Supporting Information

Electron-Rich Benzofulvenes as Effective Dipolarophiles in Copper(I)-Catalyzed Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides

Xin Chang, [1] Xue-Tao Liu,[1] Fangfang Li,[2] Yuhong Yang,[2] Lung Wa Chung,[2,*] and Chun-Jiang Wang[1,*]

[1]College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, China [2]Shenzhen Grubbs Institute, Department of Chemistry and Guangdong Provincial Key Laboratory of Catalysis, Southern University of Science and Technology, Shenzhen 518055, China

*E-mail: oscarchung@ sustech.edu.cn (L.W.C.); cjwang@whu.edu.cn (C.-J.W.)

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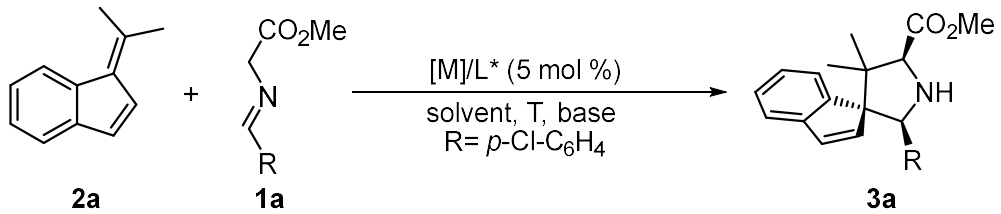
1. General Remarks

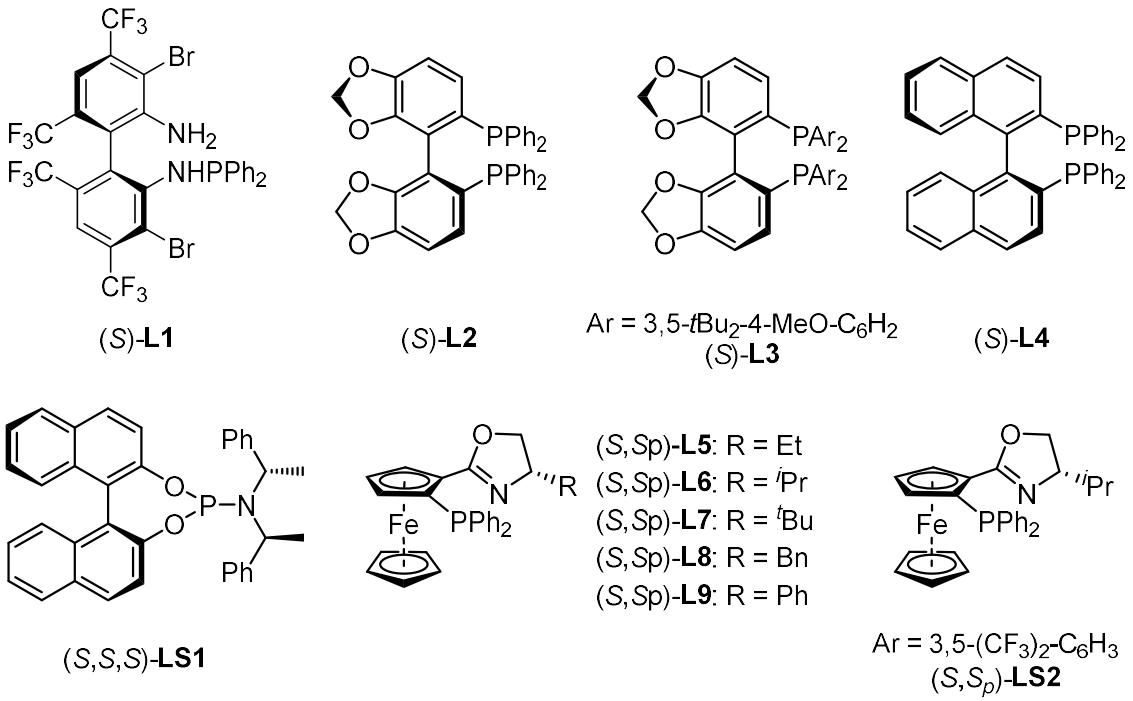
^{1}H NMR spectra were recorded on a Bruker 400 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. ^{13}C NMR spectra were recorded on a Bruker 101 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. ^{19}F NMR spectra were recorded on a Bruker 376 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal CF_3COOH signal at -76.55 ppm. The data are reported as (s = single, d = double, t = triple, q = quarter, m = multiple or unresolved, br s = broad single, coupling constant(s) in Hz, integration). High resolution mass spectra (HR-MS) were recorded on a LTQ-Orbitrap Elite mass spectrometer with MeOH as solvent mixture for the measurements. Commercially obtained reagents were used without further purification. Solvents were purified prior to use according to the standard methods. Unless otherwise noted, all reactions were carried out under nitrogen atmosphere. The enantiomeric excesses (ee) of the products were determined by high-performance liquid chromatography (HPLC) analysis performed on Agilent 1200 and 1260 Series chromatographs using a Diacel chiral column (25 cm). Optical rotations were measured on a Rudolph Research Analytical Autopol VI polarimeter with $[\alpha]_D$ values reported in degrees; concentration (c) is in g/100 mL. Benzofulvene **2a-2j** [1,2] were prepared according to the literature procedure. The imino ester **1a-1n** [3,4] was prepared according to the literature procedure. Known chiral ligands **L5-L9**, **LS2** were prepared according to the literature procedure. [5] Known chiral ligands **L1** [6] were prepared according to the literature procedure. Commercially available chiral ligands (**L2-L4**, **LS1**) were purchased and used without further purification.

2. Optimization of reaction conditions[a]



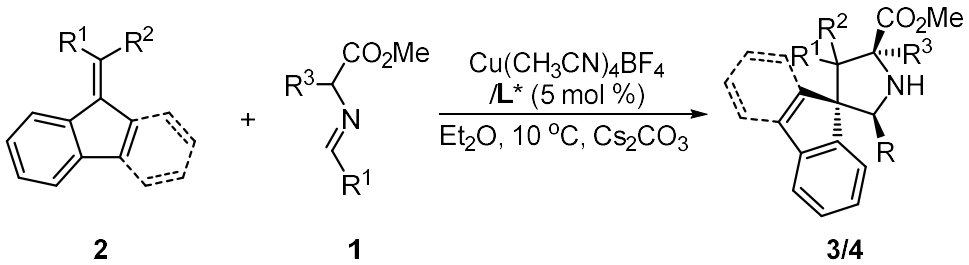
Entry	L*	M	Solvent	Base	T (°C)	Yield (%)[b]	dr[c]	Ee (%) [c]
1	**L1**	$CuBF_4$	DCM	Cs_2CO_3	25	5	--	--
2	**L2**	$CuBF_4$	DCM	Cs_2CO_3	25	88	9:1	40
3	**L3**	$CuBF_4$	DCM	Cs_2CO_3	25	40	5:1	85

4	**L4**	$CuBF_4$	DCM	Cs_2CO_3	25	93	7:1	20
5	**L5**	$CuBF_4$	DCM	Cs_2CO_3	25	29	11:1	89
6	**L6**	$CuBF_4$	DCM	Cs_2CO_3	25	98	16:1	87
7	**L7**	$CuBF_4$	DCM	Cs_2CO_3	25	56	7:1	85
8	**L8**	$CuBF_4$	DCM	Cs_2CO_3	25	93	15:1	89
9	**L9**	$CuBF_4$	DCM	Cs_2CO_3	25	98	12:1	87
10	**LS1**	$CuBF_4$	DCM	Cs_2CO_3	25	Trace	--	--
11	**LS2**	$CuBF_4$	DCM	Cs_2CO_3	25	52	5:1	91
12	**L6**	AgOAc	DCM	Cs_2CO_3	25	80	2:1	87
13	**L6**	$CuBF_4$	DCM	Cs_2CO_3	0	5	--	--
14	**L6**	$CuBF_4$	DCM	NEt_3	0	Trace	--	--
15	**L6**	$CuBF_4$	DCM	DBU	0	Trace	--	--
16	**L6**	$CuBF_4$	DCM	^{t}BuOK	0	50	20:1	95
17	**L6**	$CuBF_4$	DCM	Cs_2CO_3	10	76	14:1	96
18	**L6**	$CuBF_4$	DCE	Cs_2CO_3	10	77	20:1	87
19	**L6**	$CuBF_4$	THF	Cs_2CO_3	10	93	14:1	90
20	**L6**	$CuBF_4$	TFE	Cs_2CO_3	Trace			
21	**L6**	$CuBF_4$	CH_3CN	Cs_2CO_3	Trace			
22	**L6**	$CuBF_4$	MeOH	Cs_2CO_3	Trace			
23	**L6**	$CuBF_4$	Et_2O	Cs_2CO_3	10	81	16:1	96
24	**L6**	$CuBF_4$	Toluene	Cs_2CO_3	10	98	12:1	96
25	**L6**	CuI	Et_2O	Cs_2CO_3	25	72	19:1	96
26	**L6**	$CuPF_6$	Et_2O	Cs_2CO_3	25	45	17:1	31
27	**L6**	CuOTf1/2Ph	Et_2O	Cs_2CO_3	25	78	19:1	96
28	**L6**	CuOTf	Et_2O	Cs_2CO_3	Trace			
29	**L6**	CuOAc	Et_2O	Cs_2CO_3	25	36	18:1	95
30	**L6**	$Cu(OAc)_2$	Et_2O	Cs_2CO_3	25	74	19:1	93



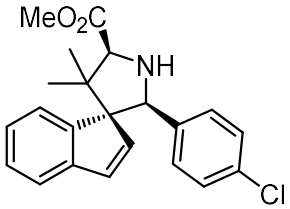
[a] All reactions were carried out with 0.4 mmol **1a** and 0.2 mmol **2a**, 0.01 mmol [M]/**L*** and 0.2 mmol of base in 2 mL of solvent for 24 h, $CuBF_4$ = $Cu(CH_3CN)_4BF_4$. [b]Yields refer to the isolated products after chromatographic purification. [c] The dr value was determined by the crude ^{1}H NMR, and the ee value was determined by HPLC analysis.

3. Typical Procedure for Cu(I)-Catalyzed 1,3-Dipolar Cycloaddition of Azomethine Ylide with Benzofulvenes



Under nitrogen atmosphere, (S,S_p)-**L6** (5.29 mg, 0.011 mmol) and $Cu(CH_3CN)_4BF_4$ (3.15 mg, 0.01 mmol) were dissolved in 2.0 mL Et_2O, which were stirred at room temperature for about 30 min. After the reaction temperature was dropped to 10 °C, the imino ester **1** (0.40 mmol) and Cs_2CO_3 (0.02 mmol) were added sequentially. Then, benzofulvenes **2** (0.2 mmol) was added. When the reaction completed (monitored by TLC), the organic solvent was removed and the residue was purified by column chromatography to give cycloadducts, which were then directly analyzed by chiral HPLC to determine the enantiomeric excess.

4. Spectral Characterization Data for the Products



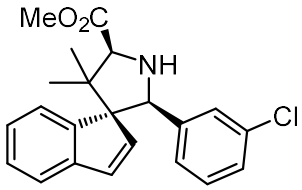
3a

Methyl (1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3a): Yield (59.5 mg, 81%); dr = 18:1; yellow solid; m.p. 60-62 ºC; $[\alpha]^{25}_{D}$ = -230.63 (*c* 0.79, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 242 nm); t_r = 7.25 and 8.87 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 6.4 Hz, 1H), 7.20 – 7.17 (m, 2H), 7.12 – 7.10 (m, 1H), 7.03 – 7.01 (m, 4H), 6.46 (d, *J* = 6.0 Hz, 1H), 6.36 (d, *J* = 6.0 Hz, 1H), 4.90 (s, 1H), 4.03 (s, 1H), 3.78 (s, 3H), 1.41 (s, 3H), 0.74 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 145.4, 144.3, 139.5, 137.7, 132.4, 130.2, 127.8, 127.4, 127.2, 124.8, 124.2, 121.2, 70.6, 70.2, 67.2, 51.7, 48.8, 29.7, 22.2.

HRMS (ESI+) Calcd. For $C_{22}H_{23}ClNO_2^+$ ($[M+H]^+$): 368.1412, found: 368.1413.



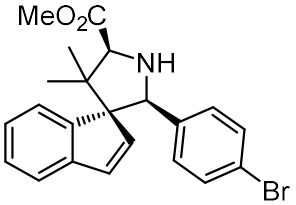
3b

Methyl (1*R*,2'*S*,5'*S*)-2'-(3-chlorophenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3b): Yield (49.2 mg, 67%); dr = 12:1; white solid; m.p. 130-132 ºC; $[\alpha]^{25}_{D}$ = -212.35 (*c* 0.51, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 95% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 242 nm); t_r = 7.81 and 11.21 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 6.4 Hz, 1H), 7.24 – 7.17 (m, 2H), 7.17 – 7.10 (m, 2H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.99 – 6.95 (m, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.44 (d, *J* = 5.6 Hz, 1H), 6.40 (d, *J* = 5.6 Hz, 1H), 4.91 (s, 1H), 4.05 (s, 1H), 3.82 (s, 3H), 1.40 (s, 3H), 0.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.7, 145.4, 144.5, 141.5, 139.5, 133.3, 130.4, 128.5, 127.3, 127.1, 126.7, 124.8, 124.7, 124.4, 121.3, 70.6, 70.3, 67.3, 51.9, 48.9, 29.6, 22.3.

HRMS (ESI+) Calcd. For $C_{22}H_{23}ClNO_2^+$ ([M+H]$^+$): 368.1412, found: 368.1408.



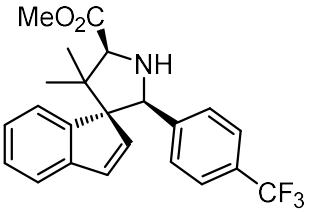
3c

Methyl (1*R*,2'*S*,5'*S*)-2'-(4-bromophenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3c): Yield (80.6 mg, 98%); dr = 20:1; yellow liquid; $[\alpha]^{25}_D$ = -213.43 (*c* 0.67, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.20 and 8.77 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 6.8 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.19 (dd, *J* =5.2 Hz, 2.0 Hz, 2H), 7.17 – 7.15 (m, 1H), 7.12 (dd, *J* = 7.2, 2.0Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.45 (d, *J* = 6.0 Hz, 1H), 6.38 (d, *J* = 6.0 Hz, 1H), 4.90 (s, 1H), 4.04 (s, 1H), 3.81 (s, 3H), 1.42 (s, 3H), 0.75 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 145.5, 144.3, 139.5, 138.2, 130.4, 130.3, 128.2, 127.3, 124.8, 124.3, 121.3, 120.7, 70.6, 70.3, 67.3, 51.8, 48.9, 29.8, 22.2.

HRMS (ESI+) Calcd. For $C_{22}H_{23}BrNO_2^+$ ([M+H]$^+$): 412.0907, found: 412.0904.



3d

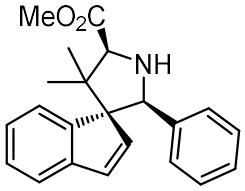
Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(4-(trifluoromethyl)phenyl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3d): Yield (77.0 mg, 96%); dr = 15:1; yellow solid; m.p. 86-88 ºC; $[\alpha]^{25}_D$ = -175.79 (*c* 0.57, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 98% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.71 and 7.77 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 6.4 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.23 – 7.18 (m, 4H), 7.13 (dd, *J* = 6.4, 2.0 Hz, 1H), 6.44 (d, *J* = 6.0 Hz, 1H), 6.37 (d, *J* = 6.0 Hz, 1H), 5.00 (s, 1H), 4.07 (s, 1H), 3.82 (s, 3H), 1.43 (s, 3H), 0.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 145.4, 144.3, 143.5, 139.1, 130.5, 129.0 (q, *J* = 32.0 Hz), 127.4, 126.8, 124.8, 124.4, 124.3 (q, *J* = 4.0 Hz), 124.2 (q, *J* = 270.0 Hz), 121.4, 70.6, 70.3, 67.3, 51.9, 49.0, 29.7, 22.2.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -62.36.

HRMS (ESI+) Calcd. For $C_{23}H_{23}F_3NO_2^+$ ($[M+H]^+$): 402.1675, found: 402.1677.



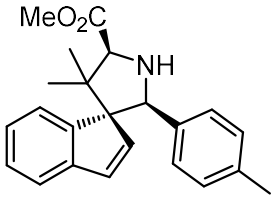
3e

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-phenylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3e): Yield (47.3 mg, 71%); dr = 10:1; yellow solid; m.p. 110-112 ºC; $[\alpha]^{25}_D$ = -170.29 (*c* 1.03, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.64 and 9.79 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 6.4 Hz, 1H), 7.22 – 7.16 (m, 2H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.09 – 7.06 (m, 5H), 6.45 (d, *J* = 6.0 Hz, 1H), 6.37 (d, *J* = 6.0 Hz, 1H), 4.94 (s, 1H), 4.04 (s, 1H), 3.81 (s, 3H), 1.41 (s, 3H), 0.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 145.4, 144.8, 139.8, 138.9, 130.0, 127.3, 127.1, 126.9, 126.5, 124.8, 124.2, 121.1, 71.0, 70.5, 67.9, 51.8, 49.1, 29.7, 22.3.

HRMS (ESI+) Calcd. For $C_{22}H_{24}BrNO_2^+$ ($[M+H]^+$): 334.1802, found: 334.1805.



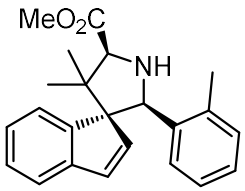
3f

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(p-tolyl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3f): Yield (61.1 mg, 88%); dr = 15:1; yellow semisolid; $[\alpha]^{25}_D$ = -135.82 (*c* 1.65, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 92% ee (Chiralpak AS-H, *i*-propanol/hexane = 1/99, flow rate 0.7 mL/min, λ = 254 nm); t_r = 11.57 and 15.92 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 6.4 Hz, 1H), 7.23 – 7.16 (m, 2H), 7.12 (dd, *J* = 7.2, 2.4 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 2H), 6.45 (d, *J* = 6.0 Hz, 1H), 6.39 (d, *J* = 6.0 Hz, 1H), 4.90 (s, 1H), 4.03 (s, 1H), 3.82 (s, 3H), 2.20 (s, 3H), 1.40 (s, 3H), 0.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 145.4, 144.9, 139.9, 136.5, 135.8, 130.0, 128.1, 127.0, 126.4, 124.8, 124.2, 121.1, 71.1, 70.5, 67.8, 51.9, 49.2, 29.8, 22.4, 21.0.

HRMS (ESI+) Calcd. For $C_{23}H_{26}NO_2^+$ ($[M+H]^+$): 348.1958, found: 348.1960.



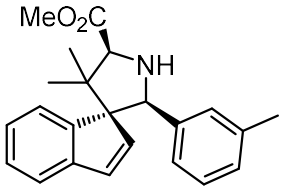
3g

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(o-tolyl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3g): Yield (52.8 mg, 76%); dr = 20:1; yellow semisolid; m.p. 120-122 °C; $[\alpha]^{25}_D$ = -97.391 (*c* 0.69, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.15 and 7.41 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.22 – 7.14 (m, 4H), 7.08 – 7.03 (m, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.47 (d, *J* = 6.0 Hz, 1H), 6.10 (d, *J* = 6.0 Hz, 1H), 5.16 (s, 1H), 4.22 (s, 1H), 3.82 (s, 3H), 1.67 (s, 3H), 1.02 (s, 3H), 0.92 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.7, 149.2, 143.8, 140.1, 139.7, 136.4, 130.4, 130.1, 126.9, 126.6, 126.3, 125.4, 124.6, 124.0, 121.2, 70.1, 63.0, 51.8, 49.1, 29.7, 25.2, 23.9, 19.7.

HRMS (ESI+) Calcd. For $C_{23}H_{26}NO_2^+$ ($[M+H]^+$): 348.1958, found: 348.1954.



3h

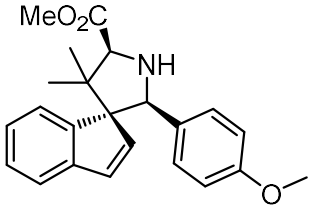
Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(m-tolyl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3h): Yield (50.0 mg, 72%); dr = 15:1; yellow solid; m.p. 100-102 °C; $[\alpha]^{25}_D$ = -218.33 (*c* 0.66, $CHCl_3$); The

product was analyzed by HPLC to determine the enantiomeric excess: 91% ee (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.34 and 7.77 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (dd, *J* = 6.4, 2.0 Hz, 1H), 7.22 – 7.15 (m, 2H), 7.12 (dd, *J* = 6.4, 2.0 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.92 – 6.88 (m, 2H), 6.81 (d, *J* = 7.6 Hz, 1H), 6.43 (d, *J* = 5.6 Hz, 1H), 6.39 (d, *J* = 5.6 Hz, 1H), 4.90 (s, 1H), 4.04 (s, 1H), 3.82 (s, 3H), 2.17 (s, 3H), 1.40 (s, 3H), 0.77 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 145.4, 145.0, 139.8, 138.8, 136.9, 130.0, 127.7, 127.22, 127.16, 127.1, 124.8, 124.2, 123.5, 121.1, 71.0, 70.5, 67.8, 51.8, 49.1, 29.7, 22.4, 21.4.

HRMS (ESI+) Calcd. For $C_{23}H_{26}NO_2^+$ ($[M+H]^+$): 348.1958, found: 348.1955.



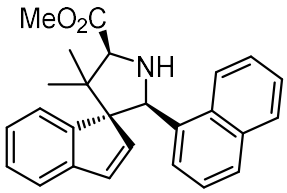
3i

Methyl (1*R*,2'*S*,5'*S*)-2'-(4-methoxyphenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3i): Yield (57.4 mg, 79%); dr = 18:1; yellow solid; m.p. 88-100 °C; $[\alpha]^{25}_D$ = -252.35 (*c* 1.02, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.47 and 12.37 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.22 – 7.15 (m, 2H), 7.11 (dd, *J* = 7.2, 2.0 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.61 (d, *J* = 8.8 Hz, 2H), 6.47 (d, *J* = 5.6 Hz, 1H), 6.39 (d, *J* = 5.6 Hz, 1H), 4.89 (s, 1H), 4.02 (s, 1H), 3.81 (s, 3H), 3.68 (s, 3H), 1.41 (s, 3H), 0.75 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 158.4, 145.5, 144.8, 139.9, 130.9, 130.0, 127.6, 127.0, 124.8, 124.1, 121.1, 112.7, 71.0, 70.5, 67.6, 55.0, 51.8, 49.1, 29.9, 22.4.

HRMS (ESI+) Calcd. For $C_{23}H_{26}NO_3^+$ ($[M+H]^+$): 364.1907, found: 364.1910.



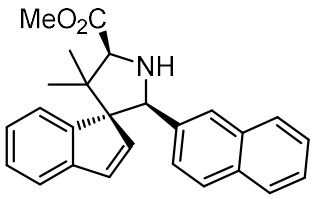
3j

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(naphthalen-1-yl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3j): Yield (42.9 mg, 56%); dr = 7:1; yellow solid; m.p. 160-162 ºC; $[\alpha]^{25}_{D}$ = -57.667 (*c* 0.60, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.03 and 11.69 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.51 – 7.47 (m, 1H), 7.32 – 7.26 (m, 3H), 7.21 – 7.16 (m, 1H), 7.01 (d, *J* = 3.2 Hz, 2H), 6.31 (d, *J* = 6.0 Hz, 1H), 5.78 (d, *J* = 6.0 Hz, 1H), 5.64 (s, 1H), 4.40 (s, 1H), 3.84 (s, 3H), 1.11 (s, 3H), 0.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.5, 150.4, 143.7, 140.0, 138.9, 133.4, 131.7, 130.9, 128.2, 127.4, 127.1, 125.23, 125.15, 125.0, 124.8, 124.0, 123.7, 121.4, 70.1, 69.8, 61.9, 51.8, 48.9, 24.2, 23.6.

HRMS (ESI+) Calcd. For $C_{26}H_{26}NO_2^+$ ($[M+H]^+$): 384.1958, found: 384.1957.



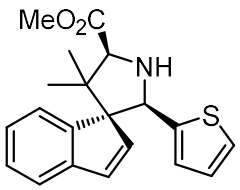
3k

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-(naphthalen-2-yl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3k): Yield (75.1 mg, 98%); dr = 10:1; yellow semisolid; $[\alpha]^{25}_{D}$ = -342.59 (*c* 1.08, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 95% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.96 and 13.84 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.65 (m, 3H), 7.60 – 7.56 (m, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.23 – 7.18 (m, 2H), 7.10 – 7.03 (m, 2H), 6.47 (d, *J* = 5.6 Hz, 1H), 6.32 (d, *J* = 5.6 Hz, 1H), 5.09 (s, 1H), 4.10 (s, 1H), 3.83 (s, 3H), 1.41 (s, 3H), 0.80 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 145.4, 145.1, 139.7, 136.9, 132.8, 132.6, 130.2, 127.9, 127.4, 127.1, 126.7, 125.6, 125.4, 125.2, 124.9, 124.8, 124.3, 121.2, 71.0, 70.5, 67.8, 51.9, 49.1, 29.5, 22.4.

HRMS (ESI+) Calcd. For $C_{26}H_{26}NO_2^+$ ($[M+H]^+$): 384.1958, found: 384.1956.



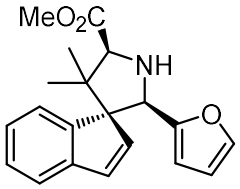
3l

Methyl (1*R*,2'*R*,5'*S*)-4',4'-dimethyl-2'-(thiophen-2-yl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3l): Yield (66.5 mg, 98%); dr = 15:1; yellow solid; m.p. 90-92 ºC; $[\alpha]^{25}_{D}$ = -136.11 (*c* 0.95, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 12.54 and 16.08 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (d, *J* = 7.2 Hz, 1H), 7.18 – 7.17 (m, 1H), 7.15 – 7.08 (m, 2H), 6.90 (dd, *J* = 4.8, 1.2 Hz, 1H), 6.65 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.50 – 6.39 (m, 3H), 5.06 (s, 1H), 3.93 (s, 1H), 3.72 (s, 3H), 1.35 (s, 3H), 0.69 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 145.8, 143.9, 142.5, 139.5, 130.8, 127.4, 126.0, 124.8, 124.4, 123.3, 123.2, 121.3, 71.0, 70.6, 64.2, 51.9, 49.3, 30.1, 22.2.

HRMS (ESI+) Calcd. For $C_{20}H_{22}NO_2S^+$ ($[M+H]^+$): 340.1366, found: 340.1362.



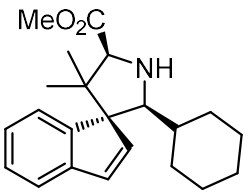
3m

Methyl (1*R*,2'*R*,5'*S*)-2'-(furan-2-yl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3m): Yield (37.5 mg, 58%); dr = 9:1; yellow solid; m.p. 80-82 ºC; $[\alpha]^{25}_{D}$ = -60.333 (*c* 2.10, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 86% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.22 and 9.42 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, *J* = 7.2 Hz, 1H), 7.25 – 7.14 (m, 4H), 6.55 (d, *J* = 5.6 Hz, 1H), 6.33 (d, *J* = 5.6 Hz, 1H), 6.16 (dd, *J* = 3.2, 1.6 Hz, 1H), 5.92 (d, *J* = 3.2 Hz, 1H), 4.80 (s, 1H), 4.05 (s, 1H), 3.81 (s, 3H), 1.14 (s, 3H), 0.91 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.8, 153.0, 146.5, 144.5, 141.4, 138.9, 130.7, 127.1, 124.7, 124.0, 121.2, 109.9, 106.4, 71.2, 70.8, 62.5, 52.0, 49.2, 27.3, 22.5.

HRMS (ESI+) Calcd. For $C_{20}H_{22}NO_3^+$ ($[M+H]^+$): 324.1594, found: 324.1594.



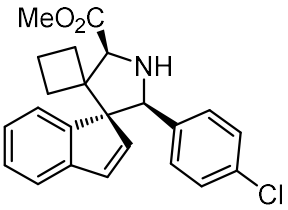
3n

Methyl (1*R*,2'*S*,5'*S*)-2'-cyclohexyl-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (3n): Yield (48.8 mg, 72%); dr = 20:1; yellow semisolid; $[\alpha]^{25}_{D}$ = 37.538 (*c* 2.64, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak OJ, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.11 and 6.20 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.18 (m, 2H), 7.12 – 7.06 (m, 1H), 6.68 (d, *J* = 6.0 Hz, 1H), 6.57 (d, *J* = 6.0 Hz, 1H), 3.78 (s, 1H), 3.76 (s, 3H), 3.49 (d, *J* = 8.8 Hz, 1H), 2.01 – 1.96 (m, 1H), 1.68 – 1.62 (m, 1H), 1.50 – 1.44 (m, 1H), 1.34 (s, 3H), 1.29 – 1.24 (m, 2H), 1.16 – 1.08 (m, 1H), 1.05 – 0.94 (m, 2H), 0.87 – 0.81 (m, 1H), 0.59 (s, 3H), 0.54 – 0.47 (m, 1H), 0.34 – 0.23 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 145.9, 145.0, 139.8, 130.2, 126.8, 124.9, 123.8, 121.3, 70.5, 70.0, 69.3, 51.9, 50.2, 41.3, 31.8, 30.8, 30.0, 26.2, 26.02, 25.96, 21.5.

HRMS (ESI+) Calcd. For $C_{22}H_{30}NO_2^+$ ($[M+H]^+$): 340.2271, found: 340.2271.



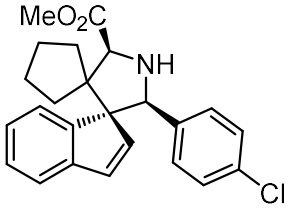
4a

Methyl (2'*S*,4'*R*,5'*S*)-5'-(4-chlorophenyl)dispiro[cyclobutane-1,3'-pyrrolidine-4',1''-indene]-2'-carboxylate (4a): Yield (74.3 mg, 98%); dr = 12:1; yellow semisolid; $[\alpha]^{25}_{D}$ = -114.52 (*c* 0.73, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.58 and 9.45 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 6.4 Hz, 1H), 7.18 – 7.14 (m, 2H), 7.14 – 7.09 (m, 1H), 7.01 – 6.96 (m, 4H), 6.46 (d, *J* = 5.6 Hz, 1H), 6.23 (d, *J* = 5.6 Hz, 1H), 4.56 (s, 1H), 4.33 (s, 1H), 3.80 (s, 3H), 2.22 – 2.13 (m, 1H), 2.11 – 1.98 (m, 1H), 1.80 – 1.69 (m, 1H), 1.66 – 1.58 (m, 1H), 1.43 – 1.36 (m, 1H), 1.34 – 1.25 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 145.2, 138.3, 137.7, 132.6, 131.5, 128.0, 127.6, 127.3, 124.7, 124.1, 121.4, 70.4, 67.2, 54.7, 52.1, 33.5, 27.8, 16.1.

HRMS (ESI+) Calcd. For $C_{23}H_{23}ClNO_2^+$ ($[M+H]^+$): 380.1412, found: 380.1408.



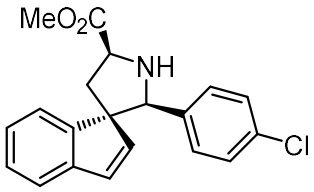
4b

Methyl (2'*S*,4'*R*,5'*S*)-5'-(4-chlorophenyl)dispiro[cyclopentane-1,3'-pyrrolidine-4',1''-indene]-2'-carboxylate (4b): Yield (45.6 mg, 58%); dr = 20:1; yellow solid; m.p. 50-52 ºC; $[\alpha]^{25}_D$ = -144.70 (*c* 1.10, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.41 and 10.30 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 6.4 Hz, 1H), 7.24 – 7.17 (m, 2H), 7.15 – 7.09 (m, 1H), 7.04 – 6.99 (m, 4H), 6.59 (d, *J* = 5.6 Hz, 1H), 6.39 (d, *J* = 5.6 Hz, 1H), 4.87 (s, 1H), 4.05 (s, 1H), 3.82 (s, 3H), 2.07 – 2.01 (m, 1H), 1.89 – 1.82 (m, 1H), 1.74 – 1.61 (m, 2H), 1.54 – 1.45 (m, 1H), 1.28 – 1.23 (m, 2H), 0.91 – 0.85 (m, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.4, 145.9, 143.9, 139.5, 137.3, 132.6, 130.2, 128.1, 127.4, 127.3, 125.2, 124.2, 121.3, 70.5, 69.5, 68.3, 60.5, 51.9, 38.9, 31.2, 23.7, 22.4.

HRMS (ESI+) Calcd. For $C_{24}H_{25}ClNO_2^+$ ($[M+H]^+$): 394.1568, found: 394.1566.



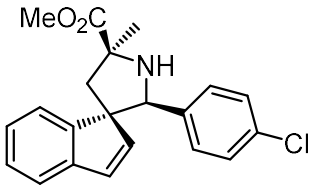
4c

Methyl (1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)spiro[indene-1,3'-pyrrolidine]-5'-carboxylate (4c): Yield (66.5 mg, 98%); dr = 5:1; yellow liquid; $[\alpha]^{25}_D$ = -246.01 (*c* 1.43, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 88% ee (Chiralpak ID, *i*-propanol/hexane = 1/99, flow rate 1.0 mL/min, λ = 254 nm); t_r = 23.79 and 36.04 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.17 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.40 (d, *J* = 5.6 Hz, 1H), 6.27 (d, *J* = 5.6 Hz, 1H), 4.72 (s, 1H), 4.33 (dd, *J* = 10.0, 4.4 Hz, 1H), 3.83 (s, 3H), 2.75 (dd, *J* = 13.2, 10.0 Hz, 1H), 2.34 (dd, *J* = 13.2, 4.4 Hz 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.2, 147.0, 144.2, 139.8, 137.0, 132.8, 130.1, 127.7, 127.4, 127.3, 125.4, 121.44, 121.39, 69.8, 63.1, 58.3, 52.4, 39.1.

HRMS (ESI+) Calcd. For $C_{20}H_{19}ClNO_2^+$ ($[M+H]^+$): 340.1099, found: 340.1099.



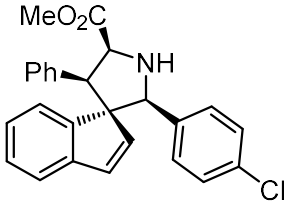
4d

Methyl (1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)-5'-methylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (4d): Yield (62.9 mg, 89%); dr = 6:1; yellow solid; m.p. 64-66 ºC; $[\alpha]^{25}_D$ = -376.39 (*c* 0.83, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (Chiralpak IE, *i*-propanol/hexane = 1/99, flow rate 0.7 mL/min, λ = 254 nm); t_r = 12.77 and 14.27 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 6.8 Hz, 1H), 7.27 – 7.20 (m, 2H), 7.14 (d, *J* = 6.8 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 6.37 (d, *J* = 5.6 Hz, 1H), 6.33 (d, *J* = 5.6 Hz, 1H), 4.84 (s, 1H), 3.83 (s, 3H), 2.62 (d, *J* = 13.6 Hz, 1H), 2.50 (d, *J* = 13.6 Hz, 1H), 1.70 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 177.7, 145.9, 144.2, 139.1, 136.3, 132.6, 130.2, 127.8, 127.6, 127.3, 127.1, 125.3, 121.3, 69.0, 65.0, 64.2, 52.7, 47.6, 28.0.

HRMS (ESI+) Calcd. For $C_{21}H_{21}ClNO_2^+$ ($[M+H]^+$): 354.1255, found: 354.1255.



4e

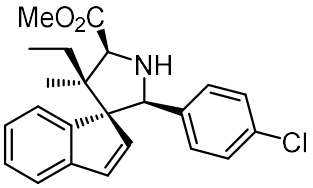
Methyl (1*S*,2'*S*,4'*R*,5'*S*)-2'-(4-chlorophenyl)-4'-phenylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (4e): Yield (81.4 mg, 98%); dr = 2:1; yellow liquid; $[\alpha]^{25}_D$ = -107.60 (*c* 0.96, $CHCl_3$); The product was

analyzed by HPLC to determine the enantiomeric excess: 85% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 242 nm); t_r = 14.05 and 19.84 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.16 (m, 2H), 7.16 – 6.99 (m, 8H), 6.99 – 6.94 (m, 2H), 6.94 – 6.84 (m, 1H), 6.44 (d, *J* = 5.6 Hz, 1H), 6.20 (d, *J* = 5.6 Hz, 1H), 4.81 (s, 1H), 4.62 (d, *J* = 8.8 Hz, 1H), 3.98 (d, *J* = 8.8 Hz, 1H), 3.72 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 146.8, 143.4, 138.8, 137.7, 132.6, 131.6, 128.4, 128.2, 128.0, 127.4, 126.9, 124.8, 124.2, 120.8, 68.7, 66.6, 64.8, 55.7, 52.3.

HRMS (ESI+) Calcd. For $C_{26}H_{23}ClNO_2^+$ ($[M+H]^+$): 416.1412, found: 416.1408.



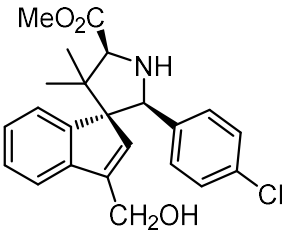
4f

Methyl (1*R*,2'*S*,4'*R*,5'*S*)-2'-(4-chlorophenyl)-4'-ethyl-4'-methylspiro[indene-1,3'-pyrrolidine]-5'-carboxylate (4f): Yield (56.4 mg, 74%); dr = 5:1; yellow solid; m.p. 88-90 ºC; $[\alpha]^{25}_D$ = -252.31 (*c* 0.78, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (Chiralpak AS-H, *i*-propanol/hexane = 1/99, flow rate 0.5 mL/min, λ = 254 nm); t_r = 16.83 and 24.08 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, *J* = 6.8 Hz, 1H), 7.15 – 7.07 (m, 2H), 7.03 (dd, *J* = 6.8, 1.6 Hz, 1H), 6.95 – 6.84 (m, 4H), 6.45 (d, *J* = 5.6 Hz, 1H), 6.26 (d, *J* = 5.6 Hz, 1H), 4.80 (s, 1H), 4.09 (s, 1H), 3.73 (s, 3H), 2.06 (q, *J* = 6.8 Hz, 1H), 1.66 (q, *J* = 6.8 Hz, 1H), 0.85 (t, *J* = 6.8 Hz, 3H), 0.64 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 145.8, 143.9, 140.3, 137.2, 132.5, 129.9, 127.9, 127.4, 127.2, 125.5, 124.1, 121.3, 71.4, 67.4, 66.3, 52.4, 51.9, 32.8, 17.8, 8.9.

HRMS (ESI+) Calcd. For $C_{23}H_{25}ClNO_2^+$ ($[M+H]^+$): 382.1568, found: 382.1567.



4g

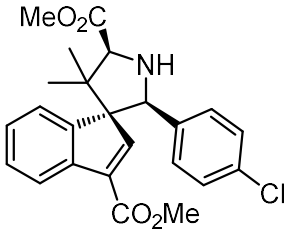
Methyl (1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)-3-(hydroxymethyl)-4',4'-dimethylspiro[indene-1,3'-pyrroli

dine]-5'-carboxylate (4g): Yield (41.0 mg, 55%); dr = 20:1; yellow semisolid; $[\alpha]^{25}_{D}$ = -233.8 (*c* 1.1, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 98% ee (Chiralpak OD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 11.59 and 15.28 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (dd, *J* = 6.4, 2.0 Hz, 1H), 7.19 – 7.13 (m, 2H), 7.12 – 7.06 (m, 1H), 6.93 (d, *J* = 2.8 Hz, 4H), 6.29 (s, 1H), 4.82 (s, 1H), 4.29 (d, *J* = 1.6 Hz, 2H), 3.96 (s, 1H), 3.73 (s, 3H), 1.35 (s, 3H), 0.69 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 145.1, 143.9, 142.3, 137.6, 135.0, 132.5, 127.8, 127.4, 127.3, 124.9, 124.8, 119.7, 70.2, 69.3, 67.5, 59.1, 51.9, 49.0, 29.8, 22.3.

HRMS (ESI+) Calcd. For $C_{23}H_{25}ClNO_3^+$ ($[M+H]^+$): 398.1517, found: 398.1516.



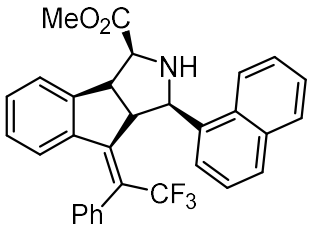
4h

Dimethyl (1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidine]-3,5'-dicarboxylate (4h): Yield (63.0 mg, 74%); dr = 7:1; yellow semisolid; $[\alpha]^{25}_{D}$ = 26.6 (*c* 0.5, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 11% ee (Chiralpak AS-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 242 nm); t_r = 11.01 and 13.83 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.53 (d, *J* = 6.4 Hz, 1H), 7.43 (s, 1H), 7.34 – 7.27 (m, 2H), 7.05 – 7.00 (m, 4H), 4.94 (s, 1H), 4.06 (s, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 1.45 (s, 3H), 0.75 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 163.9, 150.2, 143.9, 141.3, 136.6, 133.5, 132.9, 127.8, 127.7, 125.3, 124.9, 122.7, 70.2, 70.0, 67.8, 52.0, 51.5, 49.8, 30.1, 22.2.

HRMS (ESI+) Calcd. For $C_{24}H_{25}ClNO_4^+$ ($[M+H]^+$): 426.1466, found: 426.1466.



4i

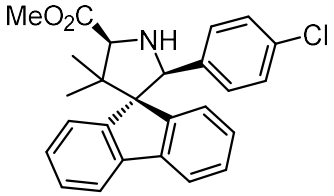
Methyl (1*R*,3*S*,3a*R*,8a*S*,E)-1-(naphthalen-1-yl)-8-(2,2,2-trifluoro-1-phenylethylidene)-1,2,3,3a,8,8a-hexahydroindeno[1,2-c]pyrrole-3-carboxylate (4i):Yield (72.0 mg, 70%); dr = 20:1; yellow semisolid; $[\alpha]^{25}_{D}$ = 8.27 (*c* 1.1, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak OD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 24.81 and 31.38 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 9.6 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.38 – 7.34 (m, 1H), 7.33 – 7.29 (m, 2H), 7.26 – 7.21 (m, 3H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 6.8 Hz, 1H), 6.88 (t, *J* = 8.0 Hz, 2H), 5.83 (d, *J* = 8.0 Hz, 1H), 5.54 (d, *J* = 9.6 Hz, 1H), 4.55 – 4.49 (m, 1H), 4.34 – 4.30 (m, 2H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 146.5, 145.1, 141.8, 134.6, 134.2, 133.7, 132.3, 130.4, 129.9, 129.3, 129.0, 128.70, 128.67, 128.4, 128.3, 127.5, 126.9, 125.8, 125.3, 124.5, 124.3, 123.8 (q, *J* = 30.3 Hz), 123.3 (q, *J* = 272.7 Hz), 64.6, 60.7, 51.9, 51.3, 51.2.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -59.51.

HRMS (ESI+) Calcd. For $C_{31}H_{25}F_3NO_2^+$ ($[M+H]^+$): 500.1831, found: 500.1829.



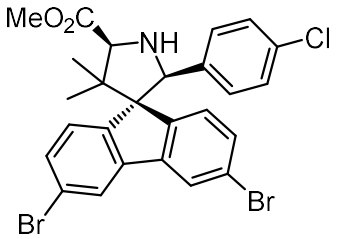
4j

Methyl (2'*S*,5'*S*)-2'-(4-chlorophenyl)-4',4'-dimethylspiro[fluorene-9,3'-pyrrolidine]-5'-carboxylate (4j): Yield (76.7 mg, 92%); dr > 20:1; white semisolid; $[\alpha]^{25}_{D}$ = -37.72 (*c* 0.79, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 98% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.33 and 13.14 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.65 (m, 2H), 7.60 (dd, *J* = 6.8, 1.6 Hz, 1H), 7.47 (d, *J* = 6.8 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.19 – 7.14 (m, 1H), 7.12 – 7.04 (m, 1H), 6.90 – 6.79 (m, 4H), 4.97 (s, 1H), 4.18 (s, 1H), 3.82 (s, 3H), 1.33 (s, 3H), 0.66 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.6, 145.4, 144.7, 142.1, 140.6, 137.2, 132.4, 128.8, 128.1, 127.6, 127.2, 127.0, 126.5, 126.3, 125.8, 119.7, 119.0, 69.9, 68.7, 67.6, 51.8, 48.4, 30.9, 24.3.

HRMS (ESI+) Calcd. For $C_{26}H_{25}ClNO_2^+$ ($[M+H]^+$): 418.1568, found: 418.1566.



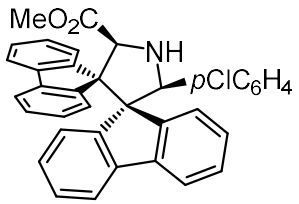
4k

Methyl (2'*S*,5'*S*)-3,6-dibromo-2'-(4-chlorophenyl)-4',4'-dimethylspiro[fluorene-9,3'-pyrrolidine]-5'-carboxylate (4k): Yield (97.4 mg, 85%); dr > 20:1; white solid; m.p. 60-62 ºC; $[\alpha]^{25}_D$ = -28.43 (*c* 0.83, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 91% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 14.76 and 20.14 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 2.0 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.42 – 7.36 (m, 1H), 7.29 – 7.24 (m, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.91 (s, 1H), 4.14 (s, 1H), 3.84 (s, 3H), 1.40 (s, 3H), 0.63 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.9, 146.7, 146.6, 140.3, 138.2, 132.8, 132.2, 131.0, 130.3, 129.7, 128.0, 127.4, 121.1, 120.3, 120.28, 120.26, 69.4, 68.6, 67.2, 51.9, 48.1, 31.3, 24.1.

HRMS (ESI+) Calcd. For $C_{26}H_{23}Br_2ClNO_2^+$ ($[M+H]^+$): 573.9779, found: 573.9776.



4l

Methyl (2'*S*,5'*S*)-5'-(4-chlorophenyl)dispiro[fluorene-9,3'-pyrrolidine-4',9''-fluorene]-2'-carboxy-

late (4l): Yield (49.6 mg, 46%); dr > 20:1; white solid; m.p. 220-222 °C; $[\alpha]^{25}_{D}$ = -241.09 (*c* 0.55, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 21.76 and 48.38 min.

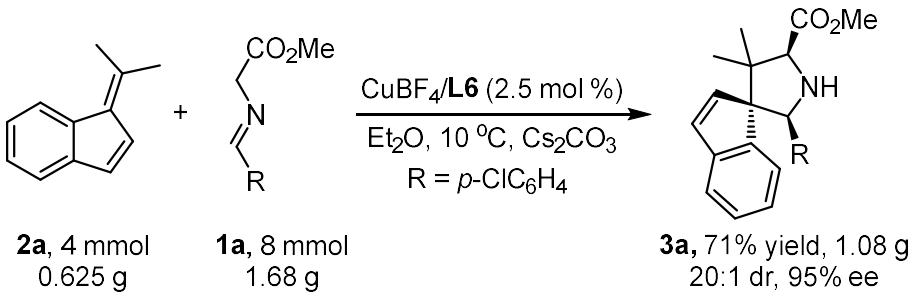
^{1}H NMR (400 MHz, Chloroform-d) δ 8.55 (d, J = 7.2 Hz, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.47 – 7.36 (m, 3H), 7.25 – 7.23 (m, 1H), 7.20 – 7.13 (m, 3H), 7.12 – 7.07 (m, 1H), 7.03 – 6.93 (m, 4H), 6.88 (d, J = 8.4 Hz, 2H), 6.76 – 6.73 (m, 1H), 6.62 (d, J = 8.4 Hz, 2H), 6.44 (d, J = 8.0 Hz, 1H), 5.84 (s, 1H), 5.08 (s, 1H), 3.36 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-d) δ 172.9, 151.9, 144.3, 142.8, 142.2, 142.0, 140.9, 140.7, 140.4, 136.6, 132.4, 129.1, 128.2, 127.9, 127.50, 127.46, 127.3, 126.6, 126.0, 125.7, 125.4, 125.32, 125.26, 125.2, 119.9, 119.0, 118.94, 118.91, 69.0, 68.2, 66.3, 65.2, 51.4.

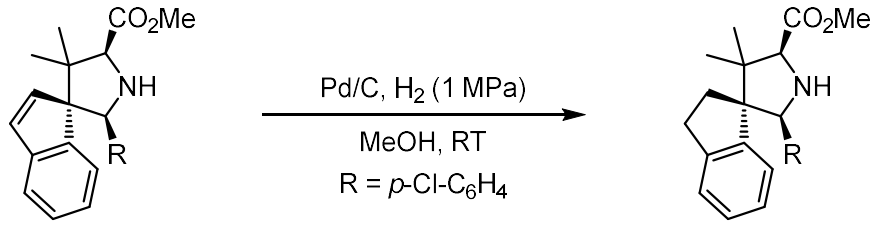
HRMS (ESI+) Calcd. For $C_{30}H_{23}NO_2^+$ ($[M+H]^+$): 540.1725, found: 540.1720.

5. Gram Scales Reaction

Under nitrogen atmosphere, (*S,S$_p$*)-**L6** (52.9 mg, 0.11 mmol) and $Cu(CH_3CN)_4BF_4$ (31.5 mg, 0.1 mmol) were dissolved in 40 mL Et_2O, which were stirred at room temperature for about 30 min. After the reaction temperature was dropped to 10 °C, the imino ester **1a** (8.00 mmol) and Cs_2CO_3 (4.00 mmol) were added sequentially. Then, the benzofulvenes **2a** (4.00 mmol) was added. When the reaction completed (monitored by TLC), the organic solvent was removed and the residue was purified by column chromatography to give cycloadducts, which were then directly analyzed by chiral HPLC to determine the enantiomeric excess.



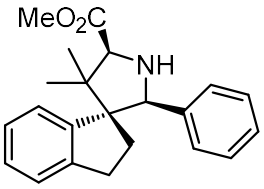
6. Synthetic Transformations



3a
20:1 dr, 95% ee

5a: 20:1 dr
59% yield, 96% ee

To a solution of cycloadduct **3a** (73.0 mg, 0.2 mmol) in MeOH (2 mL) was added Pd/C (10 mg) at room temperature. The mixtures were subsequently transferred into an autoclave, and hydrogen gas was charged. The reaction was then stirred under H_2 (1 Mpa) at 25 °C for 24 h. After the reaction completed (monitored by TLC), the solution was filtered and subsequently evaporated. The residue was purified by flash chromatography to give the product **5a**.



5a

Methyl (1*R*,2'*S*,5'*S*)-4',4'-dimethyl-2'-phenyl-2,3-dihydrospiro[indene-1,3'-pyrrolidine]-5'-carboxylate (5a): Yield (39.6 mg, 59%); dr = 20:1; yellow liquid; $[\alpha]^{25}_{D}$ = -91.64 (*c* 1.28, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.48 and 9.11 min.

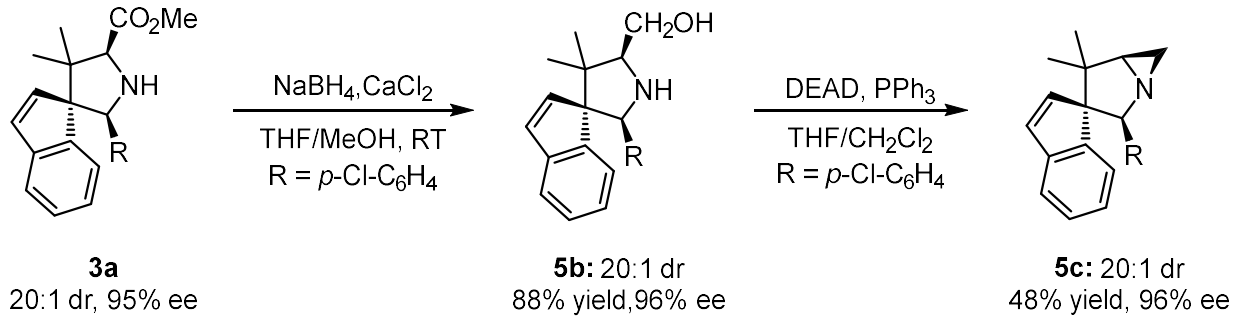
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 (d, *J* = 7.6 Hz, 1H), 7.25 – 7.09 (m, 8H), 4.90 (s, 1H), 3.87 (s, 1H), 3.81 (s, 3H), 2.77 – 2.65 (m, 1H), 2.52 – 2.45 (m, 1H), 2.02 – 1.95 (m, 1H), 1.73 – 1.63 (m, 1H), 1.15 (s, 3H), 0.97 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 145.4, 144.3, 140.4, 127.9, 127.7, 127.0, 126.9, 126.1, 125.4, 124.8, 69.1, 68.4, 65.1, 51.8, 50.5, 31.2, 29.4, 28.4, 21.5.

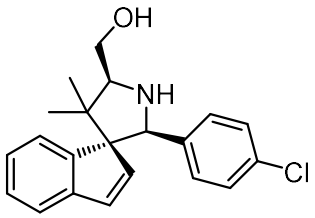
HRMS (ESI+) Calcd. For $C_{22}H_{26}NO_2^+$ ($[M+H]^+$): 336.1958, found: 336.1958.

To a solution of cycloadduct **3a** (73.0 mg, 0.2 mmol) in MeOH (1 mL) and THF (1 mL) was added $NaBH_4$ (1.0 mmol) and $CaCl_2$ (1.0 mmol) at room temperature. After 48.0 h, the solution was quenched

with a saturated aqueous NH_4Cl solution and subsequently evaporated. The residue was purified by flash chromatography to give the product **5b**.



Under nitrogen atmosphere, PPh_3 (105.0 mg, 0.4 mmol) was dissolved in dry DCM (4 mL), then DIAD (88.9 mg, 0.44 mmol) in THF (1.5 mL) was added at 0 ºC. The solution was stirred for 30 minutes at 0 ºC, followed by addition of amino alcohol **5b** (0.2 mmol) in THF (1.5 mL). The cooling bath was removed and the reaction was stirred at room temperature for 12 hours. When the reaction completed, the organic solvent was removed and the residue was purified by column chromatography to give **5c**, which was then directly analyzed by chiral HPLC to determine the enantiomeric excess.



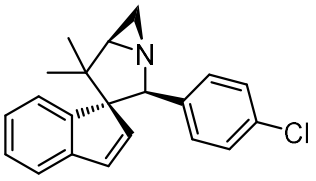
5b

((1*R*,2'*S*,5'*S*)-2'-(4-chlorophenyl)-4',4'-dimethylspiro[indene-1,3'-pyrrolidin]-5'-yl)methanol (5b): Yield (59.7 mg, 88%); dr = 20:1; white semisolid; $[\alpha]^{25}_{D}$ = -254.8 (*c* 1.48, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AS-H, *i*-propanol/hexane = 8/92, flow rate 1.0 mL/min, λ = 254 nm); t_r = 14.77 and 19.52 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 6.8 Hz, 1H), 7.23 – 7.16 (m, 2H), 7.12 (dd, *J* = 6.8, 1.6 Hz, 1H), 7.03 – 6.95 (m, 4H), 6.37 (d, *J* = 5.6 Hz, 1H), 6.30 (d, *J* = 5.6 Hz, 1H), 4.95 (s, 1H), 3.78 – 3.76 (m, 2H), 3.49 (dd, *J* = 7.2, 4.8 Hz, 1H), 1.23 (s, 3H), 0.77 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.3, 140.0, 138.5, 132.4, 130.3 127.8, 127.4, 127.2, 125.1, 124.2, 121.2, 69.9, 67.6, 65.9, 63.8, 45.5, 30.0, 21.0.

HRMS (ESI+) Calcd. For $C_{21}H_{23}ClNO^+$ ($[M+H]^+$): 340.1463, found: 340.1462.



