1.503565	0.004492
21	7	0	2.092596	1.882077	-0.090322
22	6	0	2.044619	3.040069	-1.052358
23	1	0	1.661439	2.630712	-1.990148
24	1	0	1.300654	3.739177	-0.666187
25	6	0	2.524945	2.249373	1.302310
26	1	0	2.415870	1.338265	1.895795

27	1	0	3.587186	2.500291	1.254633
28	6	0	1.692729	3.372495	1.895301
29	1	0	1.882403	4.334099	1.412761
30	1	0	0.622288	3.148708	1.834471
31	1	0	1.949281	3.478010	2.951750
32	6	0	3.393948	3.707727	-1.245740
33	1	0	4.145095	3.011654	-1.627988
34	1	0	3.281664	4.506154	-1.982585
35	1	0	3.765738	4.162145	-0.323495
36	1	0	0.239069	-0.668645	-0.671804
37	6	0	0.251982	-0.859839	1.317056
38	6	0	-1.139104	-0.584250	1.254016
39	6	0	0.826796	-1.629208	2.472808
40	1	0	1.915817	-1.671086	2.465987
41	1	0	0.485732	-1.200877	3.419303
42	1	0	0.459917	-2.662776	2.442219
43	6	0	-2.017113	-1.028177	2.403518
44	1	0	-1.792384	-2.045228	2.735671
45	1	0	-1.914100	-0.362109	3.270374
46	1	0	-3.066999	-1.007005	2.098518
47	6	0	-1.573338	-1.656616	-0.366366
48	8	0	-0.890159	-1.062850	-1.281489
49	6	0	-5.406463	1.016358	-1.203861
50	6	0	-4.821546	2.162476	-0.664748
51	6	0	-3.582778	2.074379	-0.043676
52	6	0	-2.897926	0.859821	0.044020
53	6	0	-3.502671	-0.266274	-0.506946
54	6	0	-4.749623	-0.203236	-1.121146
55	1	0	-6.377332	1.073307	-1.684895
56	1	0	-5.334476	3.116632	-0.721811
57	1	0	-3.131193	2.963751	0.391059
58	1	0	-5.178917	-1.115427	-1.521095
59	8	0	-2.942586	-1.515342	-0.370736
60	6	0	-1.537733	0.783592	0.686367
61	1	0	-0.806941	1.097925	-0.067963
62	1	0	-1.502901	1.512743	1.510509
63	6	0	-1.280617	-3.105488	-0.045326
64	1	0	-1.630884	-3.706527	-0.890337
65	1	0	-0.205004	-3.258751	0.055805
66	1	0	-1.800833	-3.437328	0.855002

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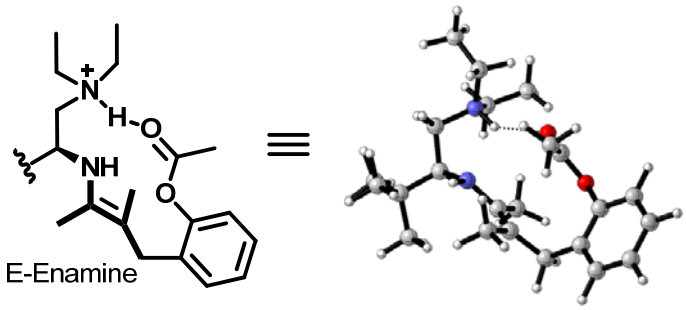
(14) Int5



E_{sol} = -1159.586895

Zero-point correction=	0.602015 (Hartree/Particle)
Thermal correction to Energy=	0.631921
Thermal correction to Enthalpy=	0.632865
Thermal correction to Gibbs Free Energy=	0.543134
Sum of electronic and zero-point Energies=	-1158.575145
Sum of electronic and thermal Energies=	-1158.545240
Sum of electronic and thermal Enthalpies=	-1158.544295
Sum of electronic and thermal Free Energies=	-1158.634026

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	396.536	115.761	188.854
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.669
Vibrational	394.759	109.799	109.526

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.060523	-2.336514	-0.094376
2	6	0	2.403498	-0.957561	0.182757
3	1	0	2.417831	-0.825557	1.269972
4	6	0	3.158872	0.223884	-0.449565
5	1	0	3.135566	0.143783	-1.540171
6	1	0	4.198597	0.290641	-0.123720
7	7	0	1.018872	-0.843559	-0.263598
8	1	0	1.458272	1.267895	0.005427
9	7	0	2.468828	1.505794	-0.079876
10	6	0	2.509100	2.543006	-1.168167
11	1	0	2.107867	2.046006	-2.055515
12	1	0	1.797850	3.318119	-0.877221
13	6	0	2.948147	2.015923	1.252557
14	1	0	2.827457	1.186906	1.954127

15	1	0	4.018592	2.209411	1.146938
16	6	0	2.192140	3.242564	1.732658
17	1	0	2.423335	4.126008	1.132005
18	1	0	1.112355	3.074165	1.718242
19	1	0	2.498205	3.455310	2.759622
20	6	0	3.899217	3.097057	-1.418961
21	1	0	4.621258	2.307830	-1.648922
22	1	0	3.858575	3.767234	-2.280587
23	1	0	4.269760	3.678209	-0.570400
24	1	0	0.886749	-1.280480	-1.169290
25	6	0	-0.090398	-1.039893	0.597738
26	6	0	-1.232342	-1.566432	0.114904
27	6	0	0.100268	-0.511148	1.993970
28	1	0	0.612156	0.457715	1.972178
29	1	0	-0.849714	-0.338820	2.494511
30	1	0	0.688891	-1.200005	2.611298
31	6	0	-1.313118	-2.117580	-1.293602
32	1	0	-0.731844	-3.044141	-1.400044
33	1	0	-2.348271	-2.356824	-1.554016
34	1	0	-0.955138	-1.417441	-2.059855
35	6	0	-2.510212	-1.661013	0.920050
36	1	0	-2.336862	-1.441502	1.975511
37	1	0	-2.871760	-2.696257	0.885799
38	6	0	-3.628866	-0.770421	0.410017
39	6	0	-4.854611	-1.308940	0.011890
40	6	0	-3.504680	0.619931	0.345361
41	6	0	-5.905836	-0.500588	-0.413581
42	1	0	-4.986417	-2.387214	0.050697
43	6	0	-4.541796	1.448204	-0.057057
44	6	0	-5.753924	0.882119	-0.441145
45	1	0	-6.846158	-0.951649	-0.712714
46	1	0	-4.392856	2.523832	-0.053978
47	1	0	-6.572980	1.520114	-0.755312
48	8	0	-2.296738	1.211650	0.742327
49	6	0	-1.380733	1.532600	-0.185123
50	6	0	-1.725523	1.356432	-1.640670
51	1	0	-2.273320	0.432599	-1.829637
52	1	0	-2.361609	2.187557	-1.963037
53	1	0	-0.798415	1.379771	-2.213686
54	8	0	-0.322114	1.999787	0.186700
55	6	0	3.054960	-2.686432	-1.587693
56	1	0	3.524133	-3.663807	-1.735510
57	1	0	2.039378	-2.763711	-1.994716
58	1	0	3.618786	-1.965665	-2.190408

59	6	0	2.260991	-3.394660	0.676592
60	1	0	2.275412	-3.191320	1.753999
61	1	0	1.215713	-3.429849	0.351874
62	1	0	2.698079	-4.385354	0.519362
63	6	0	4.507032	-2.331688	0.418888
64	1	0	4.915510	-3.346239	0.390681
65	1	0	5.163991	-1.704645	-0.193236
66	1	0	4.561680	-1.982865	1.457195

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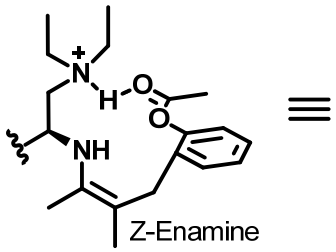
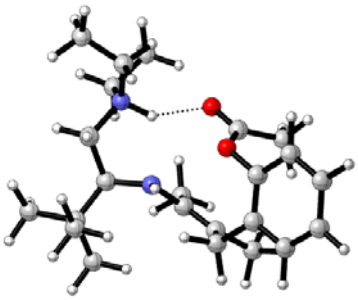
(15) Int5a





E_{sol} = -1159.587832

Zero-point correction=	0.601849 (Hartree/Particle)
Thermal correction to Energy=	0.631703
Thermal correction to Enthalpy=	0.632647
Thermal correction to Gibbs Free Energy=	0.543300
Sum of electronic and zero-point Energies=	-1158.579711
Sum of electronic and thermal Energies=	-1158.549857
Sum of electronic and thermal Enthalpies=	-1158.548913
Sum of electronic and thermal Free Energies=	-1158.638260

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	396.399	115.901	188.046
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.547
Vibrational	394.622	109.939	108.839

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.375153	2.507125	-0.624828
2	6	0	-2.115003	1.097975	-0.019858
3	1	0	-2.570256	1.100953	0.976935
4	6	0	-2.767836	-0.028359	-0.842318

5	1	0	-2.375229	-0.023742	-1.863895
6	1	0	-3.854739	0.061071	-0.888029
7	7	0	-0.715480	0.725909	0.137939
8	1	0	-1.457333	-1.250203	0.136602
9	7	0	-2.424104	-1.359707	-0.247333
10	6	0	-2.296442	-2.451742	-1.270561
11	1	0	-1.559266	-2.088411	-1.991522
12	1	0	-1.850788	-3.304617	-0.756084
13	6	0	-3.334832	-1.701170	0.898114
14	1	0	-3.273010	-0.858254	1.590830
15	1	0	-4.352458	-1.733748	0.499784
16	6	0	-2.955065	-2.996204	1.595588
17	1	0	-3.166710	-3.872412	0.977443
18	1	0	-1.896961	-3.001081	1.869676
19	1	0	-3.551050	-3.086321	2.506767
20	6	0	-3.613003	-2.805683	-1.936626
21	1	0	-4.077523	-1.938945	-2.416019
22	1	0	-3.426150	-3.550784	-2.713187
23	1	0	-4.325302	-3.240896	-1.230608
24	1	0	-0.196136	0.781475	-0.730575
25	6	0	0.061667	1.028096	1.280748
26	6	0	1.358424	1.390834	1.192059
27	6	0	-0.656967	0.784695	2.580765
28	1	0	-1.122997	-0.209755	2.569854
29	1	0	0.017898	0.830371	3.433078
30	1	0	-1.441922	1.528335	2.758450
31	6	0	2.265040	1.598425	2.382319
32	1	0	1.984697	1.016069	3.261940
33	1	0	3.293297	1.319432	2.122004
34	1	0	2.292730	2.654672	2.677387
35	6	0	2.042092	1.699358	-0.126096
36	1	0	2.544045	2.670018	-0.022688
37	1	0	1.324681	1.836282	-0.943415
38	6	0	3.096210	0.694291	-0.554030
39	6	0	4.413069	1.094127	-0.795509
40	6	0	2.805731	-0.657141	-0.749447
41	6	0	5.383627	0.193935	-1.226777
42	1	0	4.674882	2.138439	-0.646856
43	6	0	3.749933	-1.570188	-1.196569
44	6	0	5.051490	-1.141291	-1.435675
45	1	0	6.396325	0.538848	-1.406725
46	1	0	3.454874	-2.602705	-1.359009
47	1	0	5.797317	-1.846836	-1.785741
48	8	0	1.495728	-1.108446	-0.531991

49	6	0	1.191954	-1.725996	0.629378
50	6	0	2.271606	-1.925561	1.655771
51	1	0	2.960747	-2.708908	1.325267
52	1	0	2.855558	-1.015145	1.802600
53	1	0	1.796482	-2.234148	2.585963
54	8	0	0.054885	-2.122992	0.779584
55	6	0	-1.709169	2.672958	-1.995425
56	1	0	-1.909929	3.677261	-2.380662
57	1	0	-0.619956	2.568136	-1.936911
58	1	0	-2.088942	1.964109	-2.739616
59	6	0	-1.798628	3.548967	0.341899
60	1	0	-2.282513	3.486470	1.324033
61	1	0	-0.720790	3.417249	0.481797
62	1	0	-1.969273	4.557305	-0.047809
63	6	0	-3.886662	2.738098	-0.760843
64	1	0	-4.082236	3.785082	-1.011061
65	1	0	-4.332071	2.129762	-1.555507
66	1	0	-4.410310	2.520374	0.178056

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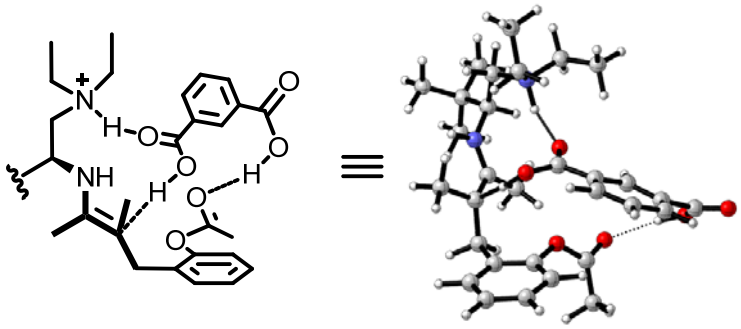
(16) TS5



E_{sol} = -1768.942138

Zero-point correction=	0.729706 (Hartree/Particle)
Thermal correction to Energy=	0.770400
Thermal correction to Enthalpy=	0.771345
Thermal correction to Gibbs Free Energy=	0.656281
Sum of electronic and zero-point Energies=	-1767.590262
Sum of electronic and thermal Energies=	-1767.549567
Sum of electronic and thermal Enthalpies=	-1767.548623
Sum of electronic and thermal Free Energies=	-1767.663687

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	483.434	156.072	242.172
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.752

Rotational	0.889	2.981	37.565
Vibrational	481.656	150.111	159.855

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.023503	0.304090	-1.339465
2	6	0	3.718092	-0.140608	-0.625258
3	1	0	3.134906	-0.740718	-1.330983
4	6	0	3.962153	-0.985067	0.632426
5	1	0	4.269393	-0.344013	1.464543
6	1	0	4.752395	-1.720872	0.475186
7	7	0	2.892285	0.993942	-0.210906
8	1	0	1.867587	-1.250633	0.579091
9	7	0	2.718456	-1.714894	1.039337
10	6	0	2.438624	-1.631810	2.512321
11	1	0	2.404451	-0.563652	2.745157
12	1	0	1.427901	-2.019662	2.658921
13	6	0	2.728415	-3.120409	0.497157
14	1	0	2.843253	-3.013006	-0.586032
15	1	0	3.626577	-3.609024	0.885453
16	6	0	1.471773	-3.906189	0.827697
17	1	0	1.402774	-4.142207	1.892825
18	1	0	0.576254	-3.364515	0.513690
19	1	0	1.507760	-4.853863	0.285141
20	6	0	3.454490	-2.375780	3.359616
21	1	0	4.477931	-2.038406	3.168249
22	1	0	3.238438	-2.192444	4.414395
23	1	0	3.406970	-3.455737	3.196593
24	1	0	3.235792	1.480008	0.610391
25	6	0	1.742631	1.463610	-0.708618
26	6	0	0.982955	2.357343	0.084752
27	6	0	1.246274	0.983622	-2.039646
28	1	0	1.737224	0.073716	-2.377690
29	1	0	0.174748	0.782652	-1.989359
30	1	0	1.431592	1.767193	-2.783905
31	6	0	1.635074	2.985966	1.309934
32	1	0	2.464000	3.656962	1.047569
33	1	0	0.887566	3.572344	1.850169
34	1	0	1.995111	2.235067	2.024180
35	6	0	-0.056759	3.262065	-0.588613
36	1	0	-0.247605	2.940668	-1.615122
37	1	0	0.353660	4.277874	-0.648230

38	6	0	-1.357981	3.301214	0.177179
39	6	0	-1.682373	4.333306	1.056250
40	6	0	-2.263947	2.245385	0.059343
41	6	0	-2.857975	4.300013	1.803402
42	1	0	-1.004267	5.178244	1.149163
43	6	0	-3.425596	2.174084	0.814631
44	6	0	-3.723893	3.217066	1.688765
45	1	0	-3.093075	5.116163	2.478229
46	1	0	-4.074267	1.307049	0.730976
47	1	0	-4.632696	3.178193	2.279945
48	8	0	-1.897510	1.211961	-0.800143
49	6	0	-2.665029	0.808063	-1.847676
50	6	0	-3.899248	1.594706	-2.197243
51	1	0	-3.752780	2.667506	-2.058743
52	1	0	-4.149693	1.367626	-3.232834
53	1	0	-4.734127	1.284909	-1.562179
54	8	0	-2.287569	-0.162199	-2.458590
55	6	0	5.911203	1.127921	-0.399190
56	1	0	6.815520	1.443211	-0.927969
57	1	0	5.407211	2.038977	-0.055752
58	1	0	6.235201	0.553385	0.476242
59	6	0	4.644354	1.152151	-2.559543
60	1	0	4.030648	0.581245	-3.265903
61	1	0	4.096869	2.055620	-2.272719
62	1	0	5.549744	1.466908	-3.086300
63	6	0	5.786312	-0.936116	-1.825578
64	1	0	6.603889	-0.628984	-2.484010
65	1	0	6.237405	-1.505515	-1.006894
66	1	0	5.136420	-1.606432	-2.400802
67	6	0	-0.403472	-0.565157	0.788180
68	8	0	-0.158942	0.459754	1.514072
69	1	0	0.378437	1.343401	0.718441
70	8	0	0.426411	-1.036749	-0.032777
71	6	0	-1.750714	-1.191481	0.900255
72	6	0	-2.205538	-1.964252	-0.166707
73	6	0	-2.588983	-0.922908	1.982859
74	6	0	-3.512523	-2.438657	-0.171922
75	1	0	-1.536384	-2.140548	-1.002577
76	6	0	-3.871283	-1.468942	2.013330
77	1	0	-2.230716	-0.282956	2.783337
78	6	0	-4.334019	-2.222389	0.937490
79	1	0	-4.517545	-1.289345	2.866651
80	1	0	-5.335817	-2.641491	0.929498
81	6	0	-4.067295	-3.184294	-1.352677

82	8	0	-4.923694	-4.019585	-1.244700
83	8	0	-3.546175	-2.857937	-2.548420
84	1	0	-3.049380	-2.019490	-2.511302

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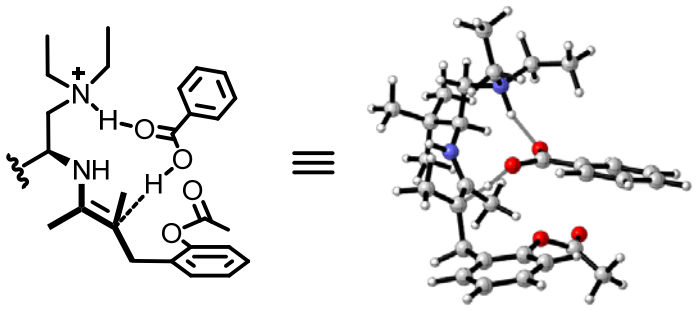
(17) TS6



E_{sol} = -1580.360747

Zero-point correction=	0.714921 (Hartree/Particle)
Thermal correction to Energy=	0.752345
Thermal correction to Enthalpy=	0.753290
Thermal correction to Gibbs Free Energy=	0.646728
Sum of electronic and zero-point Energies=	-1579.103772
Sum of electronic and thermal Energies=	-1579.066348
Sum of electronic and thermal Enthalpies=	-1579.065404
Sum of electronic and thermal Free Energies=	-1579.171965

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	472.104	145.928	224.277
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	44.500
Rotational	0.889	2.981	36.984
Vibrational	470.326	139.967	142.793

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.695411	-1.155350	0.844170
2	6	0	3.421189	-0.367943	0.428918
3	1	0	3.018776	0.124870	1.320104
4	6	0	3.695402	0.706532	-0.630292
5	1	0	3.852033	0.239471	-1.607182
6	1	0	4.592938	1.279281	-0.392345
7	7	0	2.374297	-1.230903	-0.116620
8	1	0	1.691652	1.256346	-0.233710
9	7	0	2.546057	1.661533	-0.748040

10	6	0	2.082427	1.854715	-2.163085
11	1	0	1.861566	0.852157	-2.539489
12	1	0	1.128206	2.383747	-2.108595
13	6	0	2.846890	2.946043	-0.022507
14	1	0	3.049017	2.652063	1.012200
15	1	0	3.770581	3.349689	-0.446858
16	6	0	1.715094	3.956650	-0.080742
17	1	0	1.568668	4.353824	-1.088634
18	1	0	0.780239	3.520547	0.278746
19	1	0	1.973804	4.797433	0.567399
20	6	0	3.088706	2.586949	-3.031800
21	1	0	4.060833	2.084414	-3.051920
22	1	0	2.713391	2.619361	-4.057040
23	1	0	3.238311	3.618909	-2.703310
24	1	0	2.539950	-1.540126	-1.068277
25	6	0	1.221997	-1.646474	0.426800
26	6	0	0.232449	-2.183294	-0.430858
27	6	0	0.970487	-1.458289	1.891197
28	1	0	-0.045772	-1.096317	2.061656
29	1	0	1.095741	-2.426823	2.390264
30	1	0	1.651508	-0.747390	2.354107
31	6	0	0.621558	-2.556653	-1.855257
32	1	0	1.354431	-3.374126	-1.891053
33	1	0	-0.270694	-2.884268	-2.394835
34	1	0	1.013718	-1.700750	-2.419012
35	6	0	-0.878099	-3.064626	0.153672
36	1	0	-0.913519	-2.974645	1.241426
37	1	0	-0.644998	-4.112641	-0.073466
38	6	0	-2.232712	-2.726983	-0.424016
39	6	0	-2.836967	-3.494813	-1.415665
40	6	0	-2.892108	-1.569304	0.008381
41	6	0	-4.052720	-3.112918	-1.980580
42	1	0	-2.347762	-4.408623	-1.744763
43	6	0	-4.082631	-1.149966	-0.571603
44	6	0	-4.664588	-1.936856	-1.565066
45	1	0	-4.512104	-3.727008	-2.747819
46	1	0	-4.542138	-0.215980	-0.273272
47	1	0	-5.600155	-1.618578	-2.013368
48	8	0	-2.198976	-0.859823	0.976212
49	6	0	-2.686396	-0.266495	2.110273
50	6	0	-4.169049	-0.109698	2.291910
51	1	0	-4.727705	-0.993403	1.979767
52	1	0	-4.348238	0.105253	3.344480
53	1	0	-4.503763	0.748481	1.697188

54	8	0	-1.867082	0.131012	2.893325
55	6	0	5.347667	-1.822282	-0.372850
56	1	0	6.216729	-2.404987	-0.053800
57	1	0	4.661379	-2.516911	-0.871507
58	1	0	5.703293	-1.090363	-1.106833
59	6	0	4.298704	-2.231586	1.861410
60	1	0	3.863175	-1.788730	2.764145
61	1	0	3.580202	-2.942422	1.441524
62	1	0	5.185480	-2.796041	2.164331
63	6	0	5.691199	-0.197925	1.513319
64	1	0	6.513715	-0.771201	1.950738
65	1	0	6.138606	0.511658	0.809963
66	1	0	5.216632	0.367408	2.324157
67	6	0	-0.631032	1.041059	-0.223066
68	8	0	-0.635016	0.192719	-1.183311
69	1	0	-0.227740	-0.950048	-0.690928
70	8	0	0.338319	1.172267	0.568751
71	6	0	-2.837010	1.912978	-1.029101
72	6	0	-1.832388	1.912796	-0.058537
73	6	0	-1.964767	2.693966	1.093143
74	6	0	-3.103212	3.472597	1.273454
75	6	0	-4.102081	3.480945	0.299607
76	6	0	-3.968614	2.703757	-0.851235
77	1	0	-2.720564	1.282957	-1.905414
78	1	0	-1.188547	2.646513	1.850385
79	1	0	-3.214766	4.069471	2.173072
80	1	0	-4.987874	4.093605	0.438331
81	1	0	-4.747498	2.714913	-1.607700

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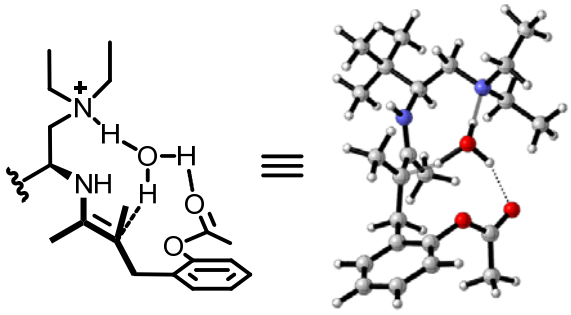
(18) TS_7



E_{sol} = -1235.987856

Zero-point correction=	0.620465 (Hartree/Particle)
Thermal correction to Energy=	0.652439
Thermal correction to Enthalpy=	0.653383
Thermal correction to Gibbs Free Energy=	0.558149

Sum of electronic and zero-point Energies= -1234.922271
Sum of electronic and thermal Energies= -1234.890298
Sum of electronic and thermal Enthalpies= -1234.889353
Sum of electronic and thermal Free Energies= -1234.984587

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	409.412	122.337	200.436
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	36.069
Vibrational	407.634	116.376	120.567

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.786651	-2.127809	0.182770
2	6	0	2.862680	-0.880902	0.275075
3	1	0	2.883392	-0.557166	1.316597
4	6	0	3.291313	0.299613	-0.609151
5	1	0	3.221838	0.003494	-1.662877
6	1	0	4.344737	0.531310	-0.404289
7	7	0	1.479937	-1.237698	-0.057931
8	1	0	0.872140	1.298712	-0.620936
9	7	0	2.458915	1.503528	-0.430127
10	6	0	2.634312	2.435330	-1.574480
11	1	0	2.381768	1.867120	-2.475715
12	1	0	1.871037	3.213242	-1.481873
13	6	0	2.731317	2.146790	0.872970
14	1	0	2.520609	1.409379	1.653897
15	1	0	3.800286	2.394337	0.954811
16	6	0	1.878715	3.381919	1.129790
17	1	0	2.137269	4.210067	0.465116
18	1	0	0.810757	3.165988	1.017870
19	1	0	2.040930	3.724641	2.154648
20	6	0	4.014883	3.067844	-1.713623
21	1	0	4.801496	2.316709	-1.831146
22	1	0	4.031795	3.702699	-2.602993
23	1	0	4.265542	3.698131	-0.855351
24	1	0	1.356669	-1.548039	-1.016583
25	6	0	0.357353	-1.106046	0.653132
26	6	0	-0.889812	-1.154043	-0.003877
27	6	0	0.448077	-0.716280	2.103407

28	1	0	0.208931	0.349152	2.217791
29	1	0	-0.277285	-1.284591	2.688184
30	1	0	1.432306	-0.902262	2.529602
31	6	0	-0.940457	-1.785664	-1.389497
32	1	0	-0.580149	-2.823167	-1.386295
33	1	0	-1.966191	-1.794358	-1.762233
34	1	0	-0.355967	-1.216141	-2.122722
35	6	0	-2.146322	-1.282094	0.866828
36	1	0	-2.092949	-0.558908	1.691103
37	1	0	-2.178567	-2.273954	1.337709
38	6	0	-3.455924	-1.083511	0.136764
39	6	0	-4.381471	-2.117904	-0.007343
40	6	0	-3.798698	0.153870	-0.410753
41	6	0	-5.590400	-1.918691	-0.670992
42	1	0	-4.148075	-3.094672	0.408161
43	6	0	-4.988762	0.376928	-1.084481
44	6	0	-5.895249	-0.672929	-1.211015
45	1	0	-6.292697	-2.739636	-0.768771
46	1	0	-5.185147	1.356869	-1.507996
47	1	0	-6.832861	-0.515531	-1.733165
48	8	0	-2.856144	1.181467	-0.337308
49	6	0	-2.754574	1.967249	0.758461
50	6	0	-3.890738	1.970946	1.739521
51	1	0	-4.039637	0.972556	2.161541
52	1	0	-3.665010	2.684280	2.529984
53	1	0	-4.820185	2.247981	1.234038
54	8	0	-1.748186	2.633545	0.862969
55	6	0	3.738795	-2.771689	-1.208752
56	1	0	4.425210	-3.623247	-1.241057
57	1	0	2.743061	-3.162485	-1.450394
58	1	0	4.047200	-2.079177	-1.999231
59	6	0	3.313851	-3.144868	1.229106
60	1	0	3.396627	-2.734320	2.242743
61	1	0	2.275071	-3.446588	1.060116
62	1	0	3.933799	-4.045214	1.186696
63	6	0	5.231526	-1.724968	0.508885
64	1	0	5.838362	-2.623552	0.655217
65	1	0	5.695253	-1.148627	-0.297018
66	1	0	5.285324	-1.135464	1.432107
67	8	0	-0.127586	1.221317	-0.886248
68	1	0	-0.604586	0.176770	-0.376509
69	1	0	-0.641134	1.953669	-0.476139

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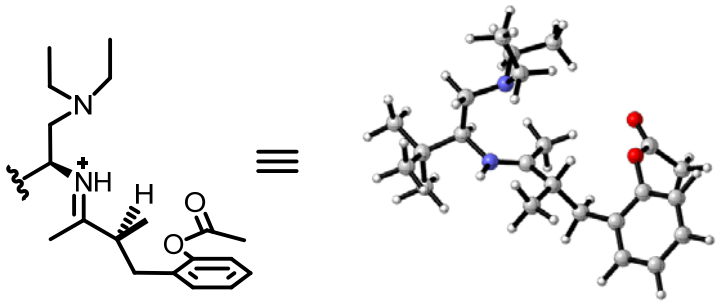
(19) Int7



E_{sol} = -1159.576987

Zero-point correction=	0.599556 (Hartree/Particle)
Thermal correction to Energy=	0.629852
Thermal correction to Enthalpy=	0.630796
Thermal correction to Gibbs Free Energy=	0.537702
Sum of electronic and zero-point Energies=	-1158.566982
Sum of electronic and thermal Energies=	-1158.536687
Sum of electronic and thermal Enthalpies=	-1158.535742
Sum of electronic and thermal Free Energies=	-1158.628836

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	395.238	116.031	195.932
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.948
Vibrational	393.460	110.070	116.324

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.083303	-1.711461	-0.507211
2	6	0	-3.052157	-0.560717	-0.456489
3	1	0	-3.022524	-0.096322	-1.445774
4	6	0	-3.289886	0.535620	0.612152
5	1	0	-3.321231	0.059644	1.599430
6	1	0	-4.279691	0.979765	0.440776
7	7	0	-1.707017	-1.083071	-0.171411
8	7	0	-2.226926	1.526220	0.575520
9	6	0	-1.681413	1.857233	1.896778
10	1	0	-1.409476	0.907721	2.377013
11	1	0	-0.744047	2.402463	1.746657
12	6	0	-2.598628	2.689506	-0.238359
13	1	0	-2.904835	2.310504	-1.223784
14	1	0	-3.484723	3.198274	0.176540

15	6	0	-1.462975	3.688918	-0.412027
16	1	0	-1.254486	4.227228	0.516945
17	1	0	-0.538653	3.200032	-0.736274
18	1	0	-1.739020	4.432894	-1.163327
19	6	0	-2.613179	2.651725	2.810464
20	1	0	-3.571617	2.139007	2.947012
21	1	0	-2.159342	2.783429	3.796205
22	1	0	-2.817326	3.646816	2.403880
23	1	0	-1.682689	-1.762333	0.587436
24	6	0	-0.568317	-0.587998	-0.535994
25	6	0	0.678201	-1.000298	0.203845
26	6	0	-0.434796	0.371438	-1.667666
27	1	0	0.356586	1.095848	-1.449266
28	1	0	-0.133503	-0.193388	-2.559728
29	1	0	-1.352087	0.909841	-1.887353
30	6	0	0.468969	-2.059723	1.283576
31	1	0	0.106259	-3.004568	0.859966
32	1	0	1.425113	-2.267457	1.769436
33	1	0	-0.218659	-1.727971	2.069395
34	6	0	1.844716	-1.389500	-0.742929
35	1	0	1.842841	-0.748736	-1.630458
36	1	0	1.697611	-2.418392	-1.090477
37	6	0	3.175364	-1.268416	-0.039838
38	6	0	3.942246	-2.373584	0.327970
39	6	0	3.659261	0.000879	0.293058
40	6	0	5.147582	-2.212209	1.008736
41	1	0	3.591045	-3.370747	0.074544
42	6	0	4.845677	0.181602	0.987114
43	6	0	5.596340	-0.937357	1.341931
44	1	0	5.732361	-3.083502	1.283323
45	1	0	5.163875	1.186131	1.247975
46	1	0	6.529405	-0.809776	1.880369
47	8	0	2.857314	1.091811	-0.031484
48	6	0	3.028688	1.768120	-1.213208
49	6	0	4.330455	1.570223	-1.940363
50	1	0	4.476743	0.516021	-2.194366
51	1	0	4.308906	2.174409	-2.845453
52	1	0	5.171951	1.870928	-1.310662
53	8	0	2.128885	2.471344	-1.583349
54	6	0	-4.139435	-2.506759	0.805198
55	1	0	-4.912368	-3.276786	0.724471
56	1	0	-3.204711	-3.040123	1.025489
57	1	0	-4.395440	-1.880444	1.665020
58	6	0	-3.704455	-2.653011	-1.658142

59	1	0	-3.688531	-2.119638	-2.615214
60	1	0	-2.719891	-3.109272	-1.505362
61	1	0	-4.435400	-3.462824	-1.739409
62	6	0	-5.466054	-1.108453	-0.789830
63	1	0	-6.180127	-1.909839	-1.000612
64	1	0	-5.851051	-0.541804	0.062977
65	1	0	-5.441421	-0.446637	-1.663082
66	1	0	0.970752	-0.052343	0.683051

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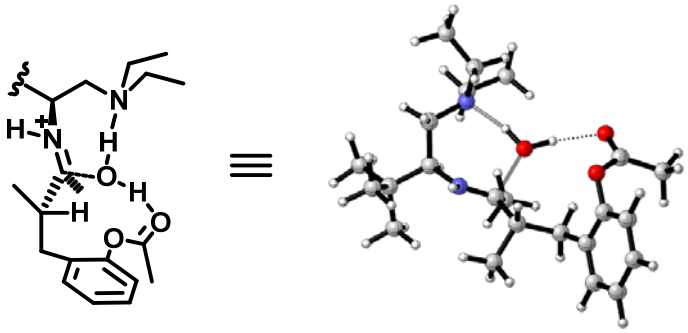
(20) TS8



E_{sol} = -1236.00794

Zero-point correction=	0.625755 (Hartree/Particle)
Thermal correction to Energy=	0.657104
Thermal correction to Enthalpy=	0.658048
Thermal correction to Gibbs Free Energy=	0.564421
Sum of electronic and zero-point Energies=	-1234.939029
Sum of electronic and thermal Energies=	-1234.907680
Sum of electronic and thermal Enthalpies=	-1234.906735
Sum of electronic and thermal Free Energies=	-1235.000363

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	412.339	121.245	197.055
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	36.155
Vibrational	410.562	115.283	117.100

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.616695	-2.210347	0.152101
2	6	0	-2.819507	-0.902470	-0.107286
3	1	0	-2.935454	-0.682595	-1.171632

4	6	0	-3.283259	0.313256	0.712550
5	1	0	-3.005874	0.156794	1.761745
6	1	0	-4.378526	0.381506	0.675710
7	7	0	-1.386302	-1.130316	0.128744
8	7	0	-2.668148	1.568406	0.257842
9	6	0	-2.536540	2.547787	1.360111
10	1	0	-1.969194	2.046587	2.151622
11	1	0	-1.902124	3.365007	1.002495
12	6	0	-3.370745	2.111238	-0.918537
13	1	0	-3.432591	1.310187	-1.664415
14	1	0	-4.409032	2.371476	-0.663347
15	6	0	-2.654219	3.307874	-1.528566
16	1	0	-2.709505	4.190865	-0.886690
17	1	0	-1.597437	3.080567	-1.708874
18	1	0	-3.114127	3.568316	-2.484775
19	6	0	-3.845733	3.102772	1.912918
20	1	0	-4.511047	2.306476	2.261760
21	1	0	-3.635979	3.755273	2.764246
22	1	0	-4.382689	3.696731	1.167807
23	1	0	-1.152373	-1.401712	1.080354
24	6	0	-0.358226	-0.795048	-0.636808
25	6	0	0.991010	-1.338390	-0.182704
26	6	0	-0.613796	-0.533149	-2.095359
27	1	0	0.287253	-0.175096	-2.589677
28	1	0	-0.927344	-1.470136	-2.571231
29	1	0	-1.397428	0.212010	-2.239867
30	6	0	0.954940	-2.873417	-0.170378
31	1	0	0.728080	-3.271495	-1.165925
32	1	0	1.932720	-3.257325	0.133486
33	1	0	0.212371	-3.264763	0.530694
34	6	0	2.174205	-0.838706	-1.041551
35	1	0	1.972446	0.180335	-1.384701
36	1	0	2.265751	-1.466279	-1.935841
37	6	0	3.468479	-0.869114	-0.263546
38	6	0	4.362877	-1.938193	-0.314761
39	6	0	3.783005	0.193228	0.589213
40	6	0	5.511462	-1.949898	0.475150
41	1	0	4.159232	-2.768184	-0.986863
42	6	0	4.909367	0.197016	1.395706
43	6	0	5.779653	-0.889654	1.335940
44	1	0	6.194906	-2.790430	0.419610
45	1	0	5.092384	1.037617	2.057548
46	1	0	6.667696	-0.901627	1.958659
47	8	0	2.877622	1.256183	0.634318

48	6	0	2.981509	2.243965	-0.292758
49	6	0	4.341783	2.552250	-0.848929
50	1	0	4.697522	1.712916	-1.454708
51	1	0	4.267825	3.446068	-1.465761
52	1	0	5.064282	2.701793	-0.043124
53	8	0	1.969202	2.821247	-0.617157
54	6	0	-3.457625	-2.698151	1.597748
55	1	0	-4.062228	-3.597490	1.749858
56	1	0	-2.422380	-2.975174	1.832463
57	1	0	-3.795274	-1.953768	2.326910
58	6	0	-3.099984	-3.287204	-0.811237
59	1	0	-3.252931	-2.986098	-1.854766
60	1	0	-2.034259	-3.489039	-0.661831
61	1	0	-3.642208	-4.224412	-0.654428
62	6	0	-5.103530	-1.967787	-0.143985
63	1	0	-5.630648	-2.925861	-0.178031
64	1	0	-5.589355	-1.358591	0.623304
65	1	0	-5.242982	-1.477839	-1.115082
66	1	0	1.132515	-0.967409	0.838833
67	8	0	-0.061045	1.029460	-0.008832
68	1	0	0.577889	1.733199	-0.269448
69	1	0	-1.015551	1.362697	-0.009007

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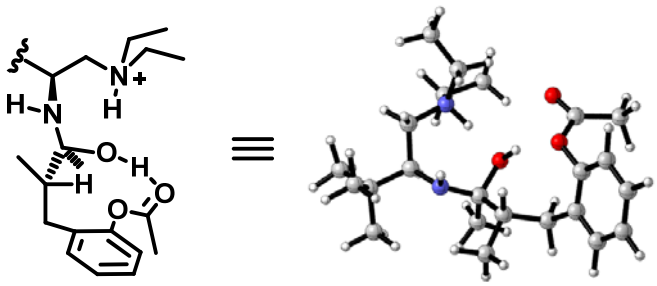
(21) Int8



E_{sol} = -1236.032121

Zero-point correction=	0.629580 (Hartree/Particle)
Thermal correction to Energy=	0.660849
Thermal correction to Enthalpy=	0.661794
Thermal correction to Gibbs Free Energy=	0.568389
Sum of electronic and zero-point Energies=	-1234.962839
Sum of electronic and thermal Energies=	-1234.931569
Sum of electronic and thermal Enthalpies=	-1234.930625
Sum of electronic and thermal Free Energies=	-1235.024030

E (Thermal)	CV	S
KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin

Total	414.689	121.245	196.587
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.986
Vibrational	412.912	115.284	116.800

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.818289	-1.824438	-0.420601
2	6	0	2.765585	-0.753128	-0.009601
3	1	0	2.907410	-0.586973	1.066096
4	6	0	2.994513	0.587538	-0.733991
5	1	0	2.715048	0.492651	-1.787906
6	1	0	4.036914	0.909234	-0.689163
7	7	0	1.404213	-1.242110	-0.202152
8	7	0	2.156093	1.682141	-0.140352
9	6	0	1.610444	2.639287	-1.162993
10	1	0	1.109153	2.014231	-1.907854
11	1	0	0.835841	3.225861	-0.665654
12	6	0	2.850255	2.349578	1.009821
13	1	0	3.174884	1.540999	1.670962
14	1	0	3.744469	2.841961	0.618473
15	6	0	1.929965	3.309070	1.744685
16	1	0	1.708129	4.201124	1.153958
17	1	0	0.986757	2.819833	2.006722
18	1	0	2.418021	3.633425	2.666423
19	6	0	2.680916	3.507473	-1.797989
20	1	0	3.487626	2.911519	-2.235591
21	1	0	2.228710	4.092971	-2.601582
22	1	0	3.112326	4.212391	-1.082668
23	1	0	1.070816	-1.125286	-1.155242
24	6	0	0.360950	-1.038477	0.772542
25	6	0	-0.936820	-1.668563	0.220621
26	6	0	0.749869	-1.581614	2.140771
27	1	0	-0.114518	-1.554056	2.809019
28	1	0	1.113705	-2.607430	2.061436
29	1	0	1.528280	-0.965606	2.599744
30	6	0	-0.825379	-3.174179	-0.010849
31	1	0	-0.666764	-3.703734	0.934431
32	1	0	-1.755801	-3.548439	-0.449553
33	1	0	-0.002339	-3.421360	-0.685678
34	6	0	-2.170055	-1.341165	1.105674

35	1	0	-1.957836	-0.475940	1.743541
36	1	0	-2.371117	-2.182732	1.776811
37	6	0	-3.397585	-1.065131	0.272782
38	6	0	-4.461590	-1.961187	0.168164
39	6	0	-3.483121	0.113485	-0.473474
40	6	0	-5.556191	-1.689606	-0.650345
41	1	0	-4.428038	-2.884782	0.739844
42	6	0	-4.549073	0.396615	-1.312988
43	6	0	-5.600089	-0.513700	-1.393412
44	1	0	-6.371498	-2.402389	-0.713750
45	1	0	-4.545252	1.308263	-1.902752
46	1	0	-6.443800	-0.304890	-2.042369
47	8	0	-2.384203	0.982565	-0.421015
48	6	0	-2.413395	2.179304	0.241318
49	6	0	-3.709383	2.622689	0.854490
50	1	0	-4.122967	1.833189	1.488426
51	1	0	-3.515263	3.519409	1.440264
52	1	0	-4.450258	2.841060	0.081156
53	8	0	-1.369817	2.778765	0.300260
54	6	0	3.667877	-2.197631	-1.899369
55	1	0	4.388419	-2.978479	-2.161817
56	1	0	2.667372	-2.592025	-2.107411
57	1	0	3.859417	-1.347969	-2.565569
58	6	0	3.581810	-3.070699	0.439090
59	1	0	3.706614	-2.843995	1.505160
60	1	0	2.575258	-3.468398	0.284354
61	1	0	4.304822	-3.849268	0.177010
62	6	0	5.239049	-1.308182	-0.153339
63	1	0	5.954250	-2.132078	-0.232850
64	1	0	5.555114	-0.545037	-0.872222
65	1	0	5.329946	-0.891649	0.857808
66	1	0	-1.096979	-1.188592	-0.758003
67	8	0	0.105246	0.381129	0.989295
68	1	0	-0.605498	0.668896	0.385444
69	1	0	1.315630	1.210182	0.293710

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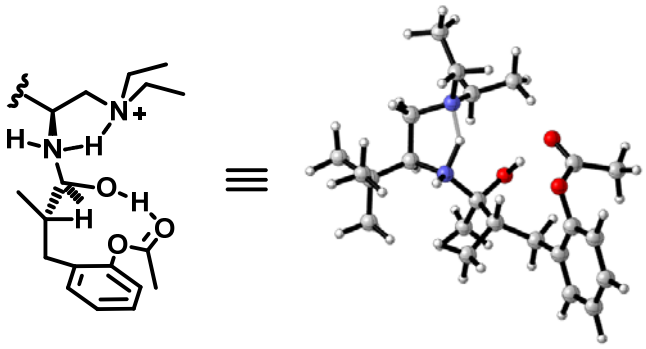
(22) TS9



E_{sol} = -1236.012111

Zero-point correction=	0.626250 (Hartree/Particle)
Thermal correction to Energy=	0.656668
Thermal correction to Enthalpy=	0.657613
Thermal correction to Gibbs Free Energy=	0.567028
Sum of electronic and zero-point Energies=	-1234.947285
Sum of electronic and thermal Energies=	-1234.916867
Sum of electronic and thermal Enthalpies=	-1234.915922
Sum of electronic and thermal Free Energies=	-1235.006507

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	412.066	119.608	190.652
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.984
Vibrational	410.288	113.646	110.867

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.378626	-2.206265	-0.458869
2	6	0	2.833205	-0.928852	0.227108
3	1	0	2.961203	-1.028018	1.309139
4	6	0	3.571886	0.368846	-0.249625
5	1	0	3.868361	0.264706	-1.296511
6	1	0	4.476832	0.532721	0.341549
7	7	0	1.391742	-0.640417	-0.022792
8	7	0	2.630373	1.491437	-0.137378
9	6	0	2.619073	2.389732	-1.313606
10	1	0	2.436032	1.755408	-2.188299
11	1	0	1.749126	3.043867	-1.211994
12	6	0	2.776076	2.178244	1.172594
13	1	0	2.570775	1.425618	1.939791

14	1	0	3.819967	2.498368	1.287620
15	6	0	1.841429	3.362416	1.355001
16	1	0	2.125720	4.208329	0.723095
17	1	0	0.803619	3.105847	1.132303
18	1	0	1.895835	3.695978	2.394112
19	6	0	3.898568	3.194664	-1.498607
20	1	0	4.773801	2.542848	-1.587636
21	1	0	3.832434	3.789850	-2.412669
22	1	0	4.068684	3.883282	-0.666041
23	1	0	1.088098	-1.077798	-0.893676
24	6	0	0.296025	-0.746484	1.041788
25	6	0	-1.003183	-1.044353	0.253107
26	6	0	0.595940	-1.754036	2.136204
27	1	0	-0.263441	-1.783864	2.810608
28	1	0	0.774731	-2.755147	1.748087
29	1	0	1.455150	-1.432369	2.729414
30	6	0	-1.067732	-2.466389	-0.308879
31	1	0	-1.111950	-3.210385	0.493474
32	1	0	-1.969628	-2.579126	-0.916712
33	1	0	-0.215843	-2.717674	-0.951919
34	6	0	-2.258404	-0.752960	1.101867
35	1	0	-2.112938	0.180173	1.659871
36	1	0	-2.375506	-1.535792	1.859884
37	6	0	-3.533413	-0.689421	0.287190
38	6	0	-4.586962	-1.578211	0.503340
39	6	0	-3.710395	0.269278	-0.717957
40	6	0	-5.757188	-1.512879	-0.250519
41	1	0	-4.484081	-2.335274	1.276154
42	6	0	-4.860108	0.351367	-1.485723
43	6	0	-5.894528	-0.550391	-1.245860
44	1	0	-6.558832	-2.218938	-0.062030
45	1	0	-4.928517	1.106727	-2.261802
46	1	0	-6.801254	-0.500313	-1.839085
47	8	0	-2.639626	1.119239	-1.012378
48	6	0	-2.274113	2.068956	-0.123155
49	6	0	-3.361957	2.714613	0.687023
50	1	0	-3.784449	1.996147	1.396318
51	1	0	-2.942660	3.561411	1.227627
52	1	0	-4.175170	3.040331	0.032887
53	8	0	-1.097513	2.352931	-0.054149
54	6	0	3.061999	-2.240062	-1.961470
55	1	0	3.558393	-3.103998	-2.413153
56	1	0	1.990413	-2.366697	-2.162974
57	1	0	3.410801	-1.352618	-2.498795

58	6	0	2.789294	-3.464987	0.186409
59	1	0	2.980887	-3.491032	1.264463
60	1	0	1.709114	-3.539128	0.021025
61	1	0	3.245793	-4.355556	-0.256347
62	6	0	4.902165	-2.227418	-0.256193
63	1	0	5.309952	-3.171787	-0.627717
64	1	0	5.406844	-1.419915	-0.795509
65	1	0	5.161784	-2.148291	0.805836
66	1	0	-1.002780	-0.338226	-0.588029
67	8	0	0.254789	0.496537	1.677700
68	1	0	-0.158190	1.154947	1.084095
69	1	0	1.577067	0.556158	-0.161659

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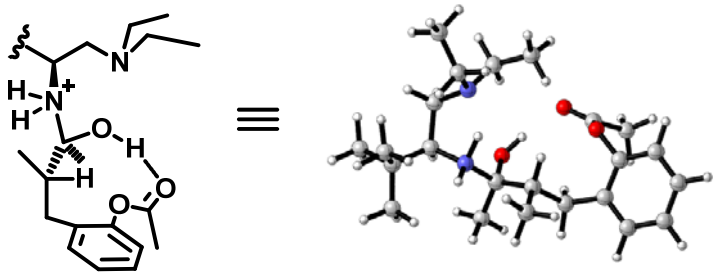
(23) Int9



