SUPPORTING INFORMATION

An Improved and Enantioselective Preparation of the Telaprevir Bicyclic [3.3.0] Proline Intermediate and Reuse of Unwanted Enantiomer

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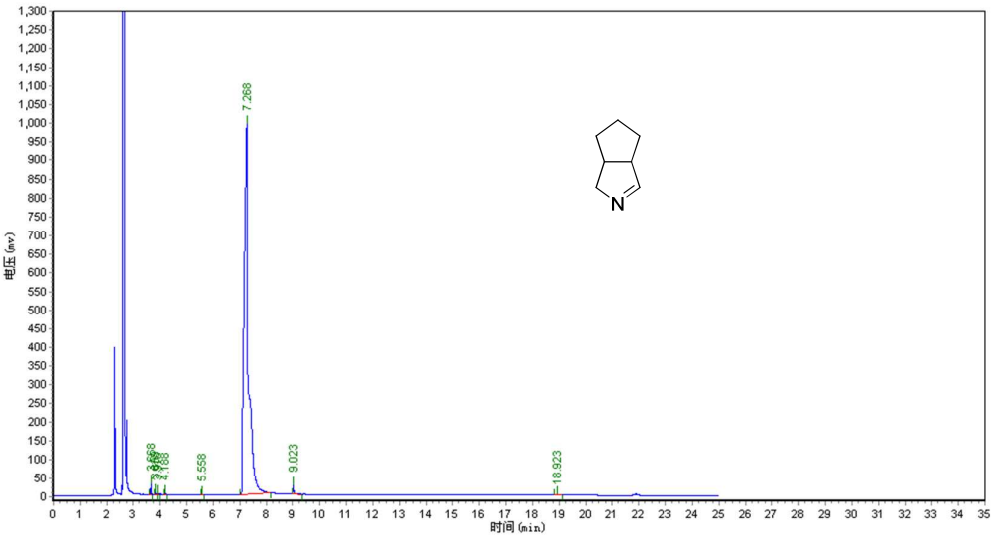
1. GC data of compounds 4, 6, 7

Operational condition:

Detectot: FID Chromatography Column: SE-54

Carrier gas: N_2 Carrier gas flow rate (mL/min): 0.1MPa

Column Temperature: temperature programming (Initial Temp: 50 °C, Heating rate: 20 °C/min, Final Temp: 250 °C)



Peak	Rt(min)	Heigth(mV*sec)	Area(mV)	Area(%)
1	3.668	28074.223	39175.602	0.3491
2	3.838	7065.706	10821.300	0.0964
3	3.918	2958.667	6487.500	0.0578
4	4.188	4474.333	7425.350	0.0662
5	5.558	2128.000	5752.100	0.0513
6	7.268	995057.813	11080857.000	98.7437
7	9.023	25176.766	61266.801	0.5460
8	18.923	2275.333	10054.800	0.0896

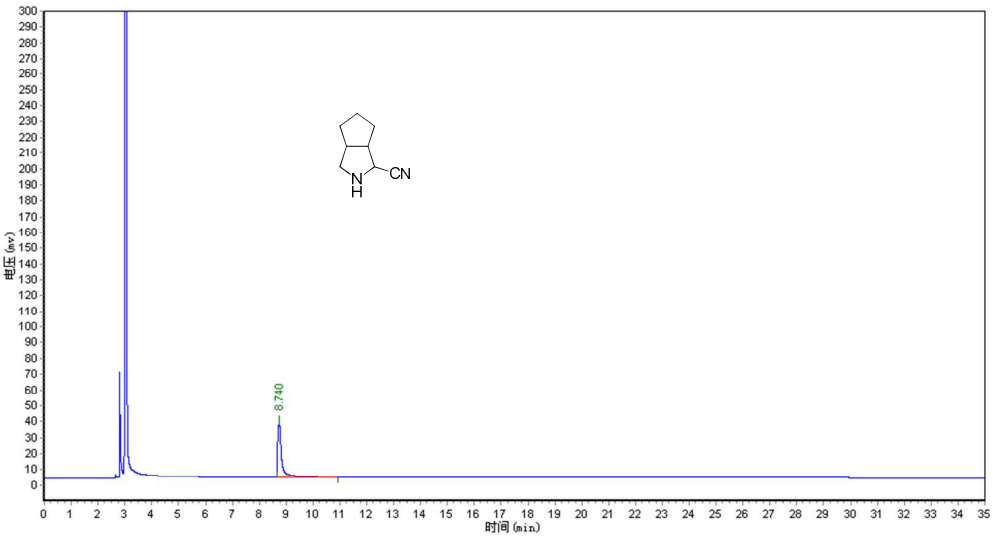
GC data of compound **4**

Operational condition:

