Supporting Information

Enantioselective Approach to Securinega Alkaloids. Total Synthesis of Securinine and (-)-Norsecurinine

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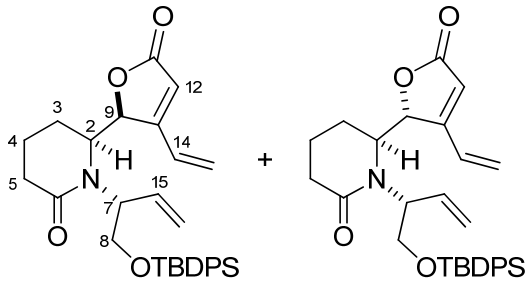
General Procedures. All reactions were carried avoiding moisture by standard procedures and under nitrogen or argon atmosphere. Commercially available reagents were used as received. The solvents were dried by distillation over the appropriate drying agents. Reactions were monitored by analytical thin-layer chromatography (TLC) using silica gel 60 F_{254} pre-coated aluminum plates (0.25 mm thickness). Flash column chromatography was performed using silica gel 60 Å, particle size 35-70 μm. IR spectra were performed by Attenuated Total Reflectance (ATR) technique. ^{1}H NMR spectra were recorded at 250, 360, 400 or 600 MHz. Proton chemical shifts are reported in ppm (δ) ($CDCl_3$ δ 7.26 ppm). ^{13}C NMR spectra were recorded at 62.5, 90 or 100 MHz with complete proton decoupling. Carbon chemical shifts are reported in ppm (δ) ($CDCl_3$, δ 77.0). NMR signals were assigned with the help of DEPT, COSY and HMQC experiments. Relative configurations were determined with the help of NOESY experiments. COSY and NOESY experiments were performed by routine methods (cosygpqf, noesygpph). Infrared peaks are reported in cm^{-1}. High resolution mass spectra (HRMS) were recorded using (ESI). Enantiomeric excess of compound **12** was determined by CHPLC using a CHIRALPACK IC 4.6 x 250 mm column (^{i}PrOH/hexanes, 1/9; 1mL/min).

(6*S*)-1-[(1*R*)-1-(*tert*-Butyldiphenylsilyloxymethyl)-2-propenyl]-6-[(2*RS*)-5-oxo-3-vinyl-2,5-dihydro-2-furyl]hexahydro-2-pyridinone (*SRS*/*SRR*-21):

(securinine numbering)

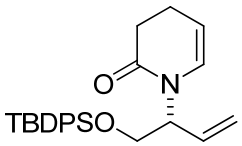


SRS-**21** *SRR*-**21**

R_f = 0.3 (hexanes:ethyl acetate 1:1); IR (ATR): 2930, 2857, 1755, 1637, 1427, 1108; ^{1}H NMR (400 MHz, CD_2Cl_2): isomers *SRS*-**21** (A, major) and *SRR*-**21** (B, minor) δ 7.60 (m, $4H_A$+$4H_B$:$4H_{PhA}$,$4H_{PhB}$), 7.41 (m, $6H_A$+$6H_B$:$6H_{PhA}$,$6H_{PhB}$), 6.51 (ddt, J = 17.8, 11.1, 0.7 Hz, $1H_A$:H_{14A}), 6.49 (bdd, J = 17.8, 11.0 Hz, $1H_B$:H_{14B}), 6.14 (ddd, J = 17.8, 10.2, 6.0 Hz, $1H_B$:H_{15B}), 6.00 (ddd, J = 17.7, 10.4, 7.4 Hz, $1H_A$:H_{15A}), 5.81 (dd, J = 1.0, 0.4 Hz, $1H_A$:H_{12A}), 5.77 (m, $1H_B$:H_{12B}), 5.72 (d, J = 17.8 Hz, $1H_A$:$H_{14'A}$), 5.64 (d, J = 11.1 Hz, $1H_A$:$H_{14'A}$), 5.61 (d, J = 11.0 Hz, $1H_B$:$H_{14'B}$), 5.54 (d, J = 17.8 Hz, $1H_B$:$H_{14'B}$), 5.20 (m, $2H_B$:$2H_{15'B}$), 5.14 (m, $1H_A$:H_{9A}), 5.14 (ddd, J = 10.4, 1.3, 1.1 Hz, $1H_A$:$H_{15'A}$), 5.12 (dt, J = 17.7, 1.3 Hz, $1H_A$:$H_{15'A}$), 5.09 (m, $1H_B$:H_{9B}), 4.24 (dd, J = 10.8, 6.5 Hz, $1H_B$:H_{8B}), 4.20 (dd, J = 10.4, 6.8 Hz, $1H_A$:H_{8A}), 3.98 (dd, J = 10.8, 6.7 Hz, $1H_B$:H_{8B}), 3.96 (m, $1H_A$:H_{2A}), 3.87 (m, $1H_B$:H_{2B}), 3.77 (dd, J = 10.4, 4.6 Hz, $1H_A$:H_{8A}), 3.68 (m, $1H_A$:H_{7A}), 3.68 (m, $1H_B$:H_{7B}), 2.28 (m, $2H_A$+$2H_B$:$2H_{5A}$,$2H_{5B}$), 1.90 (m, $3H_A$:$2H_{3A}$,H_{4A}), 1.62 (m, $1H_A$+$2H_B$:H_{4A},$2H_{3B}$), 1.04 (s, $9H_B$:$9H_{tBuB}$), 1.03 (s, $9H_A$:$9H_{tBuA}$); ^{13}C NMR (100 MHz, CD_2Cl_2): isomer *SRS*-**21** (major) δ 171.1 (C_{11}), 170.9 (C_6), 163.1 (C_{13}), 135.3 (C_{Ph}), 134.2 (C_{15}), 133.2 (C_{Ph}), 133.0 (C_{Ph}), 129.5 (C_{Ph}), 129.4 (C_{Ph}), 127.5 (C_{Ph}), 127.46 (C_{Ph}), 127.43 (C_{14}), 124.1 ($C_{14'}$), 117.2

($C_{15'}$), 117.1 (C_{12}), 82.5 (C_9), 66.0 (C_7), 65.3 (C_8), 57.9 (C_2), 31.5 (C_5), 26.4 (C_{Me}), 25.8 (C_3), 18.7 (C_{tBu}), 17.3 (C_4); HRMS (ESI+): calcd for $C_{31}H_{37}NO_4Si$: 538.2384 $[M+Na]^+$, found: 538.2397.

1-[(1*R*)-1-(1-*tert*-butyldiphenylsilyloxymethyl)-2-propenyl]-1,2,3,4-tetrahydro-2-pyridinone (26):



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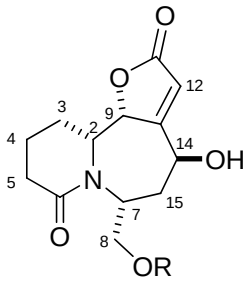
R_f = 0.3 (hexanes:ethyl acetate 1:1); $[\alpha]_D^{20}$ = -46 (*c* 0.78, $CHCl_3$); ^{1}H NMR (360 MHz, CD_2Cl_2): δ 7.65 (m, 4H:4H_{Ph}), 7.42 (m, 6H:6H_{Ph}), 6.16 (dt, *J* = 7.9, 1.6 Hz, 1H:H_6), 5.82 (ddd, *J* = 17.4, 10.7, 5.1 Hz, 1H:$H_{2'}$), 5.34 (m, 1H:$H_{1'}$), 5.23 (ddd, *J* = 10.7, 1.8, 1.2 Hz, 1H:$H_{3'}$), 5.18 (ddd, *J* = 17.4, 1.9, 1.2 Hz, 1H:$H_{3'}$), 5.14 (m, 1H:H_5), 3.81 (dd, *J* = 10.6, 5.2 Hz, 1H:$H_{1''}$), 3.77 (dd, *J* = 10.6, 7.0 Hz, 1H:$H_{1''}$), 2.57 (m, 2H:2H_3), 2.30 (m, 2H:2H_4), 1.04 (s, 9H:9H_{tBu}); ^{13}C NMR (90 MHz, $CDCl_3$): δ 169.4 (C_2), 135.6 (C_{Ph}), 133.5 ($C_{2'}$), 133.1 (C_{Ph}), 129.7 (C_{Ph}), 127.7 (C_{Ph}), 127.1 (C_6), 117.9 ($C_{3'}$), 105.6 (C_5), 63.9 ($C_{1''}$), 55.1 ($C_{1'}$), 31.7 (C_3), 26.7 (C_{Me}), 20.0 (C_4), 19.2 (C_{tBu}); HRMS (ESI+): calcd for $C_{31}H_{37}NO_4Si$: 538.2384 $[M+Na]^+$, found: 538.2397.

(4*S*,6*R*,11a*R*,11b*R*)-6-*tert*-butyldiphenylsilyloxymethyl-4-hydroxy-2,4,5,6,8,9,10,11,11a,11b-decahydrofuro[2,3-*c*]pyrido[1,2-*a*]azepine-2,8-dione (34):

(securinine numbering)

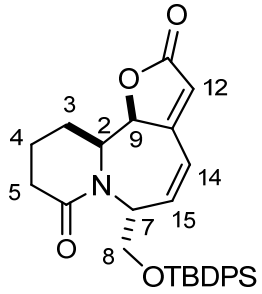


34

R_f = 0.52 (hexanes:ethyl acetate 1:1); IR (ATR): 3353, 3070, 2930, 2856, 1744, 1642, 1111; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (m, 4H:4H_{Ph}), 7.47 (m, 6H:6H_{Ph}), 5.72 (d, *J* = 2.2 Hz, 1H:H_{12}), 4.99 (dd, *J* = 8.3, 2.2 Hz, 1H:H_9), 3.84 (dd, *J* = 10.5, 4.9 Hz, 1H:H_8), 3.71 (dd, *J* = 10.5, 6.4 Hz, 1H:H_8), 3.60 (dt, *J* = 8.3, 3.2 Hz, 1H:H_2), 3.33 (d, *J* = 5.6 Hz, 1H:H_{14}), 3.25 (bqn, *J* = 6.6 Hz, 1H:H_7), 2.55 (bs, 1H:OH), 2.19 (dt, *J* = 12.9, 5.9 Hz, 1H:H_{15}), 2.04 (bdd, *J* =14.6, 6.4 Hz, 1H:H_5), 1.94 (bd, *J* = 13.8 Hz, 1H:H_3), 1.79 (dd, *J* = 12.9, 8.5 Hz, 1H:H_{15}), 1.65 (m, 2H:H_3,H_5), 1.40 (m, 1H:H_4), 1.15 (m, 1H:H_4), 1.07 (s, 9H:9H_{tBu}); ^{13}C NMR (100 MHz, $CDCl_3$): δ 174.8 (C_{11}), 173.7 (C_6), 136.0 (C_{Ph}), 135.8 (C_{Ph}), 135.6 (C_{Ph}), 133.4 (C_{Ph}), 133.3 (C_{Ph}), 130.0 (C_{Ph}), 129.9 (C_{Ph}), 127.8 (C_{Ph}), 127.7 (C_{Ph}), 111.2 (C_{12}), 92.7 (C_{13}), 78.4 (C_9), 68.0 (C_8), 65.9 (C_7), 61.8 (C_2), 50.1 (C_{14}), 34.3 (C_5), 32.7 (C_{15}), 26.9 (C_{Me}), 24.9 (C_3), 19.2 (C_{tBu}), 19.0 (C_4); HRMS (ESI+): *m/z*: calcd for $C_{29}H_{35}NO_5Si$: 506.2357 $[M+H]^+$, found: 506.2360.

(6*R*,11a*S*,11b*S*)-6-*tert*-Butyldiphenylsilyloxymethyl-2,6,8,9,10,11,11a,11b-octahydrofuro[2,3-*c*]pyrido[1,2-*a*]azepine-2,8-dione, *SRS*-28:

(securinine numbering)

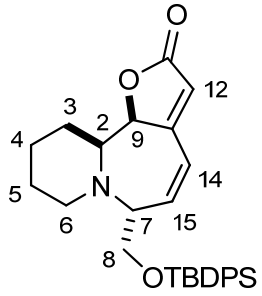


SRS-**28**

Following the same procedure described for *RRR/RRS*-**28**, a 6:1 mixture of *SRS*- and *SRR*-**21** (55 mg, 0.11 mmol) furnished *SRS*-**28** (53 mg, 0.11 mmol, 100%): R_f = 0.31 (hexanes:ethyl acetate 1:1); $[\alpha]_D^{20}$ = +87 (*c* 1.45, $CHCl_3$); **IR** (ATR): 2930, 2857, 1756, 1638, 1427, 1109; **^{1}H NMR** (360 MHz, C_6D_6): δ 7.70 (m, 4H:4H_{Ph}), 7.24 (m, 6H:6H_{Ph}), 6.03 (dt, *J* = 9.2, 4.9 Hz, 1H:H_7), 5.63 (m, 2H:H_{14},H_{15}), 5.35 (d, *J* = 1.5 Hz, 1H:H_{12}), 4.70 (dd, *J* = 7.7, 1.7 Hz, 1H:H_9), 3.78 (td, *J* = 7.8, 5.0 Hz, 1H:H_2), 3.59 (dd, *J* = 11.2, 5.5 Hz, 1H:H_8), 3.49 (dd, *J* =11.2, 8.8 Hz, 1H:H_8), 2.19 (m, 1H:H_5), 2.05 (ddd, *J* = 17.4, 8.6, 6.5 Hz, 1H:H_5), 1.59 (m, 1H:H_3), 1.35 (m, 1H:H_4), 1.25 (m, 2H:H_3,H_4), 1.10 (s, 9H:9H_{tBu}); **^{13}C NMR** (90 MHz, C_6D_6): δ 171.8 (C_{11}), 170.0 (C_6), 161.7 (C_{13}), 140.7 (C_{15}), 136.1 (C_{Ph}), 136.0 (C_{Ph}), 133.3 (C_{Ph}), 133.1 (C_{Ph}), 130.6 (C_{Ph}), 128.3 (C_{Ph}), 128.0 (C_{Ph}), 122.1 (C_{14}), 117.6 (C_{12}), 82.6 (C_9), 62.5 (C_8), 55.4 (C_2), 55.1 (C_7), 32.4 (C_5), 27.0 (C_{Me}), 23.5 (C_3), 19.4 (C_{tBu}), 18.7 (C_4); HRMS (ESI+): calcd for $C_{29}H_{33}NO_4Si$: 510.2071 $[M+Na]^+$, found: 510.2073.