E_{sol} = -1236.021767

Zero-point correction= 0.629308 (Hartree/Particle)
Thermal correction to Energy= 0.660020
Thermal correction to Enthalpy= 0.660964
Thermal correction to Gibbs Free Energy= 0.569849
Sum of electronic and zero-point Energies= -1234.951765
Sum of electronic and thermal Energies= -1234.921053
Sum of electronic and thermal Enthalpies= -1234.920108
Sum of electronic and thermal Free Energies= -1235.011224

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	414.169	120.433	191.768
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.905
Vibrational	412.391	114.471	112.063

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.115029	-1.351159	0.002061

2	6	0	2.908916	-0.543183	0.540091
3	1	0	2.743719	-0.827227	1.581771
4	6	0	3.078671	1.023404	0.486162
5	1	0	4.070447	1.269013	0.097633
6	1	0	3.029761	1.406531	1.507518
7	7	0	1.635801	-0.854394	-0.187921
8	7	0	2.033828	1.658503	-0.324027
9	6	0	2.508091	2.108220	-1.648974
10	1	0	3.023696	1.260354	-2.112623
11	1	0	1.626400	2.305896	-2.265582
12	6	0	1.292262	2.694691	0.424419
13	1	0	0.945559	2.234523	1.353736
14	1	0	1.969421	3.513438	0.707761
15	6	0	0.100376	3.238181	-0.344647
16	1	0	0.401836	3.841145	-1.205986
17	1	0	-0.546027	2.424760	-0.690363
18	1	0	-0.493384	3.872779	0.317460
19	6	0	3.419044	3.332689	-1.635849
20	1	0	4.293576	3.186526	-0.993503
21	1	0	3.779588	3.535838	-2.647500
22	1	0	2.888438	4.223440	-1.287915
23	1	0	1.785837	-1.521184	-0.947535
24	6	0	0.421692	-1.263156	0.665069
25	6	0	-0.802178	-1.212127	-0.272801
26	6	0	0.666591	-2.621114	1.297492
27	1	0	-0.211893	-2.892025	1.886568
28	1	0	0.849833	-3.399937	0.553491
29	1	0	1.514050	-2.573717	1.984270
30	6	0	-0.683211	-2.102522	-1.512676
31	1	0	-0.514286	-3.151002	-1.244917
32	1	0	-1.616303	-2.056239	-2.081108
33	1	0	0.110063	-1.783132	-2.197265
34	6	0	-2.092758	-1.552902	0.507678
35	1	0	-2.033502	-1.115714	1.513315
36	1	0	-2.156568	-2.638188	0.645547
37	6	0	-3.340818	-1.081503	-0.202980
38	6	0	-4.271176	-1.964552	-0.751840
39	6	0	-3.595804	0.285402	-0.347771
40	6	0	-5.402186	-1.495442	-1.417854
41	1	0	-4.105759	-3.034396	-0.653091
42	6	0	-4.706408	0.777270	-1.012891
43	6	0	-5.619909	-0.127302	-1.550710
44	1	0	-6.112126	-2.201465	-1.835200
45	1	0	-4.839368	1.850121	-1.110087

46	1	0	-6.496723	0.239505	-2.073626
47	8	0	-2.631328	1.170197	0.139727
48	6	0	-2.578573	1.456849	1.467414
49	6	0	-3.861705	1.393050	2.243892
50	1	0	-4.196037	0.353466	2.324848
51	1	0	-3.687030	1.800118	3.238155
52	1	0	-4.650729	1.948841	1.731369
53	8	0	-1.503170	1.752698	1.931178
54	6	0	4.458436	-0.996783	-1.450341
55	1	0	5.278262	-1.632830	-1.797456
56	1	0	3.618213	-1.161812	-2.138536
57	1	0	4.788751	0.041065	-1.557345
58	6	0	3.830385	-2.856995	0.094385
59	1	0	3.593319	-3.158728	1.119504
60	1	0	3.007140	-3.179405	-0.556557
61	1	0	4.714823	-3.418257	-0.220760
62	6	0	5.319099	-1.042170	0.903968
63	1	0	6.183683	-1.629077	0.580393
64	1	0	5.609174	0.012161	0.868312
65	1	0	5.107503	-1.303307	1.946492
66	1	0	-0.877303	-0.166163	-0.604480
67	8	0	0.352683	-0.331295	1.686990
68	1	0	-0.208215	0.438791	1.456329
69	1	0	1.396078	0.130849	-0.572333

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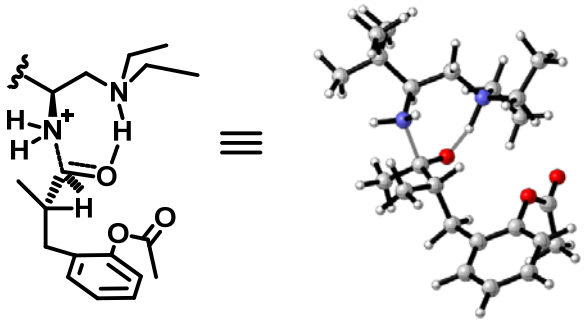
(24) TS10



E_{sol} = -1236.015972

Zero-point correction=	0.624643 (Hartree/Particle)
Thermal correction to Energy=	0.655889
Thermal correction to Enthalpy=	0.656833
Thermal correction to Gibbs Free Energy=	0.562647
Sum of electronic and zero-point Energies=	-1234.943488
Sum of electronic and thermal Energies=	-1234.912242
Sum of electronic and thermal Enthalpies=	-1234.911298
Sum of electronic and thermal Free Energies=	-1235.005484

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	411.577	120.363	198.232
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.924
Vibrational	409.799	114.401	118.508

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.382816	-1.057761	0.337673
2	6	0	-2.990852	-0.453126	0.016613
3	1	0	-2.966904	-0.195726	-1.049864
4	6	0	-2.650192	0.797665	0.839621
5	1	0	-2.335538	0.504765	1.848235
6	1	0	-3.534429	1.429354	0.953412
7	7	0	-1.884674	-1.438730	0.198197
8	7	0	-1.560461	1.600891	0.222753
9	6	0	-0.651692	2.218342	1.235390
10	1	0	-0.290496	1.392547	1.858398
11	1	0	0.214550	2.606617	0.695399
12	6	0	-2.133797	2.575200	-0.756144
13	1	0	-2.759429	1.985317	-1.433734
14	1	0	-2.788780	3.263983	-0.211223
15	6	0	-1.063011	3.309864	-1.541289
16	1	0	-0.472277	3.979601	-0.913064
17	1	0	-0.380622	2.603115	-2.020026
18	1	0	-1.545422	3.907787	-2.318311
19	6	0	-1.317965	3.288735	2.086158
20	1	0	-2.216849	2.919748	2.591349
21	1	0	-0.617615	3.618578	2.857018
22	1	0	-1.587876	4.167447	1.494085
23	1	0	-2.236262	-2.392898	0.101137
24	6	0	-0.567096	-1.229237	-0.986634
25	6	0	0.671104	-1.533727	-0.126649
26	6	0	-0.931937	-2.267620	-2.035855
27	1	0	-0.181584	-2.219621	-2.830240
28	1	0	-0.965013	-3.290004	-1.649294
29	1	0	-1.894942	-2.009617	-2.486329
30	6	0	0.700583	-2.909956	0.538766
31	1	0	0.738569	-3.710112	-0.207988

32	1	0	1.595470	-3.000722	1.160485
33	1	0	-0.158713	-3.103399	1.191533
34	6	0	1.924657	-1.332813	-1.008550
35	1	0	1.767563	-0.439193	-1.621777
36	1	0	2.030578	-2.185949	-1.689411
37	6	0	3.175402	-1.201078	-0.177657
38	6	0	4.080202	-2.251554	-0.012698
39	6	0	3.449169	-0.007055	0.493826
40	6	0	5.206883	-2.114385	0.794529
41	1	0	3.896509	-3.189508	-0.531079
42	6	0	4.559460	0.147851	1.311420
43	6	0	5.445598	-0.915565	1.460879
44	1	0	5.897324	-2.944018	0.903737
45	1	0	4.714934	1.094324	1.820344
46	1	0	6.318712	-0.805444	2.095372
47	8	0	2.541735	1.045728	0.374493
48	6	0	2.722044	2.000623	-0.586906
49	6	0	3.928799	1.878963	-1.478895
50	1	0	3.940819	0.911821	-1.989690
51	1	0	3.891764	2.688260	-2.205741
52	1	0	4.849068	1.945623	-0.892359
53	8	0	1.907892	2.881968	-0.661081
54	6	0	-4.528650	-1.372482	1.831271
55	1	0	-5.496894	-1.845532	2.019919
56	1	0	-3.756510	-2.067902	2.183649
57	1	0	-4.484668	-0.468135	2.447527
58	6	0	-4.586598	-2.340182	-0.485344
59	1	0	-4.389152	-2.170352	-1.550070
60	1	0	-3.969075	-3.181558	-0.146052
61	1	0	-5.622993	-2.675715	-0.390218
62	6	0	-5.463673	-0.055152	-0.094533
63	1	0	-6.451693	-0.510130	0.018385
64	1	0	-5.462888	0.856124	0.510005
65	1	0	-5.345532	0.226851	-1.147023
66	1	0	0.699543	-0.746062	0.642756
67	8	0	-0.657637	-0.006096	-1.418309
68	1	0	-0.948123	0.859389	-0.485340
69	1	0	-1.488816	-1.370891	1.138658

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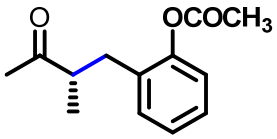
(25) *s*-Product



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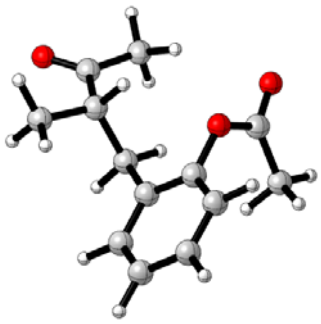

E_{sol} = -730.624107

Zero-point correction=	0.268410 (Hartree/Particle)
Thermal correction to Energy=	0.284597
Thermal correction to Enthalpy=	0.285542
Thermal correction to Gibbs Free Energy=	0.223607
Sum of electronic and zero-point Energies=	-730.122064
Sum of electronic and thermal Energies=	-730.105877
Sum of electronic and thermal Enthalpies=	-730.104932
Sum of electronic and thermal Free Energies=	-730.166867

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	178.588	59.827	130.352
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.070
Rotational	0.889	2.981	32.554
Vibrational	176.810	53.865	55.729

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.018264	-0.300344	-0.020728
2	6	0	1.635289	-0.859615	-0.342344
3	6	0	3.119384	1.195071	0.216626
4	1	0	2.354346	1.758367	-0.326700
5	1	0	2.991349	1.400961	1.285933
6	1	0	4.116933	1.533174	-0.068693
7	6	0	1.697542	-2.345994	-0.663771
8	1	0	2.073880	-2.905492	0.198373
9	1	0	0.707449	-2.727638	-0.929432
10	1	0	2.380693	-2.533176	-1.495212
11	6	0	0.661415	-0.563056	0.823628
12	1	0	0.792592	0.473571	1.158785
13	1	0	0.917700	-1.206265	1.673680

14	6	0	-0.775705	-0.790498	0.430146
15	6	0	-1.503226	-1.909494	0.836452
16	6	0	-1.418312	0.123848	-0.410168
17	6	0	-2.817140	-2.107682	0.417099
18	1	0	-1.024914	-2.636693	1.487850
19	6	0	-2.722417	-0.059118	-0.846762
20	6	0	-3.427172	-1.184307	-0.426925
21	1	0	-3.361488	-2.987500	0.744771
22	1	0	-3.162282	0.674967	-1.514780
23	1	0	-4.447410	-1.338332	-0.763033
24	8	0	-0.695163	1.218328	-0.869061
25	6	0	-0.608654	2.355875	-0.112321
26	6	0	-1.552456	2.472206	1.059816
27	1	0	-1.367841	1.678022	1.789300
28	1	0	-1.395467	3.445395	1.521673
29	1	0	-2.590145	2.372673	0.730278
30	8	0	0.190746	3.190238	-0.428997
31	1	0	1.274248	-0.295178	-1.213910
32	8	0	3.991852	-1.017093	0.042637

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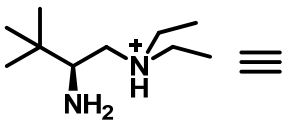
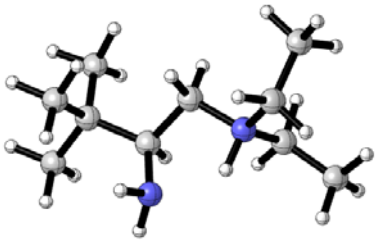
(26) Catalyst 1b





E_{sol} = -505.3966266

Zero-point correction=	0.356443 (Hartree/Particle)
Thermal correction to Energy=	0.371868
Thermal correction to Enthalpy=	0.372812
Thermal correction to Gibbs Free Energy=	0.314804
Sum of electronic and zero-point Energies=	-504.803713
Sum of electronic and thermal Energies=	-504.788288
Sum of electronic and thermal Enthalpies=	-504.787343
Sum of electronic and thermal Free Energies=	-504.845352

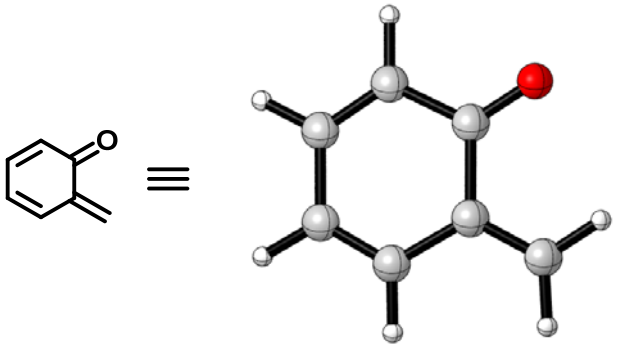
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.351	58.829	122.089
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	41.355
Rotational	0.889	2.981	31.350

Vibrational	231.573	52.867	49.384

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.373349	0.109341	0.170667
2	6	0	0.957687	-0.502239	0.001227
3	1	0	0.847897	-1.256050	0.791462
4	6	0	-0.169066	0.538150	0.180818
5	1	0	0.004276	1.408546	-0.458950
6	1	0	-0.266860	0.874914	1.214162
7	7	0	0.690609	-1.188945	-1.269355
8	7	0	-1.467005	-0.077325	-0.256853
9	6	0	-2.423329	0.912038	-0.861415
10	1	0	-1.870163	1.411267	-1.660766
11	1	0	-3.226790	0.336030	-1.324244
12	6	0	-2.069073	-0.931963	0.824301
13	1	0	-1.287987	-1.636864	1.117894
14	1	0	-2.272223	-0.277357	1.675135
15	6	0	-3.312867	-1.671512	0.363975
16	1	0	-4.161292	-1.001260	0.207486
17	1	0	-3.127812	-2.233311	-0.557053
18	1	0	-3.599432	-2.388308	1.136719
19	6	0	-2.959855	1.910948	0.148127
20	1	0	-2.156407	2.459830	0.647568
21	1	0	-3.579507	2.640412	-0.378244
22	1	0	-3.587803	1.434877	0.905898
23	1	0	1.077292	-2.128779	-1.271085
24	6	0	2.713222	1.105211	-0.945277
25	1	0	3.720056	1.500684	-0.781742
26	1	0	2.720654	0.638553	-1.937023
27	1	0	2.035980	1.965851	-0.970319
28	6	0	3.390611	-1.037994	0.143950
29	1	0	3.193293	-1.764362	0.940611
30	1	0	3.383209	-1.566318	-0.815421
31	1	0	4.401498	-0.647803	0.292556
32	6	0	2.454831	0.819023	1.528970
33	1	0	3.487017	1.117945	1.733219
34	1	0	1.845943	1.729456	1.558120
35	1	0	2.134912	0.159716	2.344852
36	1	0	-1.131039	-0.727407	-1.008623
37	1	0	1.117002	-0.692387	-2.050816

(27) Quione methide



E_{sol} = -345.4900226

Zero-point correction=	0.110538 (Hartree/Particle)
Thermal correction to Energy=	0.116938
Thermal correction to Enthalpy=	0.117882
Thermal correction to Gibbs Free Energy=	0.079969
Sum of electronic and zero-point Energies=	-345.269631
Sum of electronic and thermal Energies=	-345.263231
Sum of electronic and thermal Enthalpies=	-345.262287
Sum of electronic and thermal Free Energies=	-345.300200

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.379	24.673	79.794
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.893
Rotational	0.889	2.981	27.768
Vibrational	71.602	18.711	12.133

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.860910	-0.578138	0.000189
2	6	0	1.749612	0.875230	-0.000144
3	6	0	0.542480	1.469747	-0.000240
4	6	0	-0.682968	0.679004	-0.000063
5	6	0	-0.582107	-0.825231	-0.000102
6	6	0	0.781139	-1.383299	0.000280
7	1	0	2.857565	-1.012083	0.000363
8	1	0	2.659096	1.466830	-0.000282
9	1	0	0.448164	2.552718	-0.000428
10	1	0	0.859951	-2.465384	0.000523
11	8	0	-1.573383	-1.535435	-0.000373
12	6	0	-1.904459	1.234409	0.000329

13	1	0	-2.040962	2.312078	0.000560
14	1	0	-2.784394	0.598992	0.000750

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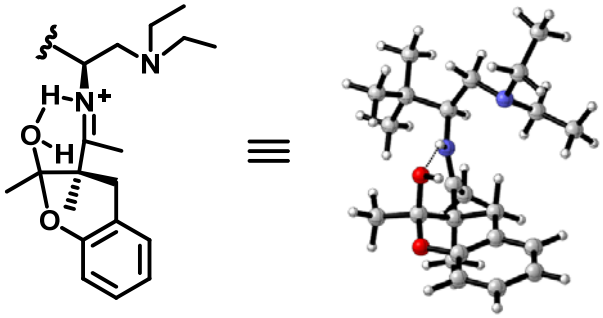
(28) Int3b



E_{sol} = -1159.578859

Zero-point correction=	0.601533 (Hartree/Particle)
Thermal correction to Energy=	0.630558
Thermal correction to Enthalpy=	0.631502
Thermal correction to Gibbs Free Energy=	0.544134
Sum of electronic and zero-point Energies=	-1158.566546
Sum of electronic and thermal Energies=	-1158.537520
Sum of electronic and thermal Enthalpies=	-1158.536576
Sum of electronic and thermal Free Energies=	-1158.623945

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	395.681	115.029	183.883
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.660
Rotational	0.889	2.981	35.544
Vibrational	393.904	109.068	104.679

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.461746	-1.468853	-0.375962
2	6	0	4.930973	-1.033980	-0.453680
3	1	0	5.300320	-0.689284	0.519029
4	1	0	5.547707	-1.883184	-0.762231
5	1	0	5.082467	-0.233996	-1.184319
6	6	0	3.354154	-2.692992	0.541103
7	1	0	3.747454	-2.479390	1.542016
8	1	0	2.319692	-3.044749	0.639991
9	1	0	3.937523	-3.521211	0.128203
10	6	0	2.957870	-1.843180	-1.776548

11	1	0	1.906482	-2.153771	-1.772899
12	1	0	3.068124	-1.025991	-2.495742
13	1	0	3.543597	-2.685479	-2.156633
14	6	0	2.638148	-0.304822	0.240450
15	1	0	2.938987	-0.188072	1.284605
16	6	0	2.794019	1.046245	-0.484457
17	1	0	2.804840	0.874212	-1.566971
18	1	0	3.779821	1.455463	-0.210008
19	7	0	1.199061	-0.618179	0.215986
20	1	0	-1.375382	-0.125417	-1.832869
21	7	0	1.696818	1.961153	-0.194028
22	6	0	1.637525	3.055760	-1.175875
23	1	0	1.547427	2.589708	-2.163580
24	1	0	0.703779	3.600364	-1.009321
25	6	0	1.738868	2.413094	1.200860
26	1	0	1.586271	1.529497	1.838186
27	1	0	2.734384	2.812496	1.464015
28	6	0	0.668801	3.441474	1.545096
29	1	0	0.868216	4.412524	1.085135
30	1	0	-0.320012	3.106359	1.215420
31	1	0	0.637944	3.591790	2.627156
32	6	0	2.819108	4.025255	-1.166162
33	1	0	3.763370	3.519415	-1.390232
34	1	0	2.672364	4.798358	-1.924841
35	1	0	2.924577	4.526598	-0.198827
36	1	0	0.734721	-0.406353	-0.680967
37	6	0	0.402142	-1.018298	1.146041
38	6	0	-1.091341	-1.056663	0.844166
39	6	0	0.882135	-1.332657	2.523479
40	1	0	1.955523	-1.211961	2.648037
41	1	0	0.358898	-0.692058	3.241548
42	1	0	0.615424	-2.365617	2.769403
43	6	0	-1.872116	-1.846486	1.903077
44	1	0	-1.537878	-2.884859	1.976329
45	1	0	-1.777316	-1.385044	2.889061
46	1	0	-2.932400	-1.854875	1.646035
47	6	0	-1.400423	-1.642363	-0.580758
48	8	0	-0.770727	-0.844379	-1.580382
49	6	0	-5.504624	0.760259	-0.858111
50	6	0	-4.992815	1.795237	-0.072791
51	6	0	-3.723243	1.680088	0.474800
52	6	0	-2.939304	0.544766	0.249036
53	6	0	-3.471804	-0.474083	-0.541774
54	6	0	-4.746750	-0.376902	-1.095365

55	1	0	-6.498341	0.840936	-1.285770
56	1	0	-5.585988	2.683315	0.116038
57	1	0	-3.323417	2.477027	1.097522
58	1	0	-5.116671	-1.199614	-1.697835
59	8	0	-2.783472	-1.648556	-0.788842
60	6	0	-1.552158	0.424766	0.829146
61	1	0	-0.836030	1.022130	0.247146
62	1	0	-1.536421	0.825695	1.850396
63	6	0	-0.928426	-3.068658	-0.778316
64	1	0	-1.138174	-3.357730	-1.809593
65	1	0	0.147514	-3.153941	-0.600670
66	1	0	-1.461872	-3.742667	-0.106605

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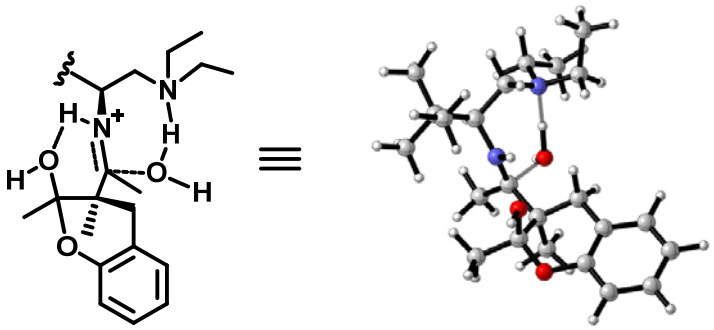
(29) TS4



E_{sol} = -1236.005853

Zero-point correction= 0.626119 (Hartree/Particle)

Thermal correction to Energy= 0.655772

Thermal correction to Enthalpy= 0.656717

Thermal correction to Gibbs Free Energy= 0.568869

Sum of electronic and zero-point Energies= -1234.929011

Sum of electronic and thermal Energies= -1234.899357

Sum of electronic and thermal Enthalpies= -1234.898413

Sum of electronic and thermal Free Energies= -1234.986261

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.809379	-2.132050	-0.911517
2	6	0	4.318904	-2.076717	-1.181845
3	1	0	4.877532	-1.786633	-0.283304
4	1	0	4.674945	-3.065343	-1.485909
5	1	0	4.574052	-1.381718	-1.987391
6	6	0	2.523227	-3.322921	0.010195
7	1	0	3.096196	-3.250784	0.942658

8	1	0	1.459654	-3.384181	0.261085
9	1	0	2.805238	-4.258523	-0.481735
10	6	0	2.047484	-2.316068	-2.229674
11	1	0	0.969310	-2.417461	-2.059740
12	1	0	2.217340	-1.486125	-2.925321
13	1	0	2.389207	-3.228197	-2.728389
14	6	0	2.351470	-0.842019	-0.183190
15	1	0	2.822996	-0.842690	0.806603
16	6	0	2.737873	0.467765	-0.892283
17	1	0	2.122547	0.581576	-1.791760
18	1	0	3.783628	0.438529	-1.215179
19	7	0	0.898829	-0.822677	0.008329
20	1	0	-1.991685	-1.983785	-1.748060
21	7	0	2.518162	1.644822	-0.018981
22	6	0	2.011431	2.821281	-0.770316
23	1	0	1.107267	2.487050	-1.290018
24	1	0	1.690727	3.565575	-0.035432
25	6	0	3.739534	1.933496	0.772273
26	1	0	3.977375	1.018336	1.327768
27	1	0	4.584030	2.119587	0.096215
28	6	0	3.567096	3.097745	1.737691
29	1	0	3.509190	4.056091	1.215528
30	1	0	2.663166	2.991043	2.346621
31	1	0	4.425421	3.141804	2.411738
32	6	0	3.003157	3.425949	-1.755730
33	1	0	3.362690	2.683994	-2.475532
34	1	0	2.517235	4.226751	-2.318171
35	1	0	3.869287	3.859400	-1.247447
36	1	0	0.356598	-0.670389	-0.838683
37	6	0	0.230369	-0.622938	1.156383
38	6	0	-1.291196	-0.387399	0.982757
39	6	0	0.707454	-1.377581	2.377216
40	1	0	1.796672	-1.397423	2.442910
41	1	0	0.303145	-0.955667	3.297026
42	1	0	0.362613	-2.413247	2.302827
43	6	0	-1.975765	-0.287129	2.351335
44	1	0	-1.943711	-1.224427	2.911810
45	1	0	-1.493414	0.494960	2.945147
46	1	0	-3.023286	-0.009610	2.224763
47	6	0	-1.954009	-1.536186	0.143366
48	8	0	-1.467951	-1.396328	-1.179460
49	6	0	-5.695881	1.163996	-1.014308
50	6	0	-4.901839	2.311232	-1.011359
51	6	0	-3.572506	2.225729	-0.618800

52	6	0	-3.006113	1.008198	-0.235584
53	6	0	-3.819002	-0.123623	-0.256067
54	6	0	-5.156193	-0.057610	-0.635616
55	1	0	-6.737780	1.220872	-1.311731
56	1	0	-5.321042	3.267146	-1.306344
57	1	0	-2.953436	3.119645	-0.600620
58	1	0	-5.748125	-0.966644	-0.625187
59	8	0	-3.349058	-1.360859	0.138699
60	6	0	-1.564962	0.920152	0.202314
61	1	0	-0.913917	0.988519	-0.679121
62	1	0	-1.322499	1.768910	0.845937
63	6	0	-1.733636	-2.953733	0.643051
64	1	0	-2.359599	-3.627172	0.050769
65	1	0	-0.689603	-3.243339	0.507244
66	1	0	-2.023779	-3.067304	1.689660
67	8	0	0.739941	1.061930	1.697373
68	1	0	1.520662	1.343224	0.958681
69	1	0	1.123089	1.057286	2.590003

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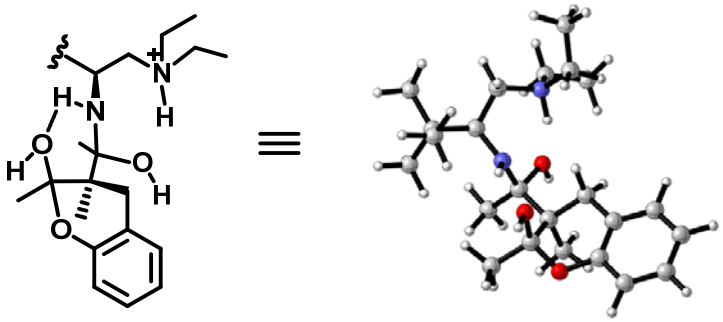
(30) Int6



E_{sol} = -1236.028894

Zero-point correction=	0.631622 (Hartree/Particle)
Thermal correction to Energy=	0.661560
Thermal correction to Enthalpy=	0.662504
Thermal correction to Gibbs Free Energy=	0.573451
Sum of electronic and zero-point Energies=	-1234.947116
Sum of electronic and thermal Energies=	-1234.917178
Sum of electronic and thermal Enthalpies=	-1234.916234
Sum of electronic and thermal Free Energies=	-1235.005287

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	415.135	120.989	187.427
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800

Rotational	0.889	2.981	35.757
Vibrational	413.358	115.028	107.870

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.147545	-1.817261	-0.809470
2	6	0	4.651132	-1.569591	-1.001485
3	1	0	5.138773	-1.310401	-0.053794
4	1	0	5.130650	-2.476348	-1.381516
5	1	0	4.853358	-0.773232	-1.725787
6	6	0	2.968179	-3.099945	0.007735
7	1	0	3.466440	-3.028101	0.981338
8	1	0	1.910297	-3.320321	0.177659
9	1	0	3.403788	-3.949024	-0.527897
10	6	0	2.487371	-2.018753	-2.181207
11	1	0	1.433597	-2.306856	-2.092715
12	1	0	2.548438	-1.131387	-2.821021
13	1	0	2.995958	-2.829650	-2.711520
14	6	0	2.509815	-0.625962	-0.034366
15	1	0	2.900027	-0.650014	0.991768
16	6	0	2.935495	0.724713	-0.665884
17	1	0	2.702782	0.721018	-1.733870
18	1	0	3.998991	0.935466	-0.540572
19	7	0	1.061368	-0.653056	0.022958
20	1	0	-1.670572	-1.798623	-2.048985
21	7	0	2.163250	1.853923	-0.049076
22	6	0	1.727765	2.884953	-1.051436
23	1	0	1.190153	2.331329	-1.825702
24	1	0	1.007354	3.533534	-0.548279
25	6	0	2.867826	2.417133	1.151012
26	1	0	3.062015	1.560635	1.799371
27	1	0	3.822711	2.820137	0.805711
28	6	0	2.033492	3.459319	1.873780
29	1	0	1.953916	4.393055	1.311414
30	1	0	1.029449	3.076585	2.080007
31	1	0	2.509642	3.691977	2.829006
32	6	0	2.884876	3.676994	-1.632366
33	1	0	3.640356	3.025936	-2.082032
34	1	0	2.503013	4.332444	-2.418280
35	1	0	3.367130	4.310615	-0.883197
36	1	0	0.582857	-1.039813	-0.782495
37	6	0	0.318231	-0.726802	1.259240

38	6	0	-1.224429	-0.632519	0.944938
39	6	0	0.700743	-1.885503	2.189521
40	1	0	1.783289	-1.893170	2.337751
41	1	0	0.233321	-1.770573	3.171750
42	1	0	0.402572	-2.855524	1.794926
43	6	0	-2.020625	-0.819530	2.246423
44	1	0	-1.979980	-1.842858	2.626350
45	1	0	-1.637980	-0.152284	3.026913
46	1	0	-3.070154	-0.561816	2.095126
47	6	0	-1.758545	-1.651835	-0.116541
48	8	0	-1.210714	-1.276873	-1.371175
49	6	0	-5.599008	1.006079	-1.064966
50	6	0	-4.886512	2.177039	-0.806601
51	6	0	-3.580373	2.096319	-0.340342
52	6	0	-2.956986	0.864308	-0.132860
53	6	0	-3.688694	-0.290348	-0.406045
54	6	0	-5.001700	-0.231182	-0.864565
55	1	0	-6.622369	1.056391	-1.422026
56	1	0	-5.351115	3.145335	-0.958733
57	1	0	-3.025725	3.006182	-0.121251
58	1	0	-5.530442	-1.159431	-1.053834
59	8	0	-3.164428	-1.548421	-0.198370
60	6	0	-1.540175	0.768186	0.375496
61	1	0	-0.844746	0.990844	-0.443656
62	1	0	-1.380841	1.516495	1.158626
63	6	0	-1.501175	-3.130835	0.128864
64	1	0	-2.100596	-3.699827	-0.587909
65	1	0	-0.447834	-3.365906	-0.038112
66	1	0	-1.797243	-3.444425	1.131569
67	8	0	0.715050	0.480248	1.952478
68	1	0	1.299914	1.400195	0.307378
69	1	0	0.451738	0.415851	2.882628

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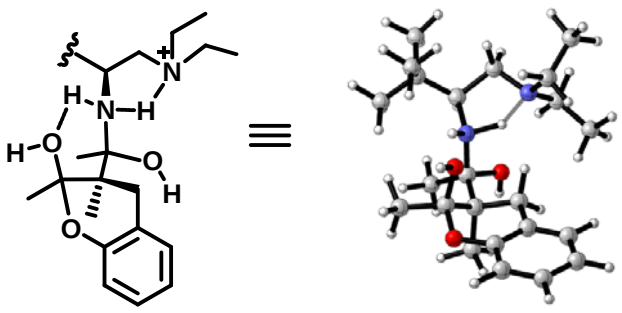
(31) TS11



E_{sol} = -1236.012858

Zero-point correction= 0.626877 (Hartree/Particle)

Thermal correction to Energy= 0.656466
Thermal correction to Enthalpy= 0.657411
Thermal correction to Gibbs Free Energy= 0.569963
Sum of electronic and zero-point Energies= -1234.939735
Sum of electronic and thermal Energies= -1234.910146
Sum of electronic and thermal Enthalpies= -1234.909202
Sum of electronic and thermal Free Energies= -1234.996649

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	411.939	119.547	184.048
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.654
Vibrational	410.161	113.585	104.594

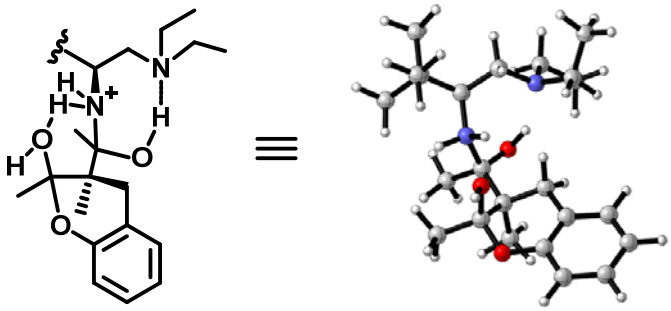
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.404521	-1.425641	-0.709390
2	6	0	4.906981	-1.098489	-0.718855
3	1	0	5.308948	-1.057975	0.300121
4	1	0	5.449937	-1.879481	-1.258632
5	1	0	5.128576	-0.147891	-1.213311
6	6	0	3.233449	-2.841684	-0.152494
7	1	0	3.611436	-2.923804	0.872114
8	1	0	2.186708	-3.159296	-0.164672
9	1	0	3.793455	-3.550173	-0.770286
10	6	0	2.860358	-1.404462	-2.145589
11	1	0	1.812929	-1.727778	-2.199766
12	1	0	2.940124	-0.422060	-2.622837
13	1	0	3.435694	-2.104777	-2.758493
14	6	0	2.697948	-0.379711	0.189097
15	1	0	3.007374	-0.520060	1.229777
16	6	0	3.056773	1.092279	-0.238165
17	1	0	3.306735	1.120447	-1.300381
18	1	0	3.929236	1.445352	0.317258
19	7	0	1.209767	-0.422136	0.159755
20	1	0	-1.228788	-1.386810	-2.281418
21	7	0	1.882225	1.943465	-0.001852
22	6	0	1.452089	2.710724	-1.193394
23	1	0	1.342567	1.984679	-2.007692
24	1	0	0.451906	3.102188	-0.987517

25	6	0	2.018514	2.741751	1.239616
26	1	0	2.251450	2.028592	2.034396
27	1	0	2.874028	3.422167	1.135816
28	6	0	0.758581	3.511551	1.594533
29	1	0	0.551686	4.318559	0.886113
30	1	0	-0.103853	2.841063	1.632467
31	1	0	0.881033	3.966002	2.580650
32	6	0	2.398975	3.834123	-1.592832
33	1	0	3.414675	3.462779	-1.764022
34	1	0	2.051881	4.298449	-2.519014
35	1	0	2.443944	4.613604	-0.827098
36	1	0	0.833152	-0.812563	-0.710709
37	6	0	0.391565	-0.848599	1.336181
38	6	0	-1.128442	-0.862541	0.914279
39	6	0	0.872912	-2.133071	2.005071
40	1	0	1.937890	-2.061598	2.233317
41	1	0	0.342269	-2.263793	2.952160
42	1	0	0.698595	-3.027239	1.410728
43	6	0	-1.958537	-1.412396	2.085904
44	1	0	-1.808679	-2.481742	2.250826
45	1	0	-1.703081	-0.883189	3.010332
46	1	0	-3.022118	-1.247196	1.905224
47	6	0	-1.469082	-1.687020	-0.372407
48	8	0	-0.870098	-0.998936	-1.465988
49	6	0	-5.540568	0.684287	-1.093089
50	6	0	-5.000700	1.841235	-0.530380
51	6	0	-3.729672	1.805924	0.028322
52	6	0	-2.972492	0.632089	0.031046
53	6	0	-3.530771	-0.504585	-0.546622
54	6	0	-4.806422	-0.494002	-1.102572
55	1	0	-6.536049	0.700098	-1.524430
56	1	0	-5.573396	2.762251	-0.520982
57	1	0	-3.308913	2.701328	0.480624
58	1	0	-5.199194	-1.410904	-1.529122
59	8	0	-2.862600	-1.713260	-0.561701
60	6	0	-1.592231	0.584569	0.635974
61	1	0	-0.893923	1.094293	-0.040313
62	1	0	-1.586050	1.139112	1.578546
63	6	0	-1.059174	-3.152476	-0.413947
64	1	0	-1.545724	-3.610842	-1.279633
65	1	0	0.021428	-3.248034	-0.540100
66	1	0	-1.379018	-3.699800	0.474510
67	8	0	0.624690	0.223253	2.236760
68	1	0	1.100881	0.788678	0.118748

69	1	0	0.412910	-0.063518	3.137087

(32) Int10



E_{sol} = -1236.02461

Zero-point correction=	0.631463 (Hartree/Particle)
Thermal correction to Energy=	0.661102
Thermal correction to Enthalpy=	0.662047
Thermal correction to Gibbs Free Energy=	0.574248
Sum of electronic and zero-point Energies=	-1234.943157
Sum of electronic and thermal Energies=	-1234.913518
Sum of electronic and thermal Enthalpies=	-1234.912574
Sum of electronic and thermal Free Energies=	-1235.000372

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	414.848	119.644	184.787
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.725
Vibrational	413.071	113.683	105.263

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.405500	-1.519980	-0.906578
2	6	0	4.854620	-1.012144	-0.964570
3	1	0	5.210367	-0.702149	0.024609
4	1	0	5.509244	-1.814427	-1.316516
5	1	0	4.972513	-0.172874	-1.654840
6	6	0	3.411486	-2.851987	-0.138916
7	1	0	3.811285	-2.724813	0.873056
8	1	0	2.423028	-3.323915	-0.054763
9	1	0	4.048173	-3.571556	-0.661083
10	6	0	2.883496	-1.746293	-2.333039
11	1	0	1.845824	-2.105521	-2.355273

12	1	0	2.939532	-0.836179	-2.938221
13	1	0	3.492687	-2.506223	-2.830932
14	6	0	2.540196	-0.484247	-0.141337
15	1	0	2.892047	-0.426289	0.893542
16	6	0	2.518147	0.918687	-0.768426
17	1	0	2.010082	0.859952	-1.739900
18	1	0	3.550510	1.231833	-0.970062
19	7	0	1.109333	-0.973795	-0.068413
20	1	0	-1.667311	-1.807653	-2.043465
21	7	0	1.822602	1.906921	0.065011
22	6	0	1.158601	2.953289	-0.740114
23	1	0	0.500380	2.440197	-1.450807
24	1	0	0.504633	3.519438	-0.069911
25	6	0	2.748443	2.453505	1.082613
26	1	0	3.142325	1.601200	1.647030
27	1	0	3.606483	2.939571	0.595030
28	6	0	2.068923	3.412352	2.048849
29	1	0	1.776425	4.347275	1.563370
30	1	0	1.179915	2.956163	2.497195
31	1	0	2.759182	3.663681	2.857379
32	6	0	2.095876	3.896935	-1.488445
33	1	0	2.776900	3.351338	-2.150249
34	1	0	1.511570	4.581963	-2.107850
35	1	0	2.696120	4.501317	-0.802661
36	1	0	0.542577	-0.514694	-0.793477
37	6	0	0.345684	-0.848960	1.292522
38	6	0	-1.188657	-0.759625	0.972429
39	6	0	0.783291	-2.014153	2.168459
40	1	0	1.874107	-2.019645	2.244244
41	1	0	0.389927	-1.847636	3.172154
42	1	0	0.438318	-2.985533	1.813586
43	6	0	-1.948880	-0.947423	2.293779
44	1	0	-1.910610	-1.976053	2.659882
45	1	0	-1.515327	-0.292364	3.054747
46	1	0	-2.998879	-0.676066	2.166176
47	6	0	-1.731159	-1.766907	-0.092888
48	8	0	-1.138109	-1.400919	-1.337756
49	6	0	-5.523793	0.947812	-1.070311
50	6	0	-4.802146	2.109063	-0.791468
51	6	0	-3.504679	2.011884	-0.306017
52	6	0	-2.900949	0.769568	-0.098705
53	6	0	-3.638936	-0.372453	-0.395245
54	6	0	-4.943855	-0.297973	-0.873310
55	1	0	-6.541003	1.013101	-1.441916

56	1	0	-5.254245	3.083211	-0.942929
57	1	0	-2.942282	2.912797	-0.071076
58	1	0	-5.479743	-1.218446	-1.079341
59	8	0	-3.125712	-1.640294	-0.200392
60	6	0	-1.496632	0.655679	0.435290
61	1	0	-0.792495	0.940834	-0.359820
62	1	0	-1.354264	1.375363	1.248197
63	6	0	-1.511982	-3.254294	0.152860
64	1	0	-2.123583	-3.805251	-0.566833
65	1	0	-0.468512	-3.537253	-0.009881
66	1	0	-1.818844	-3.558312	1.154960
67	8	0	0.793237	0.290466	1.918510
68	1	0	1.070473	-1.960861	-0.339381
69	1	0	0.898020	1.024576	1.242369

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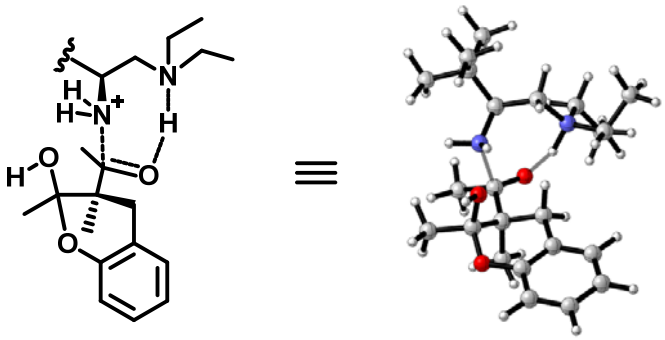
(33) TS12



E_{sol} = -1236.013568

Zero-point correction=	0.628998 (Hartree/Particle)
Thermal correction to Energy=	0.658384
Thermal correction to Enthalpy=	0.659328
Thermal correction to Gibbs Free Energy=	0.572211
Sum of electronic and zero-point Energies=	-1234.932673
Sum of electronic and thermal Energies=	-1234.903287
Sum of electronic and thermal Enthalpies=	-1234.902343
Sum of electronic and thermal Free Energies=	-1234.989461

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	413.142	118.784	183.354
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.800
Rotational	0.889	2.981	35.755
Vibrational	411.365	112.823	103.799

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.530820	-1.412602	-1.039651
2	6	0	4.916136	-0.791243	-0.809307
3	1	0	5.164185	-0.764285	0.257984
4	1	0	5.678479	-1.394215	-1.311004
5	1	0	5.003806	0.224100	-1.208279
6	6	0	3.571396	-2.846573	-0.487371
7	1	0	3.651893	-2.856463	0.606462
8	1	0	2.700677	-3.443798	-0.782494
9	1	0	4.445485	-3.368753	-0.886232
10	6	0	3.208521	-1.453198	-2.538020
11	1	0	2.204758	-1.853538	-2.725305
12	1	0	3.275823	-0.463345	-3.002854
13	1	0	3.920298	-2.102262	-3.056925
14	6	0	2.471470	-0.584042	-0.257420
15	1	0	2.822352	-0.499828	0.779222
16	6	0	2.281668	0.825568	-0.844657
17	1	0	1.546664	0.792271	-1.657318
18	1	0	3.217966	1.198443	-1.264626
19	7	0	1.156807	-1.254140	-0.172533
20	1	0	-1.804660	-2.016480	-1.923292
21	7	0	1.799739	1.821626	0.159136
22	6	0	1.074135	2.972069	-0.467354
23	1	0	0.303378	2.539340	-1.109692
24	1	0	0.563241	3.496680	0.343168
25	6	0	2.908392	2.251098	1.073167
26	1	0	3.333998	1.334530	1.485704
27	1	0	3.676337	2.742903	0.468806
28	6	0	2.402543	3.132499	2.202617
29	1	0	2.079075	4.116214	1.852567
30	1	0	1.576308	2.640661	2.724620
31	1	0	3.210721	3.287298	2.920794
32	6	0	1.970444	3.913215	-1.256213
33	1	0	2.521380	3.391436	-2.044292
34	1	0	1.346528	4.669330	-1.738278
35	1	0	2.683830	4.436846	-0.614917
36	1	0	0.547543	-1.076666	-0.976248
37	6	0	0.242705	-0.824394	1.434338
38	6	0	-1.253005	-0.725417	0.994592
39	6	0	0.668643	-2.019172	2.278981
40	1	0	1.761589	-2.042519	2.326708
41	1	0	0.310232	-1.846023	3.297070

42	1	0	0.293722	-2.984173	1.938910
43	6	0	-2.049869	-0.774532	2.315278
44	1	0	-2.048436	-1.771801	2.762853
45	1	0	-1.603323	-0.076836	3.029085
46	1	0	-3.088198	-0.480935	2.149006
47	6	0	-1.838776	-1.782749	0.006759
48	8	0	-1.270168	-1.530882	-1.274060
49	6	0	-5.504050	1.036570	-1.151748
50	6	0	-4.719378	2.176104	-0.974843
51	6	0	-3.421212	2.047164	-0.497267
52	6	0	-2.878836	0.795969	-0.198670
53	6	0	-3.680901	-0.326925	-0.391869
54	6	0	-4.987260	-0.218596	-0.860240
55	1	0	-6.522100	1.125904	-1.516184
56	1	0	-5.123067	3.158054	-1.197078
57	1	0	-2.810963	2.933910	-0.336840
58	1	0	-5.574508	-1.122486	-0.983875
59	8	0	-3.235192	-1.598099	-0.096644
60	6	0	-1.476371	0.642757	0.329922
61	1	0	-0.763960	0.756836	-0.501116
62	1	0	-1.260214	1.430069	1.059147
63	6	0	-1.682479	-3.256044	0.352732
64	1	0	-2.338196	-3.828566	-0.309381
65	1	0	-0.655956	-3.587528	0.184593
66	1	0	-1.973561	-3.473914	1.381609
67	8	0	0.767284	0.273618	1.831905
68	1	0	1.280016	-2.266114	-0.140638
69	1	0	1.127229	1.251059	0.840191

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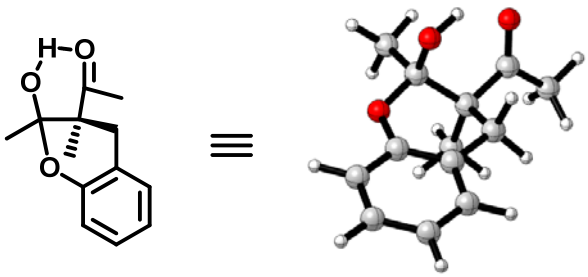
(34) Int11



E_{sol} = -730.6278829

Zero-point correction=	0.270924 (Hartree/Particle)
Thermal correction to Energy=	0.285419
Thermal correction to Enthalpy=	0.286364
Thermal correction to Gibbs Free Energy=	0.230689
Sum of electronic and zero-point Energies=	-730.123473

Sum of electronic and thermal Energies= -730.108978
Sum of electronic and thermal Enthalpies= -730.108034
Sum of electronic and thermal Free Energies= -730.163709

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	179.103	58.369	117.177
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	42.070
Rotational	0.889	2.981	32.020
Vibrational	177.326	52.407	43.088

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.572373	1.040709	-1.828085
2	6	0	-2.512215	-0.659312	-0.219352
3	6	0	-1.119084	-0.288885	0.292402
4	6	0	-3.235757	-1.807411	0.447293
5	1	0	-4.113636	-2.065409	-0.144938
6	1	0	-2.579422	-2.677845	0.547585
7	1	0	-3.547229	-1.520282	1.456977
8	6	0	-1.004326	-0.485715	1.809444
9	1	0	-1.785701	0.058831	2.348608
10	1	0	-1.084019	-1.543928	2.075522
11	1	0	-0.036239	-0.124791	2.164129
12	6	0	-0.748127	1.173592	-0.106943
13	8	0	-0.691564	1.299217	-1.502096
14	6	0	3.915756	0.158790	0.131132
15	6	0	3.683916	-1.167301	-0.232878
16	6	0	2.377935	-1.606833	-0.411209
17	6	0	1.291440	-0.747900	-0.241658
18	6	0	1.545602	0.577031	0.119468
19	6	0	2.850307	1.030056	0.309312
20	1	0	4.930357	0.516502	0.276607
21	1	0	4.513045	-1.853103	-0.372371
22	1	0	2.184641	-2.641023	-0.687838
23	1	0	2.999484	2.066492	0.593085
24	8	0	0.545959	1.477649	0.369827
25	6	0	-0.126277	-1.211993	-0.453552
26	1	0	-0.358365	-1.192394	-1.524434
27	1	0	-0.238989	-2.246074	-0.105769
28	6	0	-1.652722	2.233572	0.504685