5c

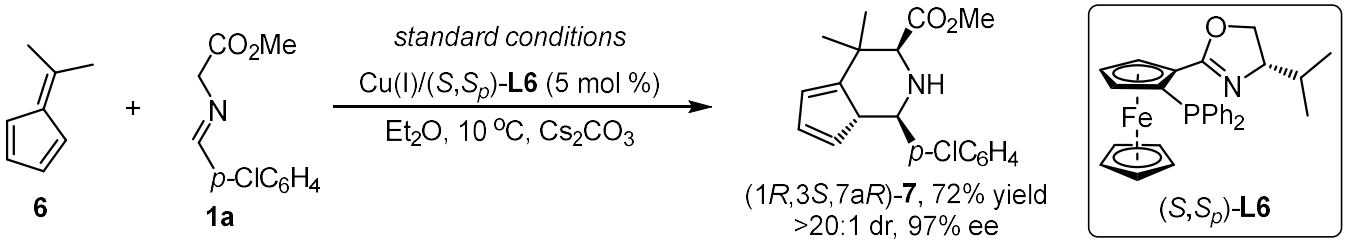
(2*S*,3*R*,5*S*)-2-(4-chlorophenyl)-4,4-dimethyl-1-azaspiro[bicyclo[3.1.0]hexane-3,1'-indene] (5c): Yield (30.8 mg, 48%); dr = 20:1; yellow semisolid; $[\alpha]^{25}_D$ = -327.35 (*c* 0.49, $CHCl_3$); The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak OJ, *i*-propanol/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm); t_r = 5.81 and 6.34 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 7.2 Hz, 1H), 7.30 – 7.28 (m, 1H), 7.26 – 7.20 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.68 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 5.6 Hz, 1H), 5.97 (d, *J* = 5.6 Hz, 1H), 5.26 (s, 1H), 2.61 – 2.59 (m, 1H), 2.17 – 2.16 (m, 1H), 1.97 (d, *J* = 5.6 Hz, 1H), 1.51 (s, 3H), 0.90 (s, 3H).

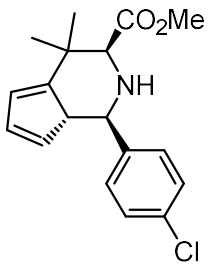
^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.1, 143.9, 142.1 137.4, 132.3, 131.3, 127.8, 127.3, 126.6, 125.8, 124.8, 121.6, 72.4, 67.5, 51.8, 45.9, 30.9, 27.4, 23.6.

HRMS (ESI+) Calcd. For $C_{21}H_{21}ClN^+$ ($[M+H]^+$): 322.1357, found: 322.1352.

7. Experimental Proof of Cu(I)-Catalyzed [3+6] Cycloaddition with Fulvene



Under nitrogen atmosphere, (*S,S*$_p$)-**L6** (5.29 mg, 0.011 mmol) and $Cu(CH_3CN)_4BF_4$ (3.15 mg, 0.01 mmol) were dissolved in 2.0 mL Et_2O, which were stirred at room temperature for about 30 min. After the reaction temperature was dropped to 10 °C, the imino ester **1a** (0.40 mmol) and Cs_2CO_3 (0.02 mmol) were added sequentially. Then, the fulvene **6** (0.2 mmol) was added. When the reaction completed (monitored by TLC), the organic solvent was removed and the residue was purified by column chromatography to give cycloadducts **7**.



7

Methyl (1*R*,3*S*,7a*R*)-1-(4-chlorophenyl)-4,4-dimethyl-2,3,4,7a-tetrahydro-1H-cyclopenta[c]pyridine-3-carboxylate (7): Yield (48 mg, 72%); dr = 20:1; yellow solid; The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak AS-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.46 and 5.55 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 8.8 Hz, 2H), 7.28 (d, *J* = 8.8 Hz, 2H), 6.38 (d, *J* = 5.6 Hz, 1H), 6.12 – 6.00 (m, 1H), 5.88 (d, *J* = 5.6 Hz, 1H), 3.67 (s, 3H), 3.10 (s, 1H), 3.00 (d, *J* = 10.8 Hz, 1H), 2.81 (d, *J* = 10.8 Hz, 1H), 1.36 (s, 3H), 1.15 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.60, 157.4, 141.1, 133.4, 132.7, 128.7, 128.4, 122.3, 69.8, 65.2, 56.1, 51.7, 38.3, 24.18, 24.15.

8. References

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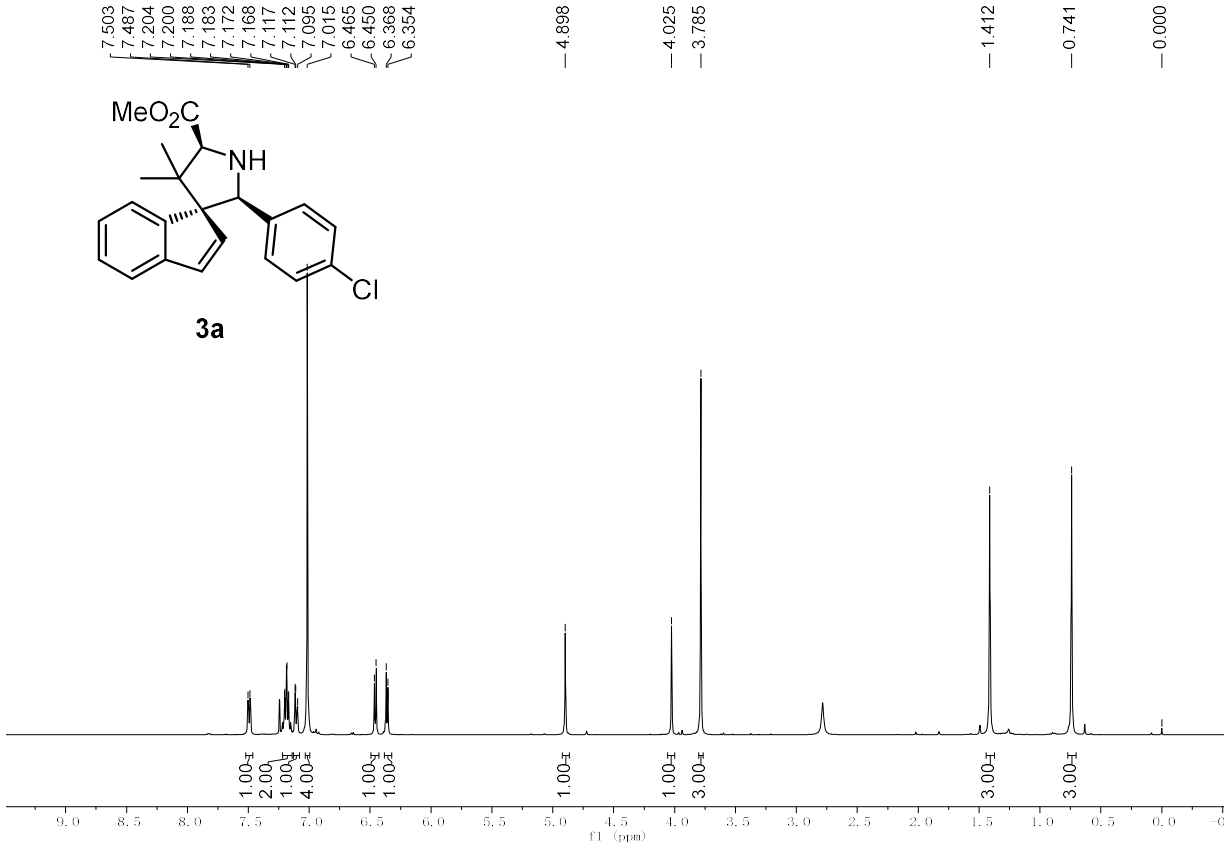
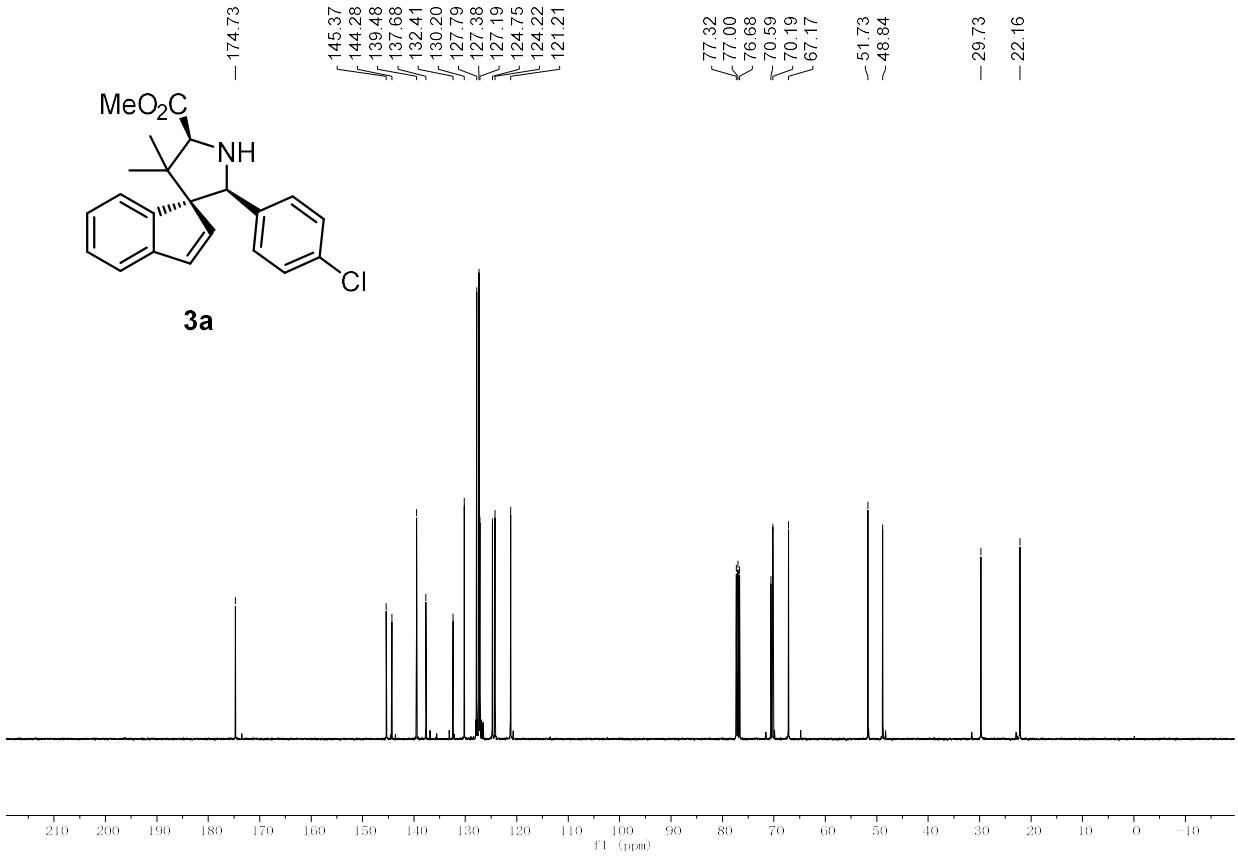
9. NMR and HPLC Spectra



^{1}H NMR (400 MHz, Chloroform-*d*) of **3a**

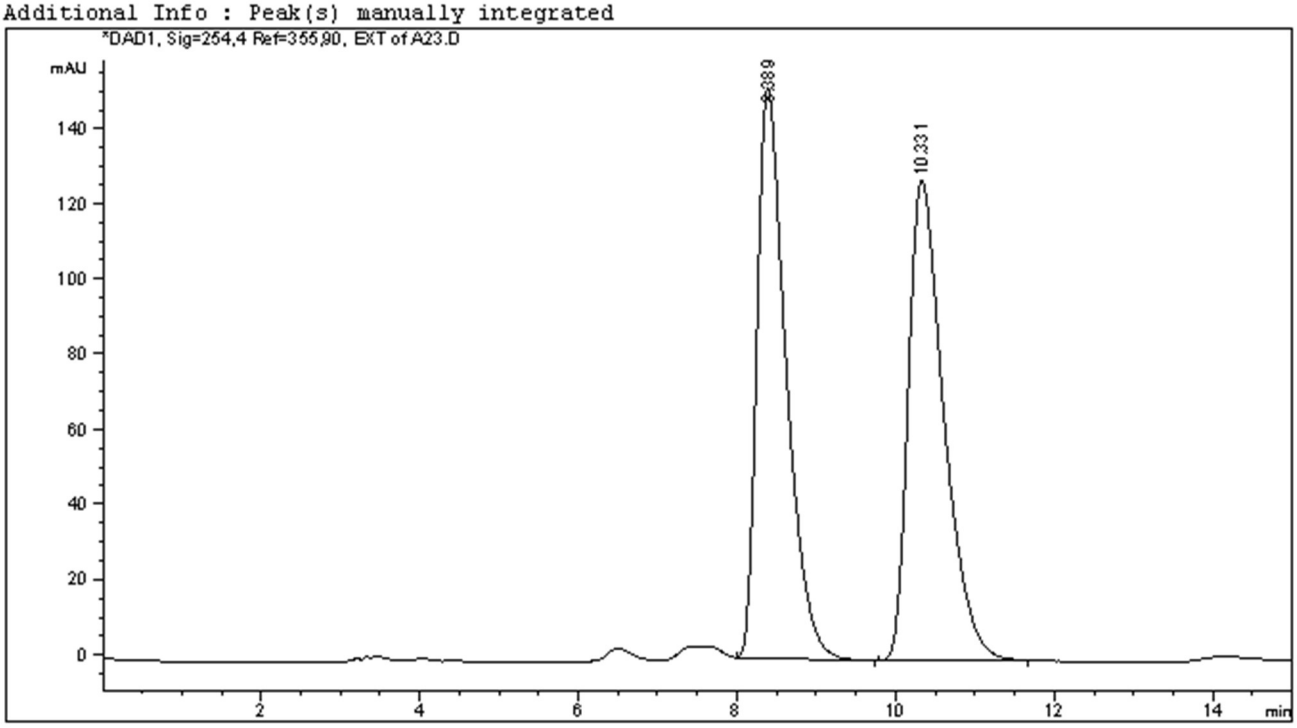


^{13}C NMR (400 MHz, Chloroform-*d*) of **3a**

Data File D:\HPLC\DATA\20230331\A 2023-03-31 09-05-46\A23.D
Sample Name: LXT-6-4-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 24
Acq. Instrument : 1260 Location : 22
Injection Date : 3/31/2023 10:41:01 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230331\A 2023-03-31 09-05-46\1-ASH-95-5-1ML-10ul-15min-ALL-nml.M
Last changed : 3/31/2023 3:21:44 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230331\A 2023-03-31 09-05-46\1-ASH-95-5-1ML-10ul-15min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:16:50 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

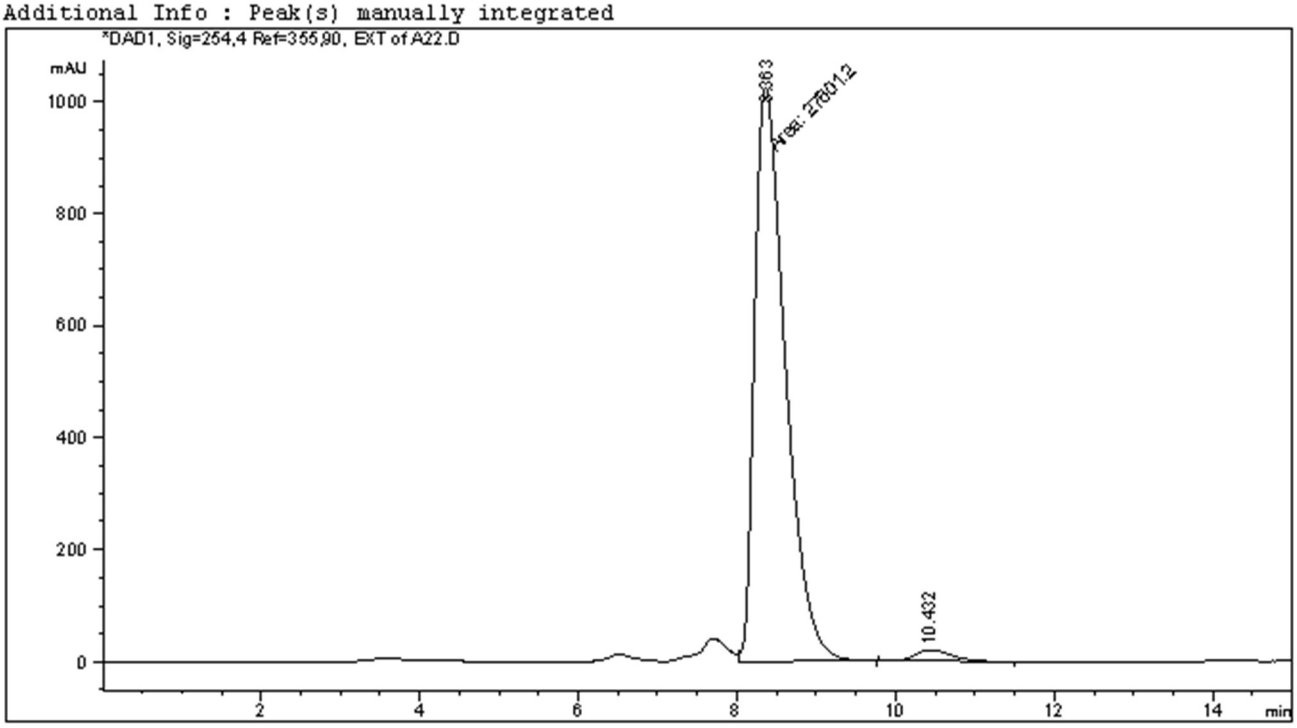
Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.389	BB	0.3775	3871.01001	151.82491	49.3745
2	10.331	BB	0.4649	3969.09546	127.58752	50.6255

Totals : 7840.10547 279.41243

Data File D:\HPLC\DATA\20230331\A 2023-03-31 09-05-46\A22.D
Sample Name: LXT-PCL-OPT

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :  23
Acq. Instrument : 1260                             Location :   21
Injection Date  : 3/31/2023 10:24:36 PM                 Inj :   1
                                                Inj Volume : 10.000 µl
Acq. Method     : D:\HPLC\Data\20230331\A 2023-03-31 09-05-46\1-ASH-95-5-1ML-10ul-15min-ALL-
                  nml.M
Last changed    : 3/31/2023 3:21:44 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230331\A 2023-03-31 09-05-46\1-ASH-95-5-1ML-10ul-15min-ALL-
                  nml.M (Sequence Method)
Last changed    : 4/10/2023 9:16:50 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

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==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.363 FM    0.4493 2.76012e4  1023.86700  97.7964
   2  10.432 BB    0.4155  621.92126   19.96250   2.2036

Totals :                  2.82231e4  1043.82951
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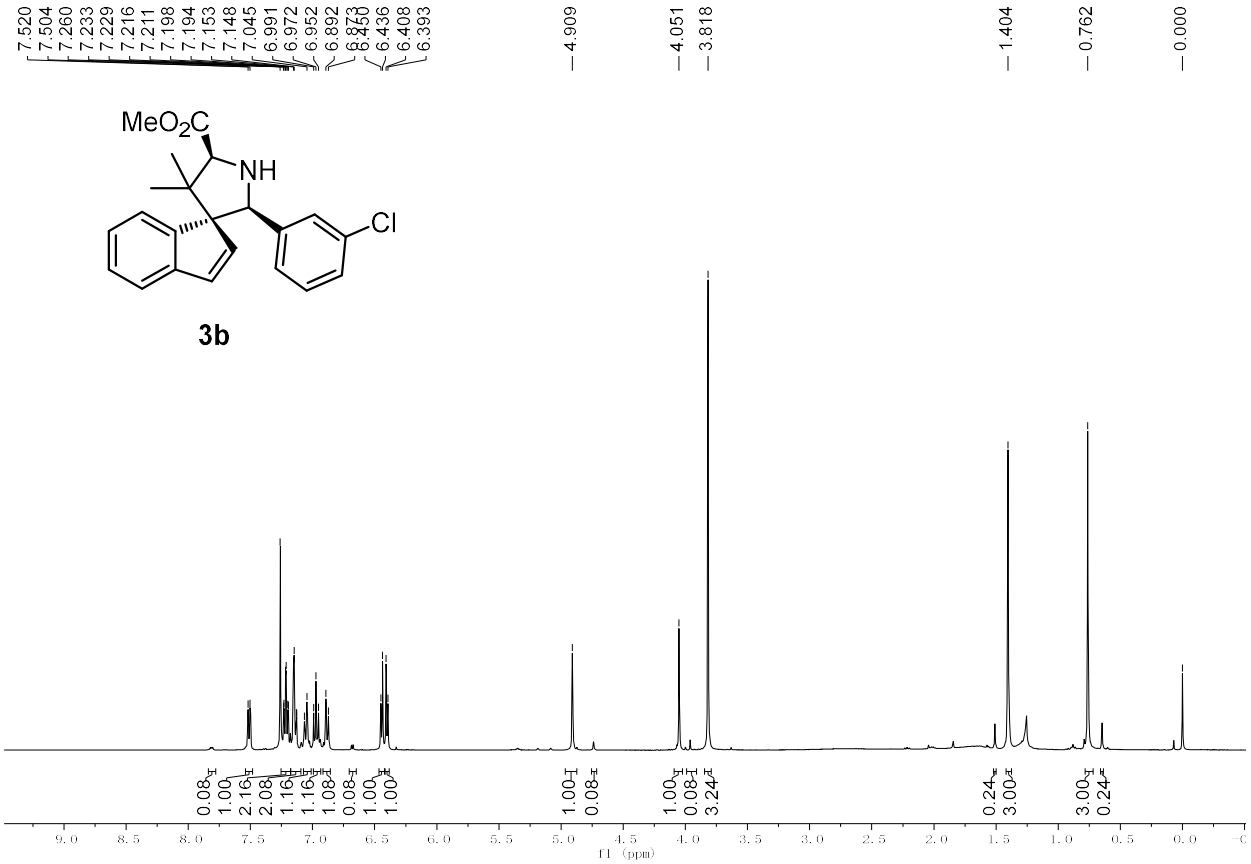
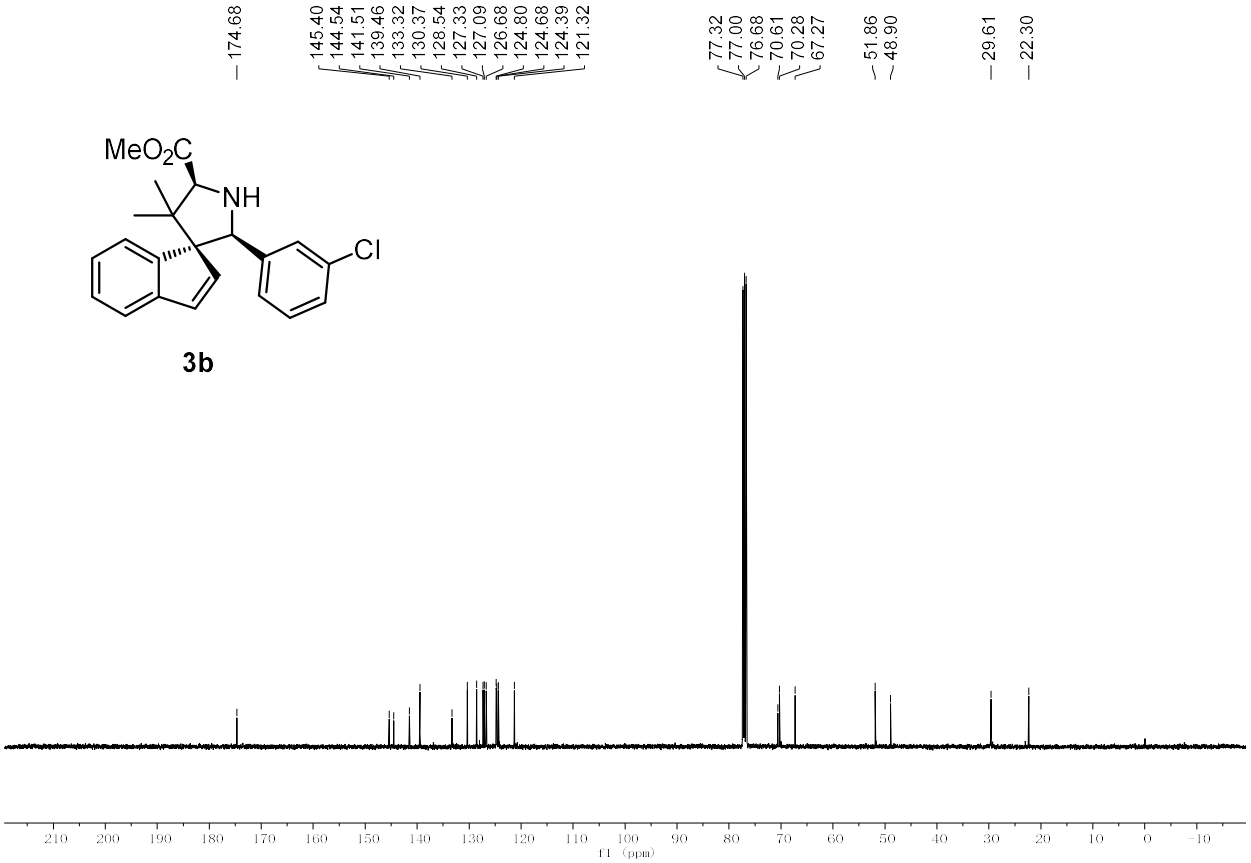


^{1}H NMR (400 MHz, Chloroform-*d*) of **3b**

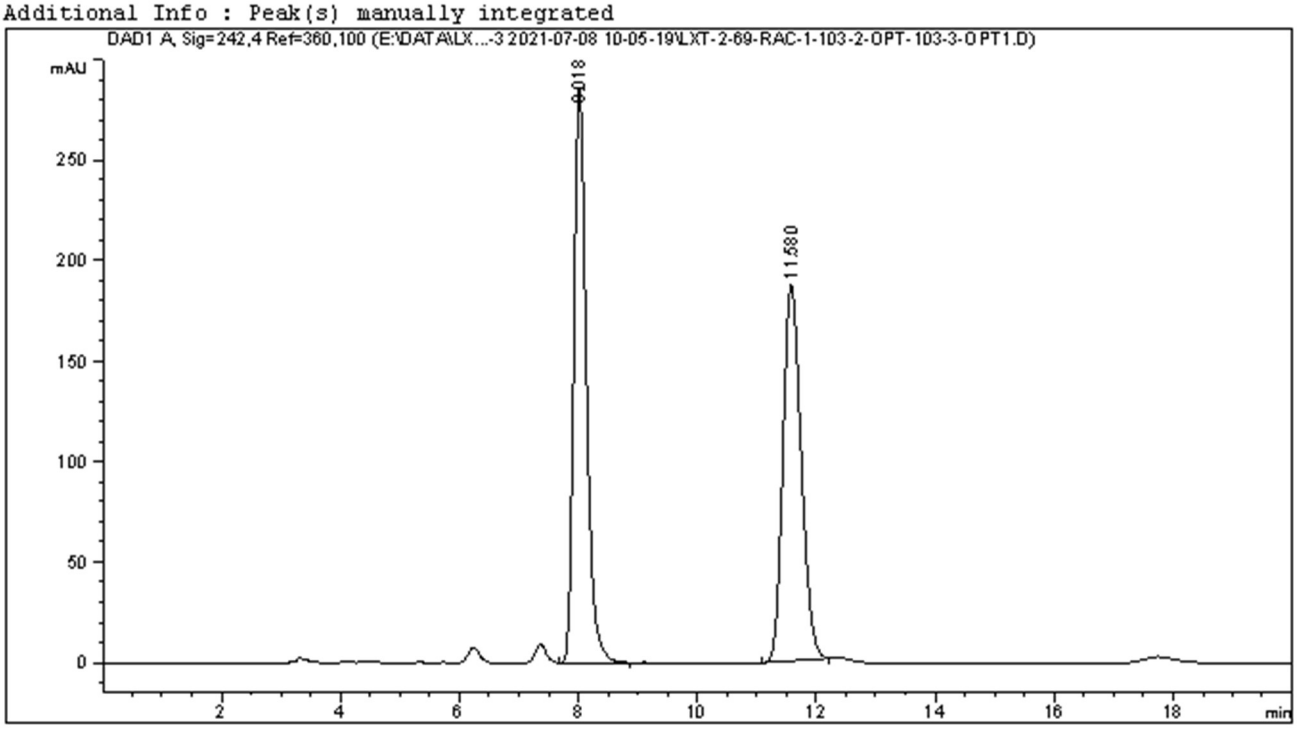


^{13}C NMR (101 MHz, Chloroform-*d*) of **3b**

Data File E:\DATA\LX...1-103-2-3 2021-07-08 10-05-19\LXT-2-69-RAC-1-103-2-OPT-103-3-OPT1.D
Sample Name: LXT-2-69-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 1
Injection Date : 7/8/2021 10:27:41 AM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-69-1-103-2-3 2021-07-08 10-05-19\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/8/2021 10:05:19 AM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-69-1-103-2-3 2021-07-08 10-05-19\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:04:32 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=242,4 Ref=360,100

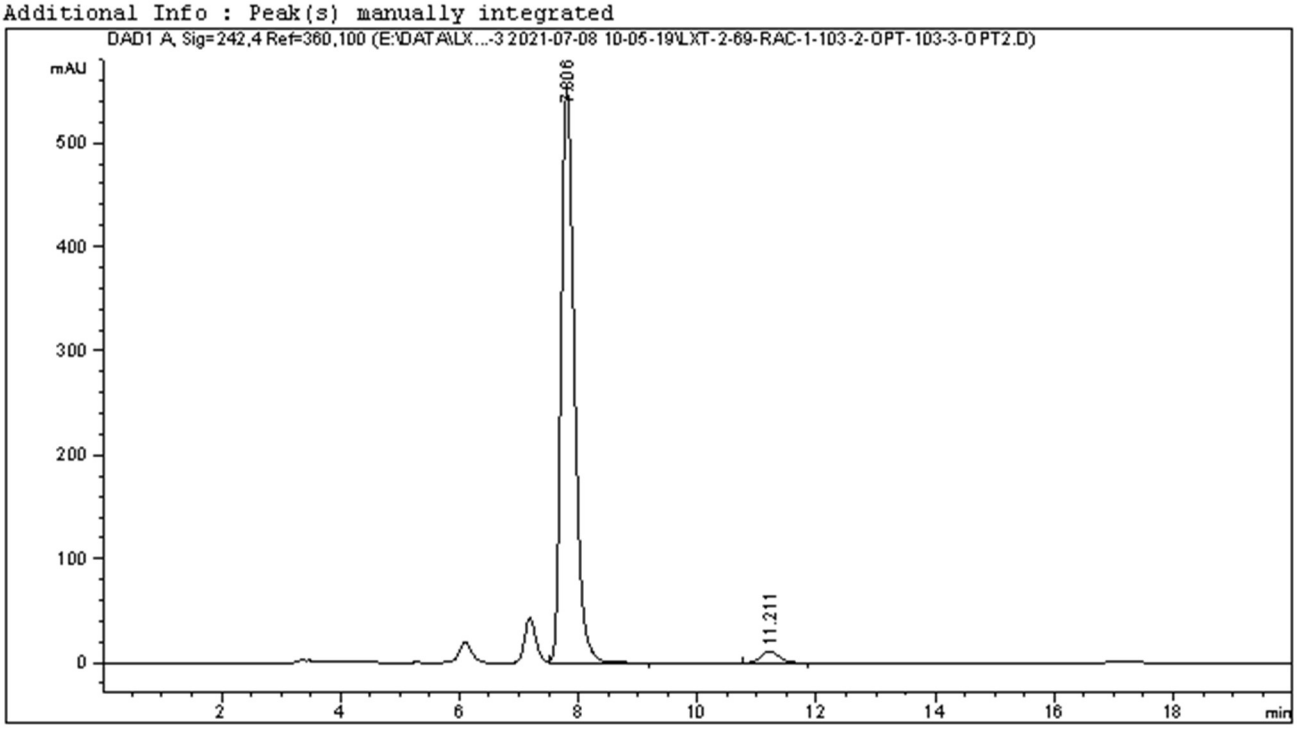
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.018	BB	0.2276	4227.33154	285.76813	51.5731
2	11.580	BB	0.3296	3969.44409	187.07130	48.4269

Totals : 8196.77563 472.83943

Data File E:\DATA\LX...1-103-2-3 2021-07-08 10-05-19\LXT-2-69-RAC-1-103-2-OPT-103-3-OPT2.D
Sample Name: LXT-1-103-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 2
Injection Date : 7/8/2021 10:49:07 AM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-69-1-103-2-3 2021-07-08 10-05-19\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/8/2021 10:05:19 AM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-69-1-103-2-3 2021-07-08 10-05-19\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:08:11 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

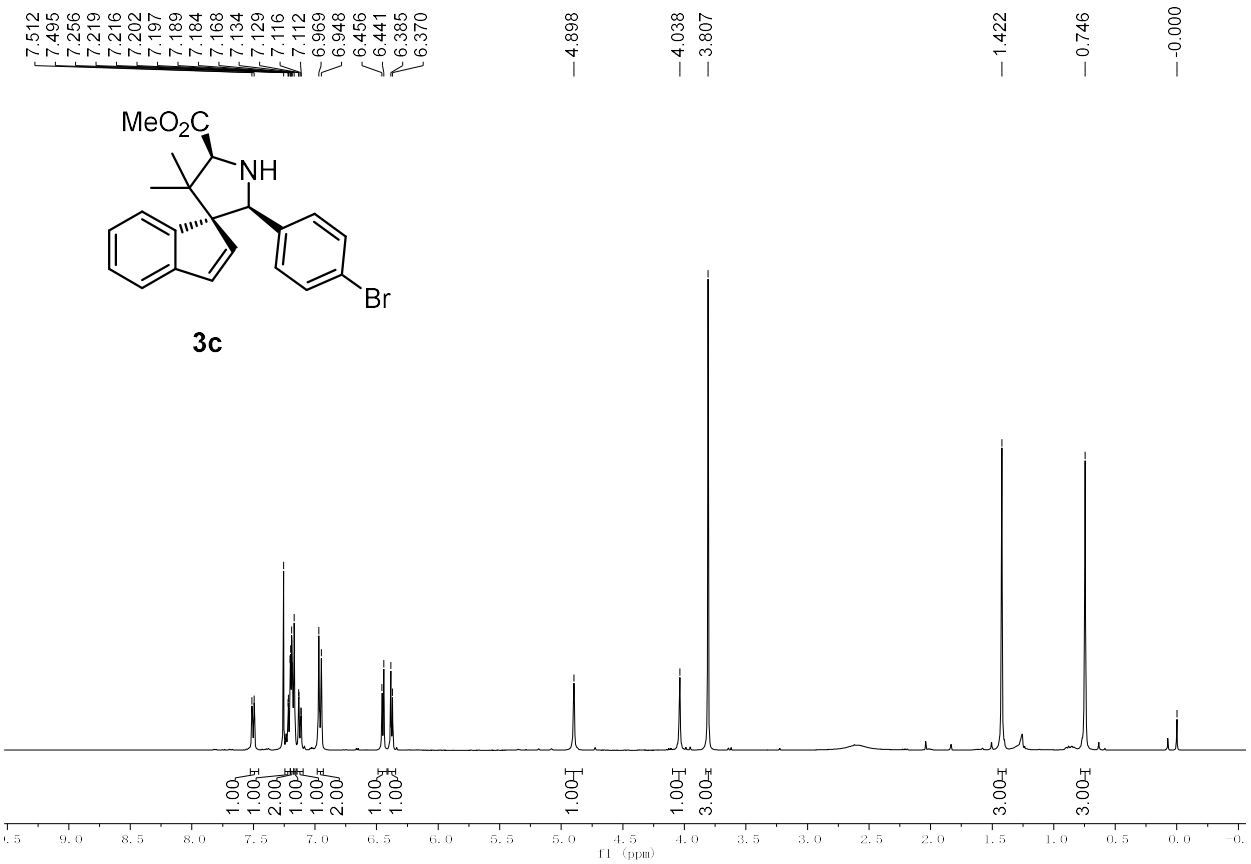
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

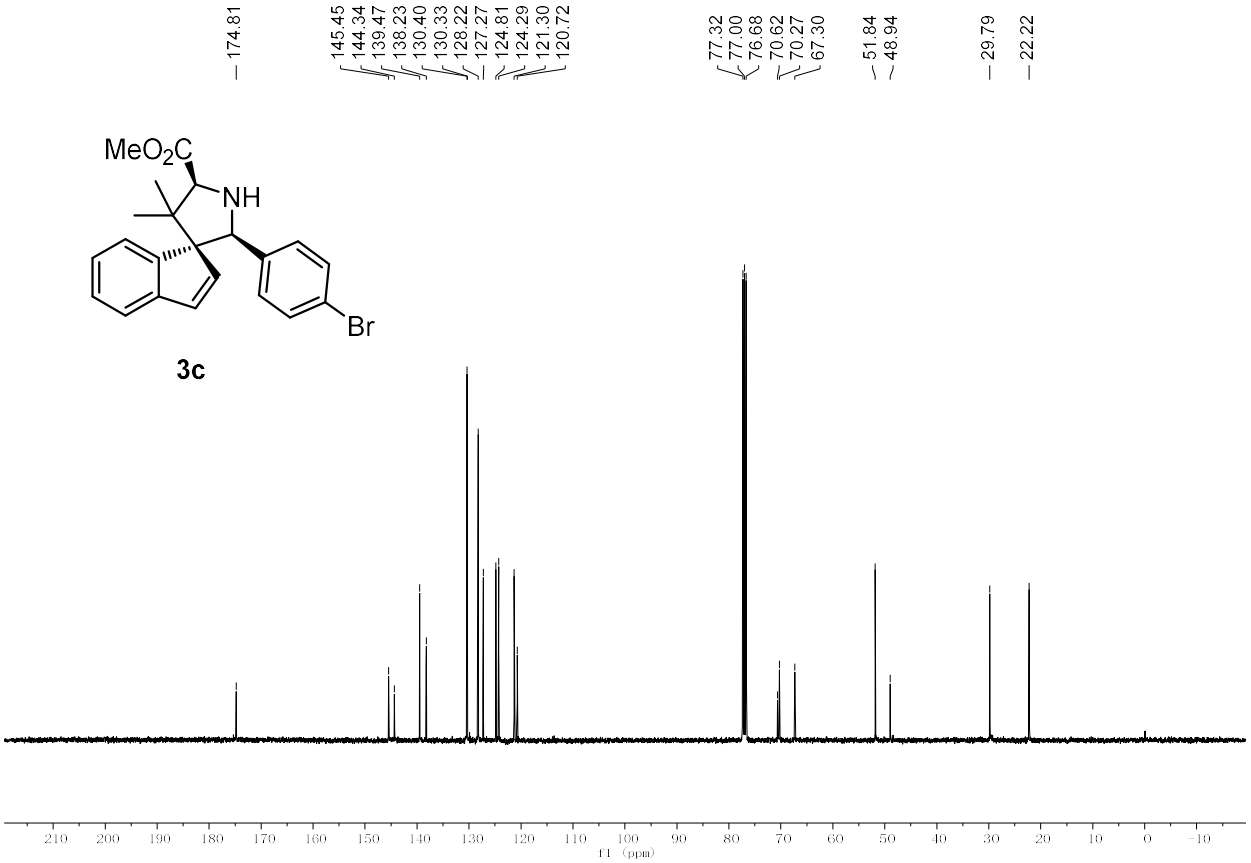
Signal 1: DAD1 A, Sig=242,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.806	VB	0.2381	8482.54492	552.66125	97.3435
2	11.211	BB	0.3118	231.49113	11.07894	2.6565

Totals : 8714.03606 563.74019



^{1}H NMR (400 MHz, Chloroform-*d*) of **3c**

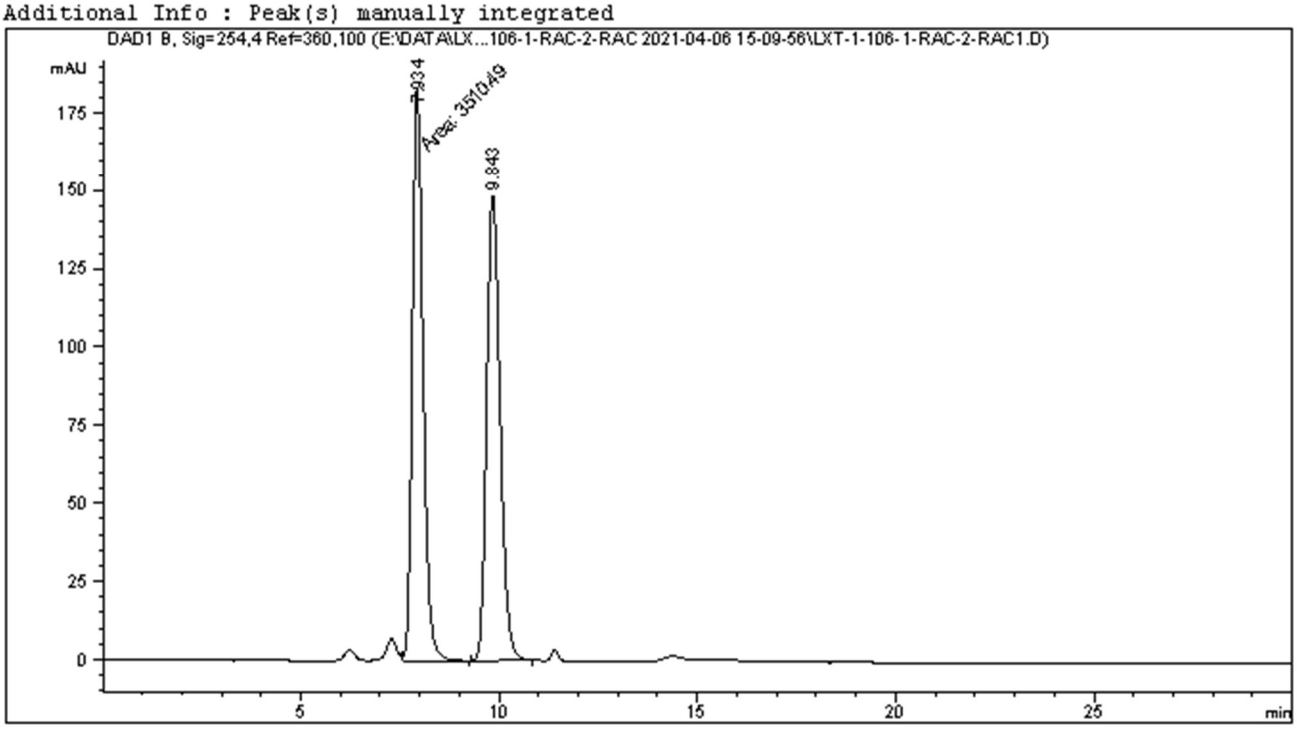


^{13}C NMR (101 MHz, Chloroform-*d*) of **3c**

Data File E:\DATA\LXT\LXT-1-106-1-RAC-2-RAC 2021-04-06 15-09-56\LXT-1-106-1-RAC-2-RAC1.D
Sample Name: LXT-1-106-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 3
Injection Date : 4/6/2021 3:22:22 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-106-1-RAC-2-RAC 2021-04-06 15-09-56\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 4/6/2021 3:09:56 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-106-1-RAC-2-RAC 2021-04-06 15-09-56\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:11:25 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.934	FM	0.3191	3510.49023	183.37376	50.0682
2	9.843	BB	0.3659	3500.92310	148.57167	49.9318

Totals : 7011.41333 331.94543

Data File E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\LXT-Z611.D
Sample Name: LXT-1-103-3-OPT

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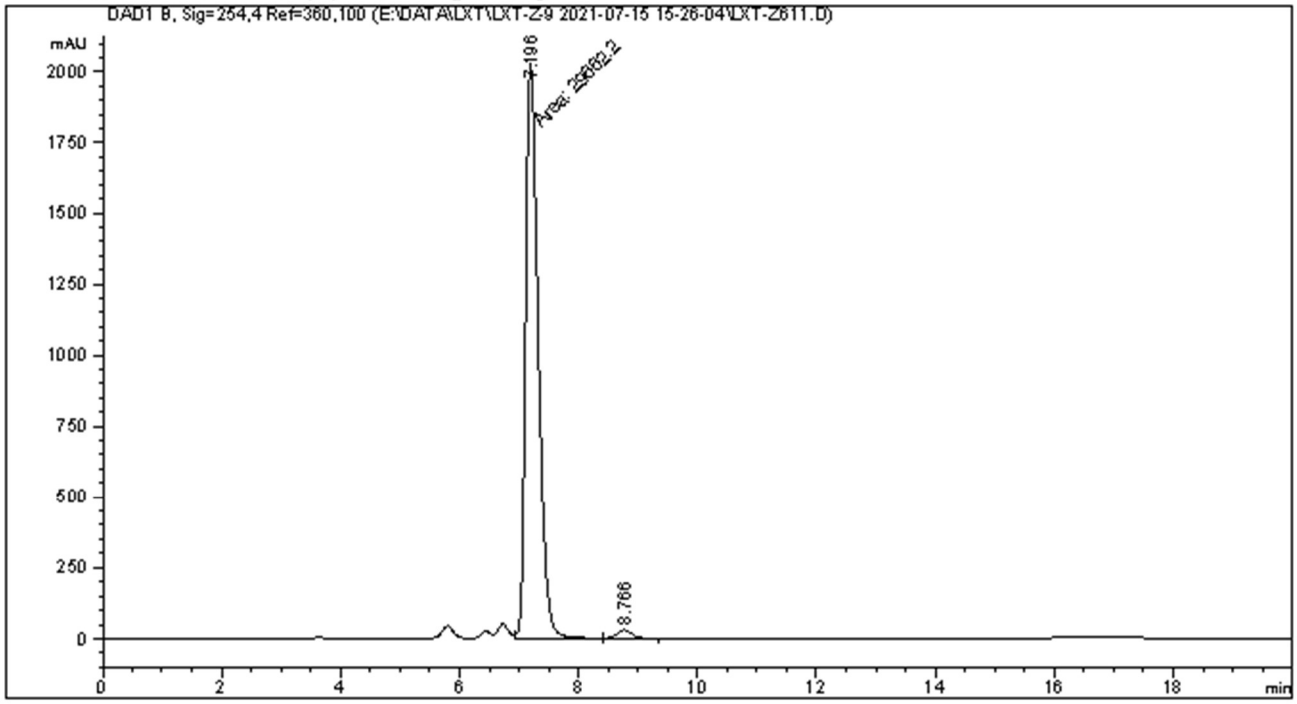
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :  12
Acq. Instrument : 1260                             Location :   9
Injection Date  : 7/15/2021 7:42:28 PM                  Inj :   1
                                                 Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed    : 7/15/2021 3:26:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
                  (Sequence Method)
Last changed    : 7/31/2021 5:26:39 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

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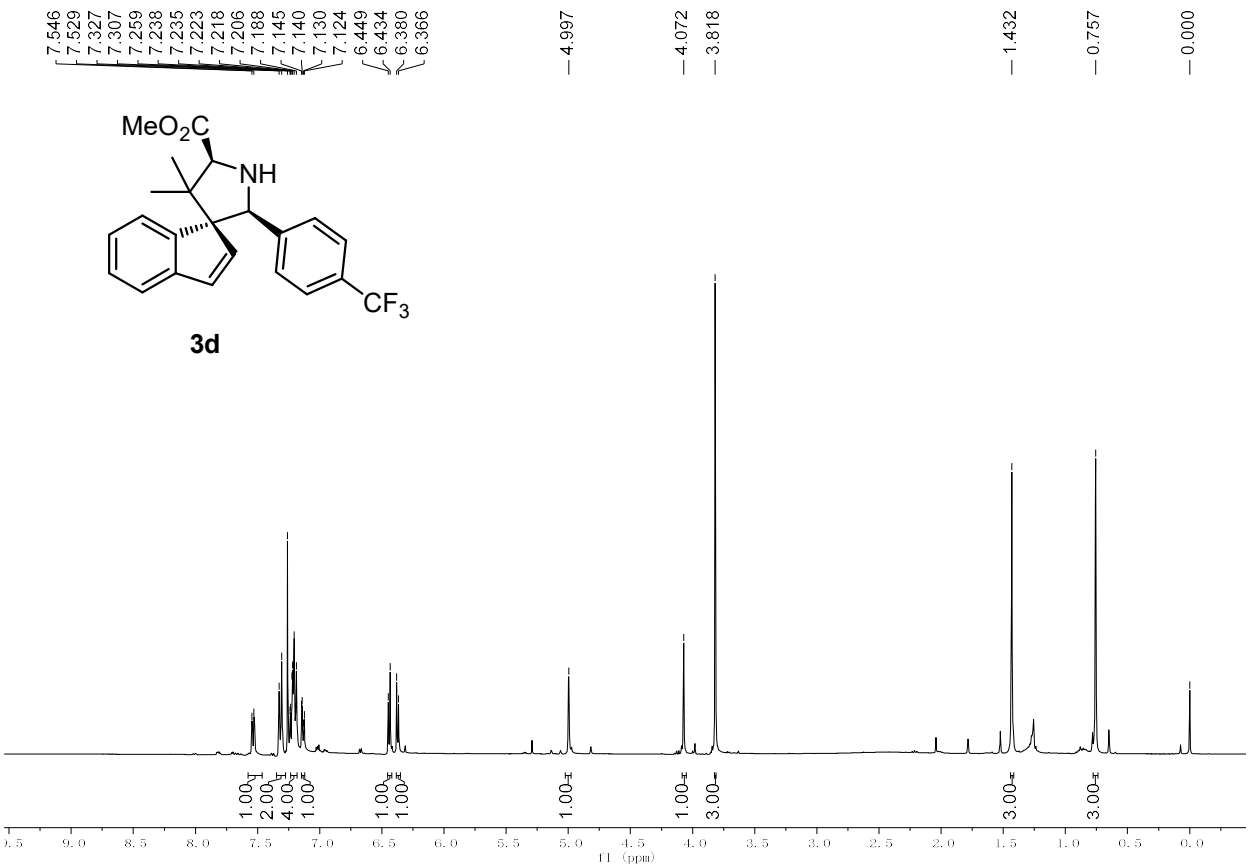
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

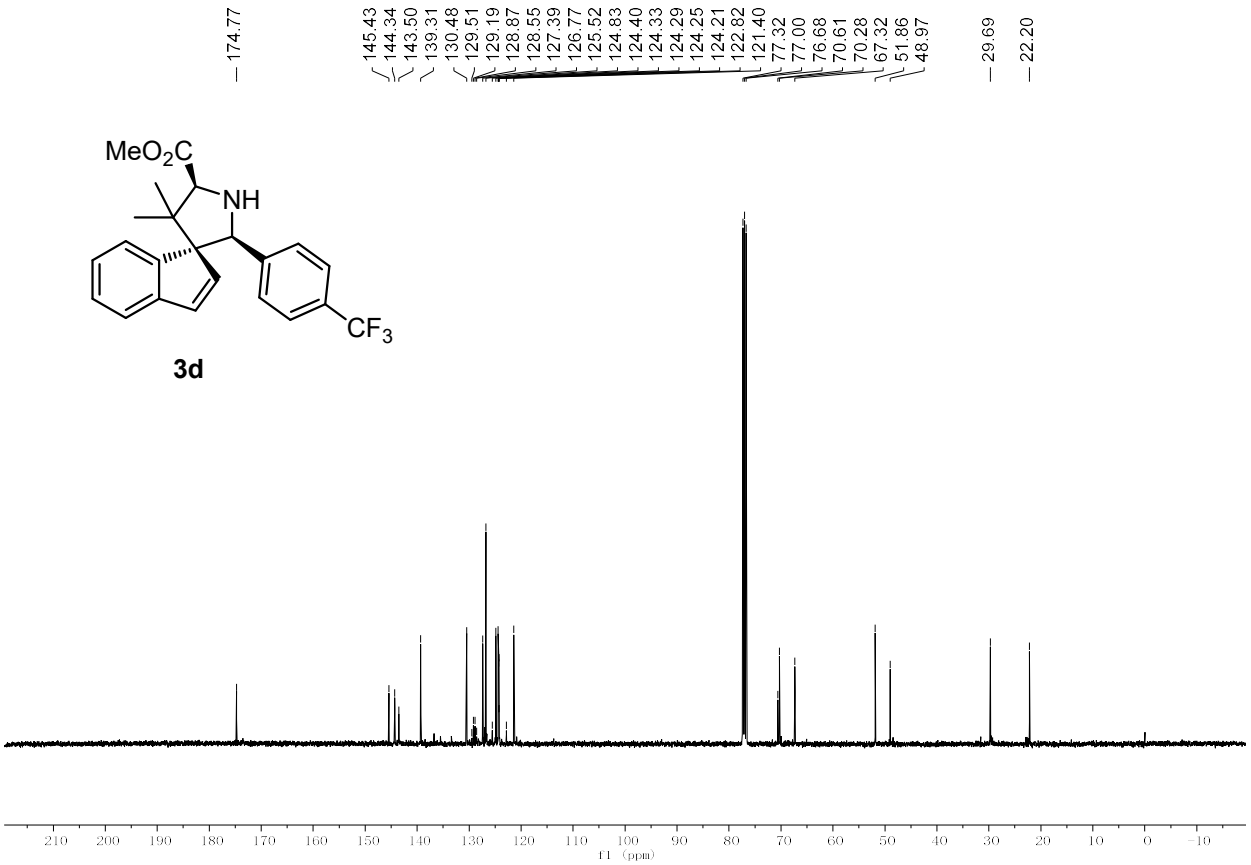

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.196 FM    0.2438 2.96622e4  2027.66748  98.4343
   2   8.766 BB    0.2536  471.81100   28.72622   1.5657