(6*R*,11a*S*,11b*S*)-6-*tert*-Butyldiphenylsilyloxymethyl-2,6,8,9,10,11,11a,11b-octahydrofuro[2,3-*c*]pyrido[1,2-*a*]azepin-2-one, *SRS*-33:

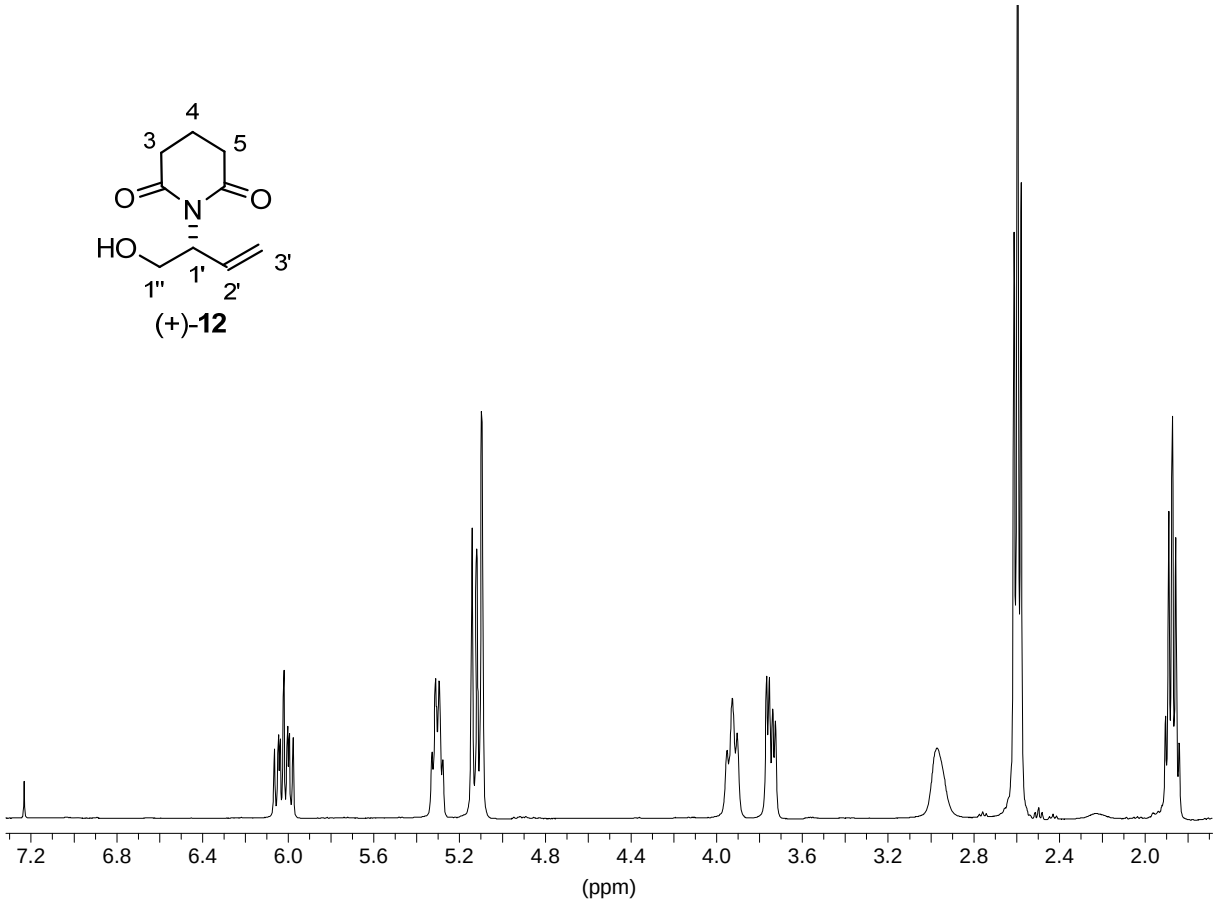
(securinine numbering)



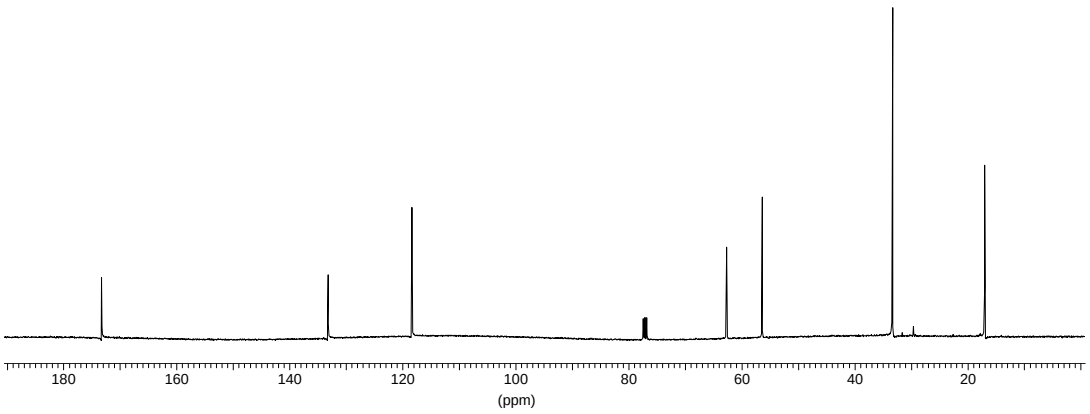
SRS-**33**

In a 10 mL schlenk vessel, lactam *SRS*-**28** (53 mg, 0.11 mmol) was dissolved in dry THF (2.1 mL) under nitrogen. The solution was cooled down to 0 ºC, a solution of BH_3·THF (1M in THF, 543 µL, 0.543 mmol) was added, and the reaction mixture was kept at the same temperature for 45 min. Then, it was treated with 1M NaOH, the aqueous phase was extracted with AcOEt (3x3 mL), and the combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The brownish oily residue was purified by flash chromatography (gradient, hexanes:ethyl acetate 4:1 to 1:1) to furnish compound *SRS*-**33** (50 mg, 0.11 mmol, 97%) as a colorless oil: R_f = 0.58 (hexanes:ethyl acetate 1:1); $[\alpha]_D^{20}$ = +63 (*c* 0.73, CH_2Cl_2); **IR** (ATR): 2926, 2855, 1754, 1427, 1260, 1109; **^{1}H NMR** (400 MHz, CD_2Cl_2): δ 7.68 (m, 4H:4H_{Ph}), 7.42 (m, 6H:6H_{Ph}), 6.45 (dd, *J* = 11.4, 0.4 Hz, 1H:H_{15}), 6.39 (dd, *J* = 11.4, 6.3 Hz, 1H:H_{14}), 5.79 (bd, *J* = 1.7 Hz, 1H:H_{12}), 5.25 (dd, *J* = 6.4, 1.7 Hz, 1H:H_9), 3.84 (dd, *J* = 10.4, 6.2 Hz, 1H:H_8), 3.80 (dd, *J* = 10.4, 6.2 Hz, 1H:H_8), 3.68 (q, *J* = 6.2 Hz, 1H:H_7), 3.35 (ddd, *J* = 11.4, 6.2, 2.4 Hz, 1H:H_2), 2.85 (m, 1H:H_6), 2.57 (dtd, *J* = 12.8, 3.5, 1.3 Hz, 1H:H_6), 1.74 (m, 1H:H_4), 1.56 (m, 1H:H_4), 1.42 (m, 1H:H_3), 1.25 (m, 2H:2H_5), 1.06 (s, 9H:9$H_{t\mathrm{Bu}}$), 0.97 (m, 1H:H_3); **^{13}C NMR** (100 MHz, CD_2Cl_2): δ 173.4 (C_{11}), 163.9 (C_{13}), 143.8 (C_{14}), 136.0 (C_{Ph}), 135.1 (C_{Ph}), 133.4 (C_{Ph}), 130.3 (C_{Ph}), 130.2 (C_{Ph}), 130.0 (C_{Ph}), 128.2 (C_{Ph}), 128.1 (C_{Ph}), 120.6 (C_{15}), 115.5 (C_{12}), 83.4 (C_9), 67.7 (C_7), 64.6 (C_8), 60.8 (C_2), 56.8 (C_6), 30.1 (C_5), 27.0 (C_{Me}), 25.1 (C_4), 24.4 (C_3), 19.3 ($C_{t\mathrm{Bu}}$): HRMS (ESI+): *m/z*: calcd. for $C_{29}H_{35}NO_3Si$: 474.2459 $[M+H]^+$, found: 474.2461.

35. Calculations using B3LYP/6-31G* as implemented by Gaussian 03, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; González, C.; Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.



^{1}H-NMR ($CDCl_3$, 250 MHz)



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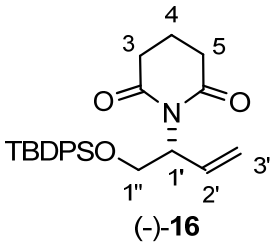
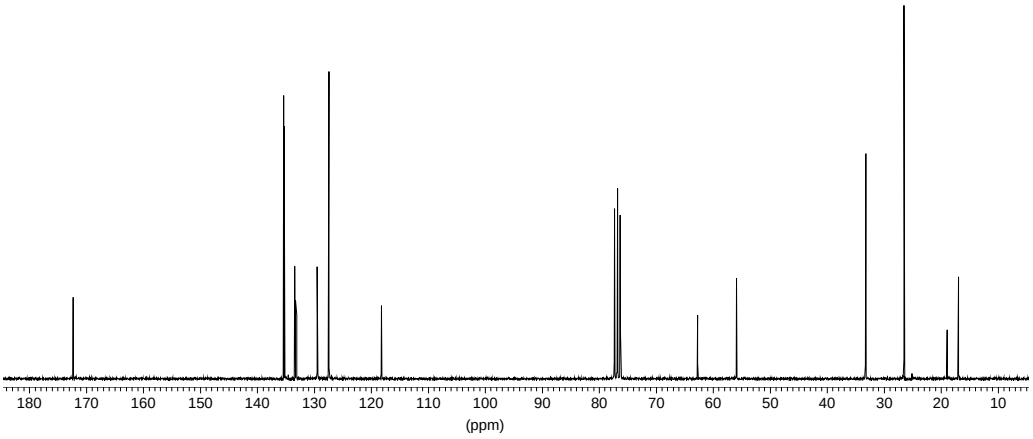
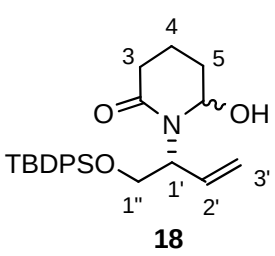


(-)-**16**

^{1}H-NMR ($CDCl_3$, 250 MHz)

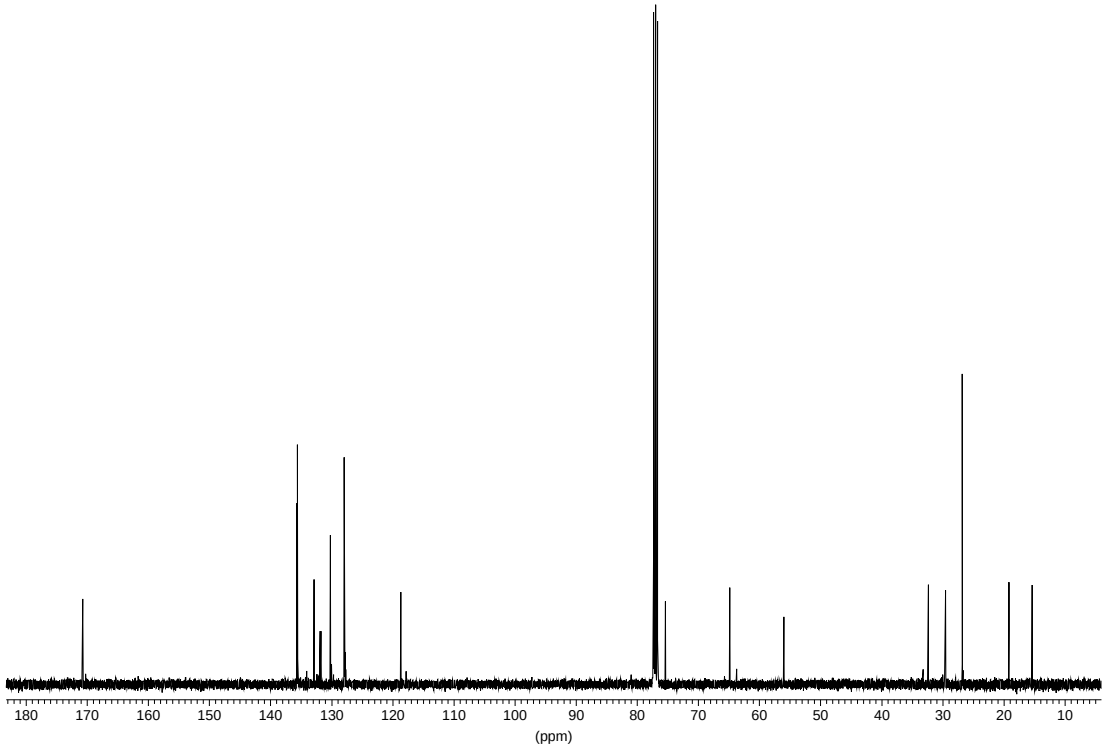


^{13}C-NMR ($CDCl_3$, 62.5 MHz)

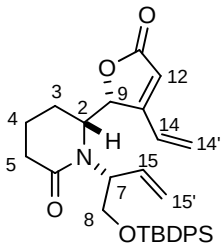


18

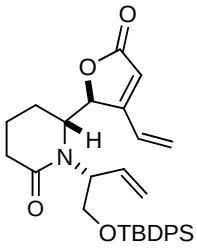
^{1}H-NMR ($CDCl_3$, 400 MHz)



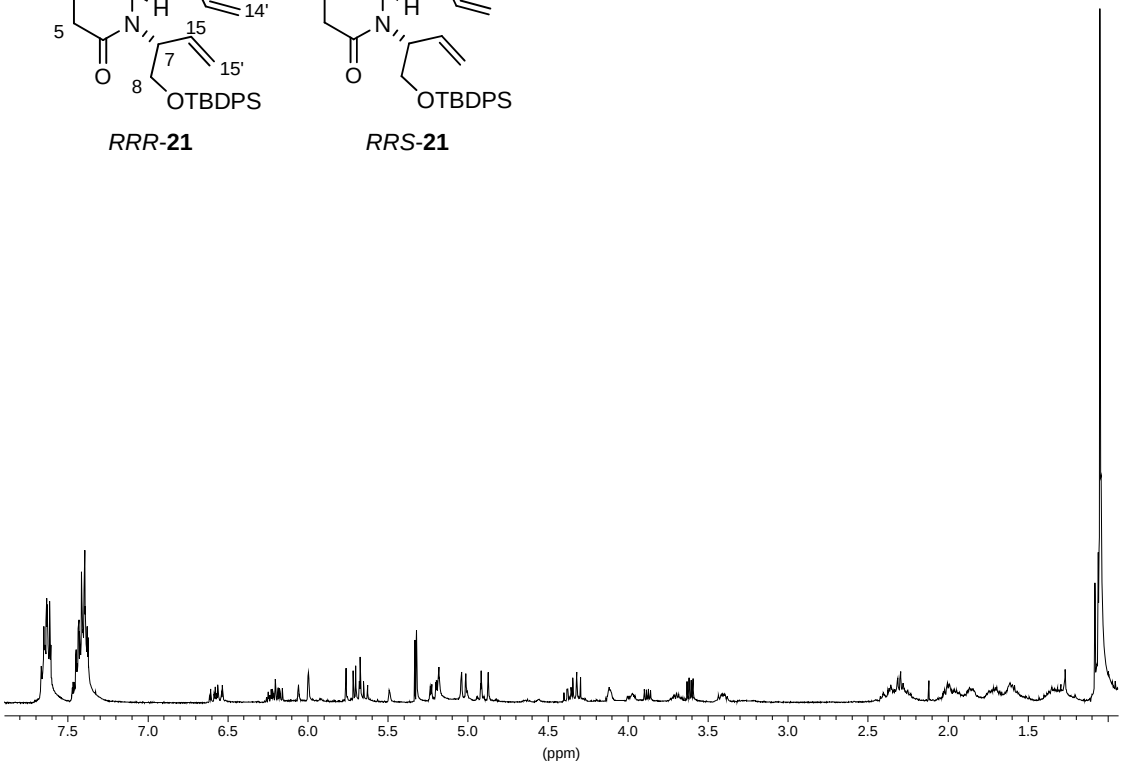
^{13}C-NMR ($CDCl_3$, 100 MHz)