Detectot: FID Chromatography Column: SE-54

Carrier gas: N_2 Carrier gas flow rate (mL/min): 0.1MPa

Column Temperature: temperature programming (Initial Temp: 50 ^{o}C, Heating rate: 20 ^{o}C/min, Final Temp: 250 ^{o}C)



Peak	Rt(min)	Heigth(mV*sec)	Area(mV)	Area(%)
1	8.740	33433.711	370236.063	100.0000

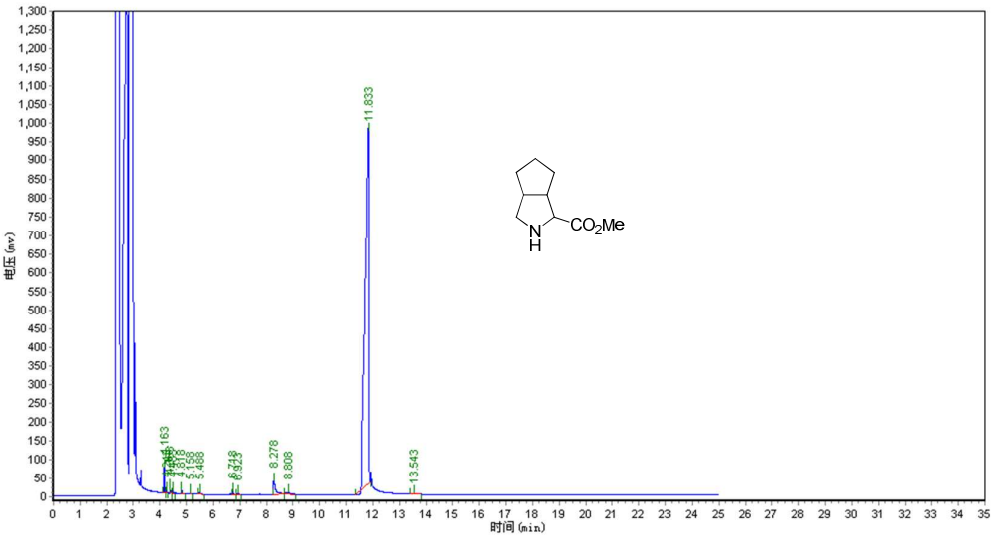
GC data of compound **6**

Operational condition:

Detectot: FID Chromatography Column: SE-54

Carrier gas: N_2 Carrier gas flow rate (mL/min): 0.1MPa

Column Temperature: temperature programming (Initial Temp: 50 °C, Heating rate: 20 °C/min, Final Temp: 250 °C)