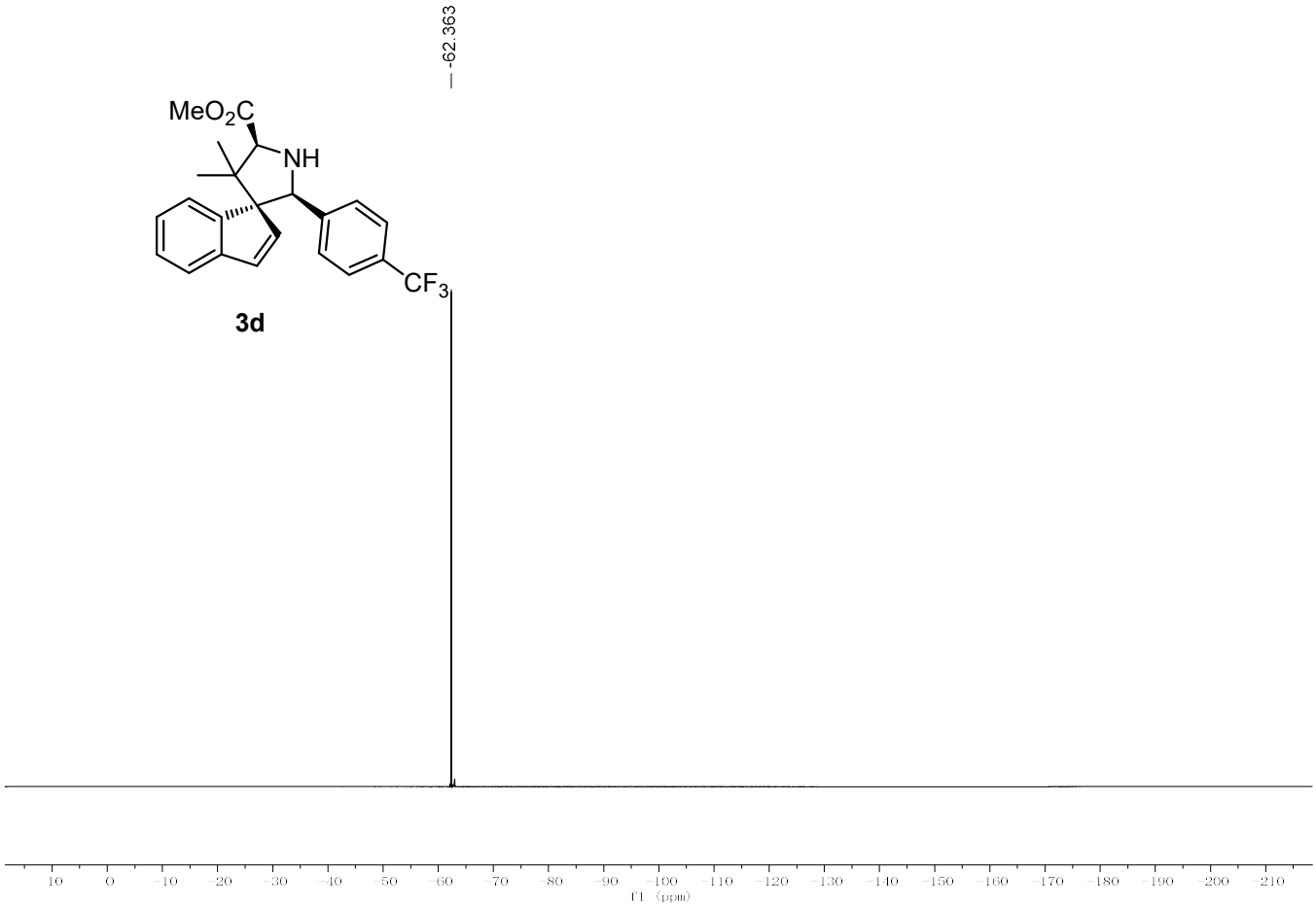
Totals :                  3.01340e4  2056.39370
```



^{1}H NMR (400 MHz, Chloroform-*d*) of **3d**



^{13}C NMR (101 MHz, Chloroform-*d*) of **3d**

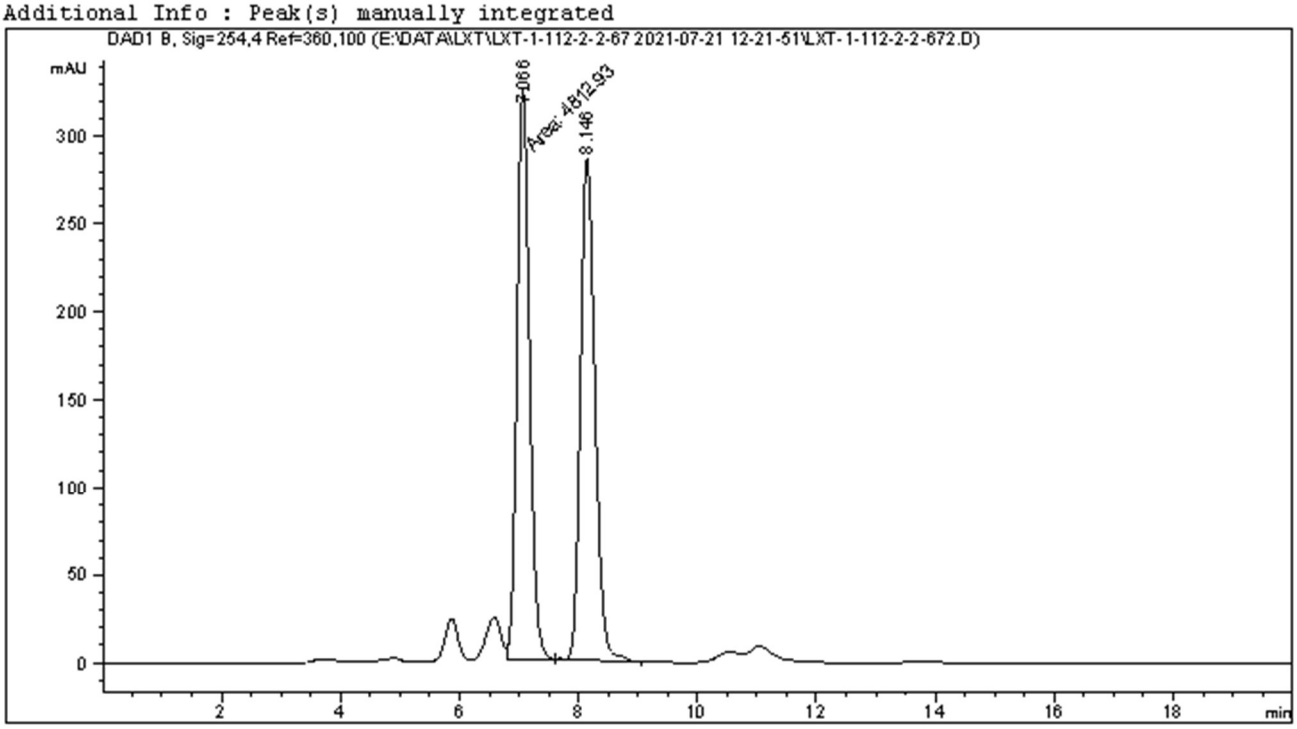


^{19}F NMR (377 MHz, Chloroform-d) of **3d**

Data File E:\DATA\LXT\LXT-1-112-2-2-67 2021-07-21 12-21-51\LXT-1-112-2-2-672.D
Sample Name: LXT-1-112-2-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 41
Injection Date : 7/21/2021 1:15:14 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-112-2-2-67 2021-07-21 12-21-51\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/21/2021 12:21:51 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-112-2-2-67 2021-07-21 12-21-51\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:17:48 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

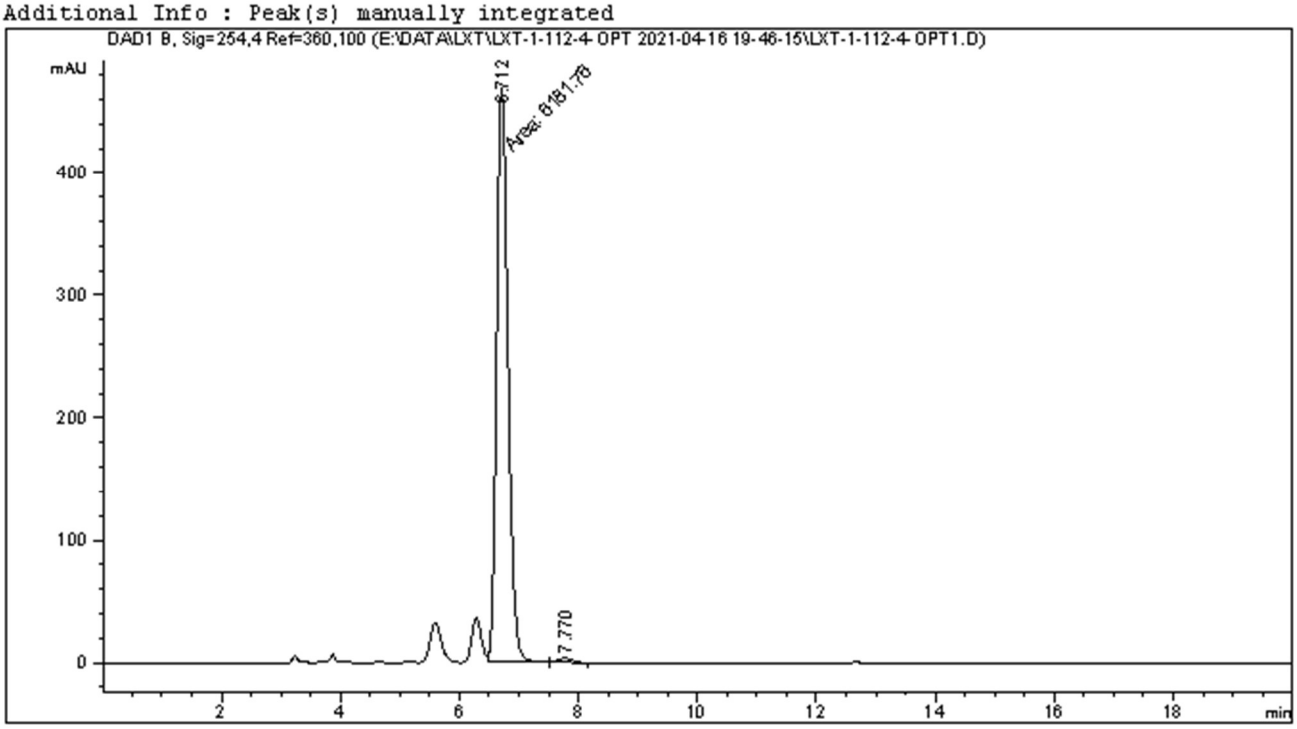
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.066	FM	0.2464	4812.93311	325.53925	49.6506
2	8.146	VB R	0.2664	4880.67383	285.61584	50.3494

Totals : 9693.60693 611.15509

Data File E:\DATA\LXT\LXT-1-112-4-OPT 2021-04-16 19-46-15\LXT-1-112-4-OPT1.D
Sample Name: LXT-1-112-4-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 11
Injection Date : 4/16/2021 7:58:45 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-112-4-OPT 2021-04-16 19-46-15\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 4/16/2021 7:46:16 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-112-4-OPT 2021-04-16 19-46-15\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:20:43 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

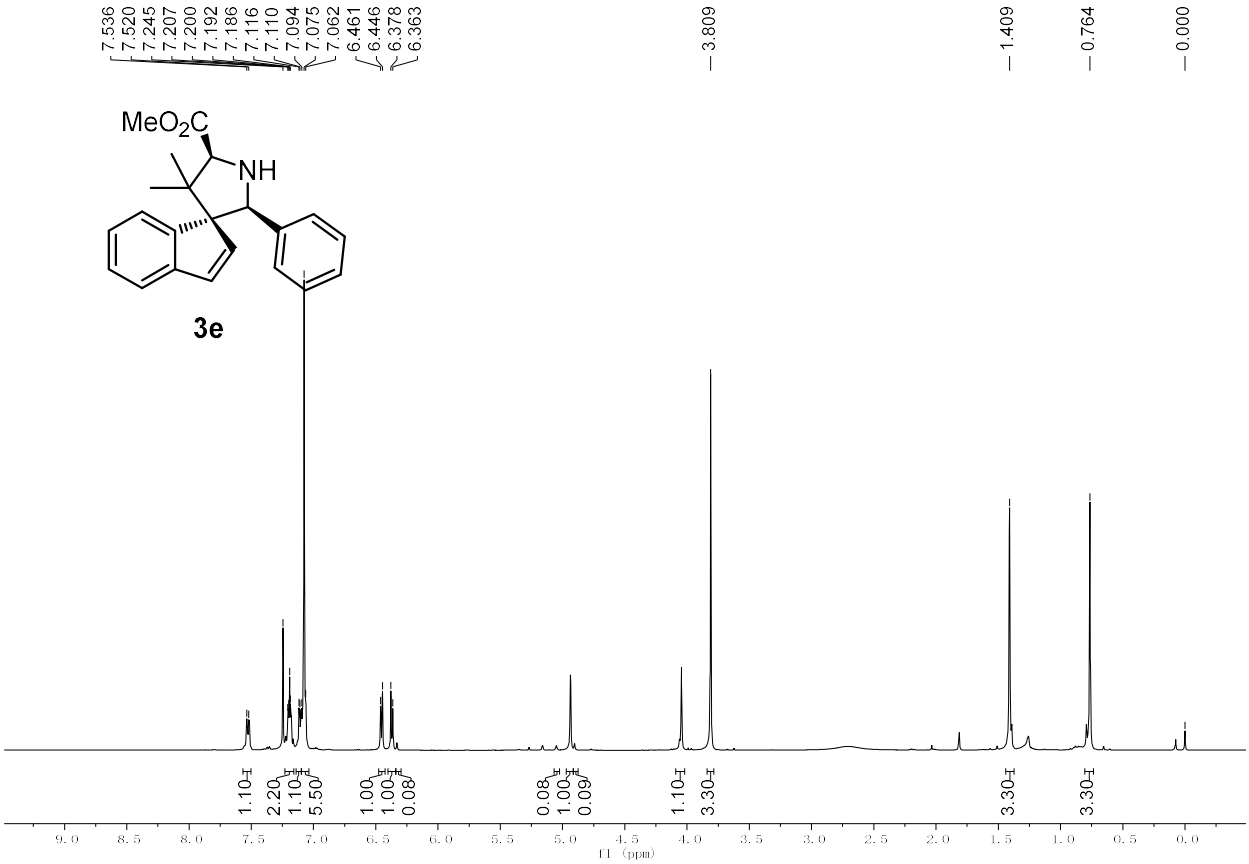
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

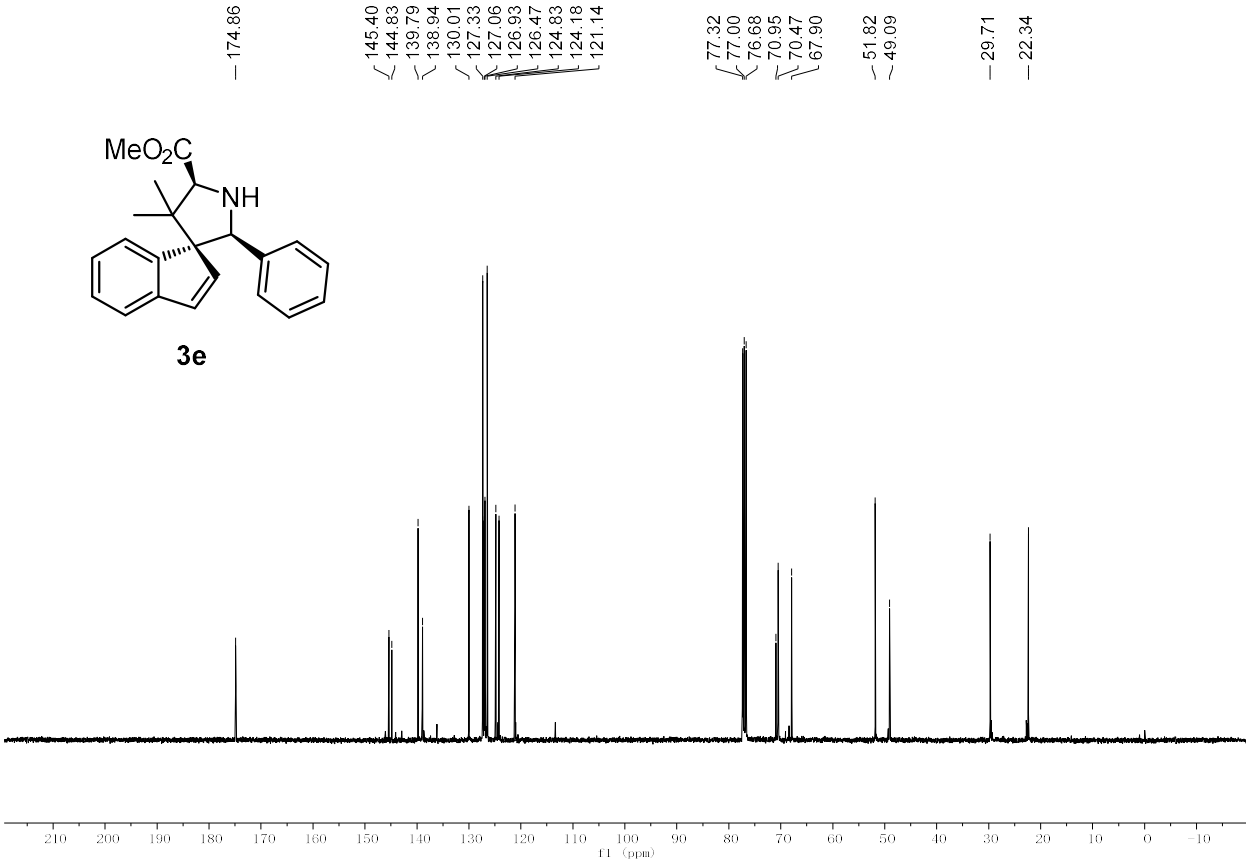
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.712	FM	0.2198	6181.76465	468.80585	99.1168
2	7.770	BB	0.2210	55.08127	3.69253	0.8832

Totals : 6236.84592 472.49838



^{1}H NMR (400 MHz, Chloroform-*d*) of **3e**

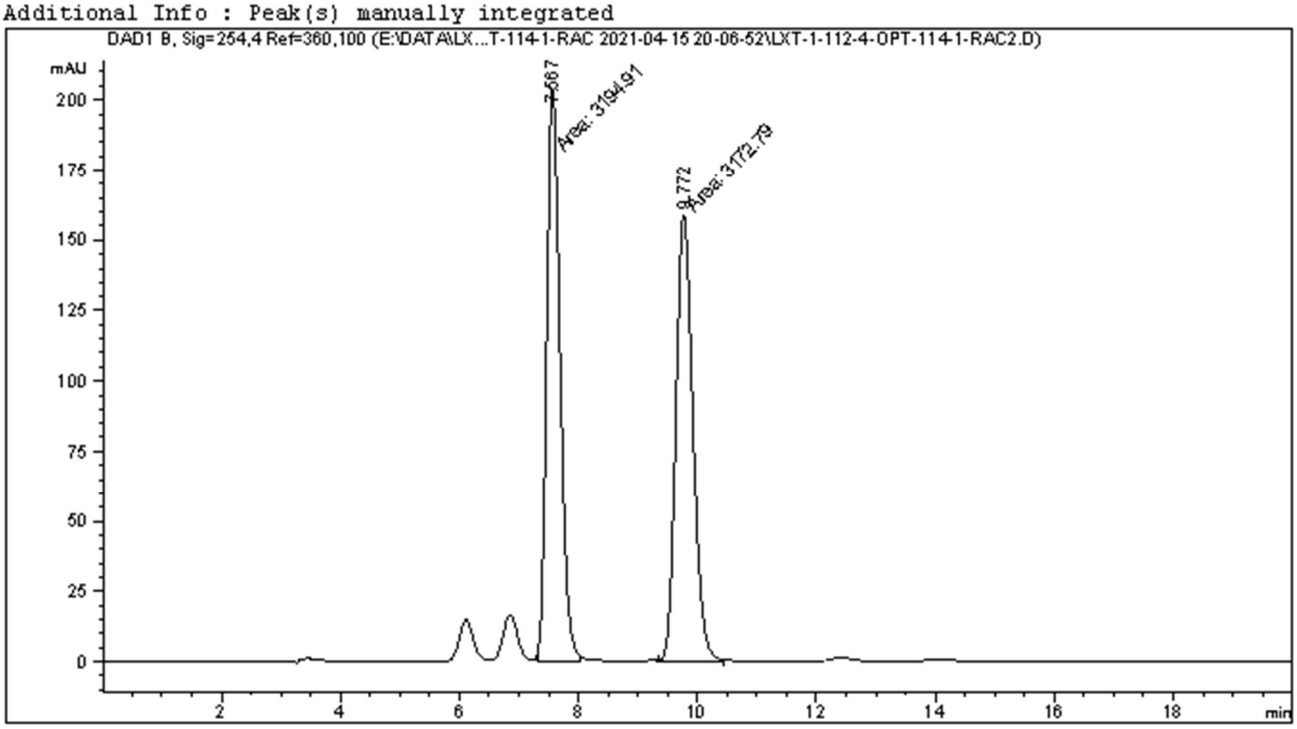


^{13}C NMR (101 MHz, Chloroform-*d*) of **3e**

Data File E:\DATA\LX...12-4-OPT-114-1-RAC 2021-04-15 20-06-52\LXT-1-112-4-OPT-114-1-RAC2.D
Sample Name: LXT-1-114-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 6
Injection Date : 4/15/2021 8:40:49 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-112-4-OPT-114-1-RAC 2021-04-15 20-06-52\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 4/15/2021 8:06:52 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-112-4-OPT-114-1-RAC 2021-04-15 20-06-52\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:15:32 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

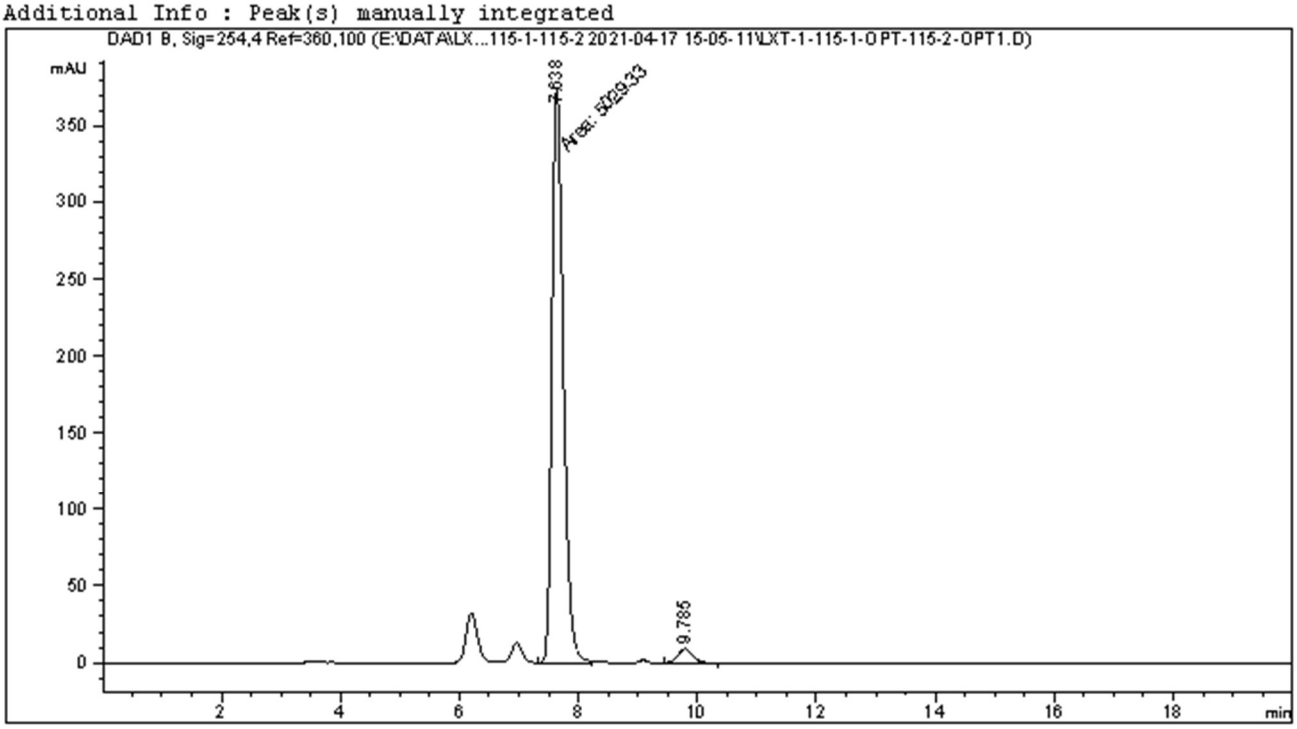
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.567	MF	0.2612	3194.90552	203.85030	50.1737
2	9.772	MF	0.3335	3172.78564	158.54521	49.8263

Totals : 6367.69116 362.39551

Data File E:\DATA\LXT\LXT-1-115-1-115-2 2021-04-17 15-05-11\LXT-1-115-1-OPT-115-2-OPT1.D
Sample Name: LXT-1-115-1-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 1
Injection Date : 4/17/2021 3:27:28 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-115-1-115-2 2021-04-17 15-05-11\1-ASH-98-2-1ML-10ul-20min -ALL-nml.M
Last changed : 4/17/2021 3:05:11 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-115-1-115-2 2021-04-17 15-05-11\1-ASH-98-2-1ML-10ul-20min -ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:19:31 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

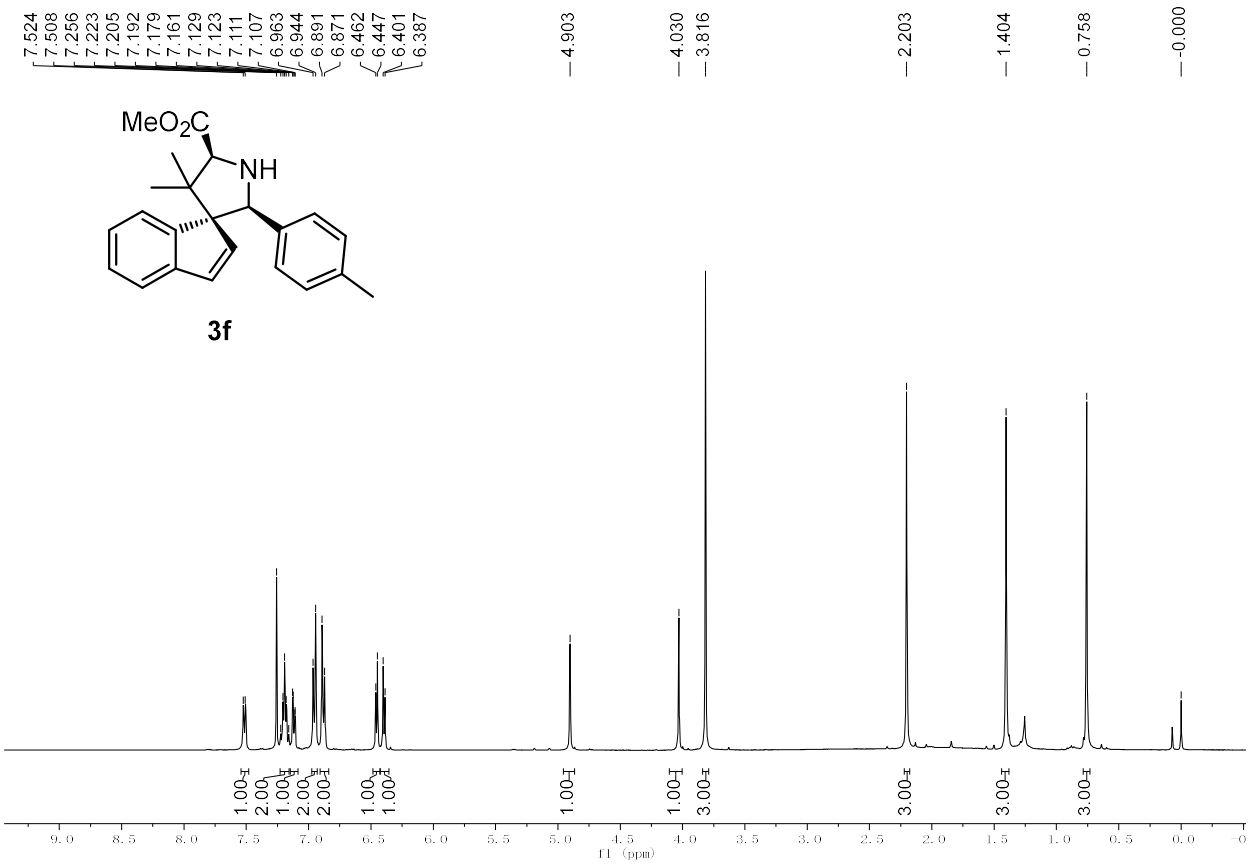
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

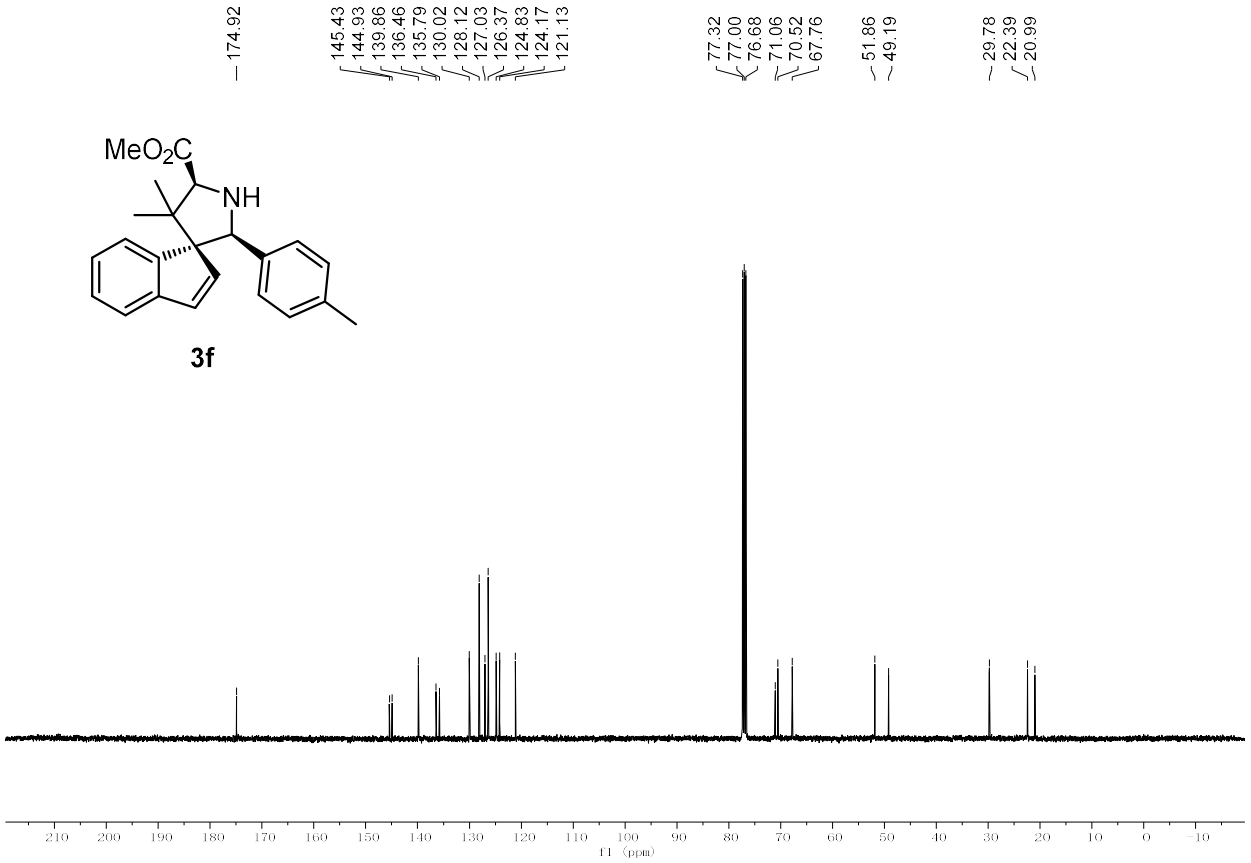
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.638	MF	0.2238	5029.32959	374.48706	97.0909
2	9.785	BB	0.2535	150.69257	8.90019	2.9091

Totals : 5180.02216 383.38725



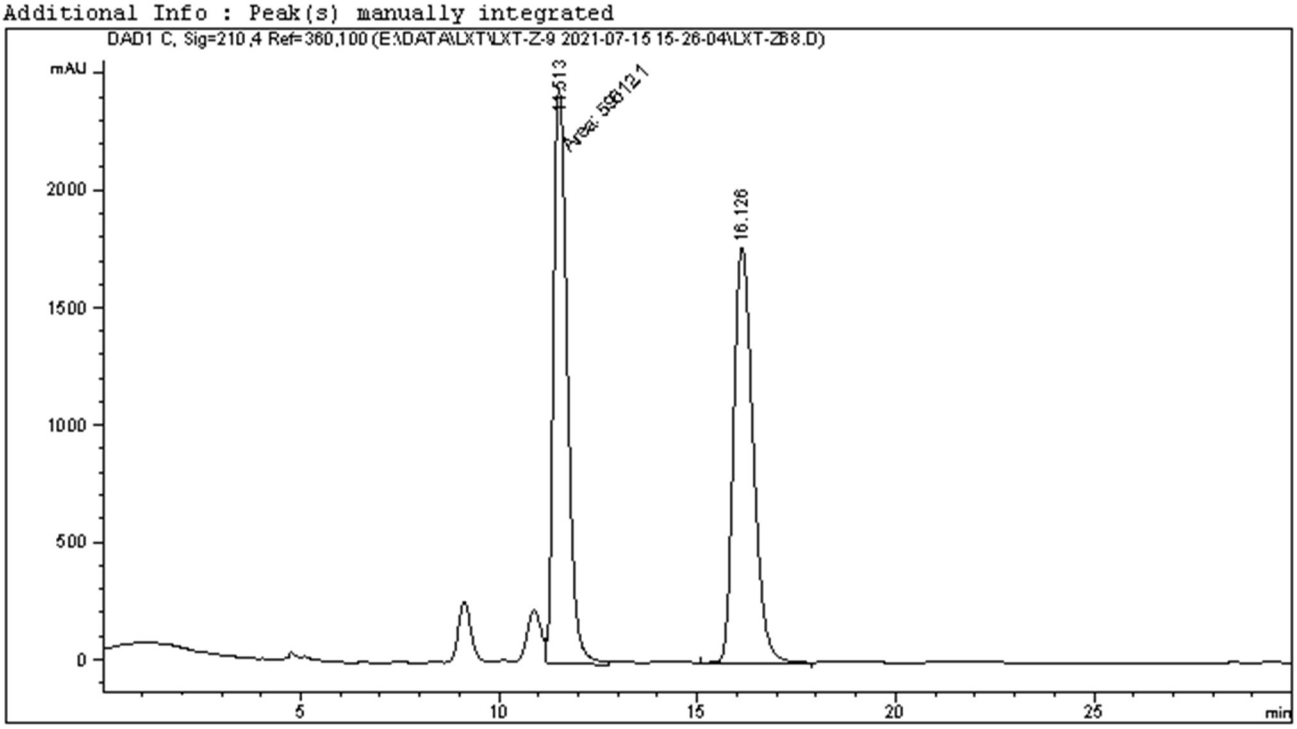
^{1}H NMR (400 MHz, Chloroform-*d*) of **3f**



^{13}C NMR (101 MHz, Chloroform-*d*) of **3f**

Data File E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\LXT-Z68.D
Sample Name: LXT-1-112-1-RAC

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   9
Acq. Instrument : 1260                           Location :   6
Injection Date  : 7/15/2021 6:17:52 PM                Inj :   1
                                               Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-99-1-0.7ML-10ul-30min-ALL-nml
                  .M
Last changed    : 7/15/2021 3:26:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-99-1-0.7ML-10ul-30min-ALL-nml
                  .M (Sequence Method)
Last changed    : 7/31/2021 5:44:48 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 C, Sig=210,4 Ref=360,100

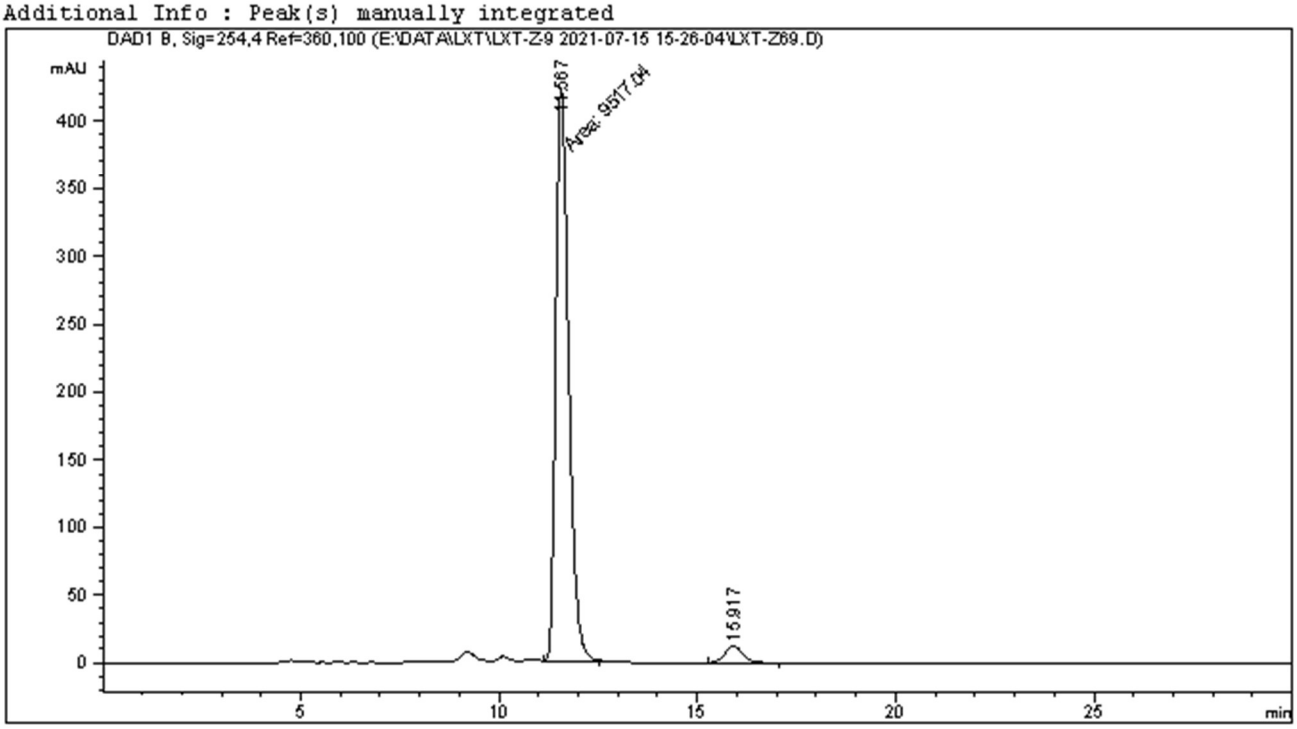
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.513 FM    0.4053 5.96121e4  2451.63062  49.5900
   2  16.126 BB    0.5364 6.05978e4  1770.10437  50.4100

Totals :                  1.20210e5  4221.73499
```

Data File E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\LXT-Z69.D
Sample Name: LXT-1-116-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 10
Acq. Instrument : 1260 Location : 7
Injection Date : 7/15/2021 6:49:23 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-99-1-0.7ML-10ul-30min-ALL-nml .M
Last changed : 7/15/2021 3:26:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-99-1-0.7ML-10ul-30min-ALL-nml .M (Sequence Method)
Last changed : 8/1/2021 11:25:15 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

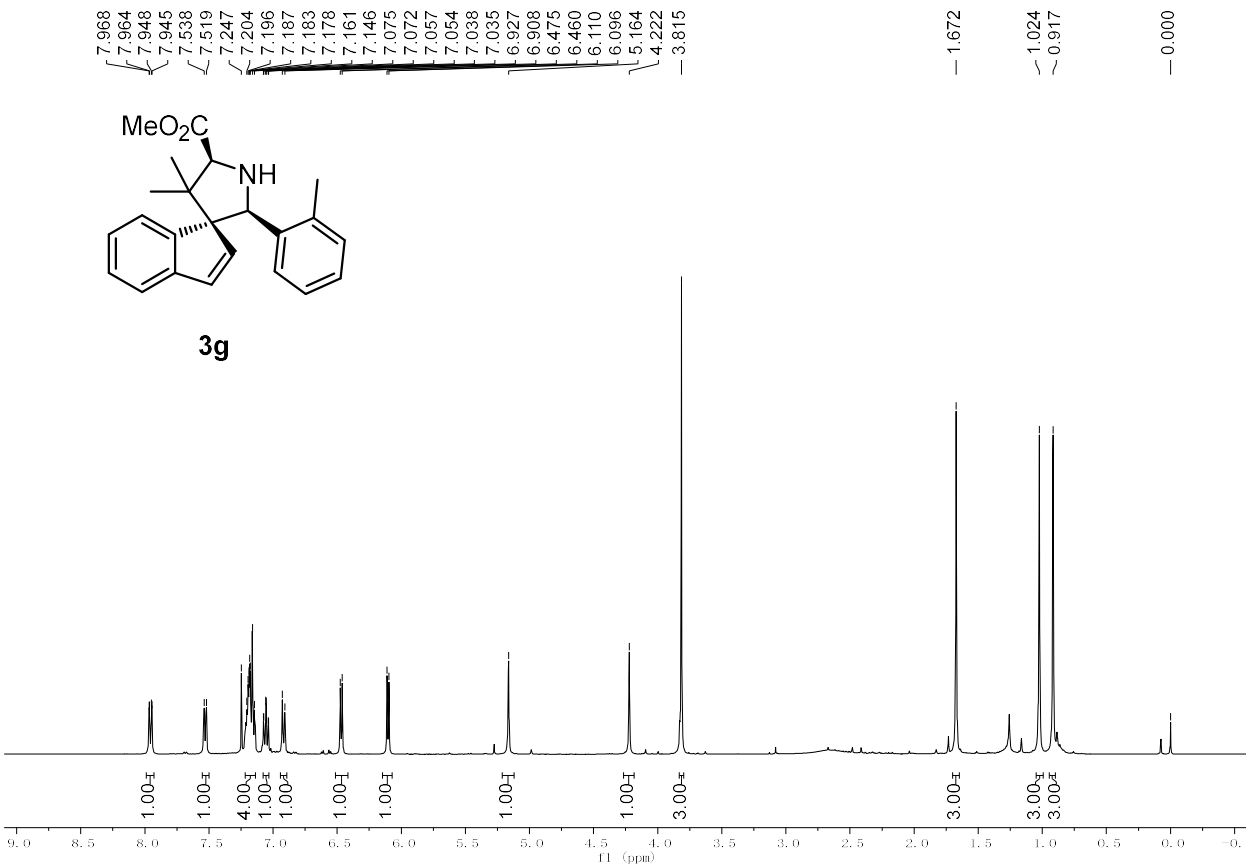
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

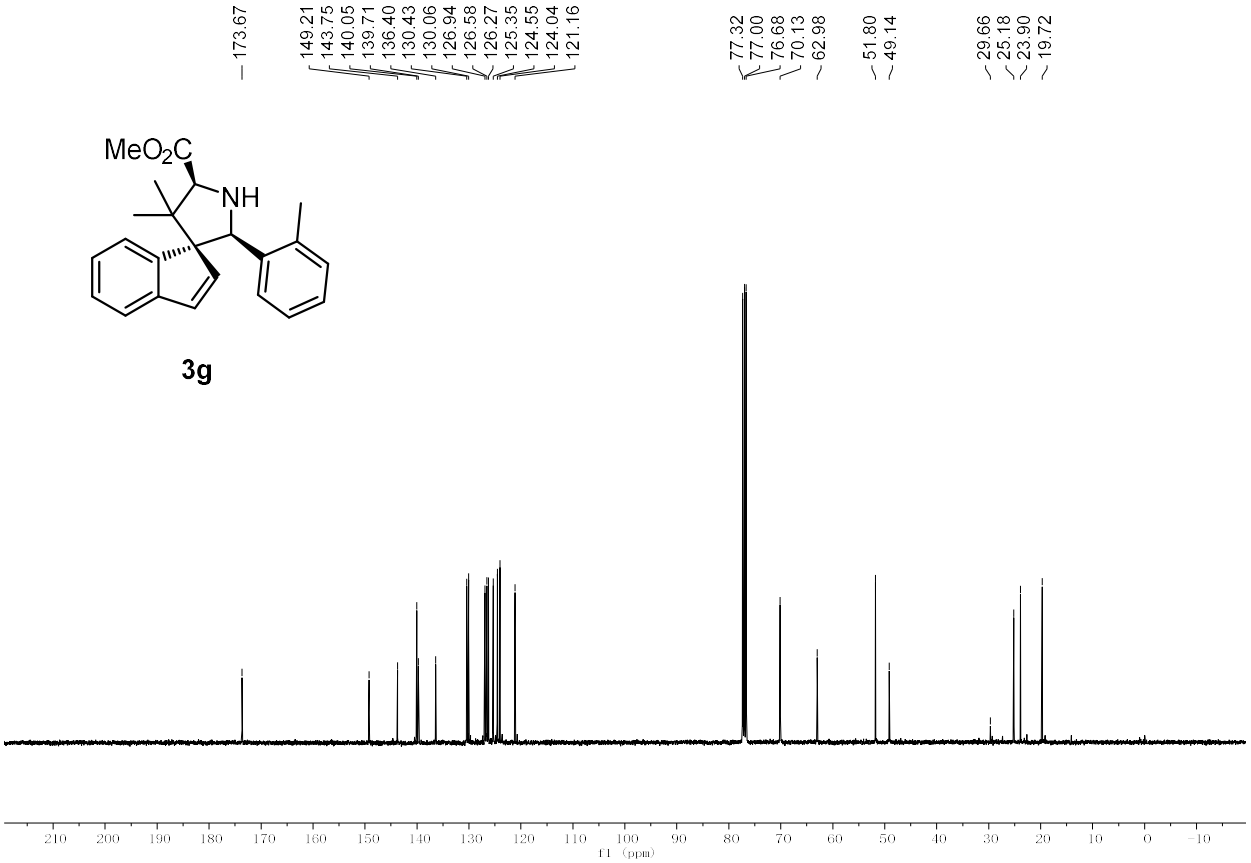
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.567	MF	0.3751	9517.04004	422.88391	96.0741
2	15.917	BB	0.4378	388.90176	12.23728	3.9259

Totals : 9905.94180 435.12119



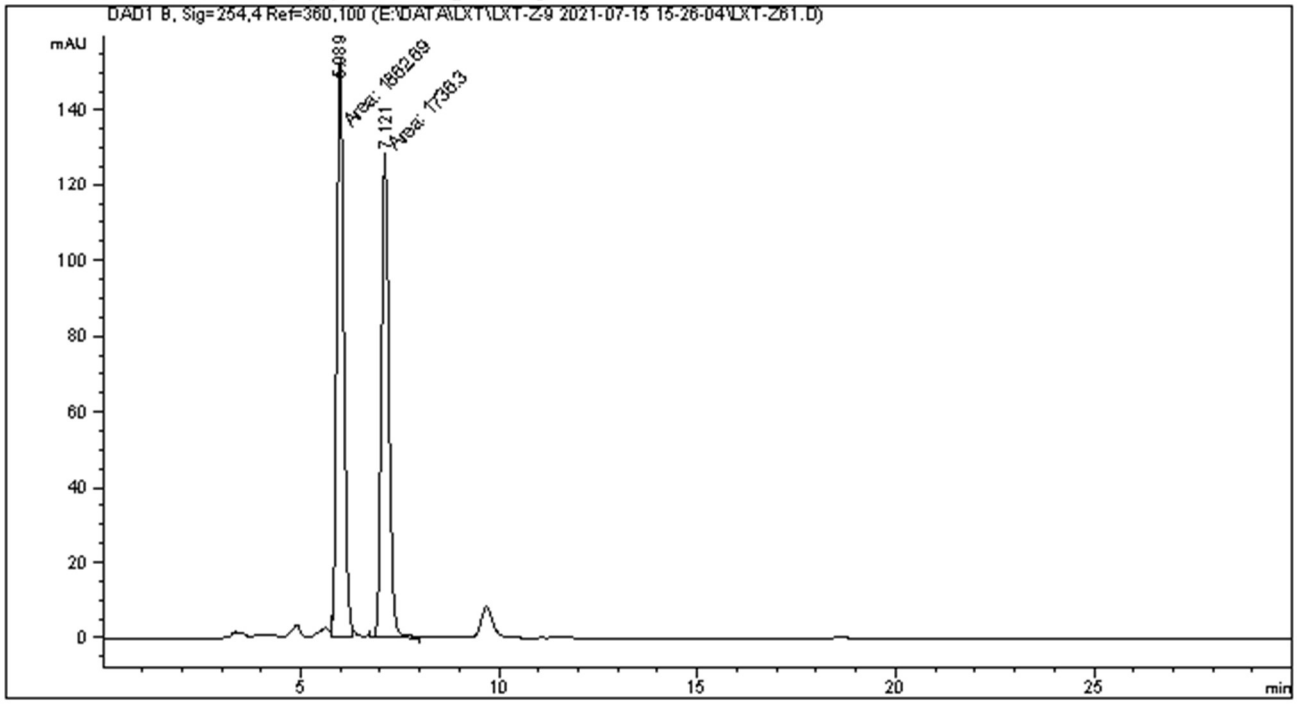
^{1}H NMR (400 MHz, Chloroform-*d*) of **3g**



^{13}C NMR (101 MHz, Chloroform-*d*) of **3g**

Data File E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\LXT-Z61.D
Sample Name: LXT-1-104-4-RAC

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :   2
Acq. Instrument : 1260                             Location :   1
Injection Date  : 7/15/2021 3:38:31 PM                  Inj :   1
                                                 Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed    : 7/15/2021 3:26:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
                  (Sequence Method)
Last changed    : 8/1/2021 11:29:44 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100

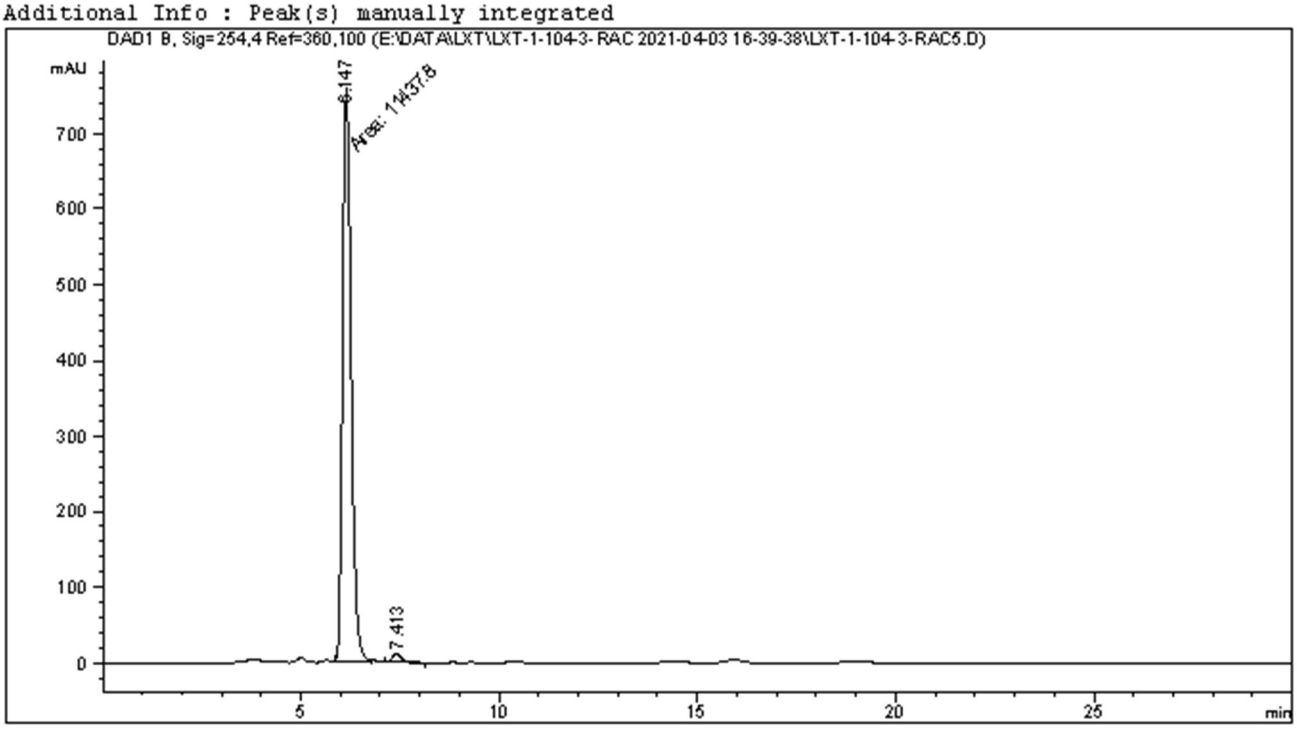
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.989 FM    0.2041 1862.68665  152.08989  51.7559
   2   7.121 MM    0.2256 1736.30017  128.27611  48.2441