RRR-**21**



RRS-**21**



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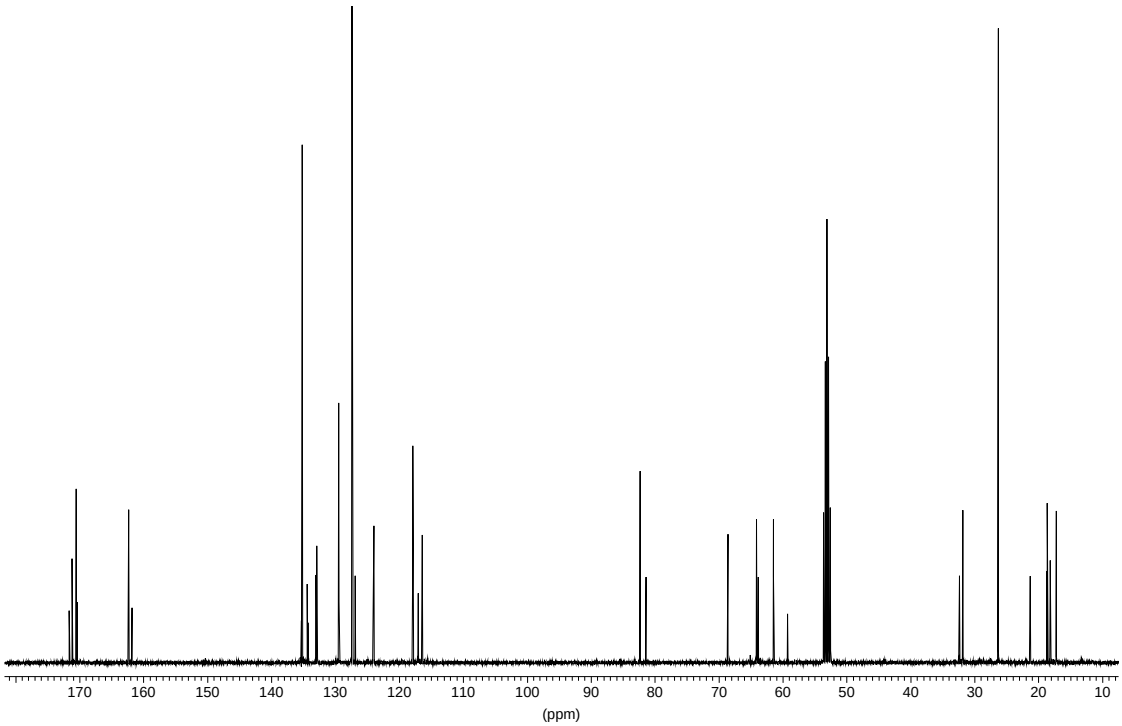
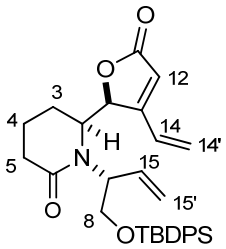
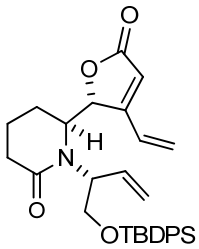


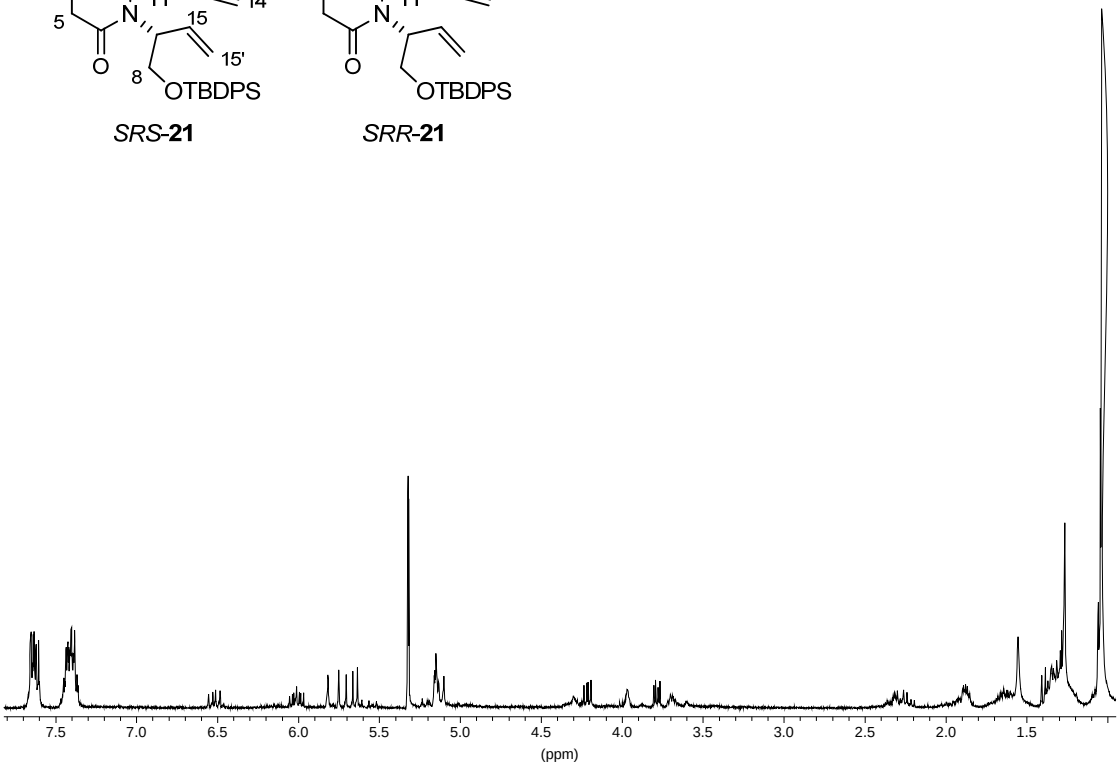
^{13}C-NMR (CD_2Cl_2, 100 MHz)



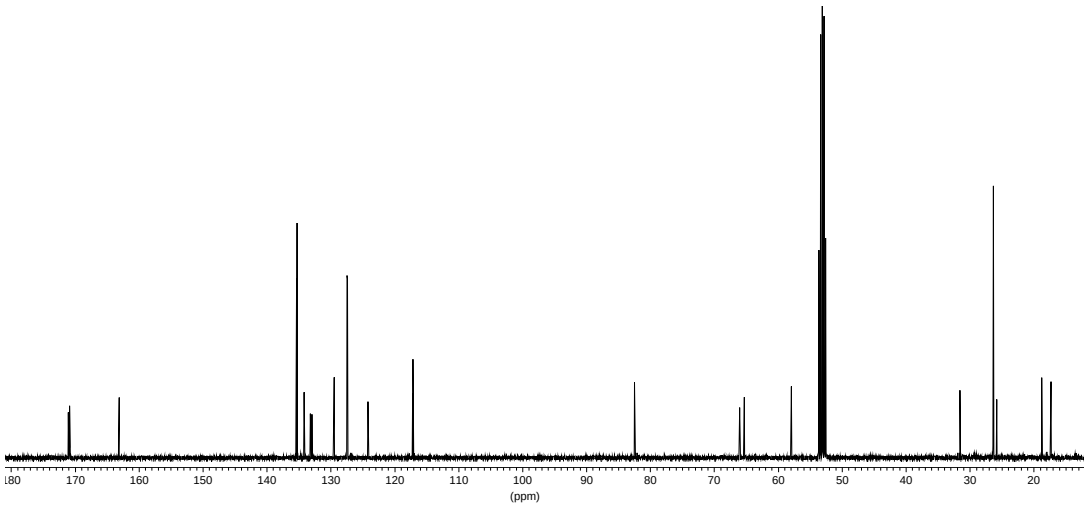
SRS-**21**



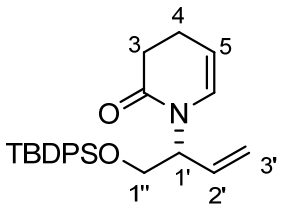
SRR-**21**



^{1}H-NMR (CD_2Cl_2, 400 MHz)



^{13}C-NMR (CD_2Cl_2, 100 MHz)



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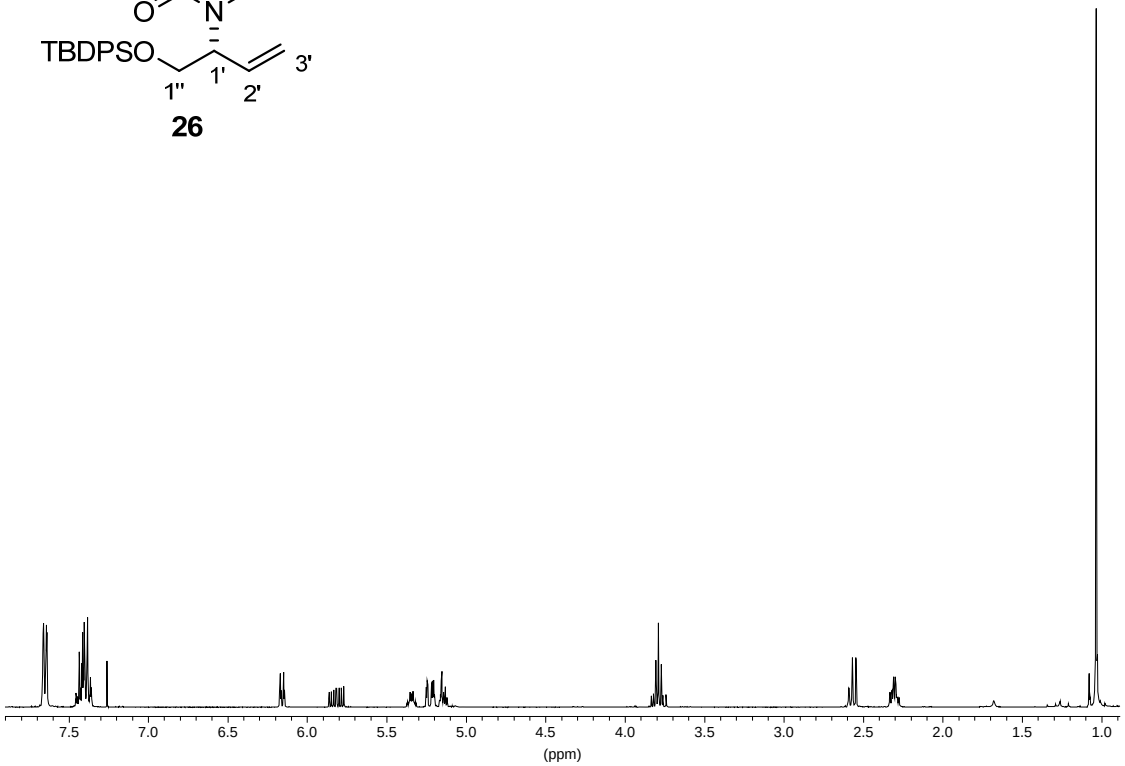
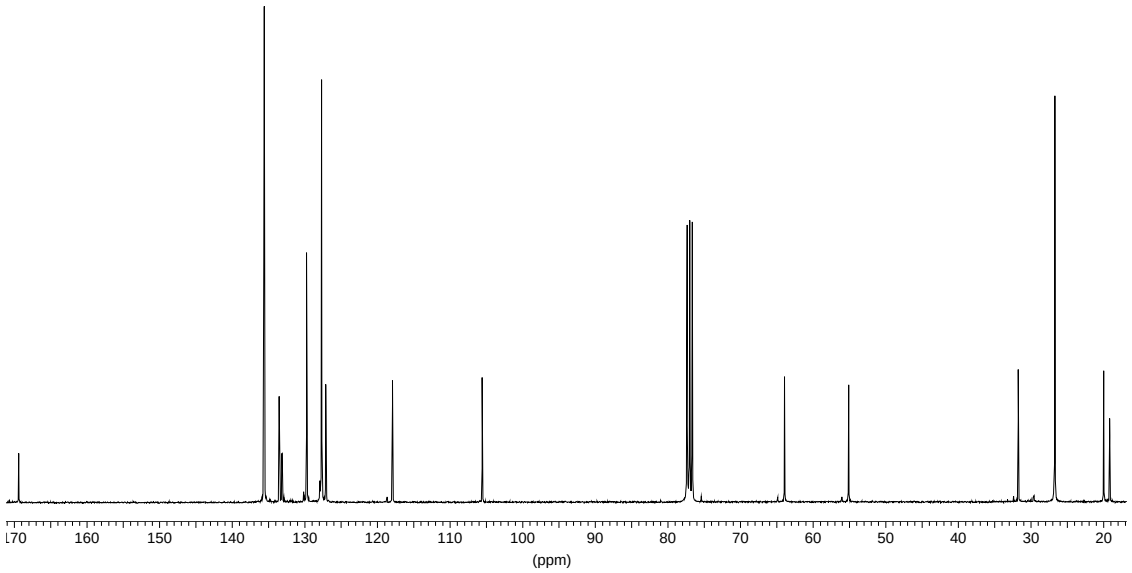
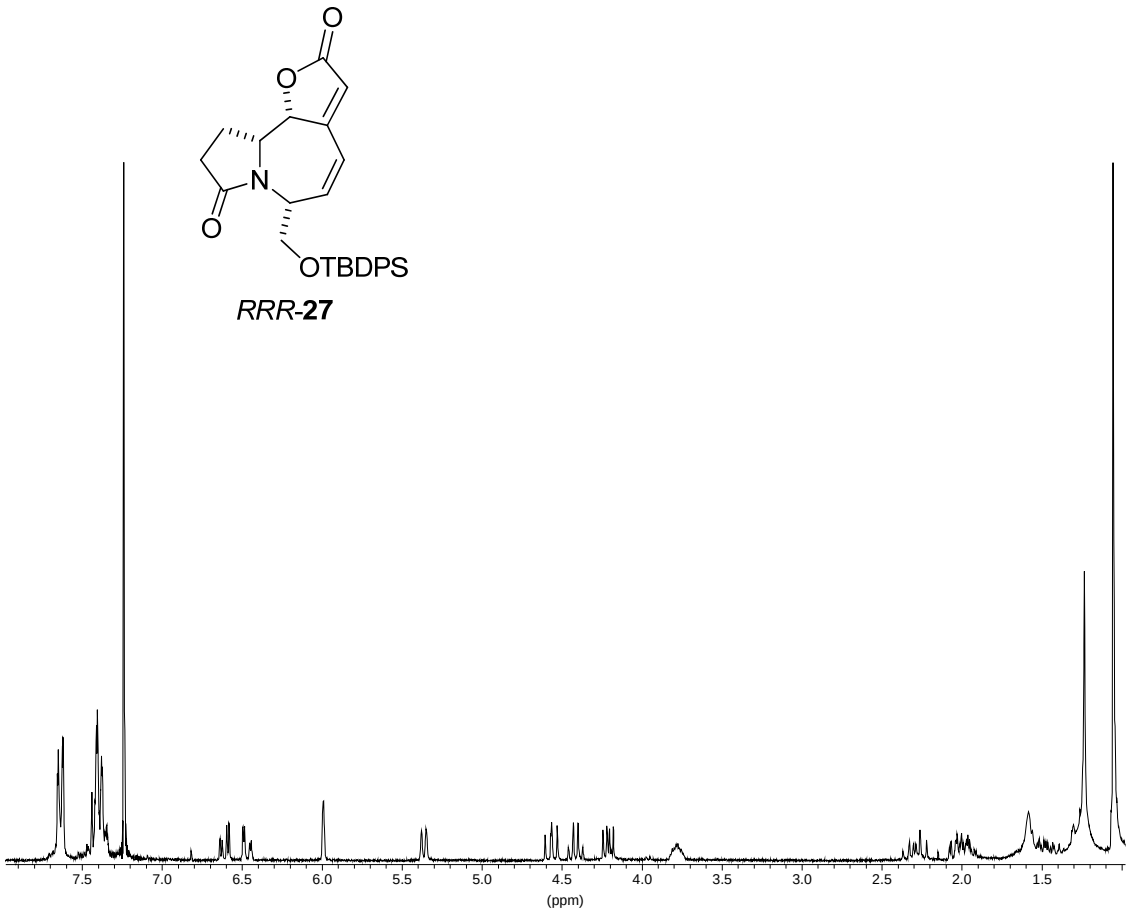