29	1	0	−1.303619	3.207597	0.155877
30	1	0	−2.685133	2.088550	0.177901
31	1	0	−1.606449	2.213214	1.595802
32	8	0	−3.018775	−0.091016	−1.169921

Reference:

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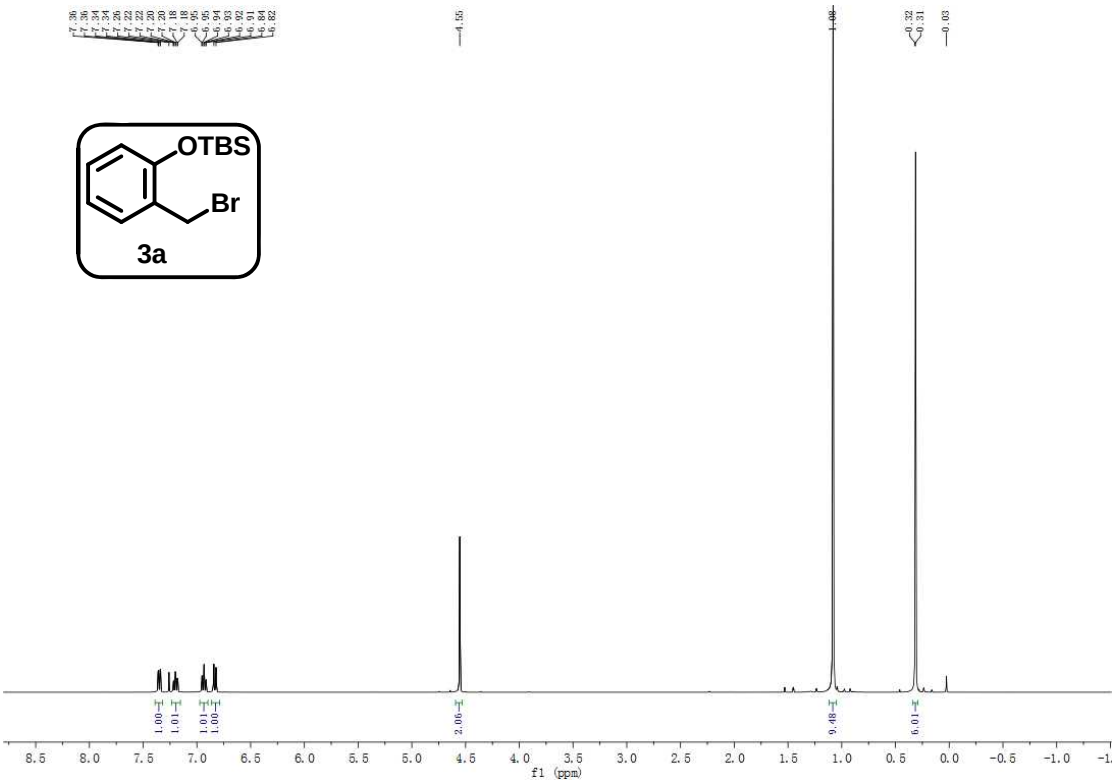
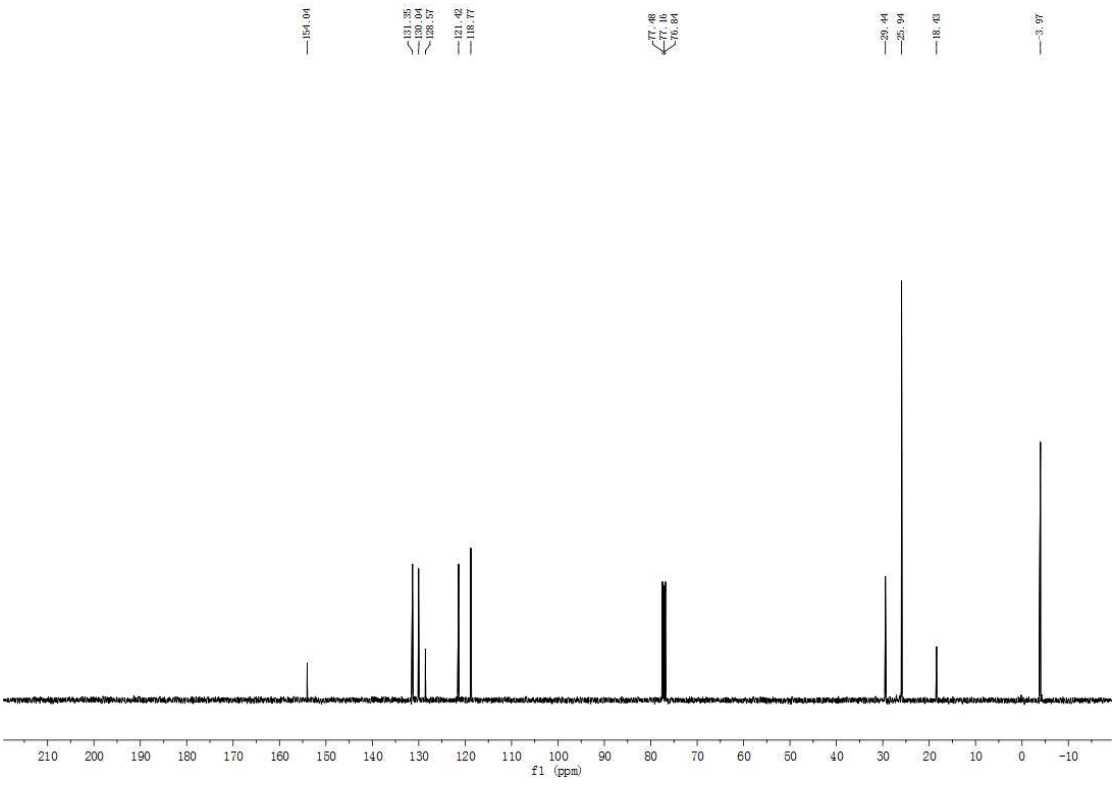
NMR spectral for new products



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Br
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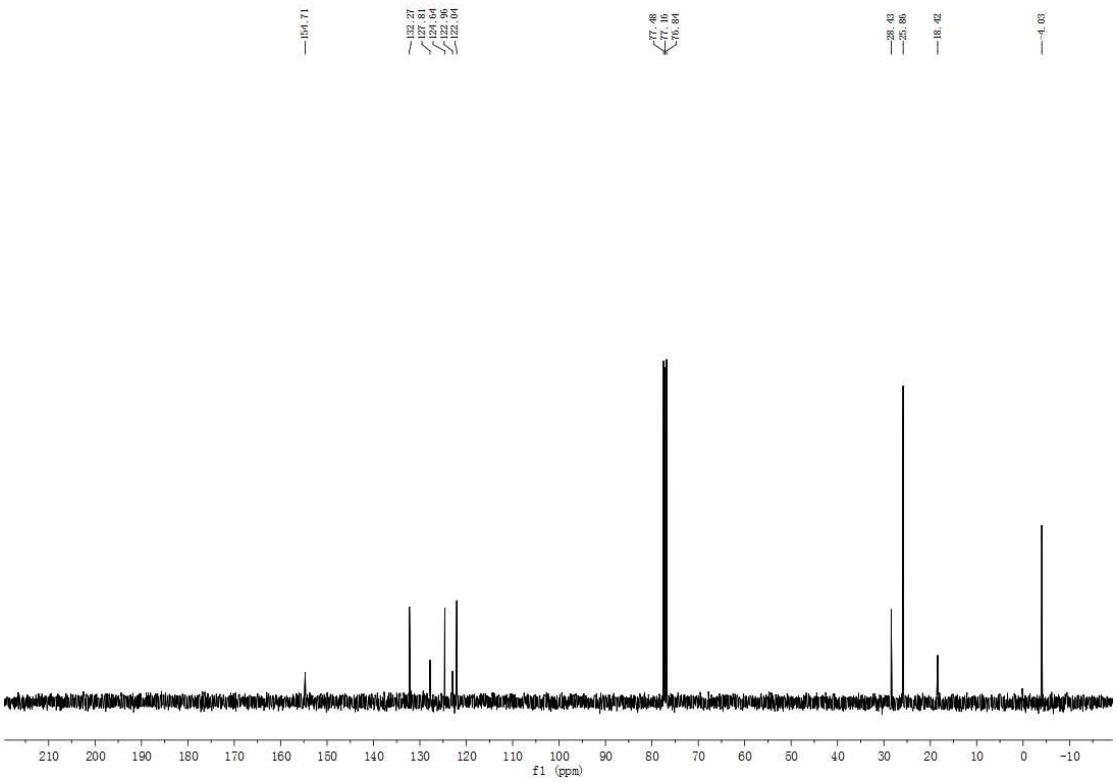
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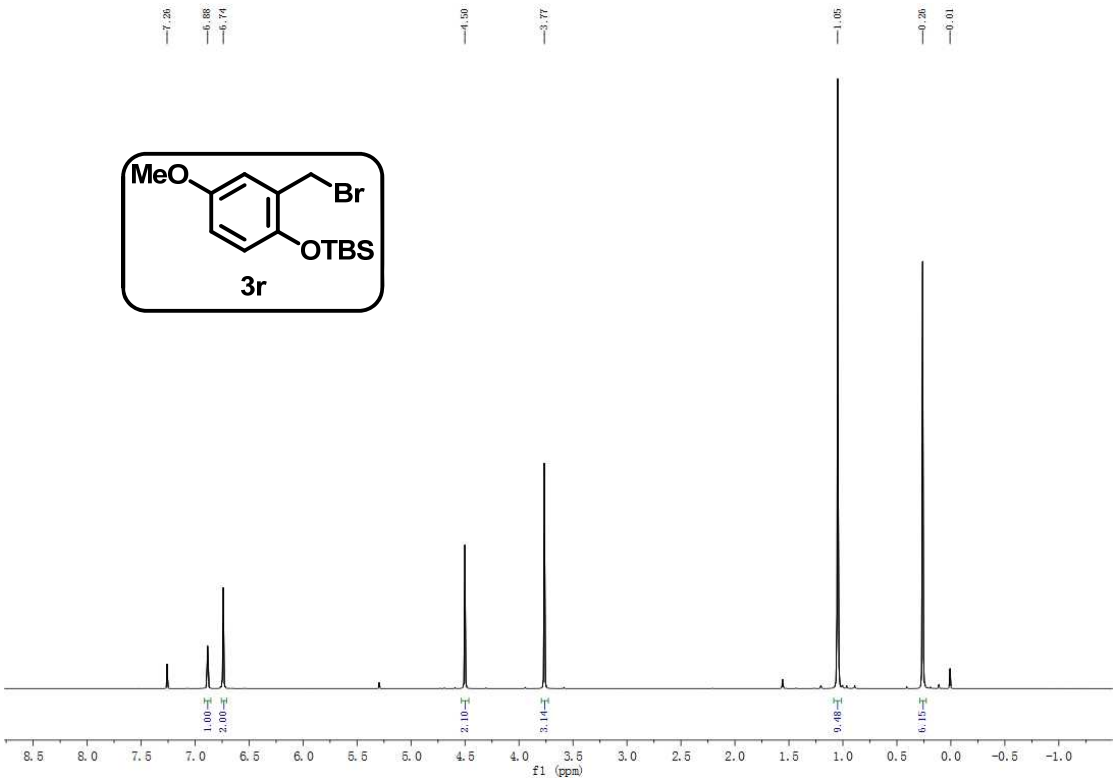
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0.01
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Br
OTBS
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2.00
2.10
3.14
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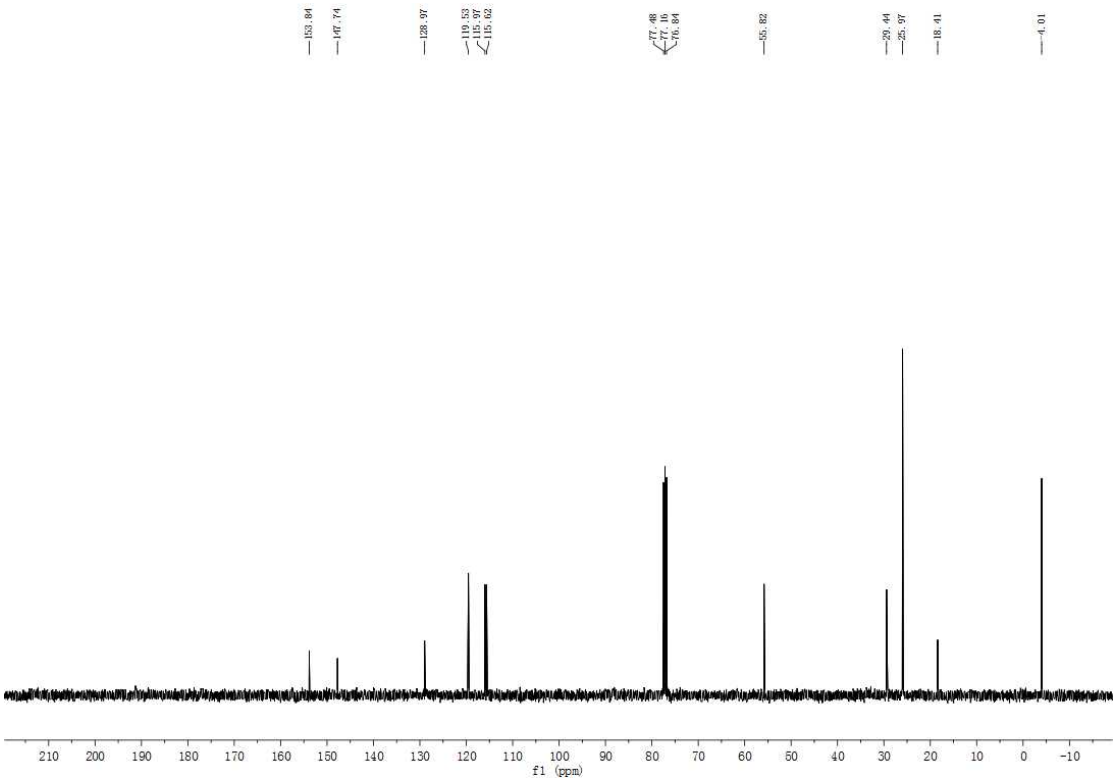
6.15
f1 (ppm)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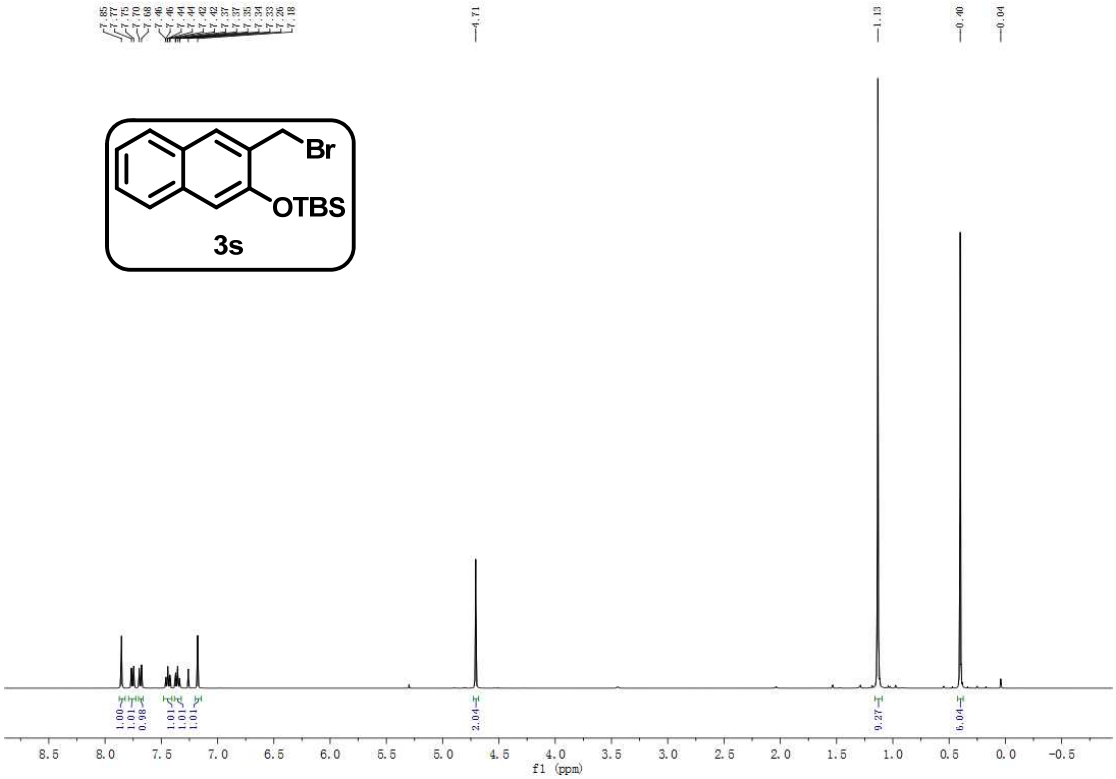
f1 (ppm)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OTBS
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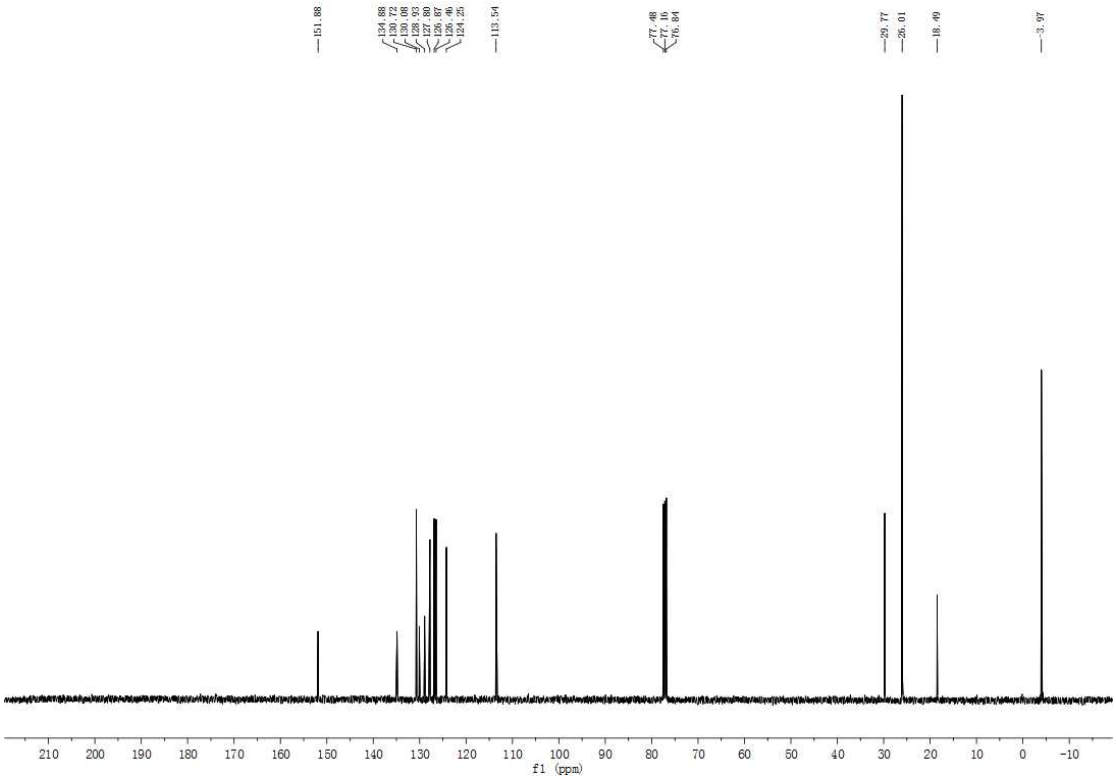
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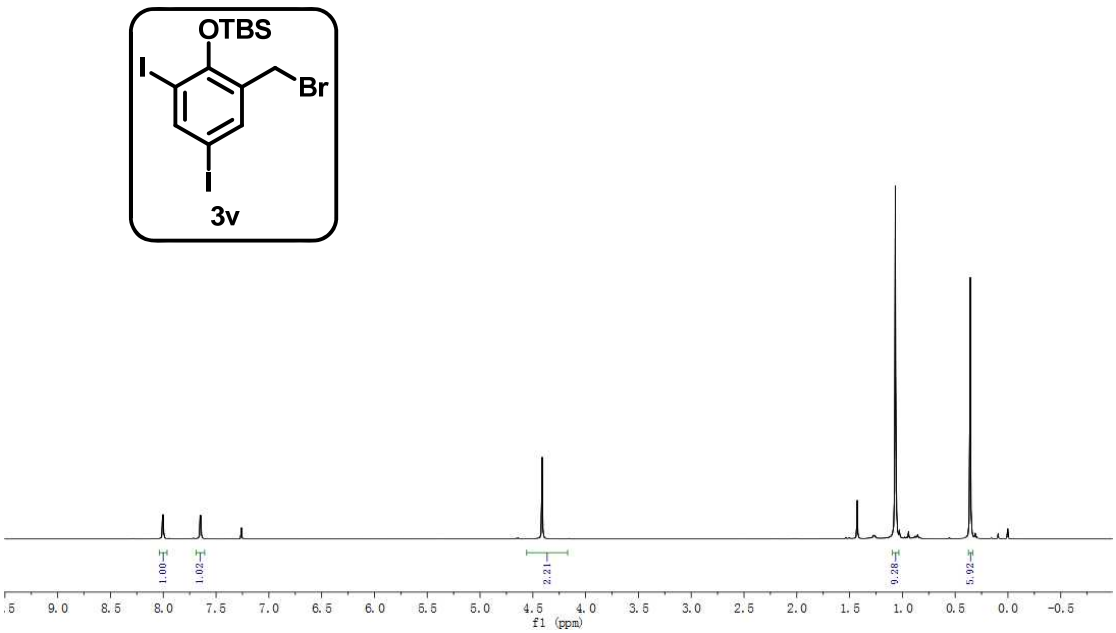
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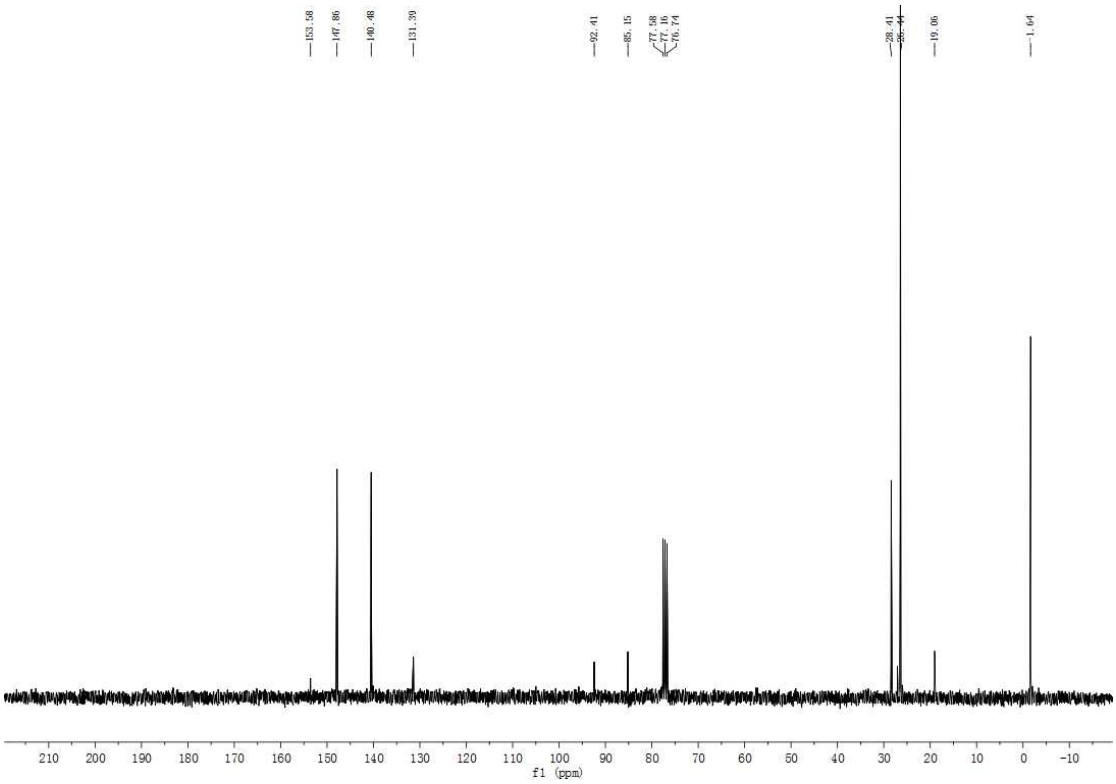
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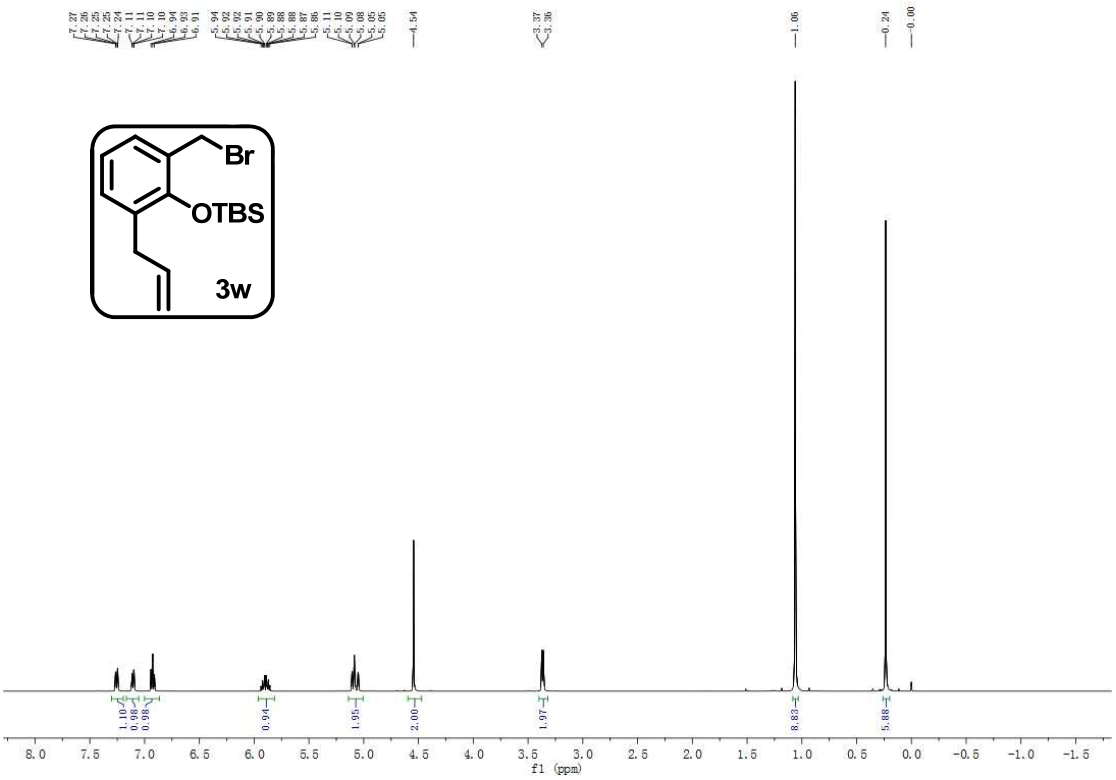
f1 (ppm)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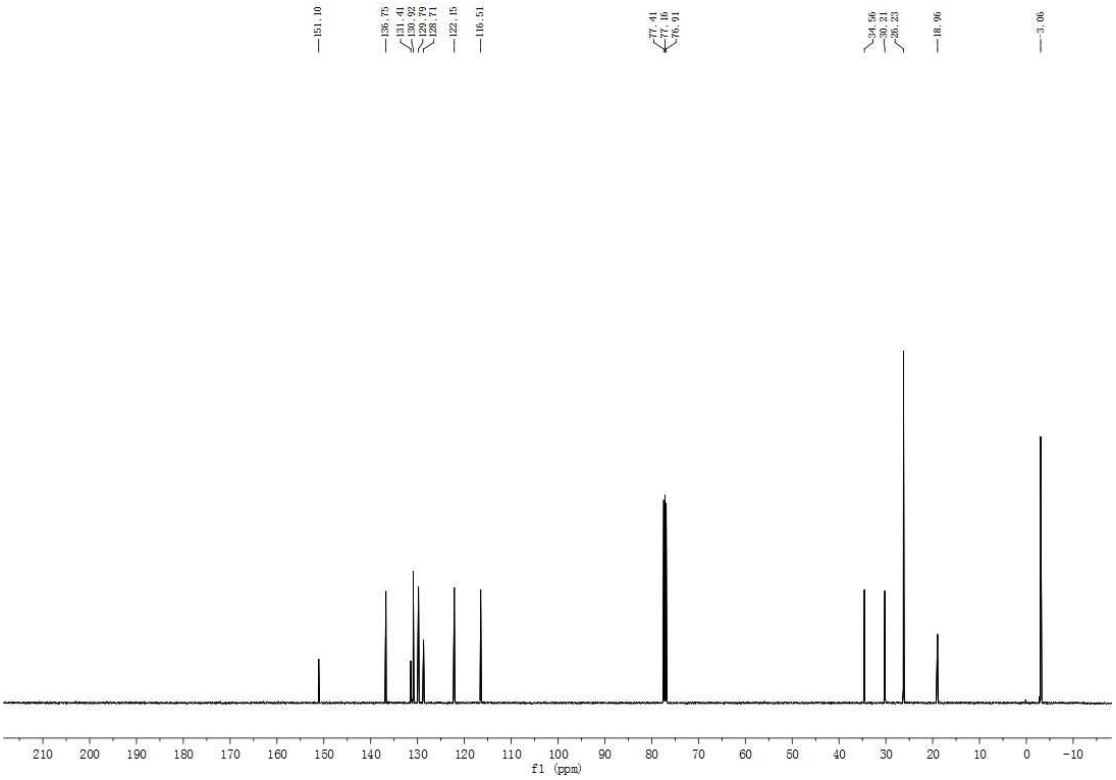
f1 (ppm)


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4.50
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F3C
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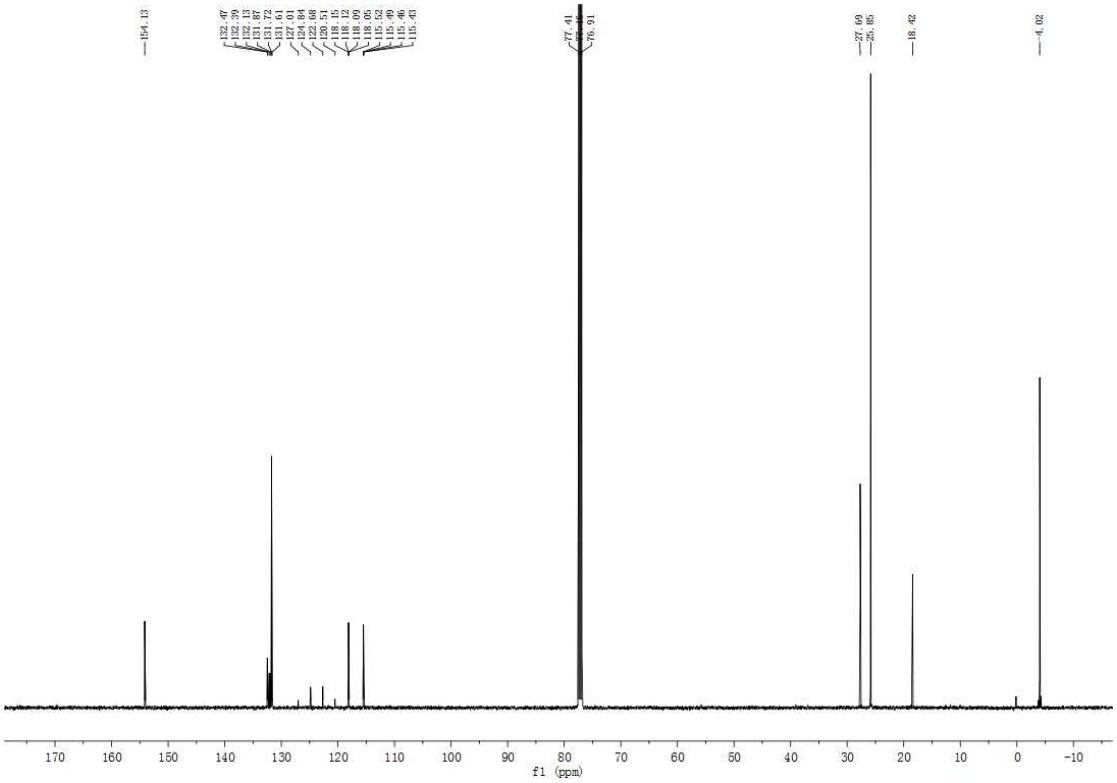
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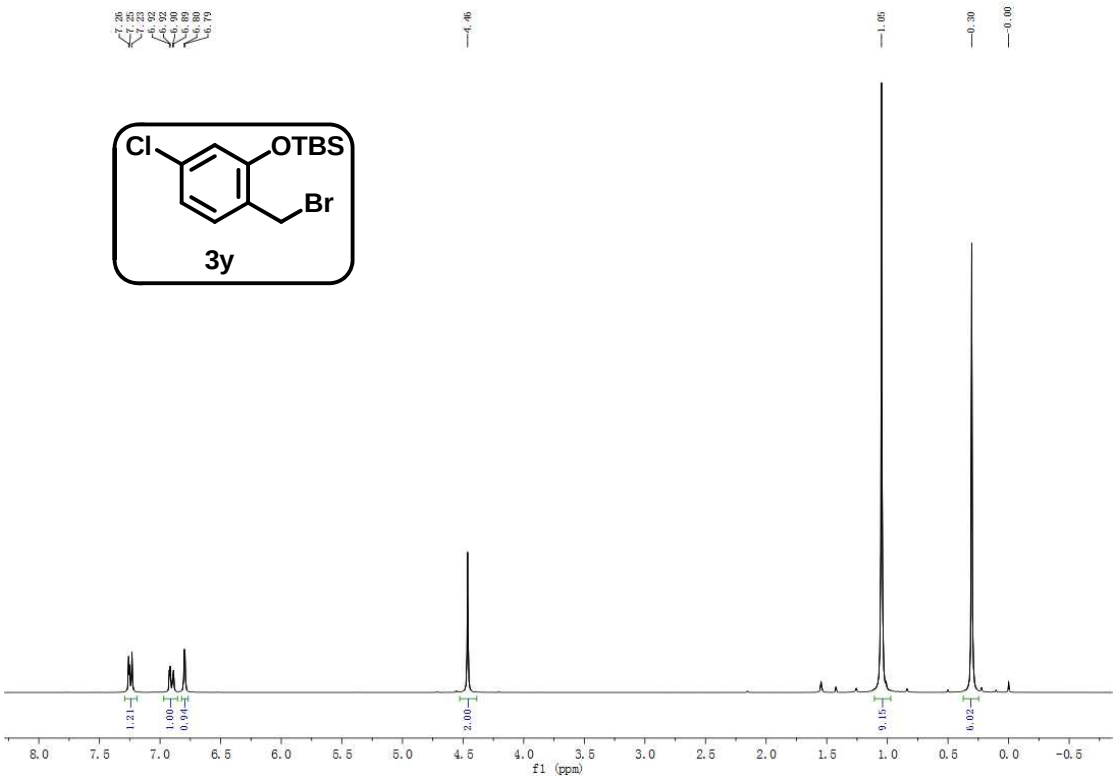
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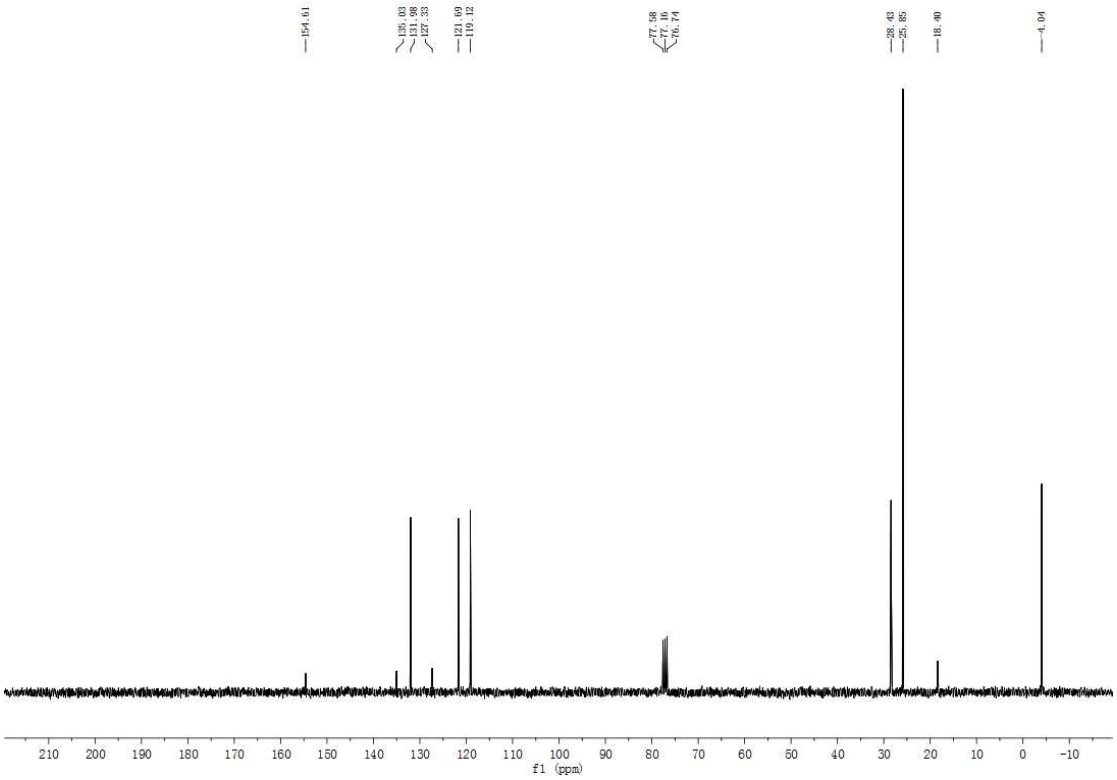
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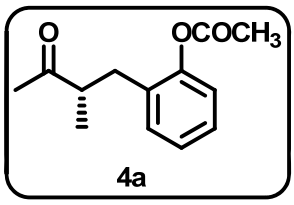
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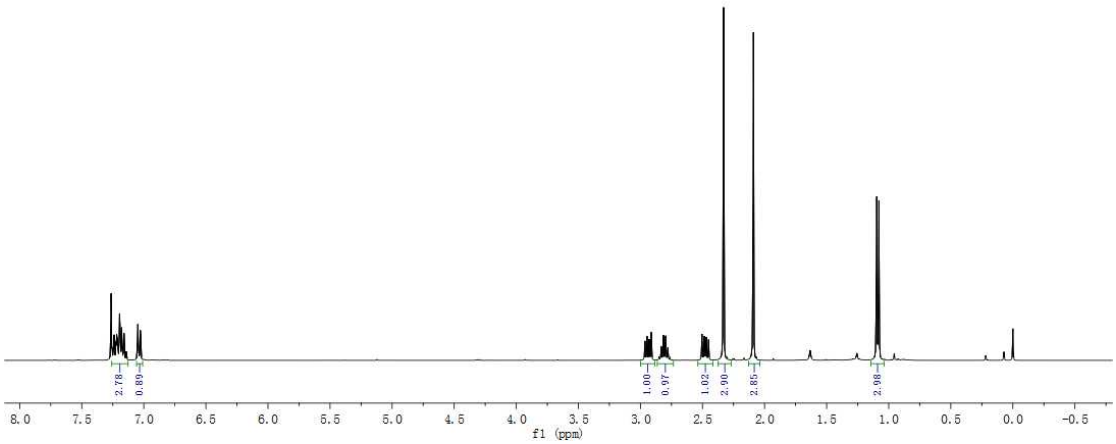
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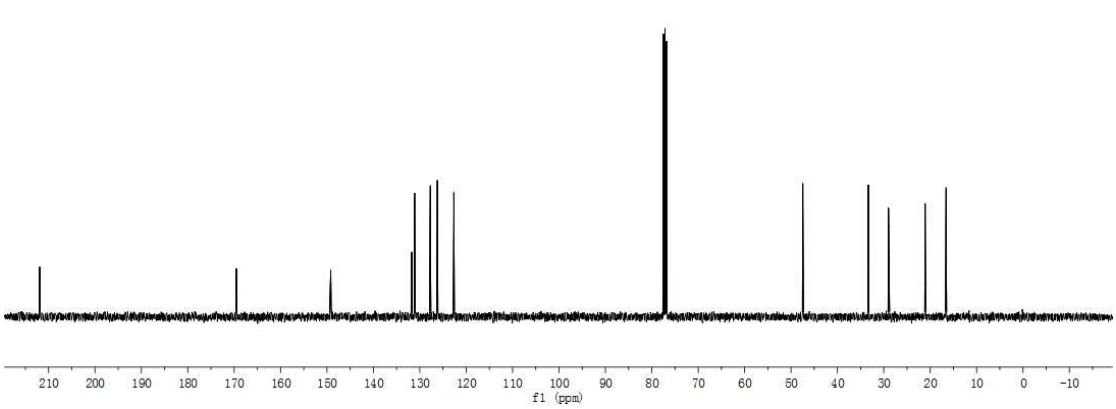
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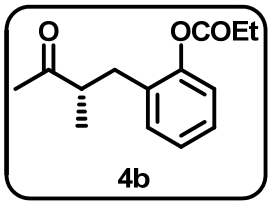
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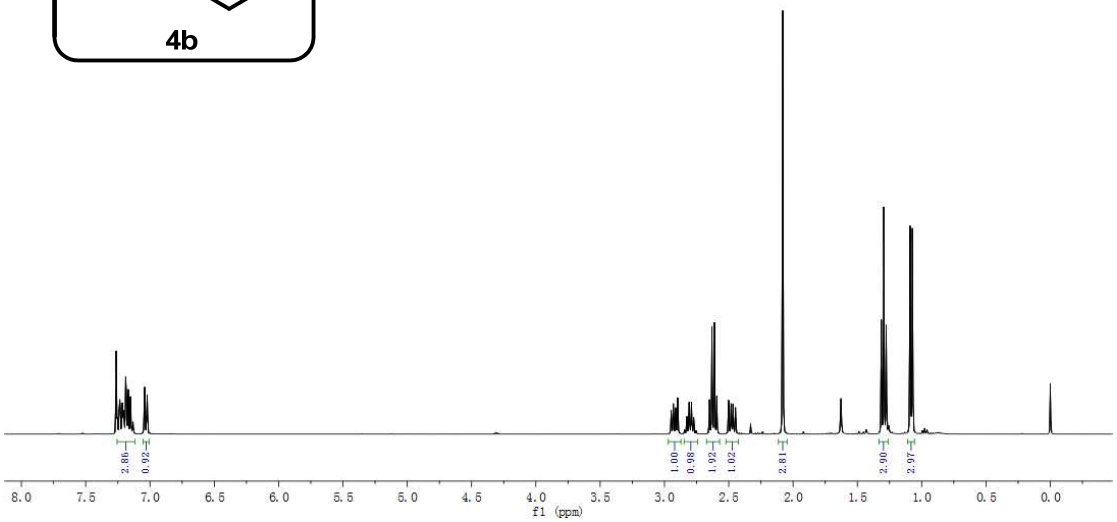
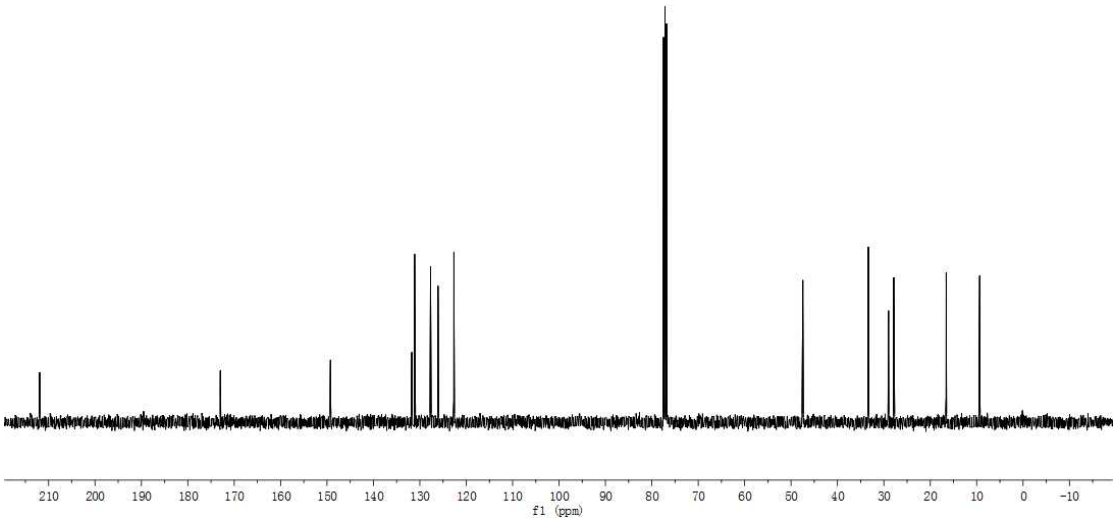
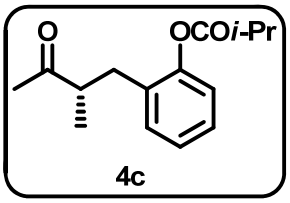
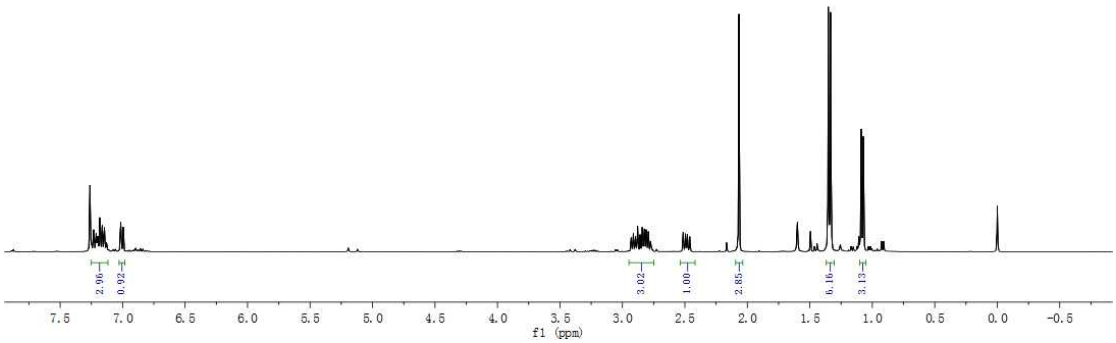
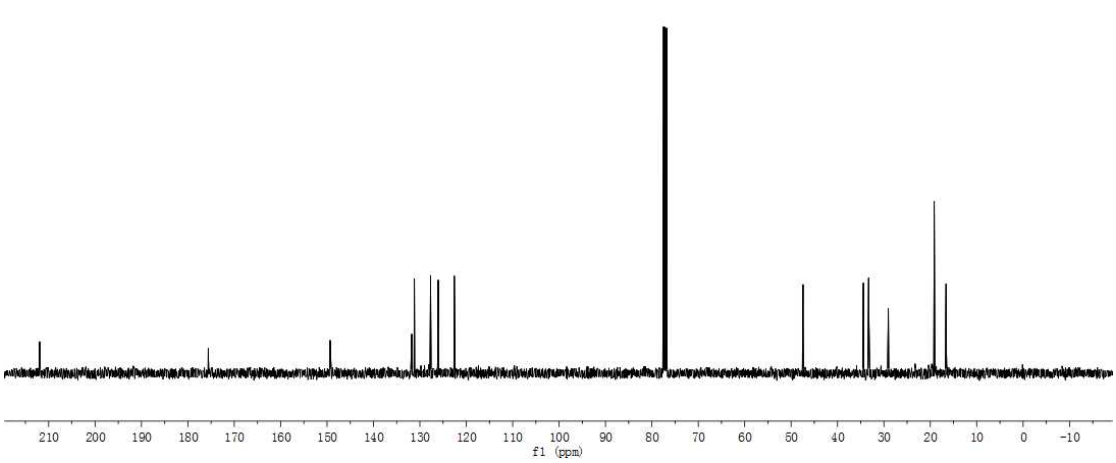
OCOEt
4b

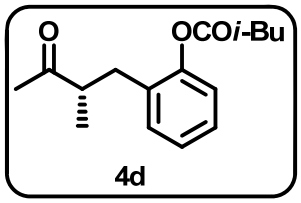

2.86
0.92
1.00
0.98
1.93
1.02
2.81
2.90
2.97
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