Totals :                  3598.98682  280.36600
```

Data File E:\DATA\LXT\LXT-1-104-3-RAC 2021-04-03 16-39-38\LXT-1-104-3-RAC5.D
Sample Name: LXT-1-104-1-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 6
Acq. Instrument : 1260 Location : 4
Injection Date : 4/3/2021 7:18:30 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-104-3-RAC 2021-04-03 16-39-38\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 4/3/2021 4:39:38 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-104-3-RAC 2021-04-03 16-39-38\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:33:44 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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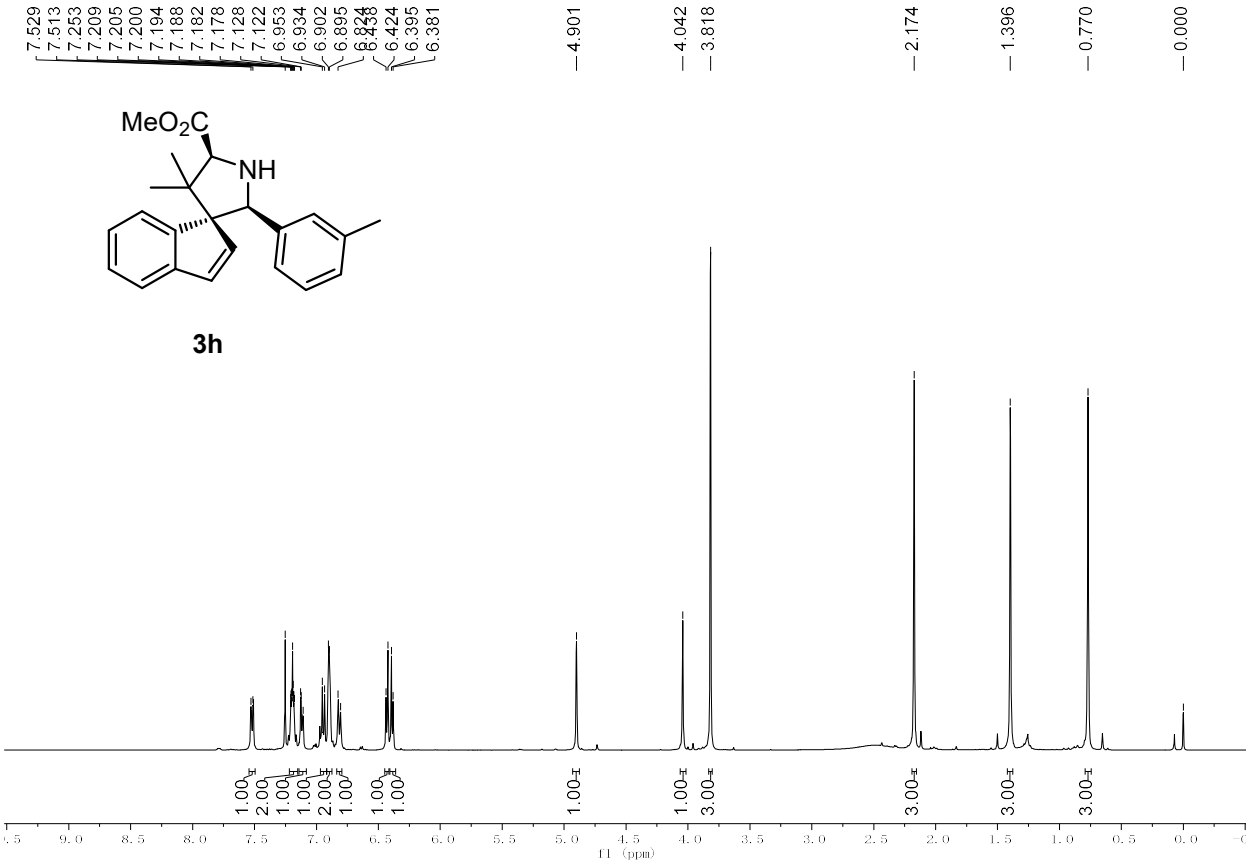
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

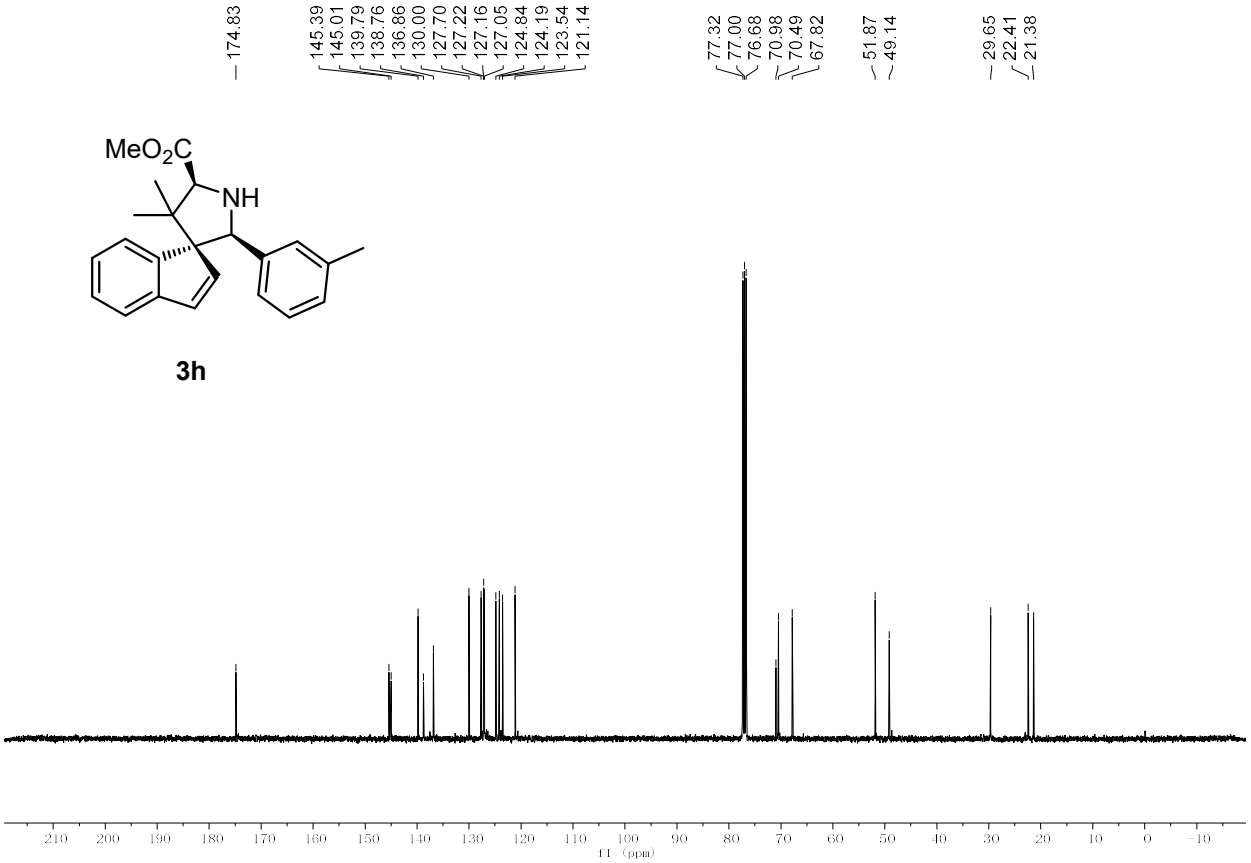
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.147	MF	0.2512	1.14378e4	758.91107	98.4454
2	7.413	BB	0.2536	180.62497	10.88670	1.5546

Totals : 1.16184e4 769.79777



^{1}H NMR (400 MHz, Chloroform-*d*) of **3h**

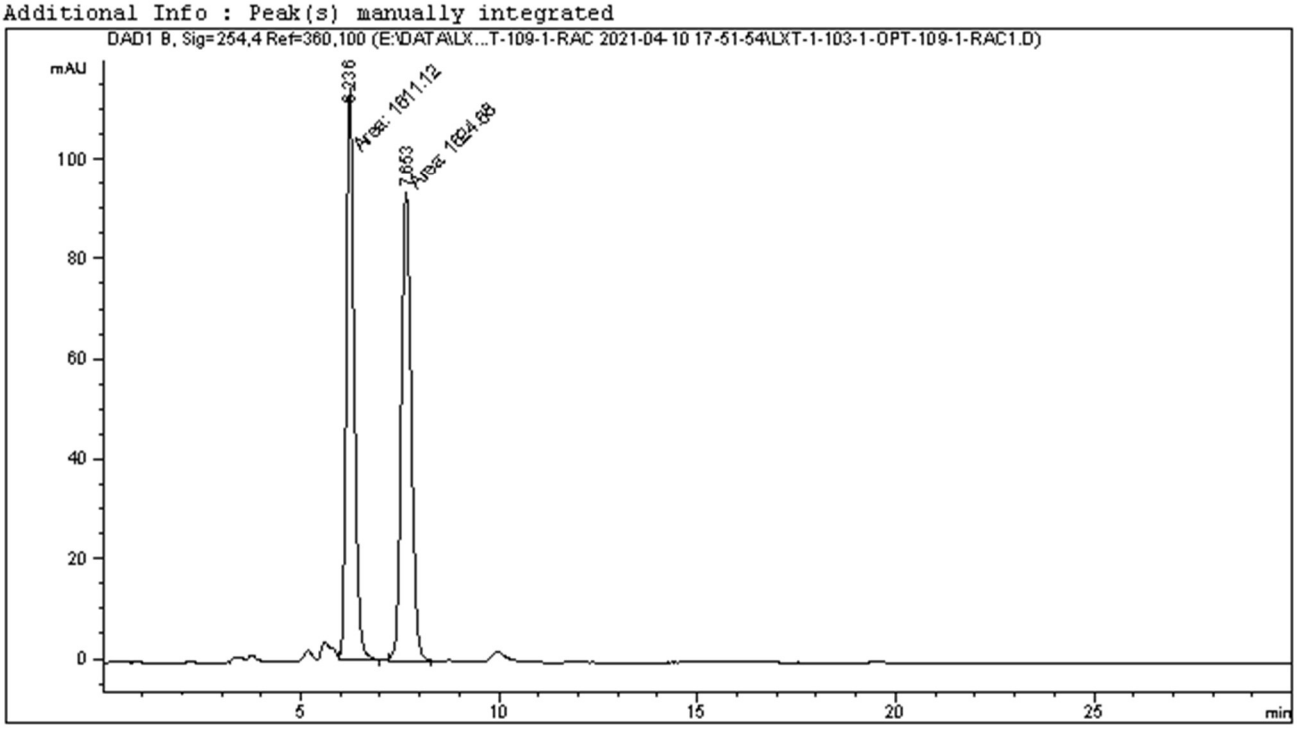


^{13}C NMR (101 MHz, Chloroform-*d*) of **3h**

Data File E:\DATA\LX...03-1-OPT-109-1-RAC 2021-04-10 17-51-54\LXT-1-103-1-OPT-109-1-RAC1.D
Sample Name: LXT-1-109-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 4
Injection Date : 4/10/2021 6:04:20 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-103-1-OPT-109-1-RAC 2021-04-10 17-51-54\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 4/10/2021 5:51:54 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-103-1-OPT-109-1-RAC 2021-04-10 17-51-54\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:43:49 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

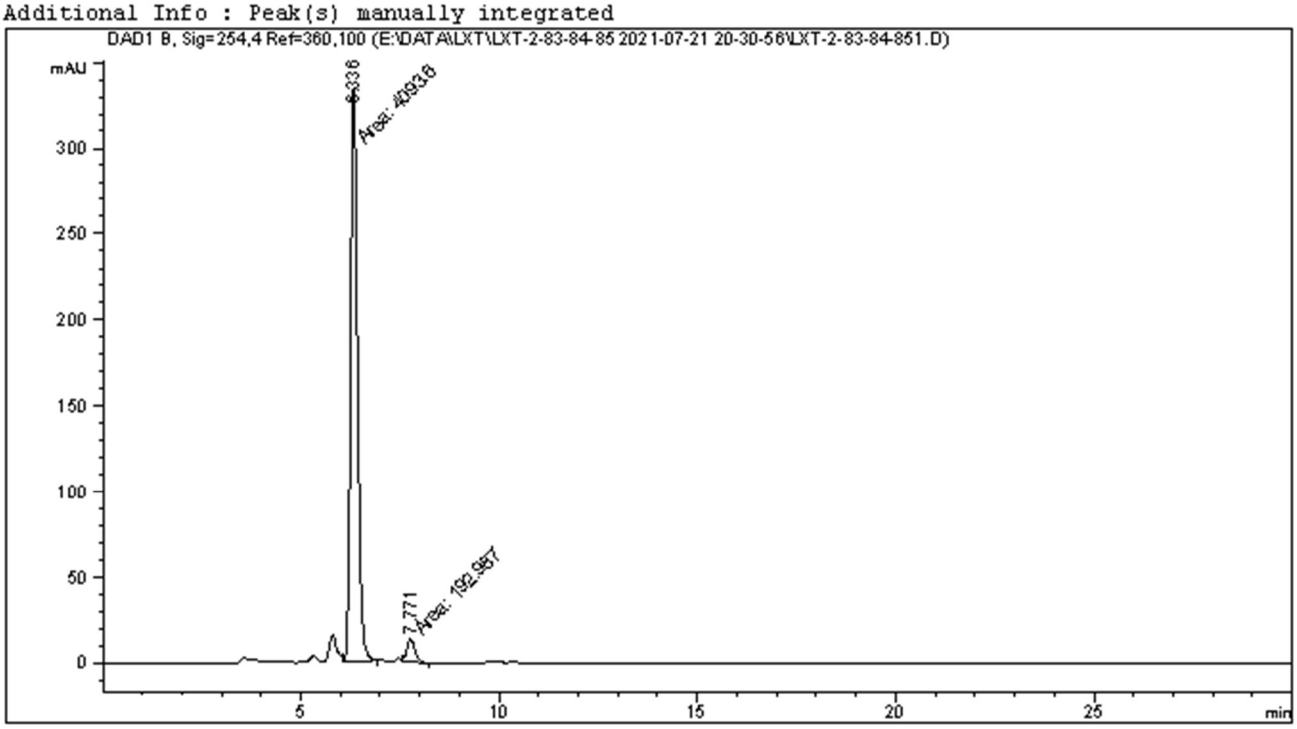
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.236	FM	0.2344	1611.12109	114.53738	49.7905
2	7.653	MF	0.2890	1624.68152	93.69435	50.2095

Totals : 3235.80261 208.23174

Data File E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\LXT-2-83-84-851.D
Sample Name: LXT-2-84-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 31
Injection Date : 7/21/2021 8:43:43 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 7/21/2021 8:30:56 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:49:34 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

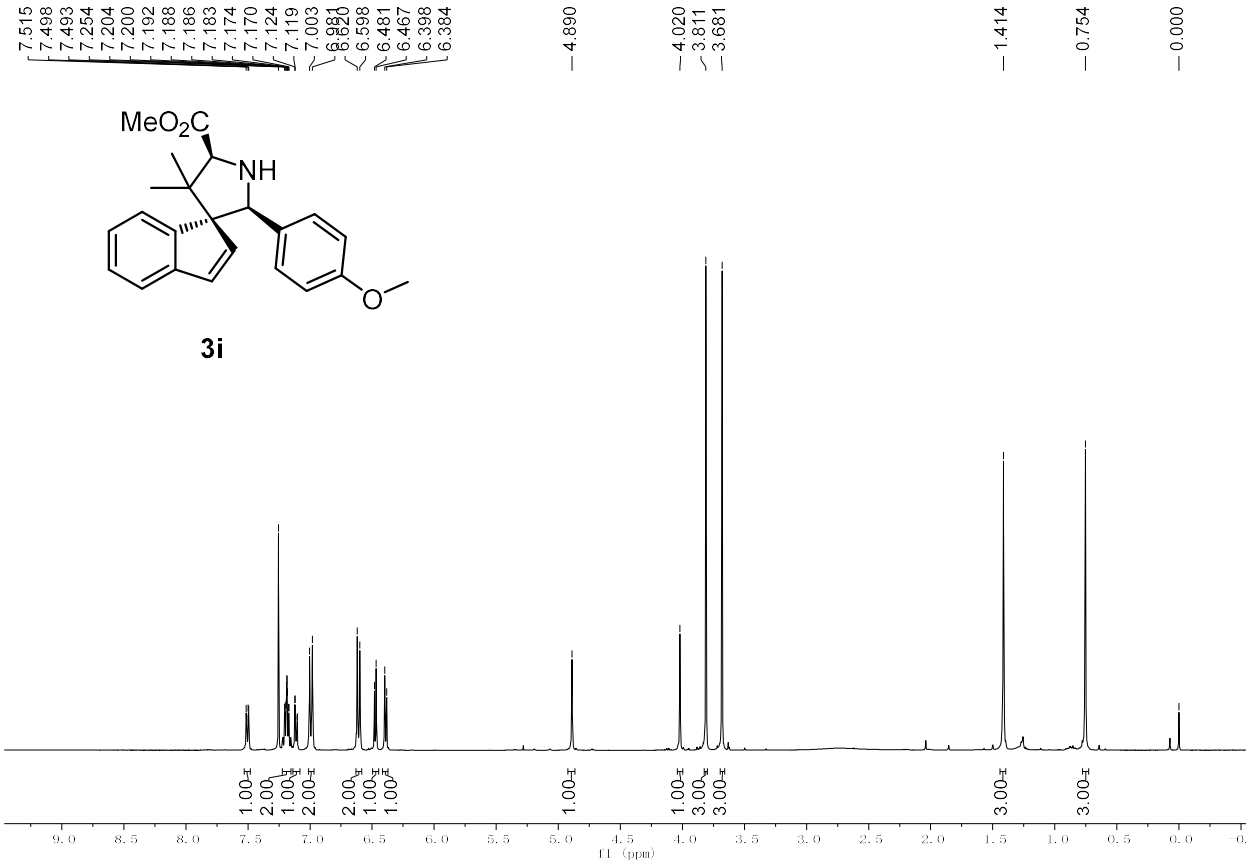
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

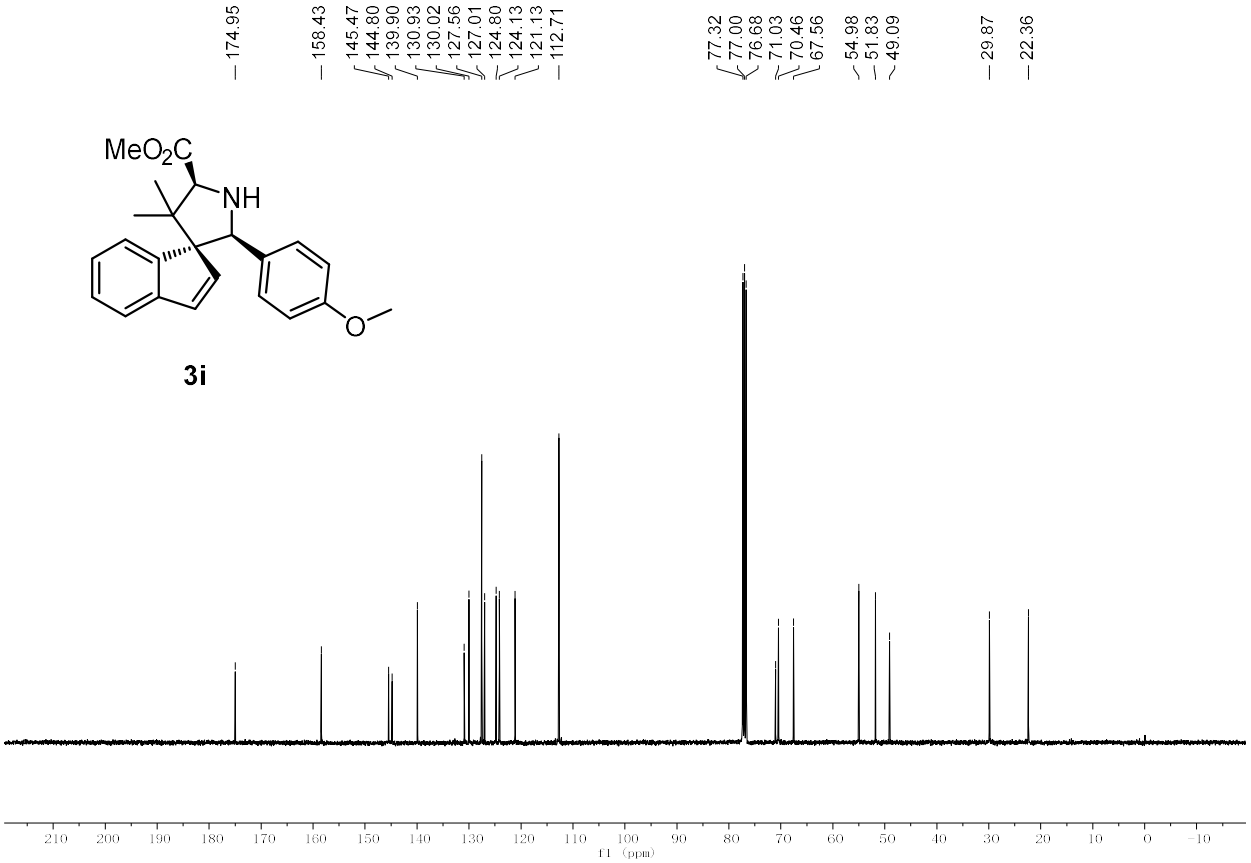
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.336	FM	0.2041	4093.59595	334.28778	95.4979
2	7.771	FM	0.2341	192.98651	13.73678	4.5021

Totals : 4286.58246 348.02457



^{1}H NMR (400 MHz, Chloroform-*d*) of **3i**

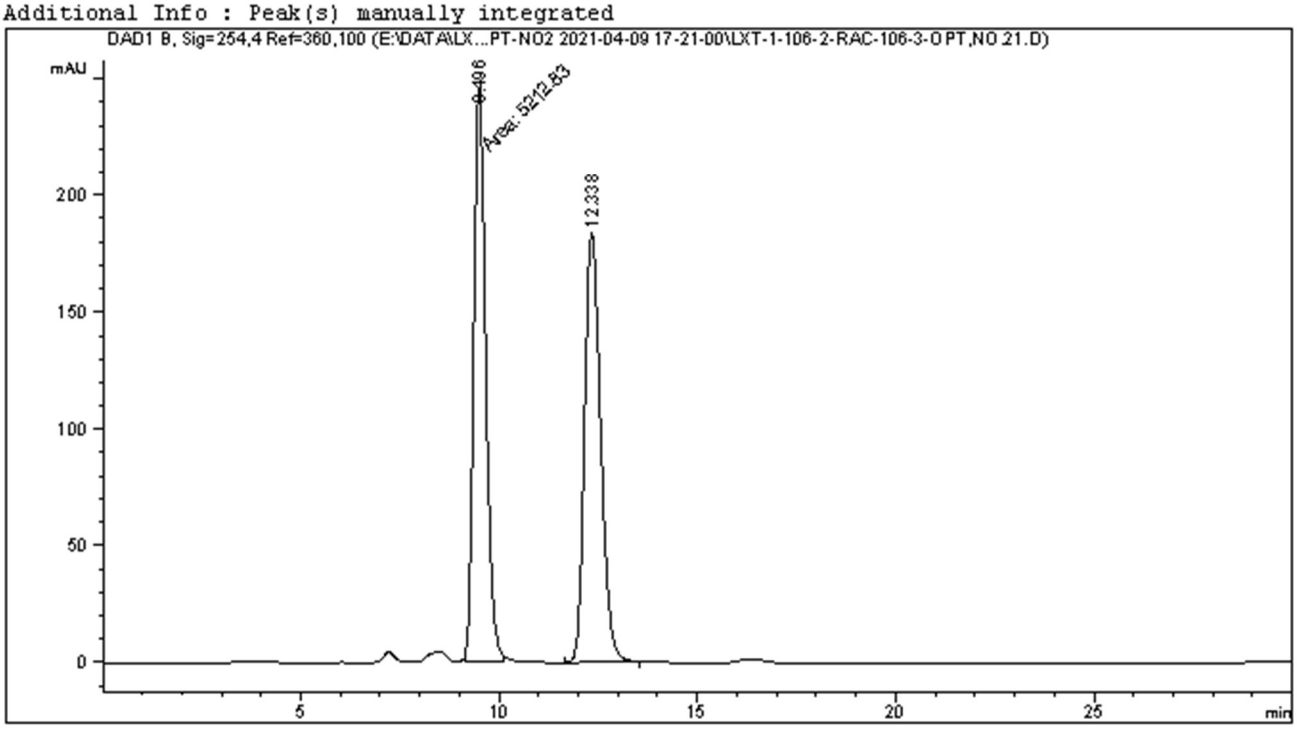


^{13}C NMR (101 MHz, Chloroform-*d*) of **3i**

Data File E:\DATA\LX...RAC-3-OPT-NO2 2021-04-09 17-21-00\LXT-1-106-2-RAC-106-3-OPT,NO.21.D
Sample Name: LXT-1-106-2-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 4
Injection Date : 4/9/2021 5:33:30 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-106-2-RAC-3-OPT-NO2 2021-04-09 17-21-00\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 4/9/2021 5:21:00 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-106-2-RAC-3-OPT-NO2 2021-04-09 17-21-00\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:54:07 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

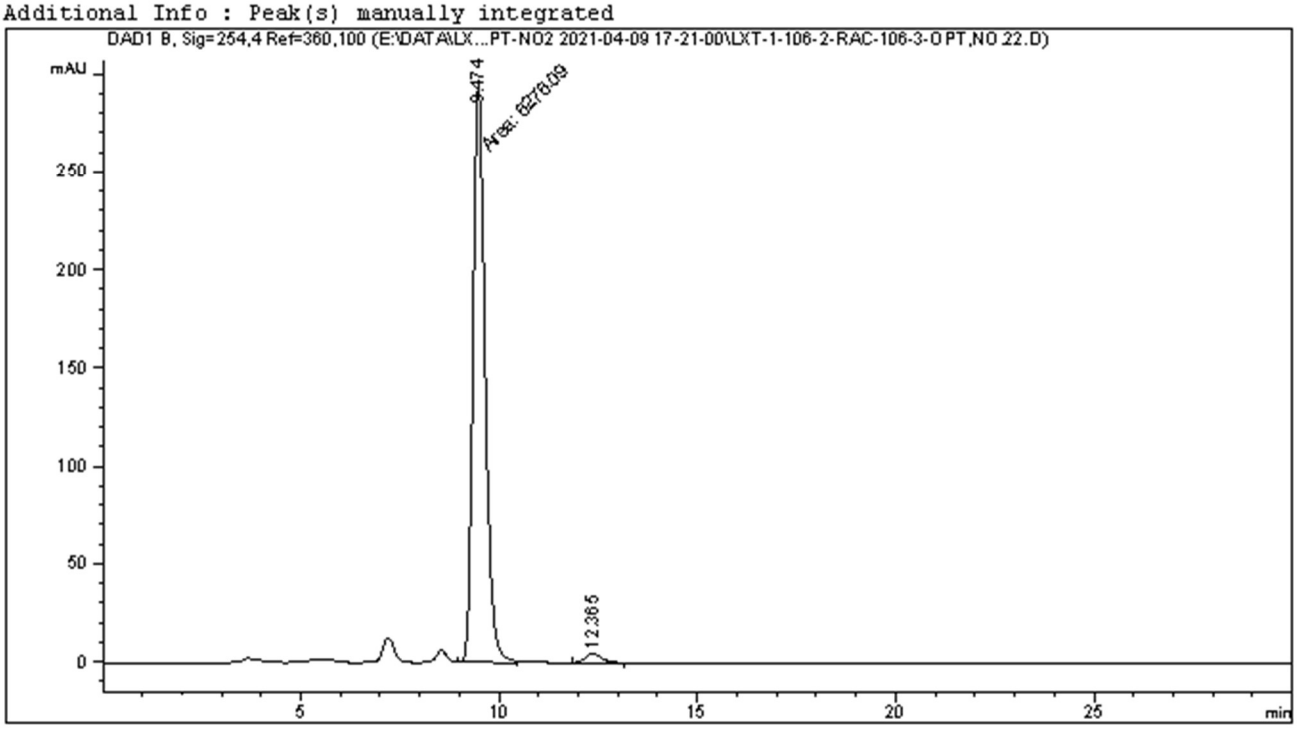
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.496	FM	0.3536	5212.83105	245.73468	50.2242
2	12.338	BB	0.4382	5166.28906	183.64671	49.7758

Totals : 1.03791e4 429.38139

Data File E:\DATA\LX...RAC-3-OPT-NO2 2021-04-09 17-21-00\LXT-1-106-2-RAC-106-3-OPT,NO.22.D
Sample Name: LXT-1-106-3-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 5
Injection Date : 4/9/2021 6:05:04 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-106-2-RAC-3-OPT-NO2 2021-04-09 17-21-00\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M
Last changed : 4/9/2021 5:21:00 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-106-2-RAC-3-OPT-NO2 2021-04-09 17-21-00\1-ASH-95-5-1ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 11:56:21 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

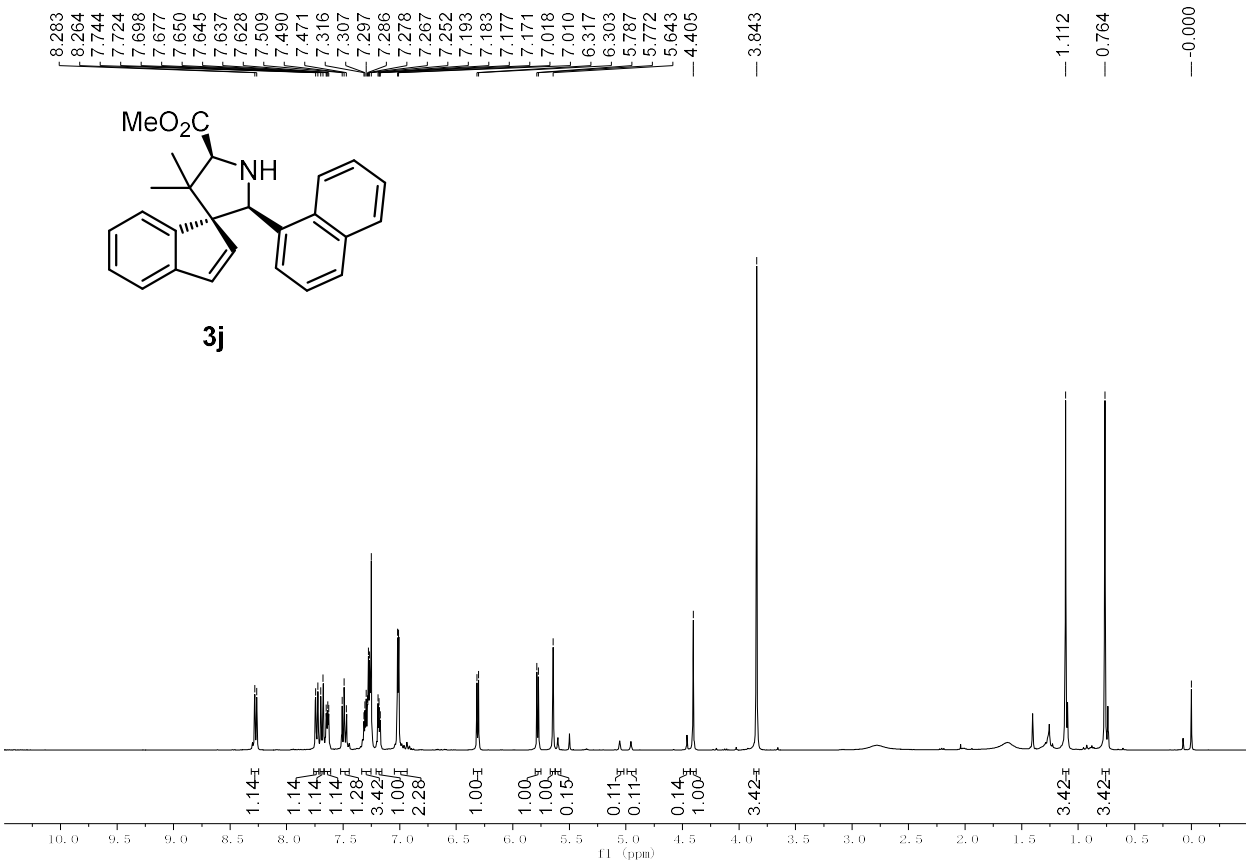
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

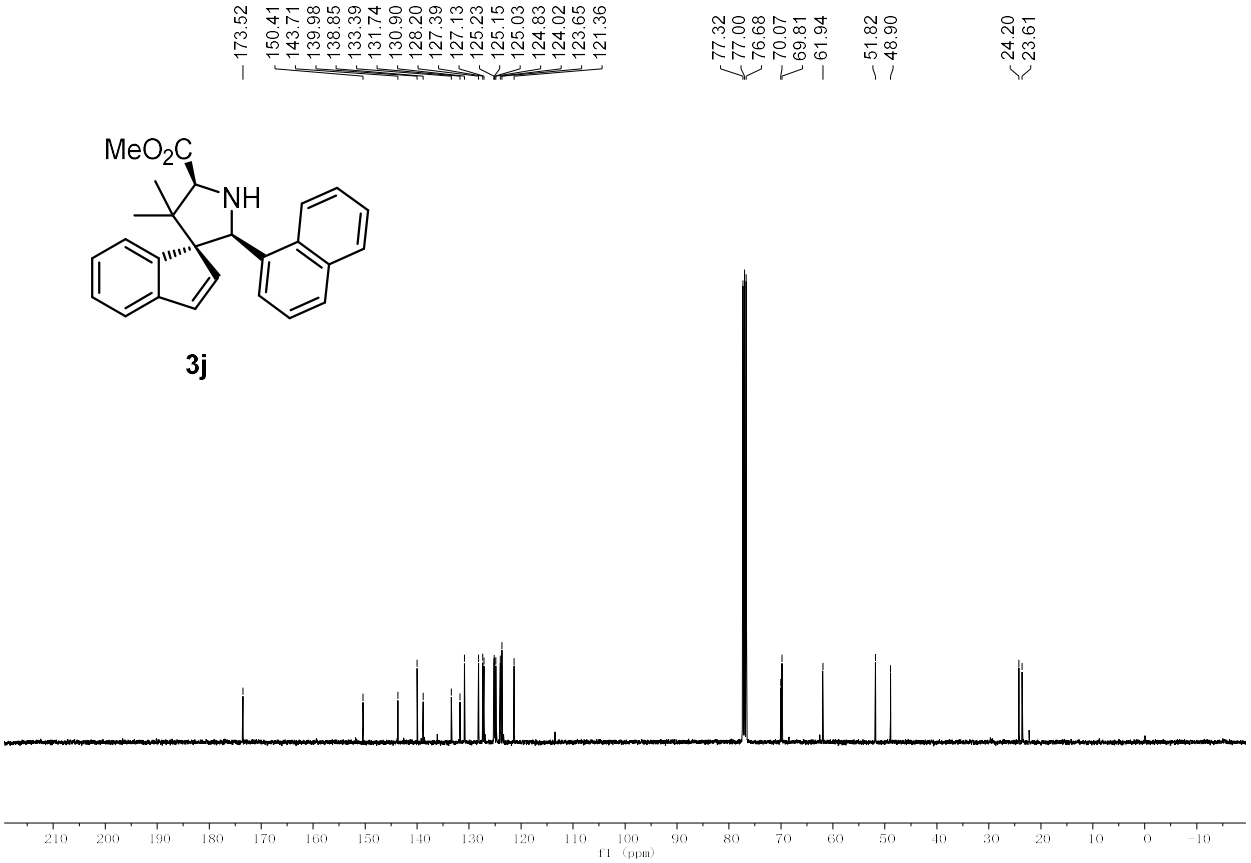
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.474	MF	0.3570	6276.08936	293.04166	98.0339
2	12.365	BB	0.3285	125.87195	4.51204	1.9661

Totals : 6401.96130 297.55370



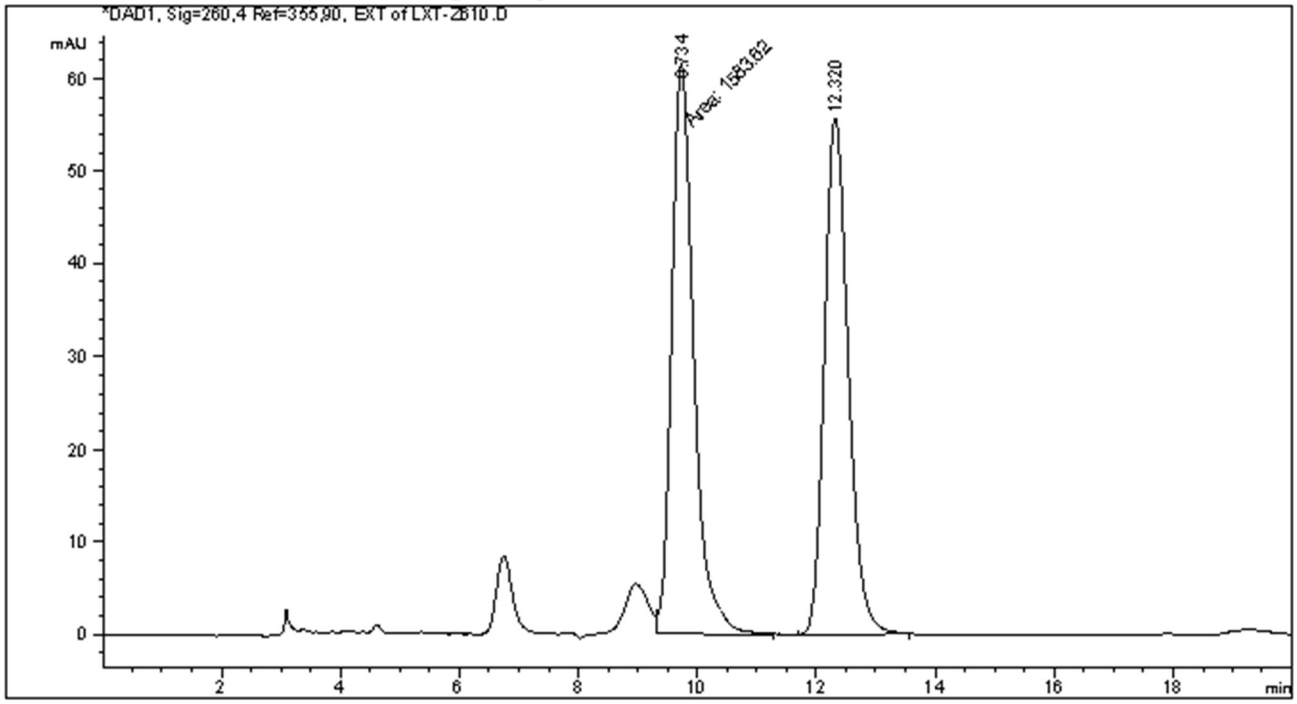
^{1}H NMR (400 MHz, Chloroform-*d*) of **3j**



^{13}C NMR (101 MHz, Chloroform-*d*) of **3j**

Data File E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\LXT-Z610.D
Sample Name: LXT-1-120-2-RAC

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :  11
Acq. Instrument : 1260                             Location :   8
Injection Date  : 7/15/2021 7:20:54 PM                  Inj :   1
                                                 Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed    : 7/15/2021 3:26:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-9 2021-07-15 15-26-04\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
                  (Sequence Method)
Last changed    : 7/31/2021 5:35:44 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

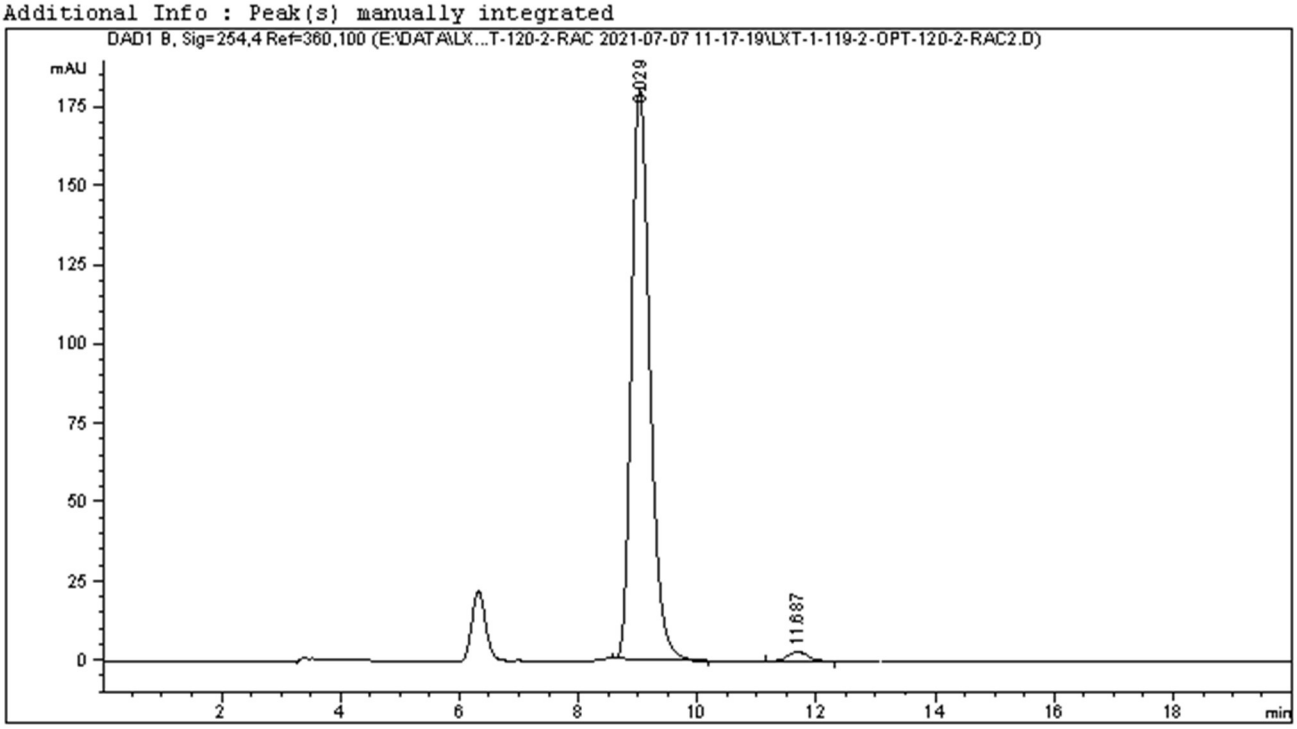

Signal 1: DAD1, Sig=260,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.734 FM    0.4287 1583.61890   61.56947  50.4932
   2  12.320 BB    0.4187 1552.68518   55.79594  49.5068

Totals :                  3136.30408  117.36541
```

Data File E:\DATA\LX...19-2-OPT-120-2-RAC 2021-07-07 11-17-19\LXT-1-119-2-OPT-120-2-RAC2.D
Sample Name: LXT-1-119-2-OPT

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1260                           Location :   32
Injection Date  : 7/7/2021 12:01:05 PM                Inj :   1
                                              Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-1-119-2-OPT-120-2-RAC 2021-07-07 11-17-19\1-ASH-98-2-1ML-
                  10ul-20min-ALL-nml.M
Last changed    : 7/7/2021 11:17:19 AM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-119-2-OPT-120-2-RAC 2021-07-07 11-17-19\1-ASH-98-2-1ML-
                  10ul-20min-ALL-nml.M (Sequence Method)
Last changed    : 8/1/2021 11:59:30 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



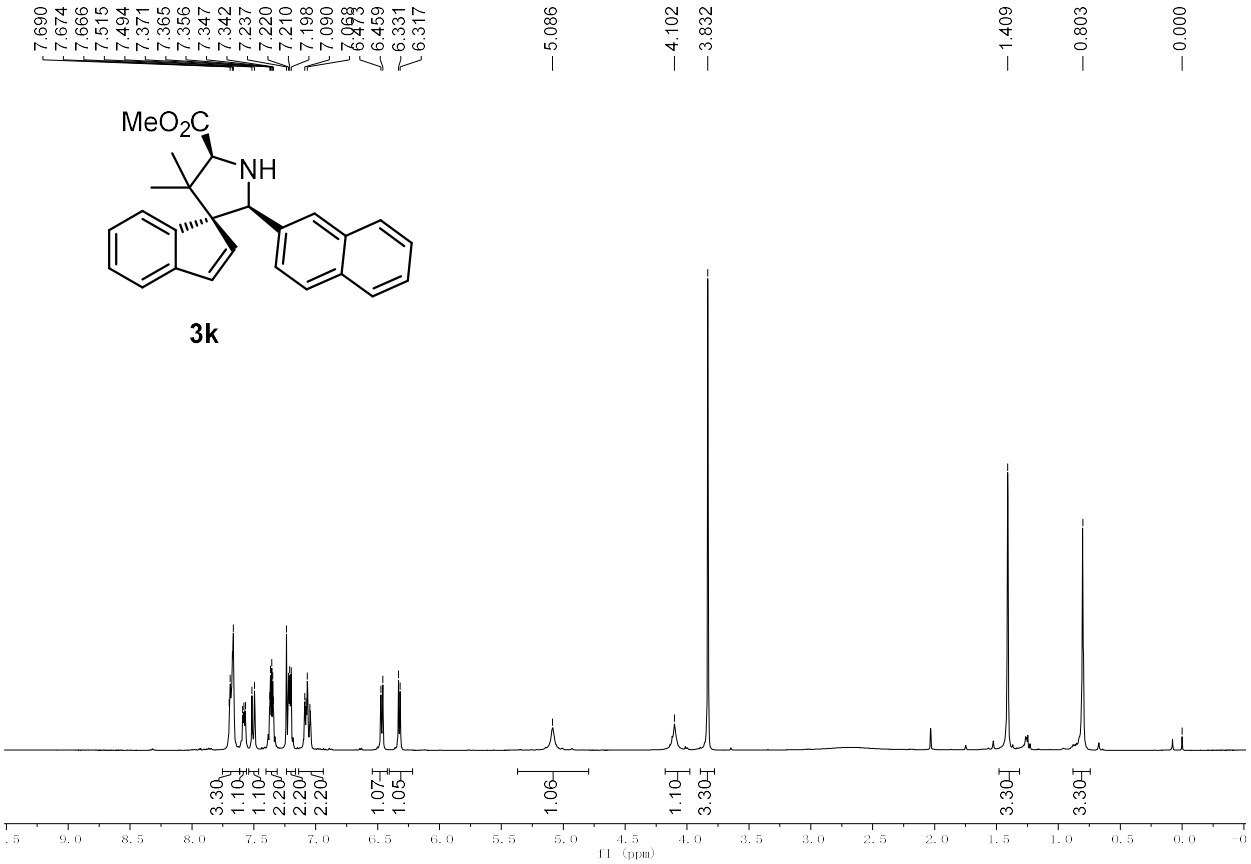

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs

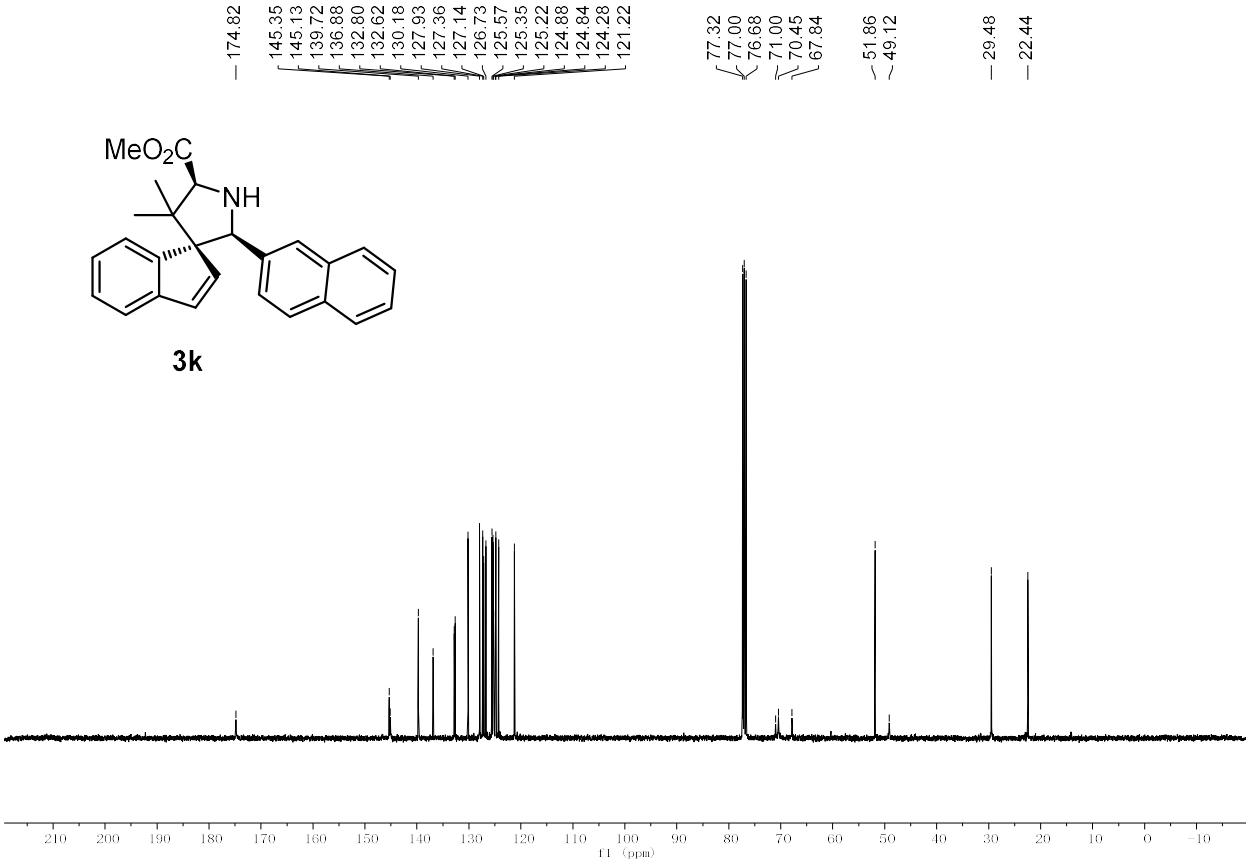

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.029 BB    0.3341 3870.81812  180.57016  98.1061
   2  11.687 BB    0.2963   74.72411    3.02438   1.8939