^{1}H-NMR ($CDCl_3$, 360 MHz)

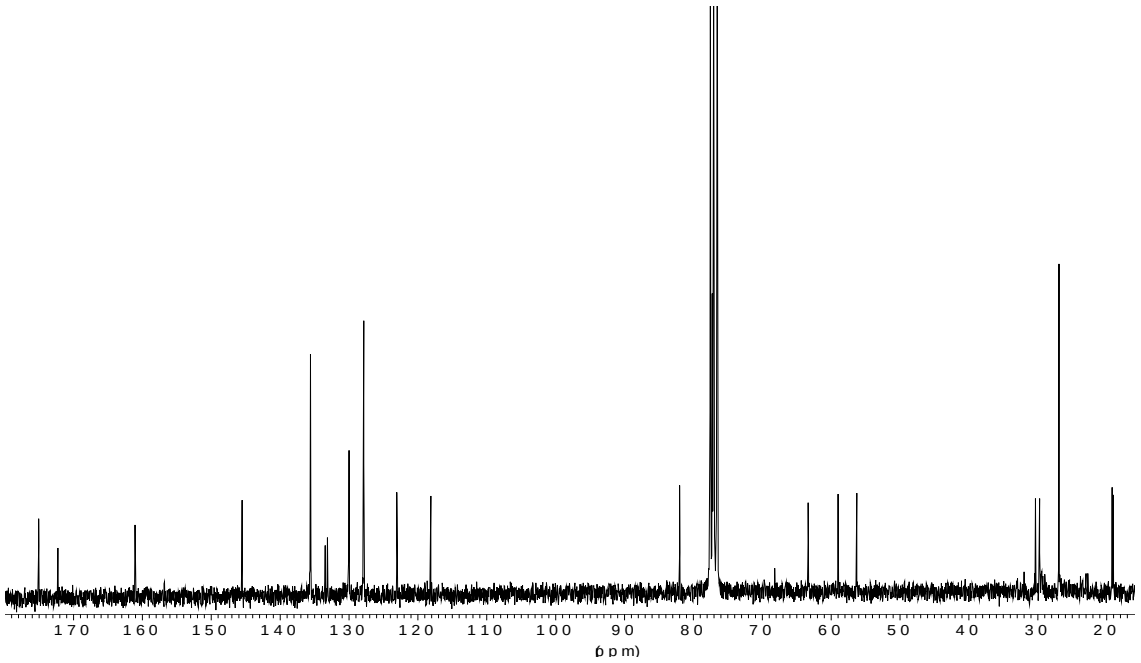


^{13}C-NMR ($CDCl_3$, 90 MHz)

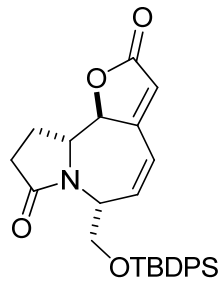


RRR-**27**

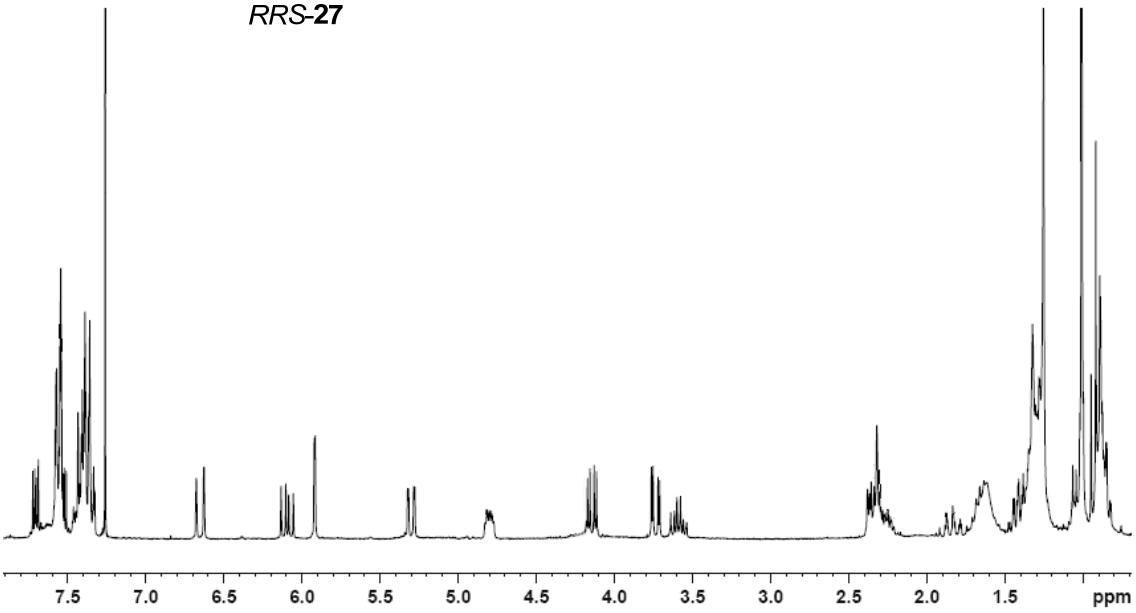
^{1}H-NMR ($CDCl_3$, 250 MHz)



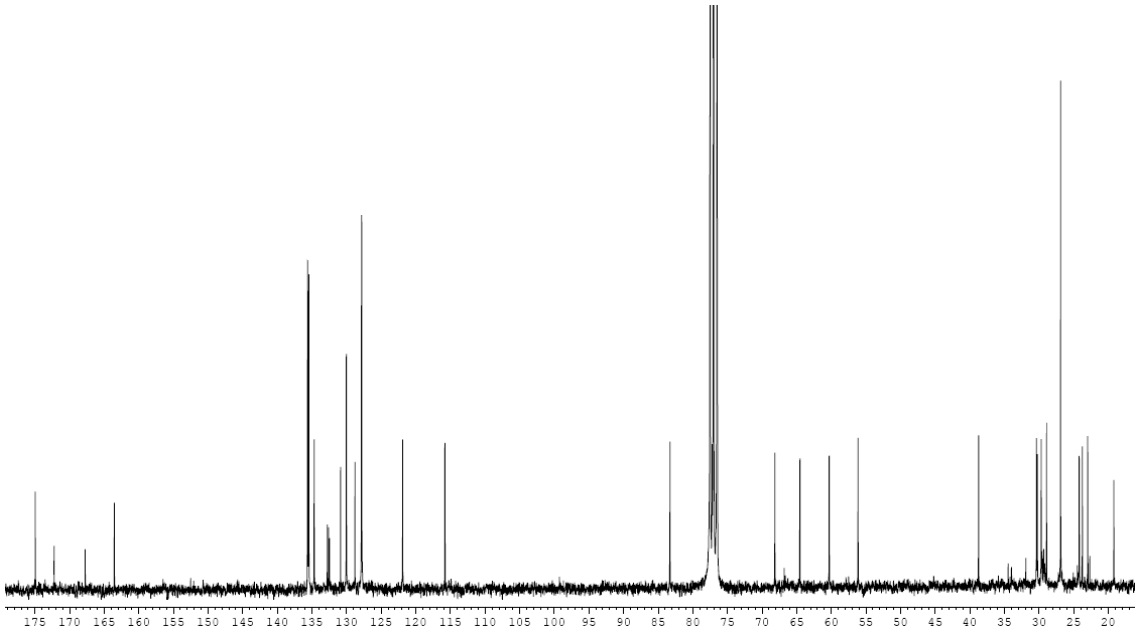
^{13}C-NMR ($CDCl_3$, 62.5 MHz)



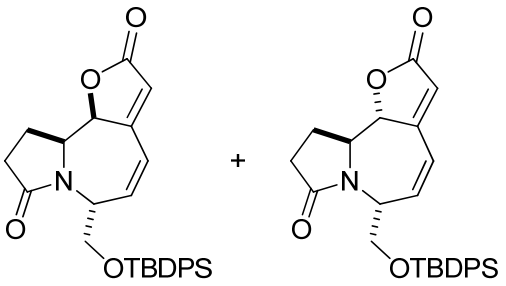
RRS-**27**



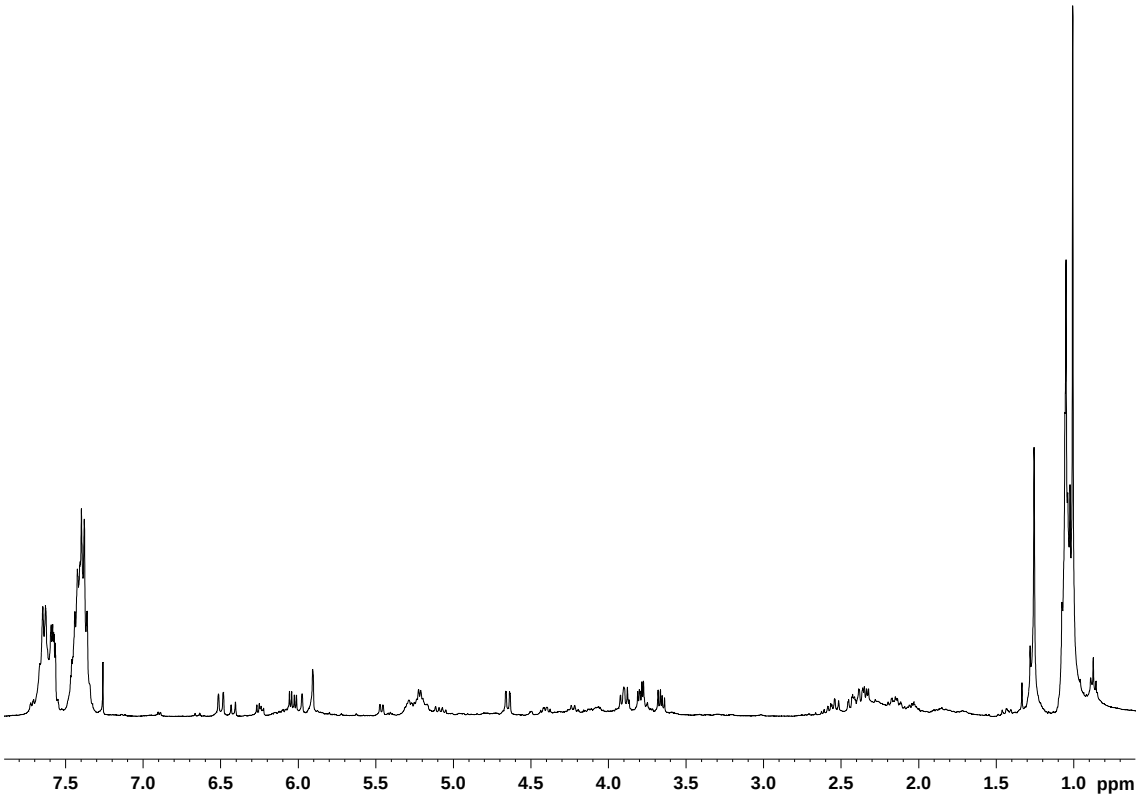
^{1}H-NMR ($CDCl_3$, 400 MHz)



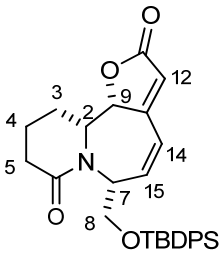
^{13}C-NMR ($CDCl_3$, 100 MHz)



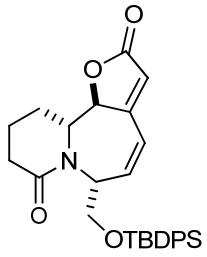
SRS-**27** *SRR*-**27**



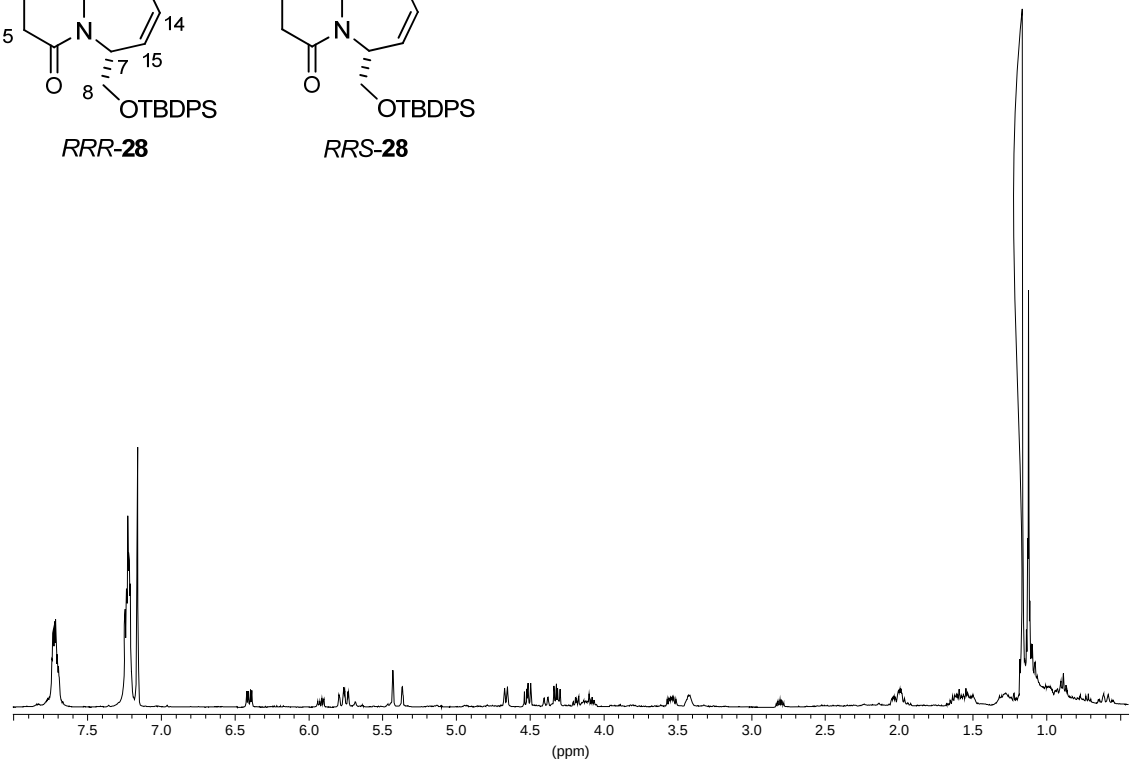
^{1}H-NMR ($CDCl_3$, 400 MHz)