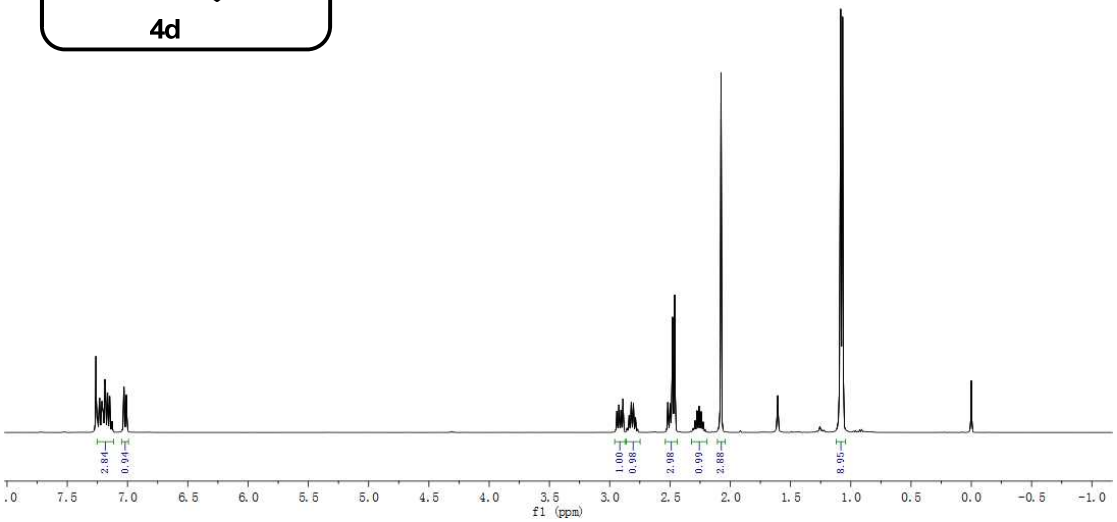

O
OCO*i*-Pr
4c

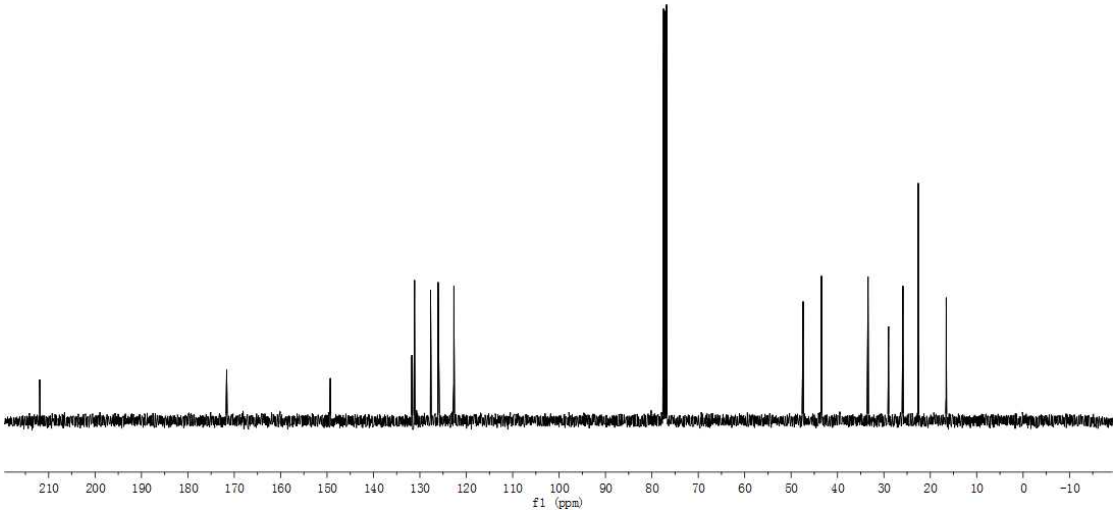

2.96
0.92
3.02
1.00
2.85
6.16
3.13
f1 (ppm)

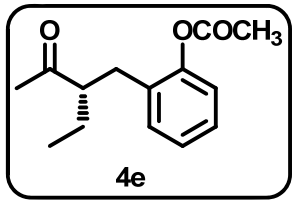

f1 (ppm)

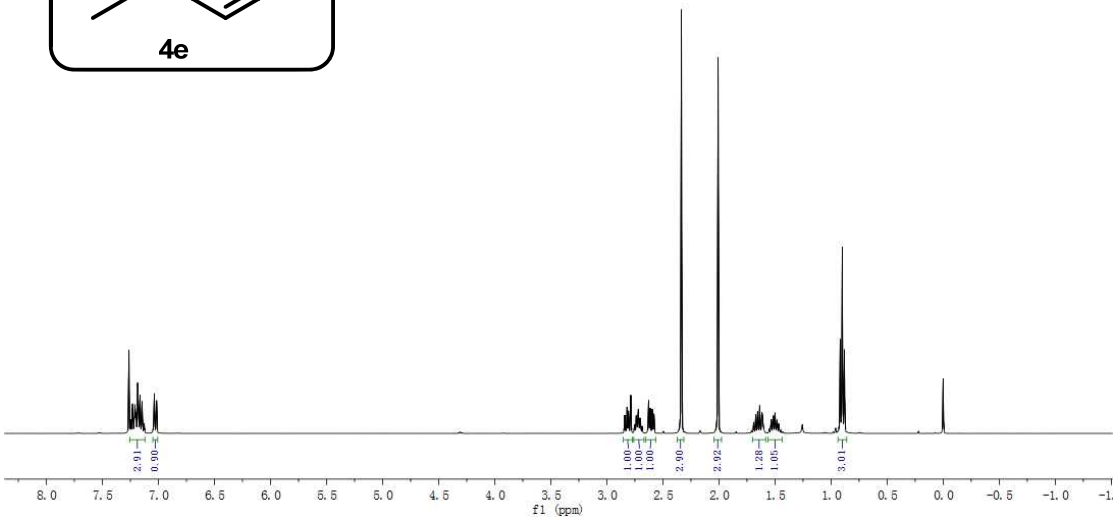


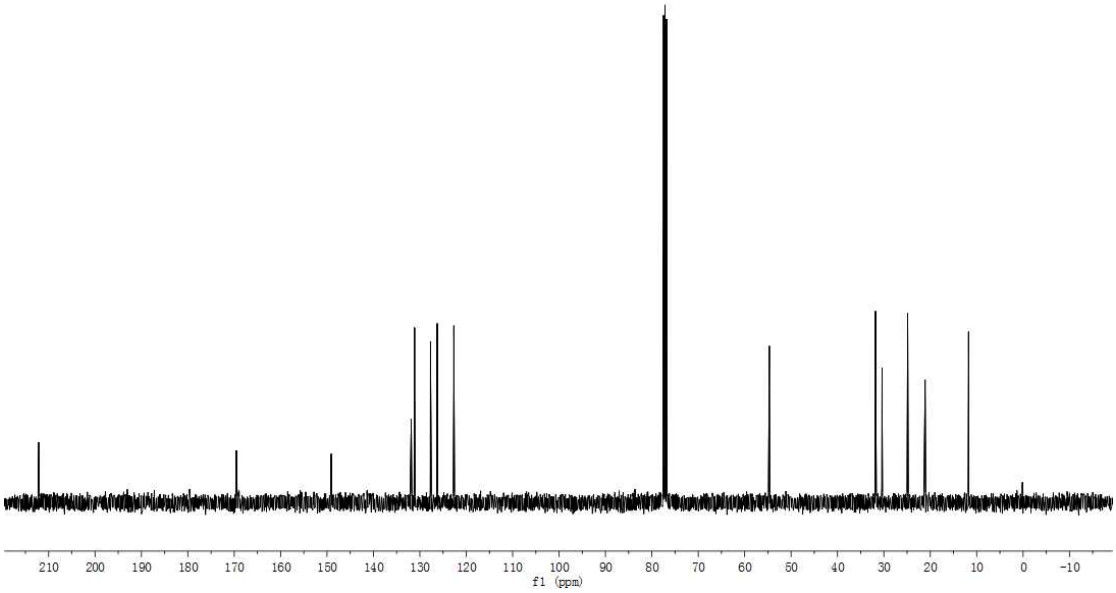
4d



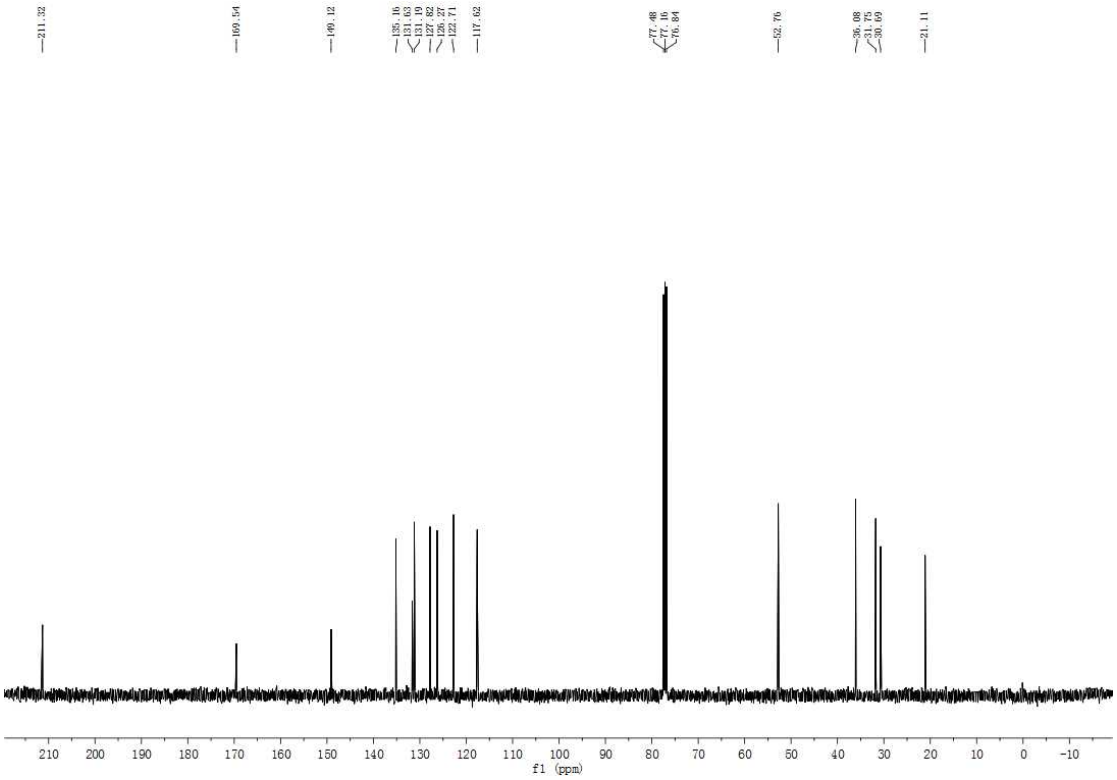



O
OCOCH3
4e

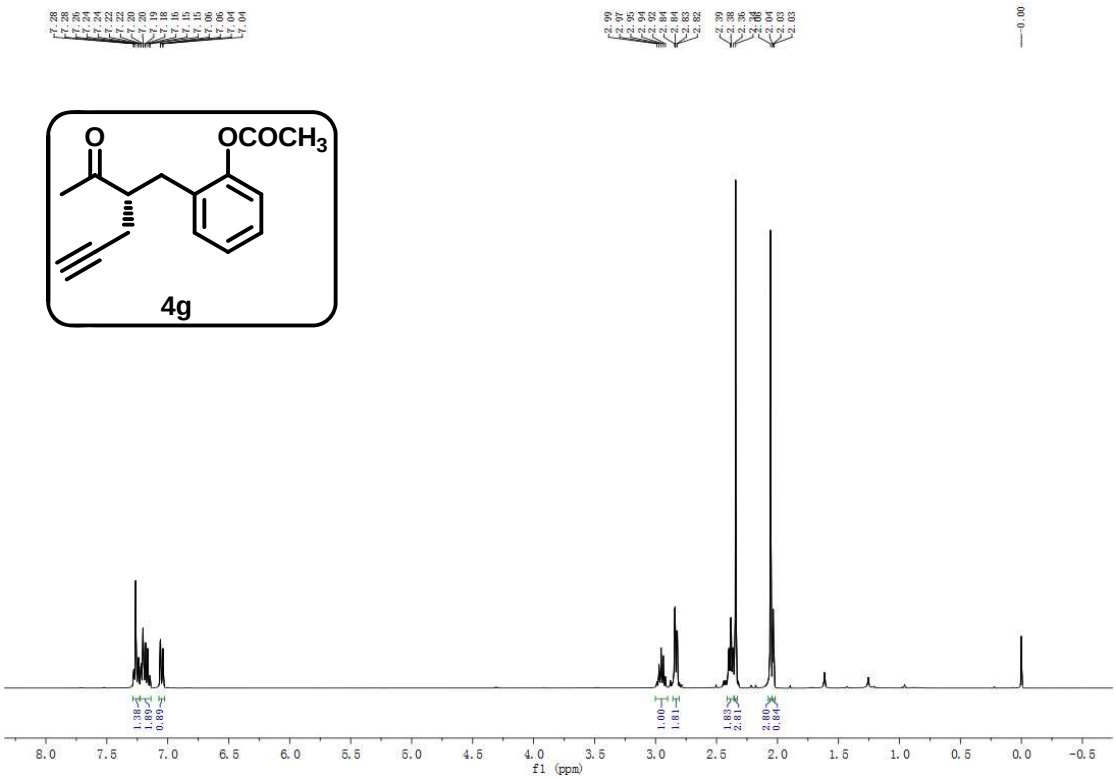

f1 (ppm)

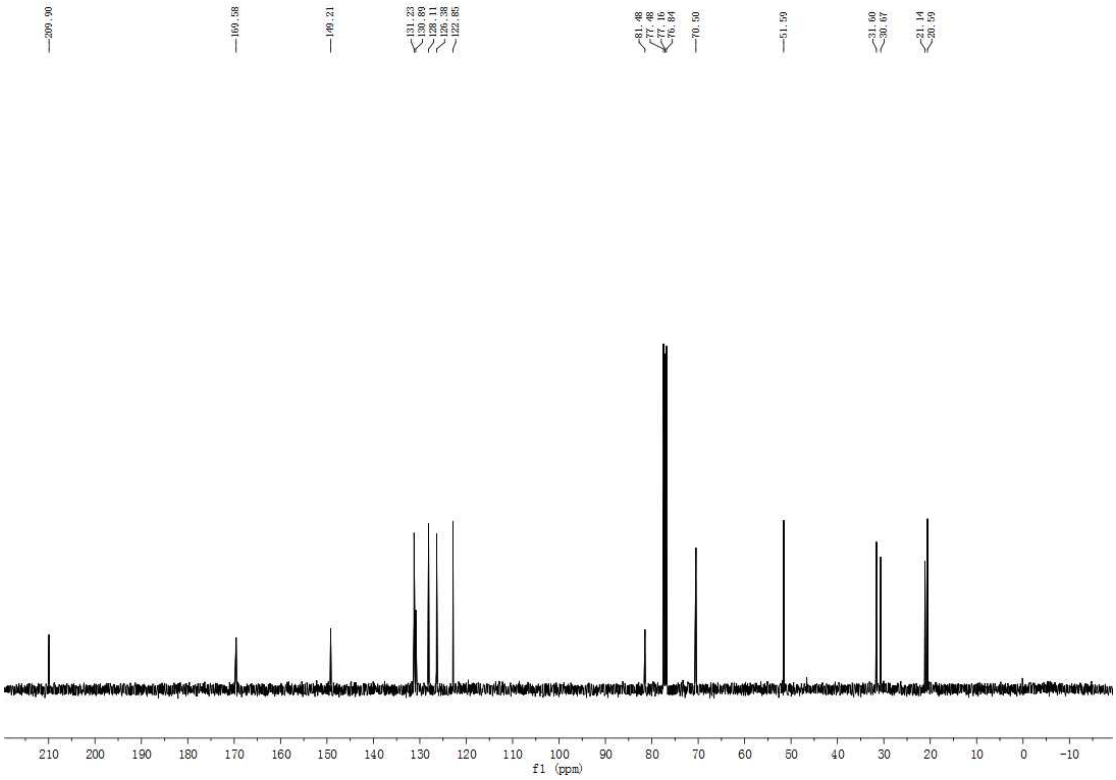

f1 (ppm)

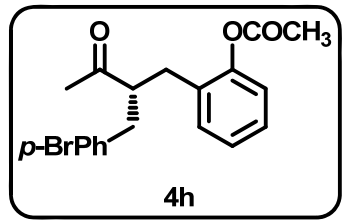

O
OCOCH3
4f
f1 (ppm)


f1 (ppm)

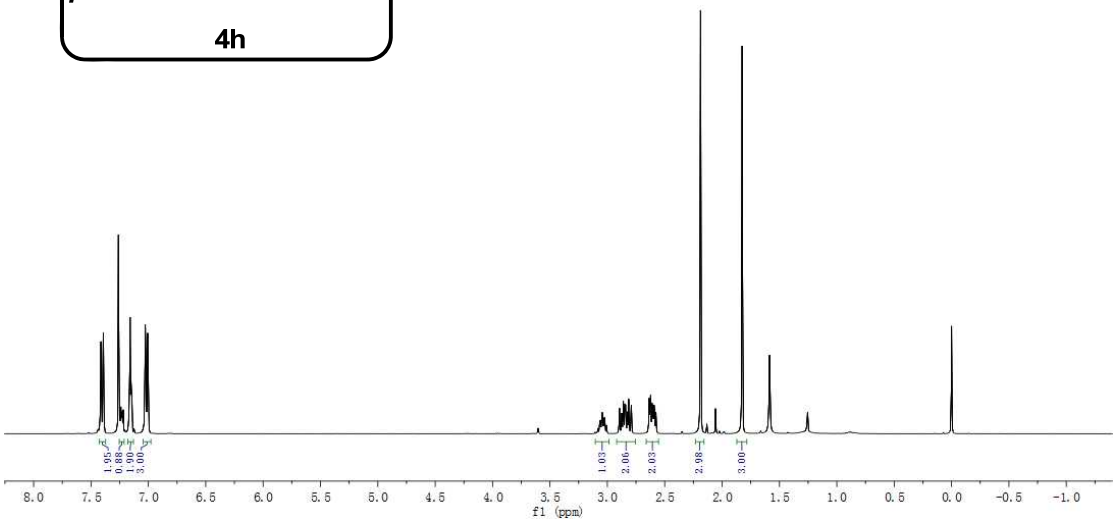
O
OCOCH3
4g

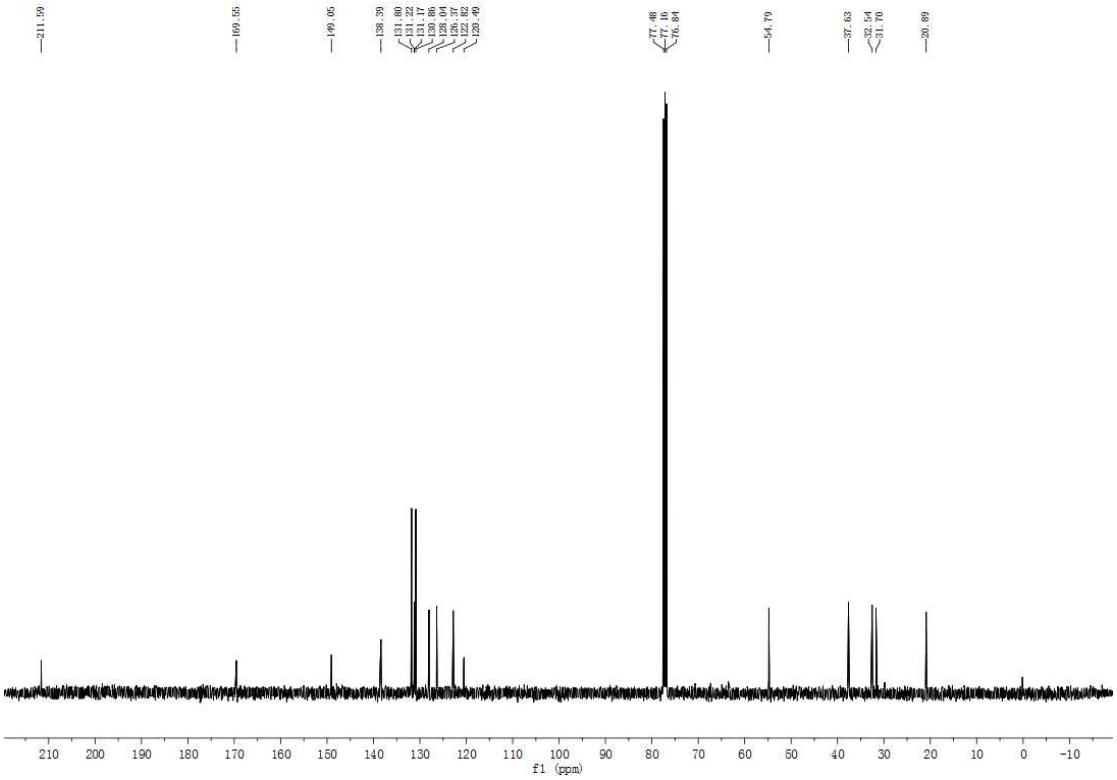

1.38
1.89
0.89
1.00
1.81
1.83
2.81
2.80
0.84
f1 (ppm)

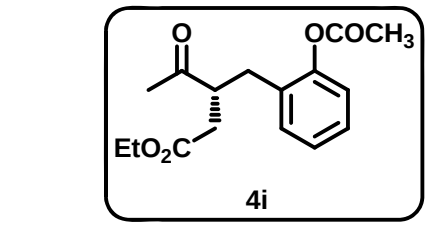

209.90
169.58
149.21
131.23
130.89
128.11
126.38
122.85
81.48
77.48
77.16
76.84
70.50
51.59
31.60
30.67
21.14
20.59
f1 (ppm)


O
OCOCH3
p-BrPh

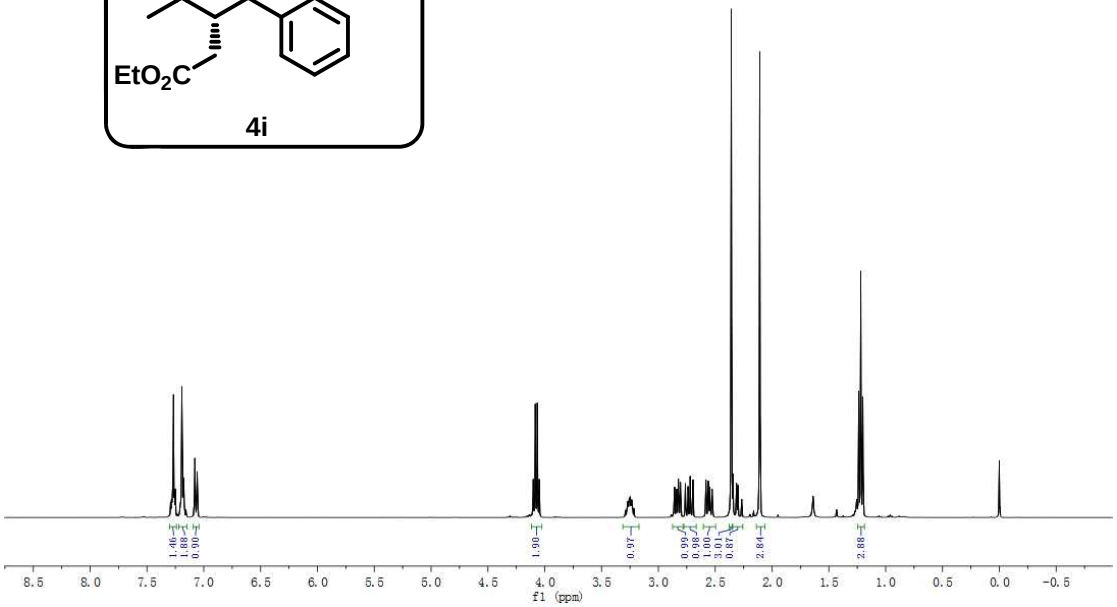
4h

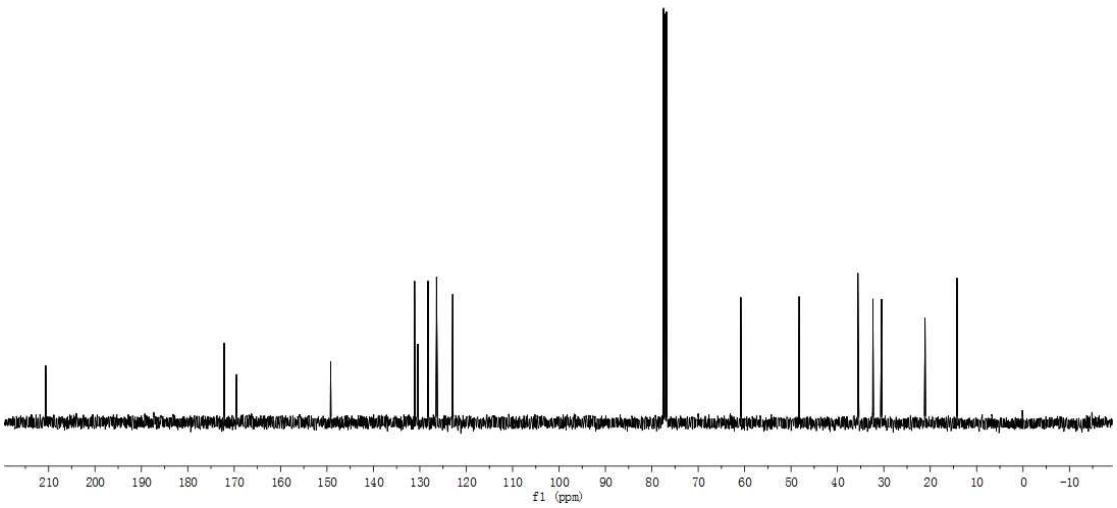

1.95
0.88
1.00
3.00
1.03
2.06
2.03
2.98
3.00
f1 (ppm)

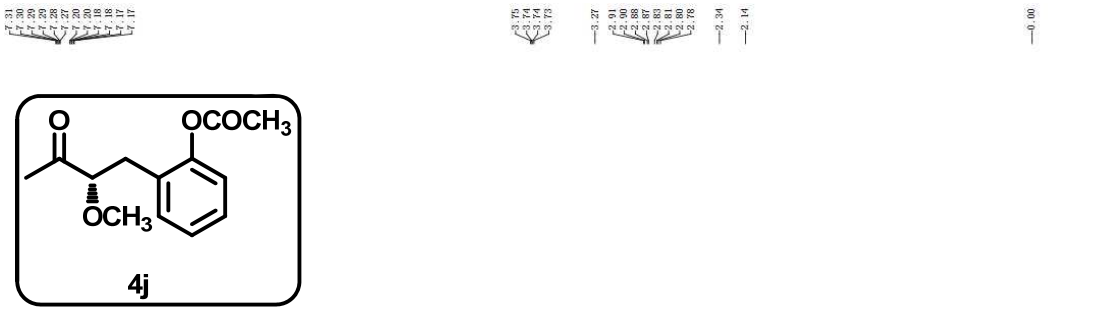

211.59
169.55
149.05
138.39
131.80
131.22
129.17
130.86
128.04
126.37
122.82
120.40
77.48
77.16
76.84
54.79
37.63
32.54
31.70
20.89
f1 (ppm)



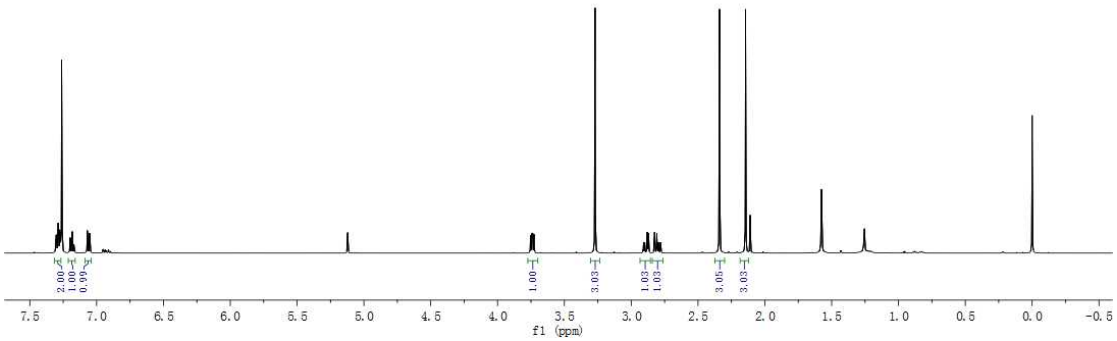
4i

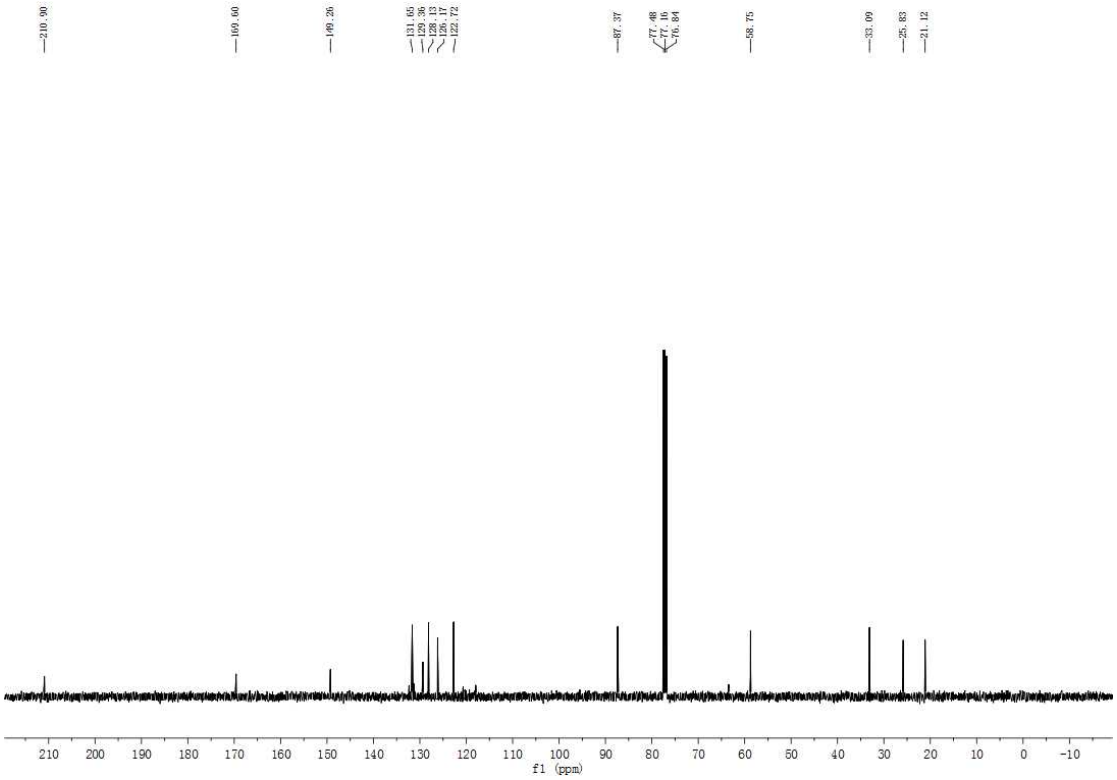




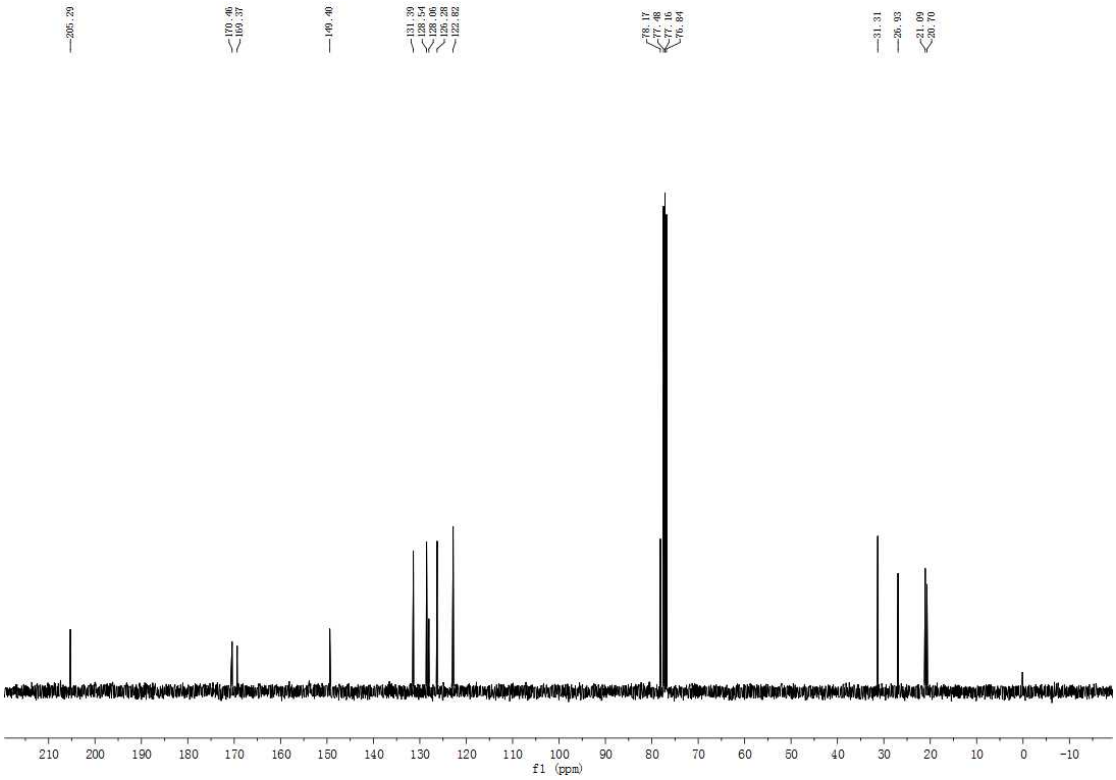


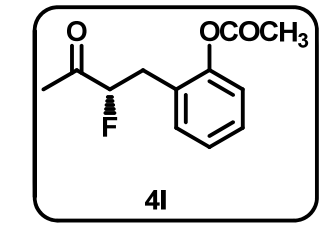
4j



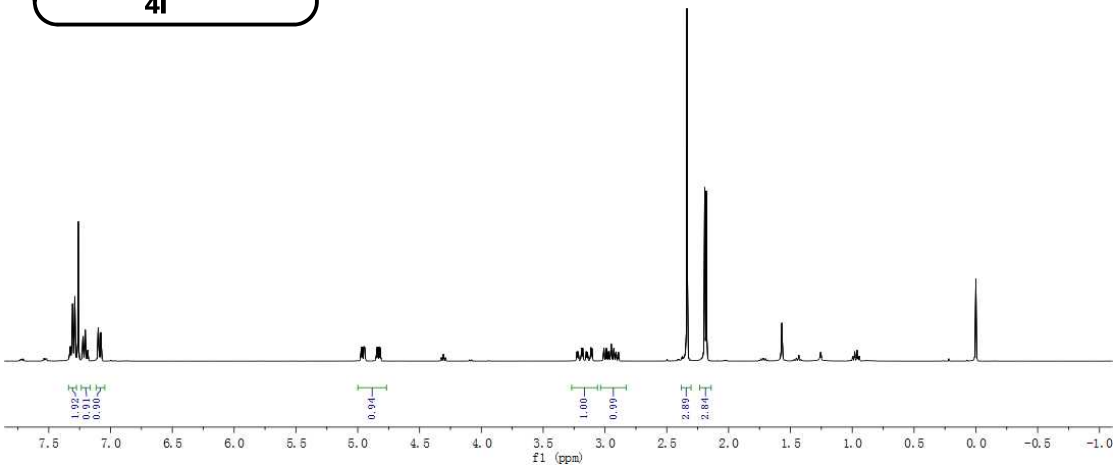


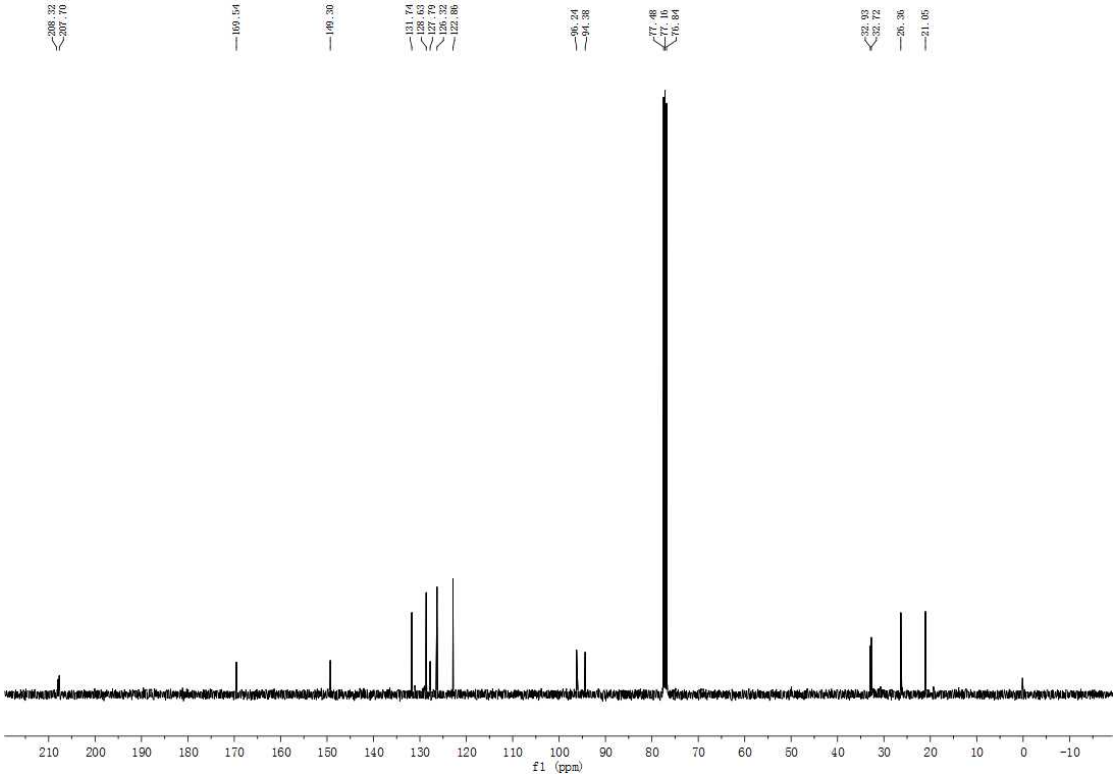
4k




O
OCOCH3
F

4l


1.92
0.91
0.94
1.00
0.99
2.89
2.84
f1 (ppm)


208.32
207.70
169.54
149.30
131.74
128.63
127.79
126.32
122.86
96.24
94.38
77.48
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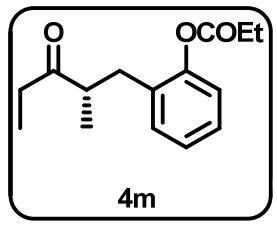
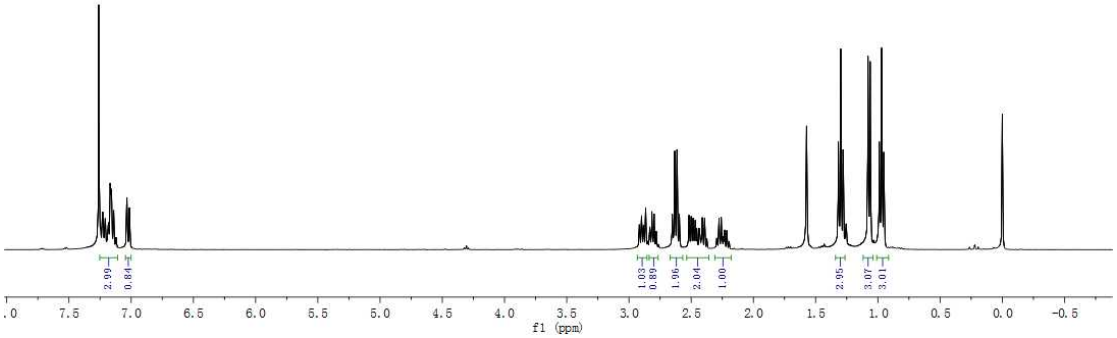
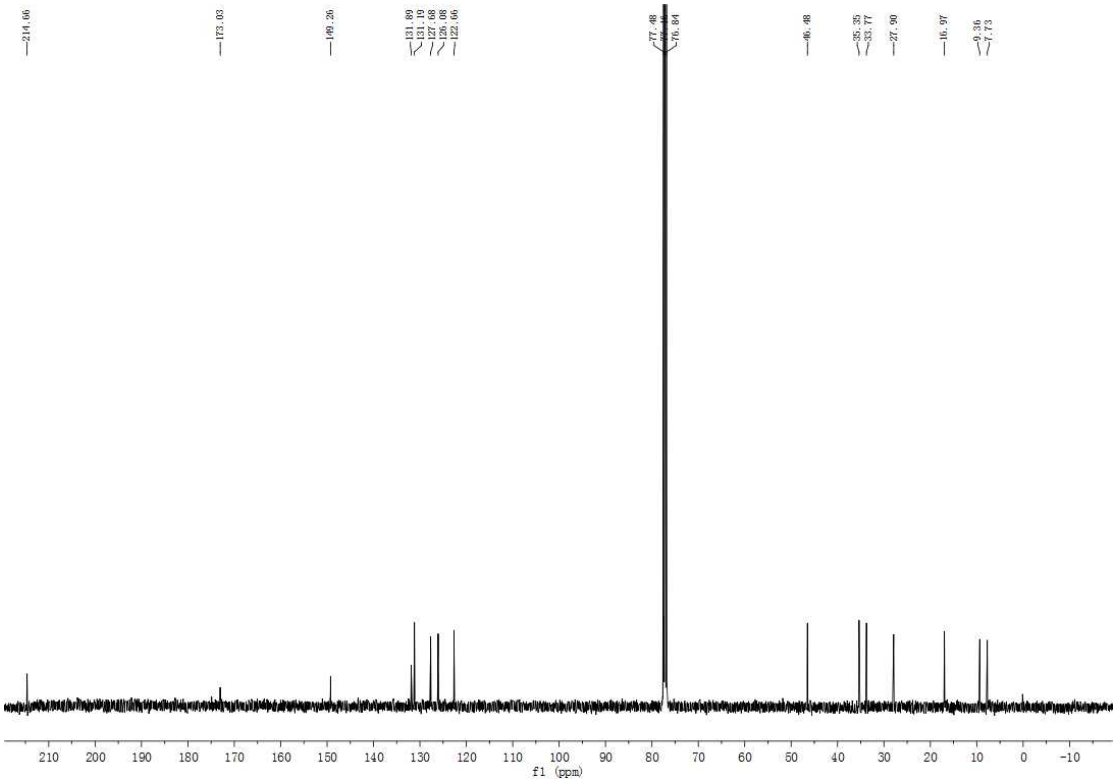
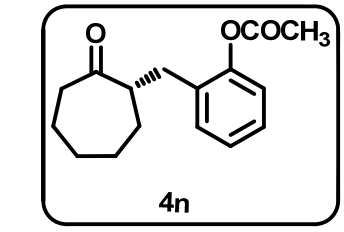
22.93
22.72
26.36
21.05
f1 (ppm)

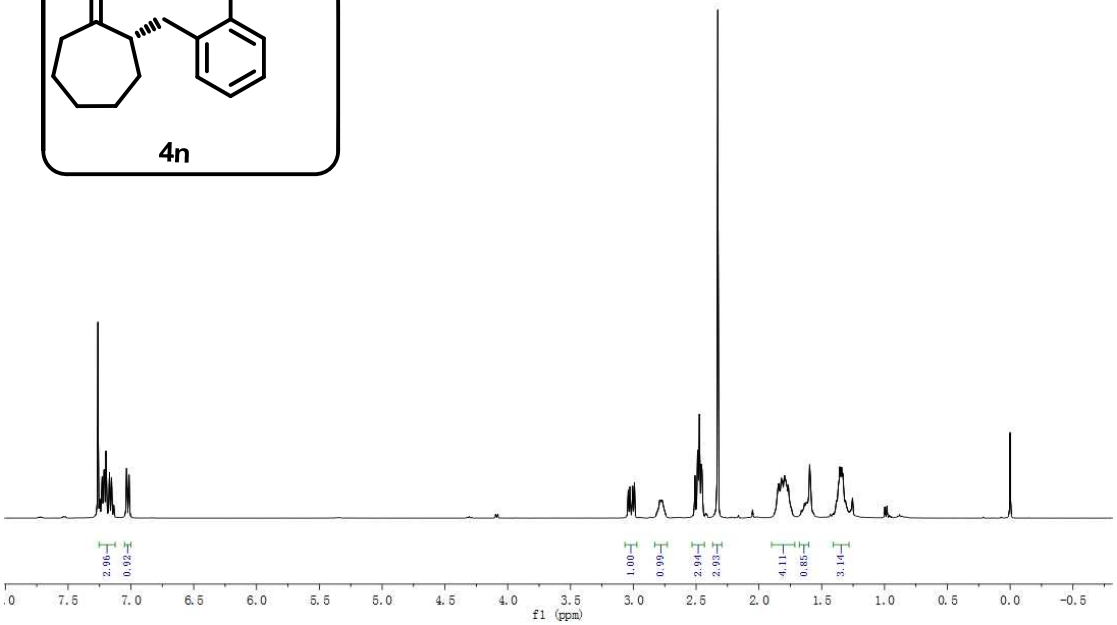

O
OCOEt
4m

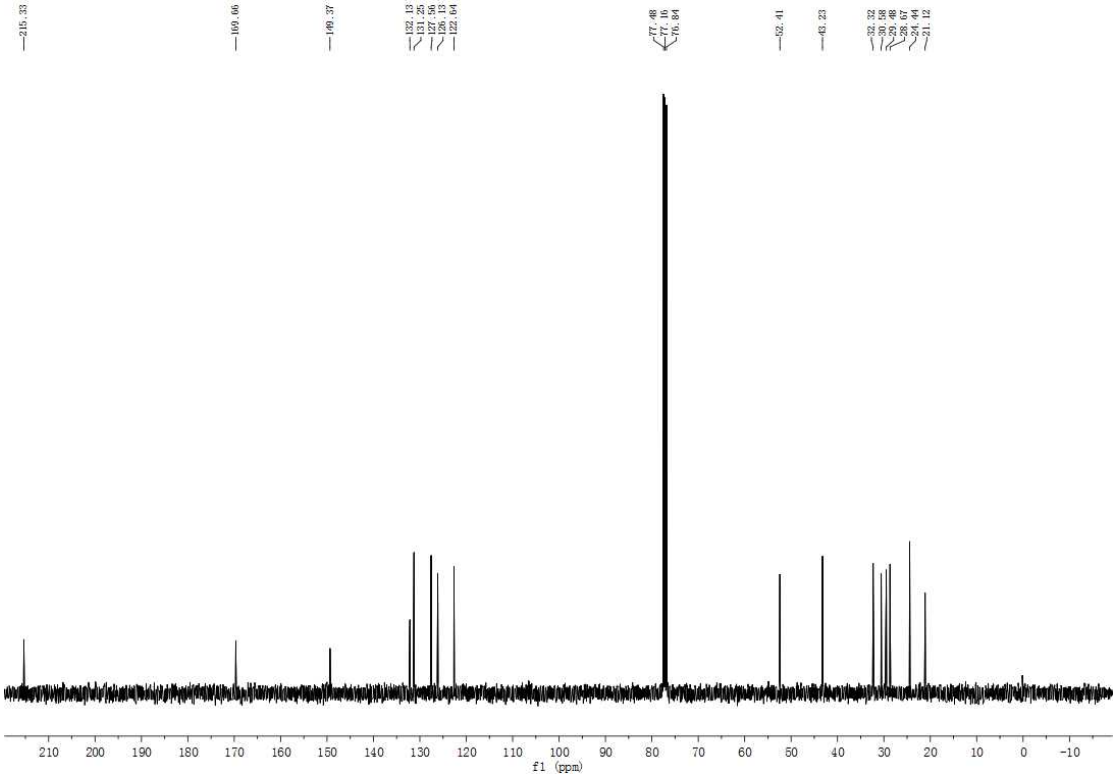

2.99
0.84
1.03
0.89
1.96
2.04
1.00
2.95
3.07
3.01
f1 (ppm)