Totals :                  3945.54222  183.59454
```



^{1}H NMR (400 MHz, Chloroform-*d*) of **3k**

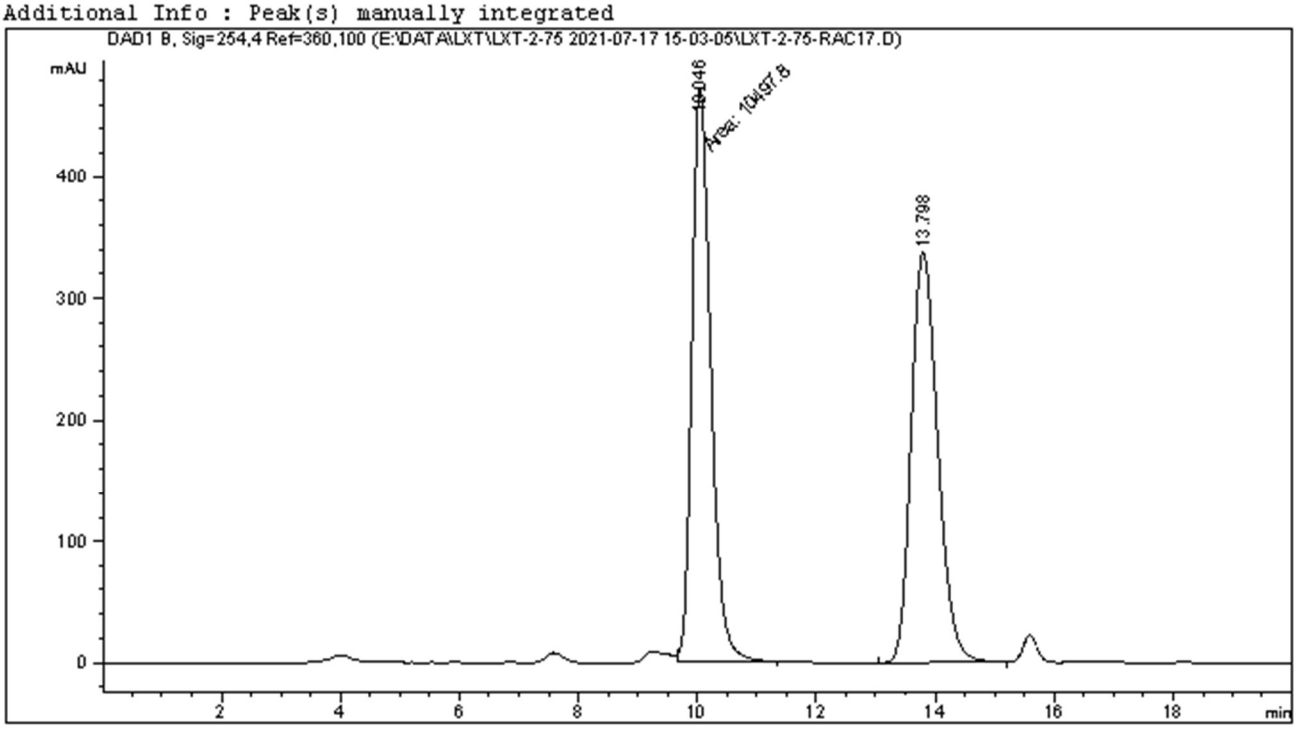


^{13}C NMR (101 MHz, Chloroform-*d*) of **3k**

Data File E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\LXT-2-75-RAC17.D
Sample Name: LXT-2-73-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 18
Acq. Instrument : 1260 Location : 21
Injection Date : 7/17/2021 8:20:31 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/17/2021 3:03:05 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:01:39 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

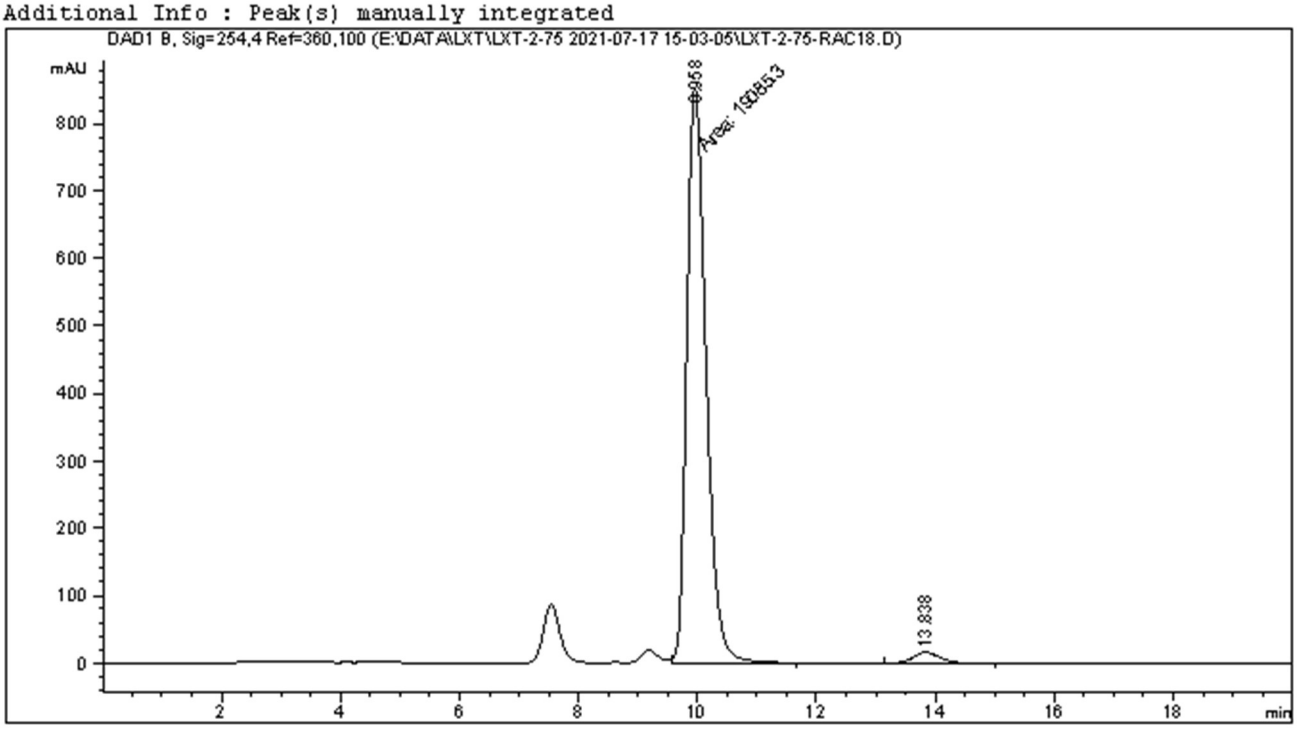
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.046	FM	0.3700	1.04978e4	472.89676	50.0655
2	13.798	BB	0.4772	1.04703e4	337.28500	49.9345

Totals : 2.09681e4 810.18176

Data File E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\LXT-2-75-RAC18.D
Sample Name: LXT-1-115-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 19
Acq. Instrument : 1260 Location : 22
Injection Date : 7/17/2021 8:41:58 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/17/2021 3:03:05 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:03:06 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

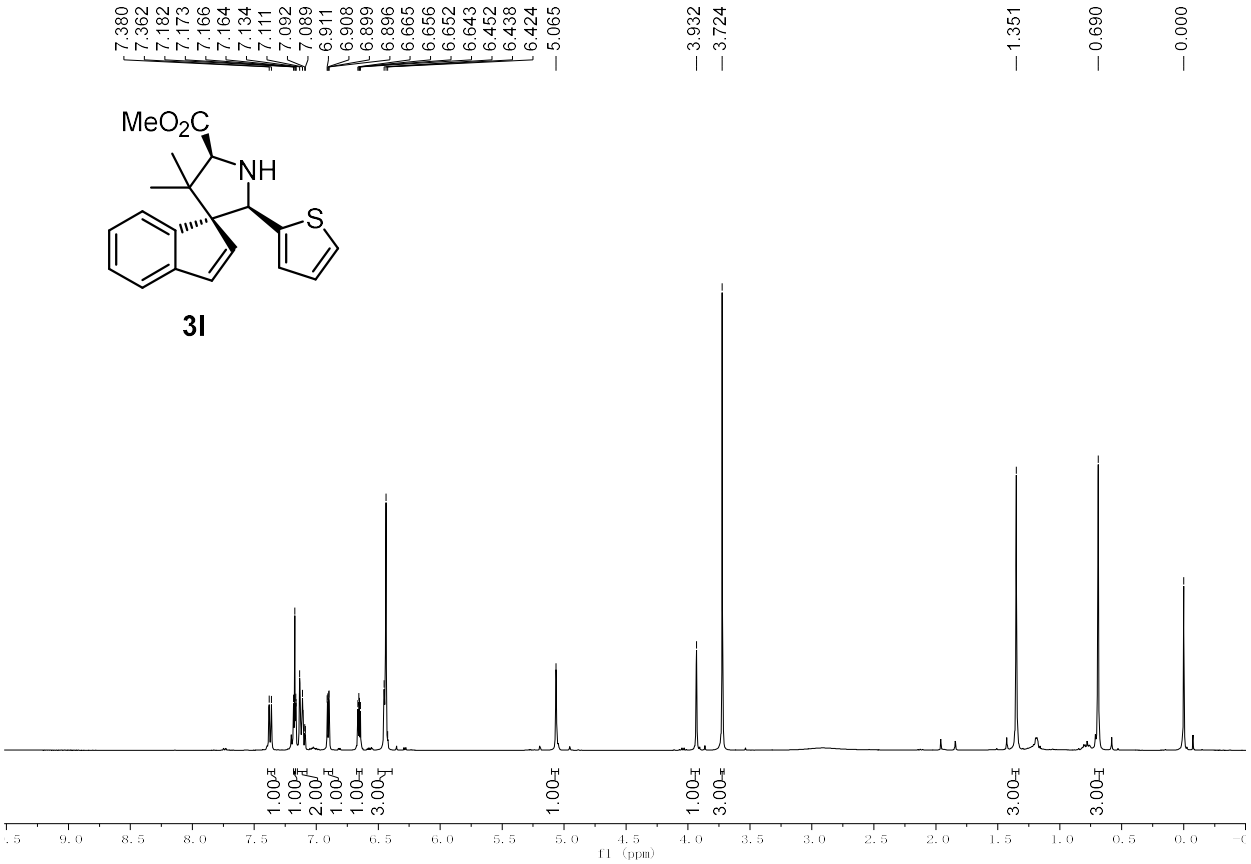
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

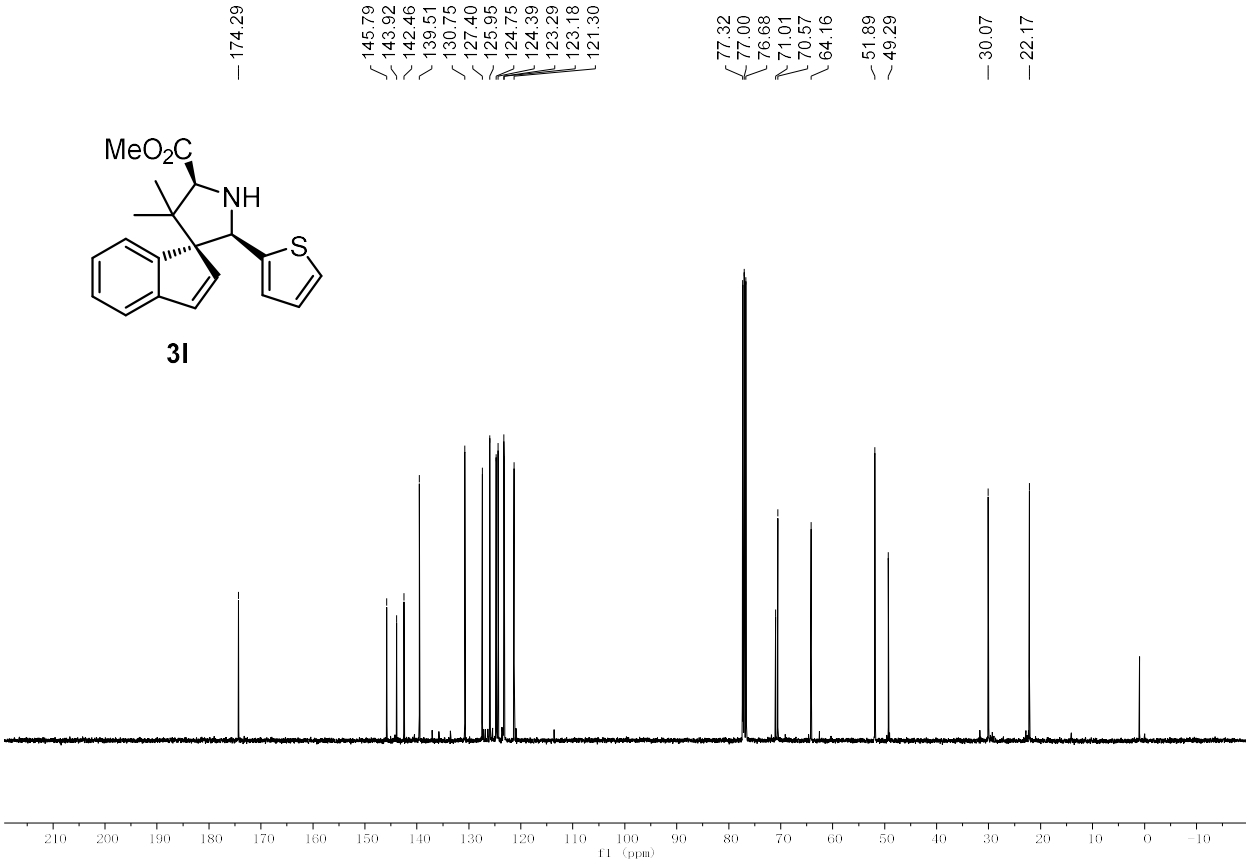
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.958	FM	0.3732	1.90853e4	852.26733	97.6073
2	13.838	BB	0.4297	467.84048	15.65163	2.3927

Totals : 1.95532e4 867.91897



^{1}H NMR (400 MHz, Chloroform-*d*) of **3l**

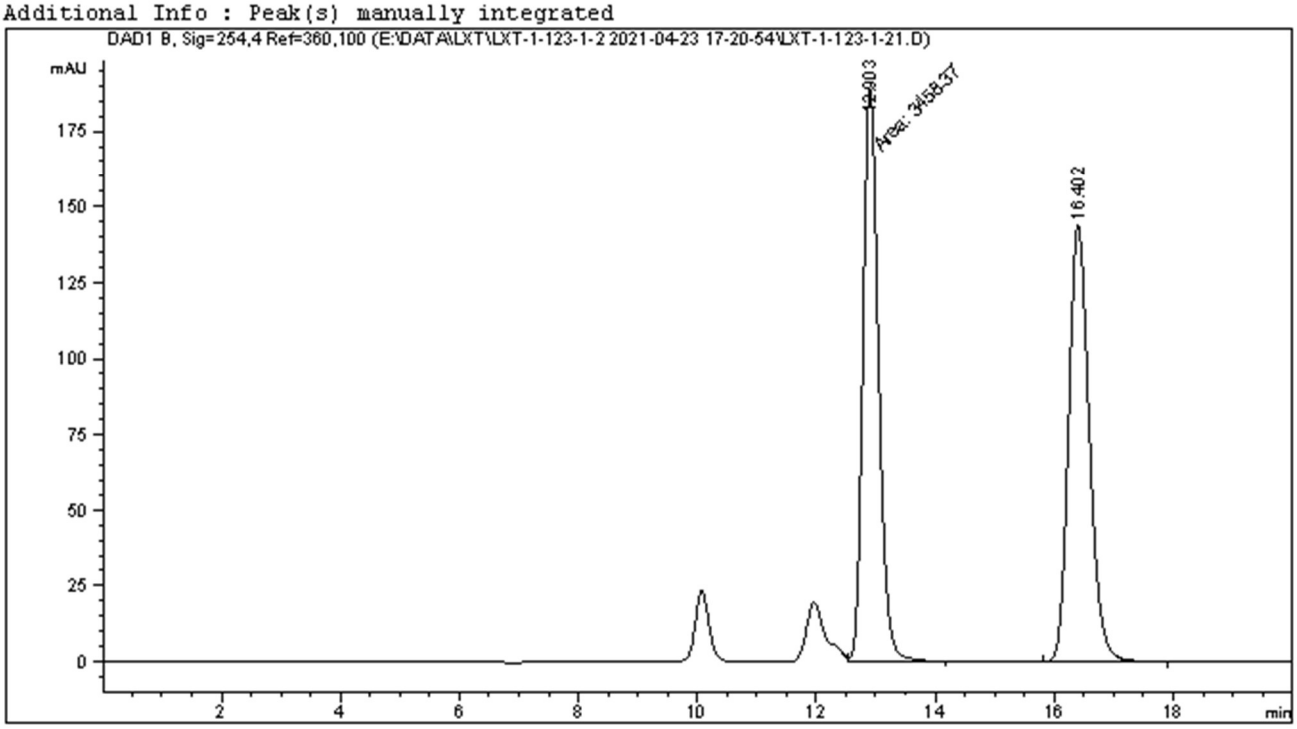


^{13}C NMR (101 MHz, Chloroform-*d*) of **3l**

Data File E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\LXT-1-123-1-21.D
Sample Name: LXT-1-123-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 6
Injection Date : 4/23/2021 5:43:16 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 4/23/2021 5:20:54 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:05:28 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

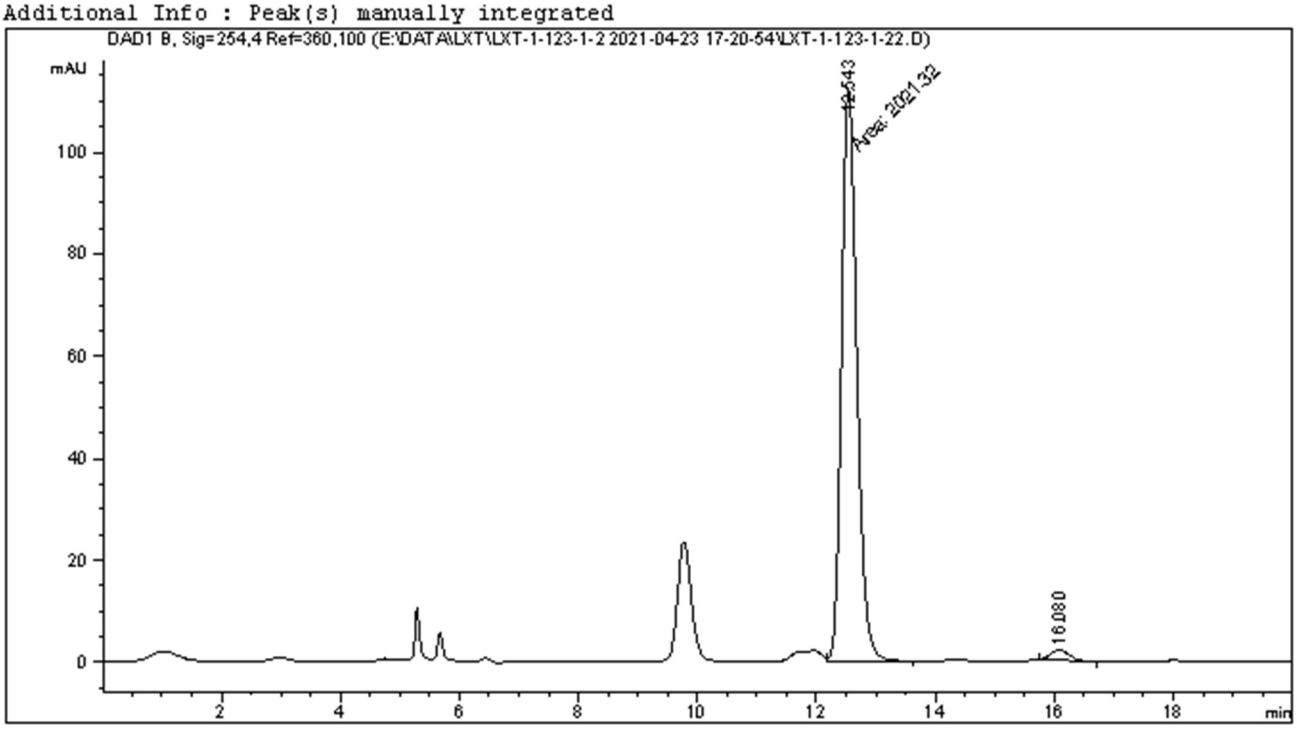
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.903	FM	0.3046	3458.36646	189.24185	49.9269
2	16.402	BB	0.3695	3468.49219	143.76036	50.0731

Totals : 6926.85864 333.00221

Data File E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\LXT-1-123-1-22.D
Sample Name: LXT-1-123-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 7
Injection Date : 4/23/2021 6:04:50 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 4/23/2021 5:20:54 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-123-1-2 2021-04-23 17-20-54\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:05:28 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

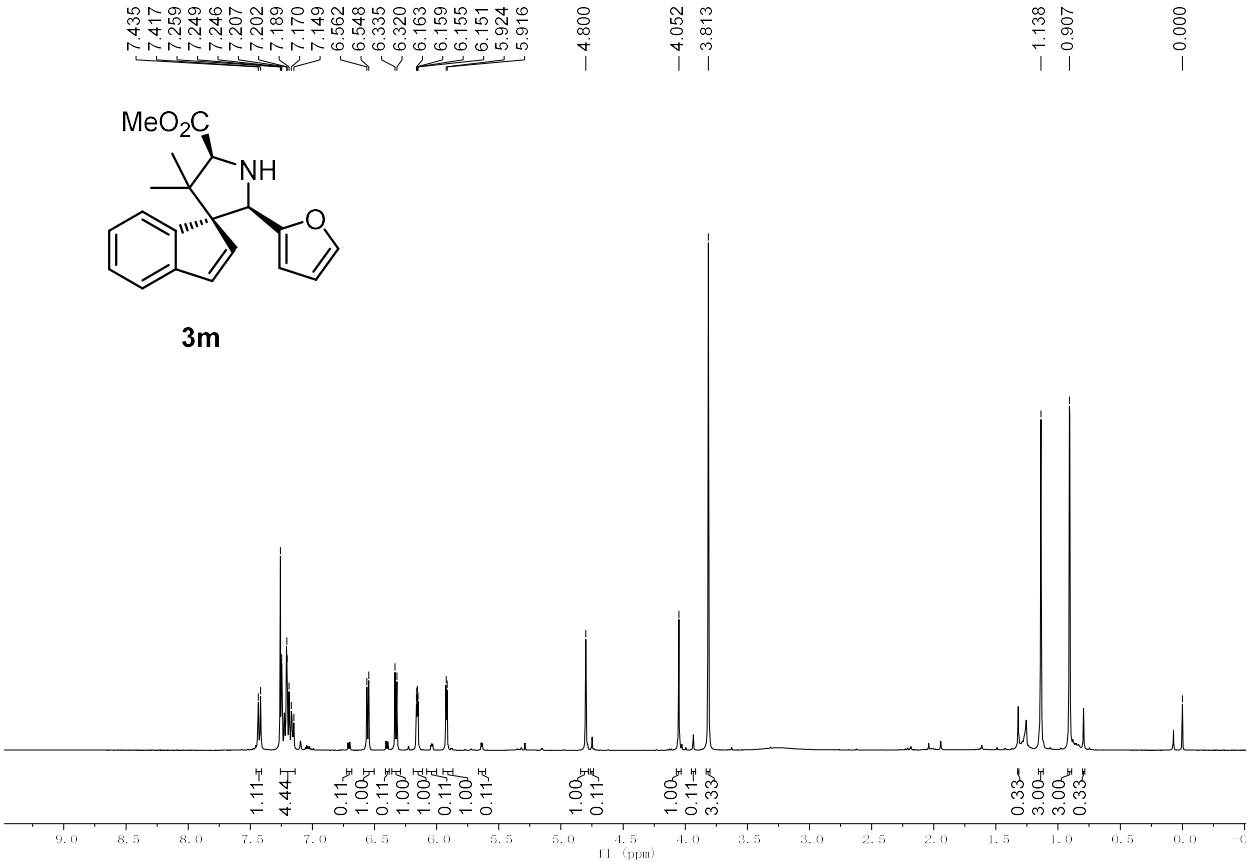
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

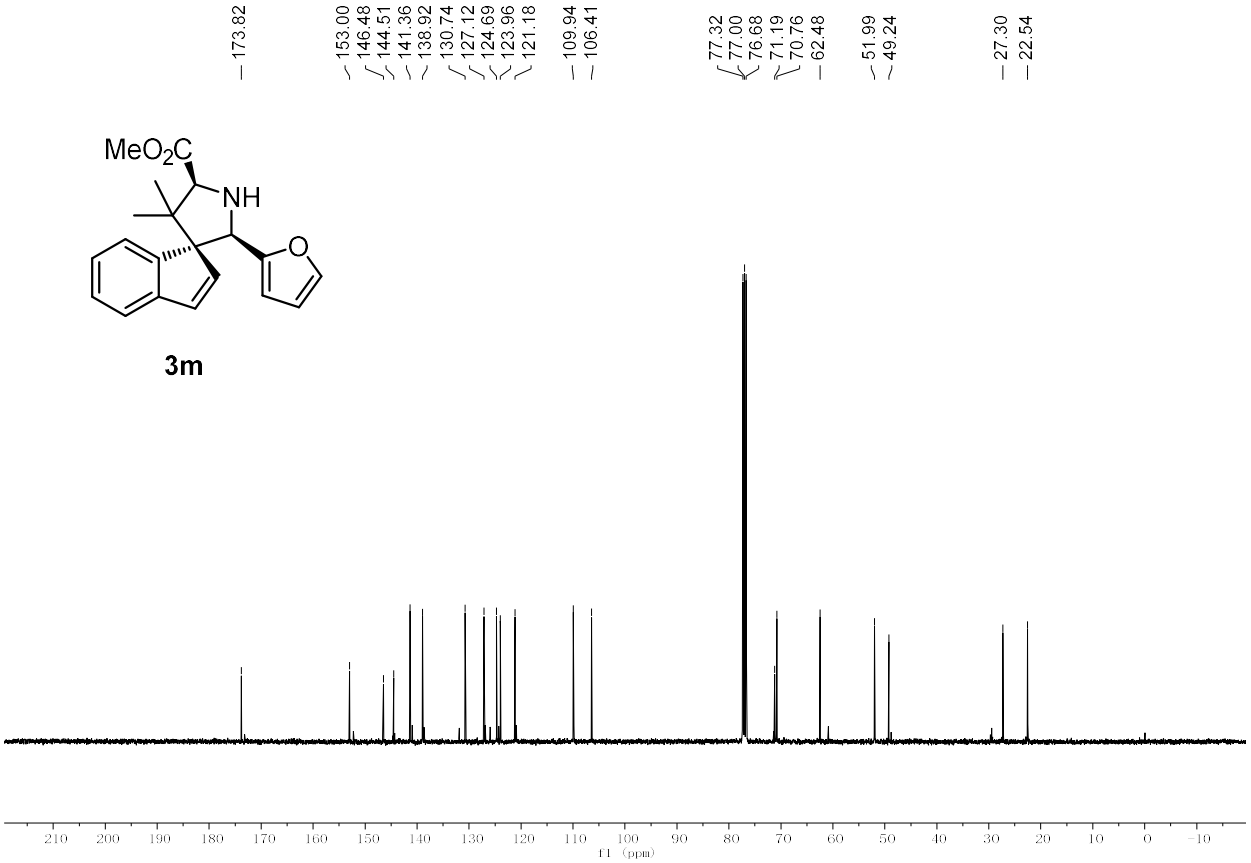
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.543	FM	0.2996	2021.31885	112.46148	98.0366
2	16.080	BB	0.2512	40.48133	1.92581	1.9634

Totals : 2061.80018 114.38729



^{1}H NMR (400 MHz, Chloroform-*d*) of **3m**

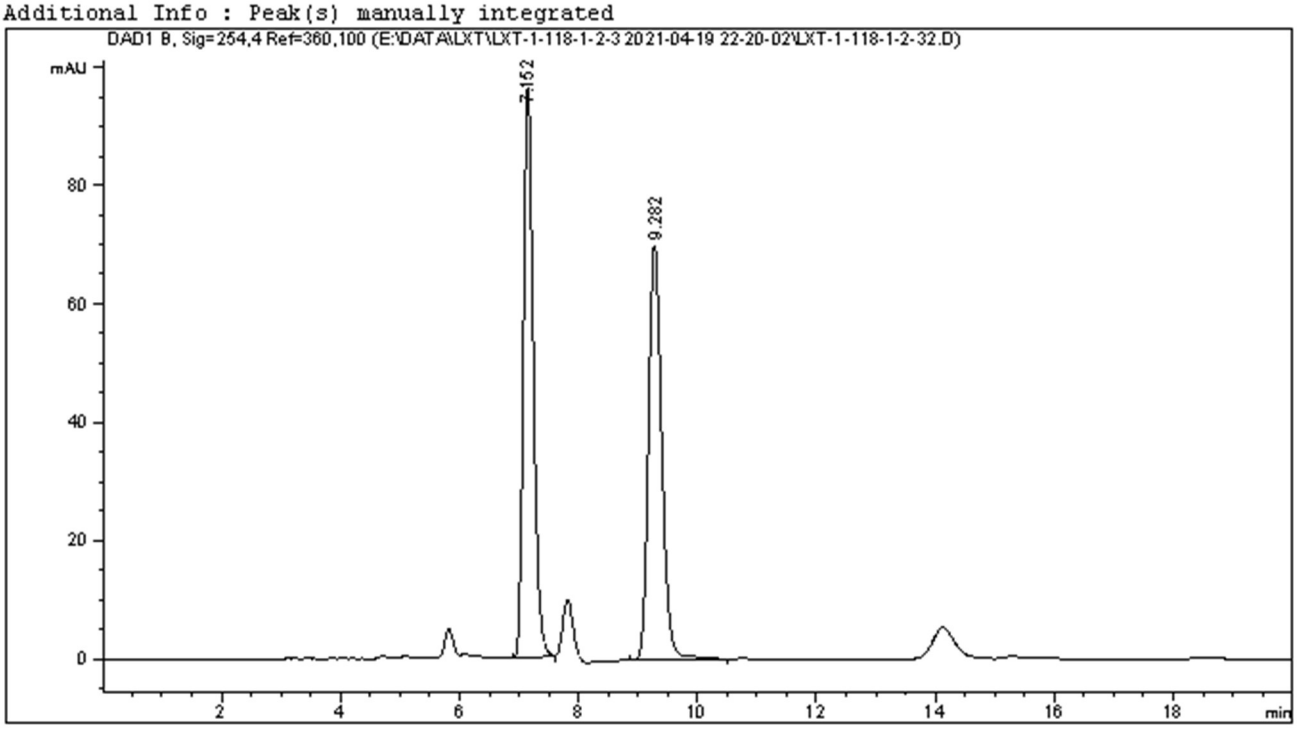


^{13}C NMR (101 MHz, Chloroform-*d*) of **3m**

Data File E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\LXT-1-118-1-2-32.D
Sample Name: LXT-1-118-2-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 12
Injection Date : 4/19/2021 11:03:54 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 4/19/2021 10:20:02 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:08:47 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

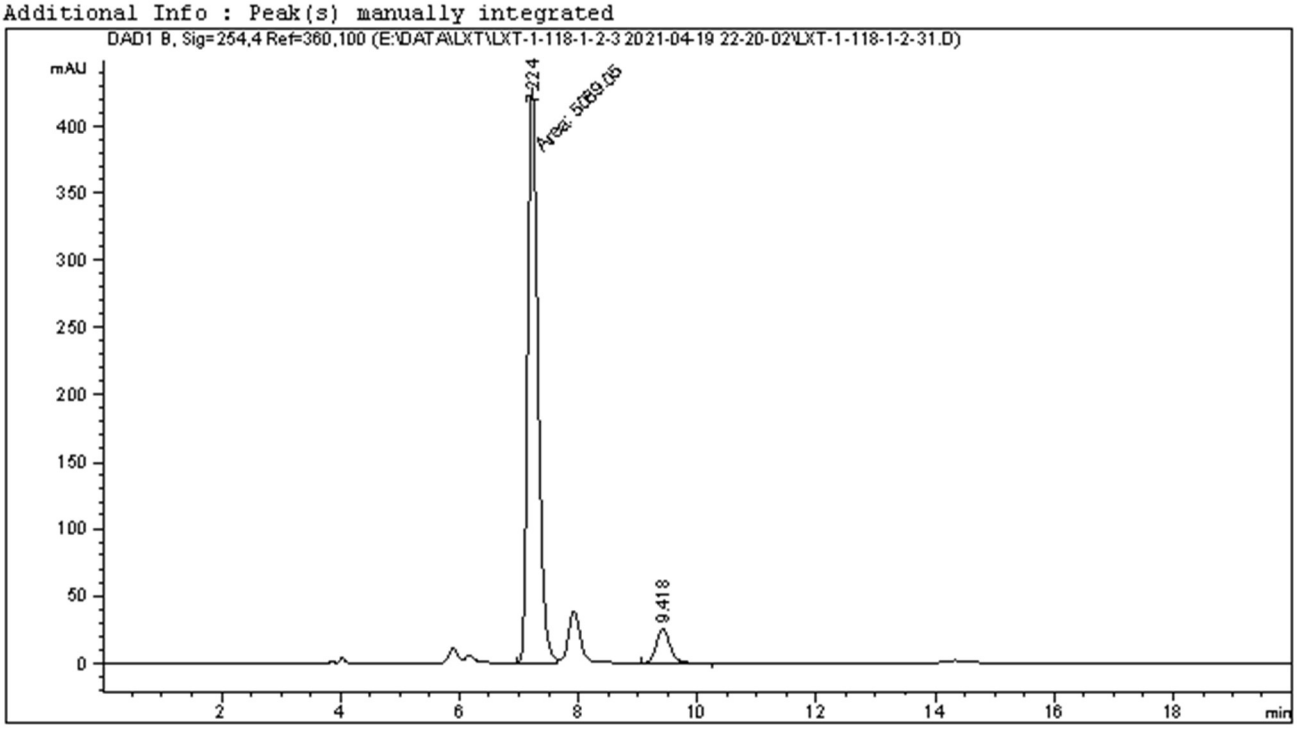
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.152	BB	0.1797	1119.08618	96.22395	50.8346
2	9.282	BB	0.2395	1082.34119	69.94288	49.1654

Totals : 2201.42737 166.16683

Data File E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\LXT-1-118-1-2-31.D
Sample Name: LXT-1-118-1-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 11
Injection Date : 4/19/2021 10:42:27 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 4/19/2021 10:20:02 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-118-1-2-3 2021-04-19 22-20-02\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:08:47 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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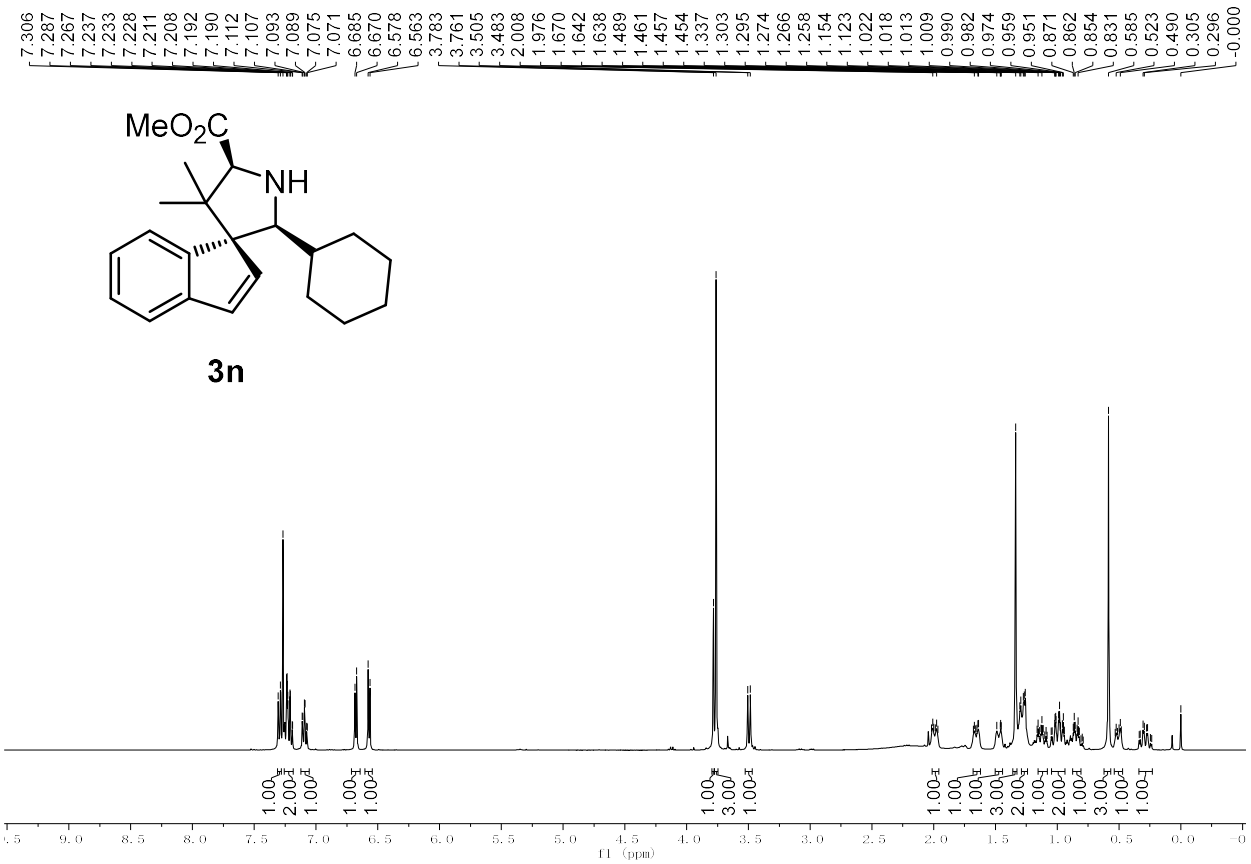
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

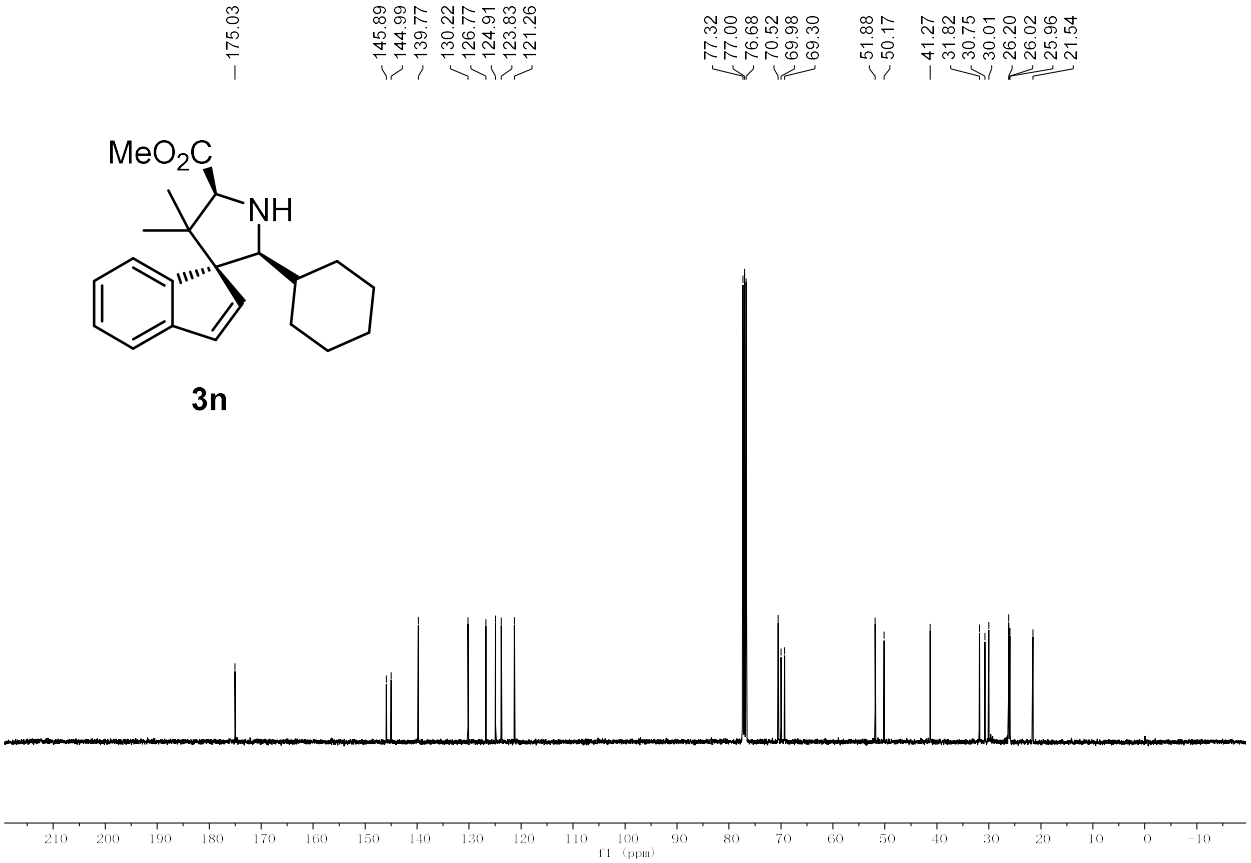
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.224	MF	0.1981	5089.04785	428.21893	92.8540
2	9.418	BB	0.2392	391.64835	25.08492	7.1460

Totals : 5480.69620 453.30385



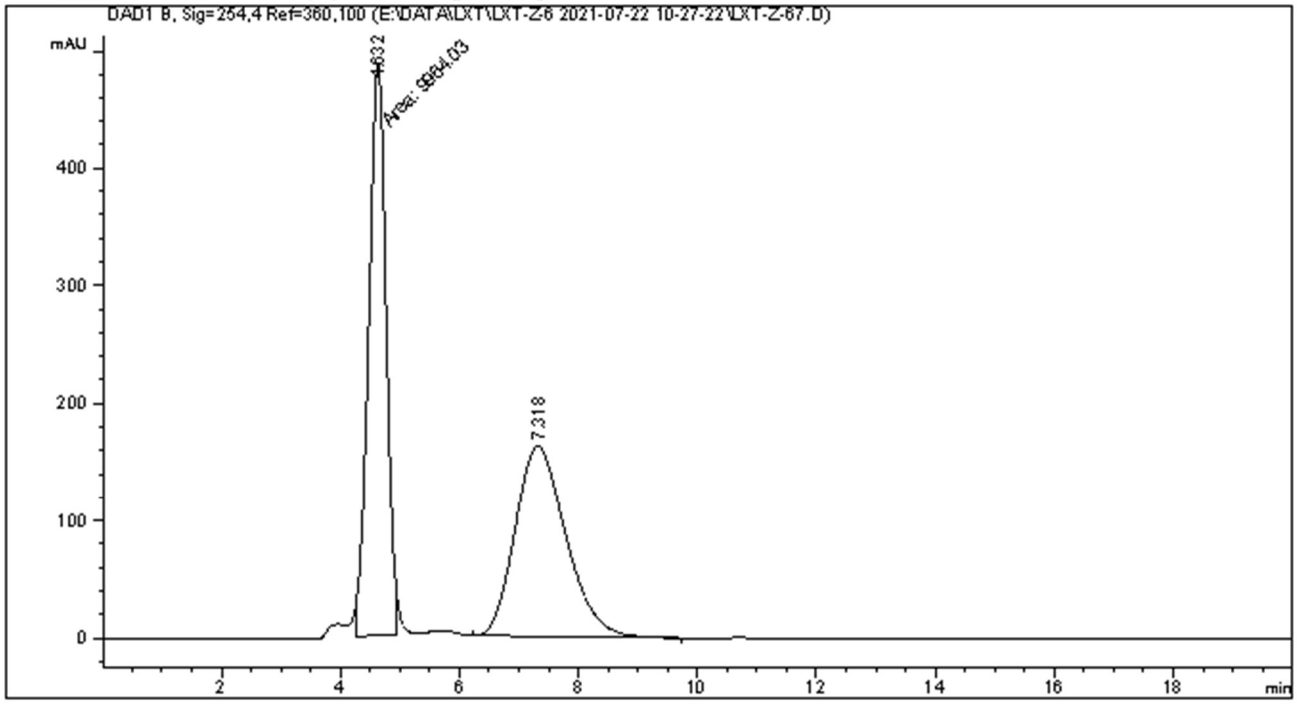
^{1}H NMR (400 MHz, Chloroform-*d*) of **3n**



^{13}C NMR (101 MHz, Chloroform-*d*) of **3n**

Data File E:\DATA\LXT\LXT-Z-6 2021-07-22 10-27-22\LXT-Z-67.D
Sample Name: LXT-2-65-RAC

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :   8
Acq. Instrument : 1260                             Location :   5
Injection Date  : 7/22/2021 12:47:51 PM                 Inj :   1
                                                Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-Z-6 2021-07-22 10-27-22\1-0J-98-2-1ML-10ul-20min-ALL-nml.M
Last changed    : 7/22/2021 10:27:23 AM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-Z-6 2021-07-22 10-27-22\1-0J-98-2-1ML-10ul-20min-ALL-nml.M
                  (Sequence Method)
Last changed    : 8/1/2021 3:14:08 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100
```

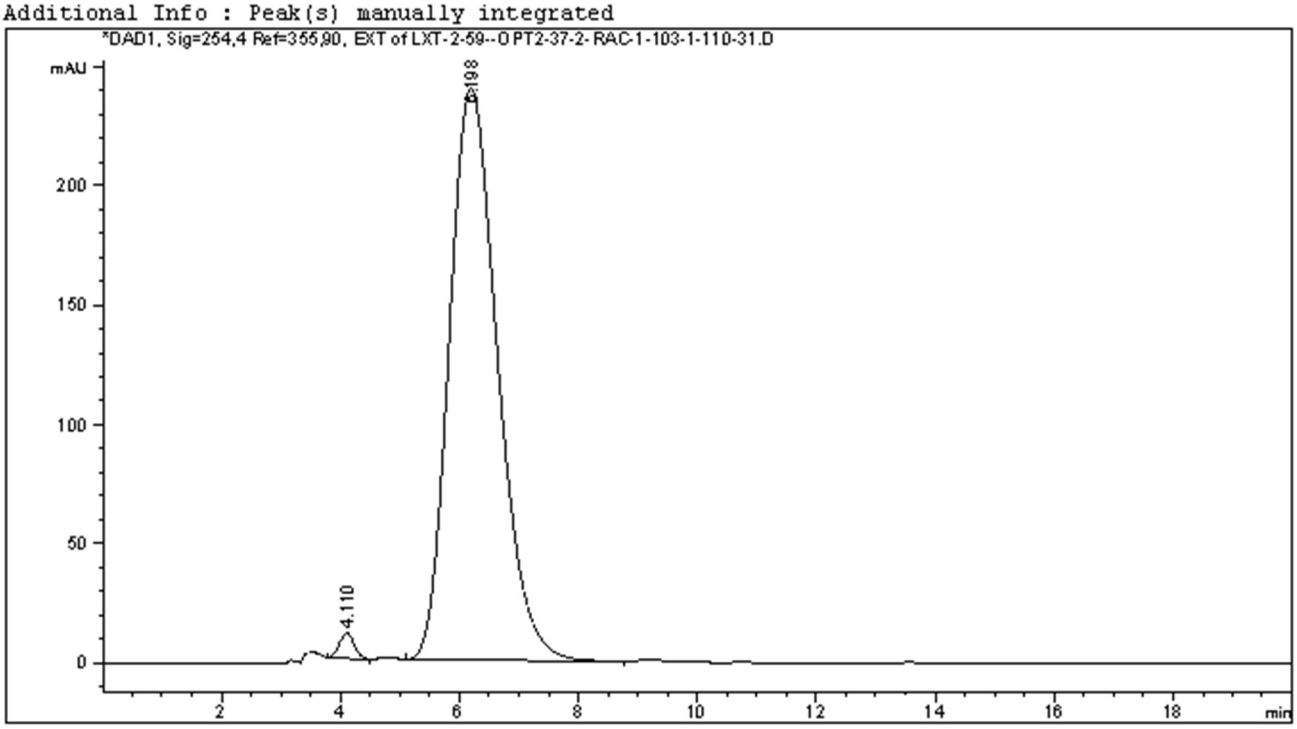
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.632	MF	0.3412	9964.03418	486.71902	50.9124
2	7.318	BB	0.8684	9606.91016	162.34944	49.0876

Totals : 1.95709e4 649.06847

Data File E:\DATA\LX...110-3- 2021-07-06 12-34-29\LXT-2-59--OPT2-37-2-RAC-1-103-1-110-31.D
Sample Name: LXT-2-59-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 3
Injection Date : 7/6/2021 12:56:53 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-59-0-237-2-R-1-103-1-0-1-110-3- 2021-07-06 12-34-29\1-0J-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/6/2021 12:34:29 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-59-0-237-2-R-1-103-1-0-1-110-3- 2021-07-06 12-34-29\1-0J-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 7/6/2021 3:24:30 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



==========

Area Percent Report

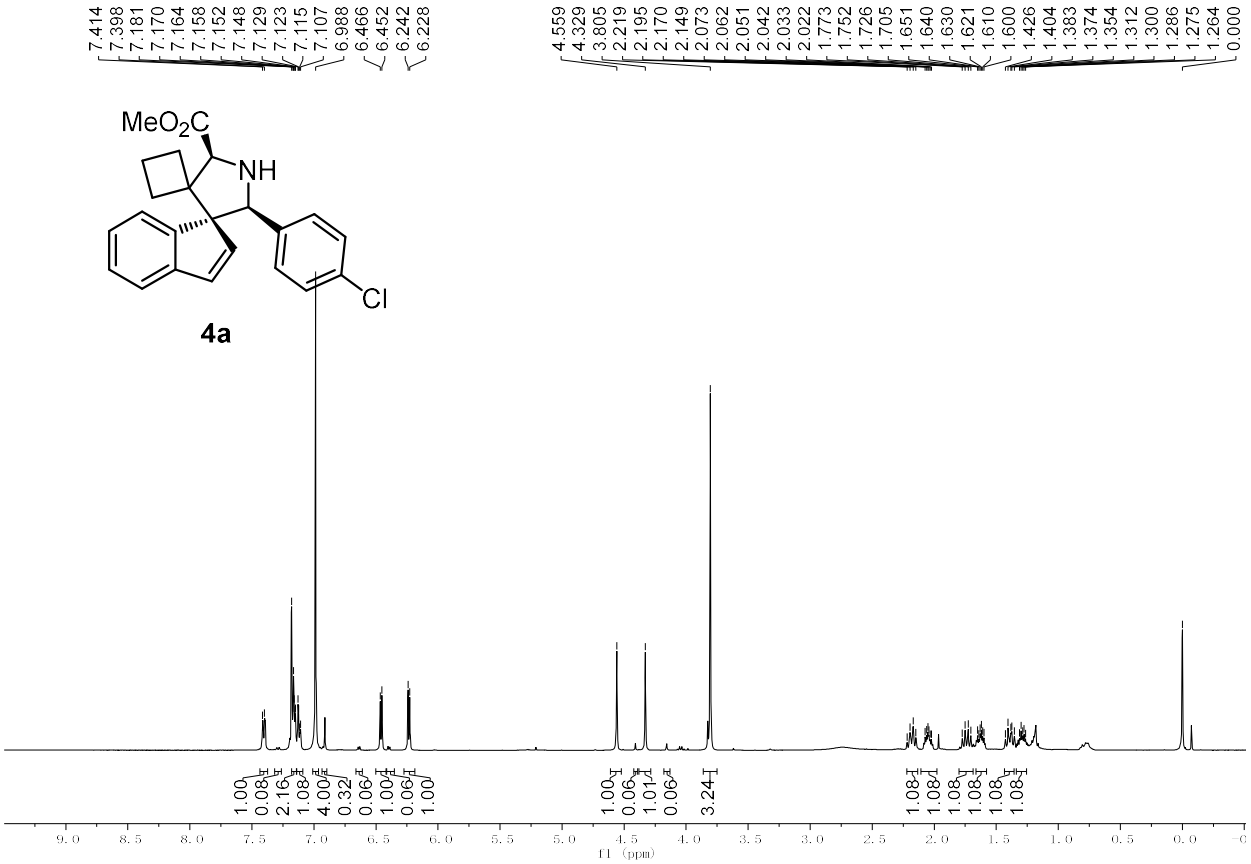
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

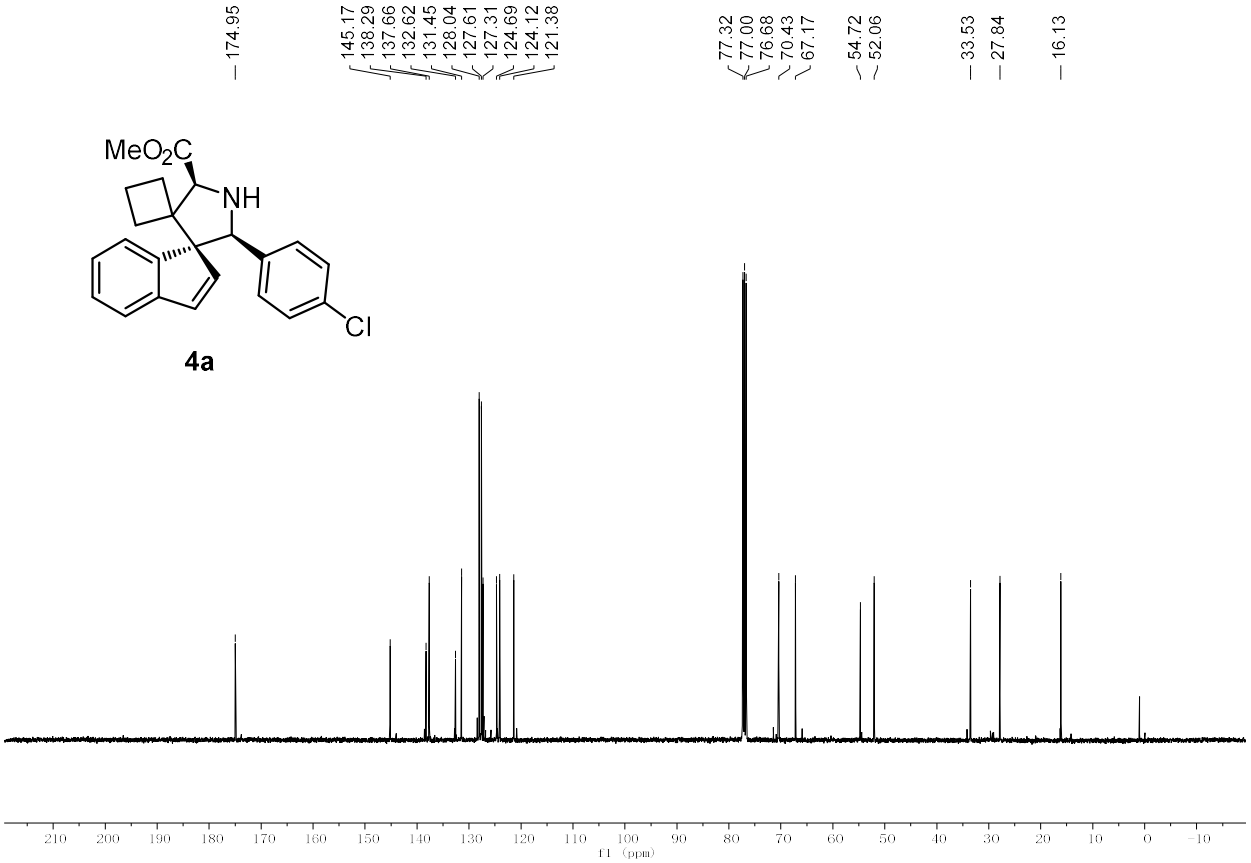
Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.110	BB	0.2606	181.61121	10.61557	1.3283
2	6.198	BB	0.8478	1.34912e4	240.02328	98.6717

Totals : 1.36728e4 250.63885



^{1}H NMR (400 MHz, Chloroform-*d*) of **4a**

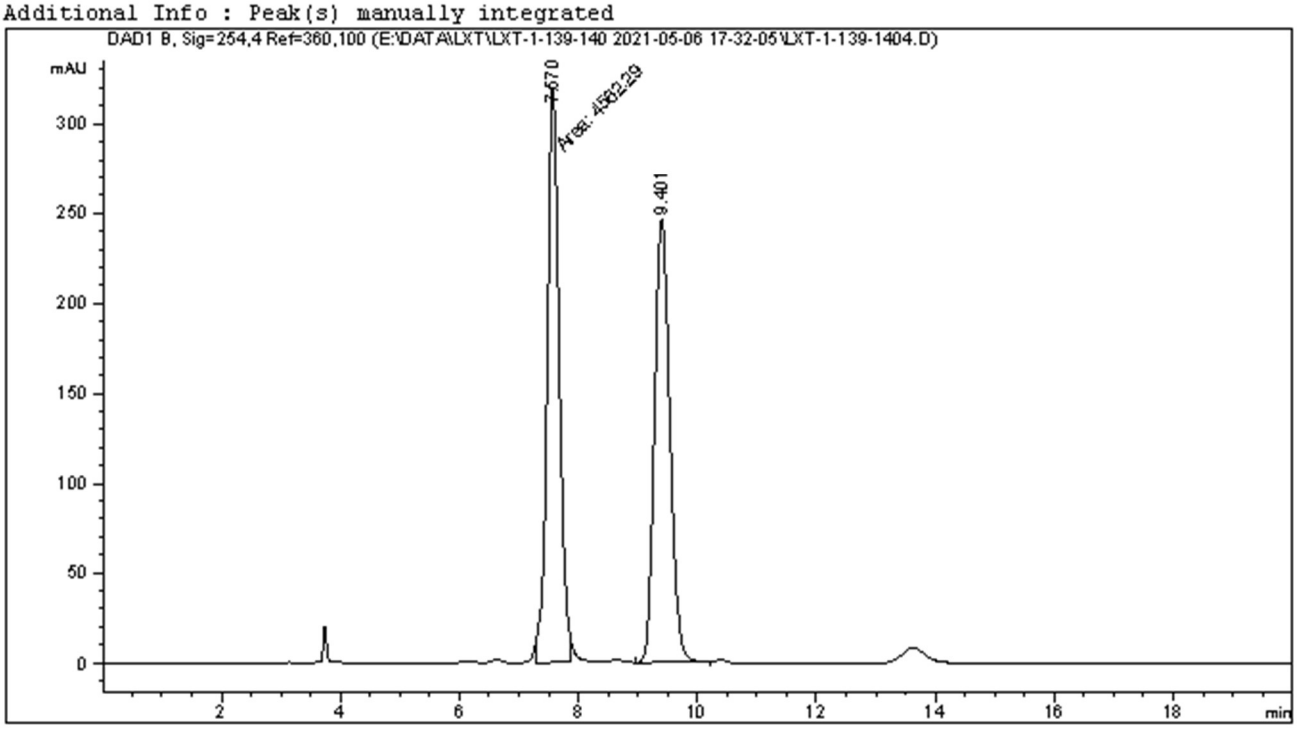


^{13}C NMR (101 MHz, Chloroform-*d*) of **4a**

Data File E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\LXT-1-139-1404.D
Sample Name: LXT-1-140-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 5
Acq. Instrument : 1260 Location : 4
Injection Date : 5/6/2021 6:58:44 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 5/6/2021 5:32:05 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:24:12 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

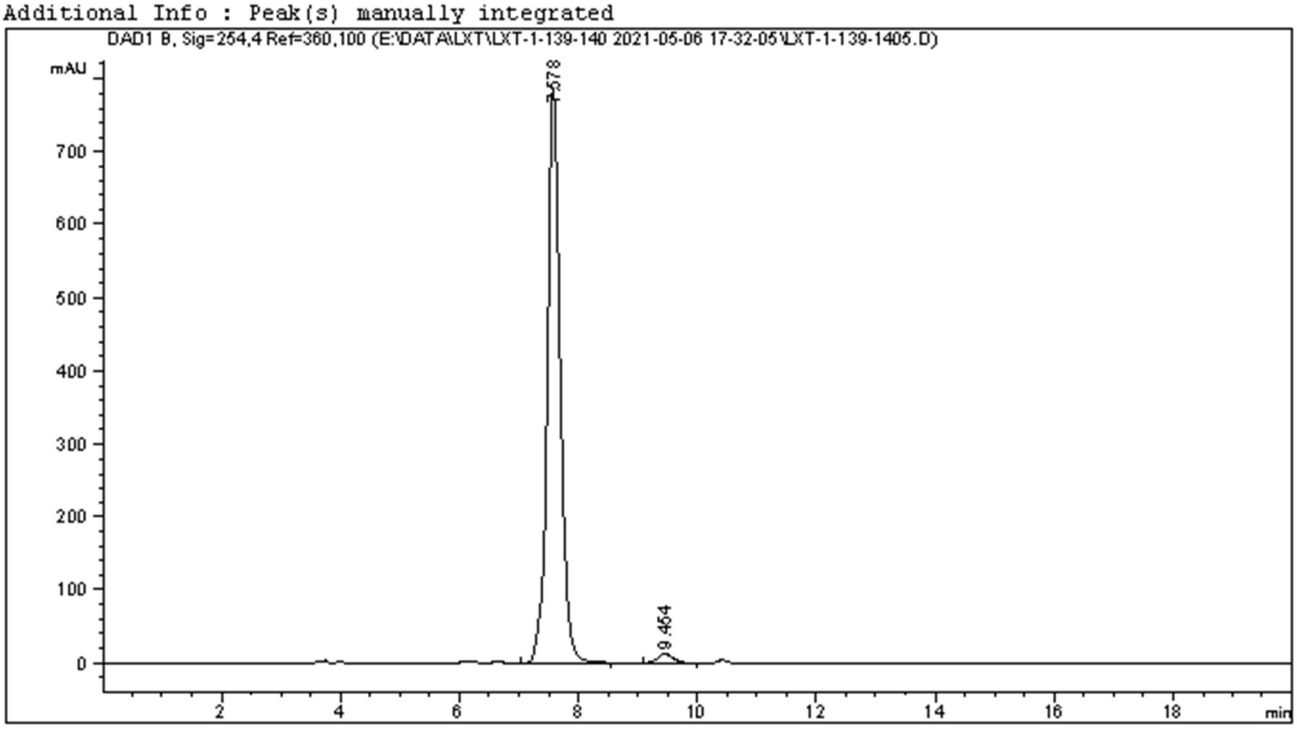
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.570	MF	0.2380	4562.29492	319.43973	50.9889
2	9.401	BB	0.2760	4385.32715	245.94644	49.0111

Totals : 8947.62207 565.38617

Data File E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\LXT-1-139-1405.D
Sample Name: LXT-1-140-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 6
Acq. Instrument : 1260 Location : 5
Injection Date : 5/6/2021 7:20:13 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 5/6/2021 5:32:05 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-139-140 2021-05-06 17-32-05\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:24:12 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

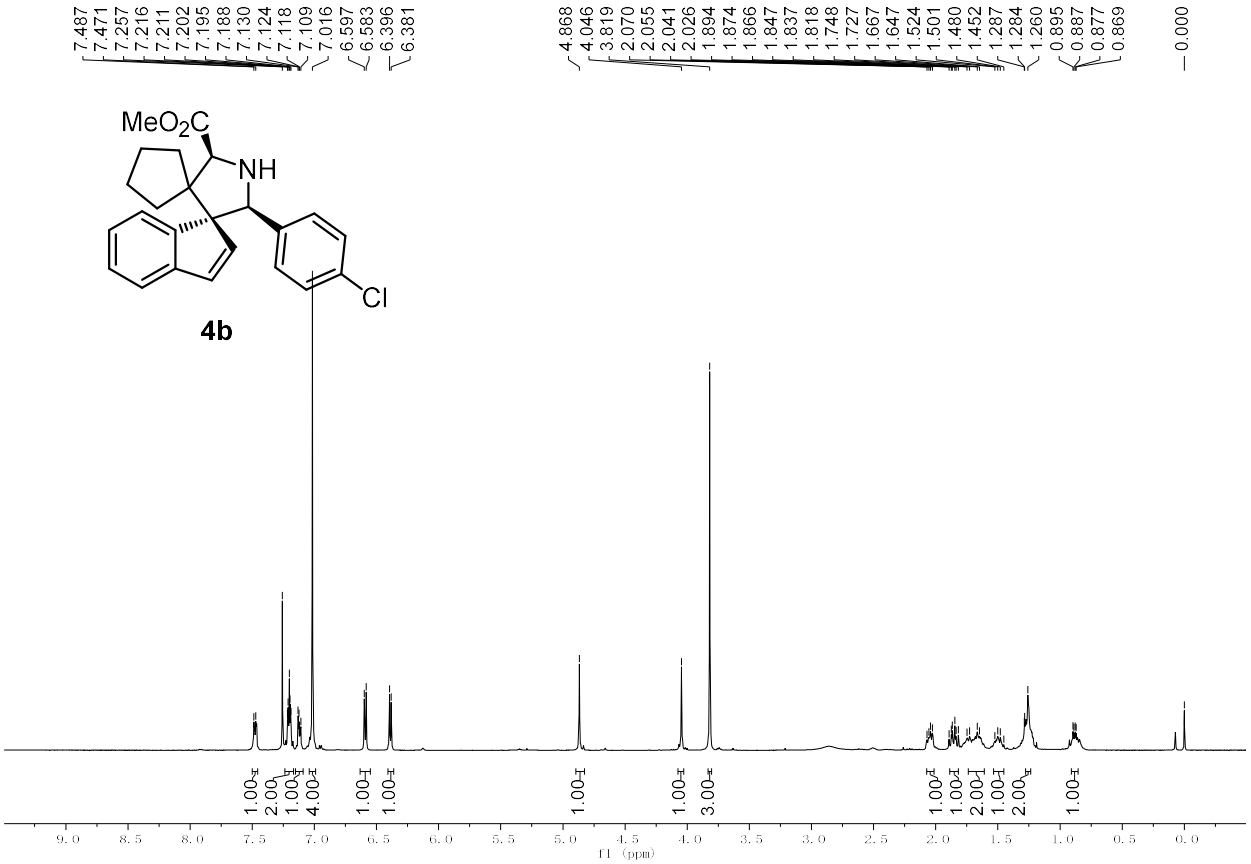
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

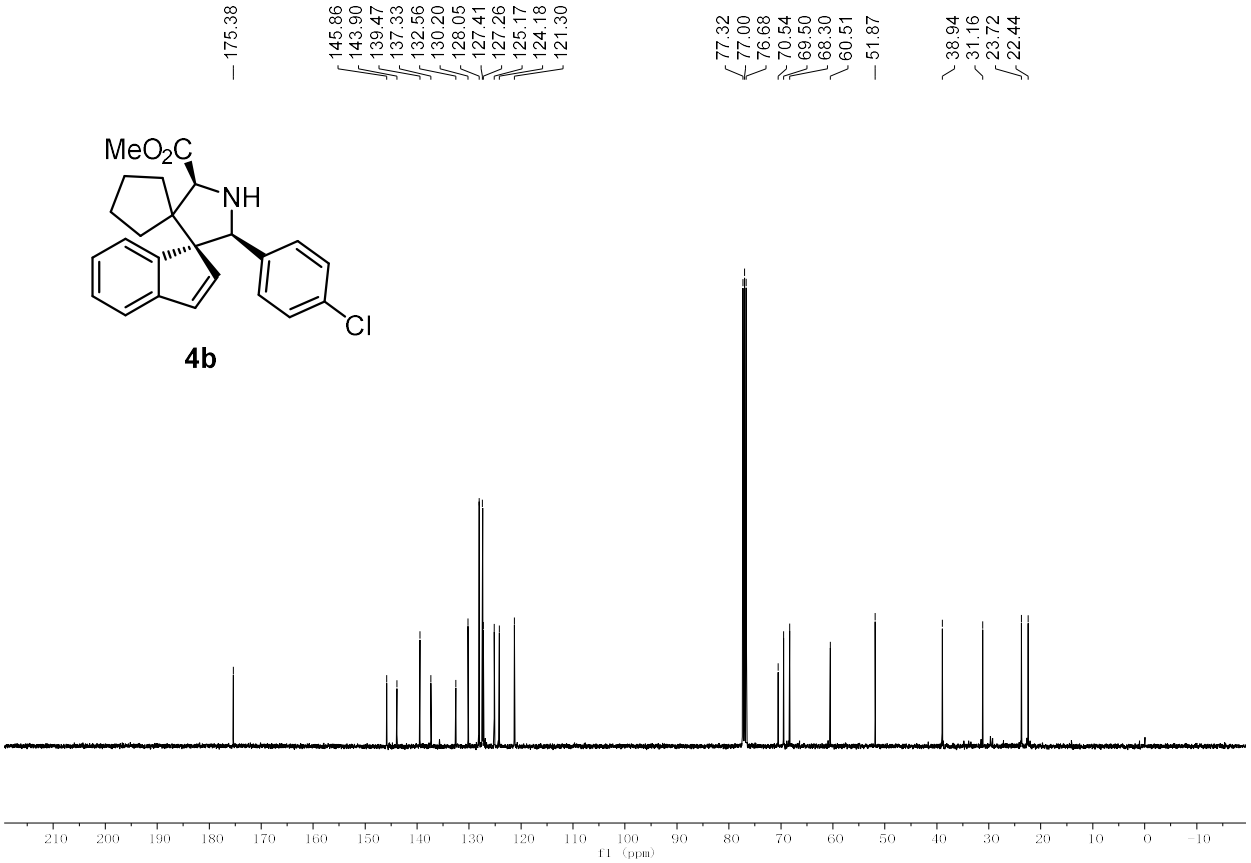
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.578	BB	0.2312	1.19520e4	786.82104	98.2380
2	9.454	BB	0.2661	214.37349	12.19398	1.7620