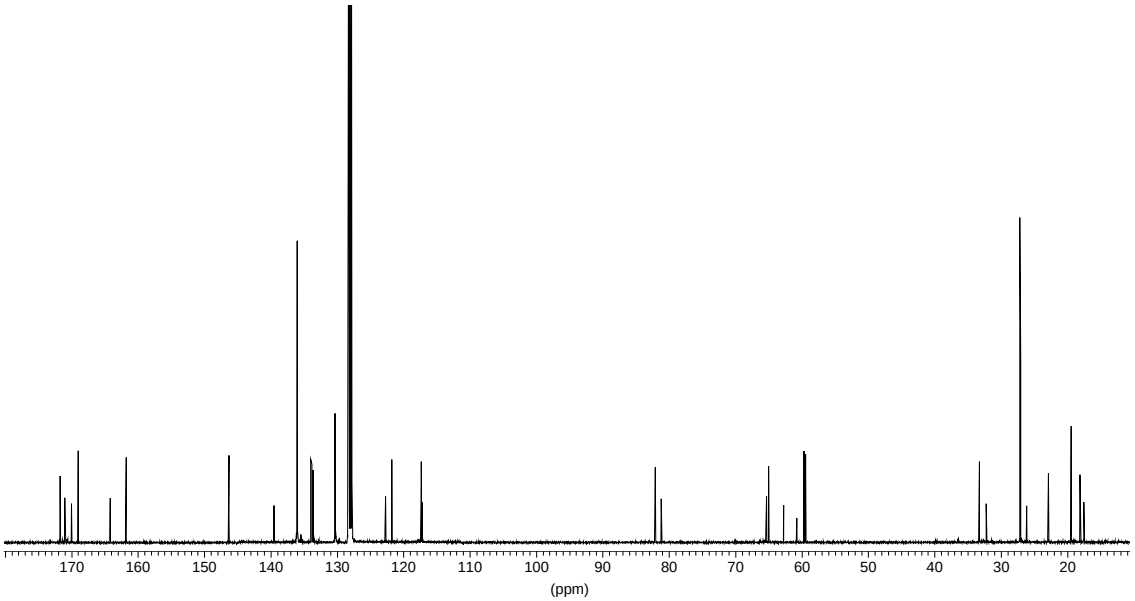
RRR-**28**



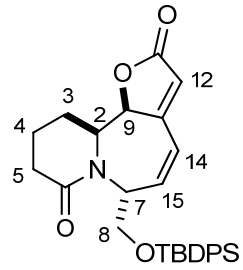
RRS-**28**



^{1}H-NMR (C_6D_6, 400 MHz)

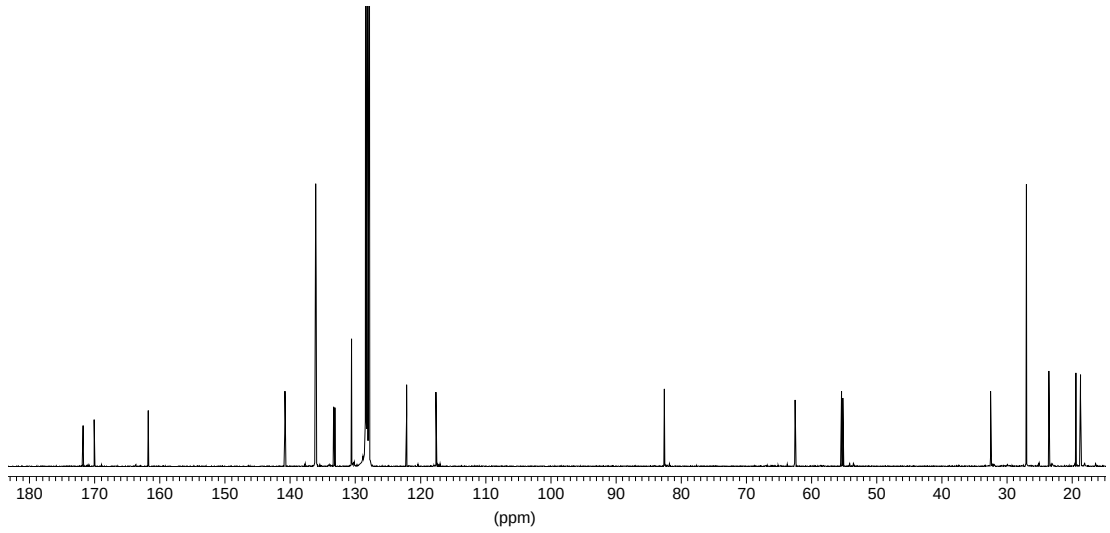


^{13}C-NMR ($CDCl_3$, 100 MHz)

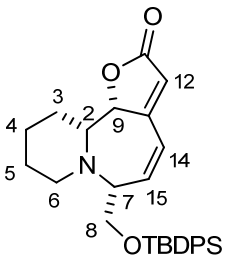


SRS-**28**

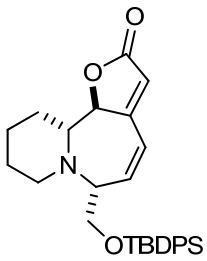
^{1}H-NMR (C_6D_6, 360 MHz)



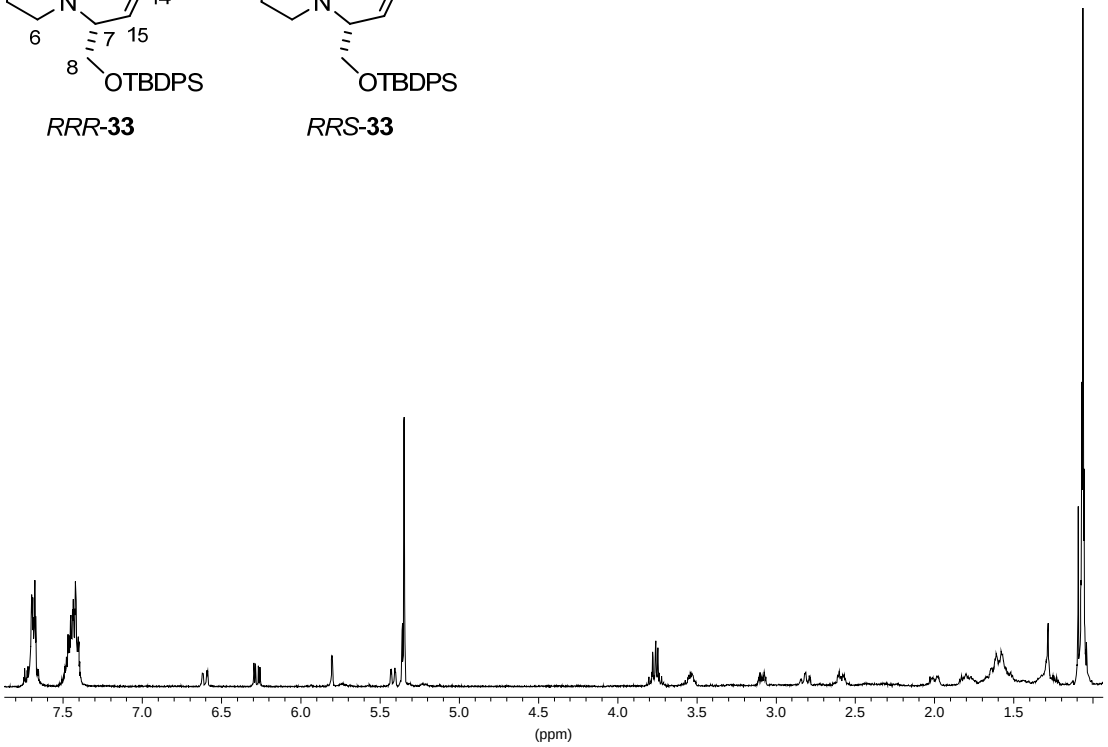
^{13}C-NMR (CD_2Cl_2, 90 MHz)



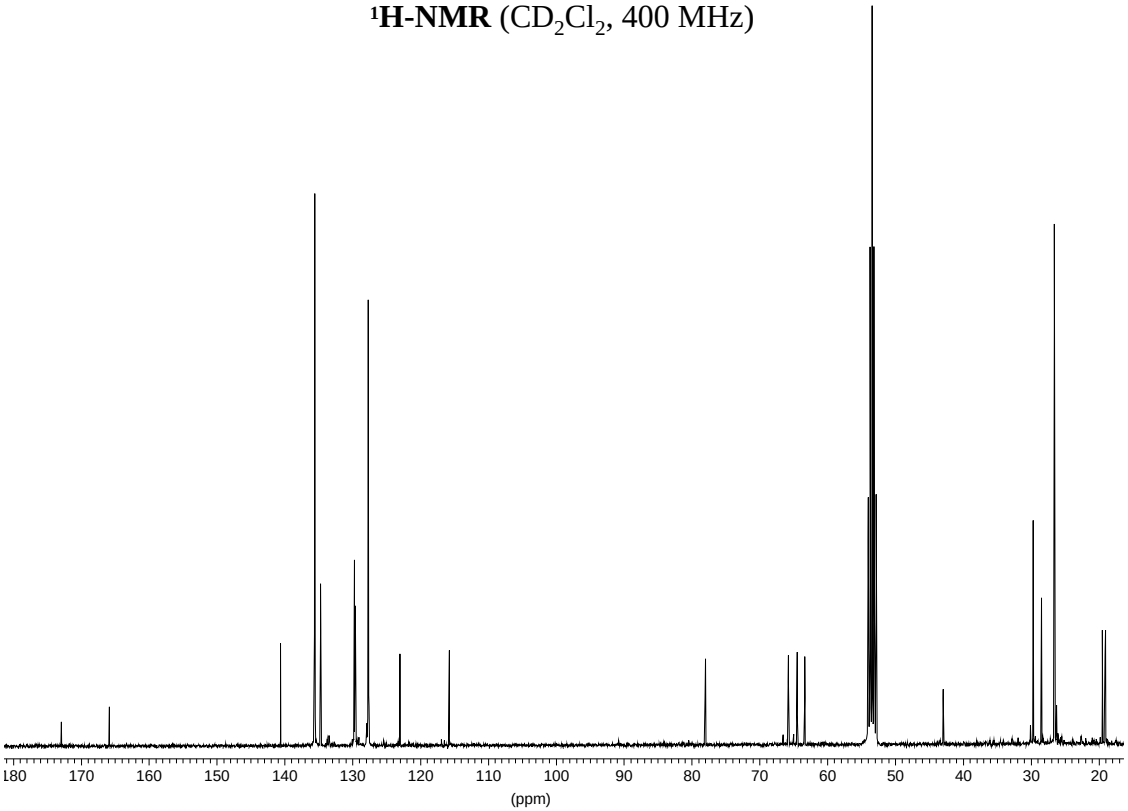
RRR-**33**



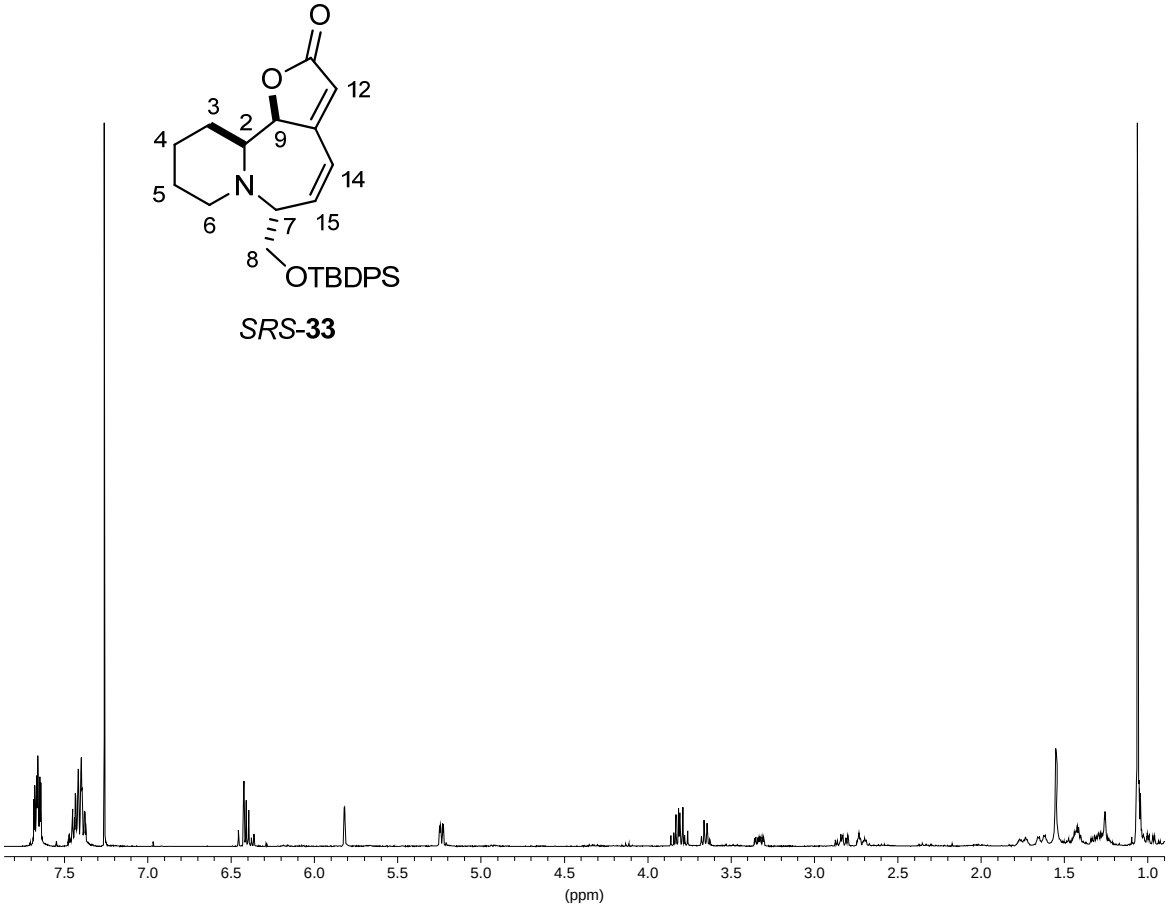
RRS-**33**



^{1}H-NMR (CD_2Cl_2, 400 MHz)

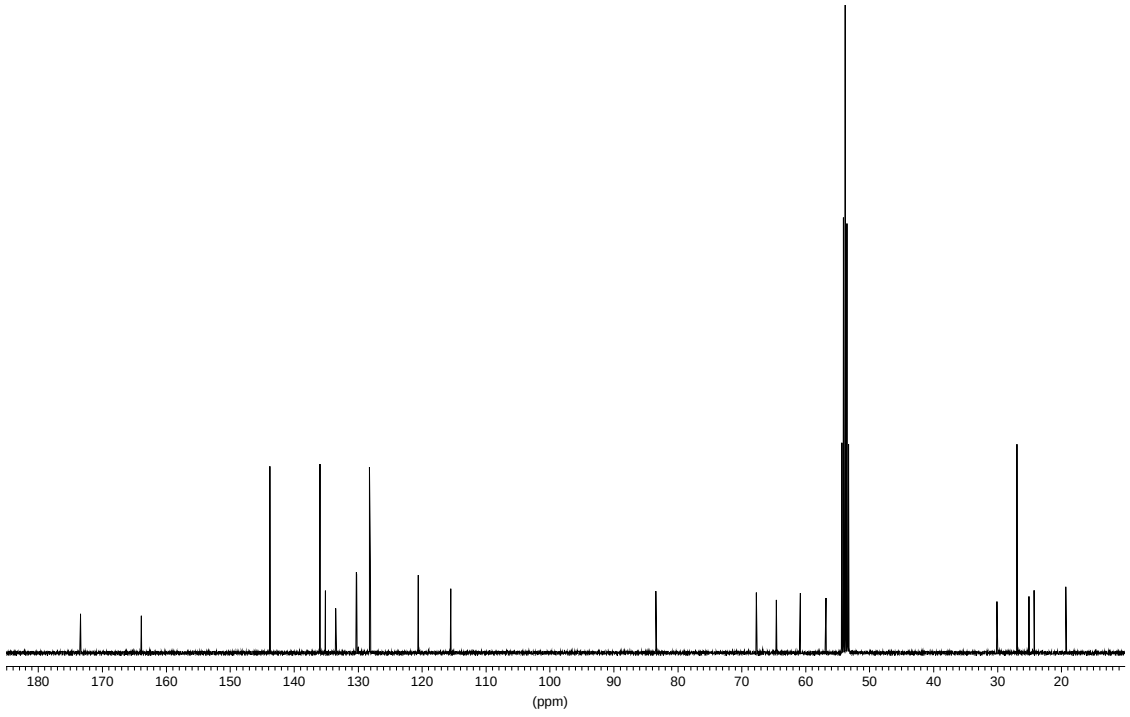


^{13}C-NMR (CD_2Cl_2, 100 MHz)