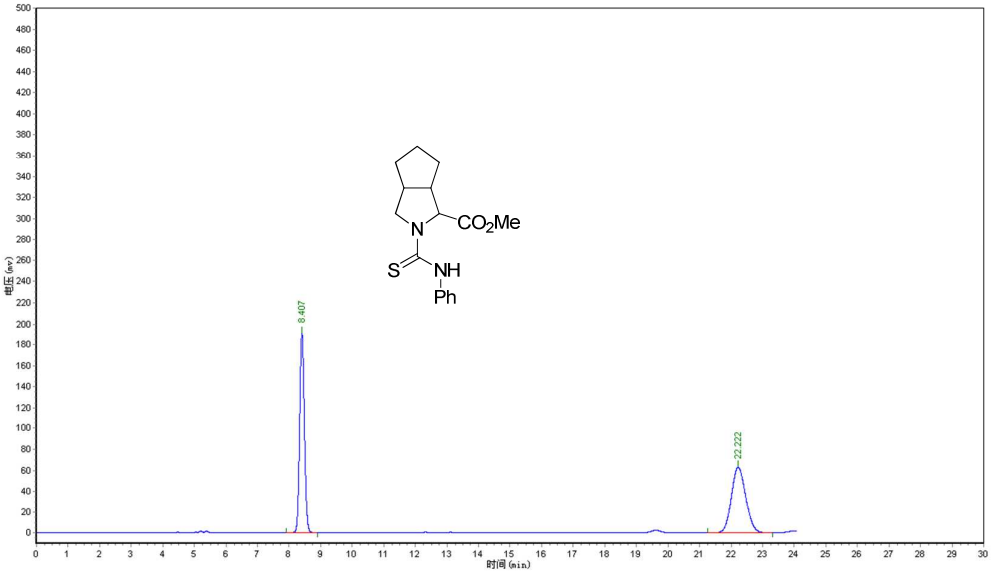


Peak	Rt(min)	Heigth(mV*sec)	Area(mV)	Area(%)
1	4.163	65466.191	107789.852	1.1472
2	4.243	4988.000	9198.400	0.0979
3	4.383	14434.000	26293.801	0.2798
4	4.483	6491.619	12893.100	0.1372
5	4.818	8993.241	19005.449	0.2023
6	5.158	2757.238	5642.250	0.0600
7	5.488	3100.213	8226.650	0.0876
8	6.718	8355.000	17980.699	0.1914
9	6.923	2905.667	7002.700	0.0745
10	8.278	35443.516	233721.406	2.4874
11	8.808	3175.542	31851.500	0.3390
12	11.833	949374.875	8903355.000	94.7549
13	13.543	1297.667	13230.500	0.1408

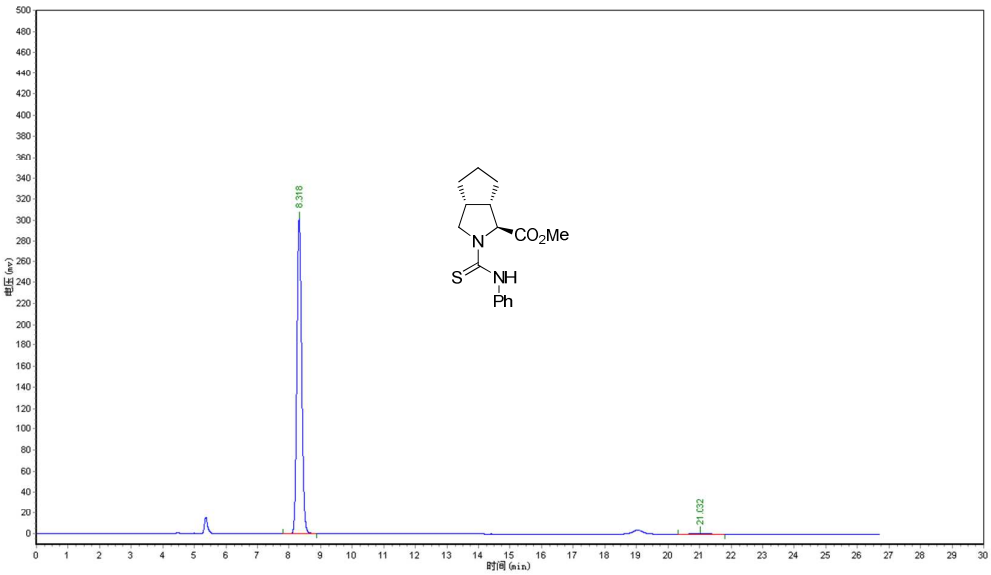
GC data of compound **7**

2. HPLC data of compound 10

Operational condition: Chiralpak AD-H column, n-hexane/ethanol = 70/30, flow rate 0.8 mL/min, 254 nm.