Totals : 1.21664e4 799.01503



^{1}H NMR (400 MHz, Chloroform-*d*) of **4b**

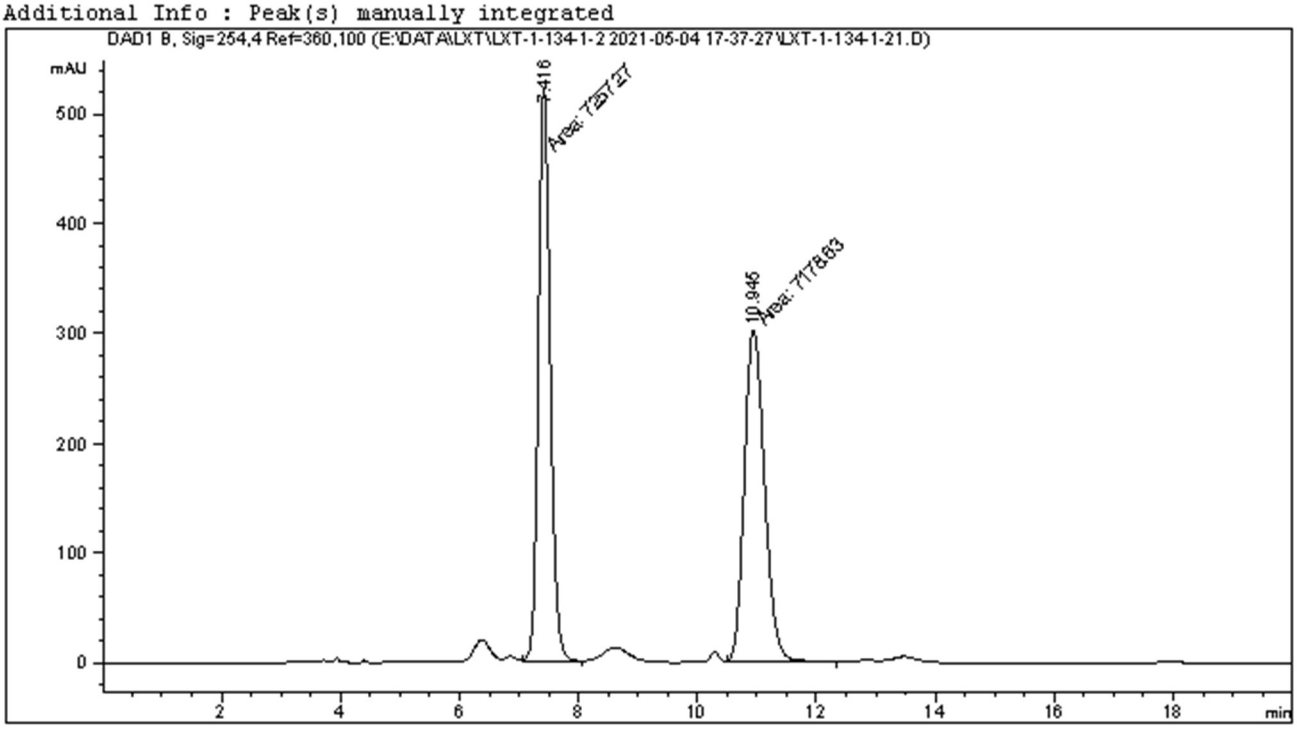


^{13}C NMR (101 MHz, Chloroform-*d*) of **4b**

Data File E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\LXT-1-134-1-21.D
Sample Name: LXT-1-134-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 5
Injection Date : 5/4/2021 5:59:54 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 5/4/2021 5:37:27 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:27:12 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

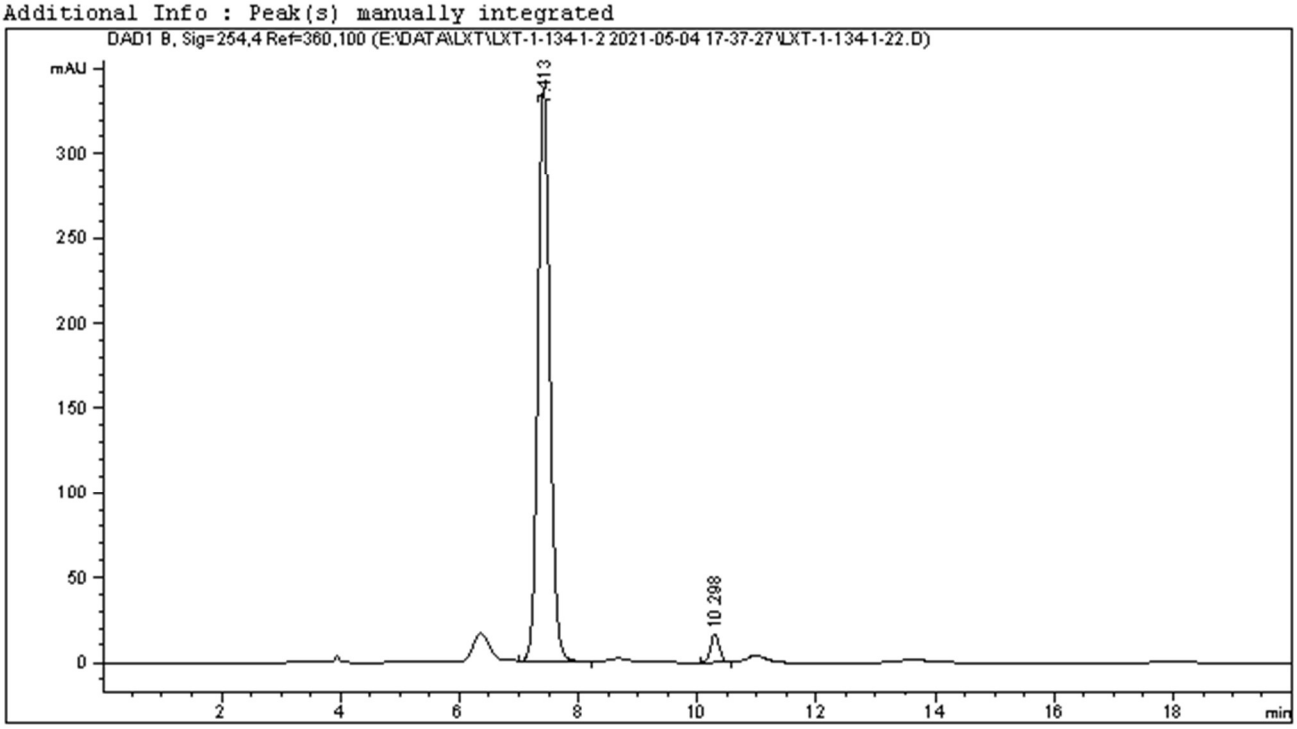
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.416	FM	0.2315	7257.27100	522.38721	50.2724
2	10.945	FM	0.3943	7178.63135	303.43472	49.7276

Totals : 1.44359e4 825.82193

Data File E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\LXT-1-134-1-22.D
Sample Name: LXT-1-134-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 6
Injection Date : 5/4/2021 6:21:22 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 5/4/2021 5:37:27 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-134-1-2 2021-05-04 17-37-27\1-ASH-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:27:12 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

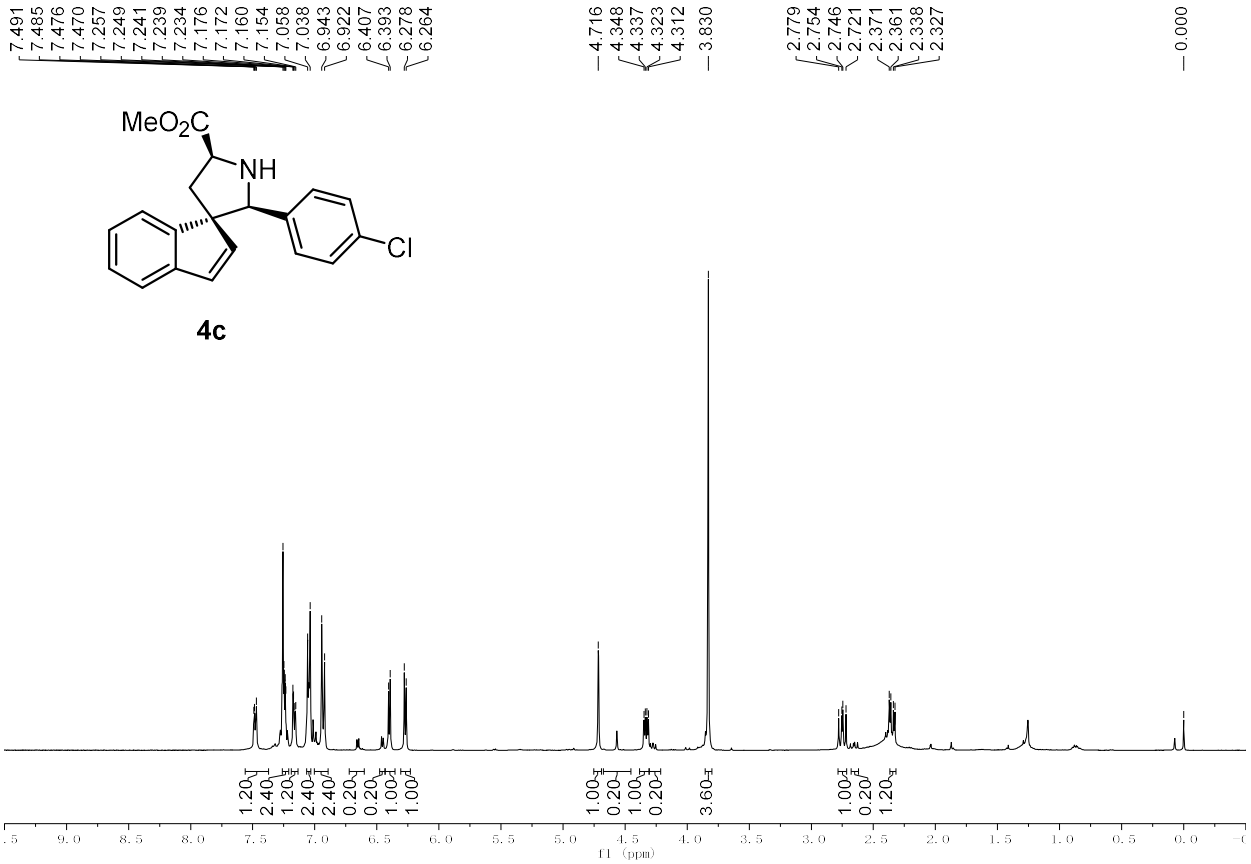
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

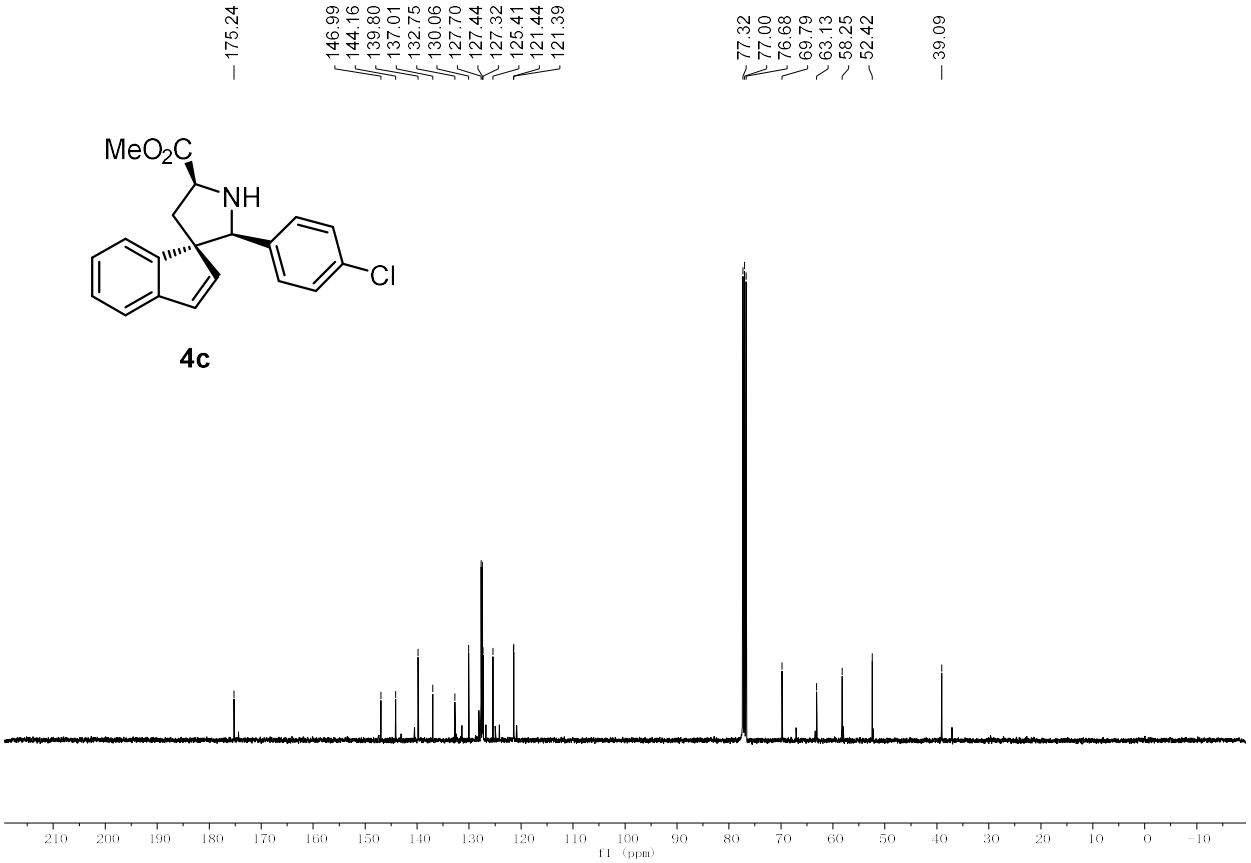
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.413	VB	0.2156	4745.57324	338.31546	96.5298
2	10.298	BB	0.1547	170.59984	17.05873	3.4702

Totals : 4916.17308 355.37419



^{1}H NMR (400 MHz, Chloroform-*d*) of **4c**

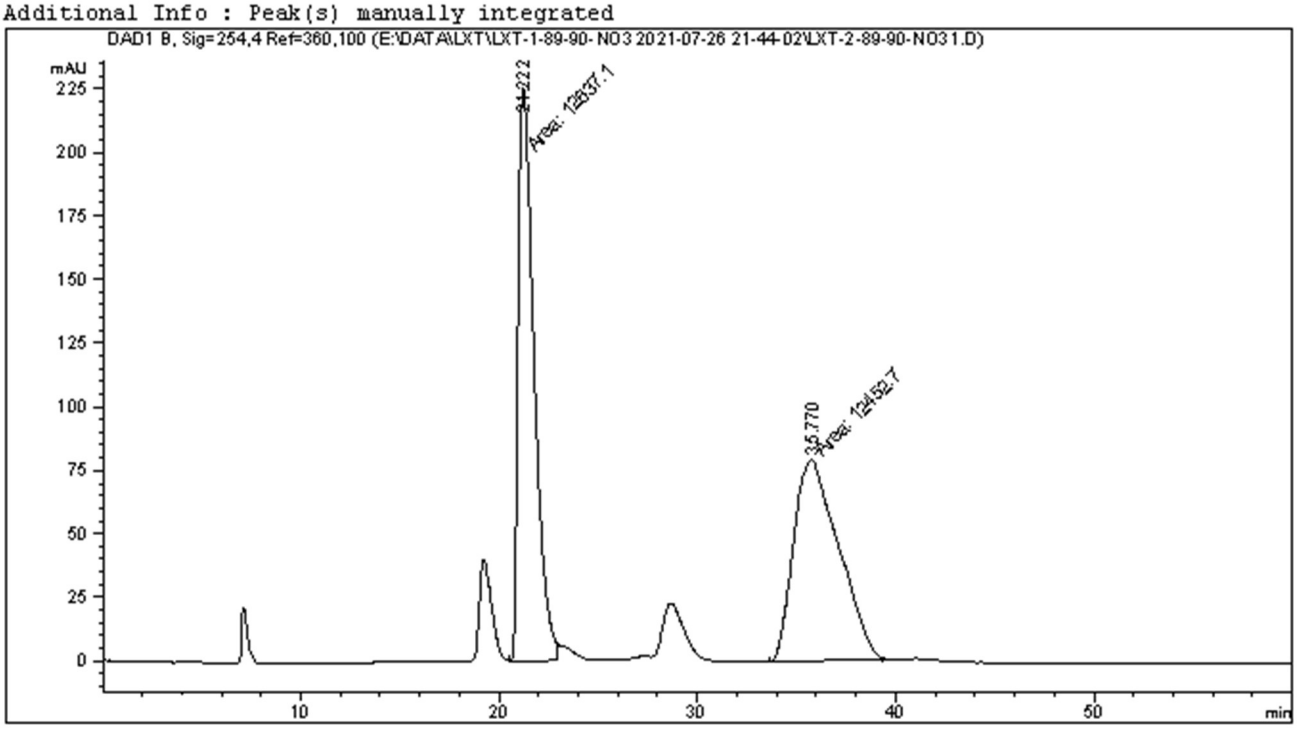


^{13}C NMR (101 MHz, Chloroform-*d*) of **4c**

Data File E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\LXT-2-89-90-N031.D
Sample Name: LXT-2-89-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 21
Injection Date : 7/26/2021 10:06:28 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\1-ID-99-1-1ML-10ul-60min-ALL-nml.M
Last changed : 7/26/2021 9:44:03 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\1-ID-99-1-1ML-10ul-60min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 4:01:30 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

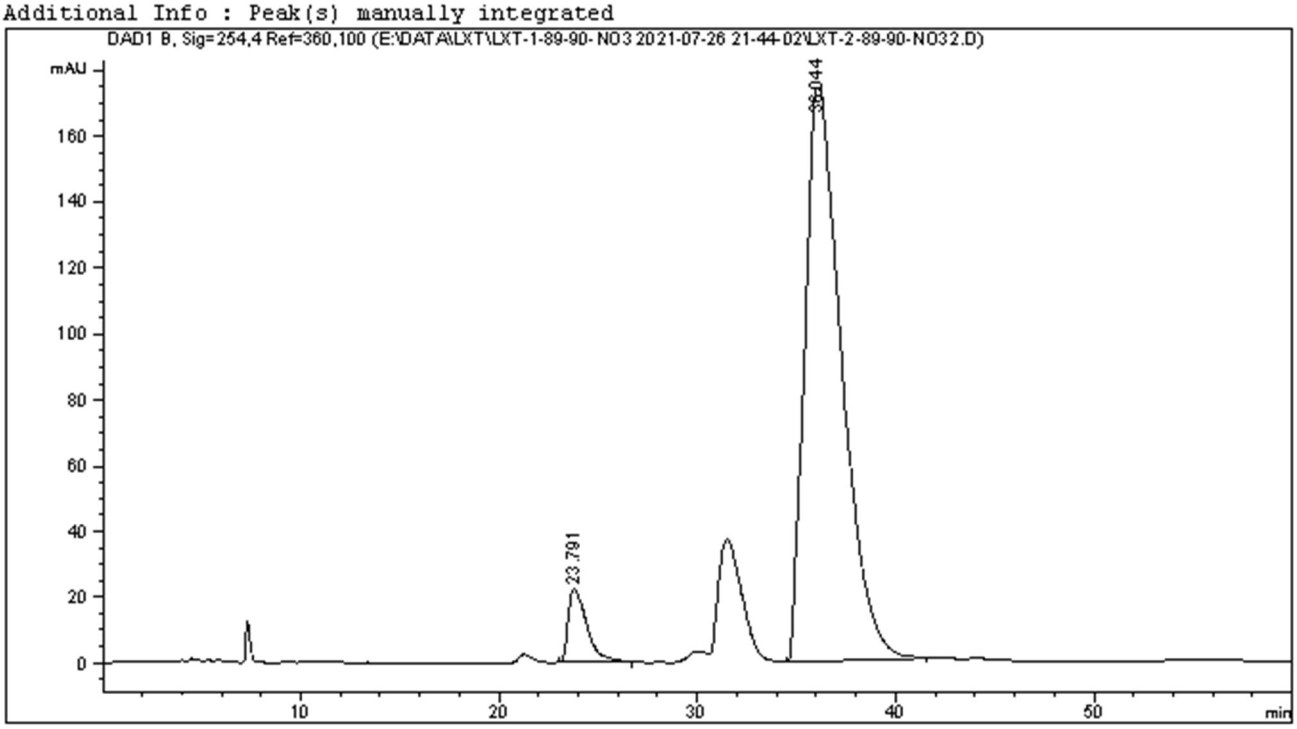
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.222	MF	0.9354	1.26371e4	225.17052	50.3674
2	35.770	MM	2.6140	1.24527e4	79.39778	49.6326

Totals : 2.50898e4 304.56830

Data File E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\LXT-2-89-90-N032.D
Sample Name: LXT-2-90-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 22
Injection Date : 7/26/2021 11:08:00 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\1-ID-99-1-1ML-10ul-60min-ALL-nml.M
Last changed : 7/26/2021 9:44:03 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-89-90-N03 2021-07-26 21-44-02\1-ID-99-1-1ML-10ul-60min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 4:08:06 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

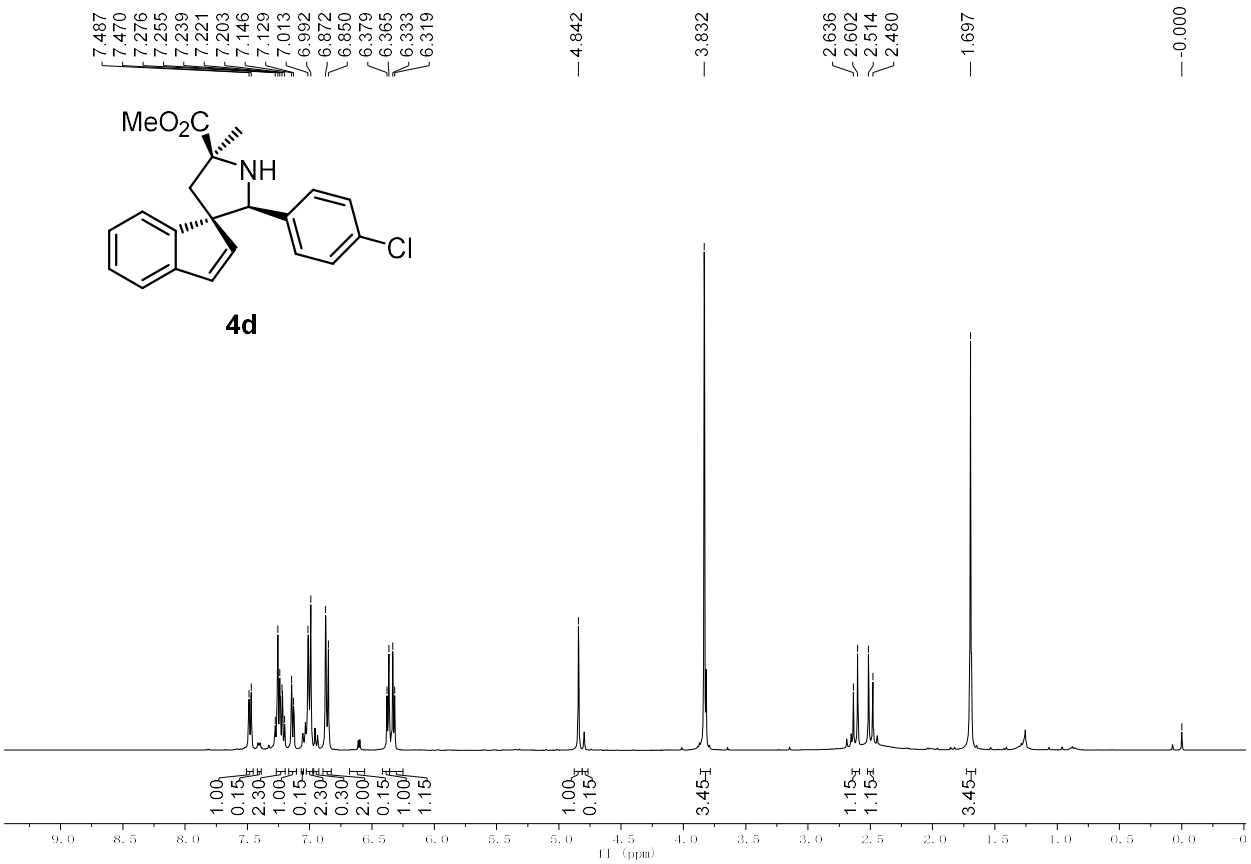
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

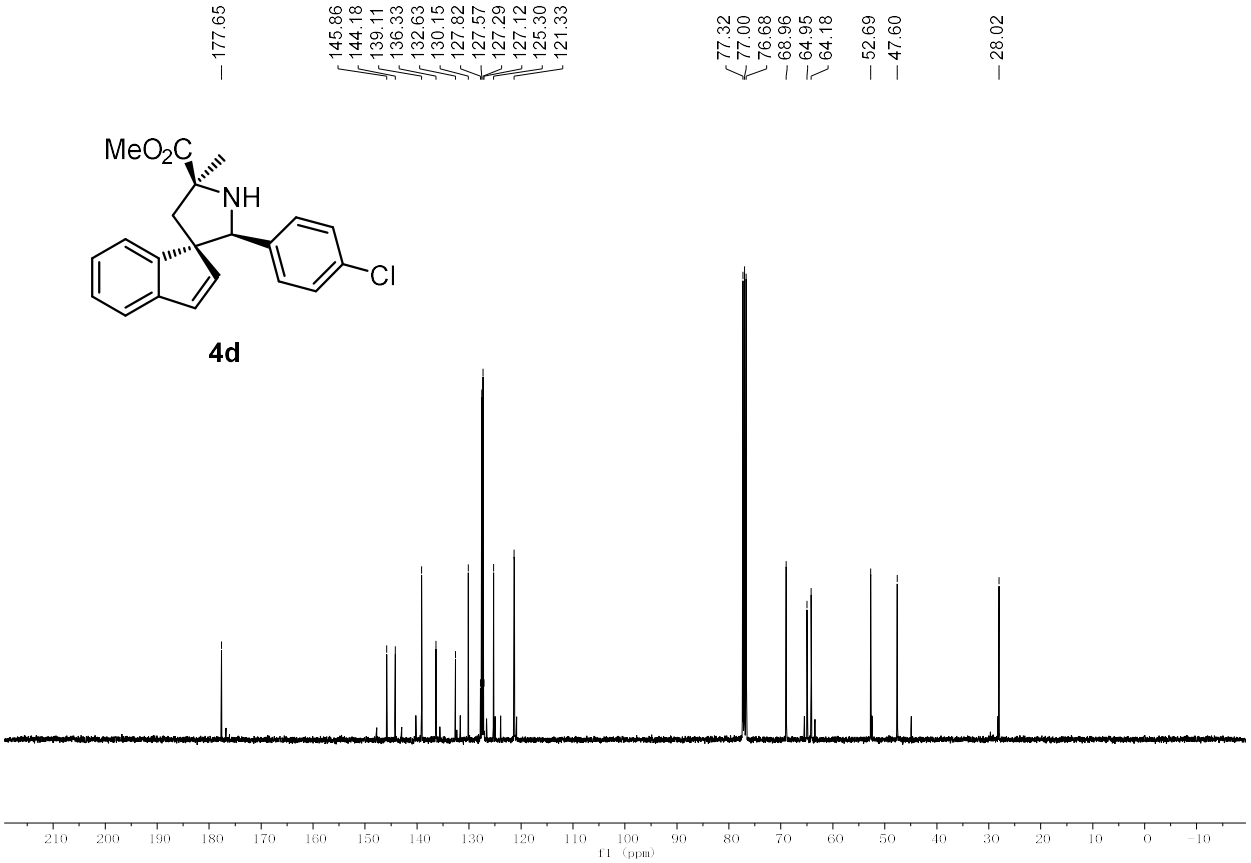
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.791	BB	0.7732	1459.53198	22.13574	6.0944
2	36.044	BB	1.5974	2.24893e4	174.05887	93.9056

Totals : 2.39488e4 196.19460



^{1}H NMR (400 MHz, Chloroform-*d*) of **4d**



^{13}C NMR (101 MHz, Chloroform-*d*) of **4d**

Data File E:\DATA\LXT\LXT-2-41-48 2021-07-21 16-10-39\LXT-2-41-482.D
Sample Name: LXT-2-41-RAC

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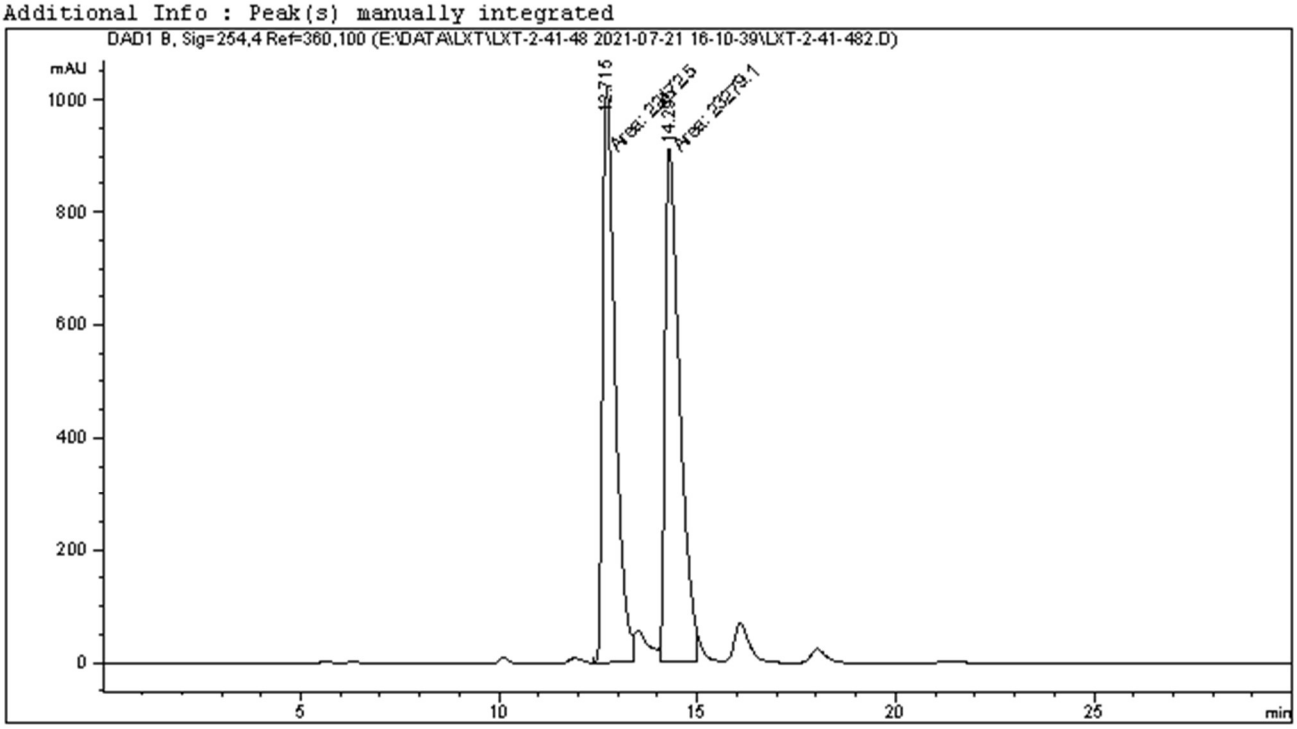
Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 4
Injection Date : 7/21/2021 4:54:36 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-41-48 2021-07-21 16-10-39\1-IE-99-1-0.7ML-10ul-30min-ALL-nml.M
Last changed : 7/21/2021 4:10:39 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-41-48 2021-07-21 16-10-39\1-IE-99-1-0.7ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 4:22:12 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

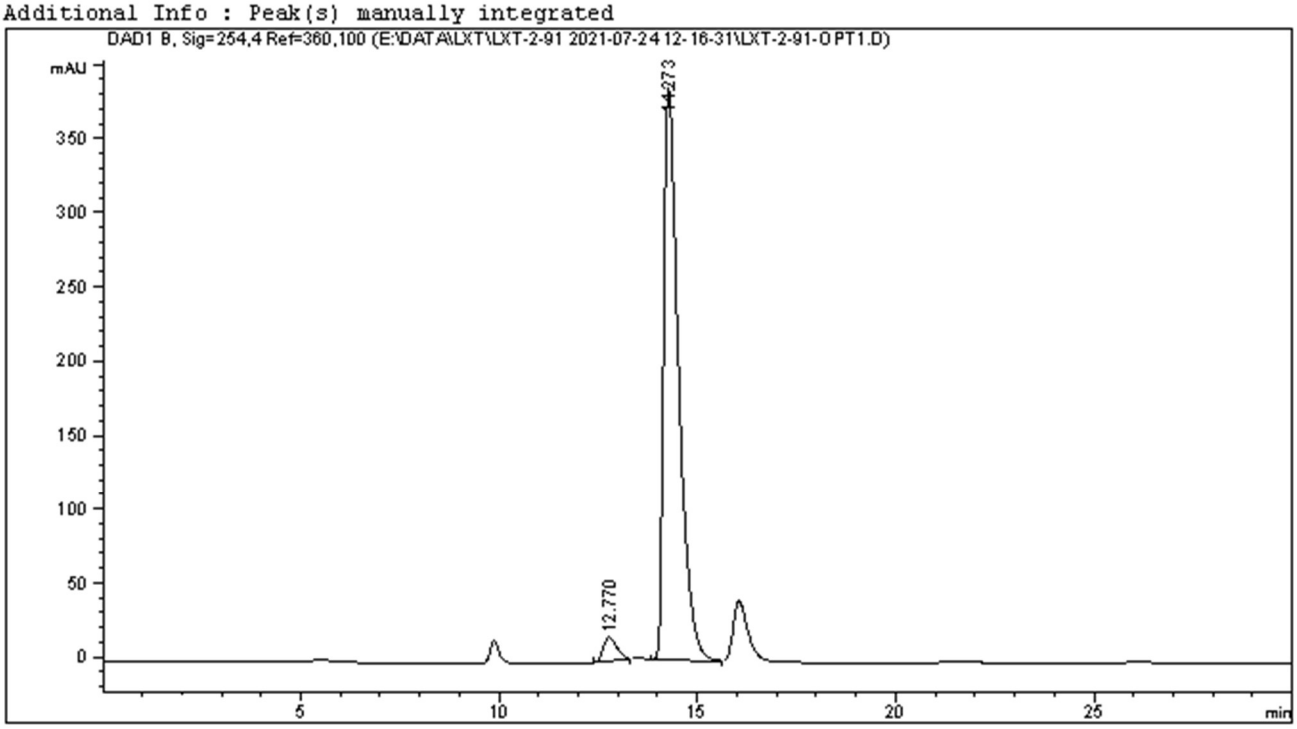
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.715	MF	0.3674	2.24725e4	1019.31366	49.1185
2	14.295	FM	0.4258	2.32791e4	911.28888	50.8815

Totals : 4.57516e4 1930.60254

Data File E:\DATA\LXT\LXT-2-91 2021-07-24 12-16-31\LXT-2-91-OPT1.D
Sample Name: LXT-2-91-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 11
Injection Date : 7/24/2021 12:39:01 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-91 2021-07-24 12-16-31\1-IE-99-1-0.7ML-10ul-30min-ALL-nml .M
Last changed : 7/24/2021 12:16:31 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-91 2021-07-24 12-16-31\1-IE-99-1-0.7ML-10ul-30min-ALL-nml .M (Sequence Method)
Last changed : 8/1/2021 4:17:39 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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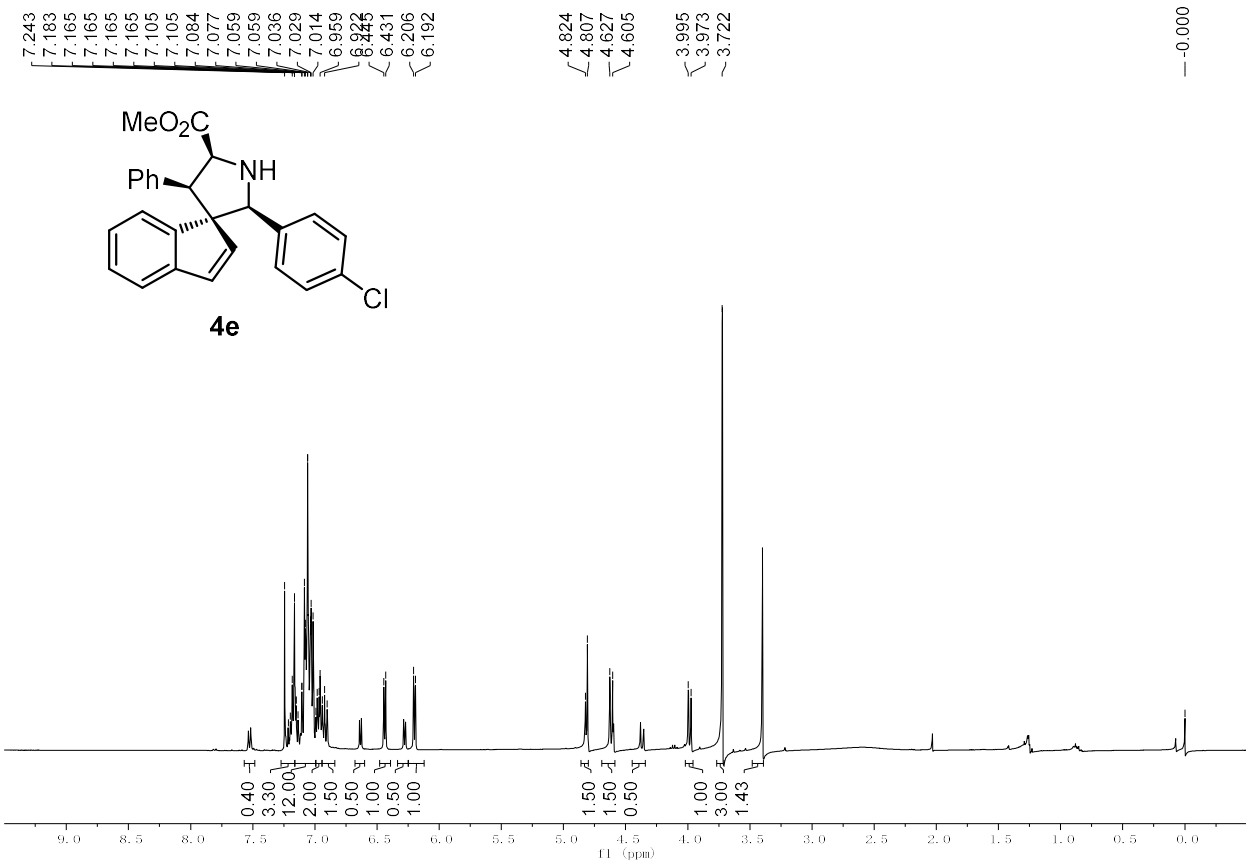
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

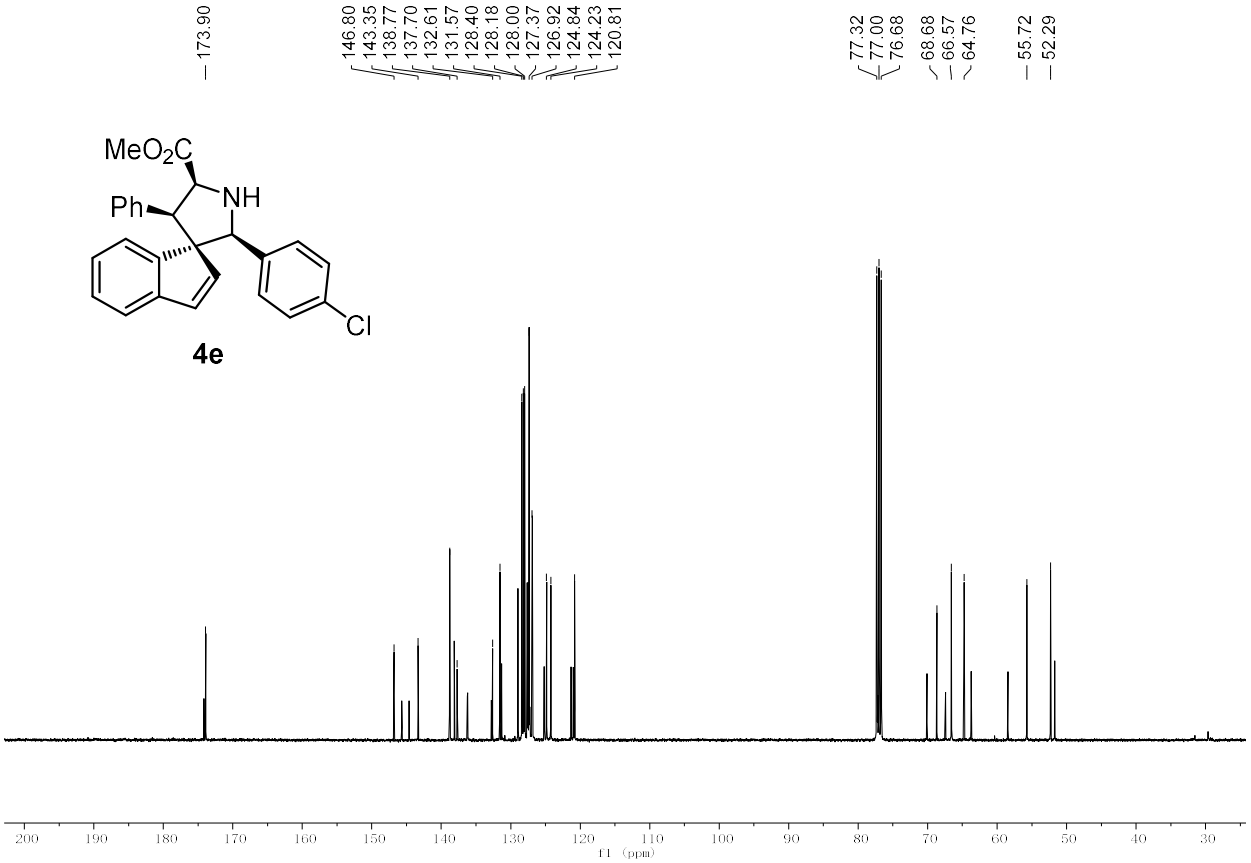
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.770	BB	0.3512	375.98056	15.88419	3.5755
2	14.273	BB	0.3974	1.01395e4	386.11749	96.4245

Totals : 1.05154e4 402.00168



^{1}H NMR (400 MHz, Chloroform-*d*) of **4e**

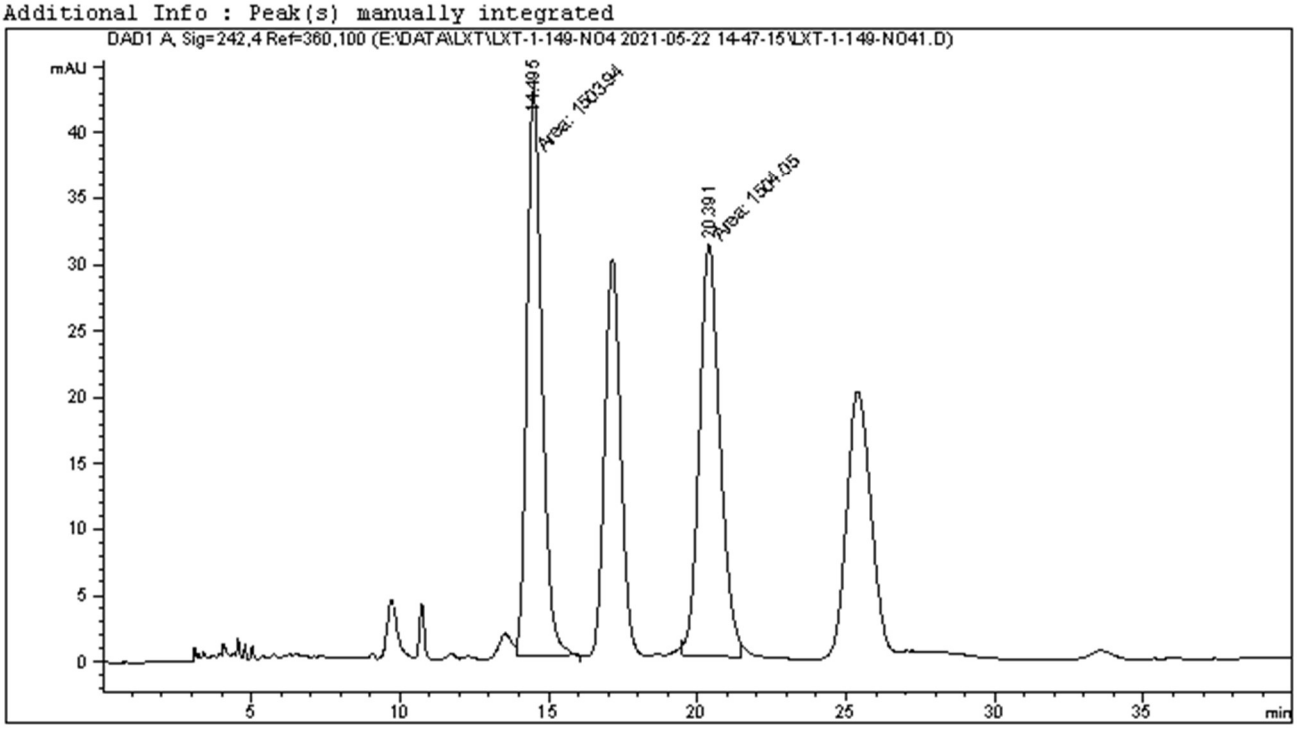


^{13}C NMR (101 MHz, Chloroform-*d*) of **4e**

Data File E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\LXT-1-149-N041.D
Sample Name: LXT-1-149-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 6
Injection Date : 5/22/2021 2:59:51 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\1-ASH-98-2-1ML-10ul-40min-ALL -nml.M
Last changed : 5/22/2021 2:47:15 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\1-ASH-98-2-1ML-10ul-40min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:36:02 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=242,4 Ref=360,100

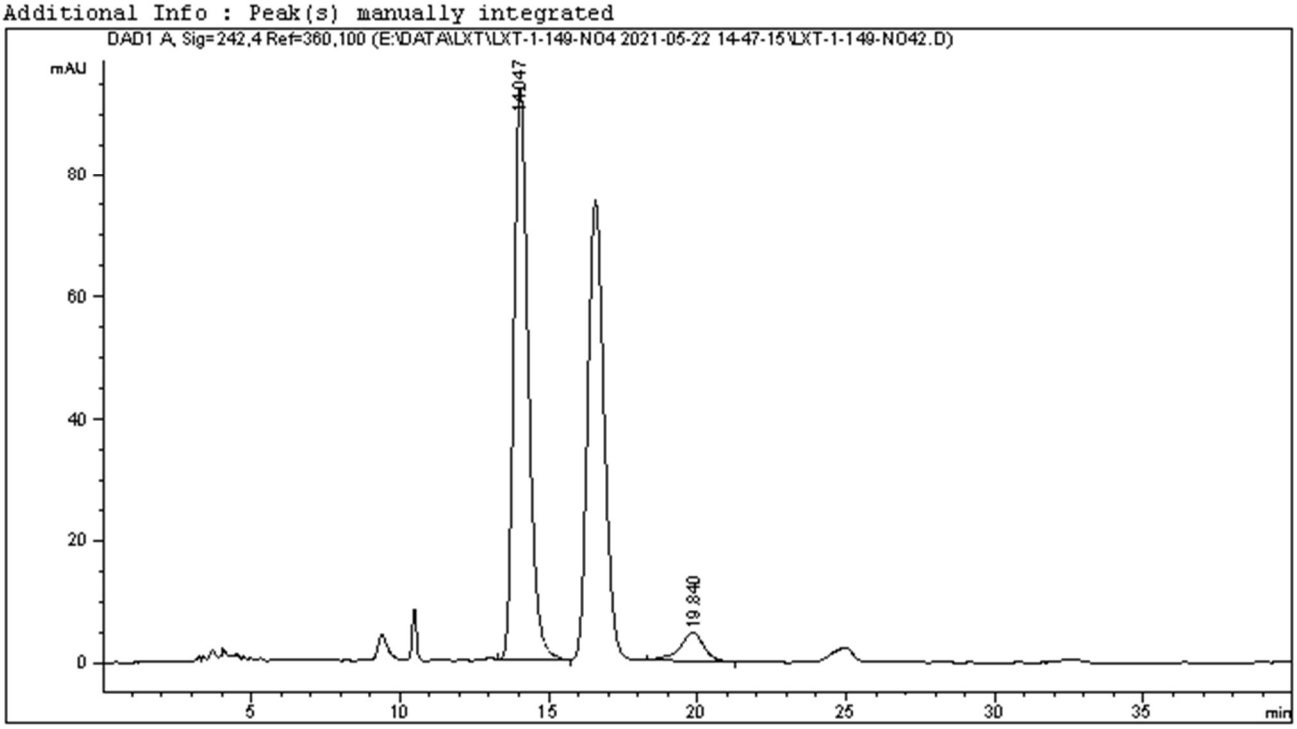
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.495	MM	0.5843	1503.93835	42.90088	49.9981
2	20.391	MF	0.8071	1504.05432	31.05901	50.0019

Totals : 3007.99268 73.95988

Data File E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\LXT-1-149-N042.D
Sample Name: LXT-1-149-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 7
Injection Date : 5/22/2021 3:41:19 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\1-ASH-98-2-1ML-10ul-40min-ALL -nml.M
Last changed : 5/22/2021 2:47:15 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-1-149-N04 2021-05-22 14-47-15\1-ASH-98-2-1ML-10ul-40min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 3:36:02 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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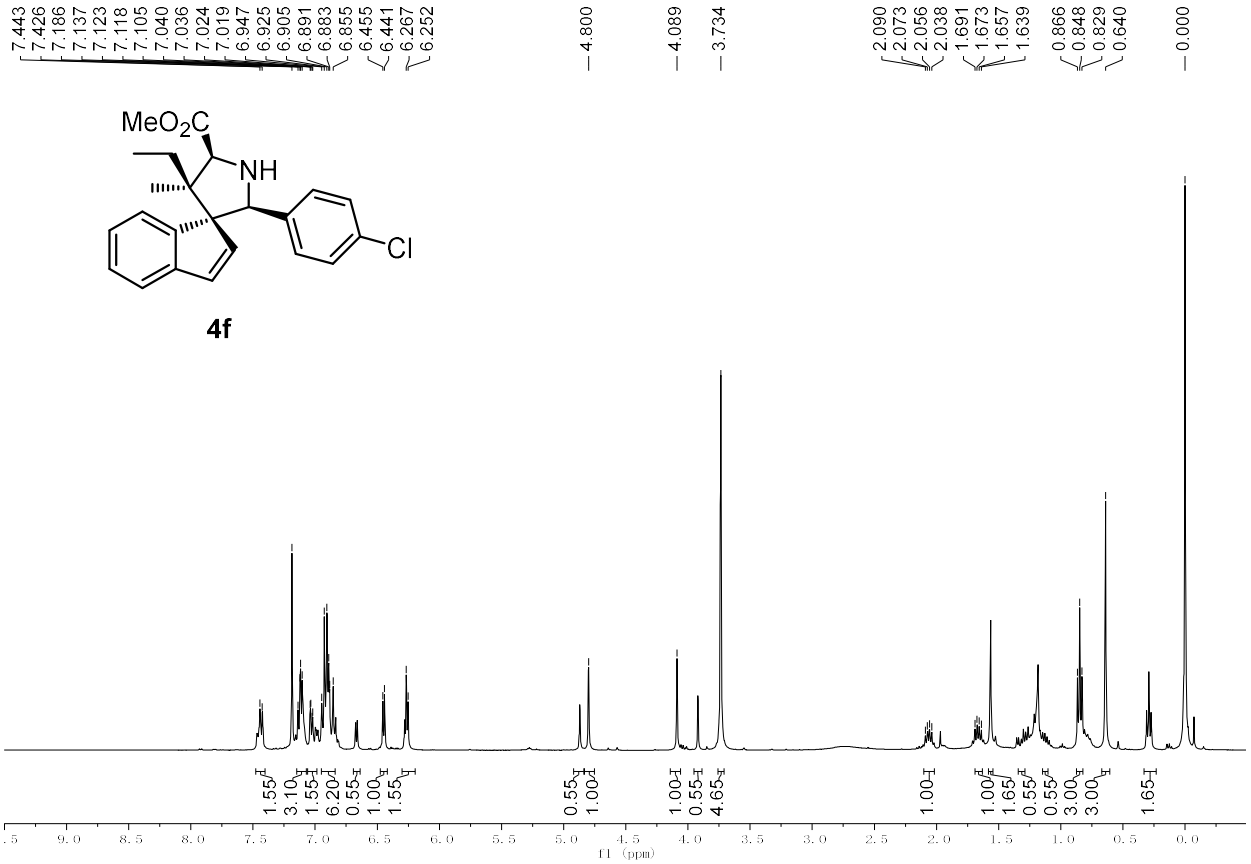
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

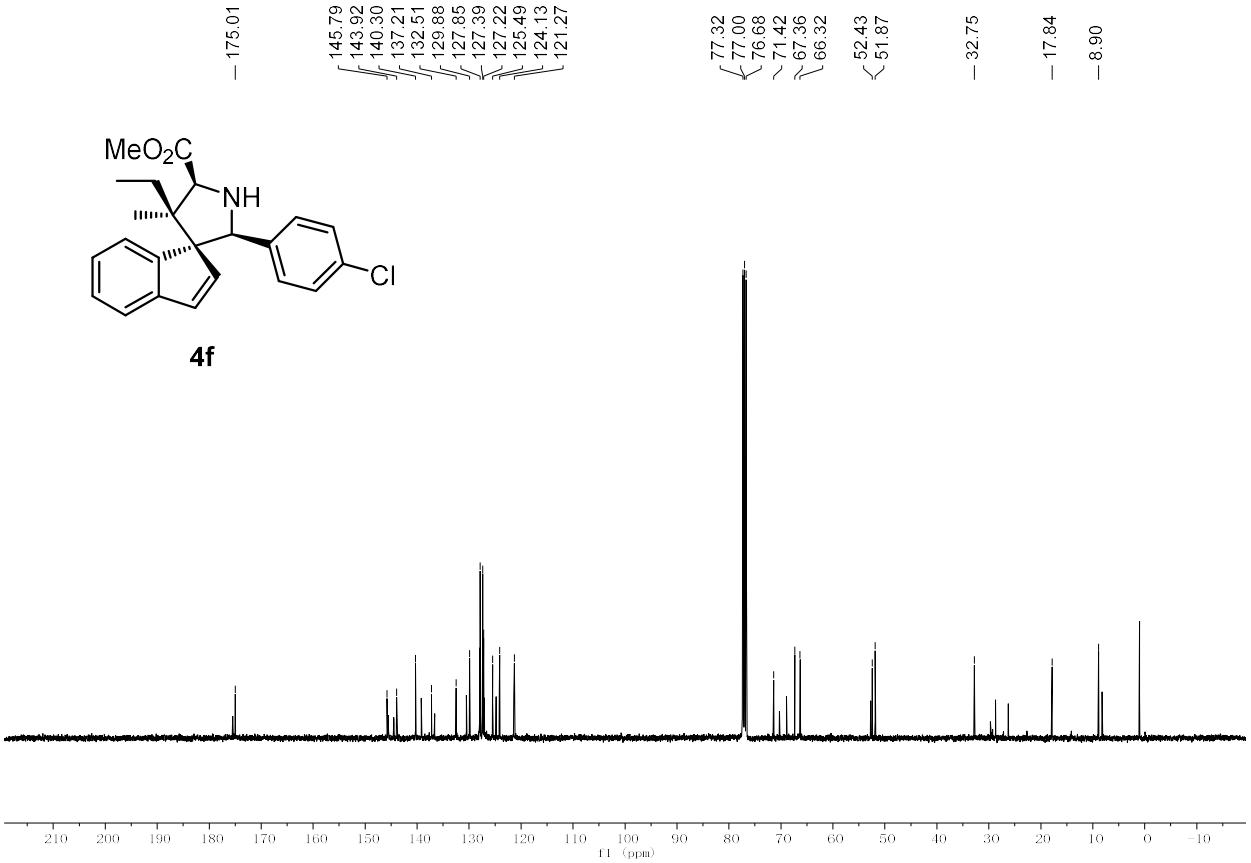
Signal 1: DAD1 A, Sig=242,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.047	BB	0.5225	3208.11206	93.68336	92.4947
2	19.840	BB	0.6669	260.31570	4.58136	7.5053