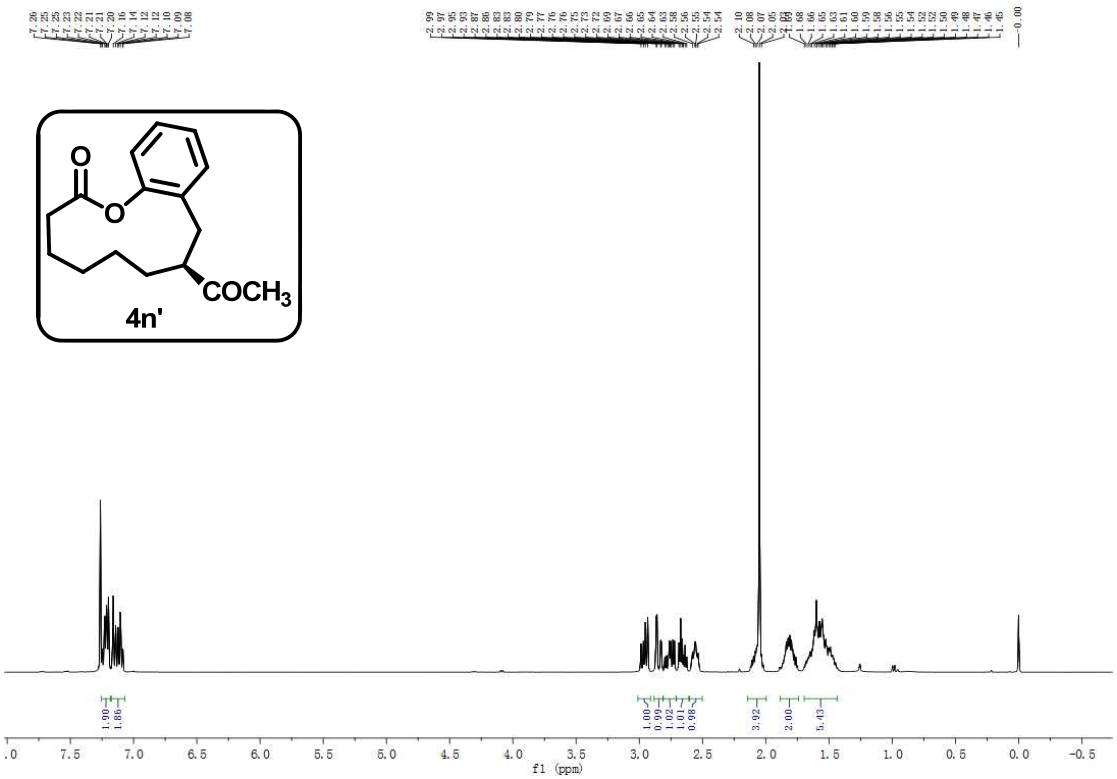

214.66
173.03
149.26
131.89
131.19
127.68
126.08
122.66
77.48
77.16
76.84
46.48
35.26
33.77
27.90
16.97
9.36
7.73
f1 (ppm)

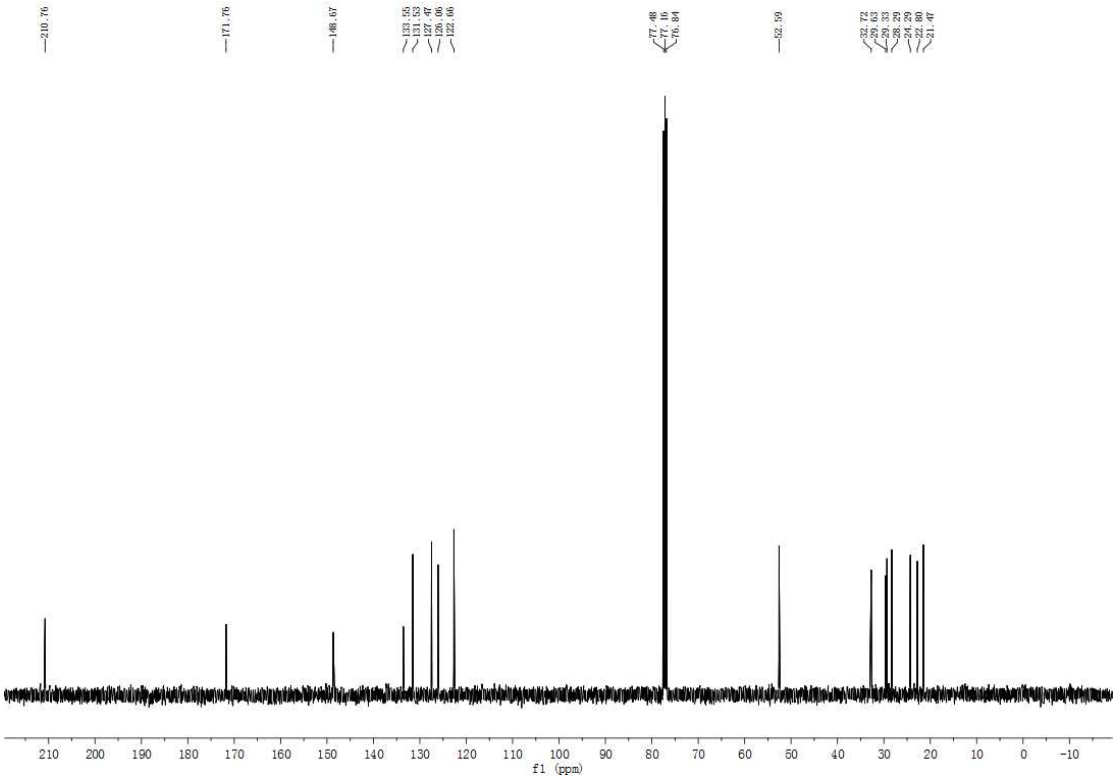

O
OCOCH3

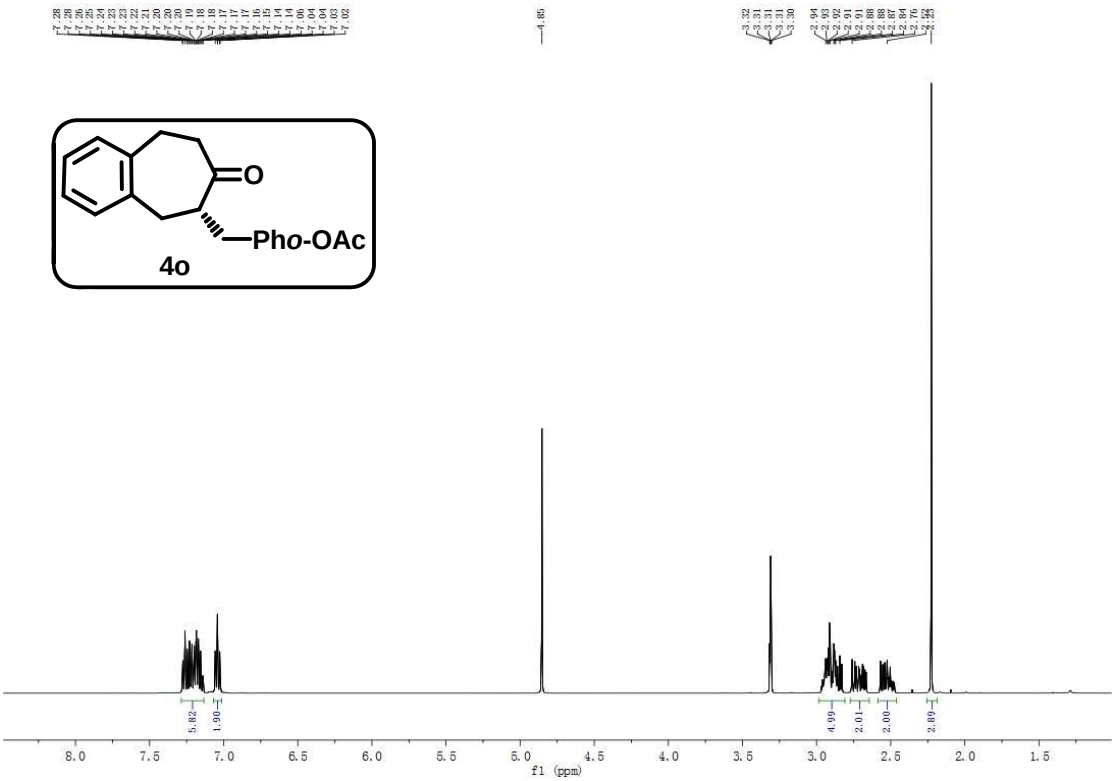
4n

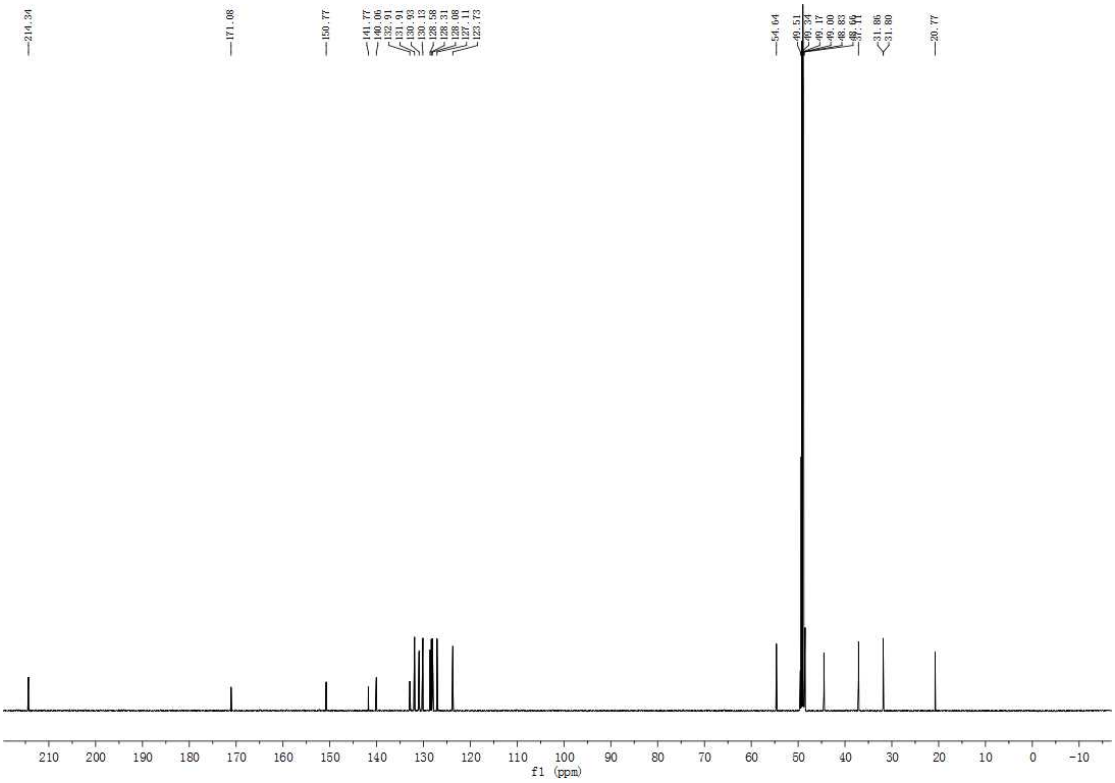

2.96
0.92
1.00
0.99
2.94
2.93
4.11
0.85
3.14
f1 (ppm)

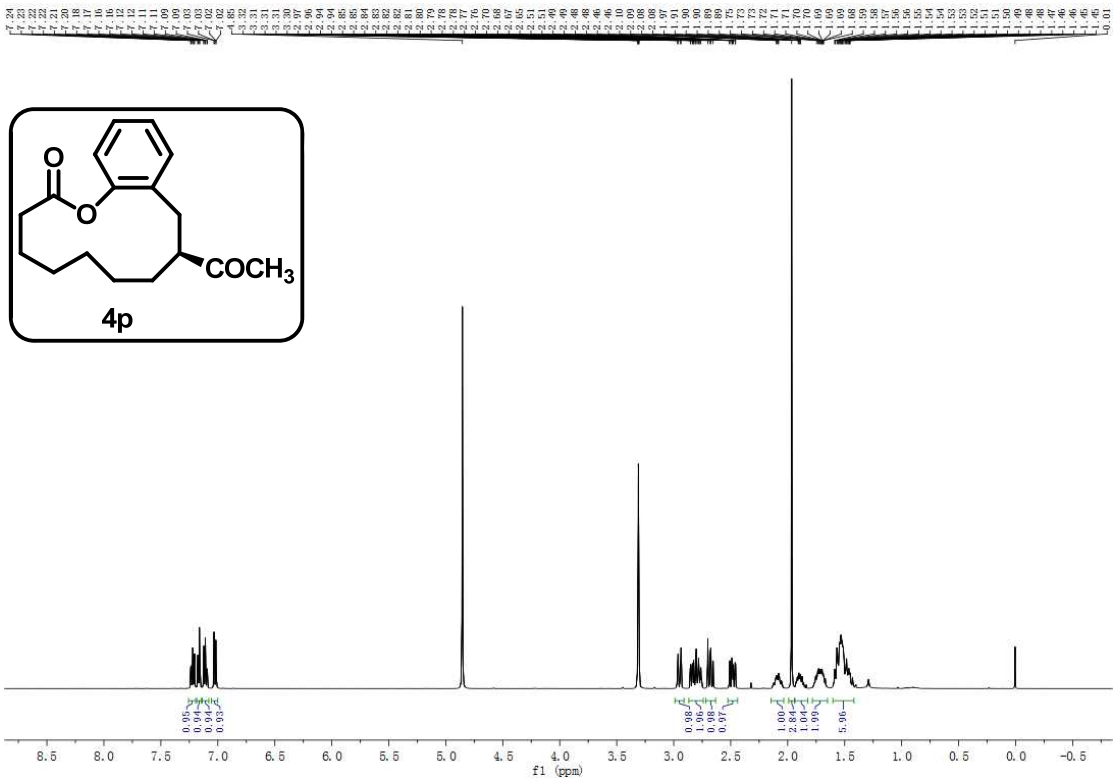

215.33
169.66
149.37
132.13
131.25
127.56
126.13
122.64
77.48
77.16
76.84
52.41
43.23
32.32
30.38
29.48
28.07
24.44
21.12
f1 (ppm)

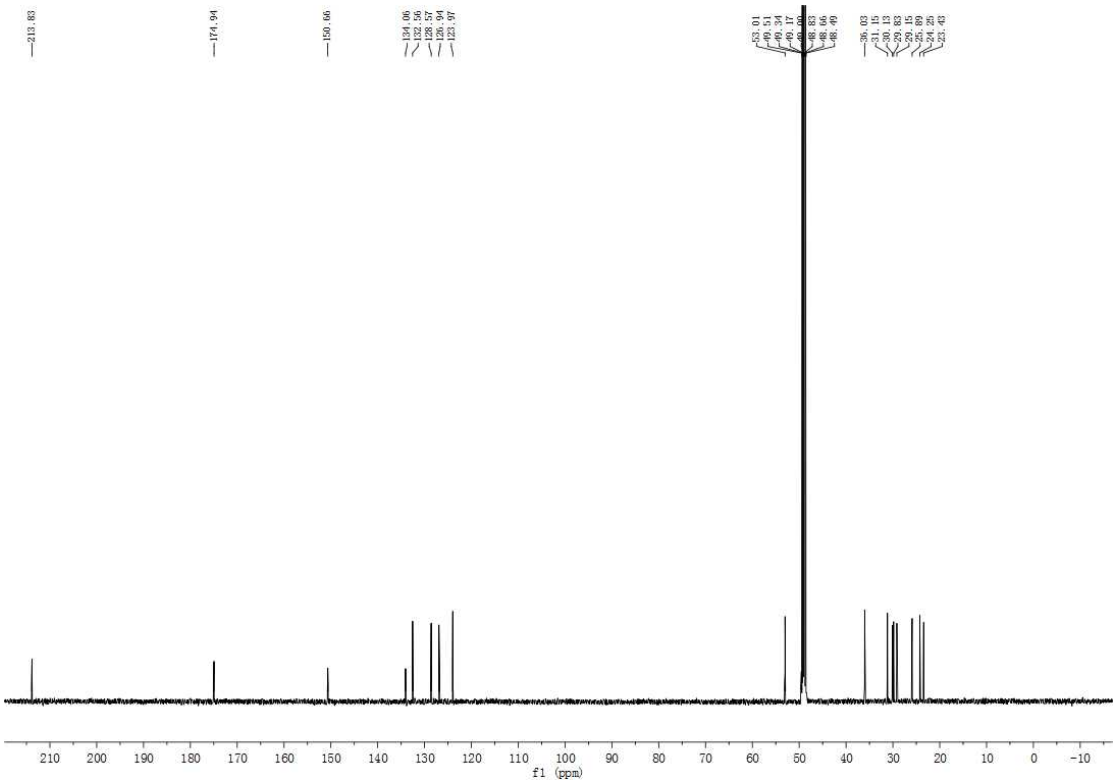

O
O
COCH3
4n'
f1 (ppm)


f1 (ppm)

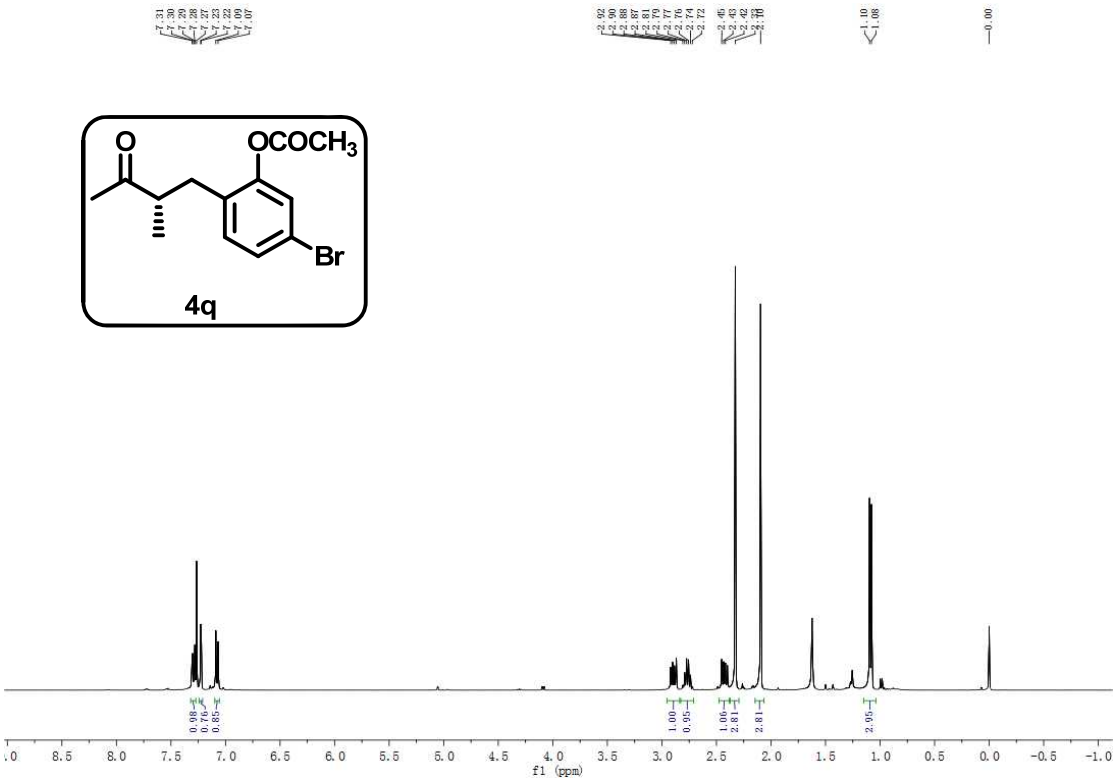

O
Pho-OAc
4o
f1 (ppm)

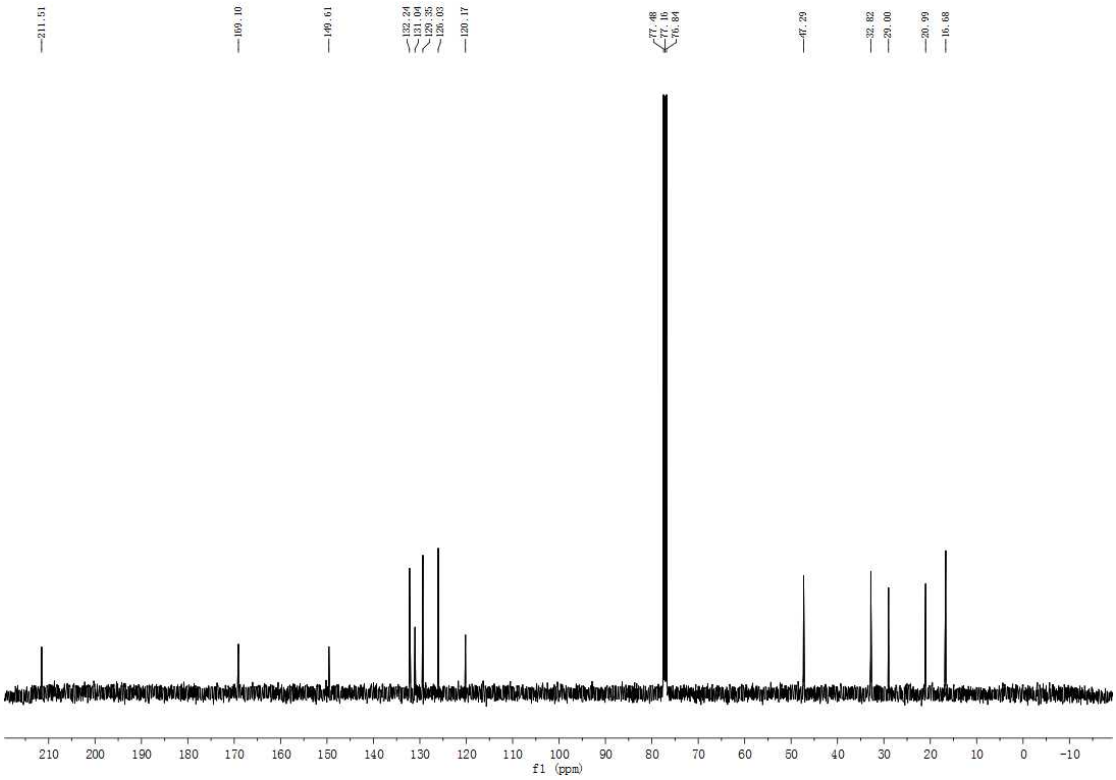

f1 (ppm)

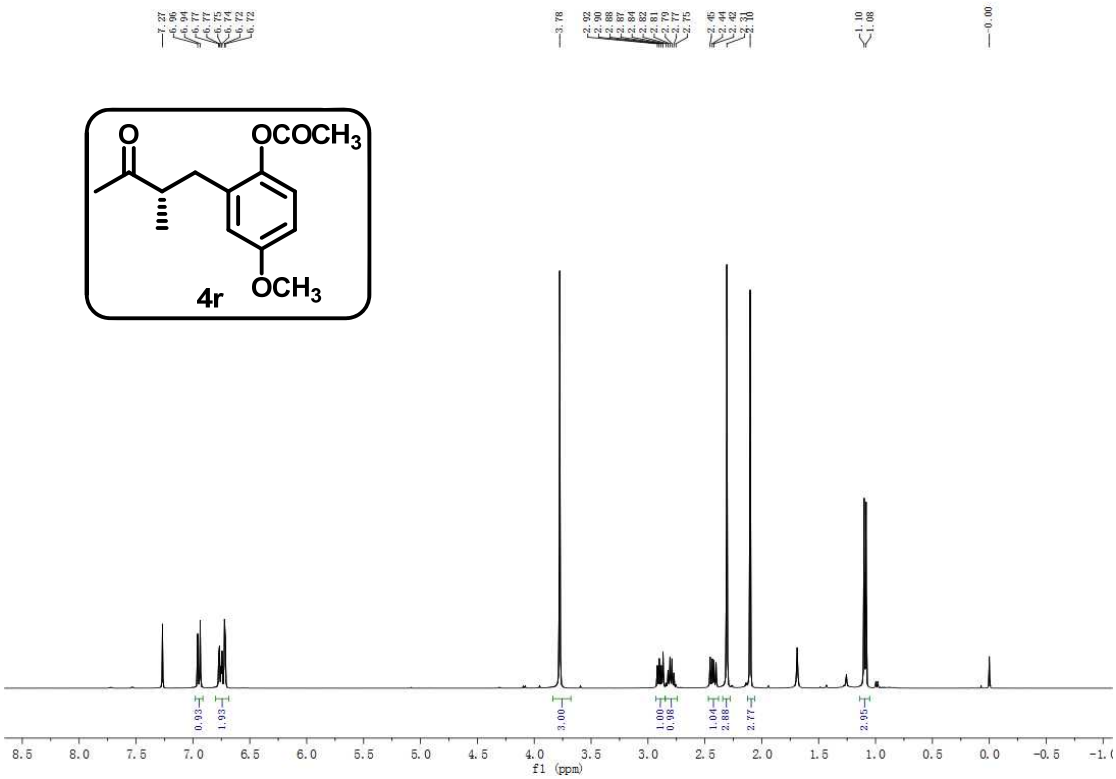

O
O
COCH3
4p
f1 (ppm)

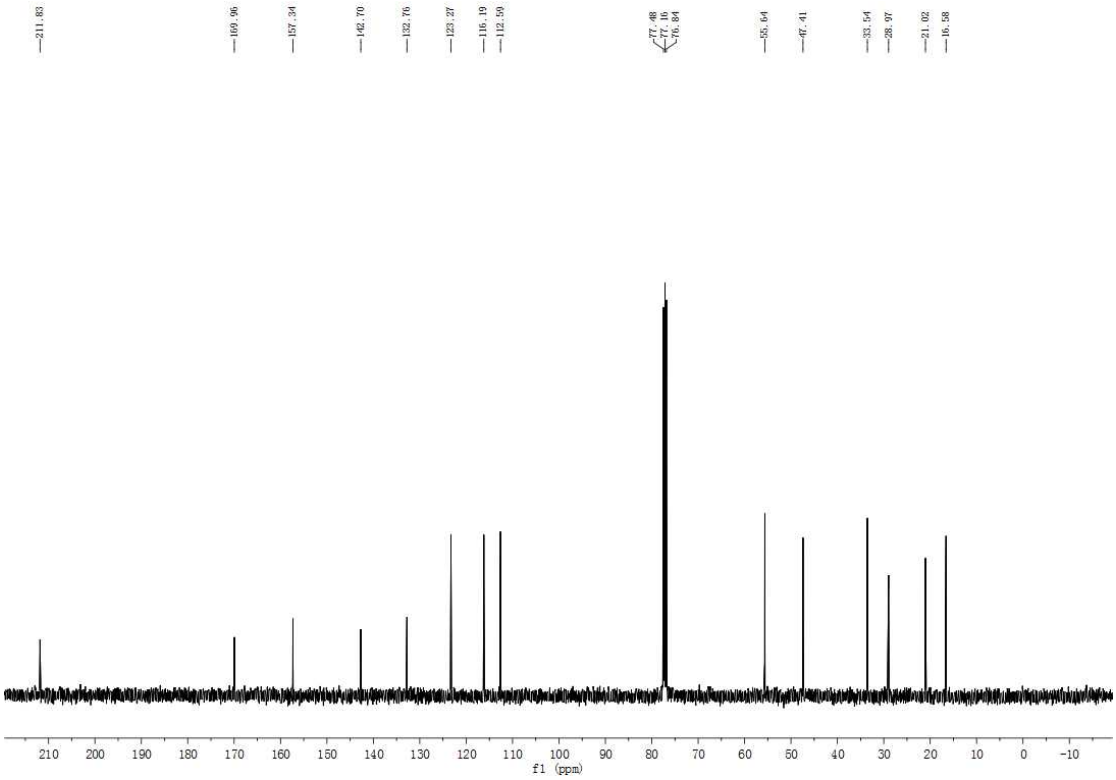

f1 (ppm)

4q

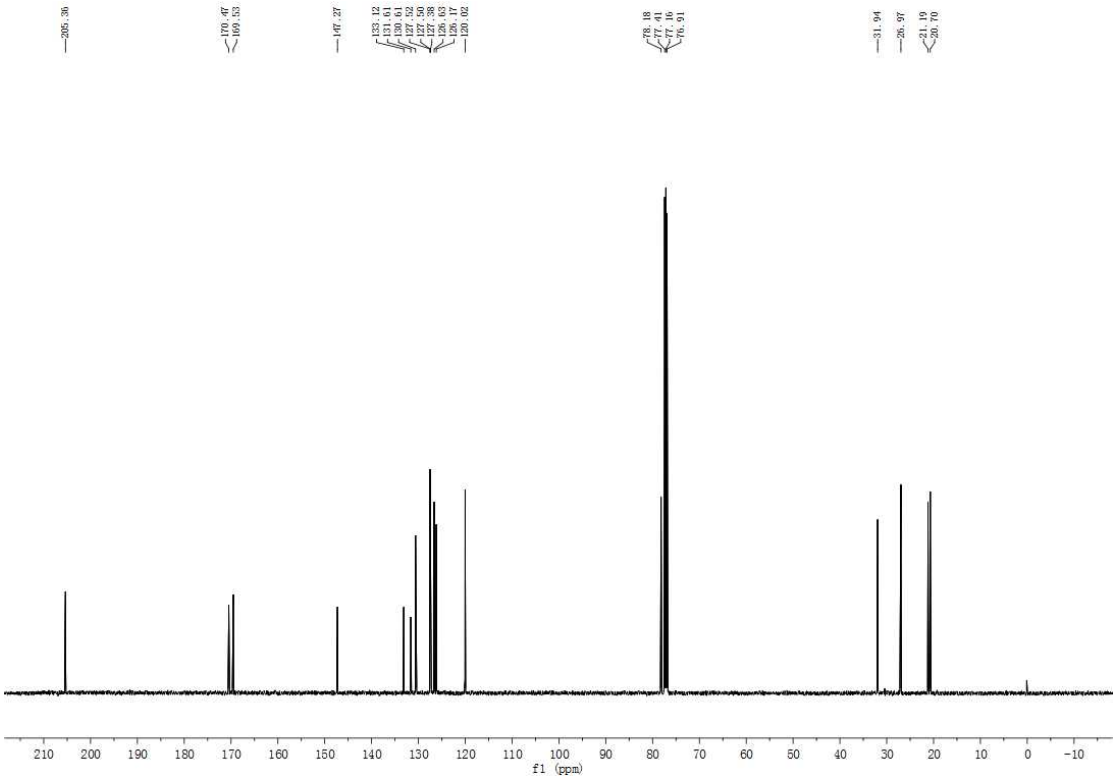


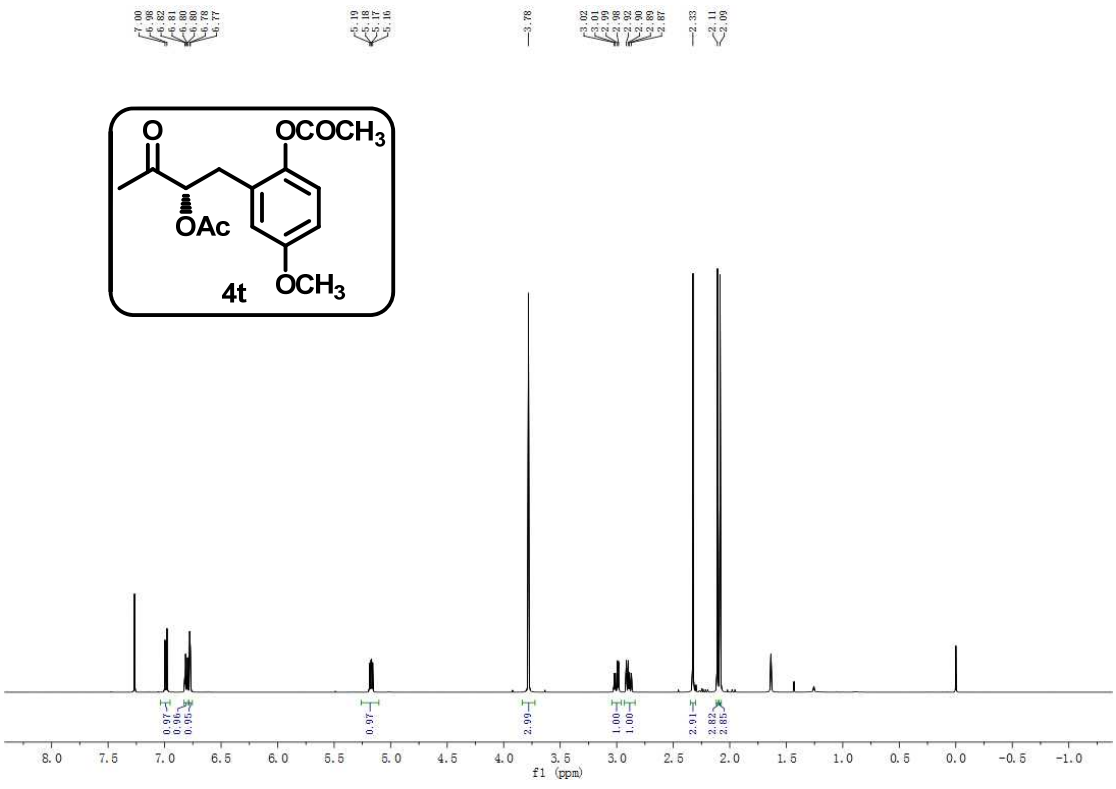


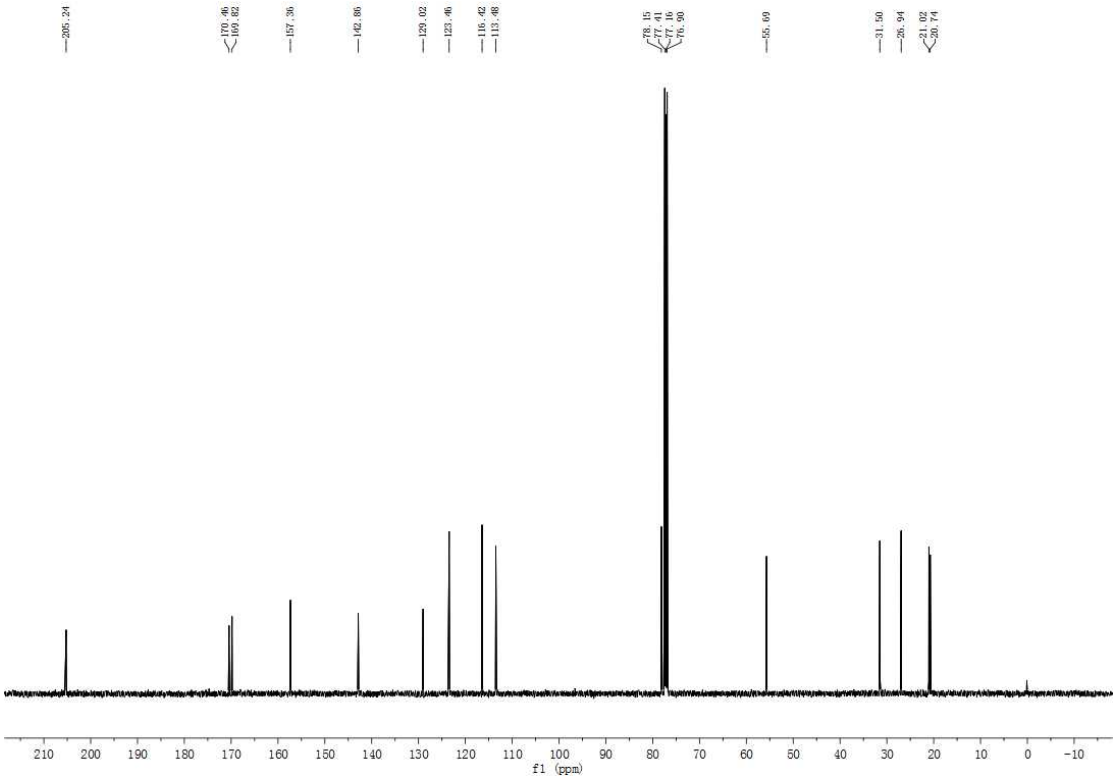

O
OCOCH3
OCH3
4r
f1 (ppm)


f1 (ppm)

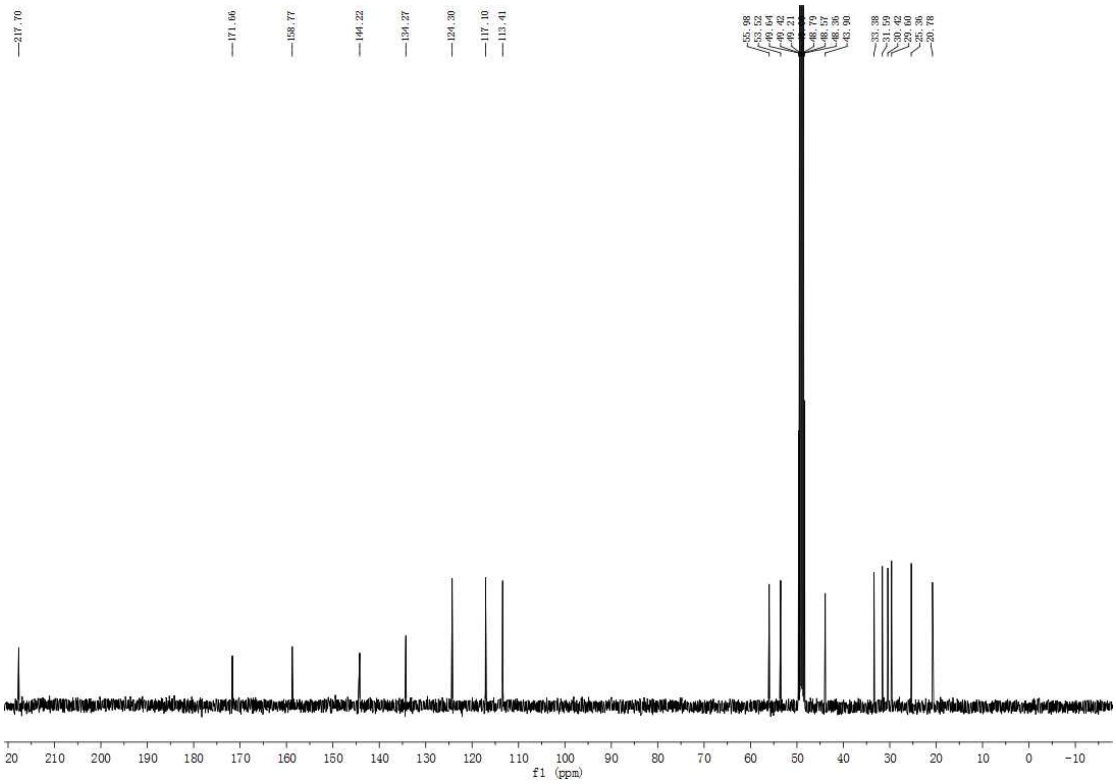
O
OCOCH3
OAc
4s



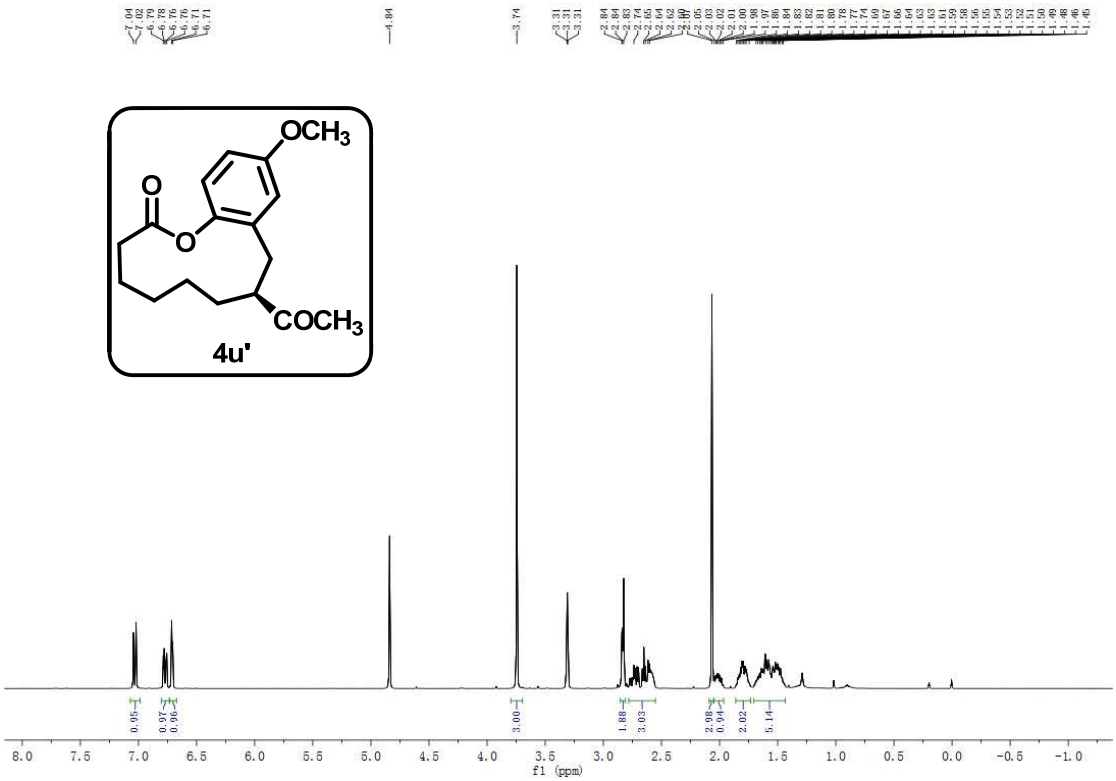

O
OCOCH3
OAc
4t
OCH3
f1 (ppm)

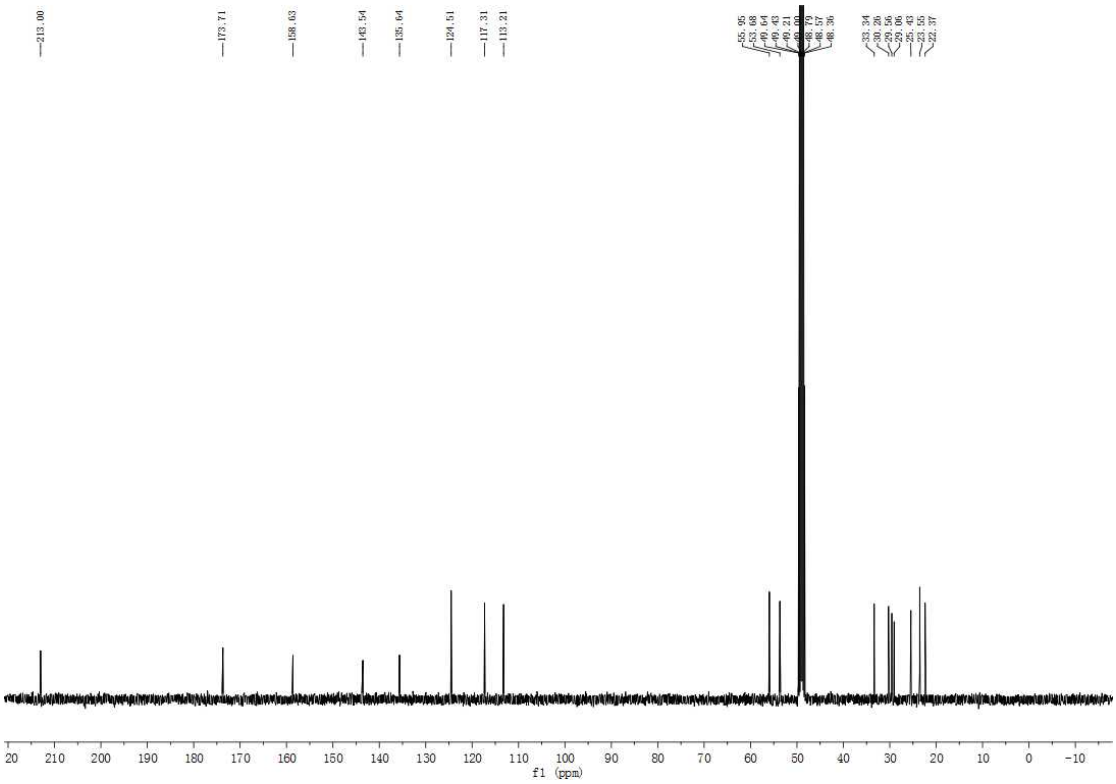

f1 (ppm)

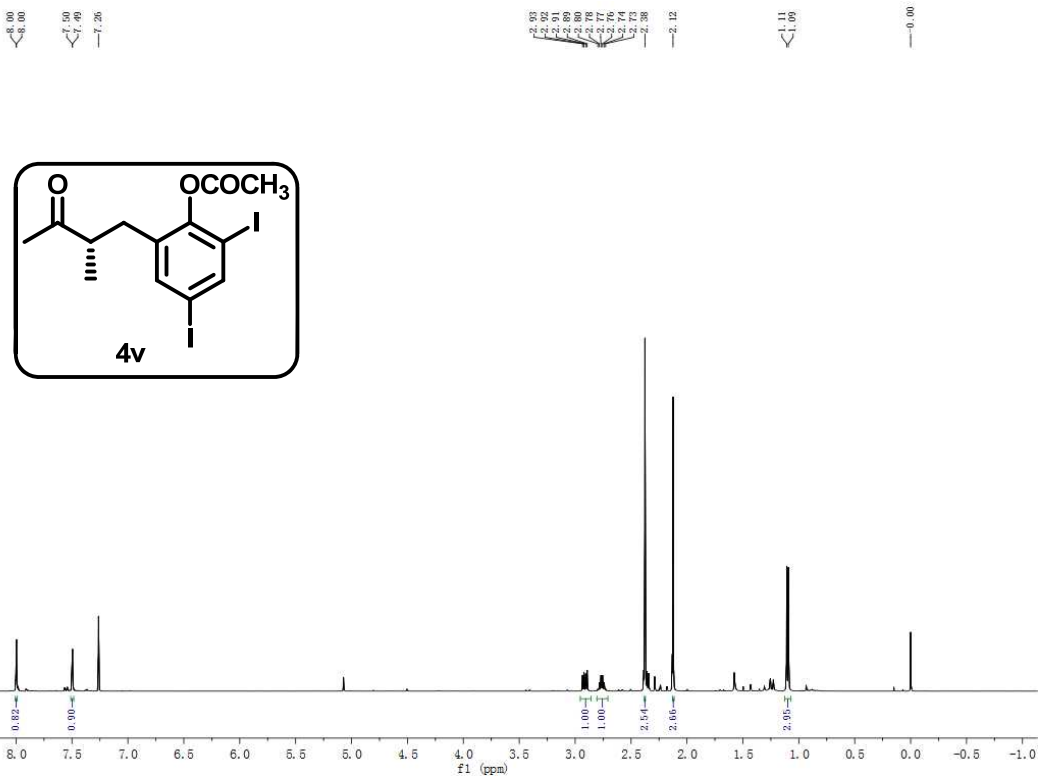

O
OCOCH3
OCH3
4u
f1 (ppm)

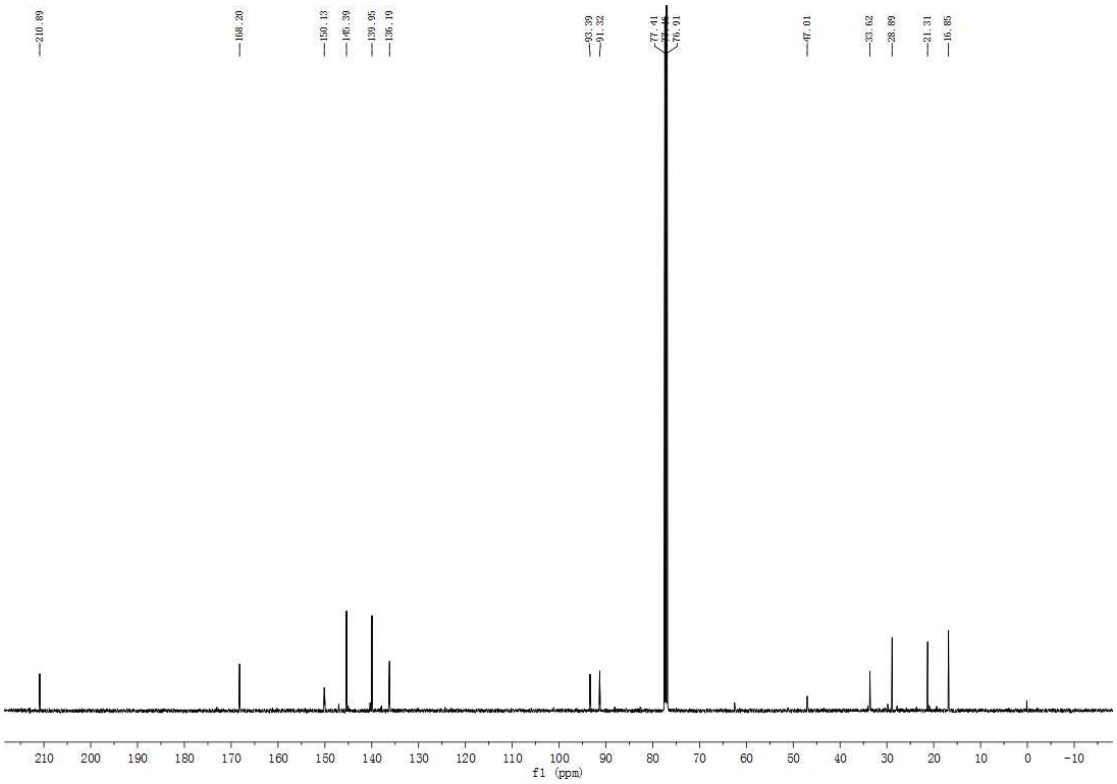

f1 (ppm)

4u'






8.00
8.00
7.50
7.49
7.26
2.93
2.92
2.91
2.89
2.80
2.78
2.77
2.76
2.74
2.73
2.38
2.12
1.11
1.09
0.00
O
OCOCH3
I
I
4v
0.82
0.90
1.00
1.00
2.54
2.66
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