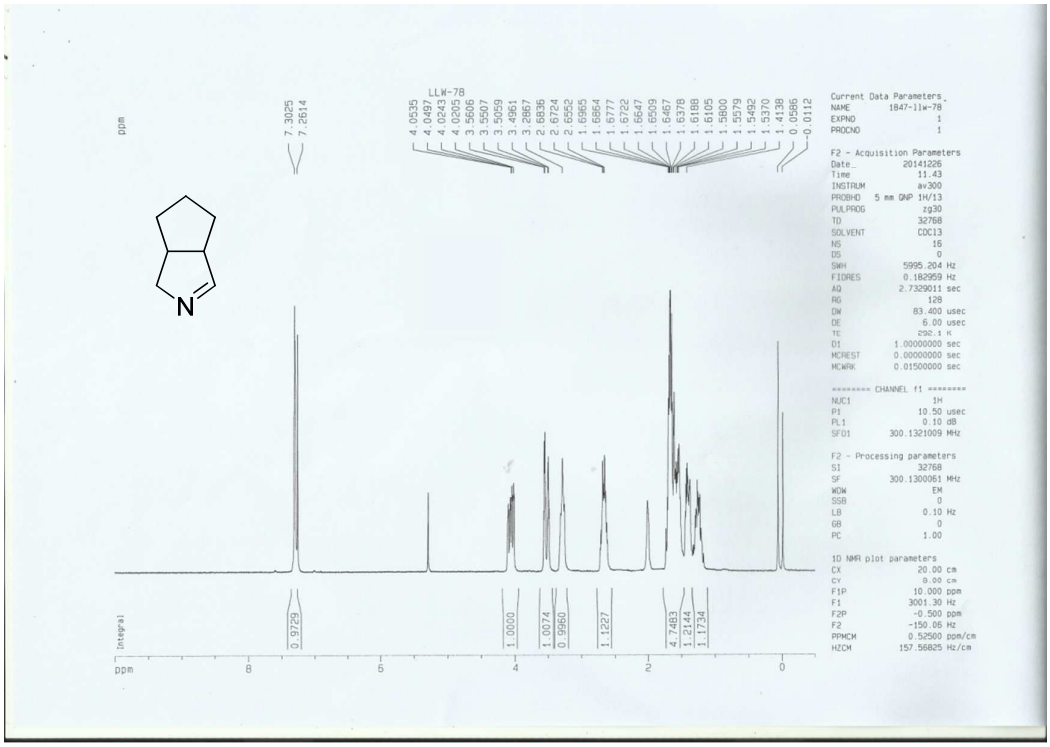


Peak	Rt(min)	Heigth(mV*sec)	Area(mV)	Area(%)
1	8.407	190890.031	1998661.750	50.1055
2	22.222	62866.004	1990248.125	49.8945