Totals : 3468.42776 98.26472



^{1}H NMR (400 MHz, Chloroform-*d*) of **4f**

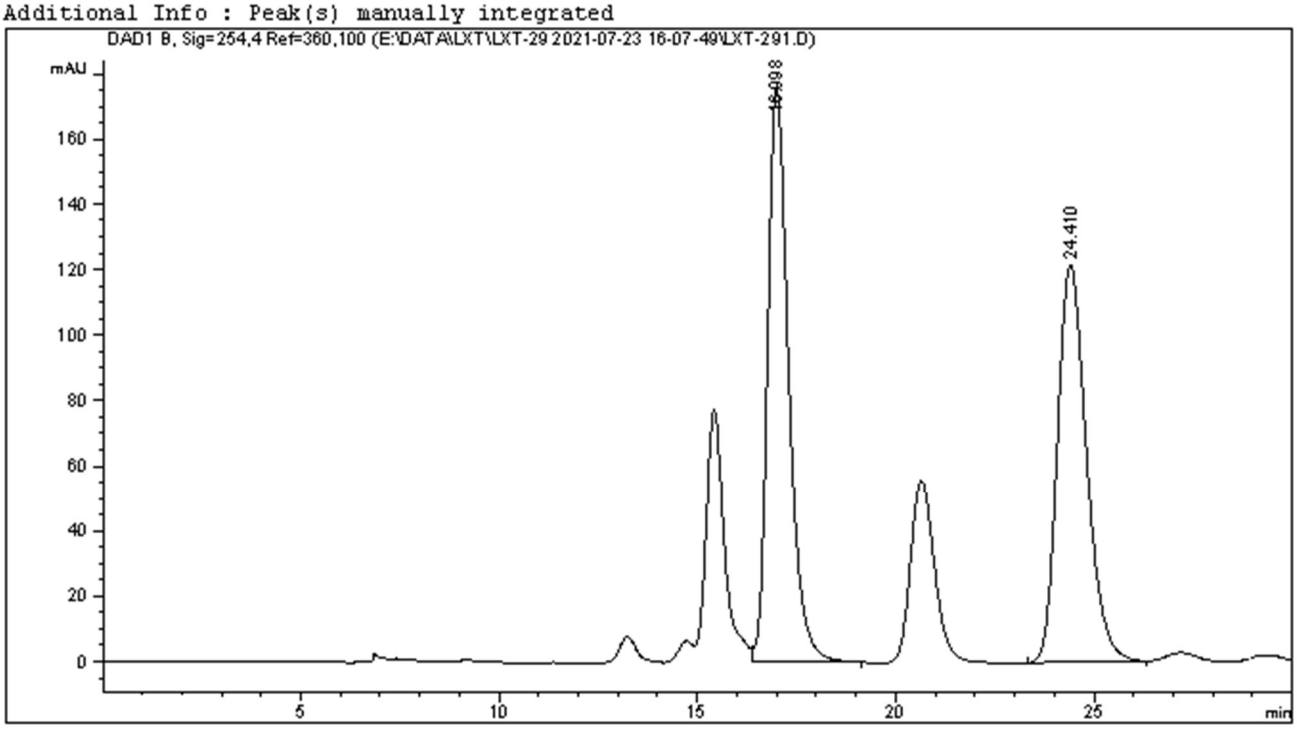


^{13}C NMR (101 MHz, Chloroform-*d*) of **4f**

Data File E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\LXT-291.D
Sample Name: LXT-2-29-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 31
Injection Date : 7/23/2021 4:30:23 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\1-ASH-99-1-0.5ML-10ul-30min-ALL-nml.M
Last changed : 7/23/2021 4:07:49 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\1-ASH-99-1-0.5ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:53:28 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

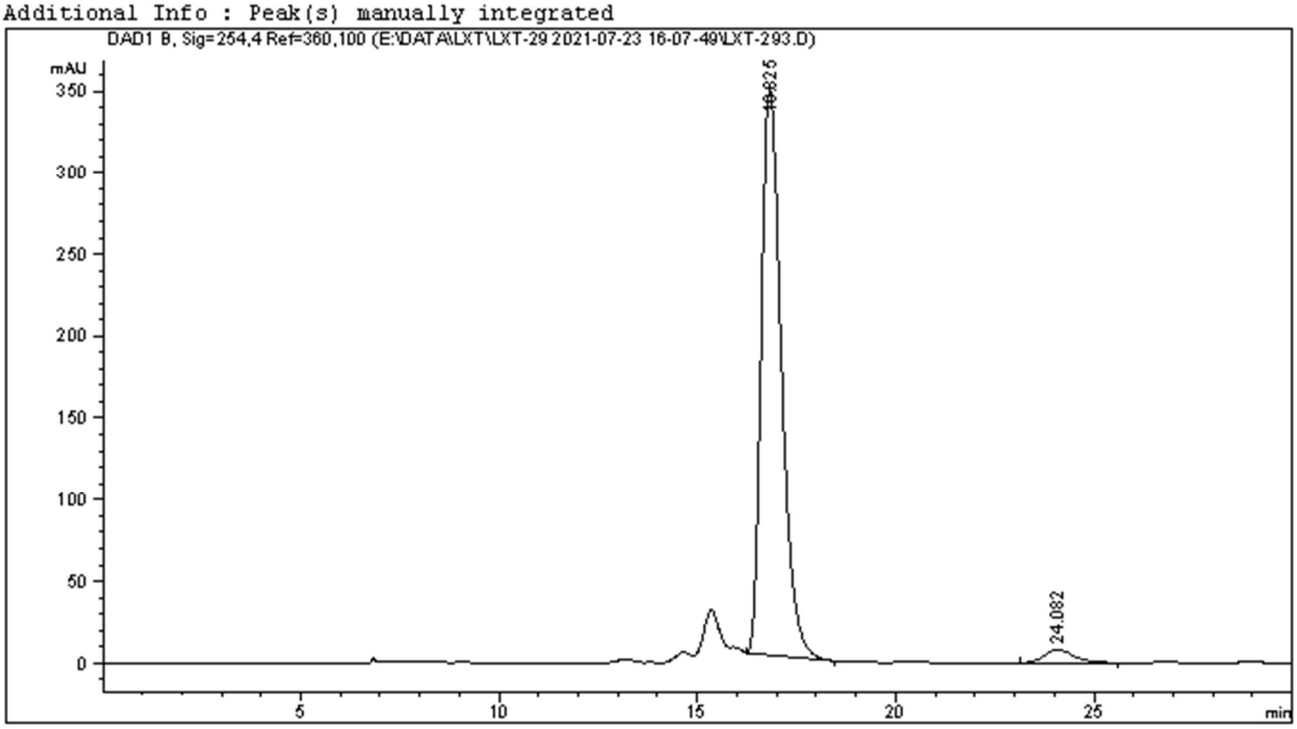
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.998	VB	0.5585	6487.63574	175.81052	51.2194
2	24.410	BB	0.7507	6178.73682	121.62289	48.7806

Totals : 1.26664e4 297.43341

Data File E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\LXT-293.D
Sample Name: LXT-2-29-2-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 4
Acq. Instrument : 1260 Location : 32
Injection Date : 7/23/2021 5:12:54 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\1-ASH-99-1-0.5ML-10ul-30min-ALL-nml.M
Last changed : 7/23/2021 4:07:49 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-29 2021-07-23 16-07-49\1-ASH-99-1-0.5ML-10ul-30min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:53:28 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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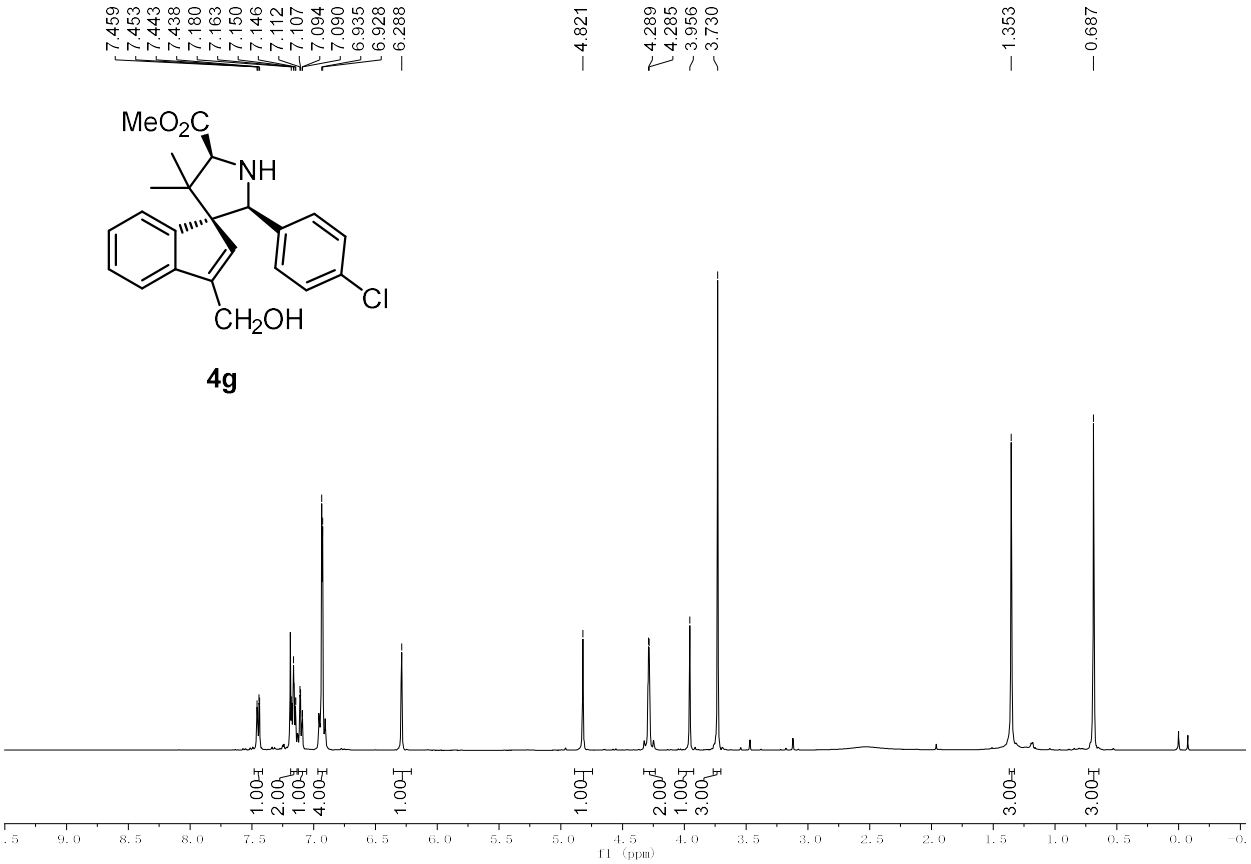
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

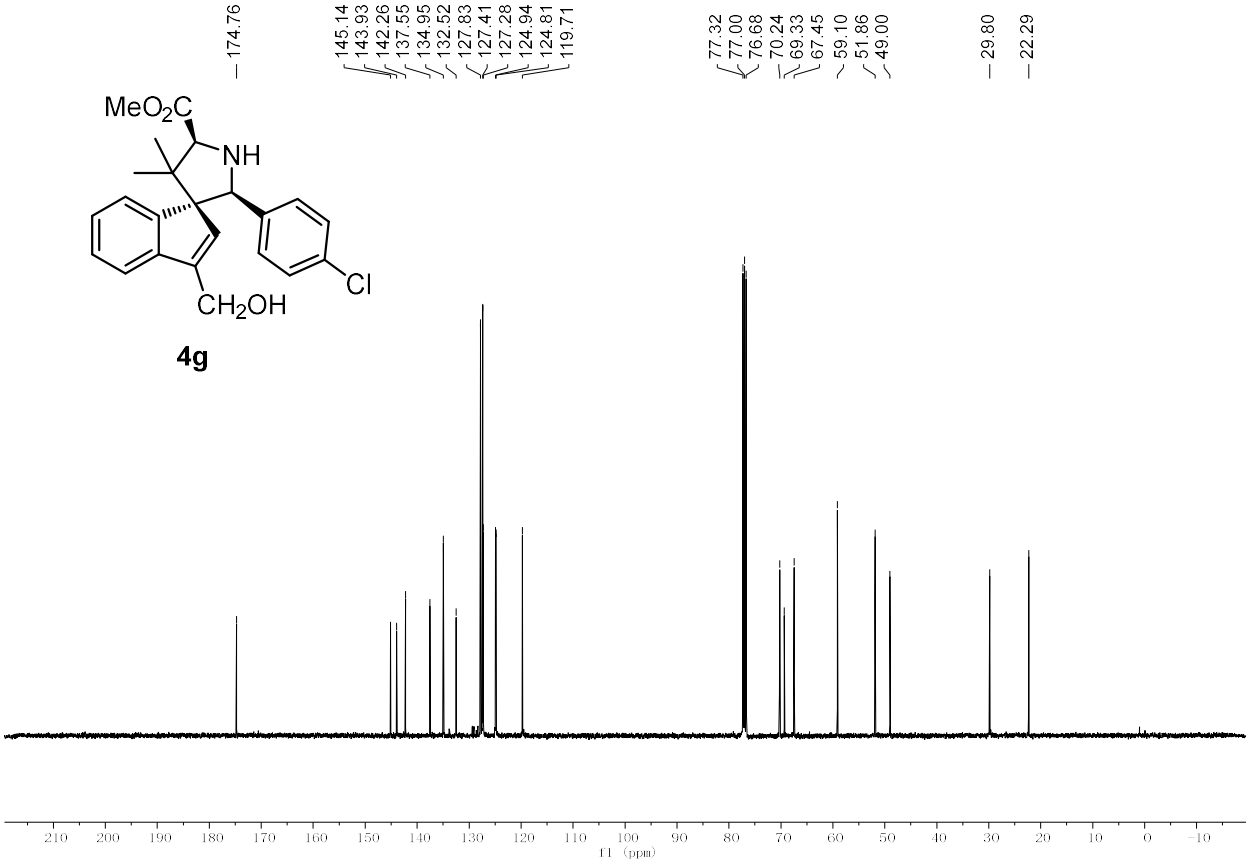
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.825	BB	0.5443	1.21983e4	346.83093	96.8099
2	24.082	BB	0.5930	401.96222	7.97579	3.1901

Totals : 1.26002e4 354.80672



^{1}H NMR (400 MHz, Chloroform-*d*) of **4g**



^{13}C NMR (400 MHz, Chloroform-*d*) of **4g**

Data File D:\HPLC\DATA\20230403\B 2023-04-03 11-04-06\B16.D
Sample Name: LXT-6-19-RAC

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :  17
Acq. Instrument : 1260                             Location :   31
Injection Date  : 4/3/2023 6:08:38 PM                   Inj :   1
                                                 Inj Volume : 10.000 µl
Acq. Method     : D:\HPLC\Data\20230403\B 2023-04-03 11-04-06\1-0D-90-10-1ML-10ul-20min-ALL-
                  nml.M
Last changed    : 4/3/2023 3:29:14 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230403\B 2023-04-03 11-04-06\1-0D-90-10-1ML-10ul-20min-ALL-
                  nml.M (Sequence Method)
Last changed    : 4/10/2023 9:10:11 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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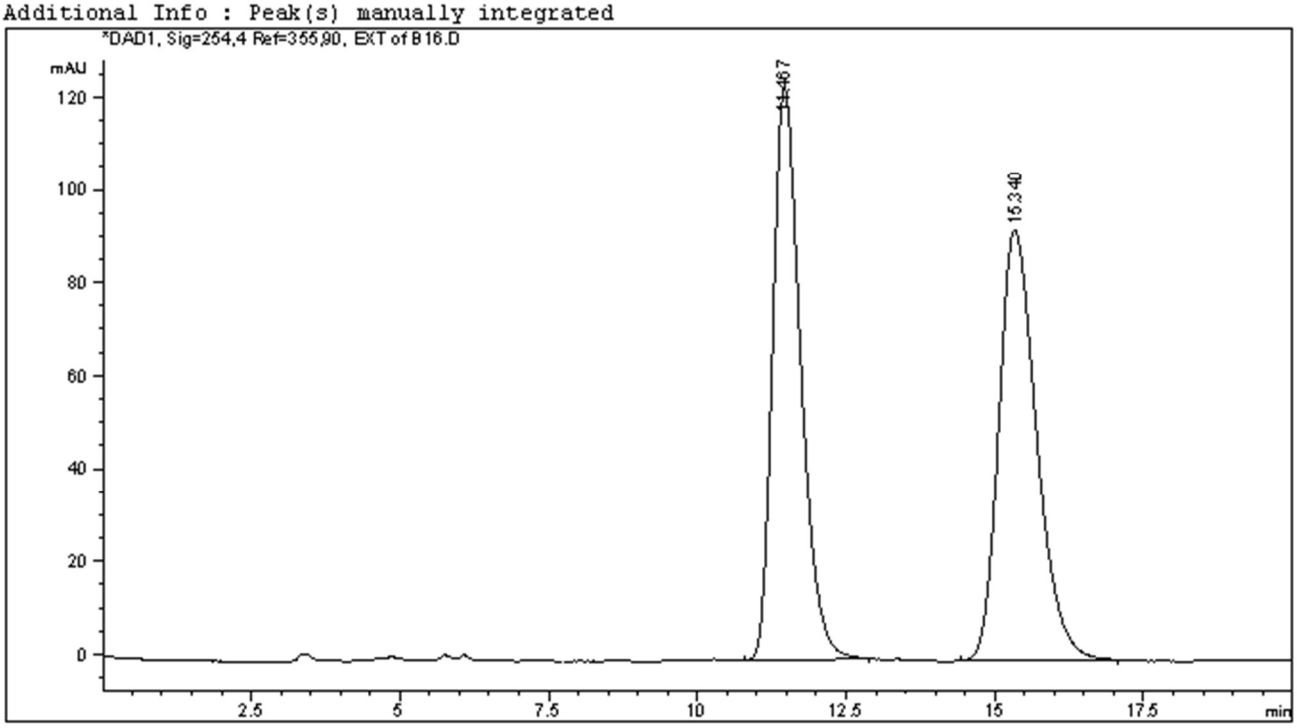


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==================================================================
                         Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

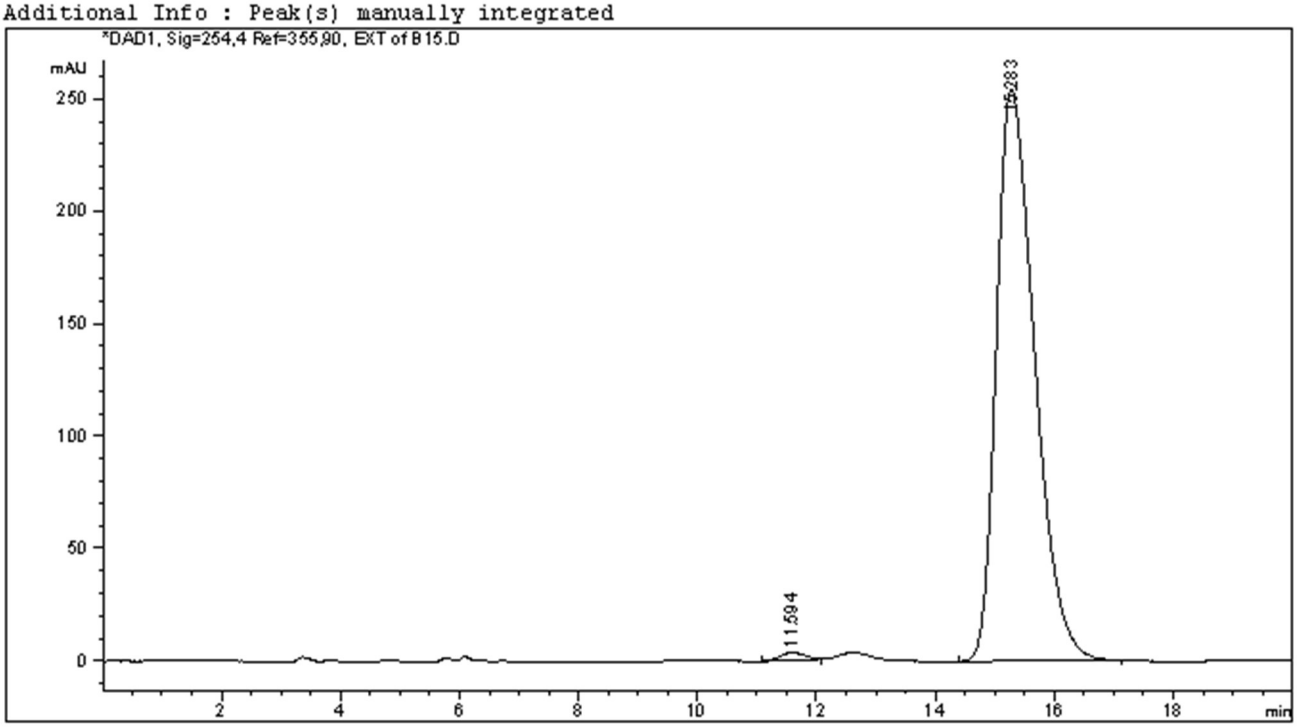
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.467 BB    0.4847 4041.36768  123.19960  49.7316
   2  15.340 BB    0.6426 4084.98706   92.61632  50.2684

Totals :                  8126.35474  215.81592
```

Data File D:\HPLC\DATA\20230403\B 2023-04-03 11-04-06\B15.D
Sample Name: LXT-6-19-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 16
Acq. Instrument : 1260 Location : 32
Injection Date : 4/3/2023 5:47:08 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230403\B 2023-04-03 11-04-06\1-0D-90-10-1ML-10ul-20min-ALL-nml.M
Last changed : 4/3/2023 3:29:14 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230403\B 2023-04-03 11-04-06\1-0D-90-10-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:10:11 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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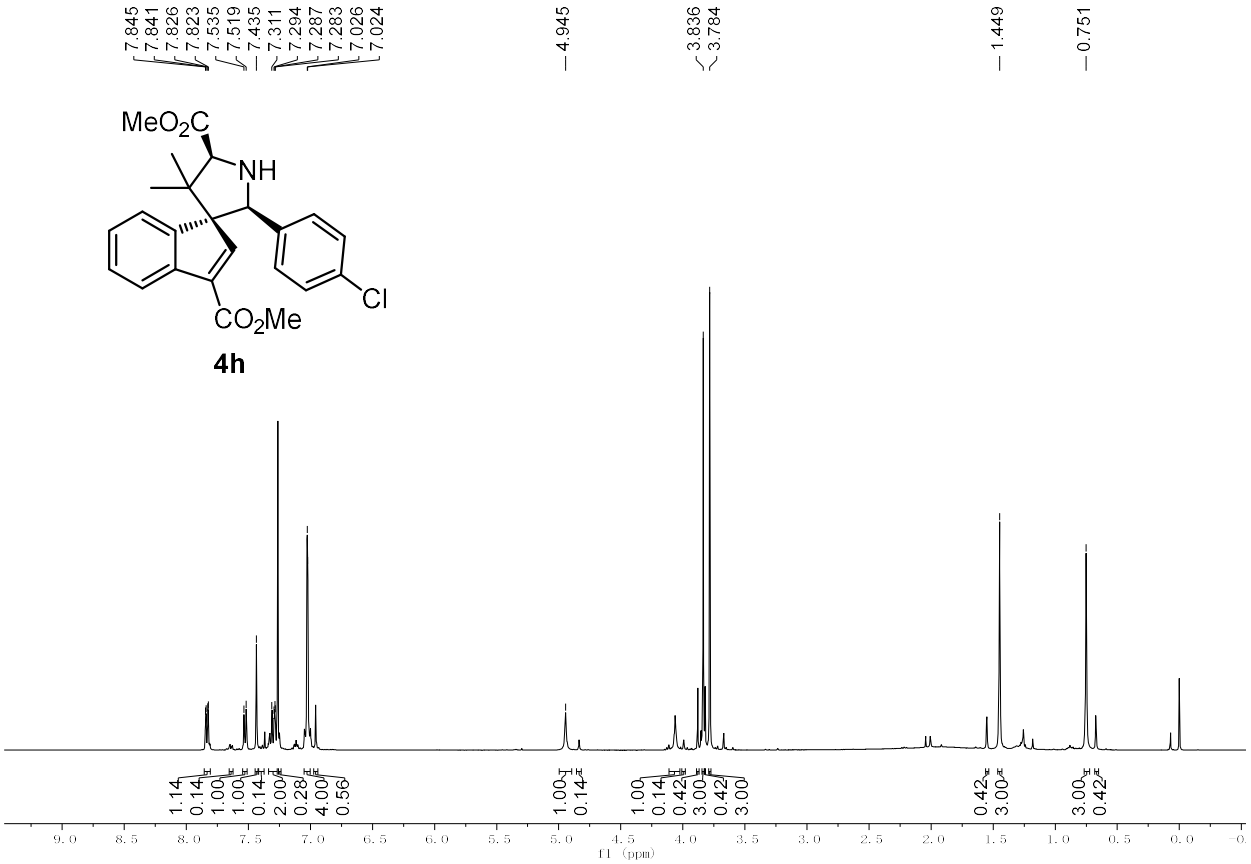
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

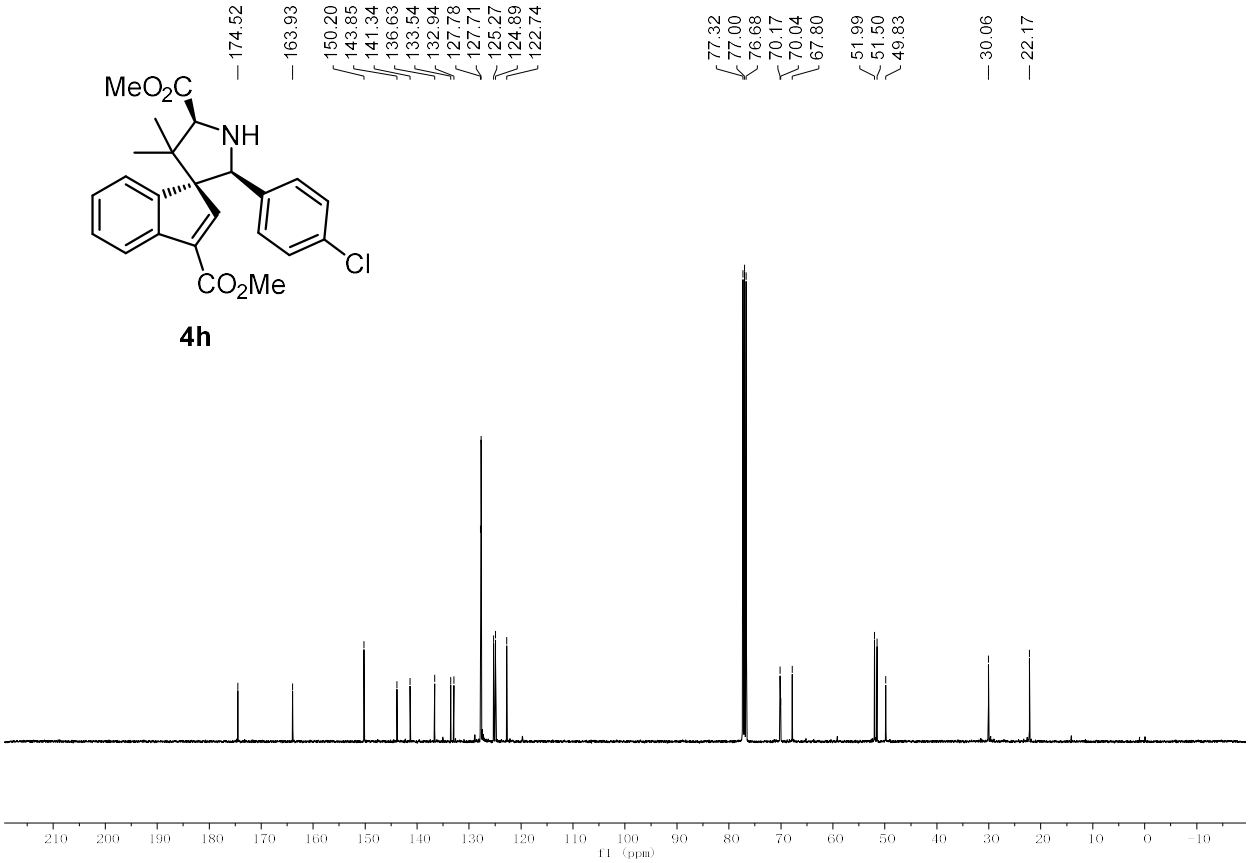
Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.594	BB	0.3327	94.81008	3.37574	0.8286
2	15.283	BB	0.6504	1.13475e4	254.88110	99.1714

Totals : 1.14423e4 258.25685



^{1}H NMR (400 MHz, Chloroform-*d*) of **4h**

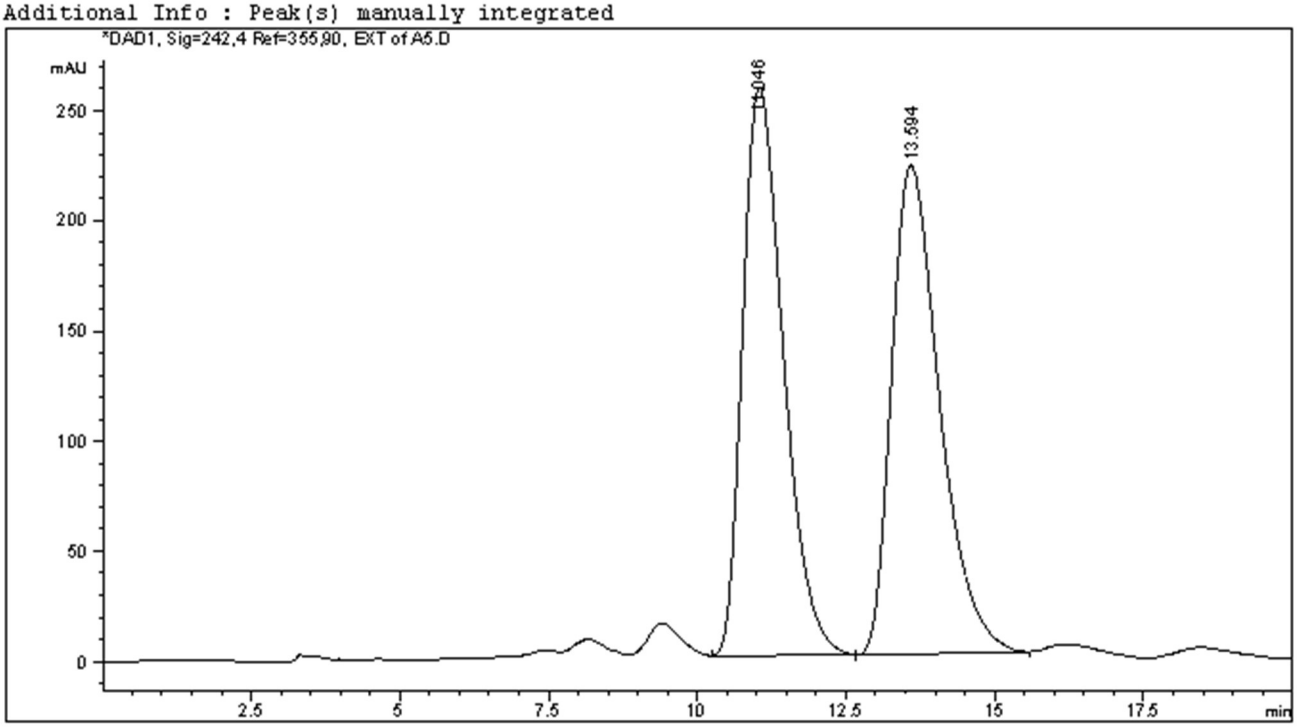


^{13}C NMR (400 MHz, Chloroform-*d*) of **4h**

Data File D:\HPLC\DATA\20230404\A 2023-04-04 10-58-02\A5.D
Sample Name: LXT-6-16-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 6
Acq. Instrument : 1260 Location : 41
Injection Date : 4/4/2023 11:42:33 AM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230404\A 2023-04-04 10-58-02\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M
Last changed : 4/4/2023 11:09:43 AM by SYSTEM
Analysis Method : D:\HPLC\Data\20230404\A 2023-04-04 10-58-02\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:21:51 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1, Sig=242,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

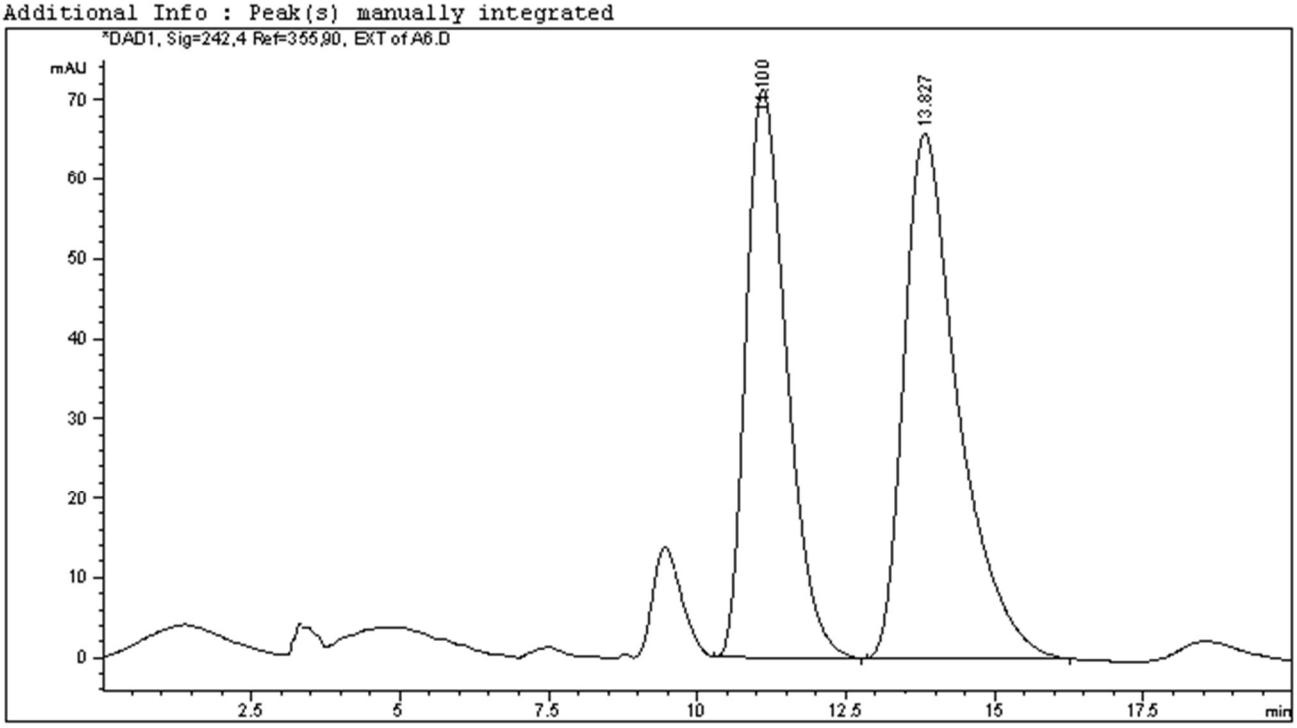
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.046	BB	0.7185	1.22629e4	257.53787	49.6566
2	13.594	BB	0.8411	1.24325e4	221.76202	50.3434

Totals : 2.46954e4 479.29990

Data File D:\HPLC\DATA\20230404\A 2023-04-04 10-58-02\A6.D
Sample Name: LXT-6-16-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 7
Acq. Instrument : 1260 Location : 42
Injection Date : 4/4/2023 12:04:00 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230404\A 2023-04-04 10-58-02\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M
Last changed : 4/4/2023 11:09:43 AM by SYSTEM
Analysis Method : D:\HPLC\Data\20230404\A 2023-04-04 10-58-02\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:21:51 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

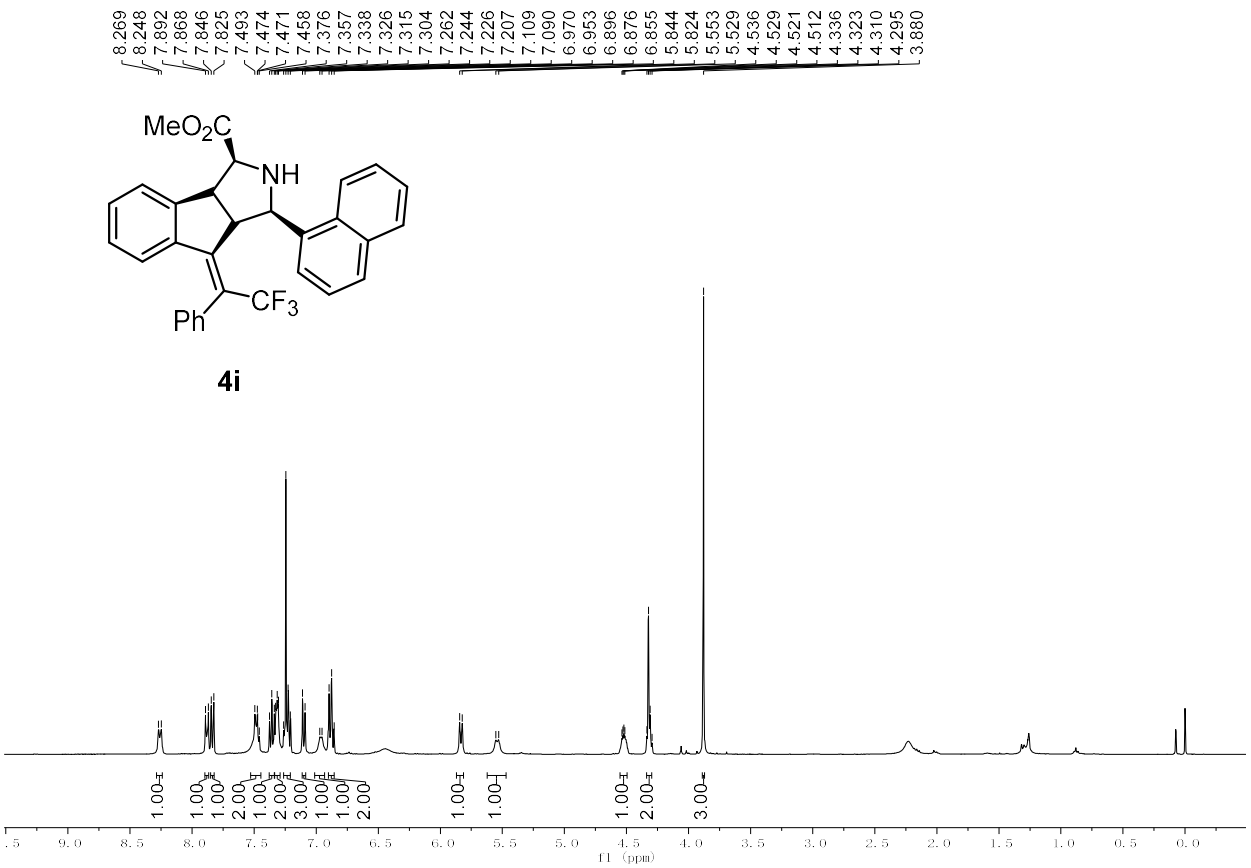
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

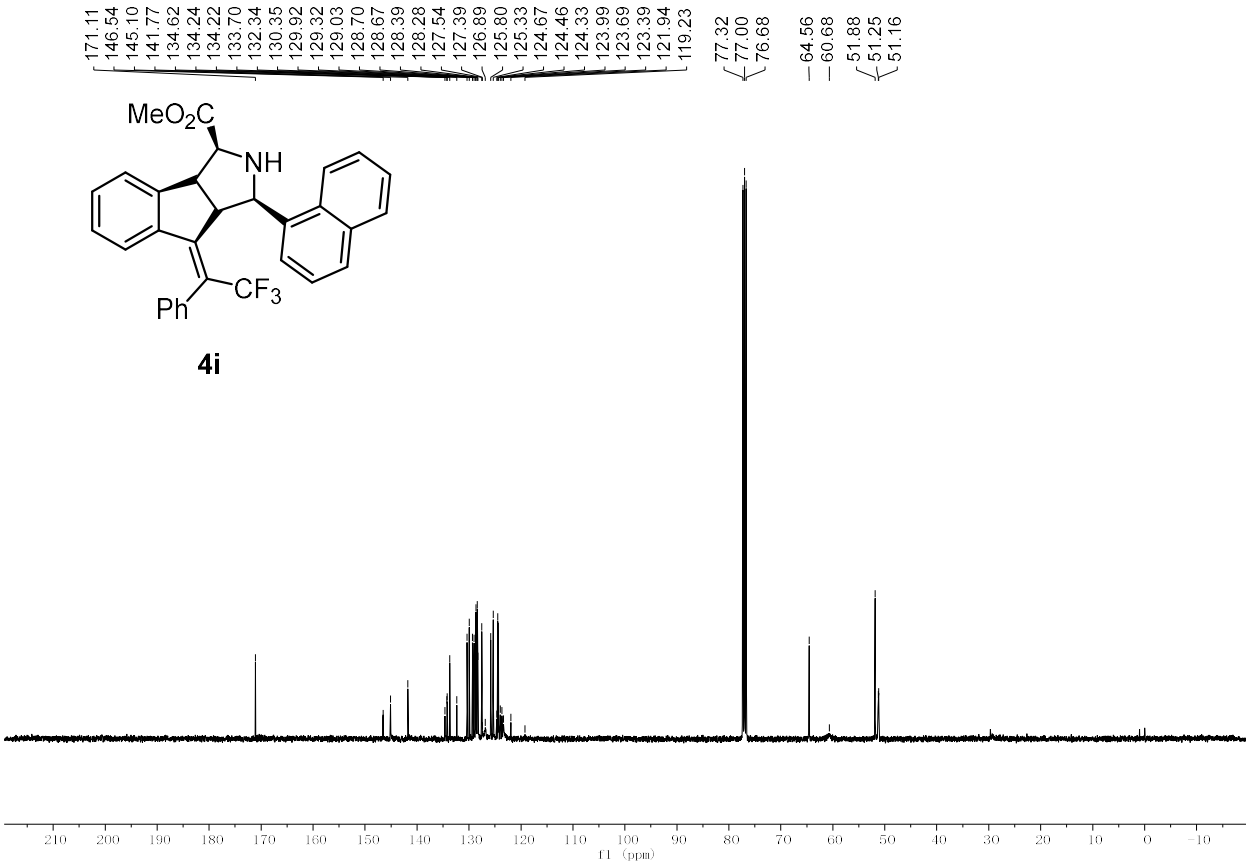
Signal 1: DAD1, Sig=242,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.100	BB	0.6754	3383.09717	71.45516	44.7554
2	13.827	BB	0.7733	4175.99121	65.89890	55.2446

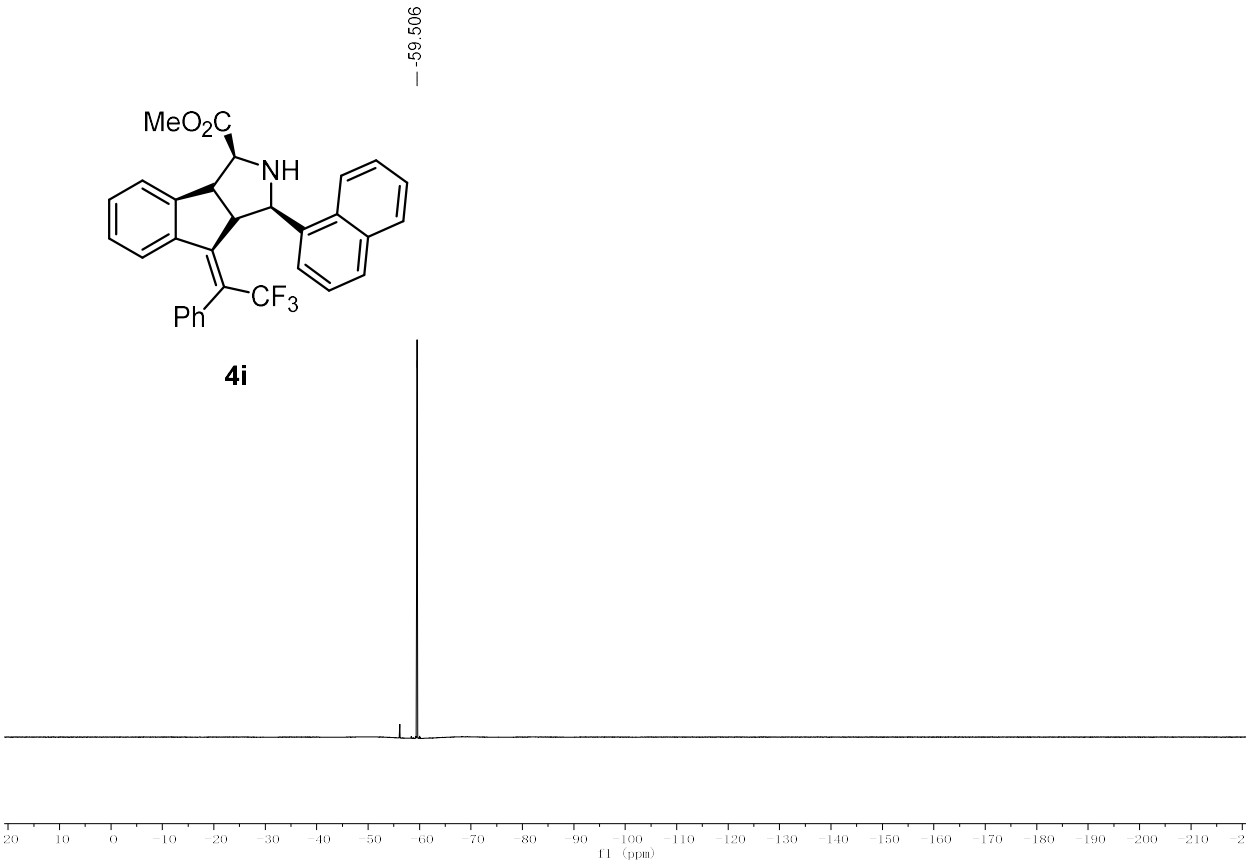
Totals : 7559.08838 137.35406



^{1}H NMR (400 MHz, Chloroform-*d*) of **4i**



^{13}C NMR (400 MHz, Chloroform-*d*) of **4i**

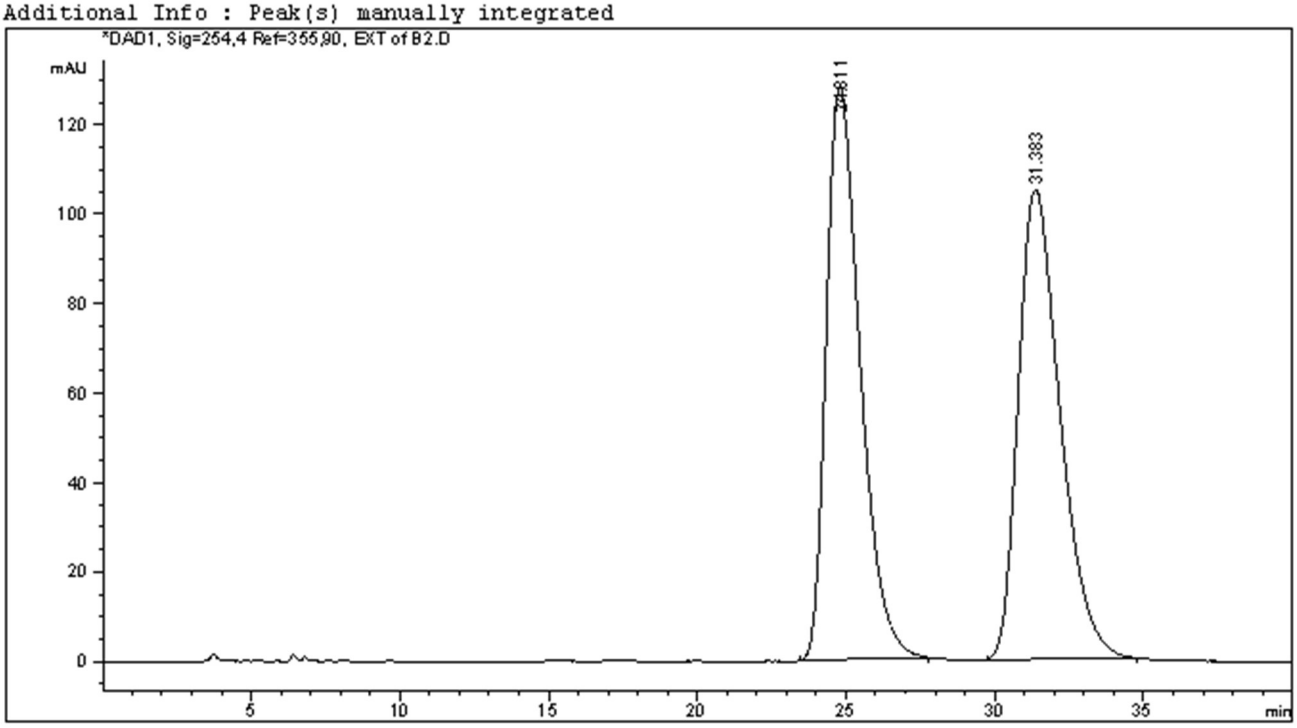


^{19}F NMR (377 MHz, Chloroform-d) of **4i**

Data File D:\HPLC\DATA\20230407\B 2023-04-07 14-52-15\B2.D
Sample Name: LXT-6-26-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 1
Injection Date : 4/7/2023 3:46:06 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230407\B 2023-04-07 14-52-15\1-0D-90-10-1ML-10ul-40min-ALL-nml.M
Last changed : 4/7/2023 2:52:15 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230407\B 2023-04-07 14-52-15\1-0D-90-10-1ML-10ul-40min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:03:49 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

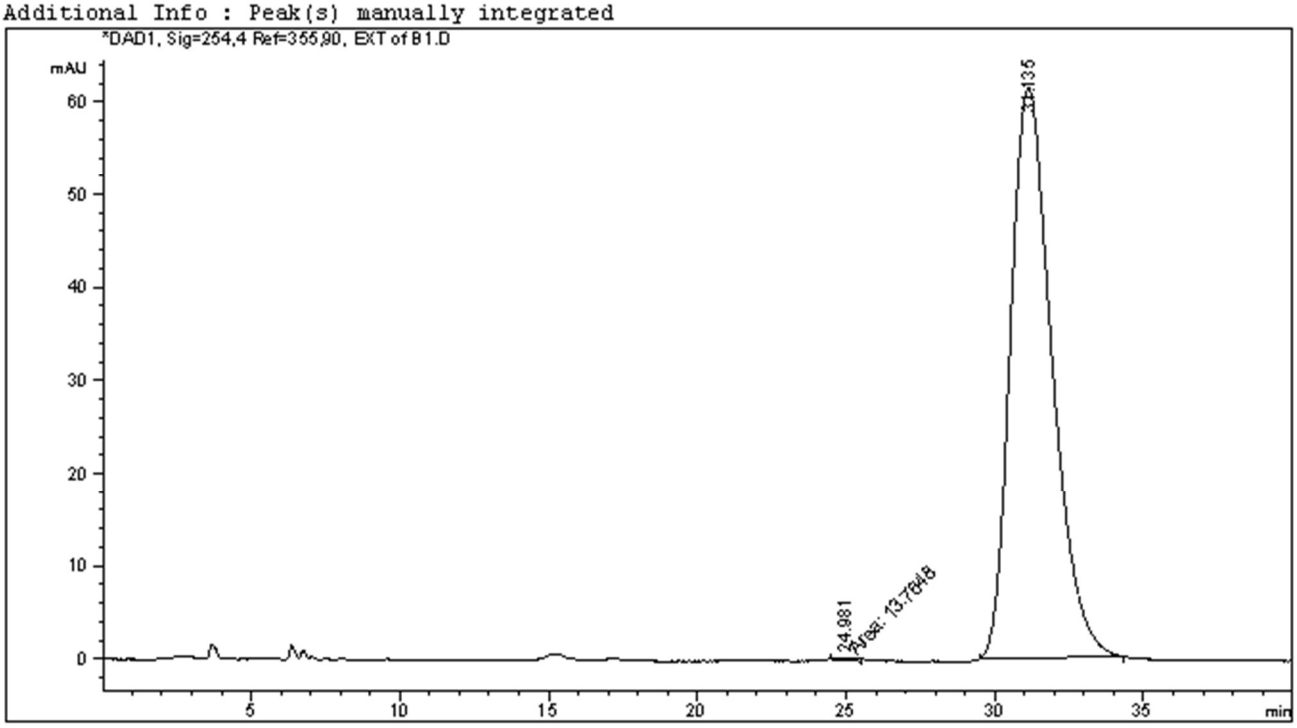
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.811	BB	0.9485	1.01410e4	127.83653	49.7700
2	31.383	BB	1.1511	1.02347e4	104.91816	50.2300

Totals : 2.03757e4 232.75469

Data File D:\HPLC\DATA\20230407\B 2023-04-07 14-52-15\B1.D
Sample Name: LXT-6-26-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 2
Injection Date : 4/7/2023 3:04:40 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20230407\B 2023-04-07 14-52-15\1-0D-90-10-1ML-10ul-40min-ALL-nml.M
Last changed : 4/7/2023 2:52:15 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20230407\B 2023-04-07 14-52-15\1-0D-90-10-1ML-10ul-40min-ALL-nml.M (Sequence Method)
Last changed : 4/10/2023 9:03:49 AM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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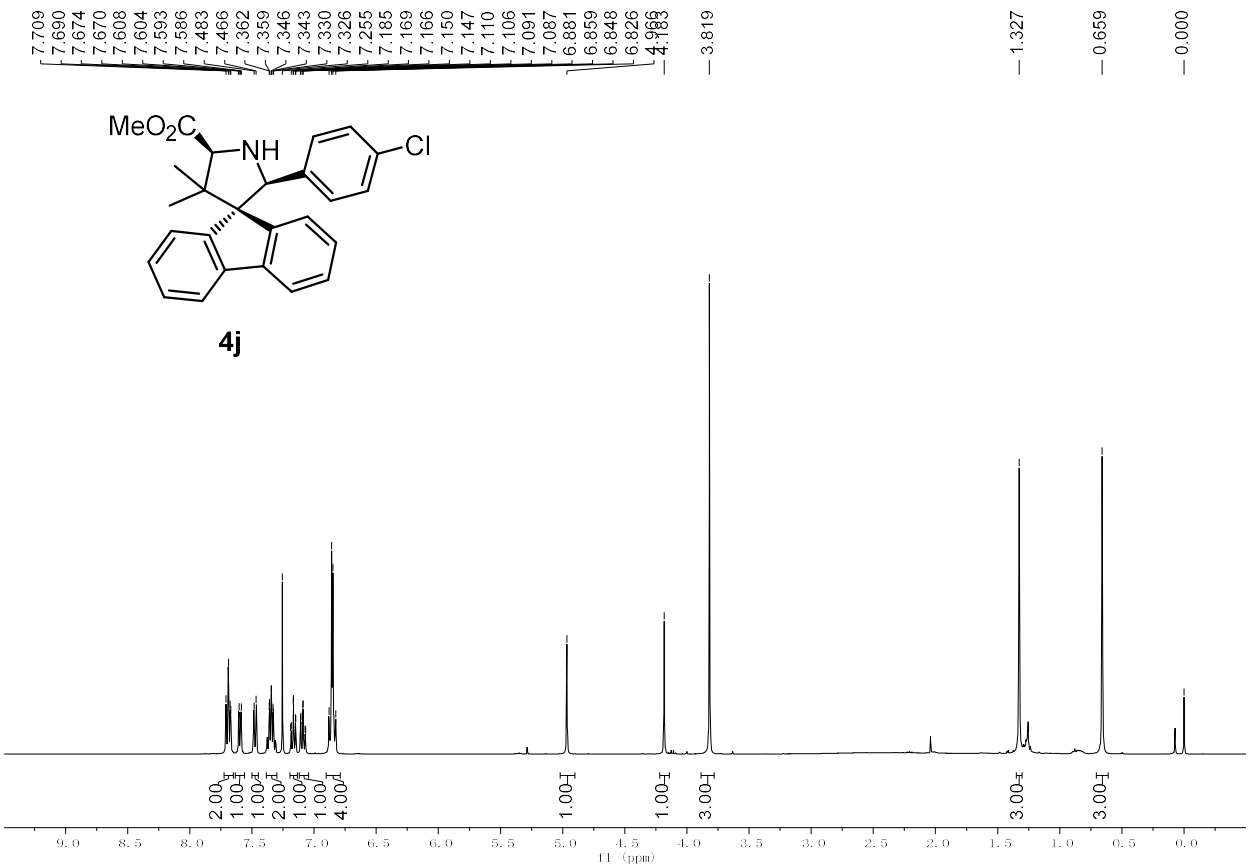
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

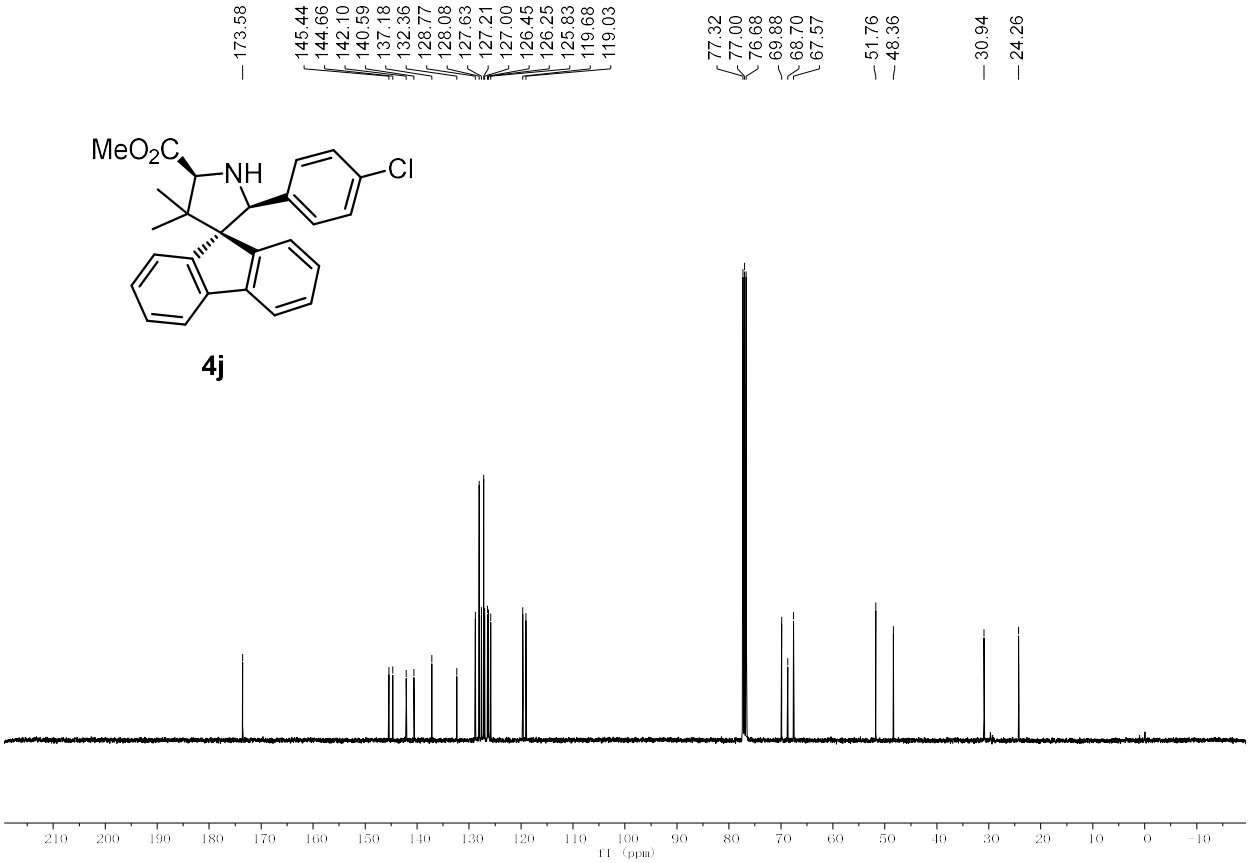
Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.981	MM	0.7782	13.76484	2.94791e-1	0.2314
2	31.135	BB	1.1344	5935.10352	61.36396	99.7686

Totals : 5948.86835 61.65875



^{1}H NMR (400 MHz, Chloroform-*d*) of **4j**



^{13}C NMR (101 MHz, Chloroform-*d*) of **4j**

Data File E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\LXT-2-46-561.D
Sample Name: LXT-2-46-RAC