210.89
168.20
150.13
145.39
139.95
136.19
93.39
91.32
77.41
77.16
76.91
47.01
33.62
28.89
21.31
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200
190
180
170
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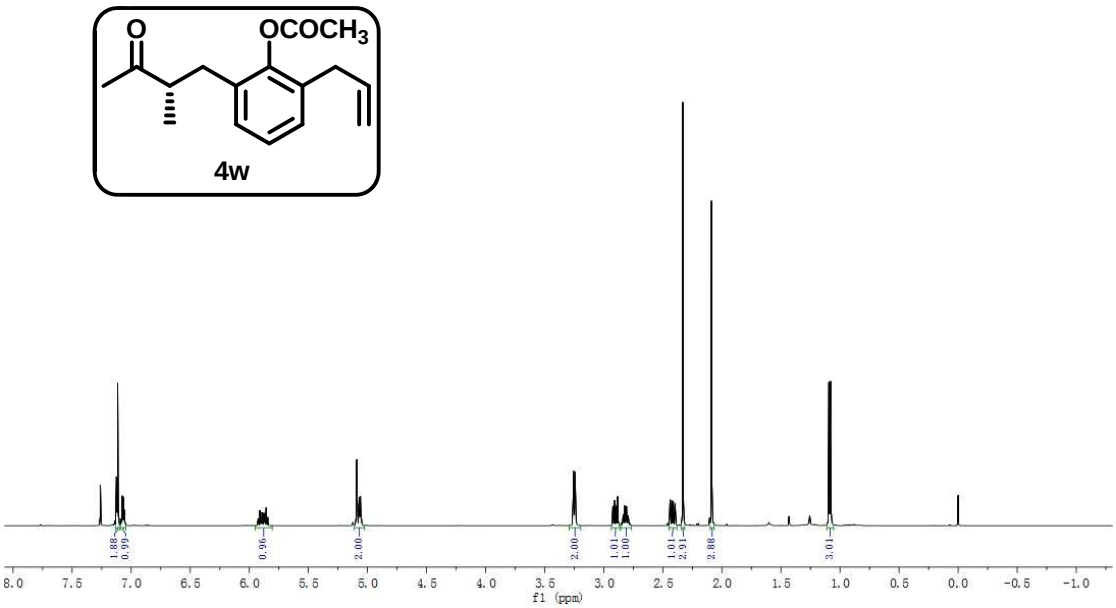
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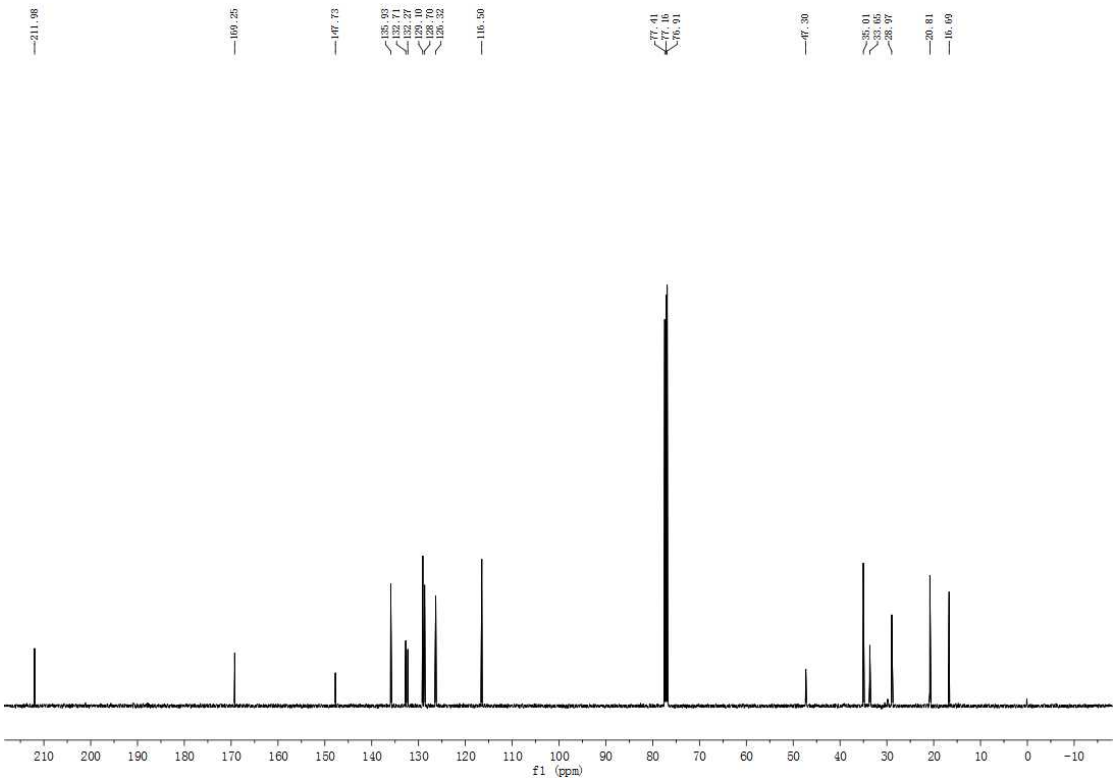
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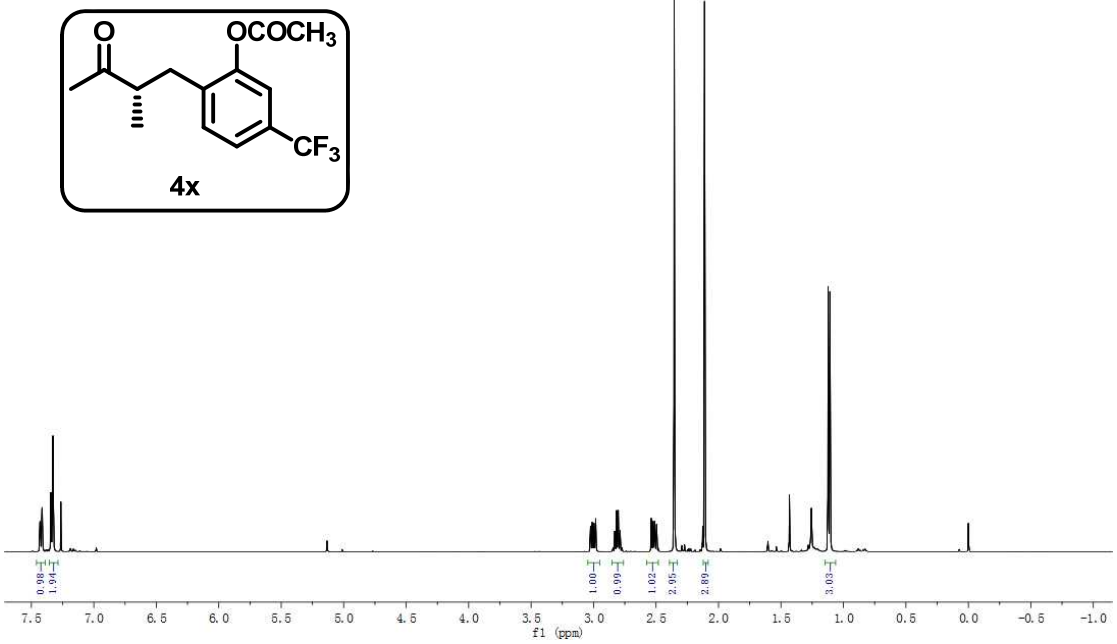
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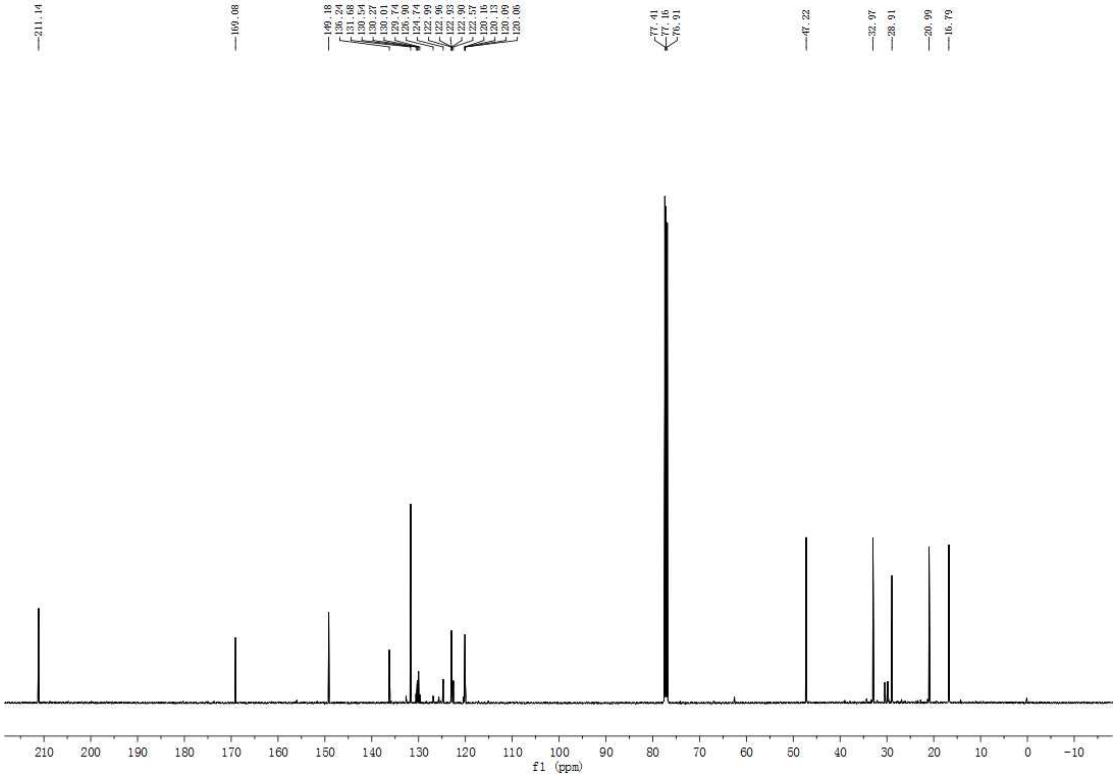
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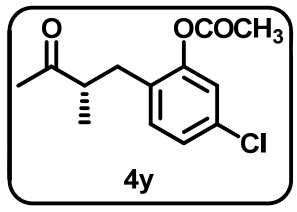

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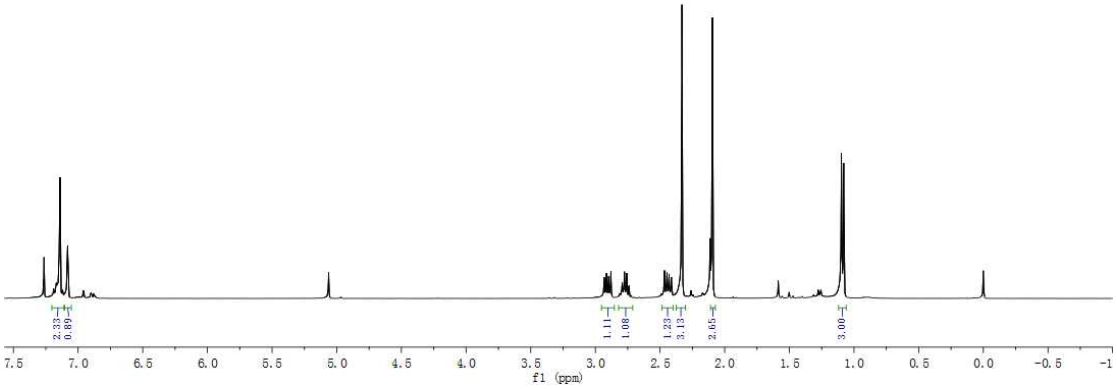

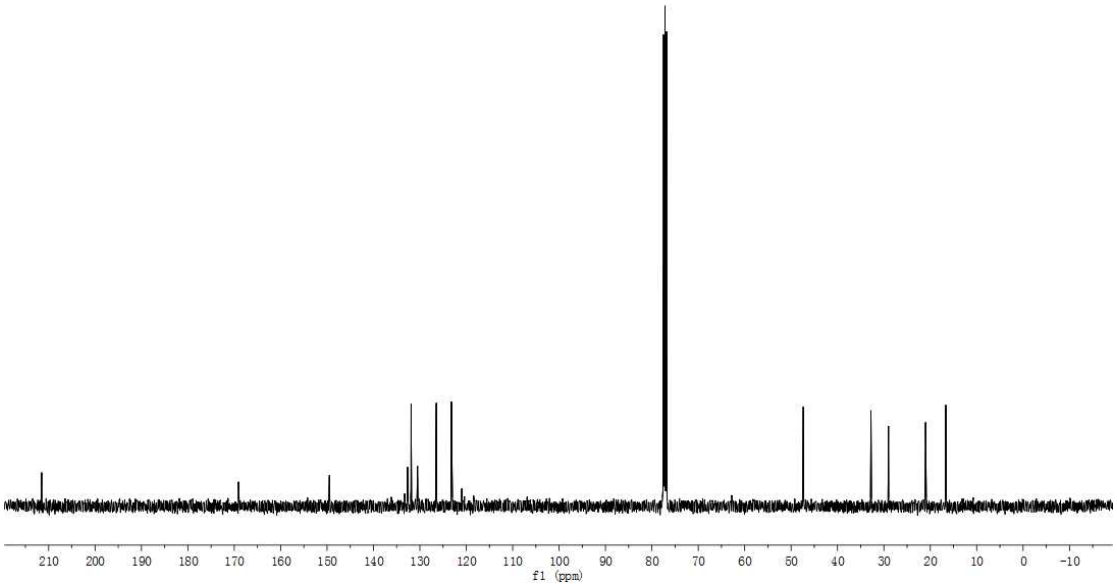

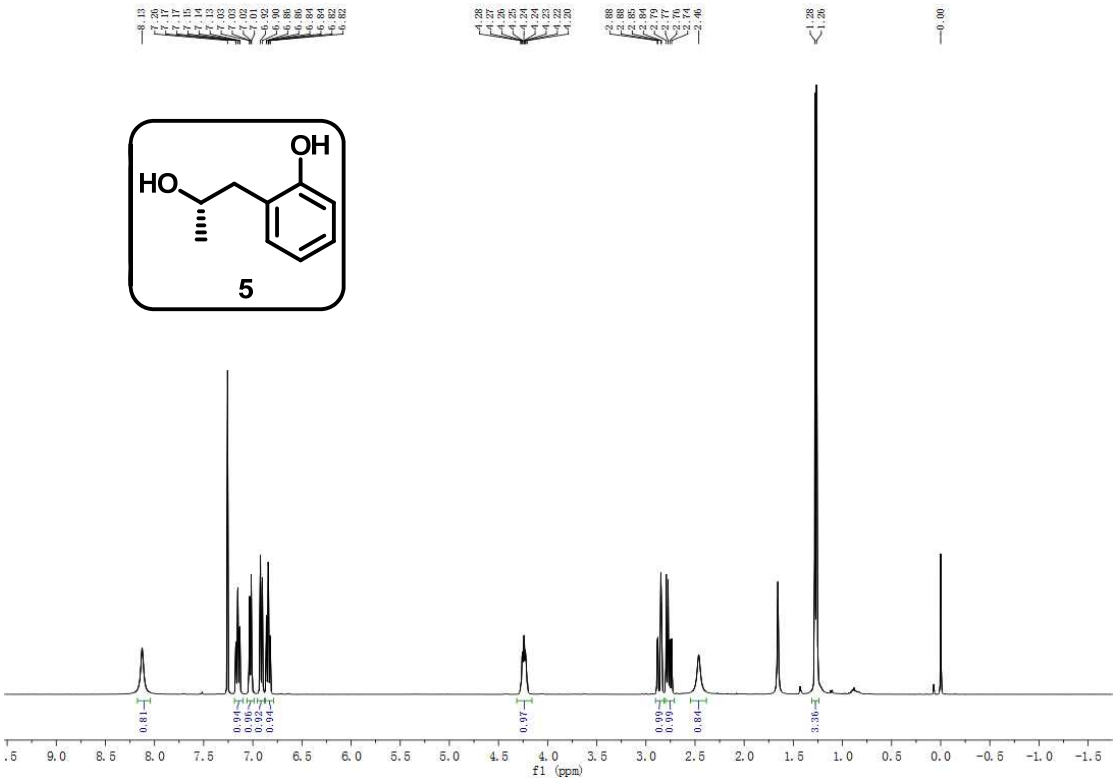
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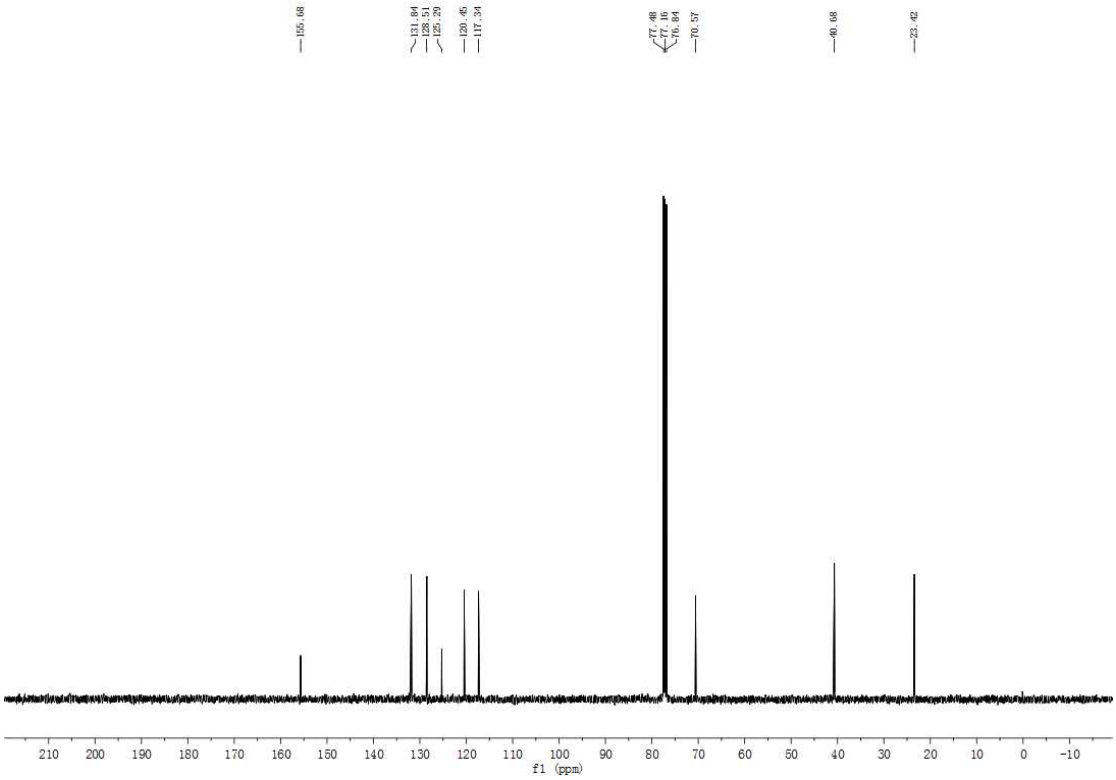
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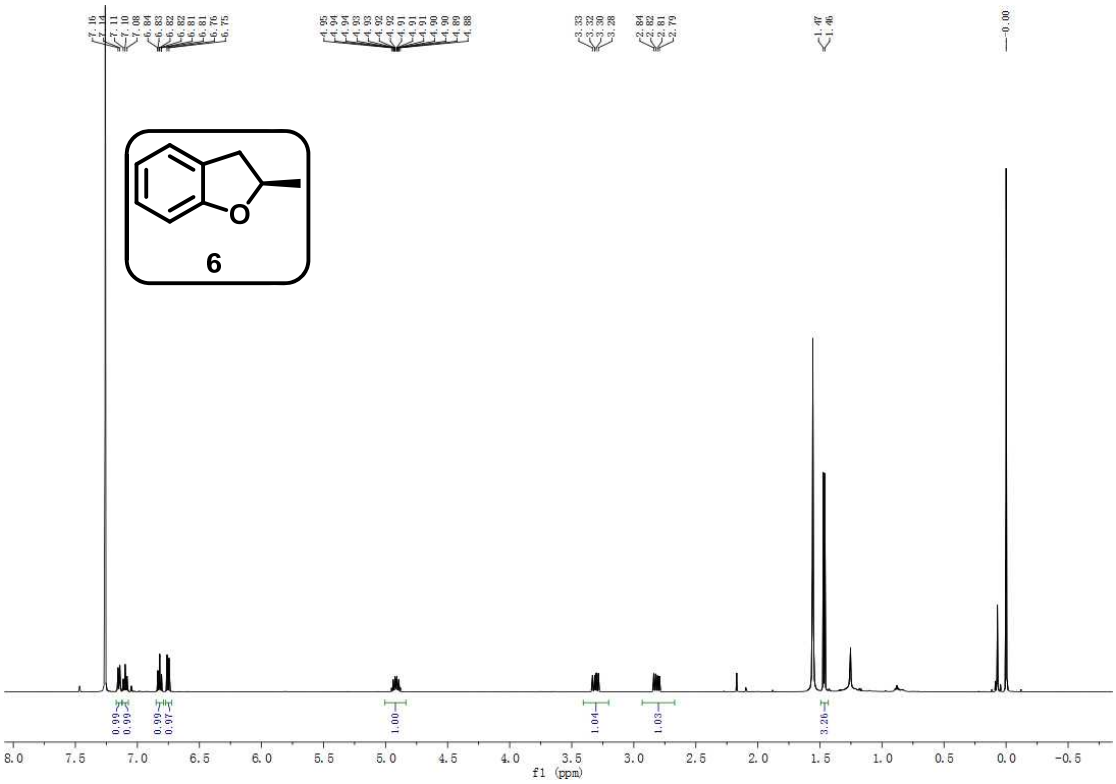
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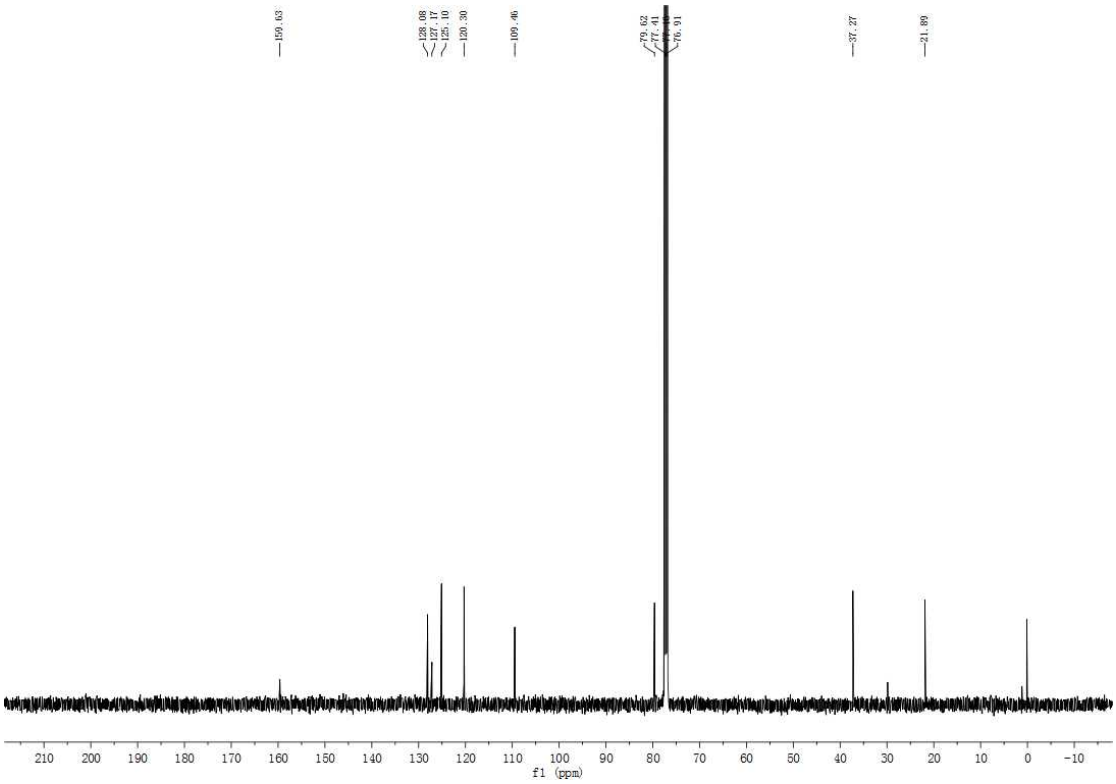
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2.40
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0.93
0.92
0.00
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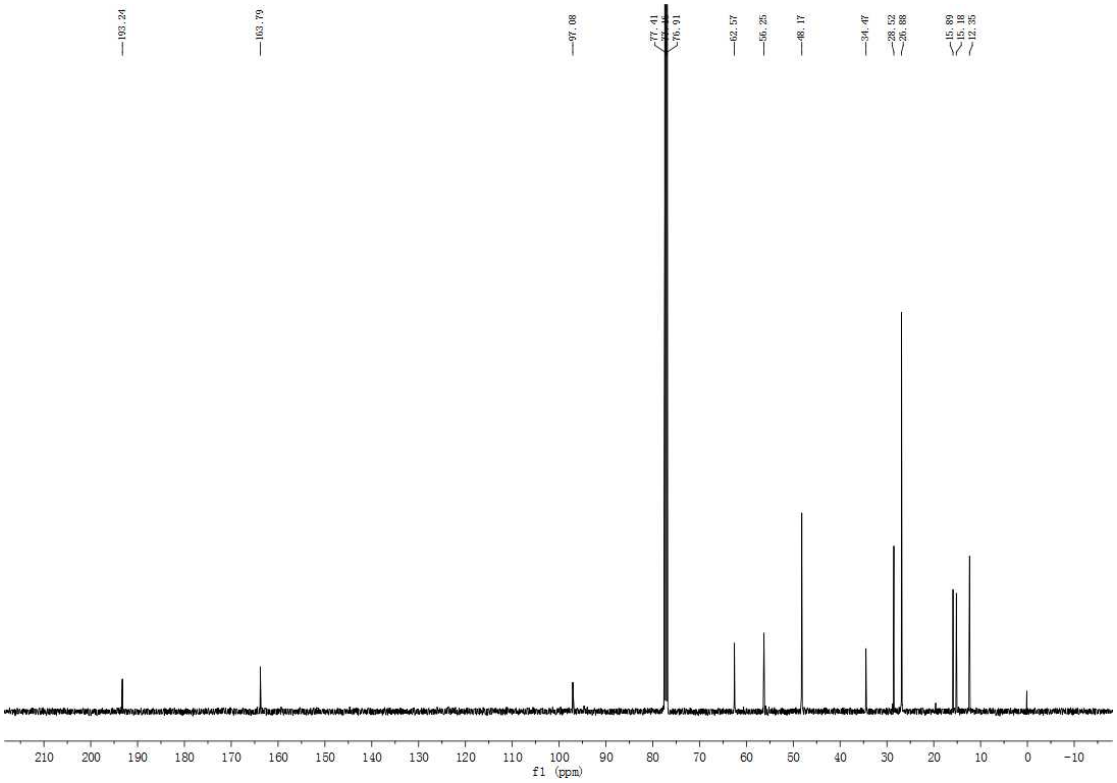
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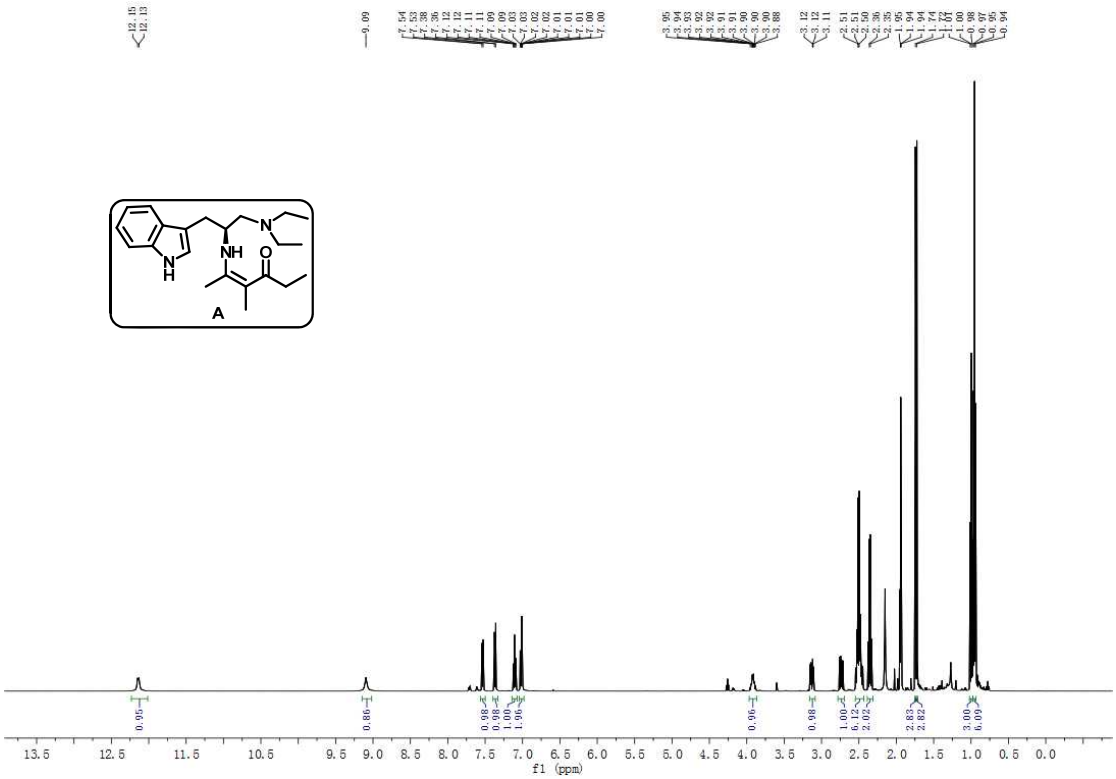
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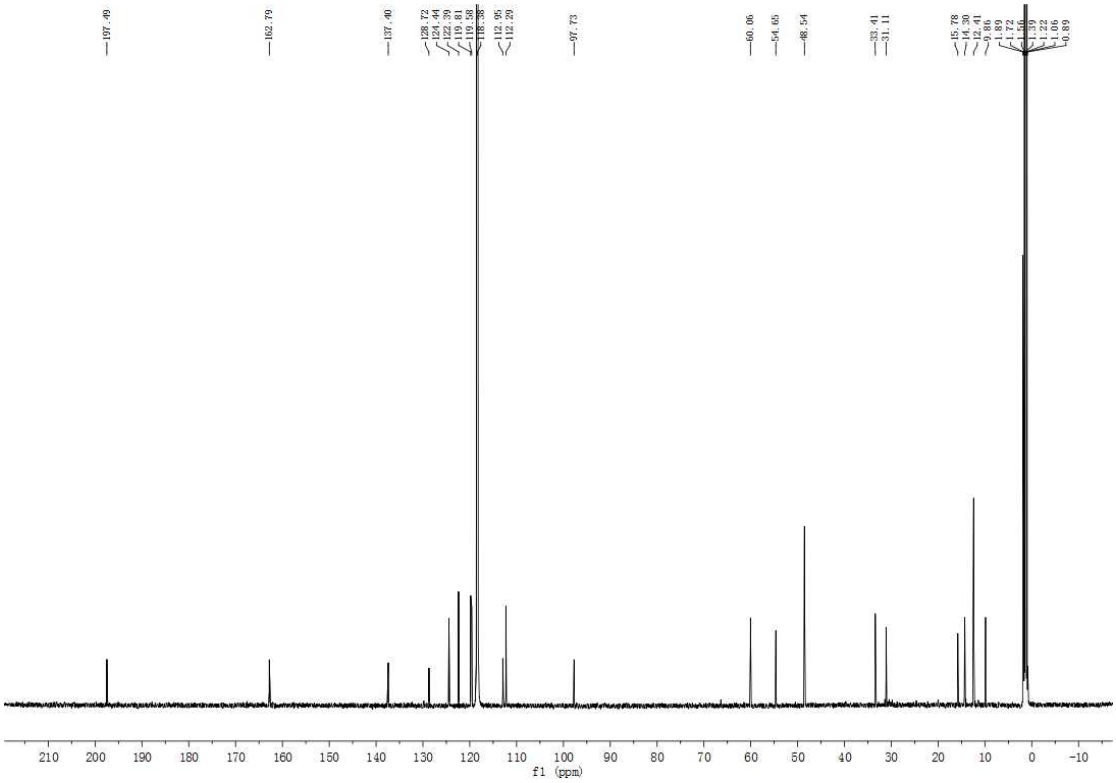
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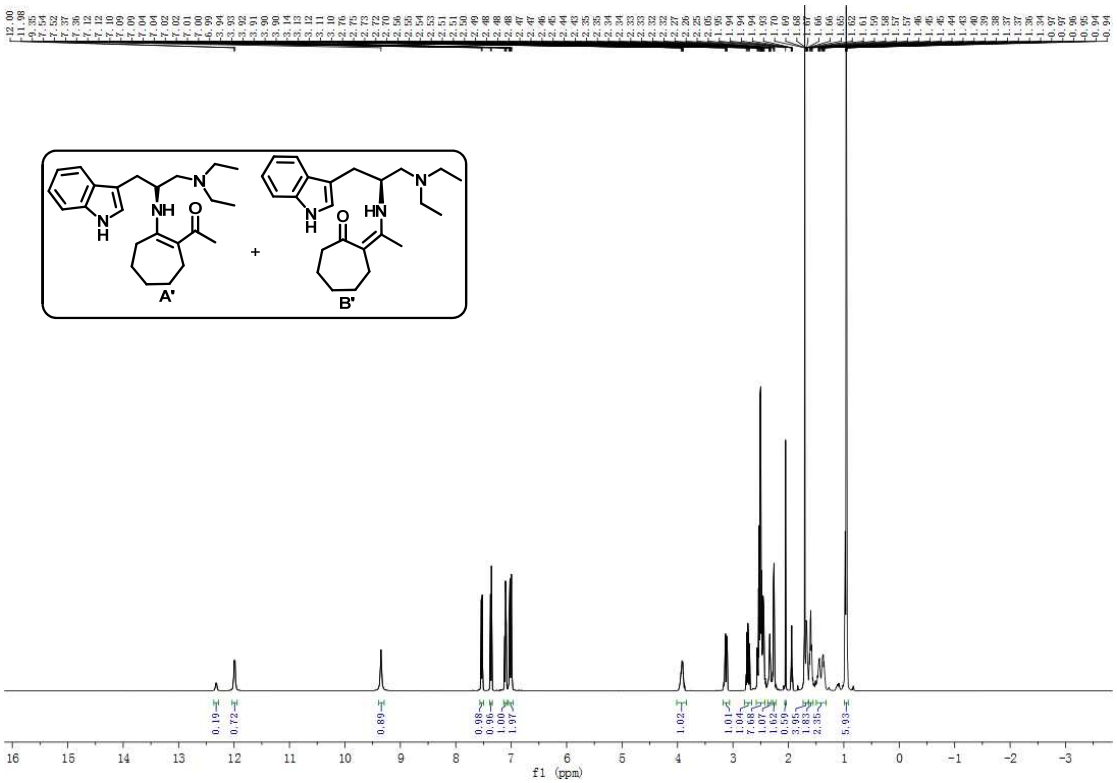
A'
B'
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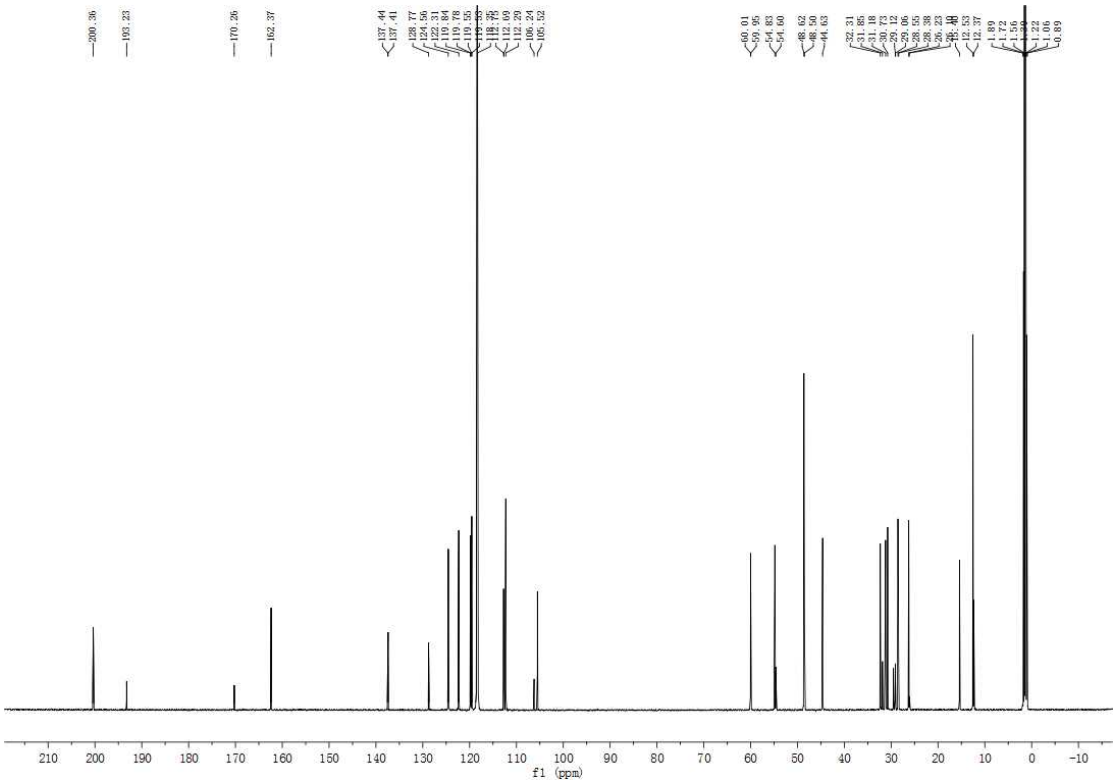
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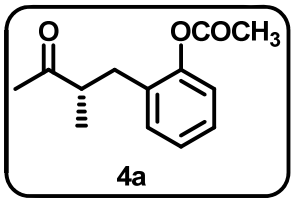
HPLC charts



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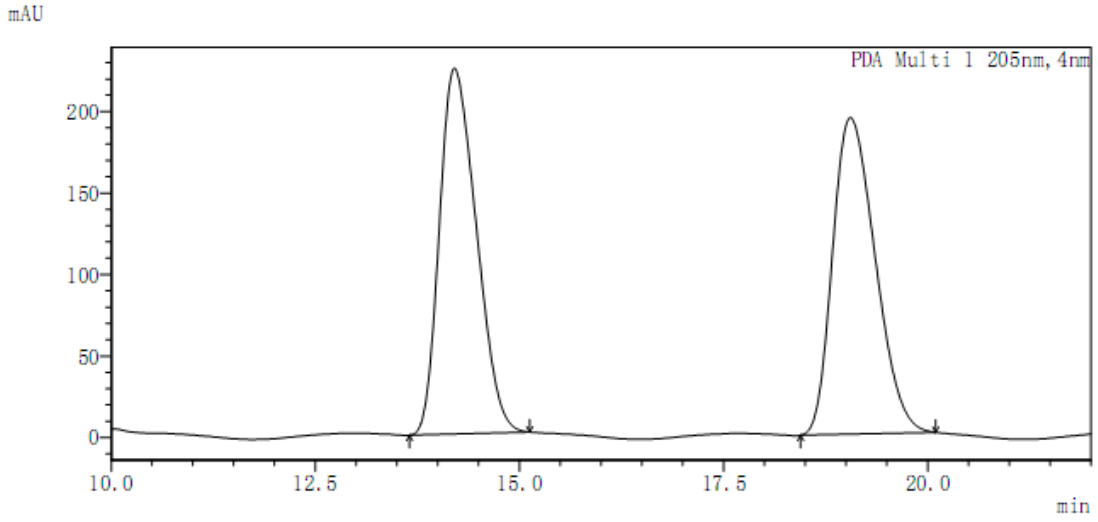

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	14.204	224384	7056826	50.014
2	19.053	194253	7052921	49.986

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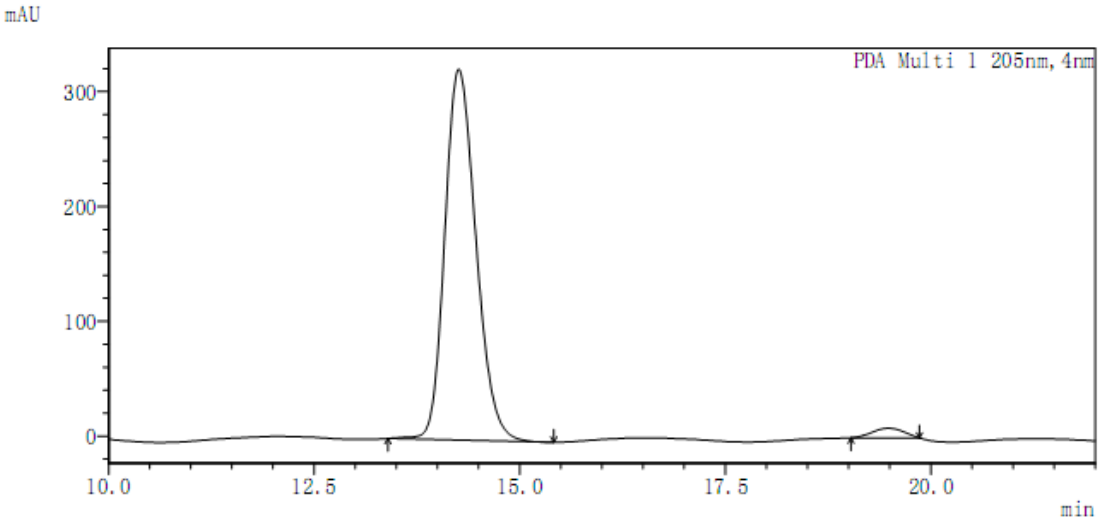
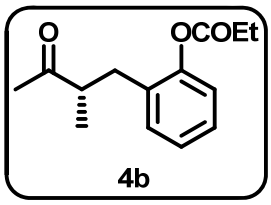


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	14.258	322657	8498734	97.433
2	19.479	8419	223953	2.567



4b

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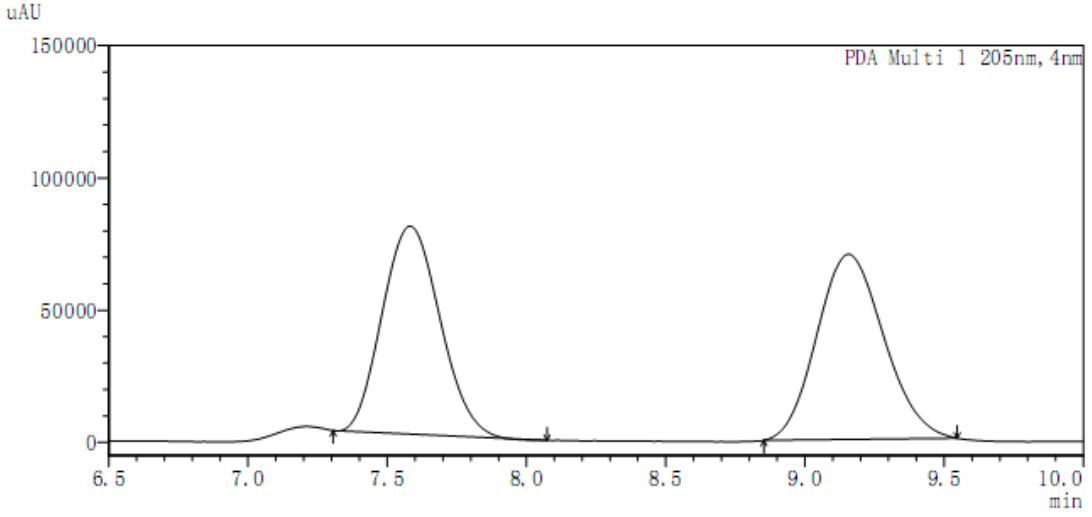

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.582	78745	1134462	49.219
2	9.156	70005	1170471	50.781

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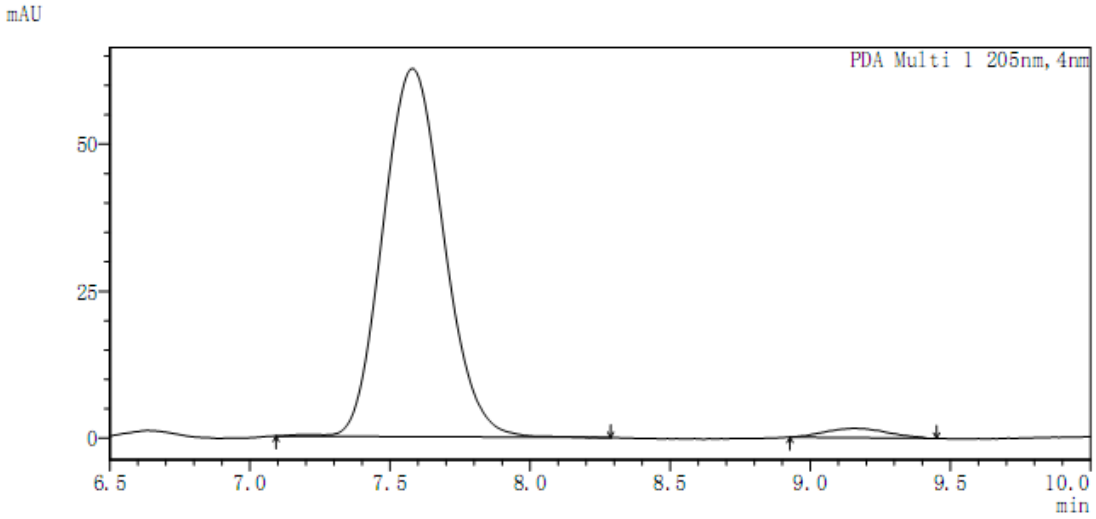
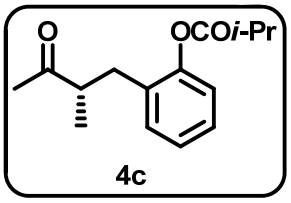


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.580	62667	945925	97.446
2	9.161	1624	24796	2.554



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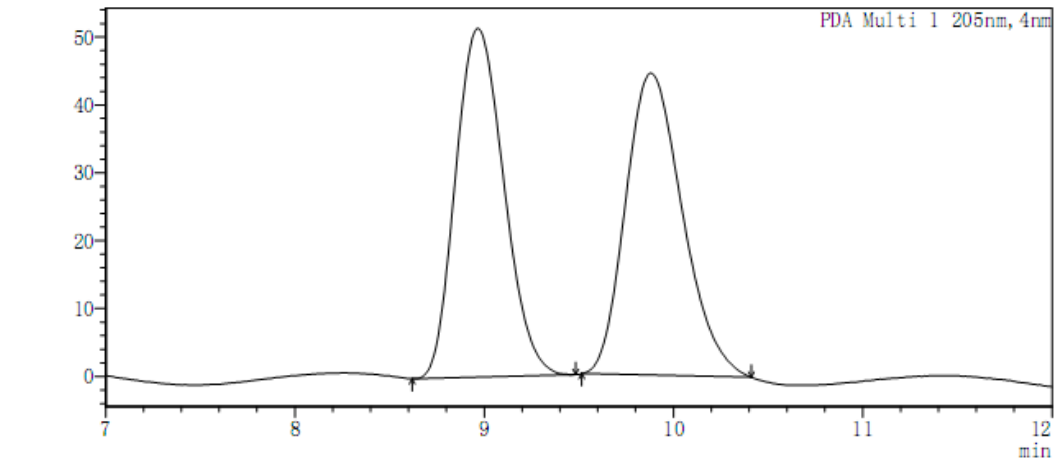

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.966	51368	912207	49.525
2	9.880	44523	929724	50.475

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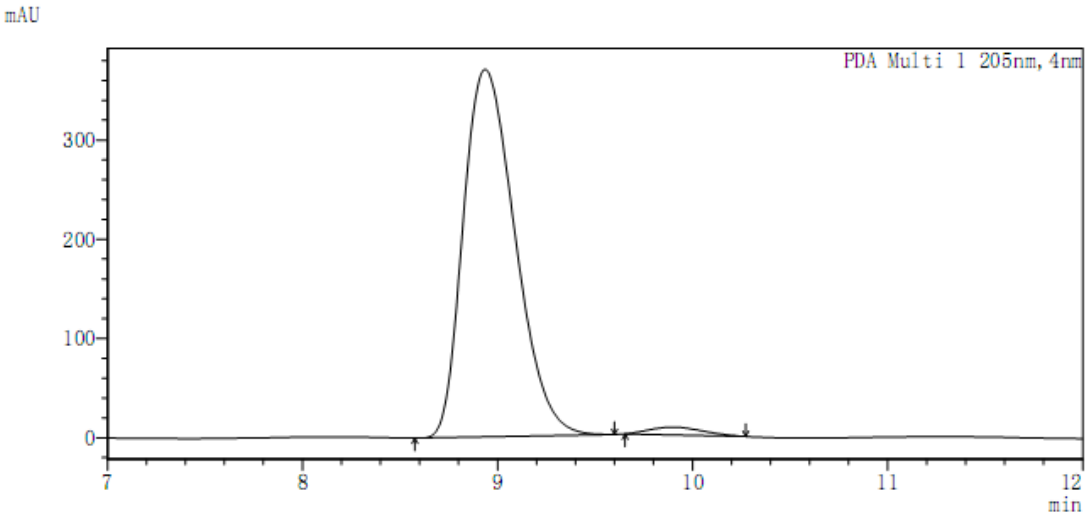
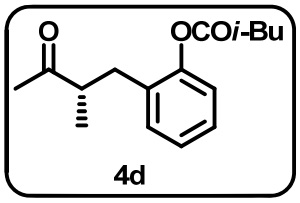