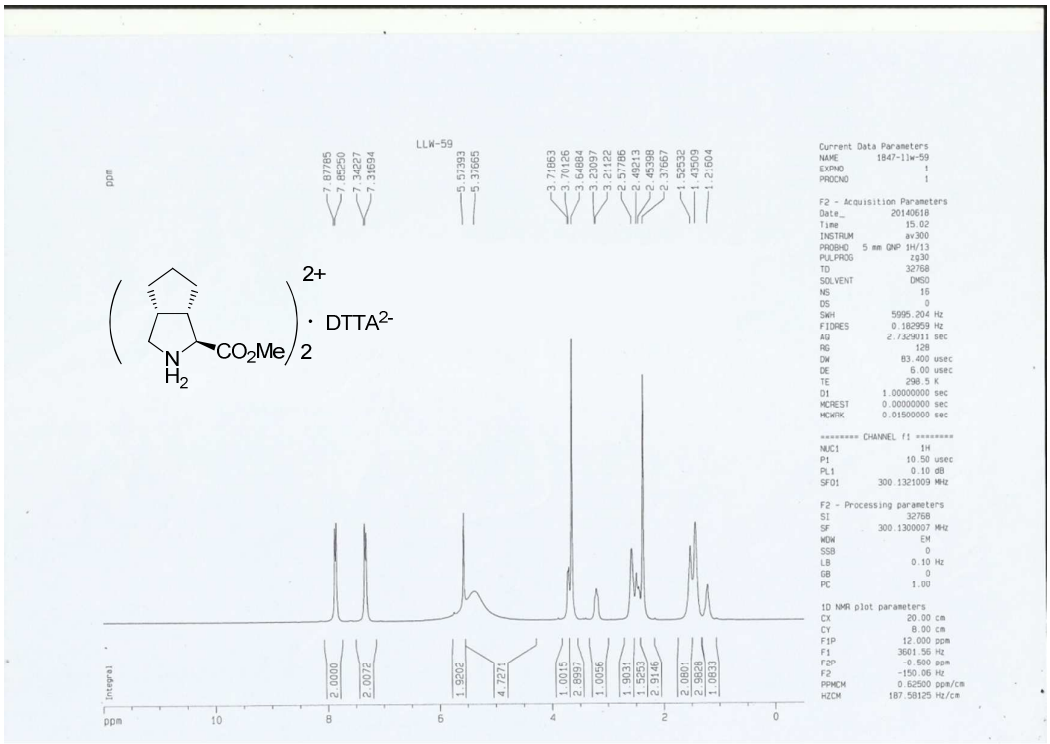


Peak	Rt(min)	Heigth(mV*sec)	Area(mV)	Area(%)
1	8.318	301127.875	3146880.500	99.6978
2	21.032	321.295	9537.851	0.3022