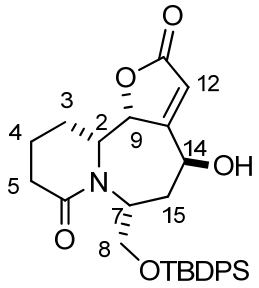


SRS-**33**

^{1}H-NMR ($CDCl_3$, 400 MHz)



^{13}C-NMR (CD_2Cl_2, 100 MHz)



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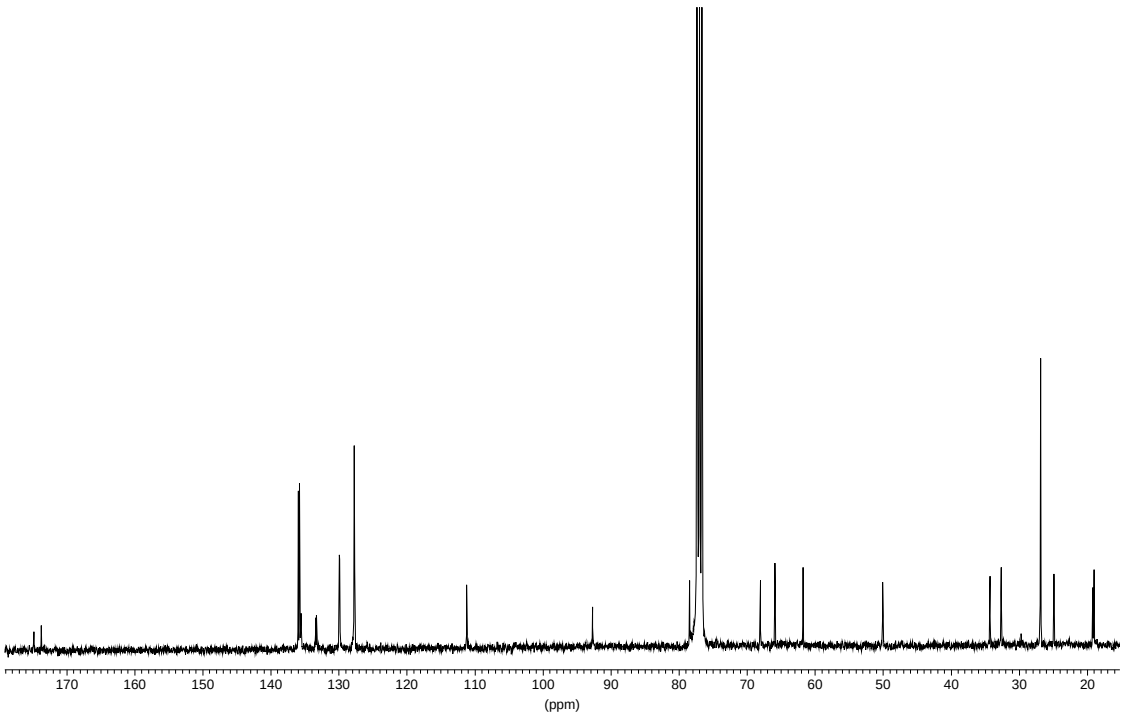
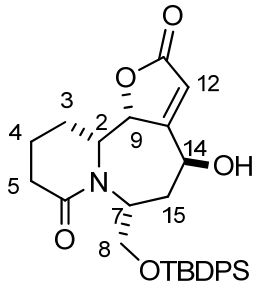
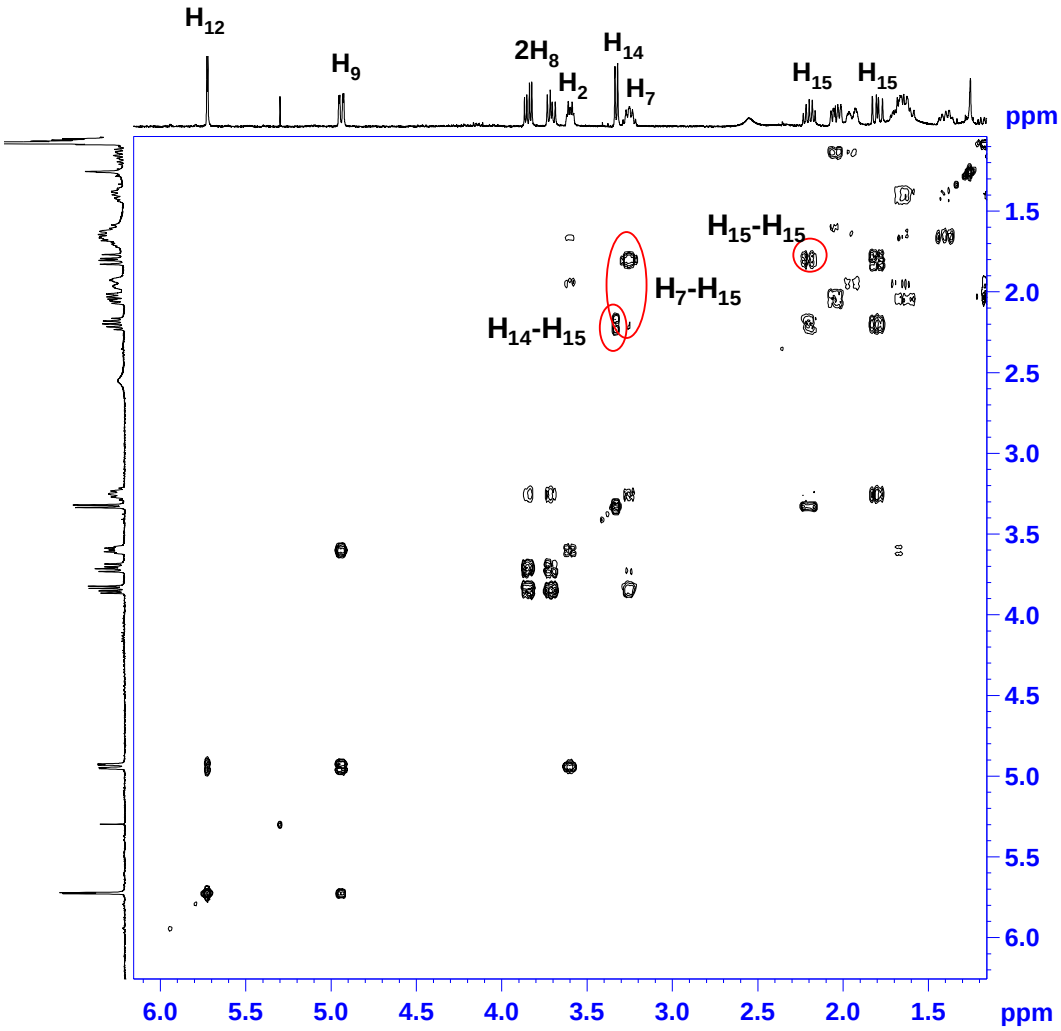
^{1}H-NMR ($CDCl_3$, 400 MHz)



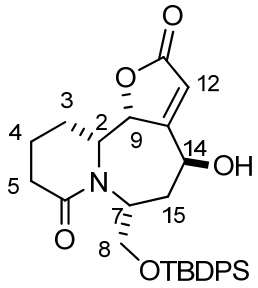
^{13}C-NMR (CD_2Cl_2, 100 MHz)



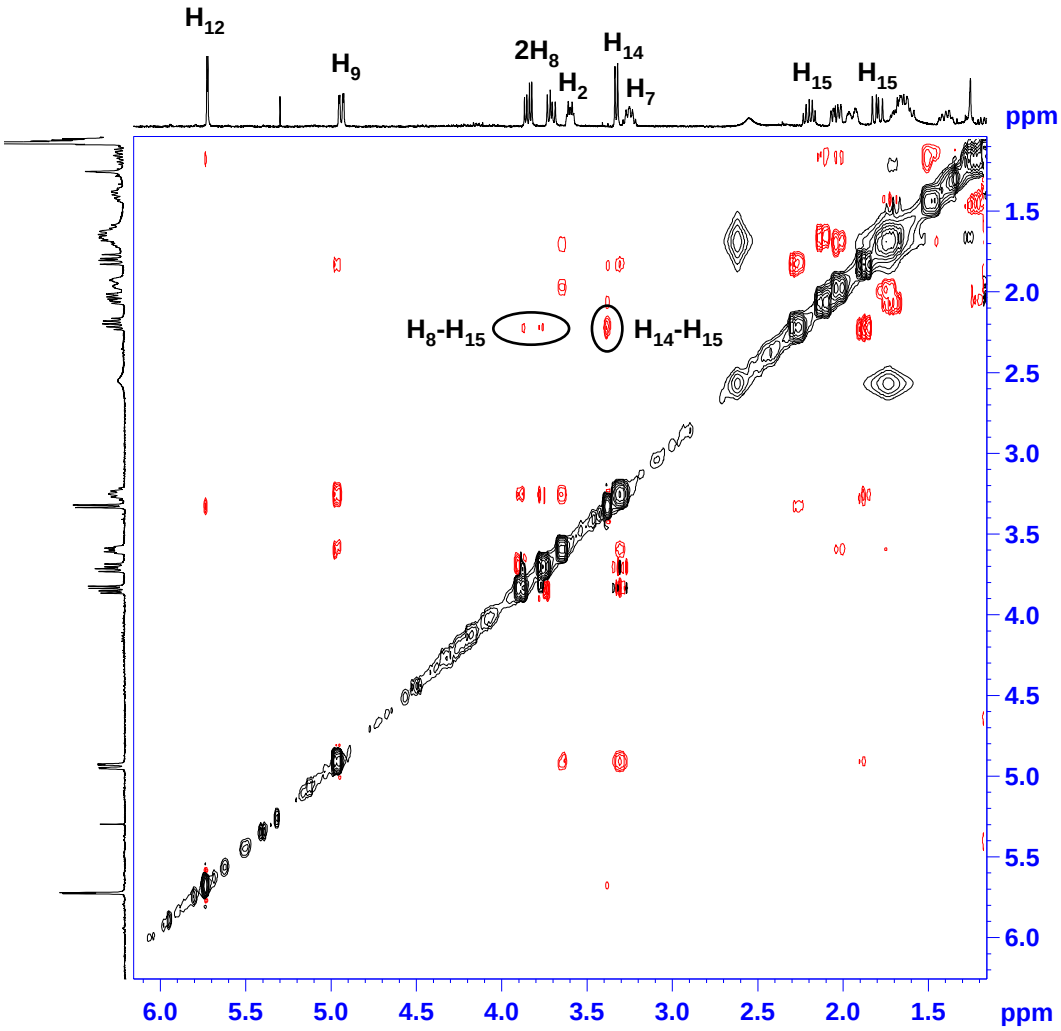
34



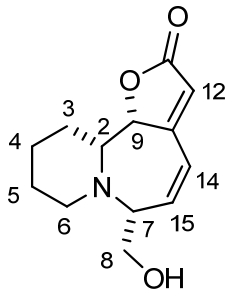
COSY ($CDCl_3$, 400 MHz)



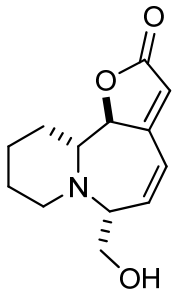
34



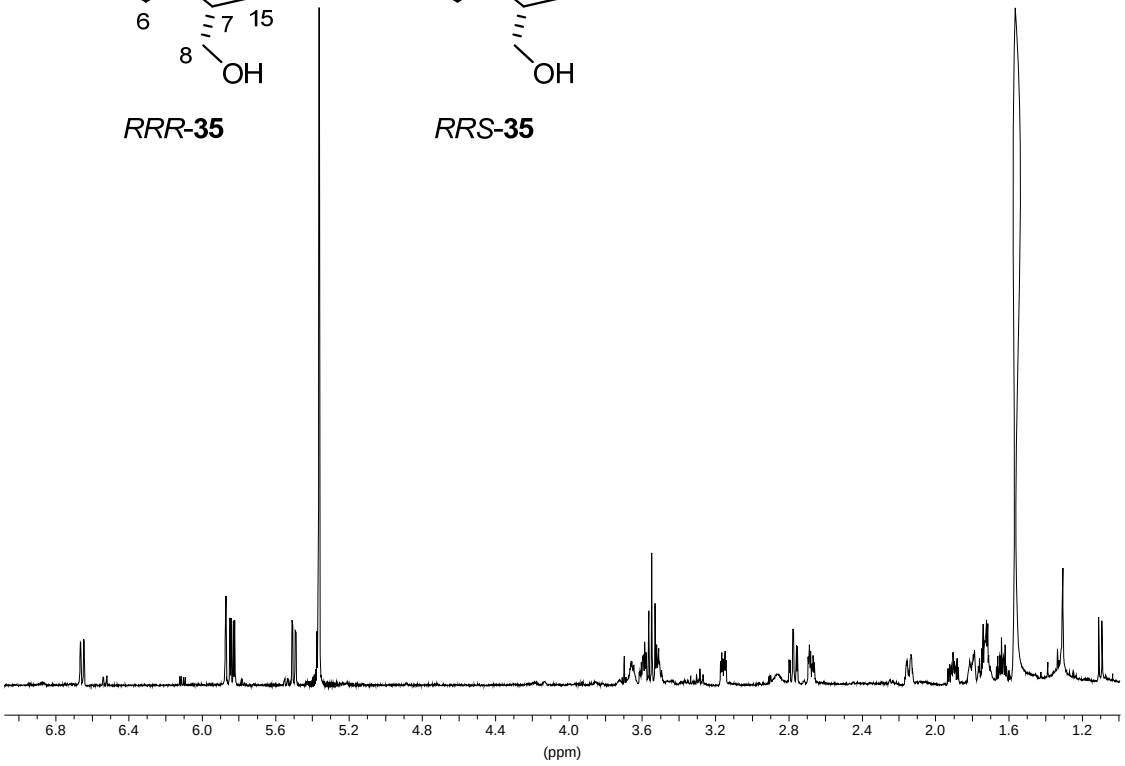
NOESY ($CDCl_3$, 400 MHz)