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.936	370416	6842805	97.873
2	9.893	7774	148679	2.127



4d

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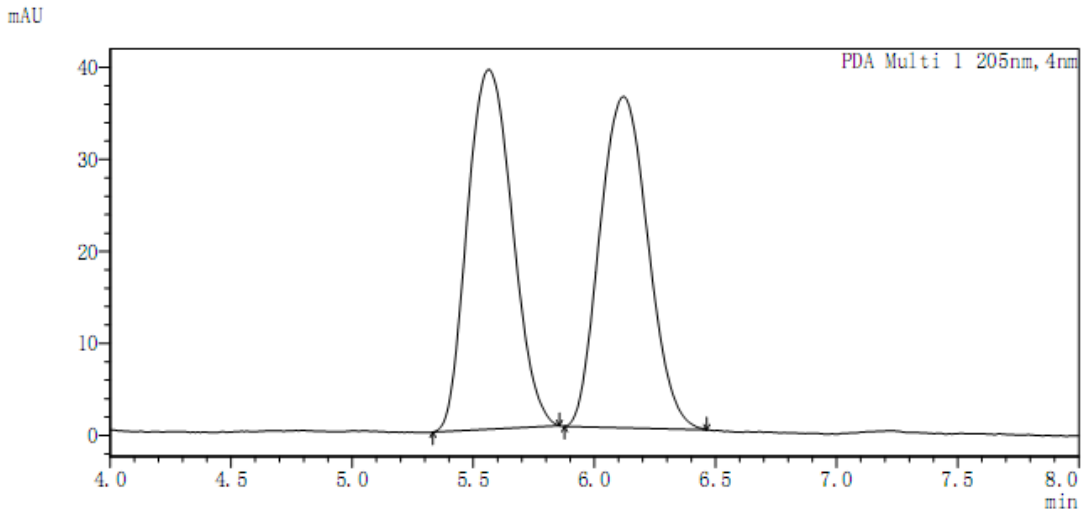

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.564	39084	505673	50.324
2	6.120	36030	499160	49.676

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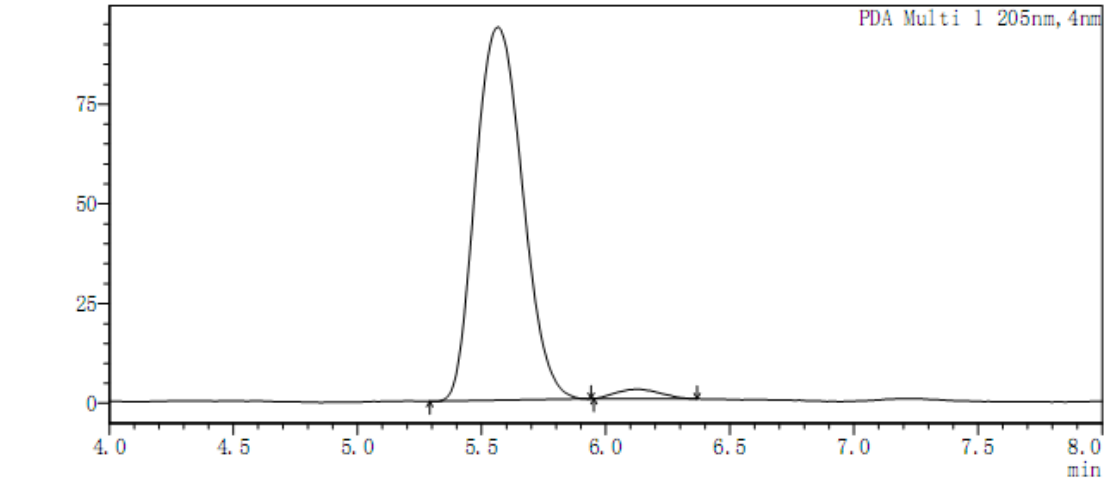
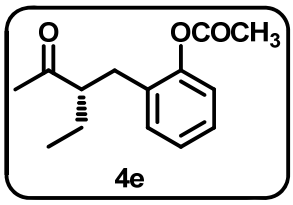


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.566	93611	1231639	97.664
2	6.132	2403	29455	2.336



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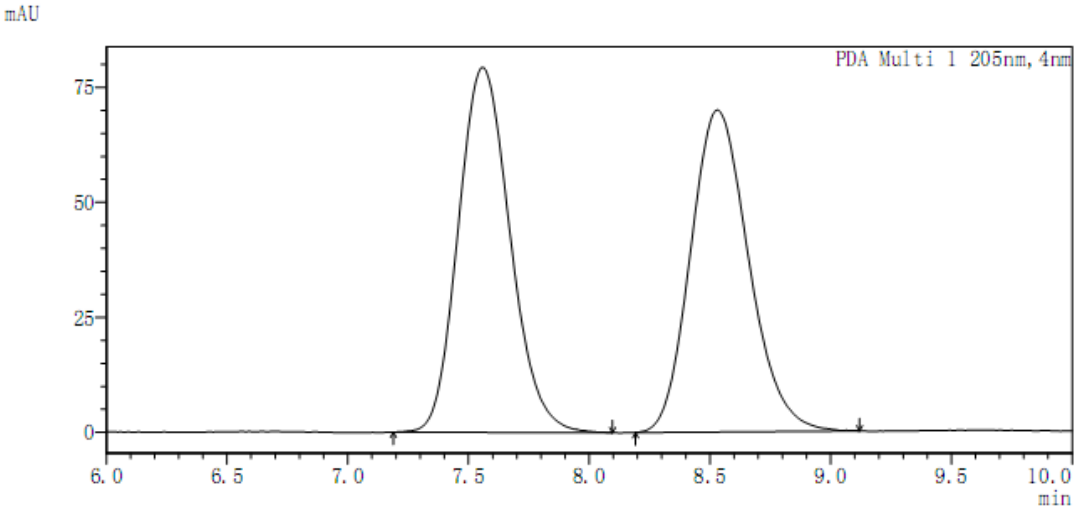

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.559	79378	1186739	50.283
2	8.531	70054	1173375	49.717

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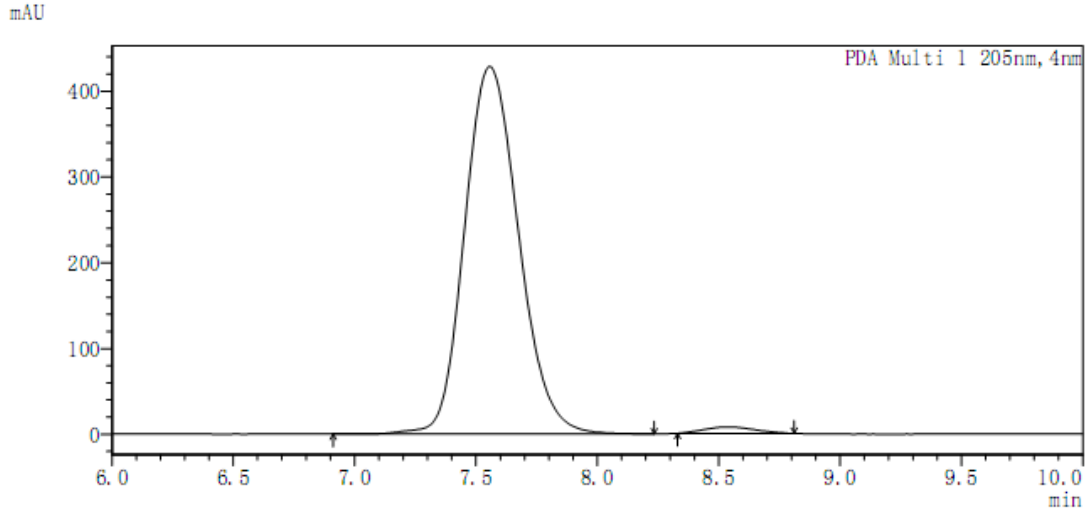
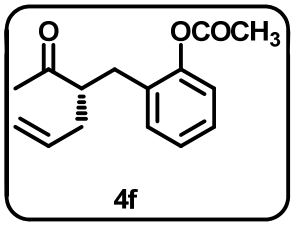


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.557	428367	6640737	98.429
2	8.538	7228	105985	1.571



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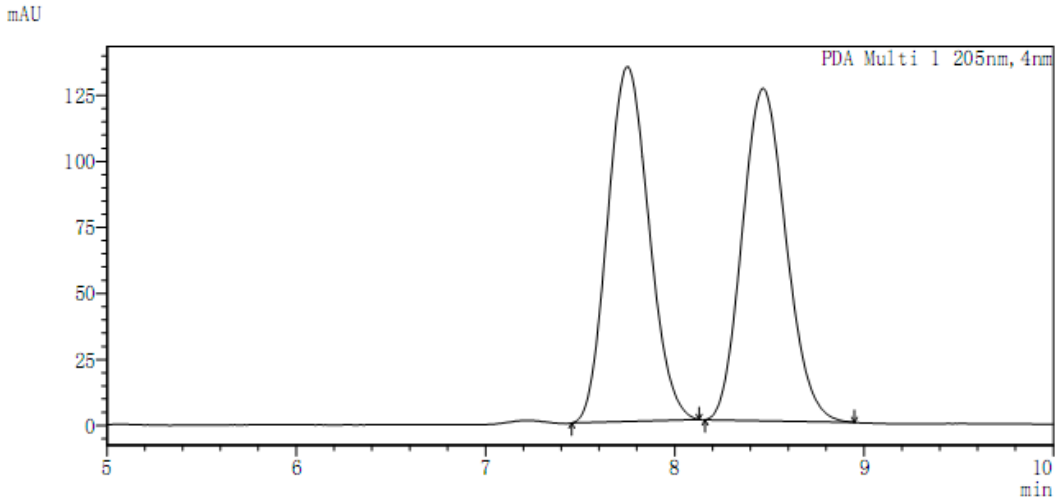

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.750	134357	2039989	50.082
2	8.466	125935	2033327	49.918

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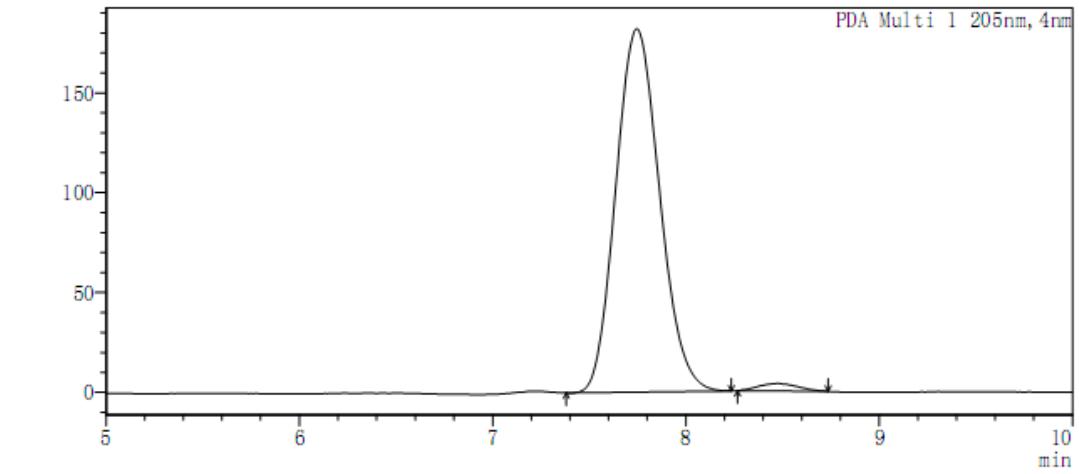
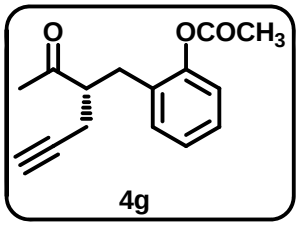


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.746	181937	2863752	98.192
2	8.471	3704	52721	1.808



4g

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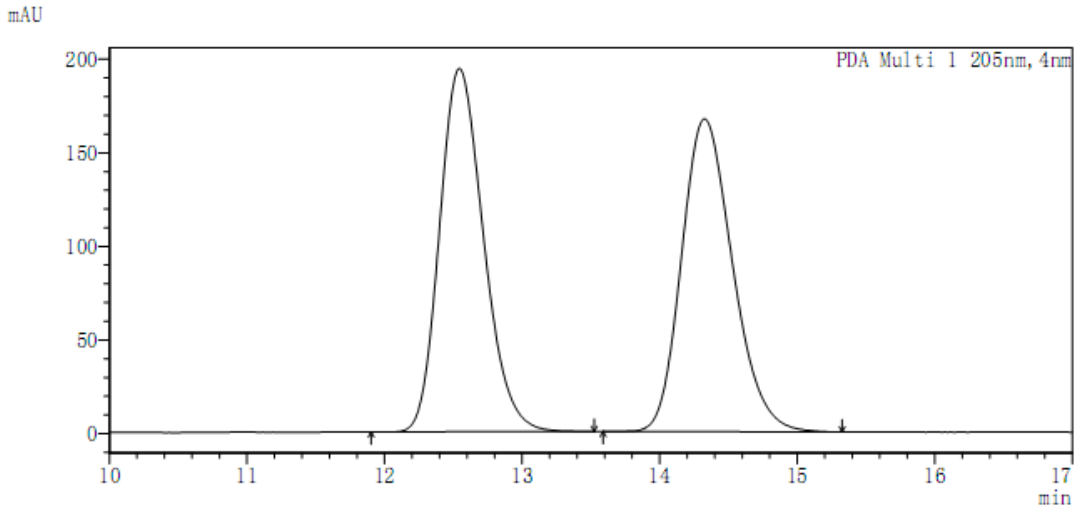

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.545	194123	4309413	49.994
2	14.326	167179	4310400	50.006

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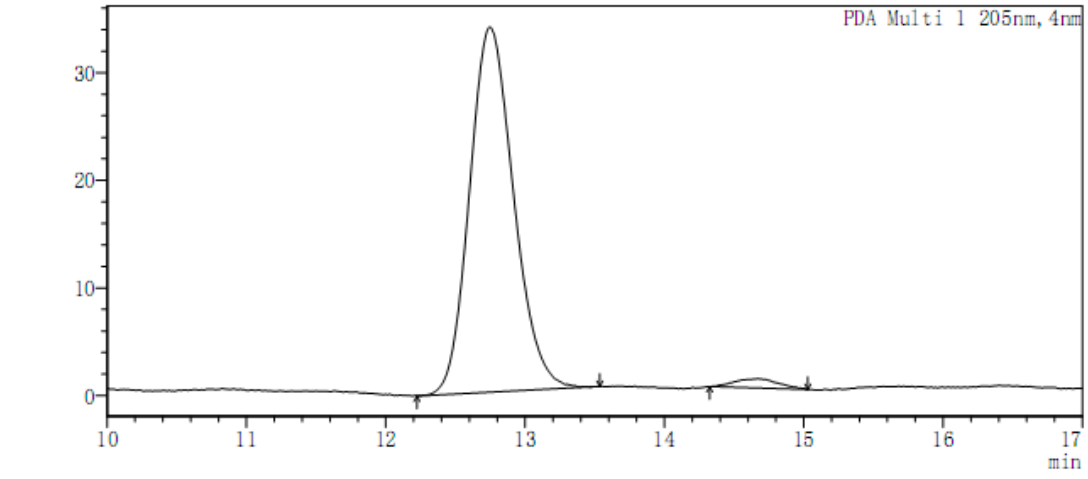
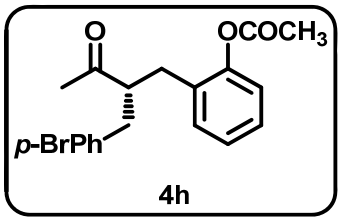


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.748	33940	746401	97.538
2	14.673	863	18844	2.462



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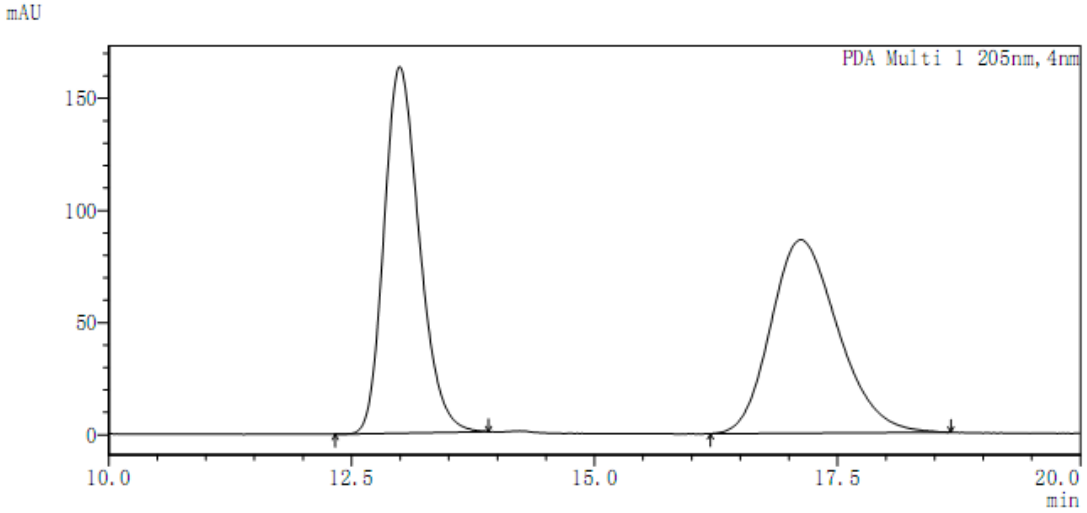

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.994	163425	4134607	49.890
2	17.122	86208	4152847	50.110

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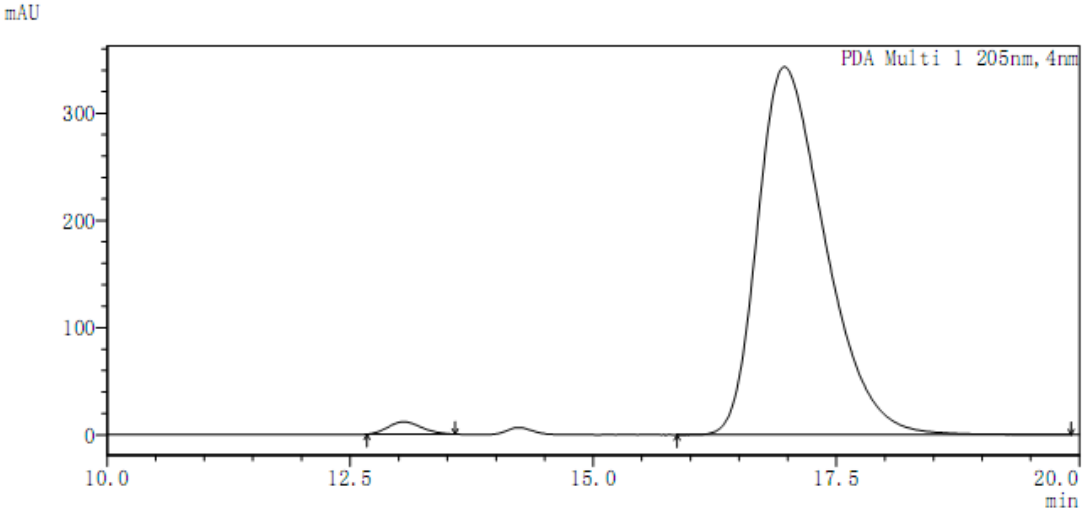
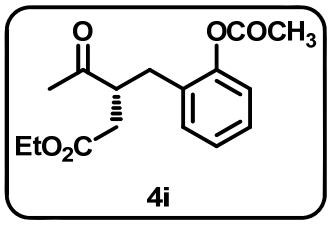


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.047	11493	274650	1.625
2	16.965	343231	16627564	98.375



4i

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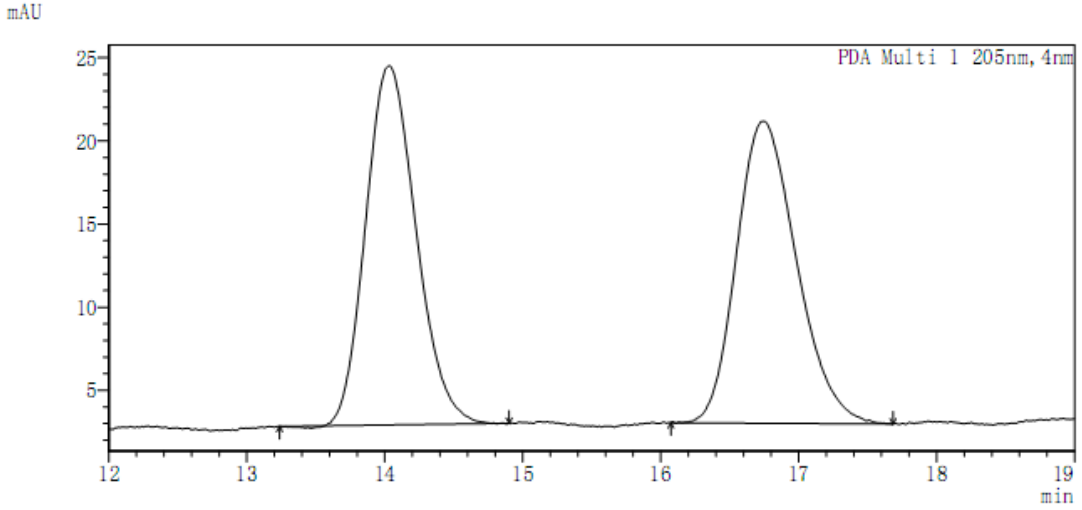

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	14.034	21607	547486	49.882
2	16.749	18161	550079	50.118

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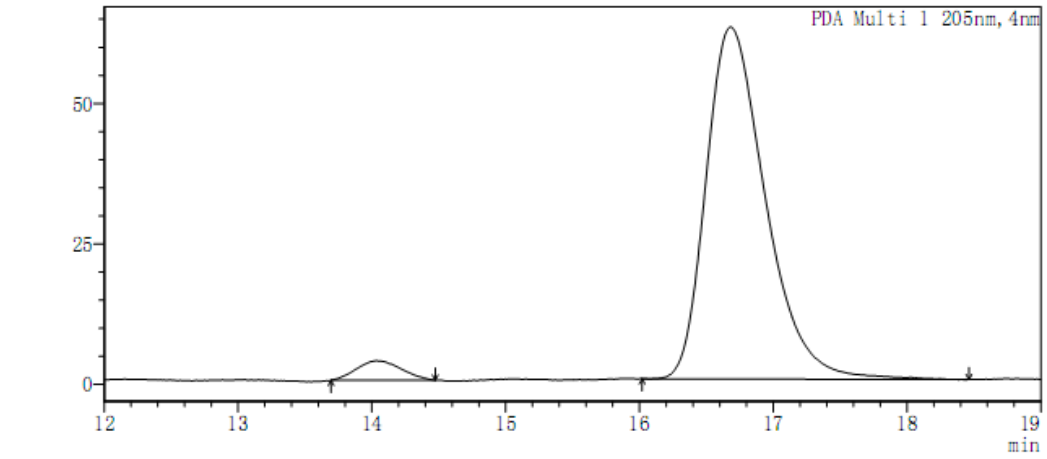
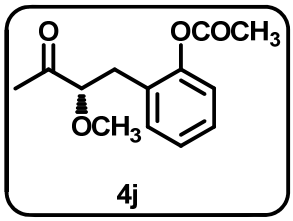


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	14.037	3486	80510	3.995
2	16.681	62659	1934668	96.005



4j

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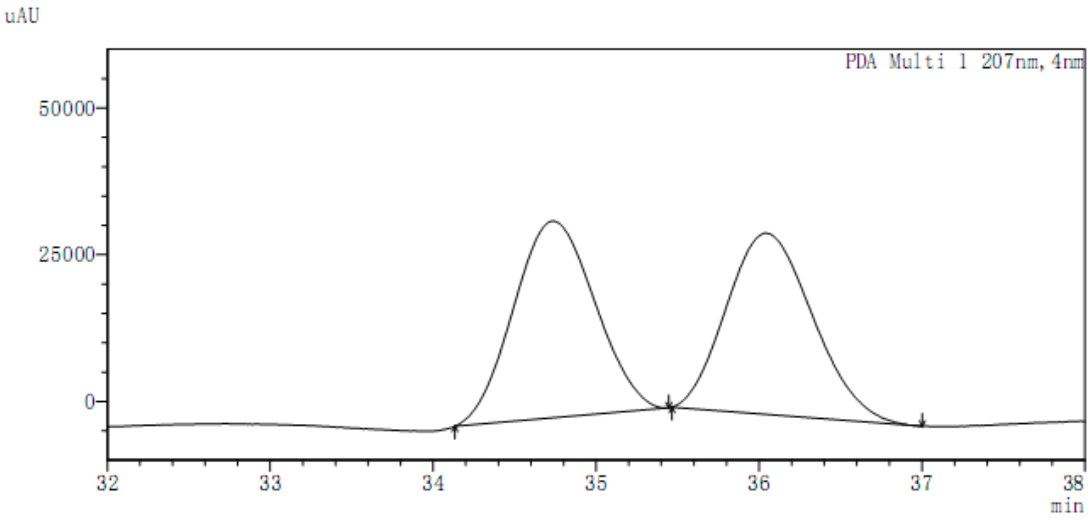

<Peak Results>

PDA Ch1 207nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	34.737	33517	1163174	50.656
2	36.041	30876	1133057	49.344

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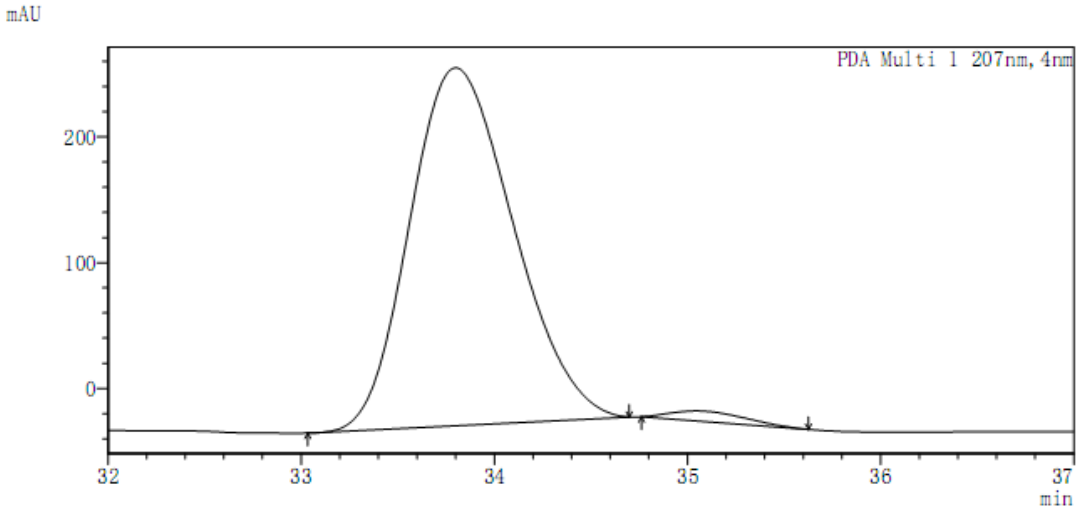
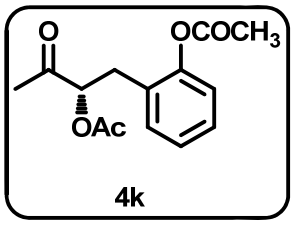


<Peak Results>

PDA Ch1 207nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	33.800	284357	10595699	97.985
2	35.044	7852	217875	2.015



4k

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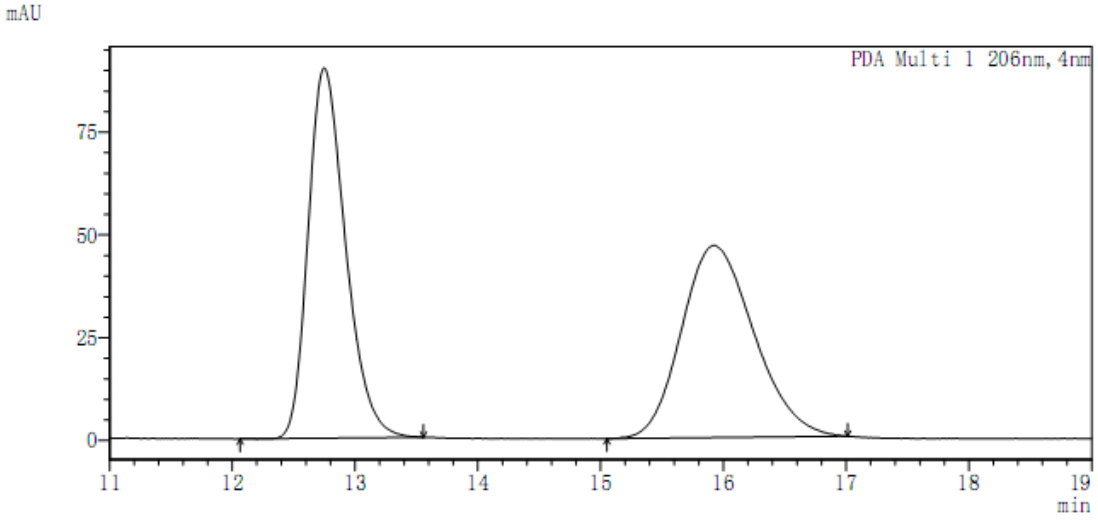

<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.748	90125	1905769	49.844
2	15.924	46723	1917727	50.156

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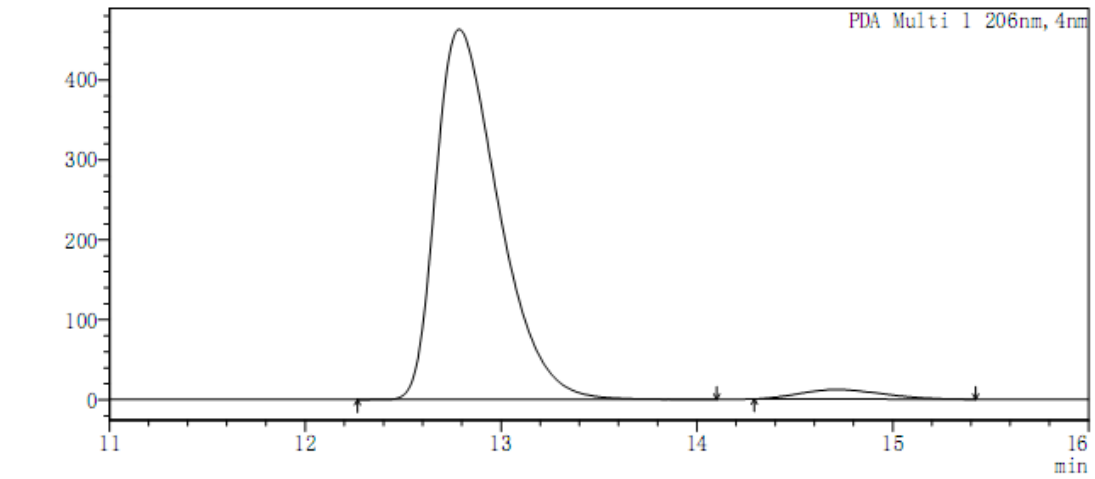
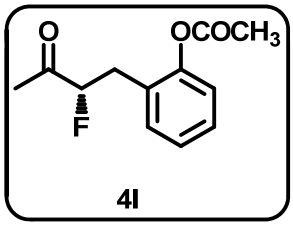


<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.787	463150	10304310	96.743
2	14.713	11854	346881	3.257



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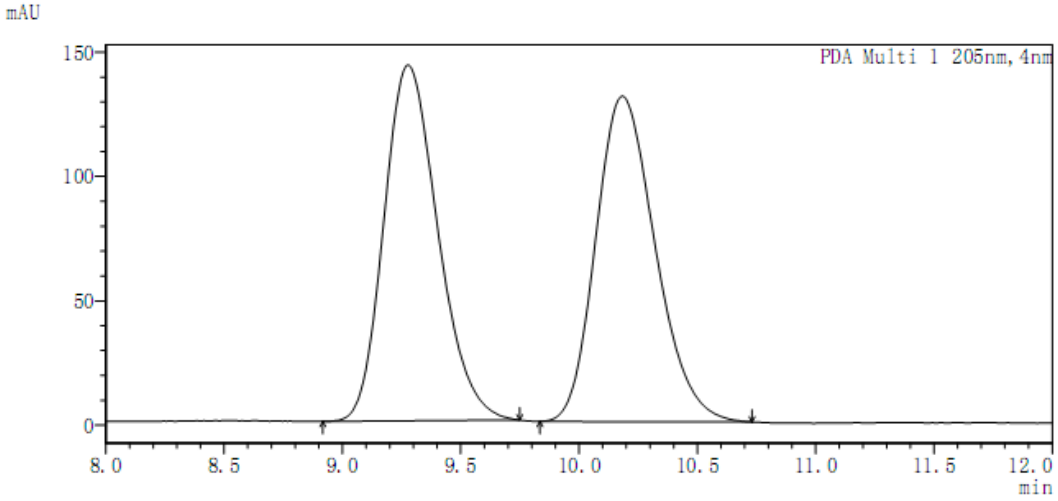

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.277	143095	2272812	49.870
2	10.184	130868	2284683	50.130

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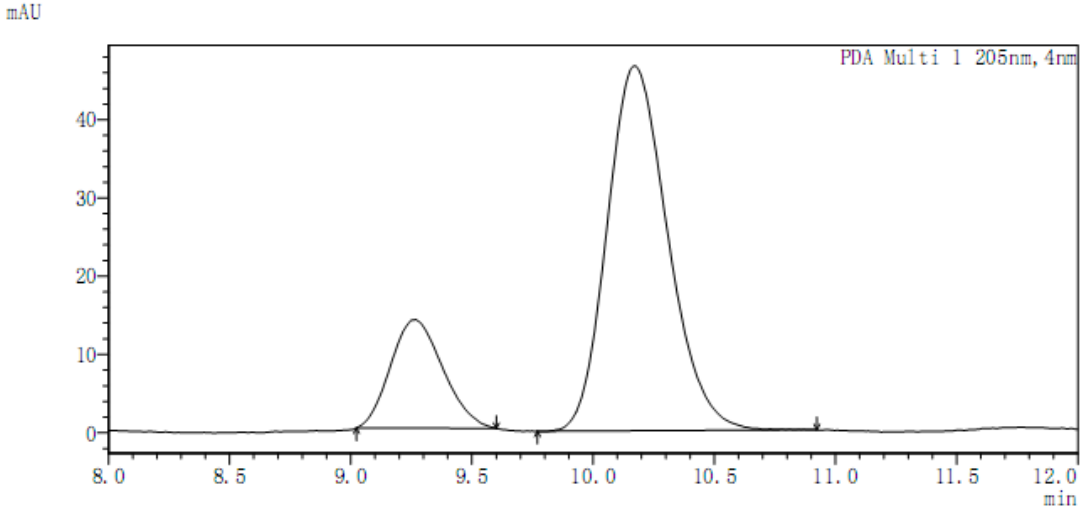
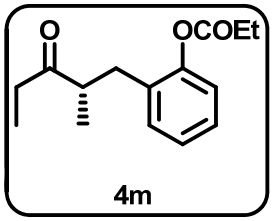


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.265	13852	207738	20.358
2	10.171	46601	812671	79.642



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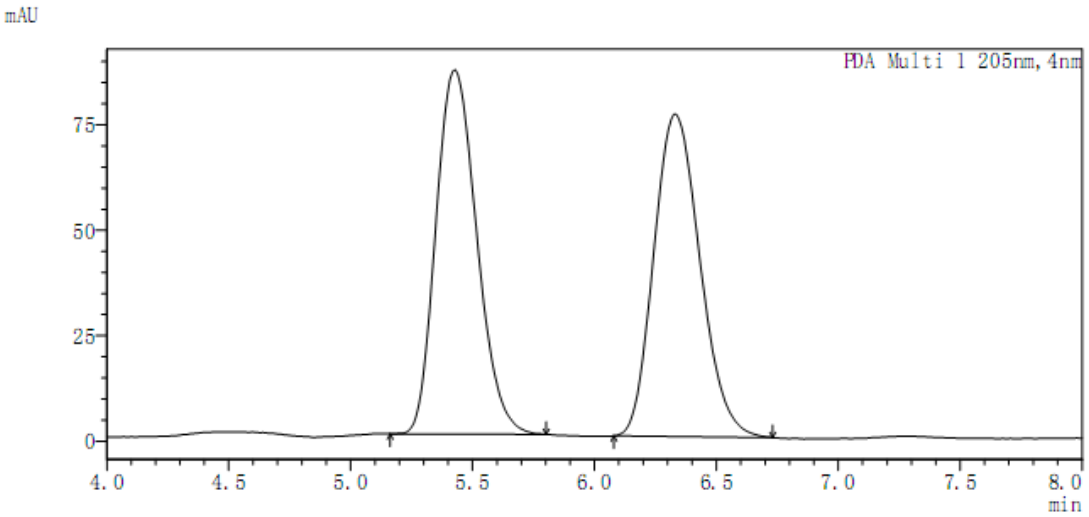

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.427	86394	1007652	50.015
2	6.331	76392	1007037	49.985

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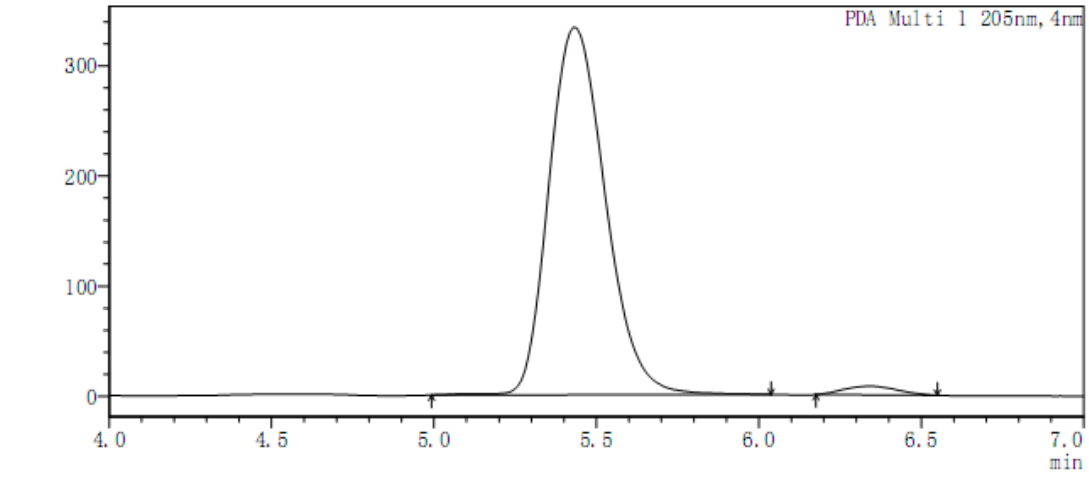
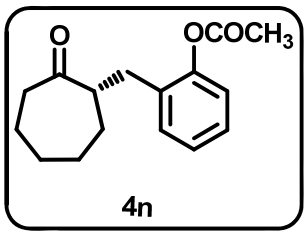


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	5.433	333834	4029867	97.804
2	6.338	7864	90487	2.196



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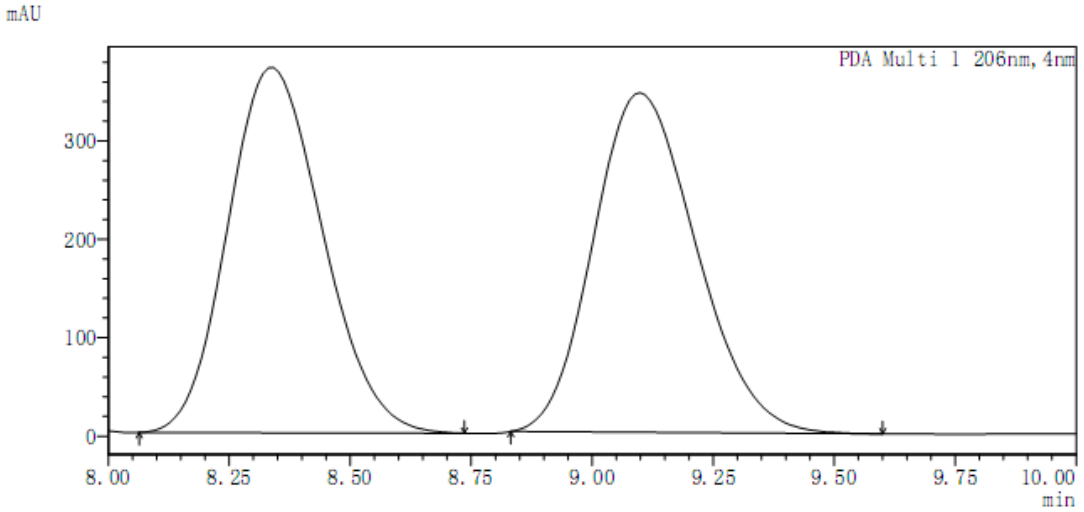

<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.337	371280	5064215	49.812
2	9.098	345160	5102395	50.188

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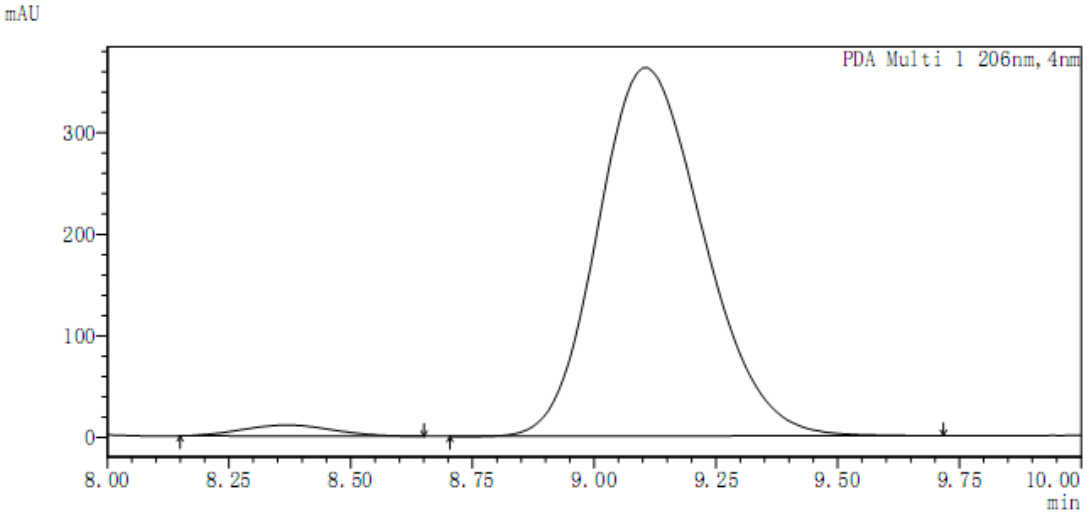
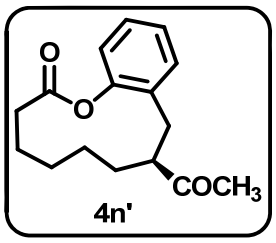


<Peak Results>

PDA Ch1 206nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.369	10852	140697	2.502
2	9.105	362639	5483515	97.498



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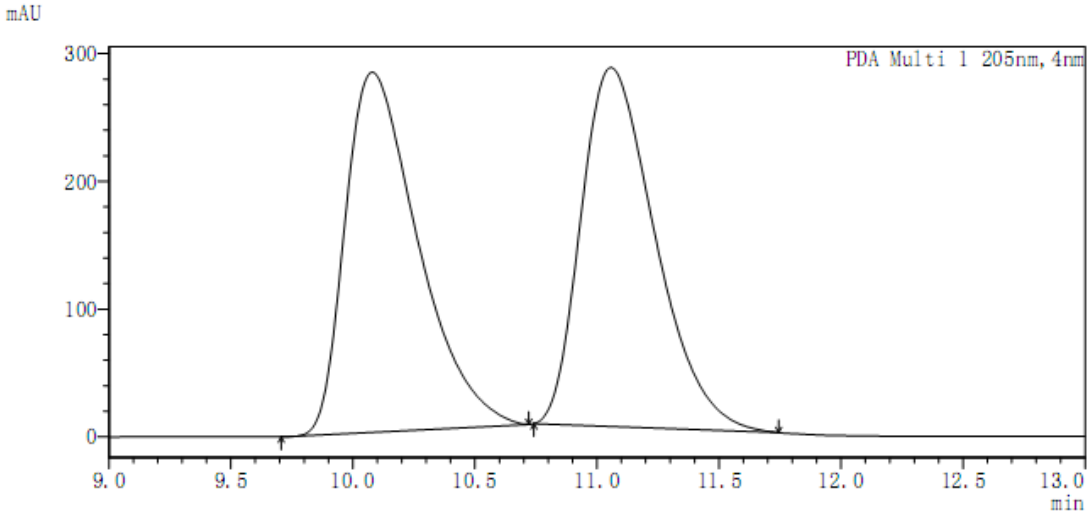
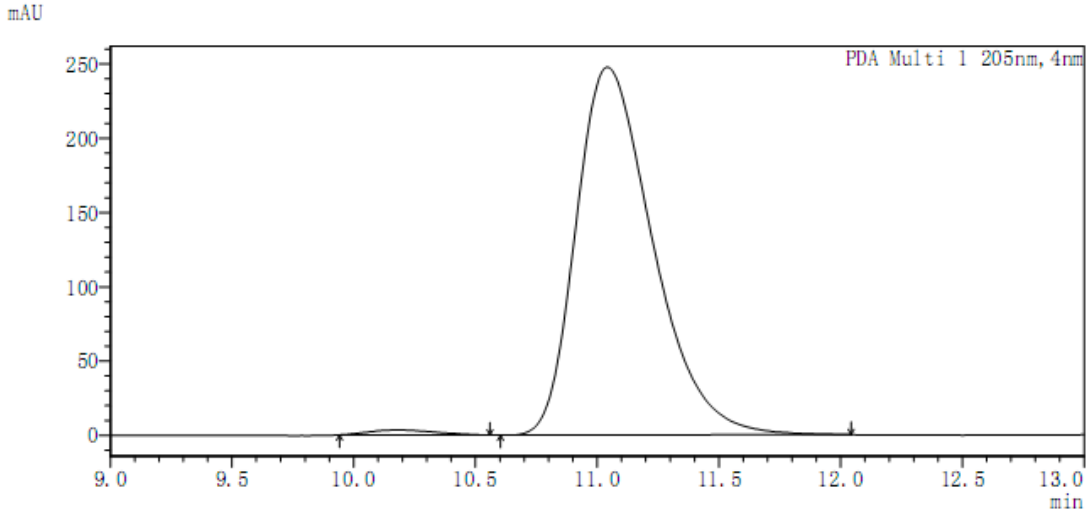


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.079	282079	5862855	49.634
2	11.057	281000	5949399	50.366

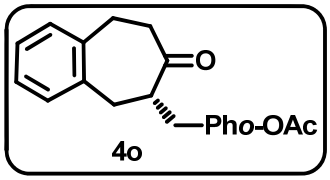
<Chromatogram>



<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.184	3354	63072	1.145
2	11.042	247692	5444367	98.855



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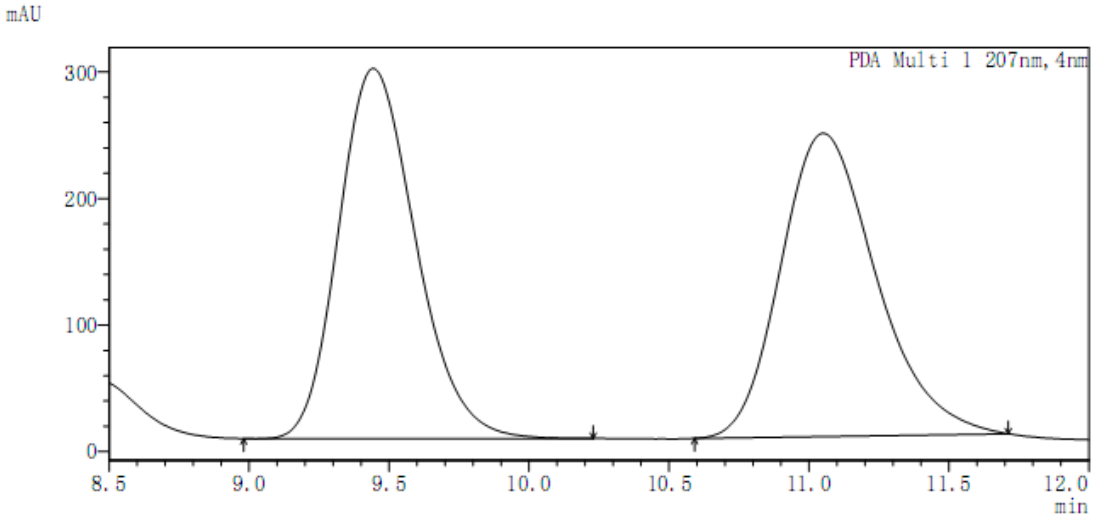