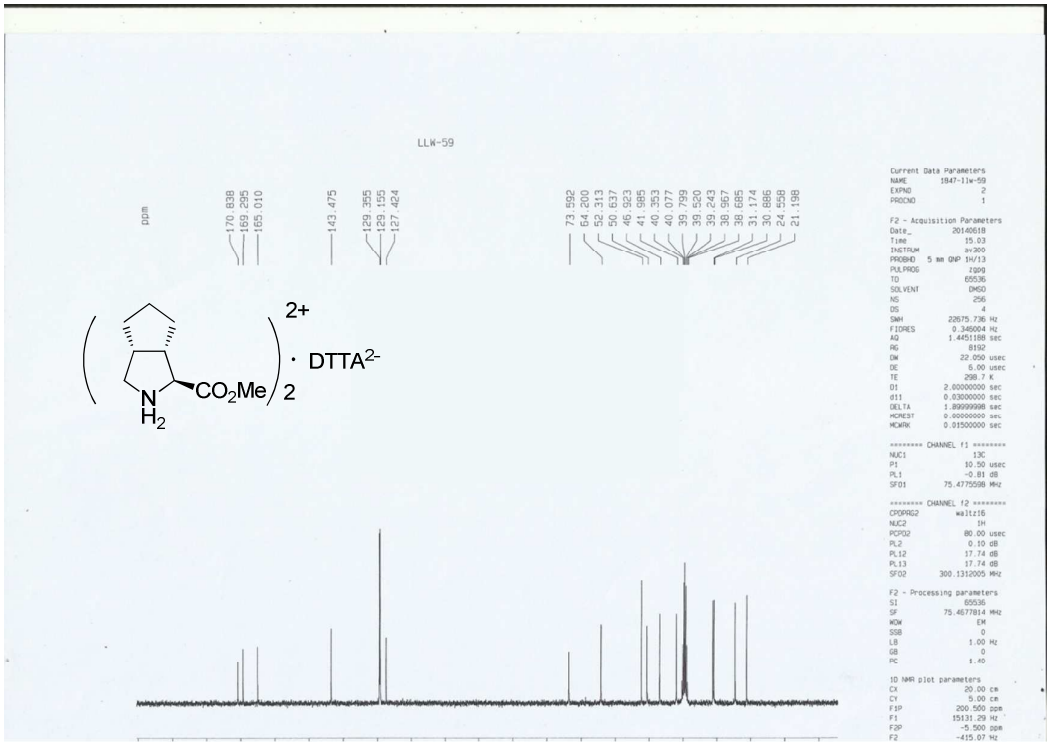
3. NMR data of compound 4, 8, 9, 10



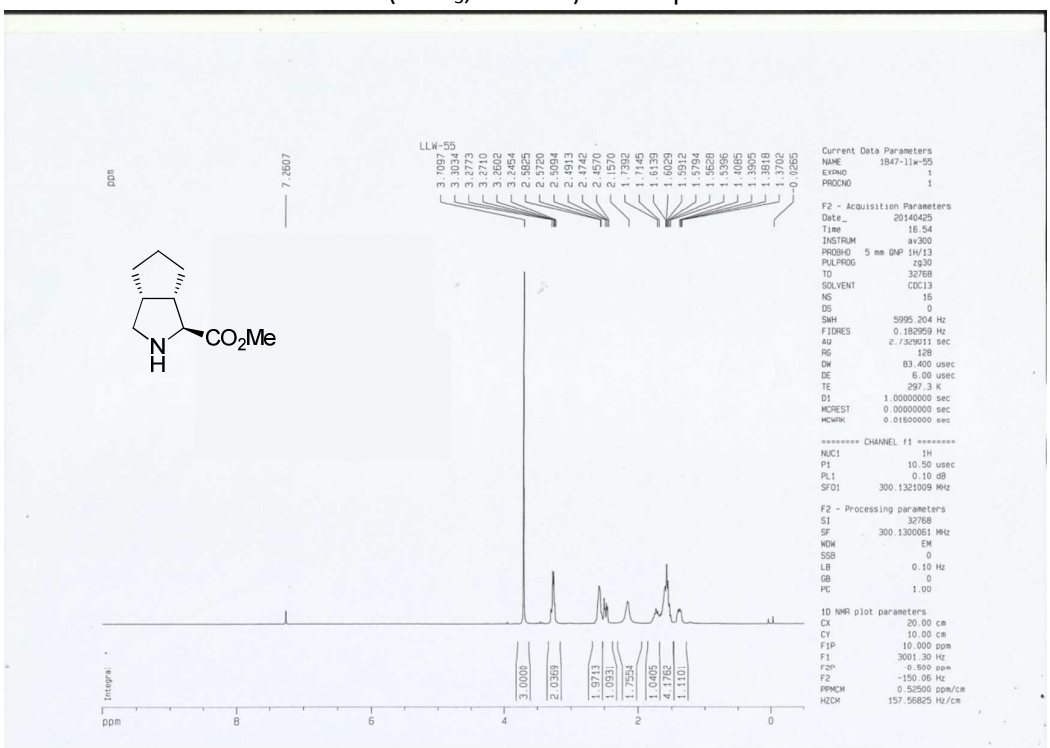
^{1}H NMR ($CDCl_3$, 300 MHz) of compound **4**



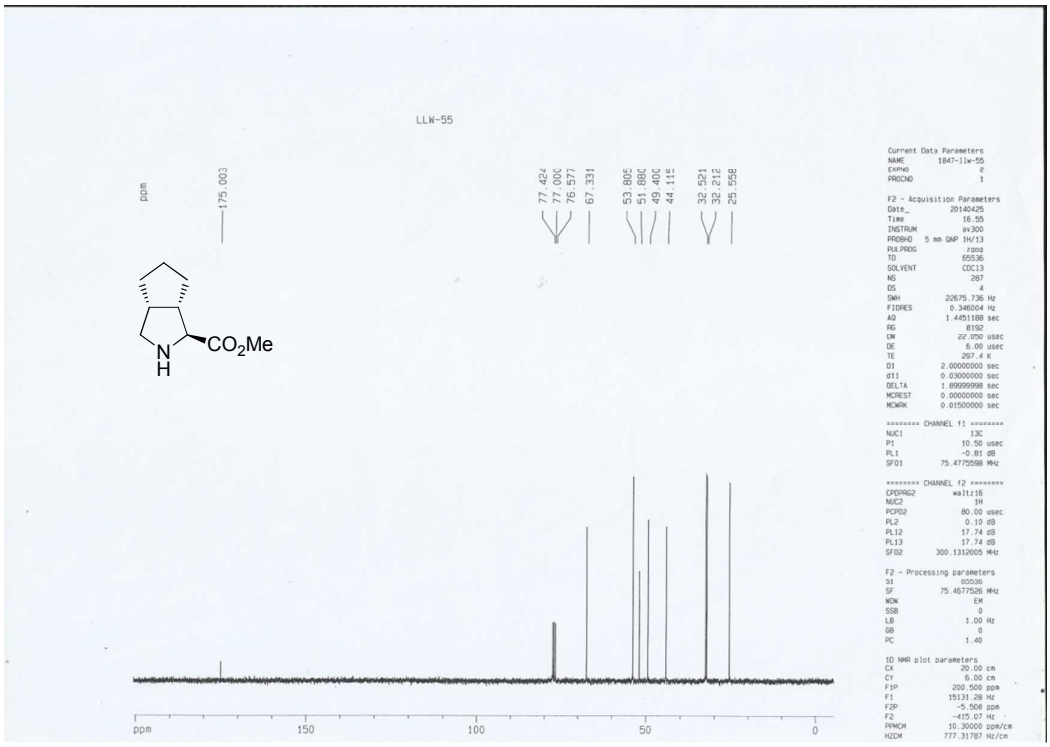
^{1}H NMR ($CDCl_3$, 300 MHz) of compound **8**