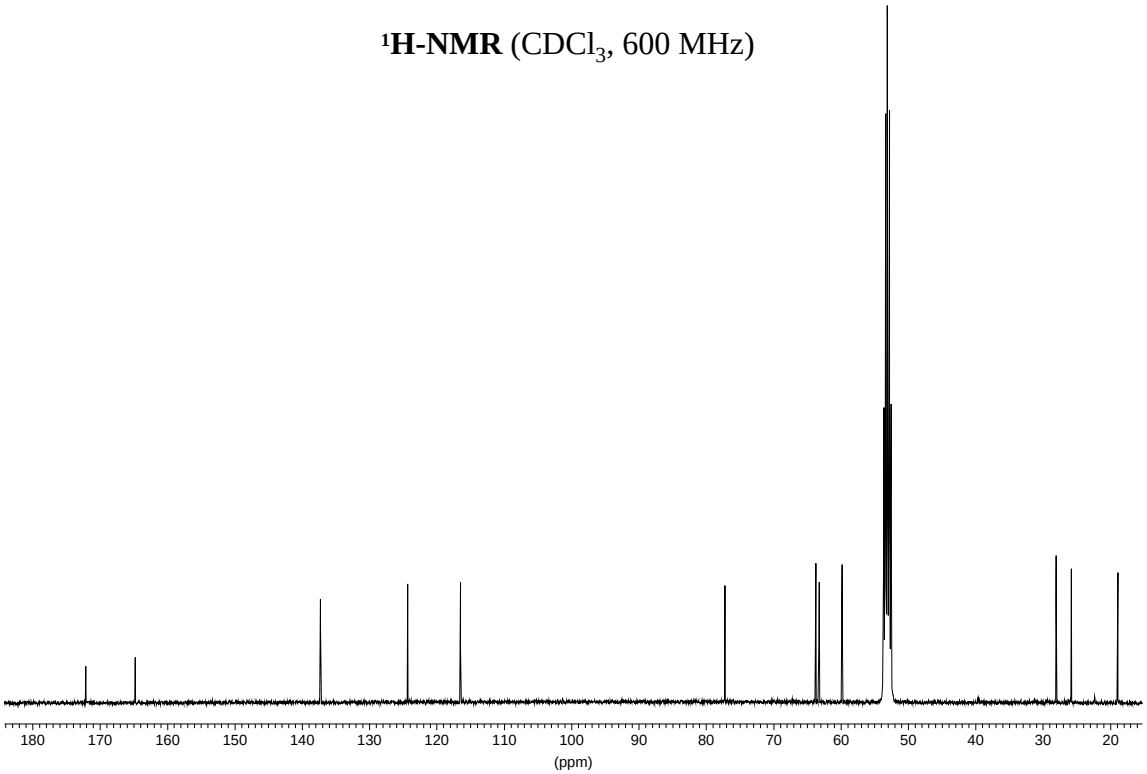
RRR-**35**



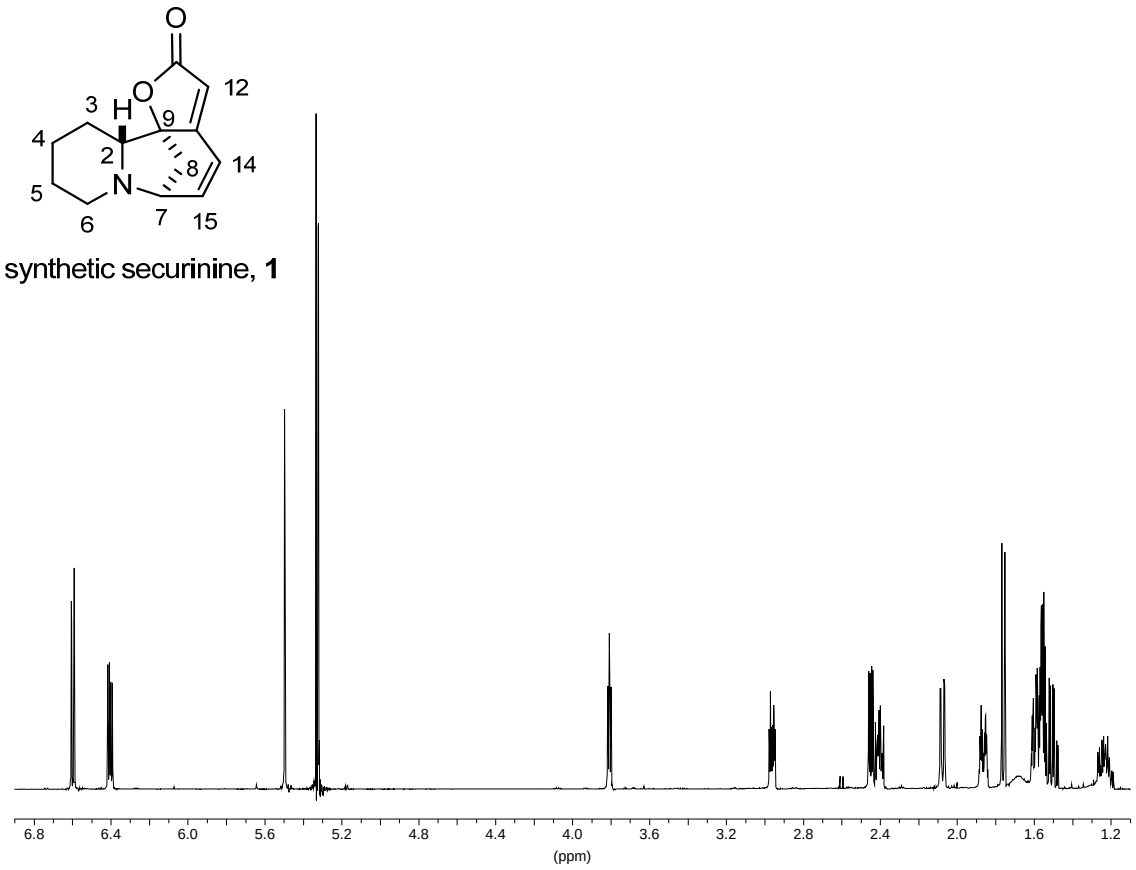
RRS-**35**



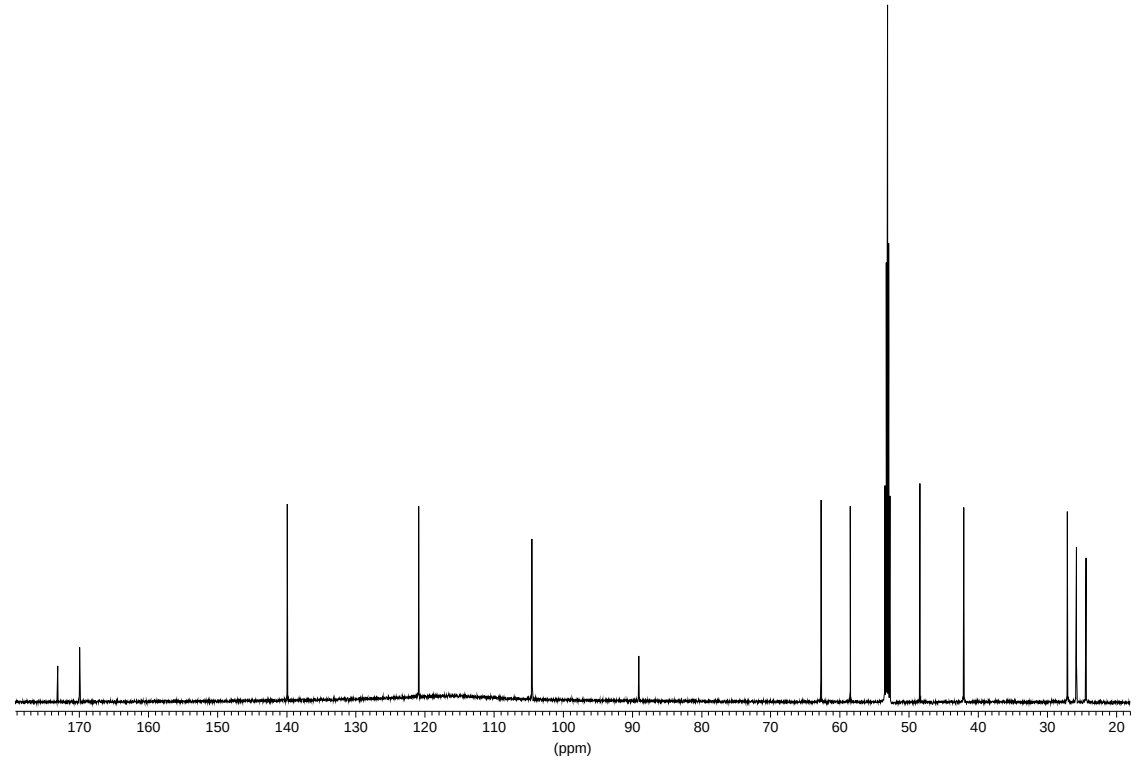
^{1}H-NMR ($CDCl_3$, 600 MHz)



^{13}C-NMR (CD_2Cl_2, 100 MHz)

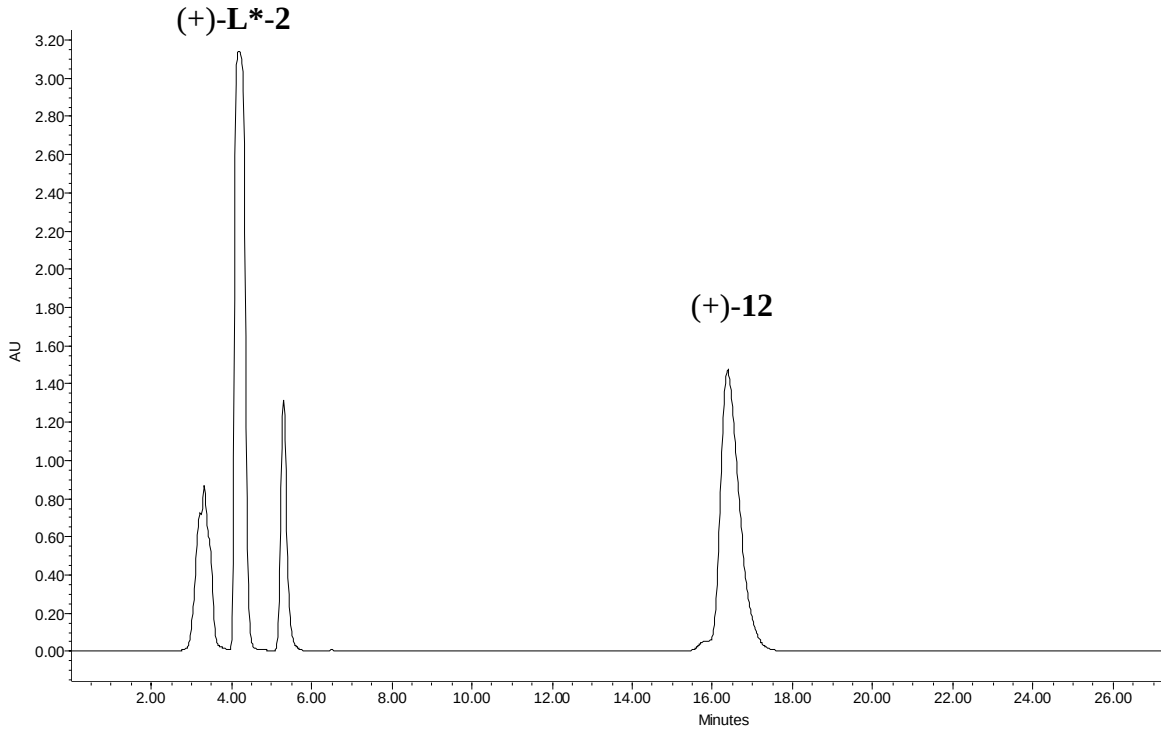


^{1}H-NMR (CD_2Cl_2, 600 MHz)

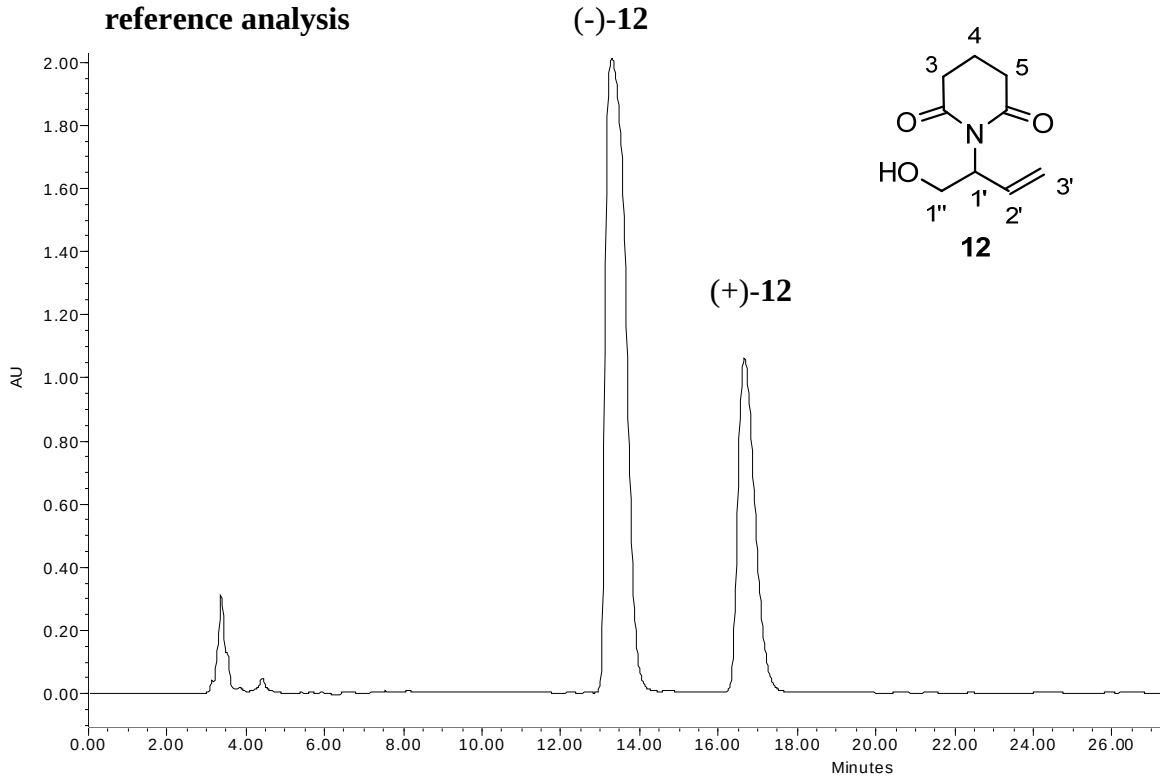


^{13}C-NMR (CD_2Cl_2, 100 MHz)

HPLC analysis of the asymmetric allylation of glutarimide (crude material)



reference analysis



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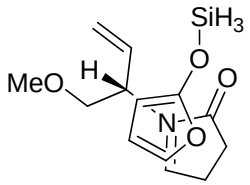
ORIENTATION A



A

E = -1152.28703556 a.u.