<Peak Results>

PDA Ch1 207nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.444	292799	5622010	49.663
2	11.051	239905	5698413	50.337

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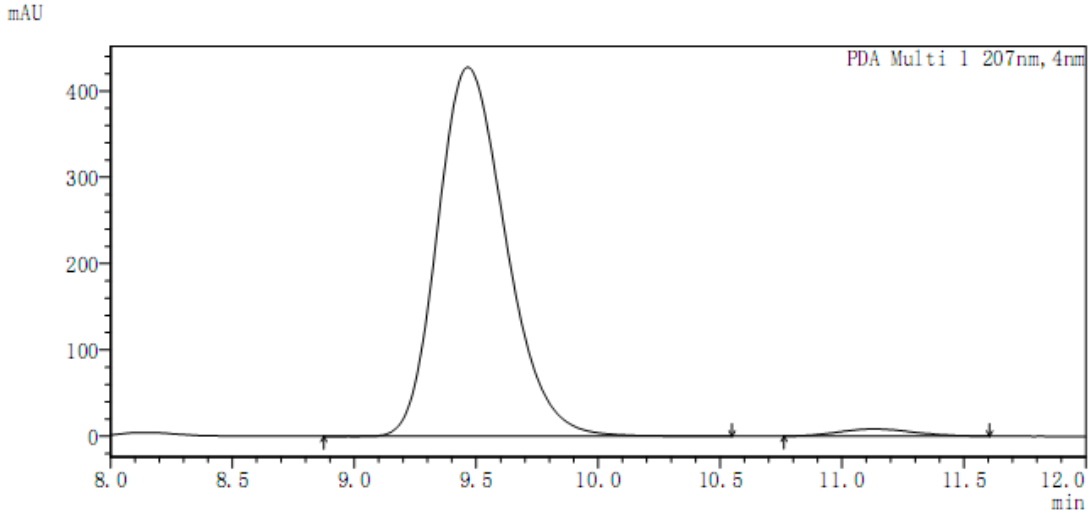
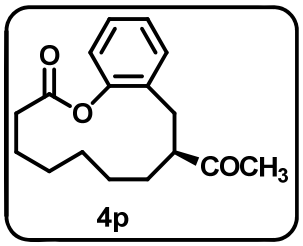


<Peak Results>

PDA Ch1 207nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	9.465	427869	8341515	97.869
2	11.133	8339	181647	2.131



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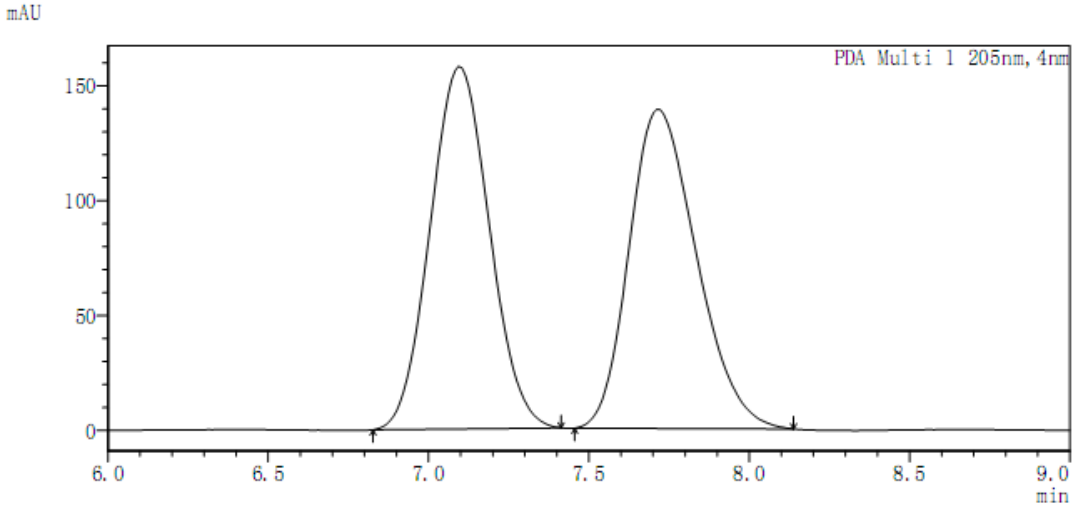

<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.096	157921	2029266	50.003
2	7.716	138945	2029028	49.997

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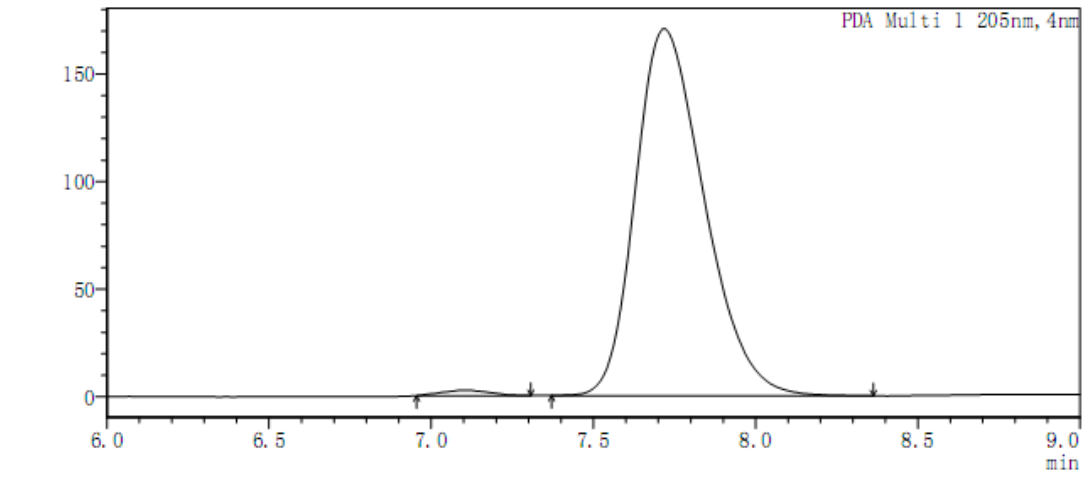
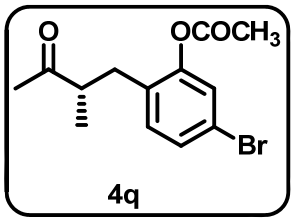


<Peak Results>

PDA Ch1 205nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.104	2438	25705	1.010
2	7.717	170343	2518049	98.990



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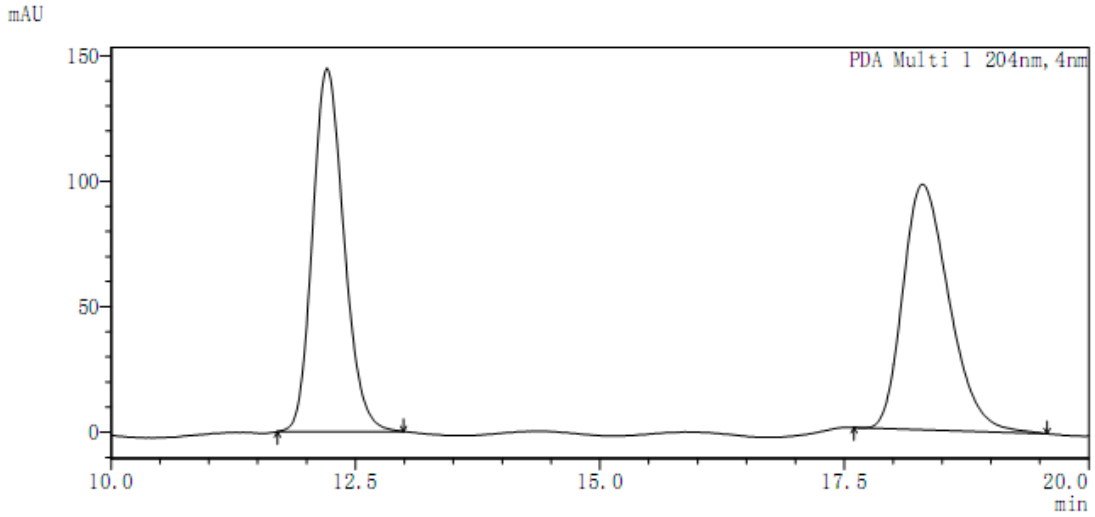
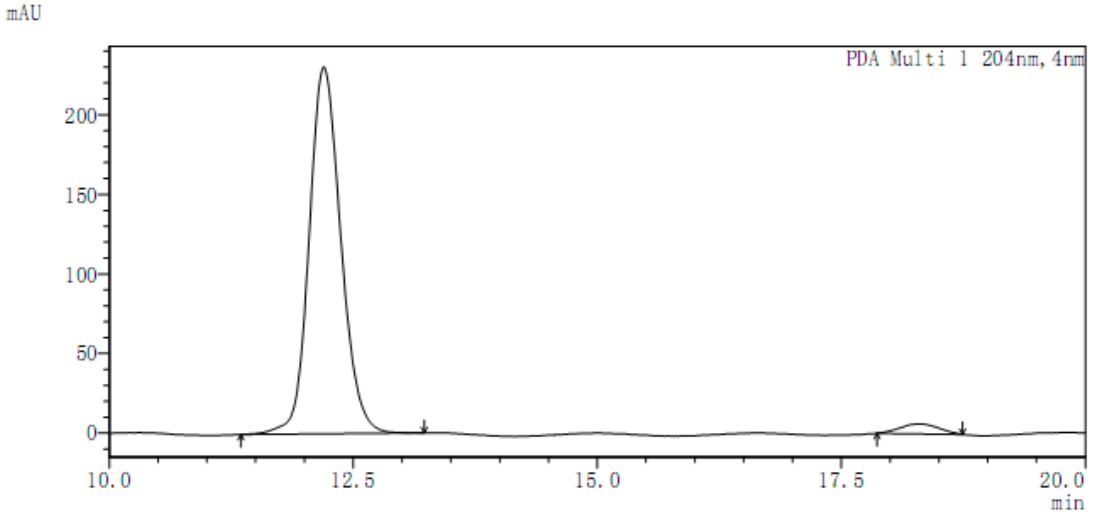


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.208	144729	3235759	50.099
2	18.296	97815	3222988	49.901

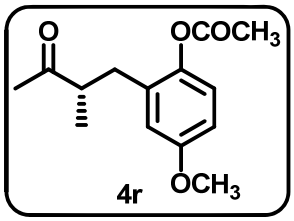
<Chromatogram>



<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	12.199	230431	5209167	96.812
2	18.284	6236	171511	3.188



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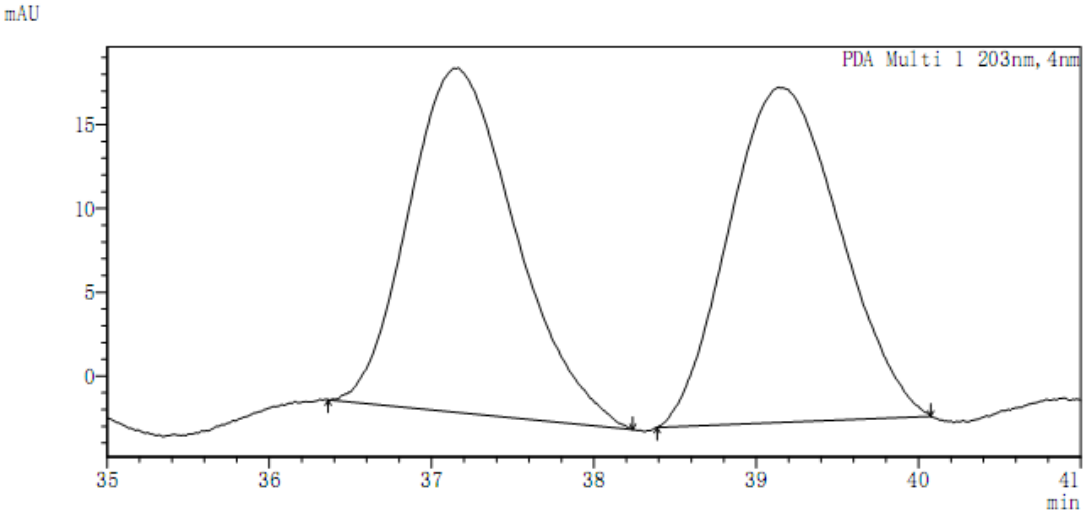

<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	37.163	20571	942363	49.683
2	39.136	20020	954380	50.317

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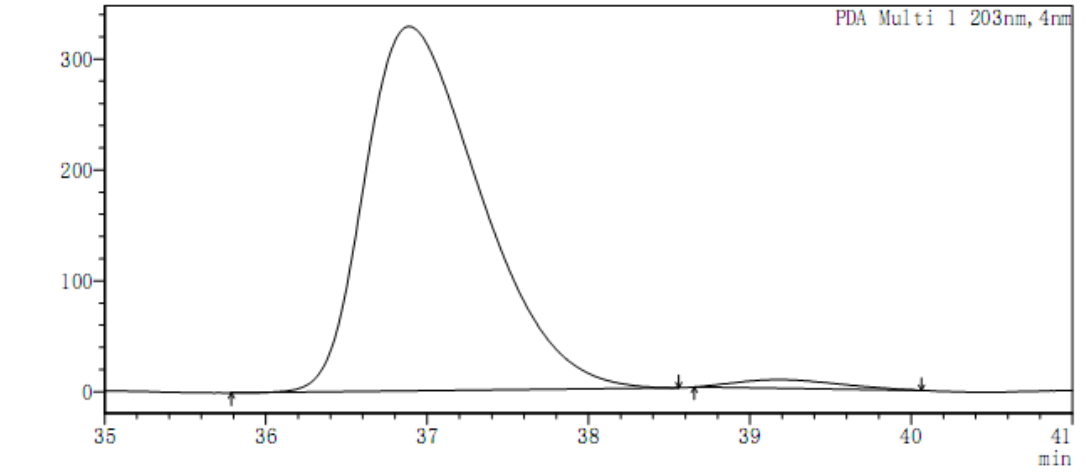
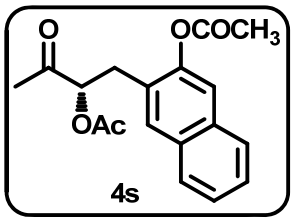


<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	36.889	328545	16389651	97.915
2	39.204	7823	348956	2.085



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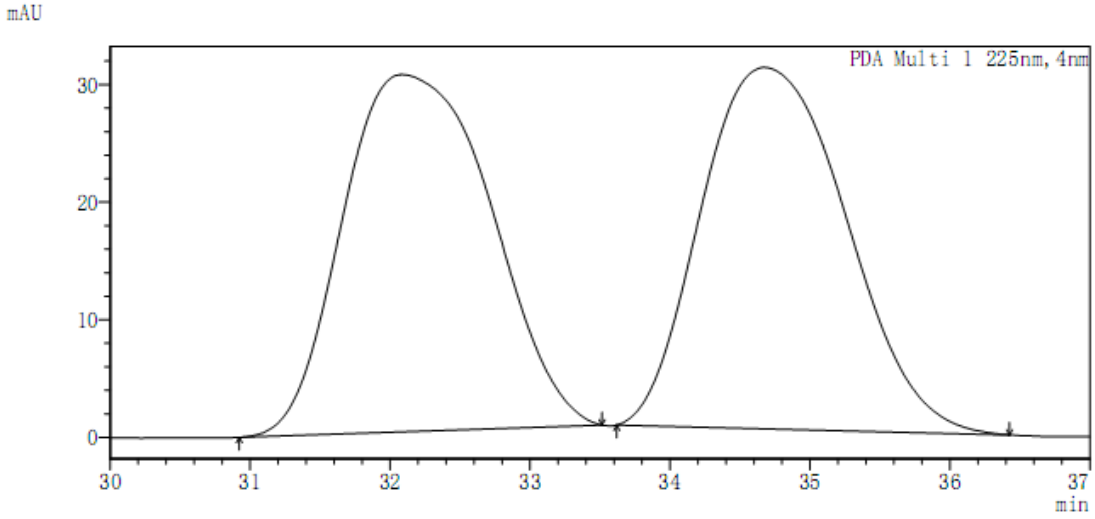

<Peak Results>

PDA Ch1 225nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	32.085	30376	2232080	50.200
2	34.671	30730	2214260	49.800

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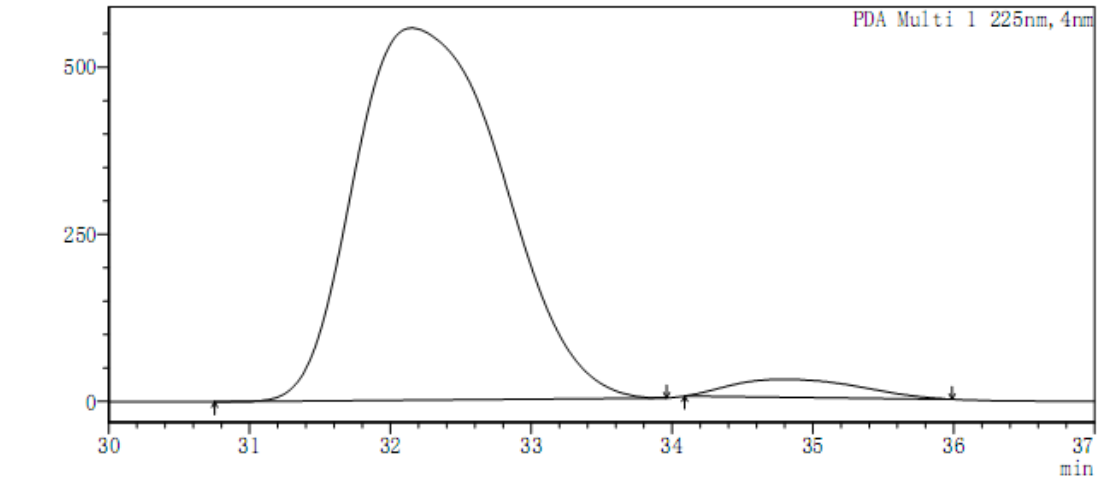
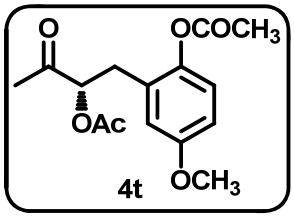


<Peak Results>

PDA Ch1 225nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	32.152	556225	40593863	95.952
2	34.792	26842	1712566	4.048



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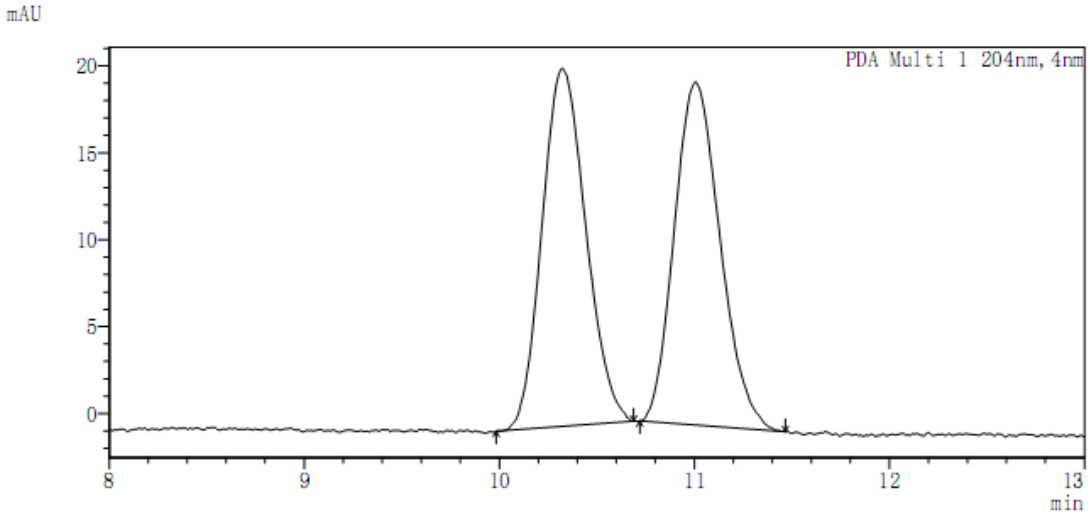

<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.323	20609	321425	49.973
2	11.006	19754	321773	50.027

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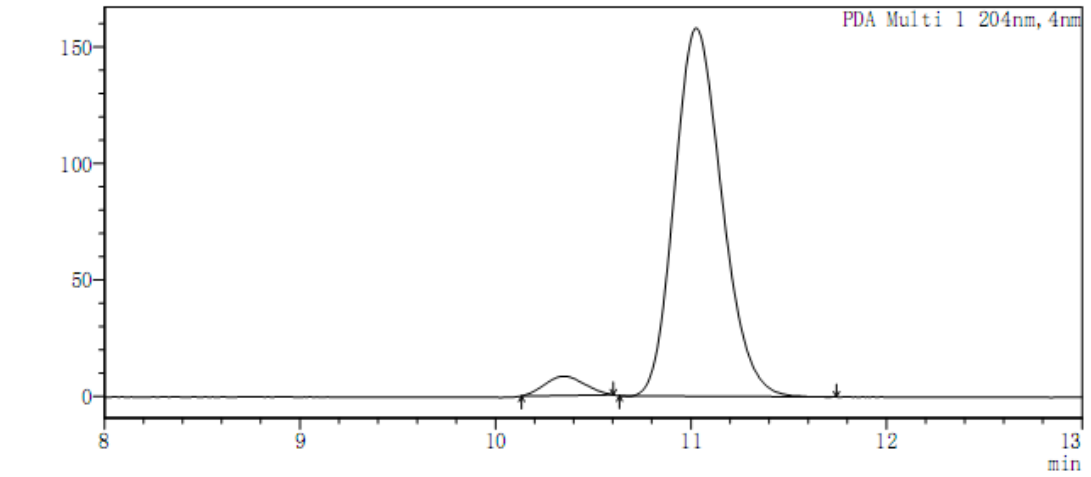
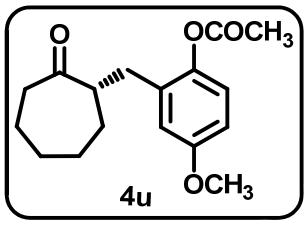


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	10.349	8220	116976	4.203
2	11.026	158150	2666327	95.797



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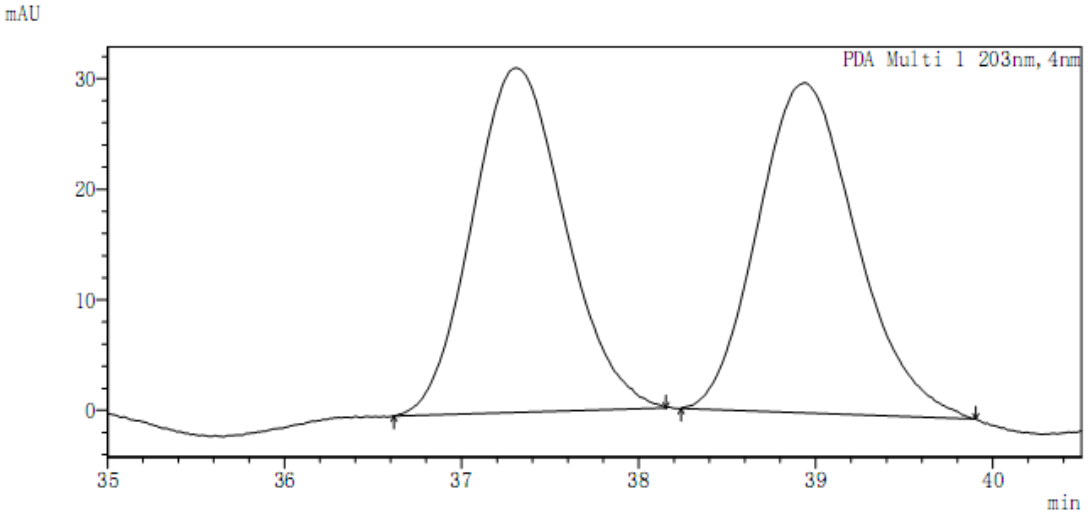

<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	37.310	31156	1132304	49.449
2	38.937	29840	1157518	50.551

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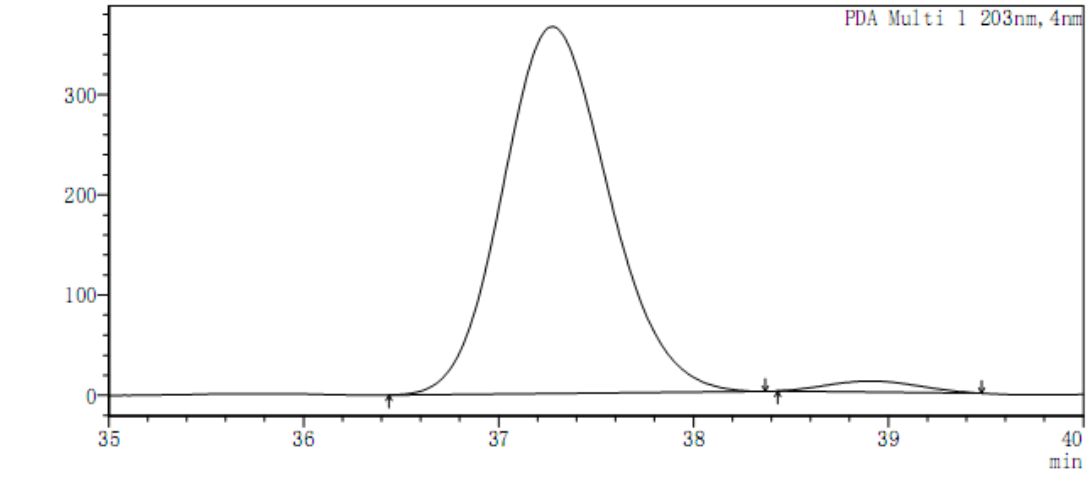
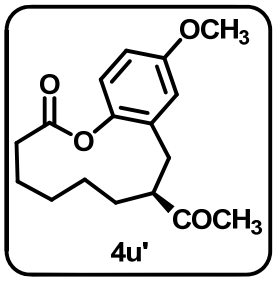


<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	37.277	365926	13850964	97.492
2	38.907	10918	356365	2.508



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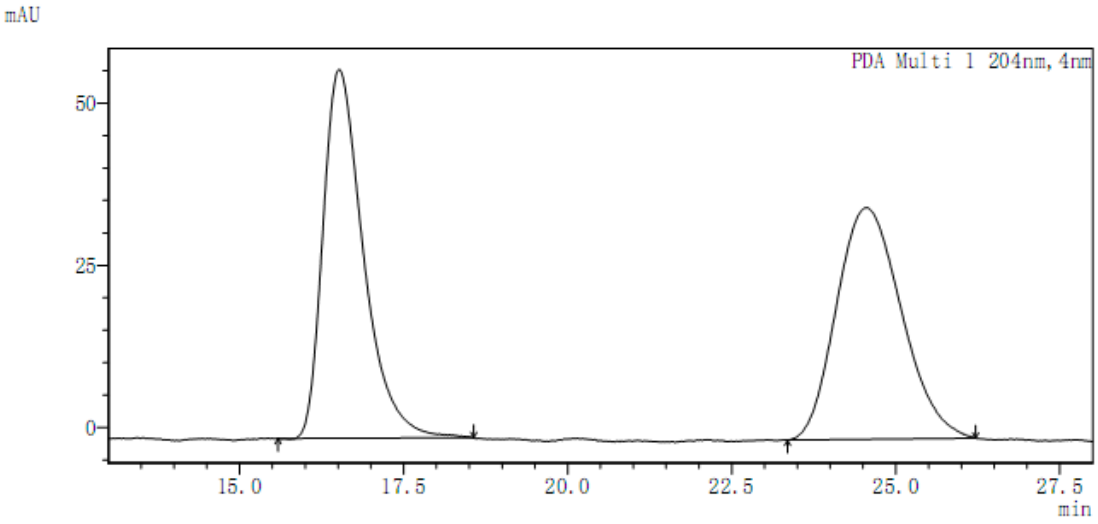

<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	16.518	56840	2433573	49.722
2	24.551	35695	2460832	50.278

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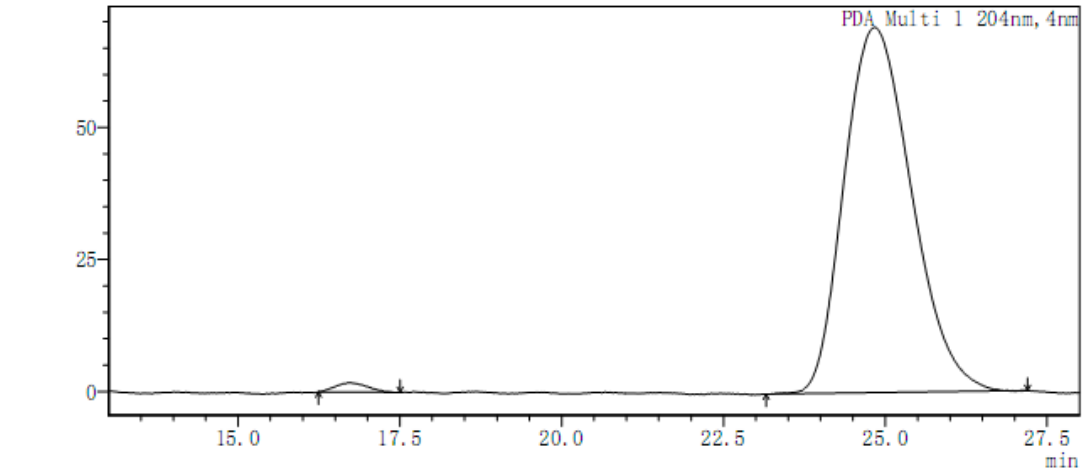
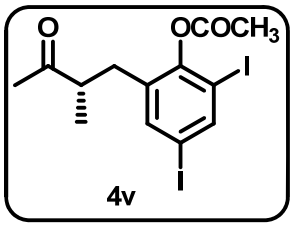


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	16.718	1791	61836	1.219
2	24.842	69187	5009941	98.781



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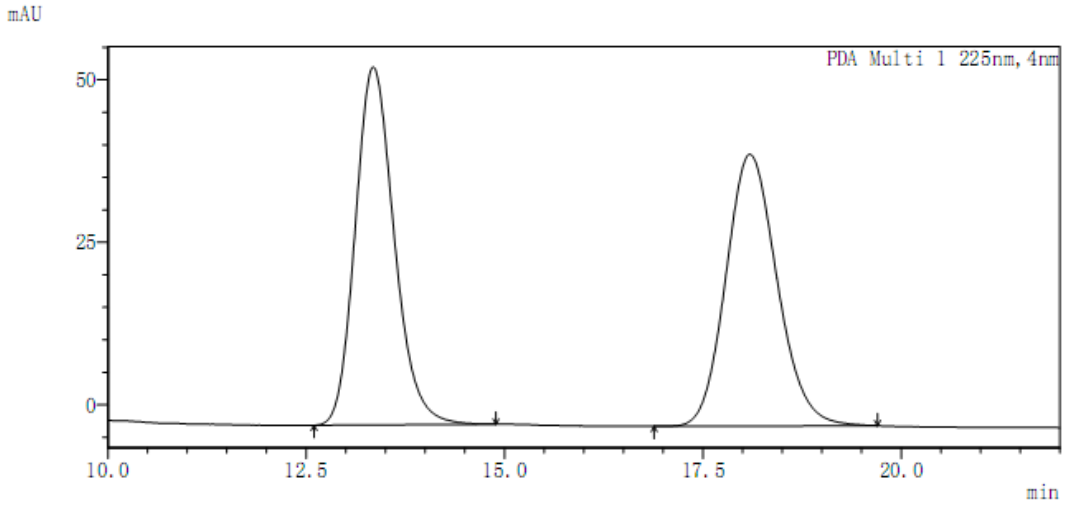

<Peak Results>

PDA Ch1 225nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.345	55057	1881201	50.051
2	18.092	41813	1877373	49.949

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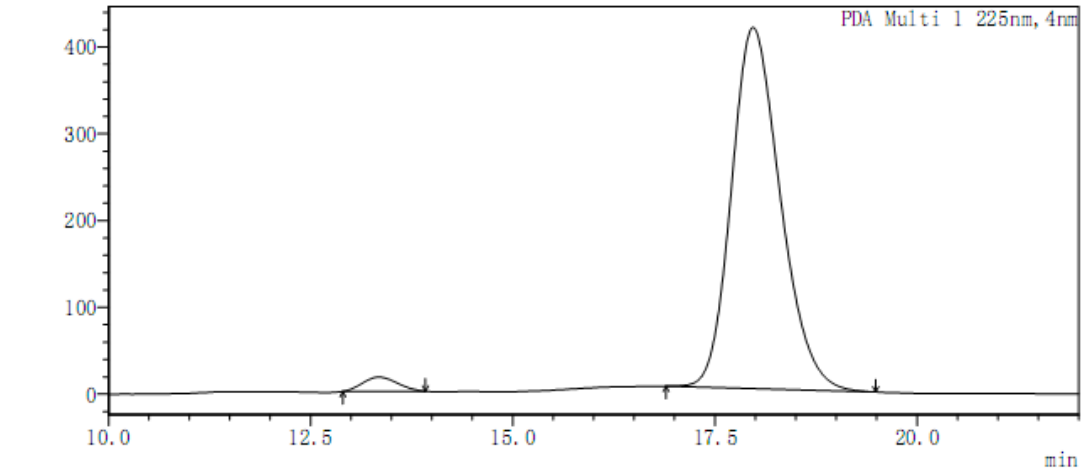
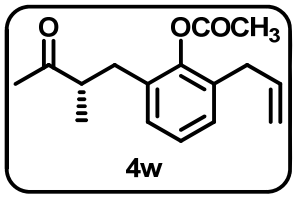


<Peak Results>

PDA Ch1 225nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	13.347	16349	490812	2.717
2	17.972	416294	17570907	97.283



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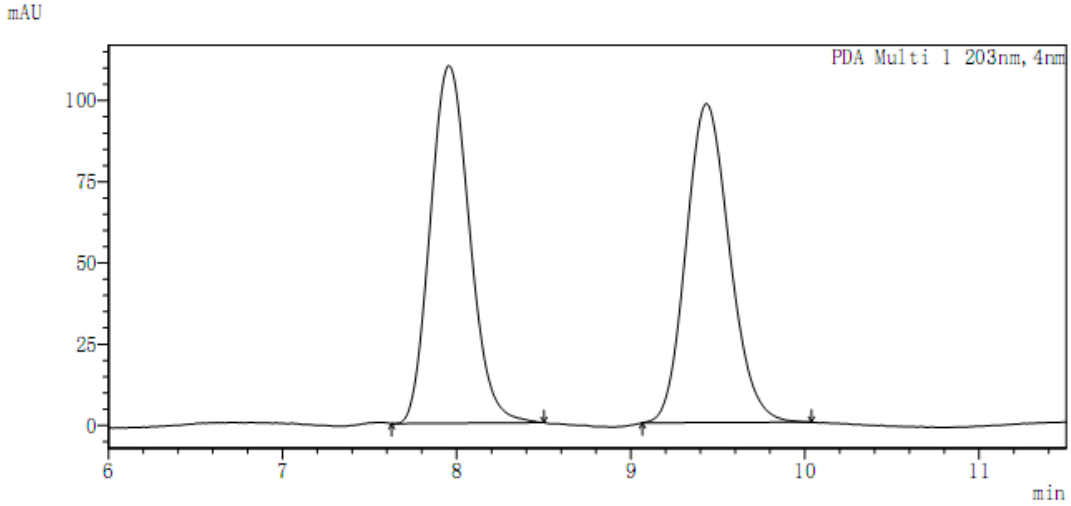

<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.956	110054	1728031	50.327
2	9.434	98084	1705555	49.673

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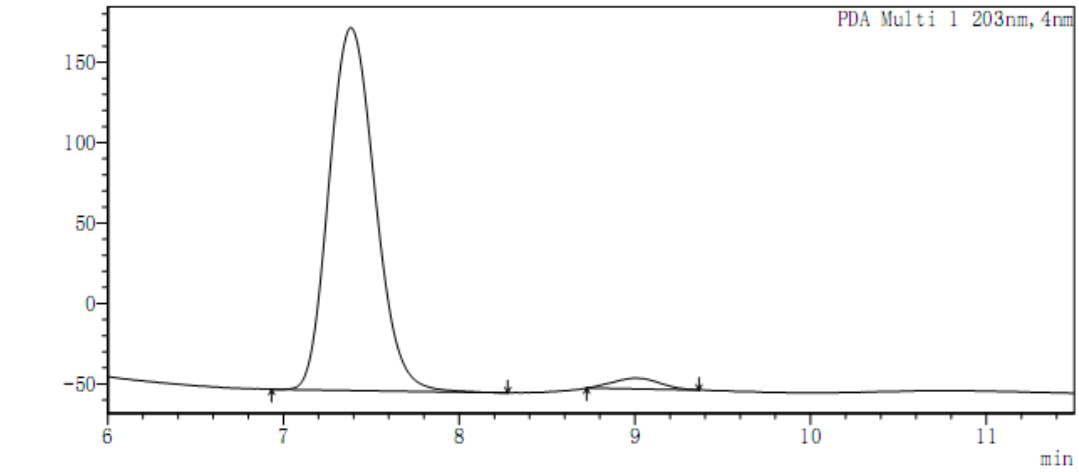
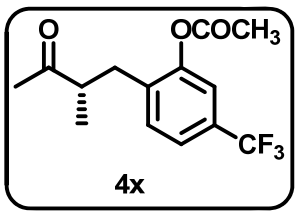


<Peak Results>

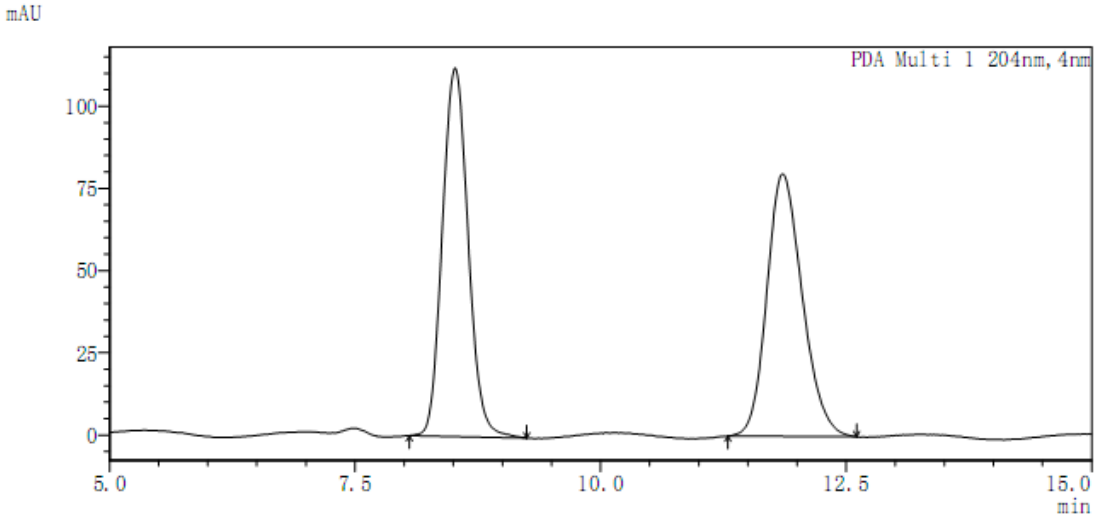
PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	7.384	225772	4092905	97.051
2	9.004	6635	124352	2.949



4x

<Chromatogram>

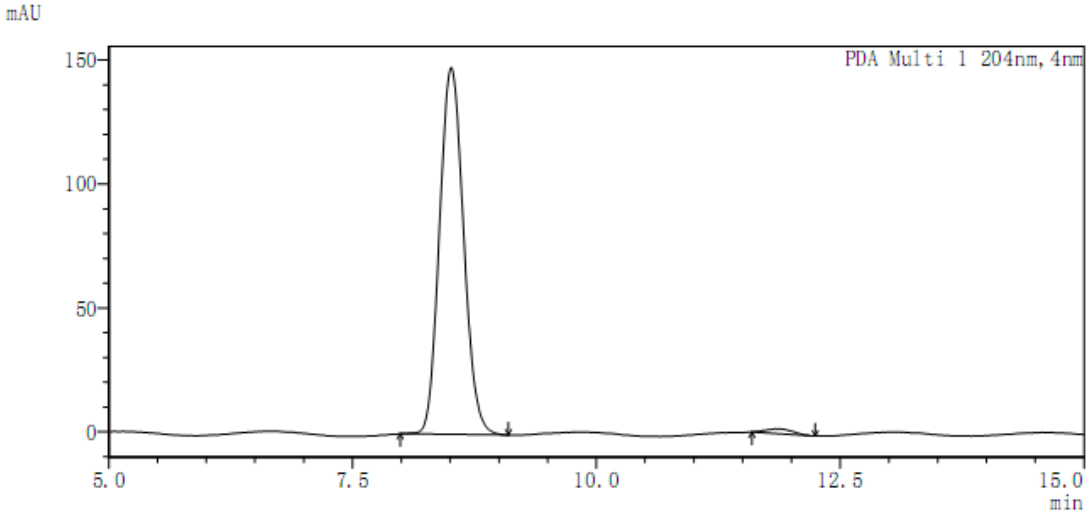


<Peak Results>

PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.518	112032	2044082	50.545
2	11.854	79736	2000037	49.455

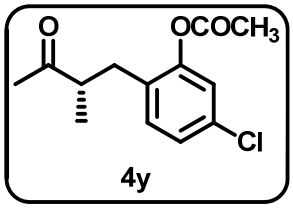
<Chromatogram>



<Peak Results>

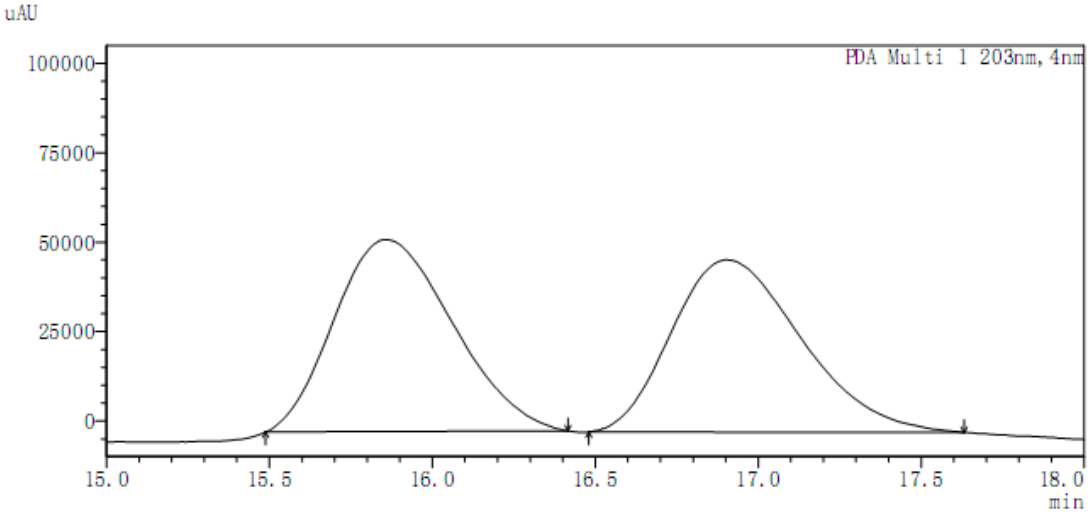
PDA Ch1 204nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	8.512	148097	2541464	98.582
2	11.833	1882	36564	1.418



4y

<Chromatogram>

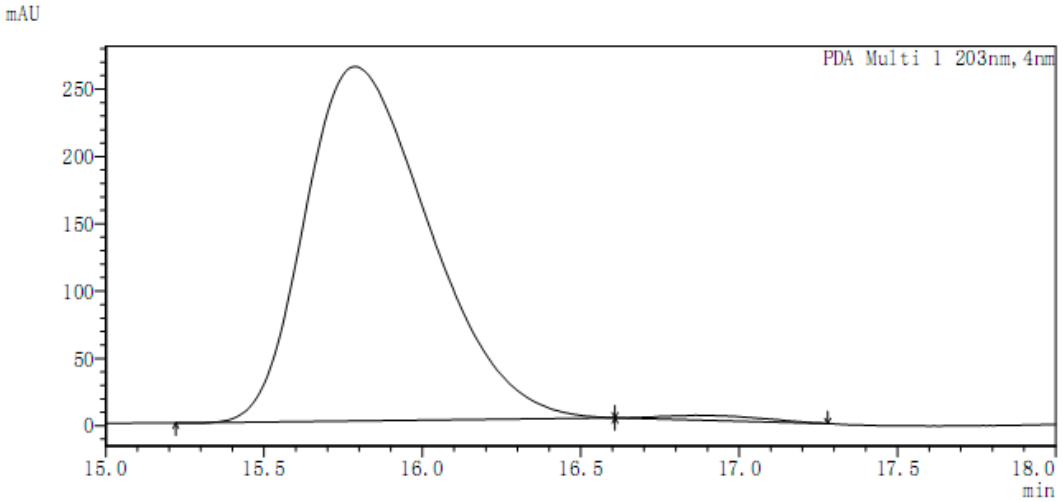


<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	15.859	53689	1358084	50.403
2	16.904	48206	1336383	49.597

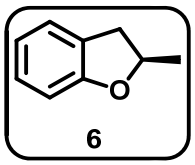
<Chromatogram>



<Peak Results>

PDA Ch1 203nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	15.788	263220	7188828	98.913
2	16.865	3504	79038	1.087



6

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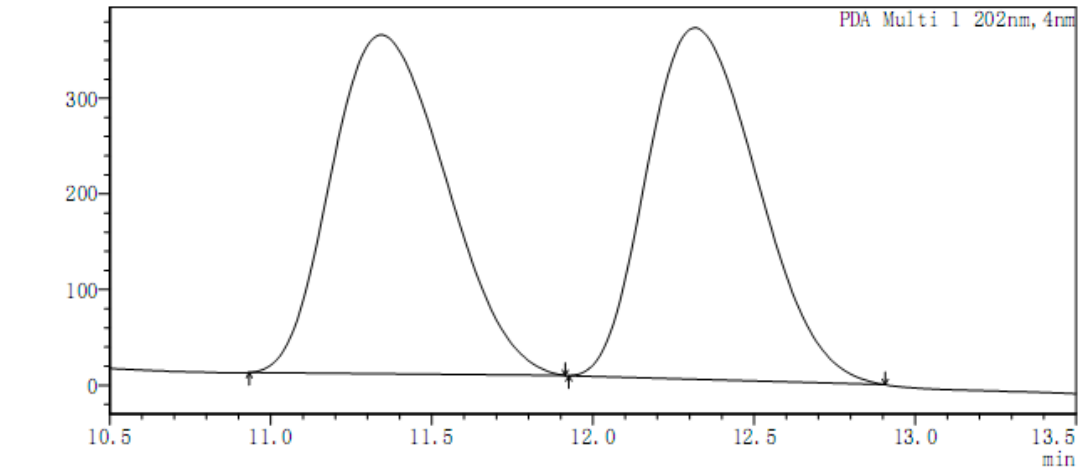
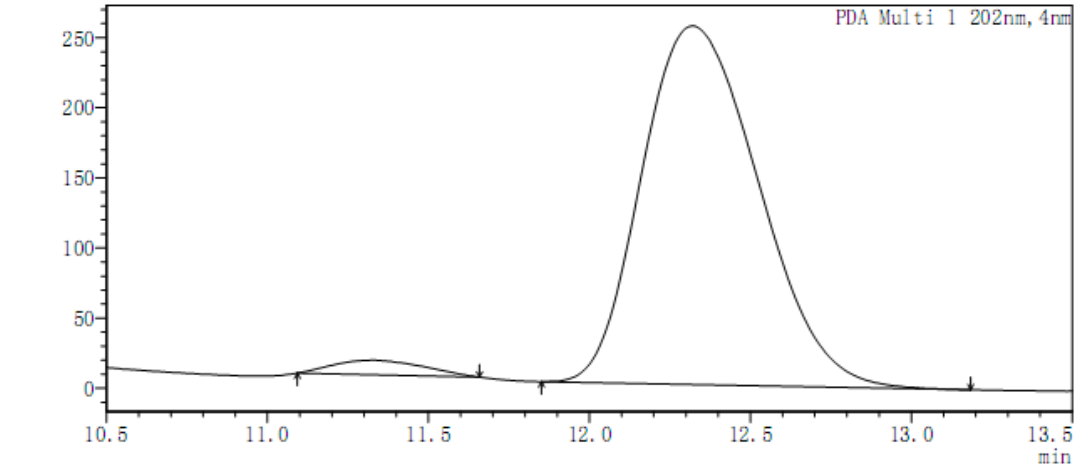


<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	11.343	354305	8772573	49.939
2	12.317	367652	8793979	50.061

<Chromatogram>



<Peak Results>

PDA Ch1 202nm

Index	Time/min	Height/mAU	Quantity/Area	Area %/%
1	11.325	10284	203090	3.048
2	12.321	255812	6459836	96.952