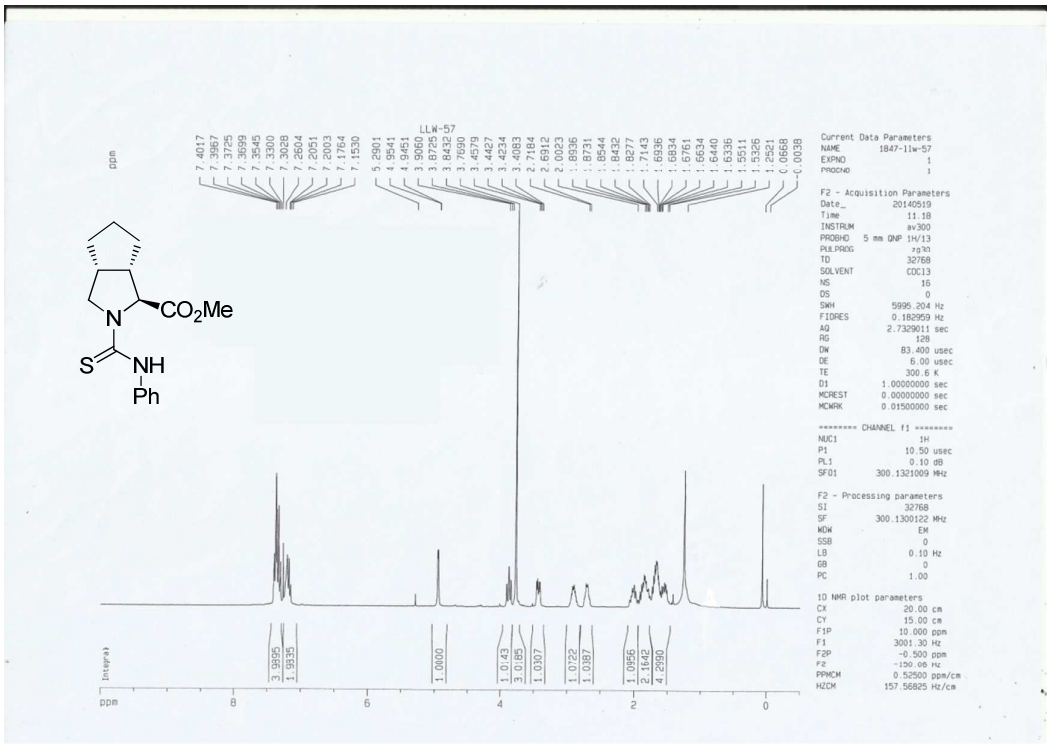
^{13}C NMR ($CDCl_3$, 75 MHz) of compound **8**