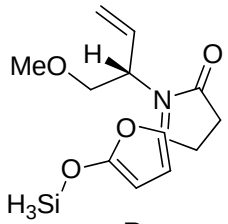
ν_i = -122.134003 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	-0.554318	-3.395777	-0.039241
6	-1.072221	-2.534673	-0.463630
1	-2.107520	-2.847523	-0.661386
6	-0.408178	-1.952187	-1.720573
1	0.648599	-2.226316	-1.796524
1	-0.894557	-2.236800	-2.656658
6	-1.155509	-1.359864	0.471119
1	-1.712253	-1.353994	1.397337
6	-0.503556	-0.449372	-1.538733
7	-0.924692	-0.217565	-0.161248
6	-1.402669	1.097174	0.368500
1	-1.408617	0.977172	1.456032
8	-0.314608	0.435976	-2.326467
6	0.869594	-1.784672	1.747778
1	0.559983	-2.768290	2.067599
8	1.659335	-1.755612	0.608370
6	1.065505	-0.610444	2.453729
1	0.631957	-0.373228	3.416641
6	1.908885	0.210718	1.679728
1	2.233856	1.217638	1.893770
6	2.237874	-0.538891	0.558516
8	2.949076	-0.319808	-0.522110

14	3.942211	1.036744	-0.879629
1	3.098534	2.251691	-0.814716
1	5.022888	1.088494	0.129653
1	4.430282	0.754993	-2.239373
6	-2.862322	1.278375	-0.093793
1	-3.251375	2.191593	0.379644
1	-2.903315	1.417653	-1.185528
8	-3.585823	0.136193	0.307732
6	-4.976772	0.216502	0.003259
1	-5.430301	-0.714218	0.349063
1	-5.446851	1.062797	0.521816
1	-5.141117	0.323148	-1.077948
6	-0.546492	2.281738	-0.001307
1	-0.350484	2.436099	-1.056766
6	-0.134119	3.166067	0.907473
1	-0.335643	3.045511	1.970331
1	0.408182	4.061088	0.617211

ORIENTATION B



B

E = -1152.27876095 a.u.

ν_i = -159.522003 cm^{-1}

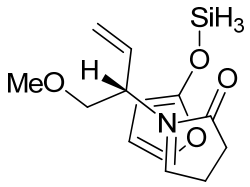
Atomic number and coordinates (x, y, z in Armstrong):

1	0.253875	-3.351409	-1.079664
6	-0.582836	-2.682824	-1.278482
1	-0.688962	-2.620737	-2.370807

6	-1.903526	-3.097066	-0.611171
1	-1.747008	-3.748803	0.256696
1	-2.604375	-3.607586	-1.275633
6	-0.351453	-1.279170	-0.773108
1	0.390950	-0.608303	-1.191603
6	-2.505066	-1.791243	-0.124585
7	-1.478026	-0.776689	-0.271475
6	-1.666243	0.635787	0.179747
1	-0.729565	1.147628	-0.055328
8	-3.600446	-1.554784	0.304713
6	1.177482	-1.307532	0.984133
1	0.433290	-1.460185	1.751764
8	1.598848	0.014405	0.855718
6	2.198265	-2.130431	0.518715
1	2.198377	-3.212470	0.547660
6	3.205663	-1.309306	-0.012337
1	4.121670	-1.612674	-0.498284
6	2.792425	-0.002172	0.234001
8	3.296569	1.175487	-0.025069
14	4.863641	1.547015	-0.639221
1	4.989852	0.895722	-1.963268
1	5.857736	1.012288	0.316282
1	4.858772	3.016082	-0.720881
6	-2.775638	1.313202	-0.652849
1	-2.664102	1.036100	-1.716809
1	-3.767378	0.976547	-0.319362
8	-2.598128	2.691367	-0.460287
6	-3.624630	3.473907	-1.055397
1	-3.391828	4.516798	-0.833030
1	-3.654843	3.334184	-2.146226

1	-4.610412	3.224650	-0.637433
6	-1.913859	0.689003	1.668537
1	-2.841393	0.239425	2.014510
6	-1.089358	1.297122	2.521802
1	-0.169367	1.775282	2.195186
1	-1.322173	1.358601	3.581025

ORIENTATION C



C

E = -1152.2862571 a.u.

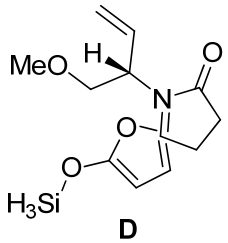
ν_i = -177.796005 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	-0.295342	-2.663582	1.996774
6	-0.821717	-2.294998	1.115867
1	-1.828481	-2.735653	1.133730
6	-0.103668	-2.587583	-0.212735
1	0.956078	-2.819761	-0.077280
1	-0.550717	-3.405402	-0.784593
6	-1.020284	-0.797621	1.102938
1	-1.666212	-0.272438	1.791879
6	-0.230645	-1.299692	-1.004249
7	-0.837101	-0.316592	-0.124303
6	-1.446789	0.915168	-0.706806
1	-0.831810	1.155359	-1.577022
8	0.062189	-1.048789	-2.142802
6	0.895591	-0.220262	2.327116

1	0.617930	-0.772594	3.212940
8	1.757225	-0.893257	1.464788
6	1.066468	1.144611	2.134761
1	0.577891	1.926072	2.700243
6	1.938626	1.314945	1.049025
1	2.249931	2.240554	0.587838
6	2.327613	0.032595	0.673141
8	3.084164	-0.454007	-0.277098
14	3.939218	0.402237	-1.502315
1	2.983132	1.334282	-2.143003
1	5.044442	1.139721	-0.852712
1	4.403287	-0.661571	-2.406645
6	-2.857610	0.525091	-1.193968
1	-3.321607	1.414274	-1.646201
1	-2.791420	-0.255229	-1.969127
8	-3.584591	0.071632	-0.073427
6	-4.940969	-0.247009	-0.374005
1	-5.398781	-0.591215	0.555221
1	-5.482670	0.635638	-0.739473
1	-5.004409	-1.043097	-1.129167
6	-1.506693	2.086080	0.238613
1	-2.136492	1.969771	1.117939
6	-0.952695	3.266961	-0.036844
1	-0.357348	3.430704	-0.932705
1	-1.092010	4.124629	0.615065

ORIENTATION D



D

E = -1152.28001252 a.u.

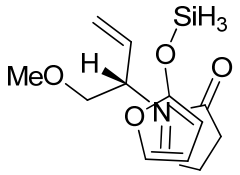
ν_i = -150.985001 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	-1.559573	1.418337	-0.738830
6	-0.484701	1.561339	-0.878851
1	-0.337047	1.830144	-1.934113
6	0.137976	2.595079	0.072735
1	-0.488080	2.773913	0.954533
1	0.337646	3.566737	-0.385530
6	0.306385	0.314103	-0.608408
1	0.241988	-0.577781	-1.218491
6	1.438349	1.960643	0.534411
7	1.435194	0.596166	0.039056
6	2.609654	-0.291159	0.281483
1	3.003518	0.017141	1.253388
8	2.339798	2.408570	1.186734
6	-1.146005	-0.916620	0.763990
1	-0.352366	-1.634572	0.911686
8	-2.074111	-1.257156	-0.214101
6	-1.757579	-0.053072	1.664683
1	-1.304943	0.338387	2.566846
6	-3.052929	0.214144	1.188506
1	-3.799069	0.865538	1.620411
6	-3.196673	-0.560011	0.038266

8	-4.157865	-0.723642	-0.832441
14	-5.780423	-0.153302	-0.743172
1	-5.728575	1.324121	-0.645438
1	-6.401859	-0.744904	0.461483
1	-6.378969	-0.621943	-2.002885
6	3.679653	0.022891	-0.785904
1	3.287103	-0.230678	-1.788560
1	3.907363	1.100911	-0.776189
8	4.800367	-0.746636	-0.458649
6	5.907832	-0.522649	-1.322397
1	6.714808	-1.165754	-0.967537
1	5.663885	-0.786502	-2.361861
1	6.236354	0.525986	-1.286836
6	2.244313	-1.752184	0.303664
1	2.006597	-2.211296	-0.656691
6	2.296497	-2.505576	1.403363
1	2.582152	-2.094512	2.368932
1	2.086491	-3.570851	1.371111

ORIENTATION E



E

E = -1152.2775687 a.u.

ν_i = -142.063004 cm^{-1}

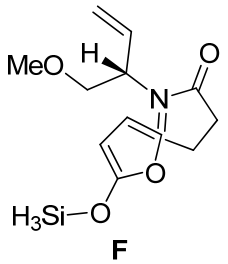
Atomic number and coordinates (x, y, z in Armstrong):

1	-0.926627	3.341023	-1.367040
6	-1.531597	2.491006	-1.047675

1	-2.370855	2.411460	-1.753432
6	-2.028755	2.566201	0.401823
1	-1.403234	3.217071	1.023589
1	-3.060091	2.909835	0.506998
6	-0.794106	1.179016	-1.086503
1	-0.431411	0.717824	-1.997452
6	-1.906138	1.145588	0.929429
7	-1.130799	0.402105	-0.065547
6	-0.912340	-1.086981	-0.049257
1	0.055646	-1.243587	-0.535241
8	-2.322855	0.674913	1.945556
6	1.451999	1.909428	-0.941361
1	1.375734	2.402330	-1.899820
6	1.592397	2.439254	0.335780
1	1.239577	3.411725	0.653981
6	2.257913	1.490871	1.129212
1	2.509012	1.543191	2.177825
6	2.584332	0.451124	0.270579
8	2.126398	0.686995	-0.977994
8	3.210306	-0.674172	0.501475
14	4.006412	-1.691774	-0.646077
1	4.699343	-2.671011	0.207558
1	2.976309	-2.324004	-1.500954
1	4.924453	-0.847942	-1.439828
6	-2.006127	-1.728494	-0.923594
1	-1.871414	-2.820961	-0.892301
1	-1.887970	-1.410543	-1.976206
6	-0.880198	-1.678829	1.338771
1	-1.836519	-1.767936	1.840378
6	0.235886	-2.139124	1.901874

1	1.208727	-2.062217	1.422219
1	0.216151	-2.613424	2.878508
8	-3.253026	-1.335397	-0.414684
6	-4.352344	-1.987682	-1.041562
1	-4.299102	-3.076170	-0.902614
1	-5.256583	-1.607034	-0.563821
1	-4.387456	-1.766516	-2.118354

ORIENTATION F



F

E = -1152.27994061 a.u.

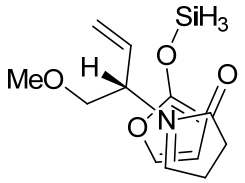
ν_i = -124.552002 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	1.179007	-2.181364	-0.951884
6	0.175299	-2.072155	-0.539072
1	0.107586	-2.764259	0.312548
6	-0.966417	-2.296546	-1.540487
1	-0.639613	-2.195769	-2.581815
1	-1.454961	-3.269787	-1.450717
6	-0.093946	-0.690328	-0.006326
1	0.437625	-0.253016	0.832131
6	-1.971722	-1.193818	-1.248030
7	-1.329374	-0.299821	-0.277541
6	-1.972116	0.892459	0.362597
1	-1.138573	1.516209	0.704313
8	-3.061296	-1.016865	-1.704064

6	1.519026	0.544034	-1.263596
1	1.228817	0.130665	-2.218065
6	1.377846	1.822262	-0.742545
1	0.624917	2.536373	-1.049183
6	2.365352	1.998834	0.245616
1	2.540809	2.853814	0.880990
6	3.121885	0.837699	0.229023
8	2.645759	-0.038478	-0.688511
8	4.152170	0.490983	0.953930
14	5.185362	-0.875977	0.761289
1	6.206920	-0.667914	1.800465
1	4.381342	-2.096993	0.999022
1	5.735412	-0.854101	-0.610902
6	-2.739591	0.421039	1.611897
1	-3.197019	1.307459	2.079135
1	-2.029220	-0.010983	2.341196
6	-2.820258	1.691130	-0.596510
1	-3.704296	1.200350	-0.986114
6	-2.545572	2.960353	-0.898080
1	-3.197308	3.540611	-1.544268
1	-1.678254	3.482436	-0.496655
8	-3.698060	-0.521734	1.218456
6	-4.556389	-0.929753	2.278087
1	-5.118140	-0.077070	2.683912
1	-5.254550	-1.653227	1.854130
1	-3.988913	-1.403522	3.092575

ORIENTATION G



G

E = -1152.28231201 a.u.

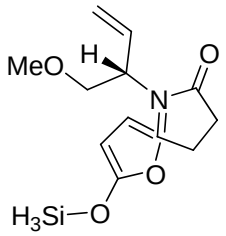
ν_i = -221.112000 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	0.771288	3.313195	1.433070
6	1.329196	2.509846	0.951144
1	2.337031	2.508887	1.388813
6	1.394387	2.594085	-0.581360
1	0.592968	3.205822	-1.007768
1	2.339837	2.986763	-0.964373
6	0.753860	1.136860	1.199711
1	0.757684	0.664380	2.173158
6	1.215137	1.158760	-1.053279
7	0.925184	0.362747	0.123492
6	0.966909	-1.137339	0.129578
1	0.079292	-1.495657	-0.400750
8	1.271874	0.706714	-2.163975
6	-1.469396	1.401396	1.439360
1	-1.475599	1.417923	2.520367
6	-1.779827	2.428404	0.540506
1	-1.622946	3.483989	0.721200
6	-2.284797	1.848418	-0.626063
1	-2.586240	2.324505	-1.547239
6	-2.370411	0.484996	-0.357105
8	-1.933528	0.204122	0.885800
8	-2.778855	-0.485358	-1.124908

14	-3.521375	-1.989139	-0.716176
1	-4.087014	-2.444246	-1.996316
1	-2.474074	-2.904854	-0.214075
1	-4.539706	-1.714179	0.319754
6	2.227243	-1.607691	-0.626424
1	2.136014	-1.418931	-1.702036
1	2.315745	-2.694145	-0.469475
6	0.999293	-1.664194	1.543669
1	1.946573	-1.520514	2.061347
6	0.009719	-2.343631	2.123122
1	-0.937013	-2.529284	1.623285
1	0.121078	-2.760157	3.120154
8	3.324663	-0.912003	-0.076034
6	4.570333	-1.311069	-0.638881
1	4.593321	-1.128899	-1.722343
1	5.343050	-0.711081	-0.154287
1	4.768565	-2.375637	-0.451376

ORIENTATION H



H

E = -1152.28273159 a.u.

ν_i = -121.383003 cm^{-1}

Atomic number and coordinates (x, y, z in Armstrong):

1	1.007551	-1.897621	-1.204384
6	-0.033556	-1.810443	-0.895732
1	-0.221734	-2.605690	-0.159459

6	-1.060965	-1.866995	-2.035953
1	-0.632648	-1.569709	-3.000671
1	-1.524237	-2.846236	-2.175802
6	-0.351691	-0.512411	-0.196900
1	0.101425	-0.202468	0.737759
6	-2.115212	-0.850590	-1.642173
7	-1.568021	-0.099416	-0.515326
6	-2.452985	0.836689	0.236722
1	-3.352029	0.878850	-0.381837
8	-3.193919	-0.621624	-2.107538
6	1.406536	0.787146	-1.203671
1	1.102007	0.536800	-2.208982
6	1.380027	1.997375	-0.525340
1	0.690443	2.804470	-0.728722
6	2.374840	1.961270	0.468868
1	2.622956	2.710728	1.205234
6	3.026291	0.749431	0.300702
8	2.478829	0.040169	-0.714091
8	4.018927	0.225589	0.969973
14	4.940751	-1.180378	0.589062
1	5.966467	-1.200850	1.644815
1	4.040818	-2.354817	0.656413
1	5.503665	-1.013640	-0.767937
6	-2.806035	0.189750	1.587861
1	-3.645597	0.754375	2.020664
1	-1.957568	0.276163	2.291477
6	-1.880024	2.218960	0.408329
1	-1.065953	2.325920	1.124330
6	-2.375266	3.295132	-0.204708
1	-1.978814	4.288866	-0.015936

1	-3.203261	3.228468	-0.906662
8	-3.136868	-1.157711	1.358729
6	-3.690741	-1.801530	2.502002
1	-4.621972	-1.313444	2.820058
1	-3.906264	-2.830859	2.209900
1	-2.982681	-1.802176	3.343527