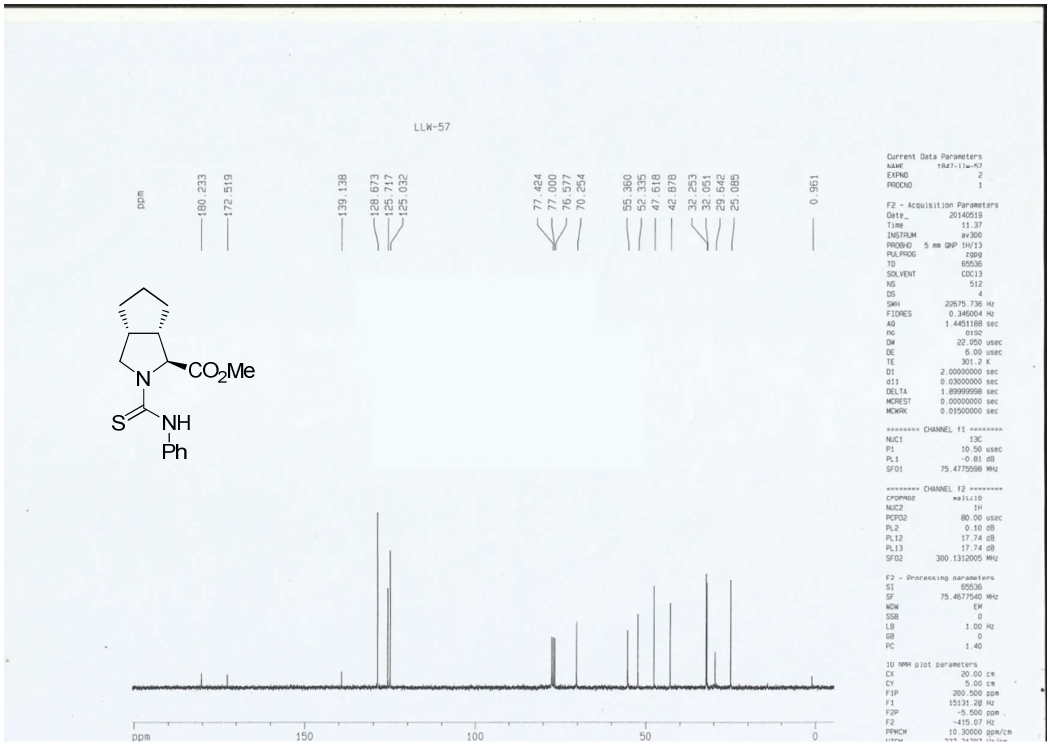
^{1}H NMR ($CDCl_3$, 300 MHz) of compound **9**



^{13}C NMR ($CDCl_3$, 75 MHz) of compound **9**



^{1}H NMR ($CDCl_3$, 300 MHz) of compound **10**



^{13}C NMR ($CDCl_3$, 75 MHz) of compound **10**

5. Mass spectrum of compound

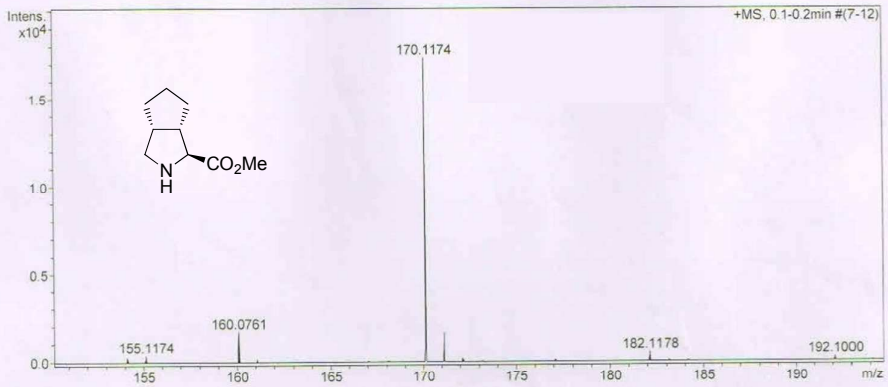
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\USER-2013\LLW-0.d	Acquisition Date	11/4/2013 3:47:10 PM
Method	lc-ms-20130131.m	Operator	Ma
Sample Name	LLW-0	Instrument / Ser#	micrOTOF-Q II 10203
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
170.1174	1	C 9 H 16 N O 2	100.00	170.1176	1.1	0.9	3.9	2.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 11/4/2013 5:30:45 PM Page 1 of 1

HRMS (ESI+): m/z 170 ($M+H^+$) (calculated for $C_9H_{16}NO_2$169)