```
==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :   2
Acq. Instrument : 1260                             Location :   3
Injection Date  : 6/25/2021 4:51:30 PM                  Inj :   1
                                                Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\1-ASH-98-2-1ML-10ul-20min-ALL-
                  nml.M
Last changed    : 6/25/2021 4:39:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\1-ASH-98-2-1ML-10ul-20min-ALL-
                  nml.M (Sequence Method)
Last changed    : 8/1/2021 3:44:16 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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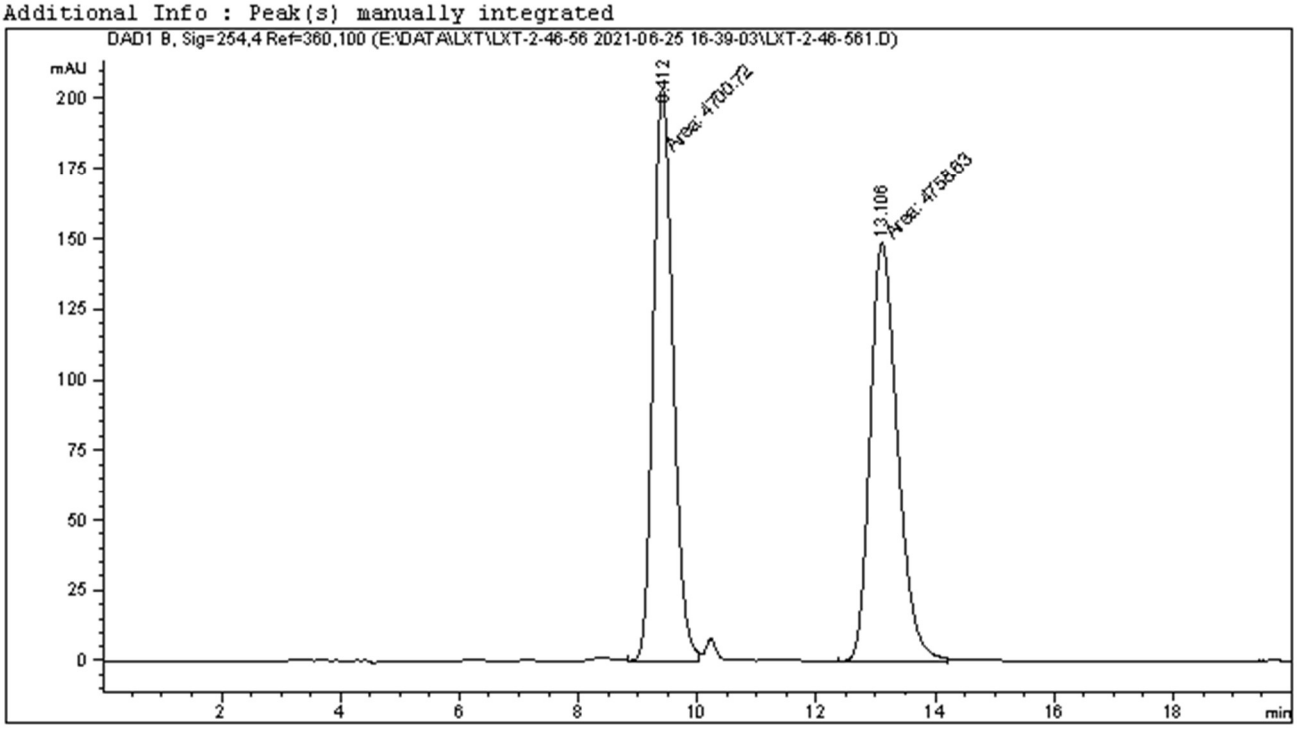


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==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100

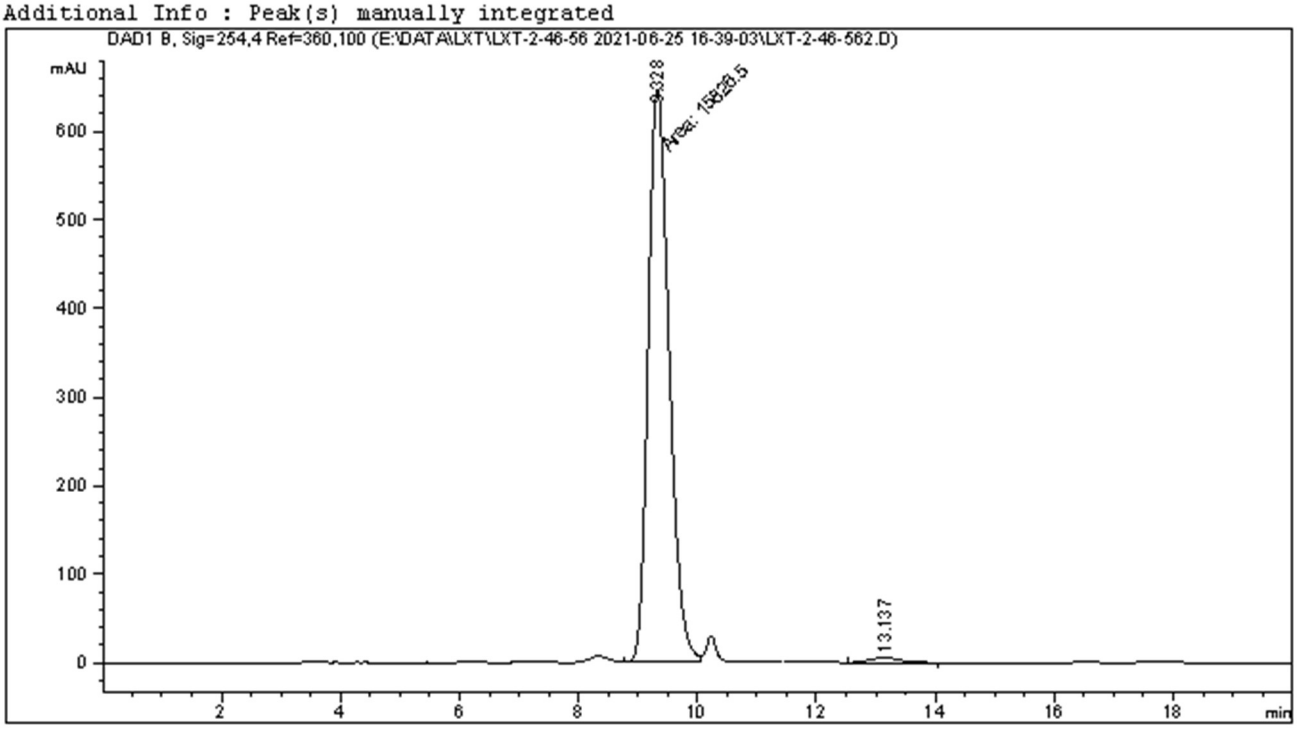
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.412 MF    0.3849 4700.71924  203.55023  49.6939
   2  13.106 MF    0.5339 4758.62793  148.55513  50.3061

Totals :                  9459.34717  352.10536
```

Data File E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\LXT-2-46-562.D
Sample Name: LXT-2-56-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 4
Injection Date : 6/25/2021 5:12:57 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 6/25/2021 4:39:04 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-46-56 2021-06-25 16-39-03\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 3:44:16 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

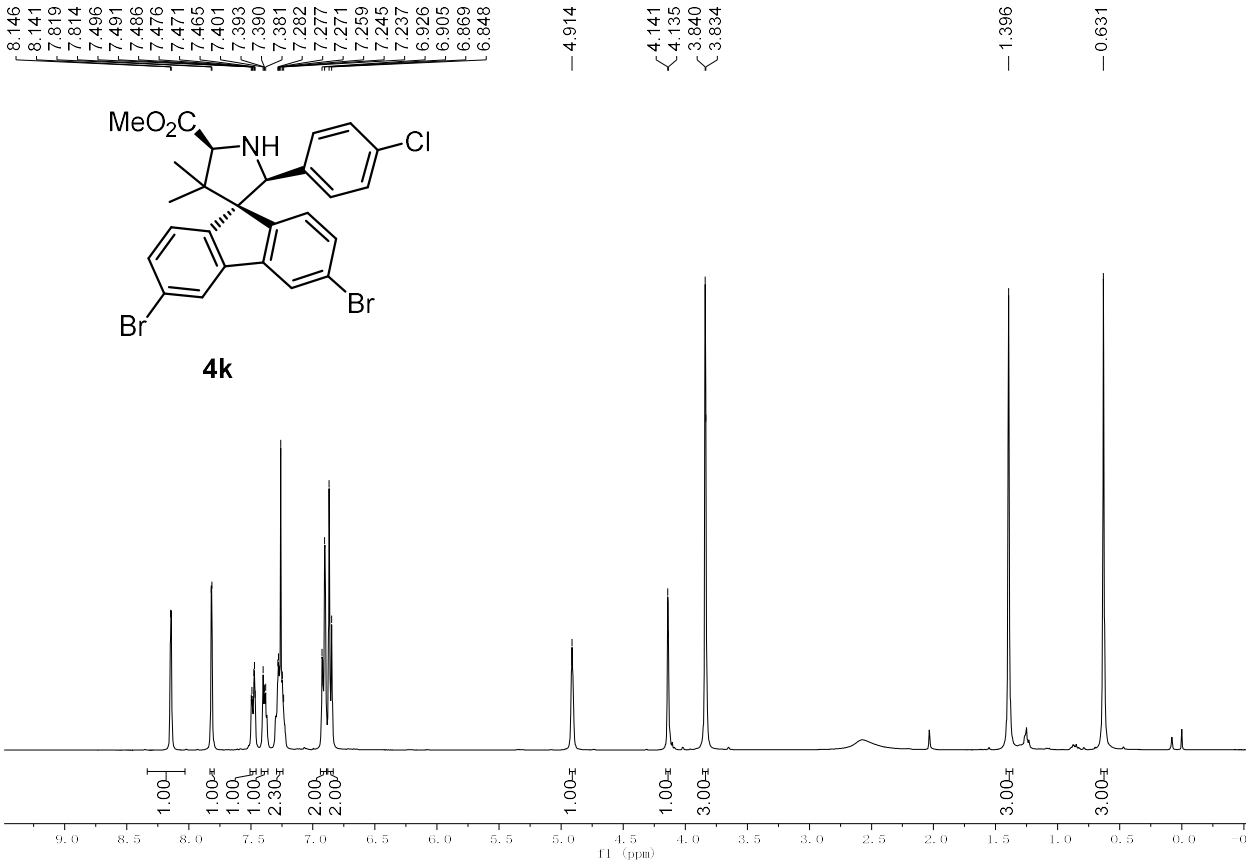
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

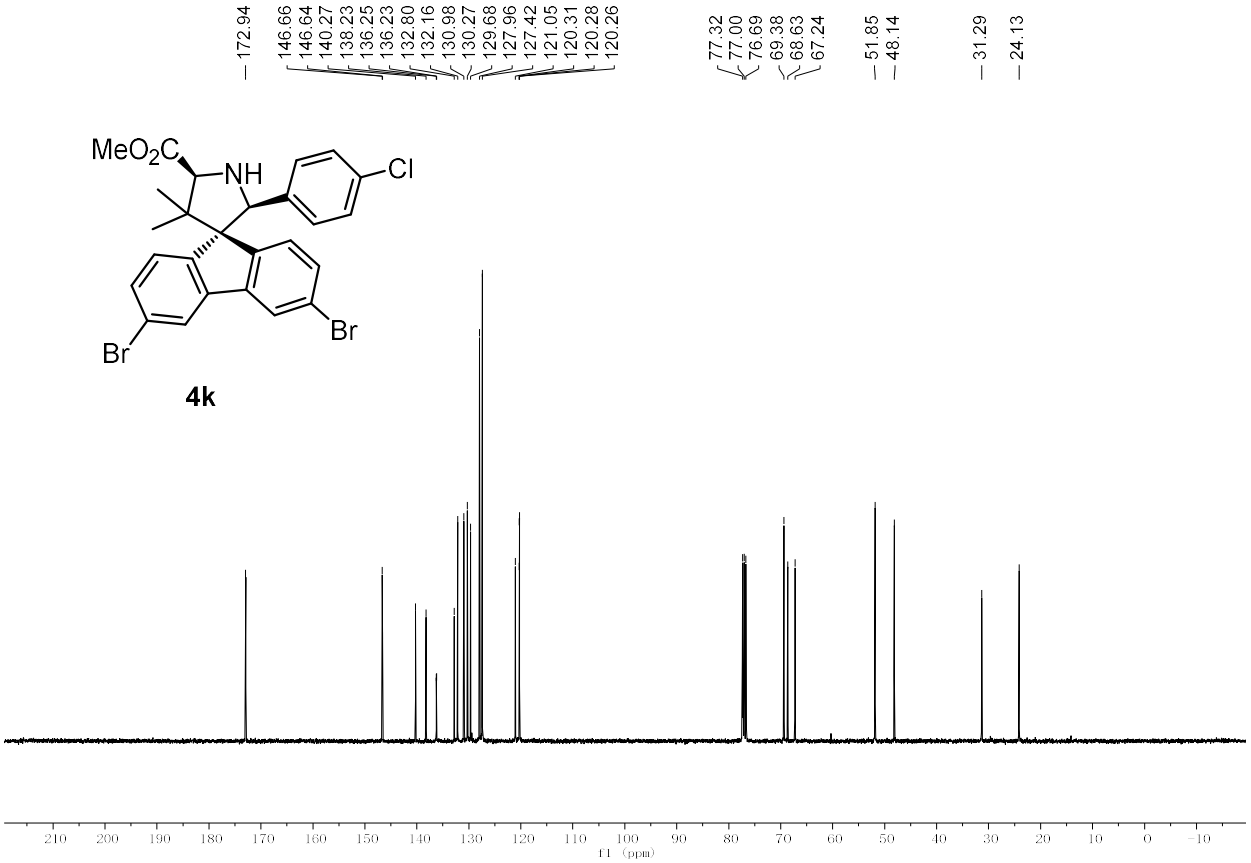
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.328	MF	0.4068	1.58265e4	648.44427	98.8990
2	13.137	BB	0.3913	176.18407	5.33443	1.1010

Totals : 1.60026e4 653.77870



^{1}H NMR (400 MHz, Chloroform-*d*) of **4k**

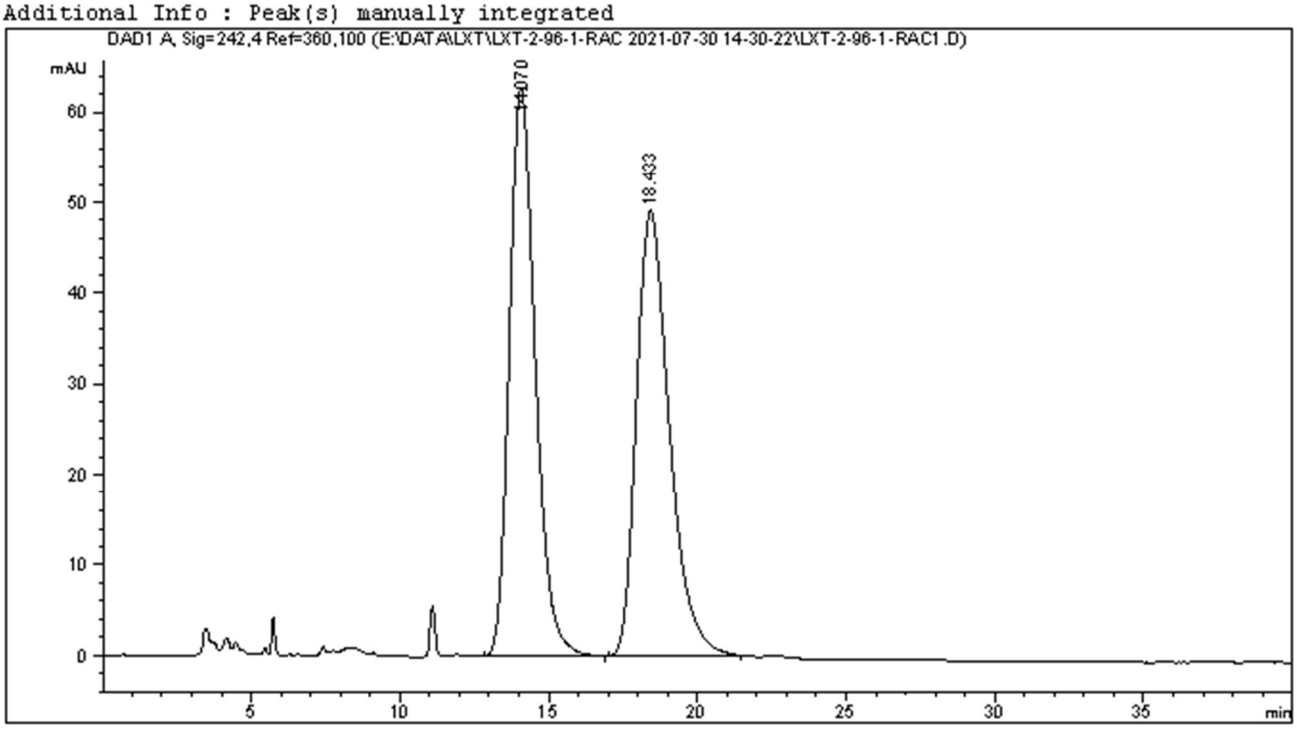


^{13}C NMR (101 MHz, Chloroform-*d*) of **4k**

Data File E:\DATA\LXT\LXT-2-96-1-RAC 2021-07-30 14-30-22\LXT-2-96-1-RAC1.D
Sample Name: LXT-2-96-1-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 23
Injection Date : 7/30/2021 2:52:47 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-96-1-RAC 2021-07-30 14-30-22\1-ASH-98-2-1ML-10ul-40min-ALL-nml.M
Last changed : 7/30/2021 2:30:22 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-96-1-RAC 2021-07-30 14-30-22\1-ASH-98-2-1ML-10ul-40min-ALL-nml.M (Sequence Method)
Last changed : 7/30/2021 10:07:47 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=242,4 Ref=360,100

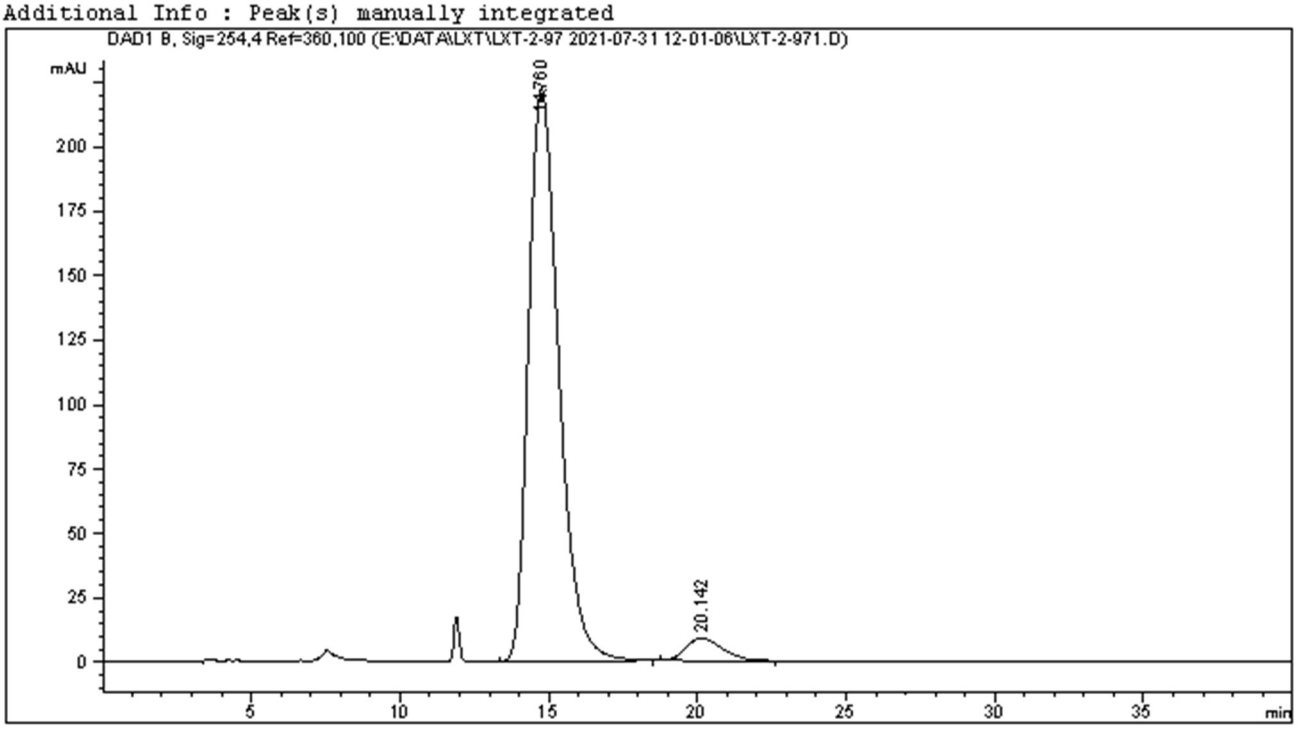
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.070	BB	0.8598	3805.64551	62.72746	50.1634
2	18.433	BB	0.9769	3780.84595	49.12714	49.8366

Totals : 7586.49146 111.85461

Data File E:\DATA\LXT\LXT-2-97 2021-07-31 12-01-06\LXT-2-971.D
Sample Name: LXT-2-97-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 2
Acq. Instrument : 1260 Location : 22
Injection Date : 7/31/2021 12:23:50 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-97 2021-07-31 12-01-06\1-ASH-98-2-1ML-10ul-40min-ALL-nml.M
Last changed : 7/31/2021 12:01:06 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-97 2021-07-31 12-01-06\1-ASH-98-2-1ML-10ul-40min-ALL-nml.M (Sequence Method)
Last changed : 8/1/2021 4:25:35 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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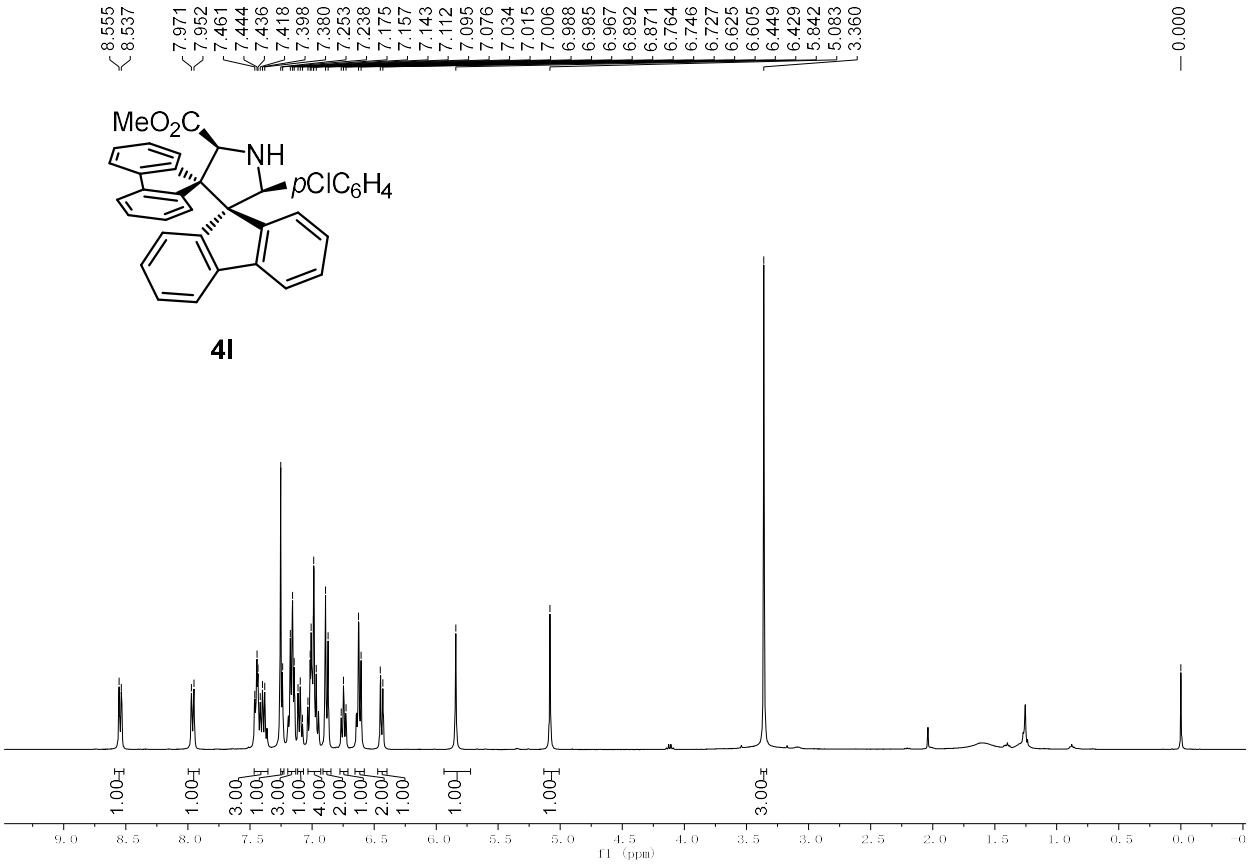
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

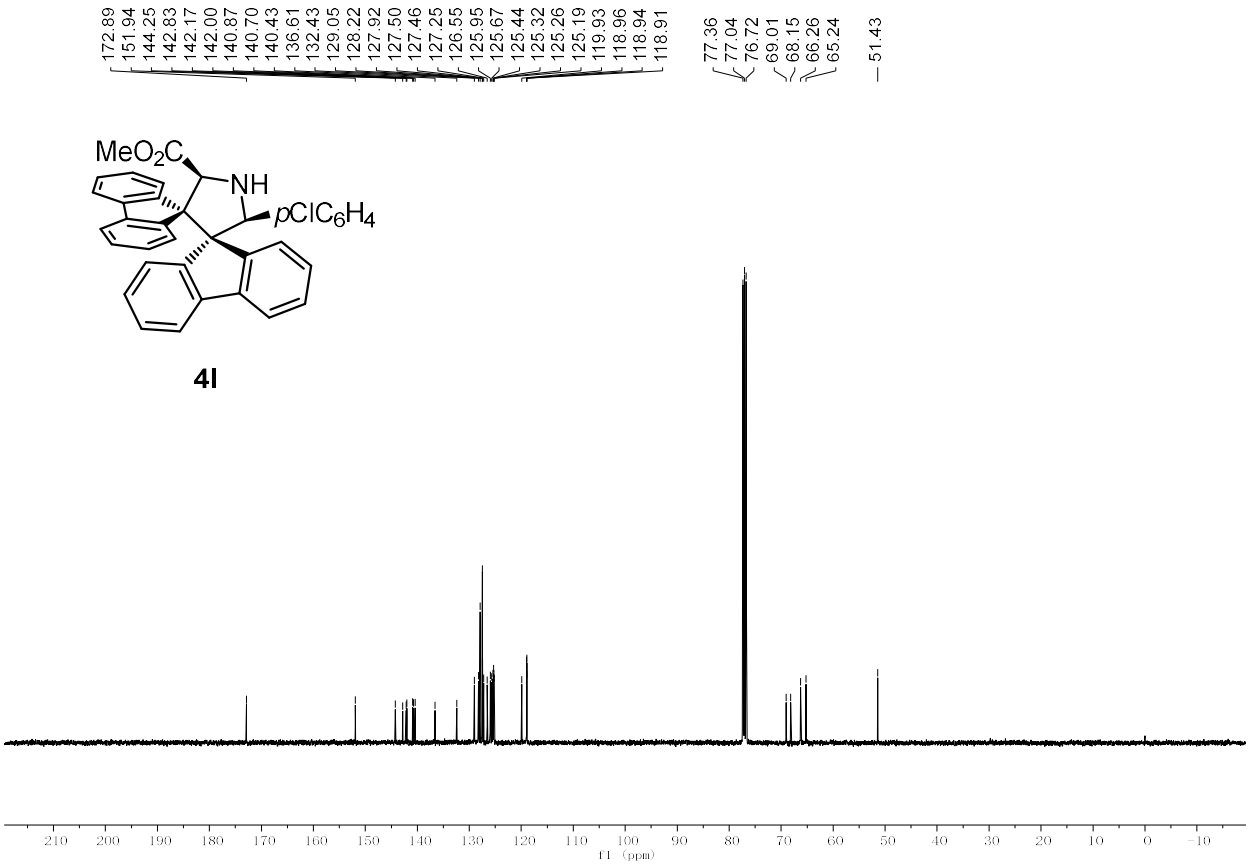
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.760	BB	1.0364	1.56996e4	222.43683	95.4850
2	20.142	BB	1.0008	742.36194	8.69699	4.5150

Totals : 1.64420e4 231.13382



^{1}H NMR (400 MHz, Chloroform-*d*) of **4l**

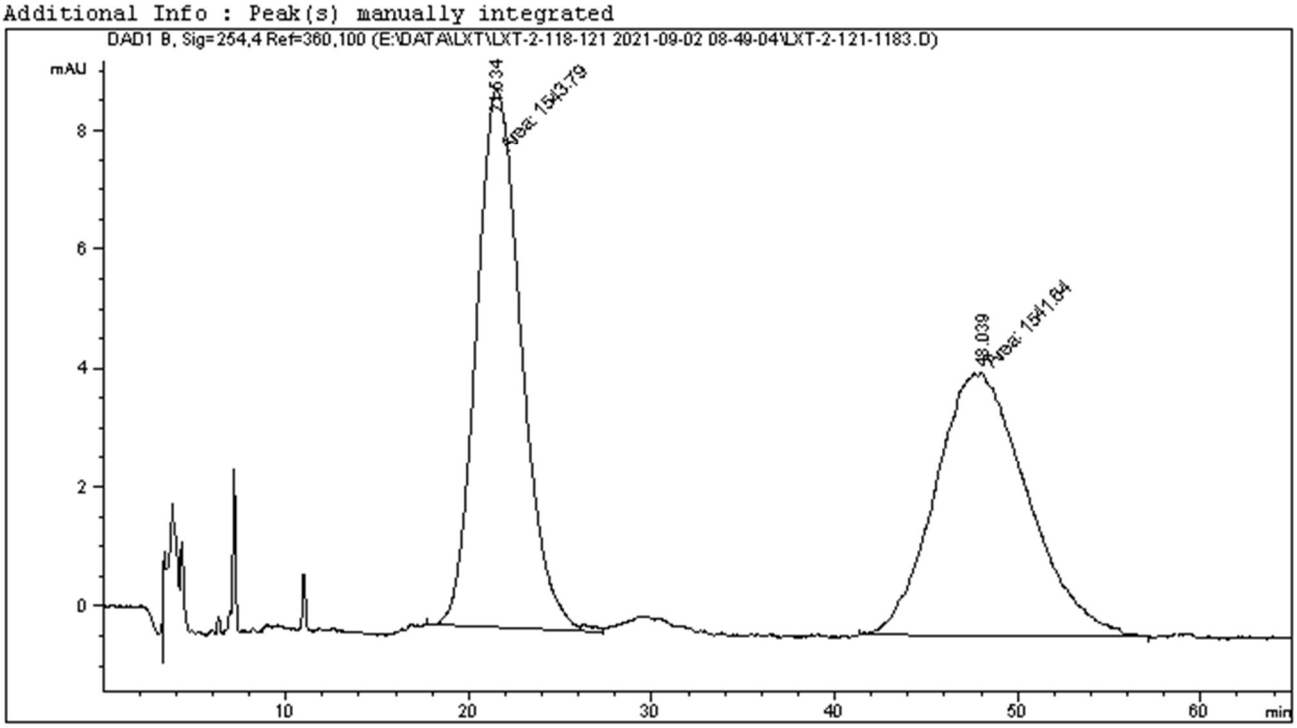


^{13}C NMR (101 MHz, Chloroform-*d*) of **4l**

Data File E:\DATA\LXT\LXT-2-118-121 2021-09-02 08-49-04\LXT-2-121-1183.D
Sample Name: LXT-2-116

==========

Acq. Operator : SYSTEM Seq. Line : 4
Acq. Instrument : 1260 Location : 4
Injection Date : 9/2/2021 10:04:32 AM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-118-121 2021-09-02 08-49-04\1-ASH-98-2-1ML-10ul-60min-ALL -nml.M
Last changed : 9/2/2021 10:57:20 AM by SYSTEM (modified after loading)
Analysis Method : E:\DATA\LXT\LXT-2-118-121 2021-09-02 08-49-04\1-ASH-98-2-1ML-10ul-60min-ALL -nml.M (Sequence Method)
Last changed : 1/4/2022 9:21:51 AM by SYSTEM (modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

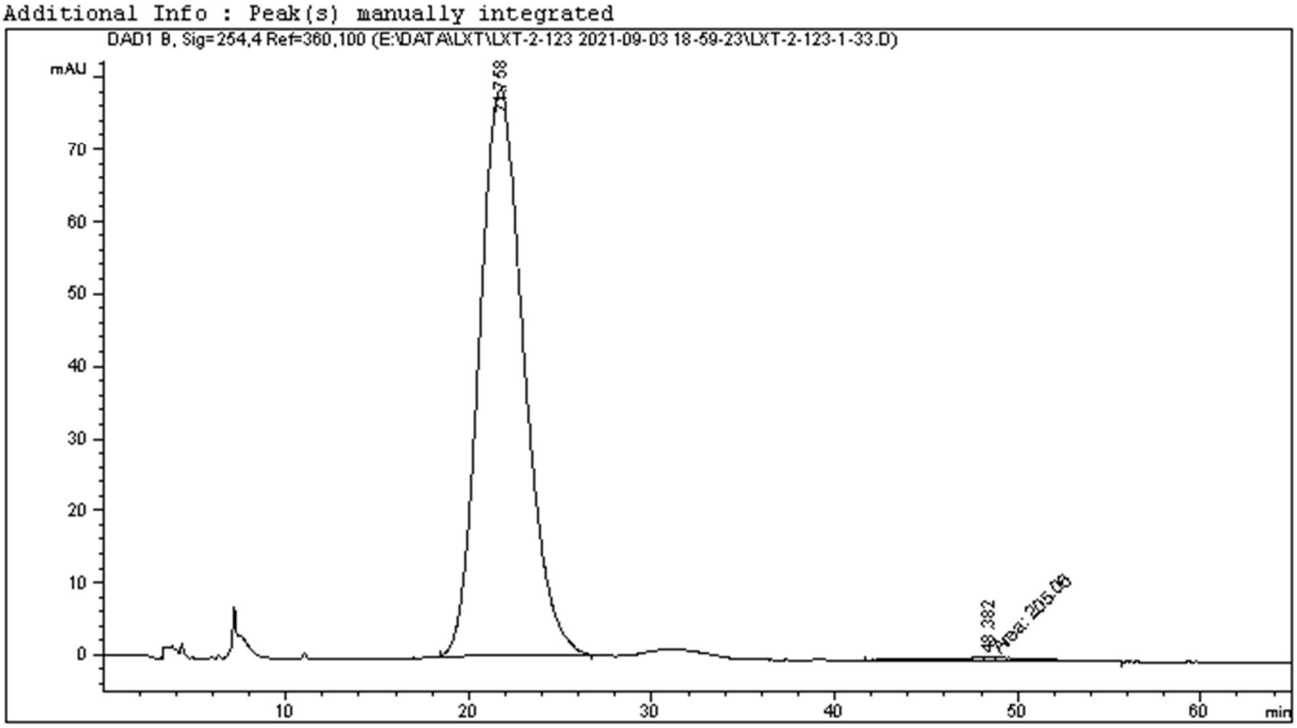
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.534	MM	2.8422	1543.79053	9.05291	50.0348
2	48.039	MM	5.8015	1541.64124	4.42883	49.9652

Totals : 3085.43176 13.48174

Data File E:\DATA\LXT\LXT-2-123 2021-09-03 18-59-23\LXT-2-123-1-33.D
Sample Name: LXT-2-113

==========

Acq. Operator : SYSTEM Seq. Line : 4
Acq. Instrument : 1260 Location : 23
Injection Date : 9/3/2021 8:14:55 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-123 2021-09-03 18-59-23\1-ASH-98-2-1ML-10ul-60min-ALL-nml .M
Last changed : 9/3/2021 8:24:39 PM by SYSTEM (modified after loading)
Analysis Method : E:\DATA\LXT\LXT-2-123 2021-09-03 18-59-23\1-ASH-98-2-1ML-10ul-60min-ALL-nml .M (Sequence Method)
Last changed : 1/4/2022 9:16:51 AM by SYSTEM (modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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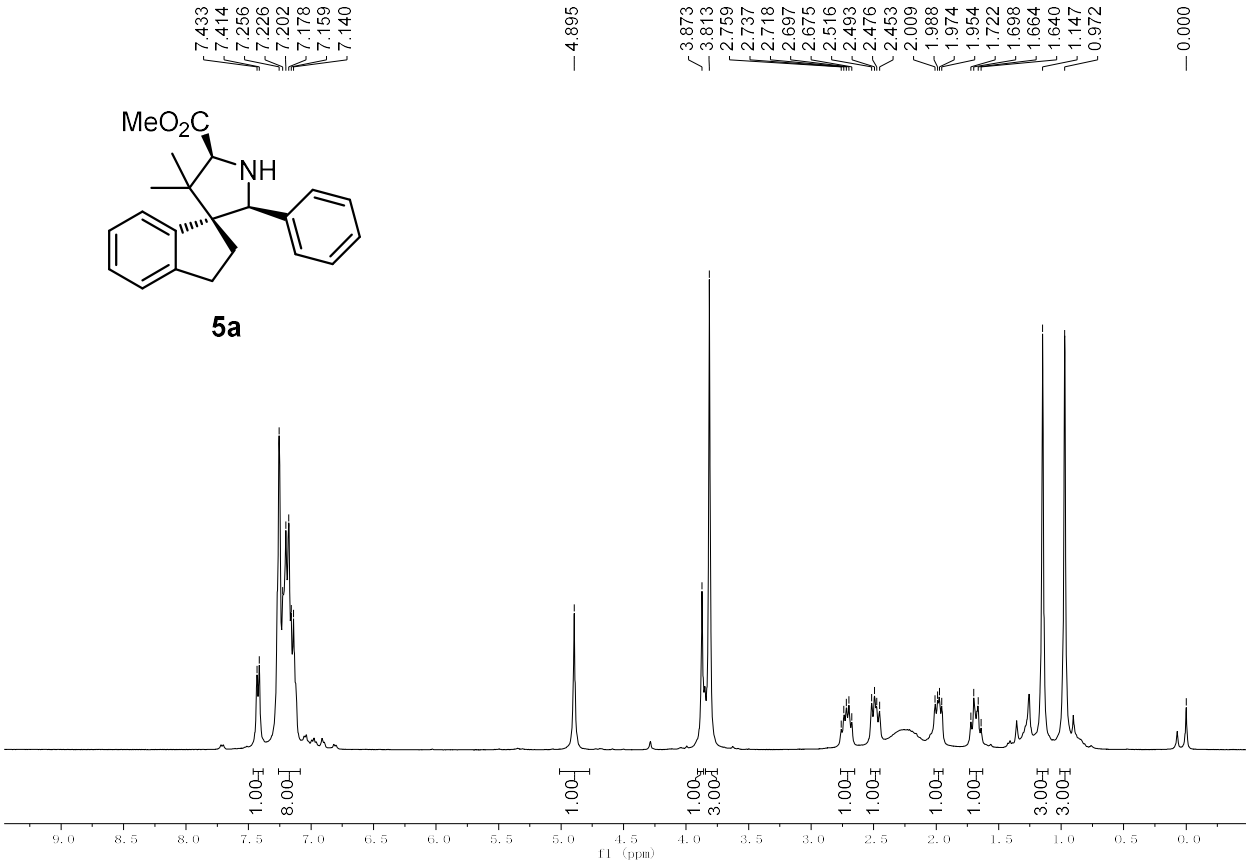
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

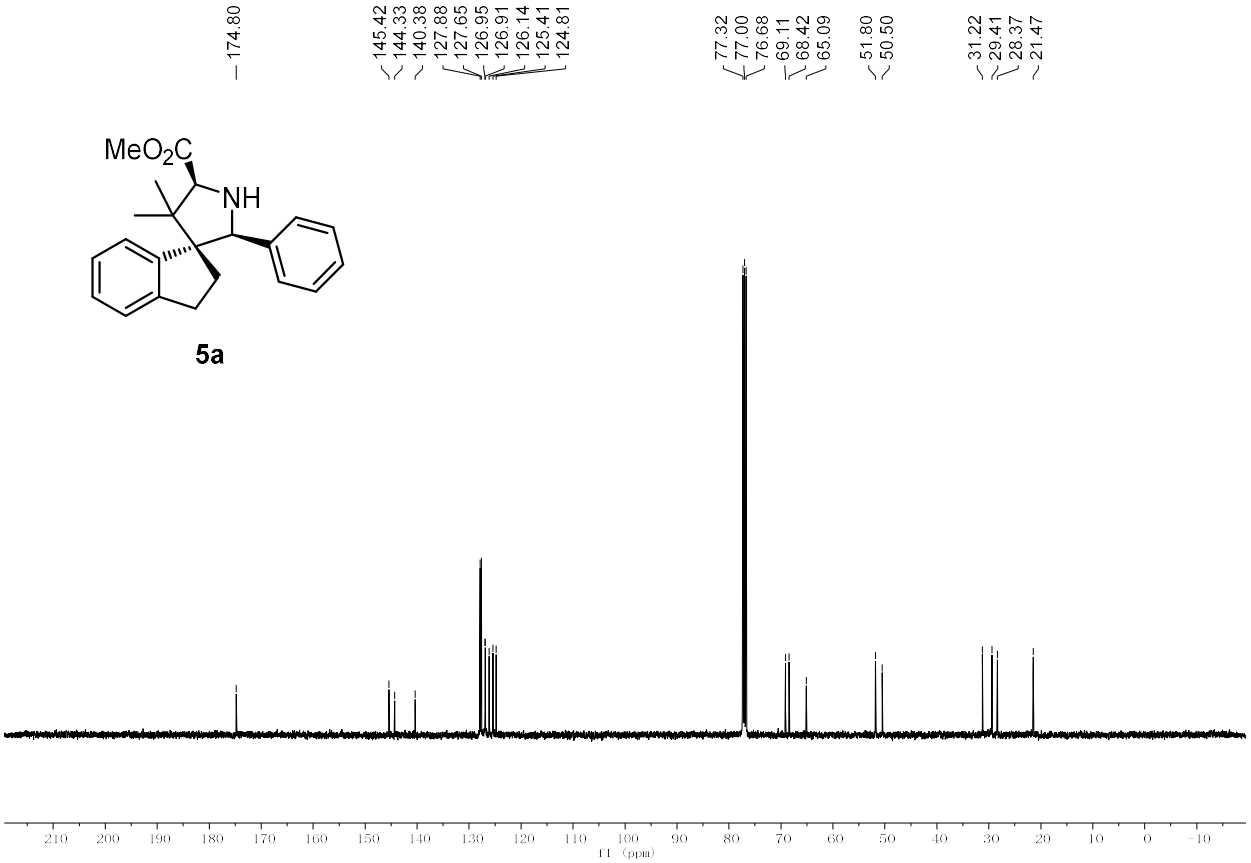
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.758	BB	1.9653	1.31950e4	78.52912	98.4697
2	48.382	MM	6.6045	205.06017	5.17479e-1	1.5303

Totals : 1.34000e4 79.04660



^{1}H NMR (400 MHz, Chloroform-*d*) of **5a**



^{13}C NMR (101 MHz, Chloroform-*d*) of **5a**

Data File E:\DATA\LXT\LXT-2-88-OPT 2021-07-25 18-03-22\LXT-2-88-OPT2.D
Sample Name: LXT-2-82-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 3
Acq. Instrument : 1260 Location : 52
Injection Date : 7/25/2021 6:47:33 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-88-OPT 2021-07-25 18-03-22\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/25/2021 6:03:23 PM by SYSTEM
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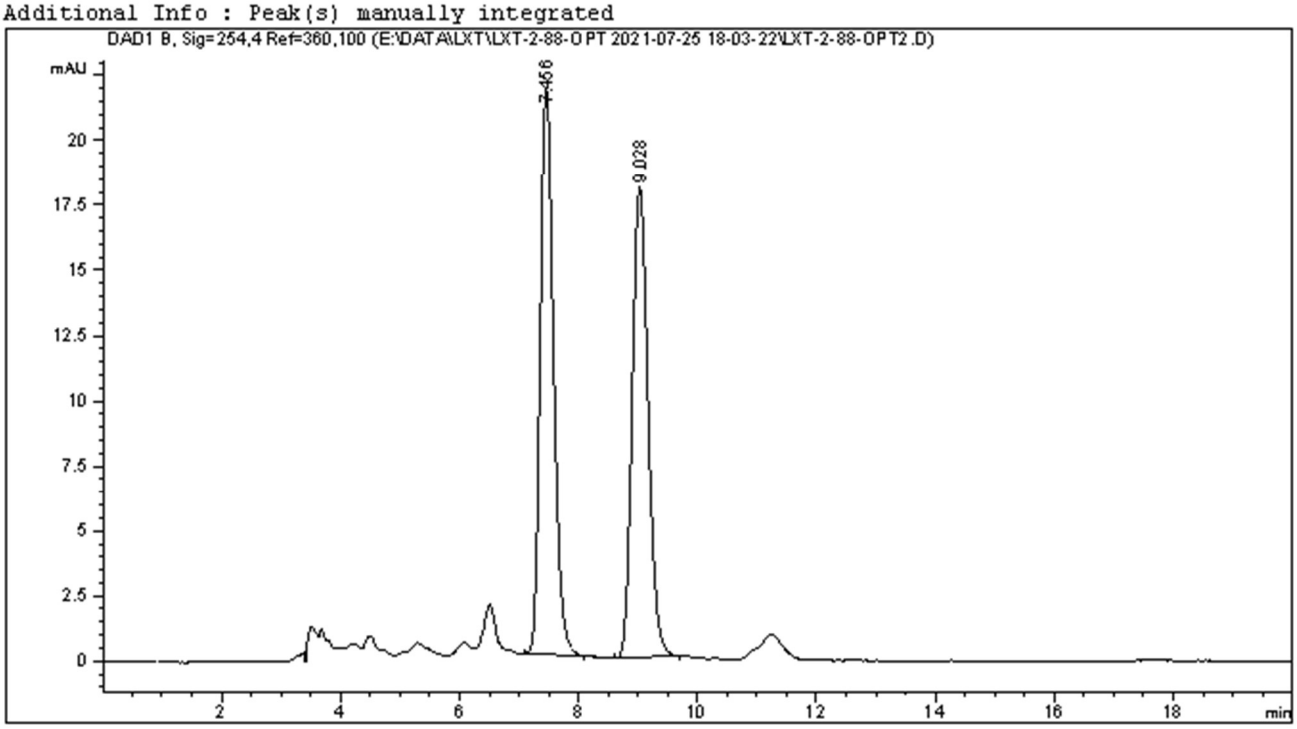

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Area Percent Report

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Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.456	BB	0.2436	340.25430	21.73787	50.4134
2	9.028	BB	0.2825	334.67352	18.03796	49.5866

Totals : 674.92783 39.77584

Data File E:\DATA\LXT\LXT-2-88-OPT 2021-07-25 18-03-22\LXT-2-88-OPT1.D
Sample Name: LXT-2-88-OPT

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Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-88-OPT 2021-07-25 18-03-22\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M
Last changed : 7/25/2021 6:03:23 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-88-OPT 2021-07-25 18-03-22\1-ASH-98-2-1ML-10ul-20min-ALL-nml.M (Sequence Method)
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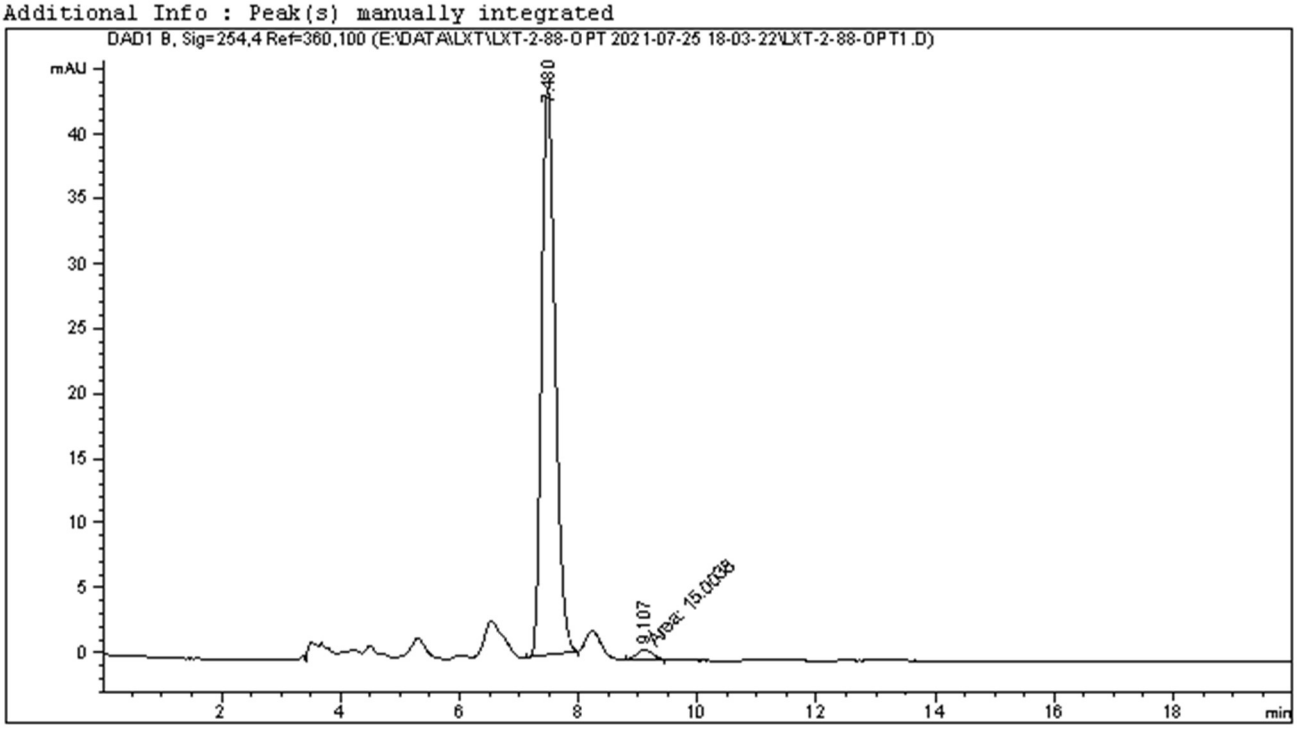
Additional Info : Peak(s) manually integrated



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Area Percent Report

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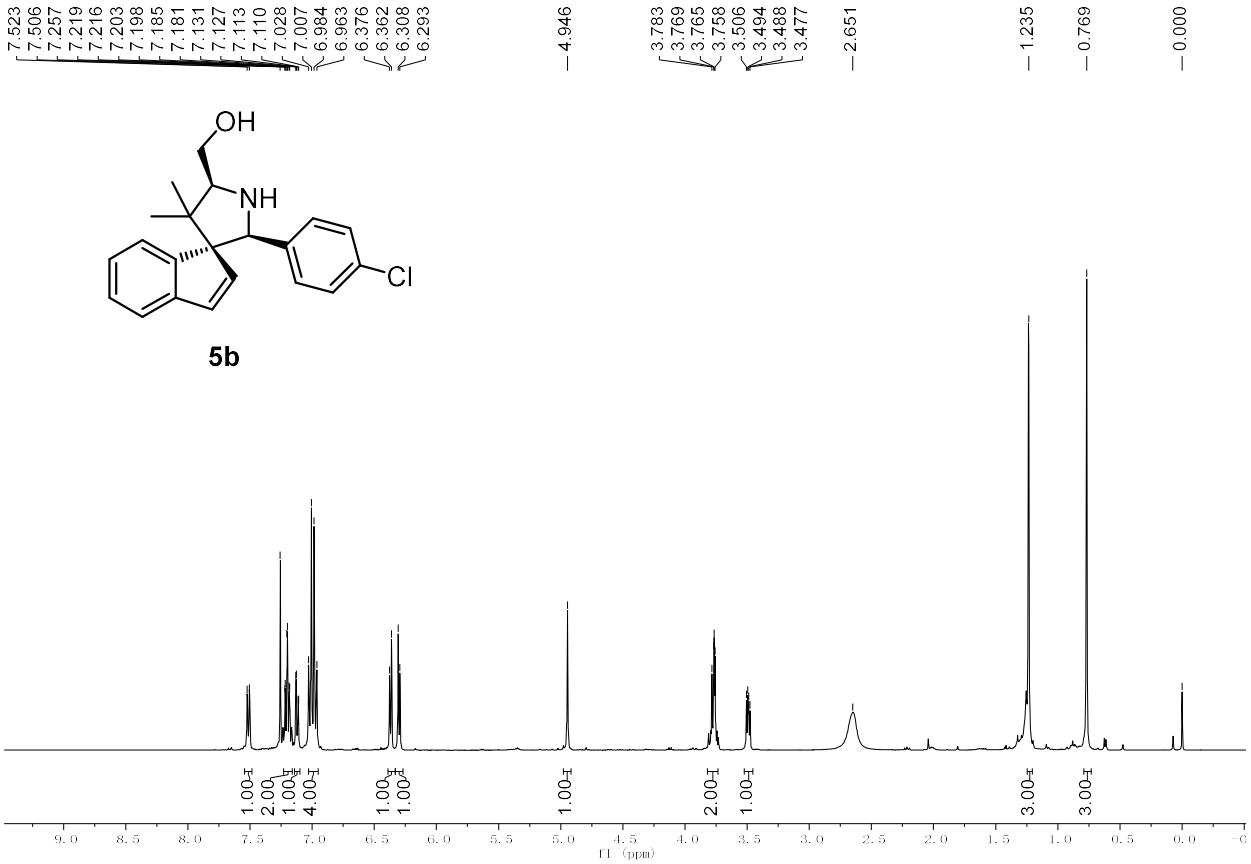
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

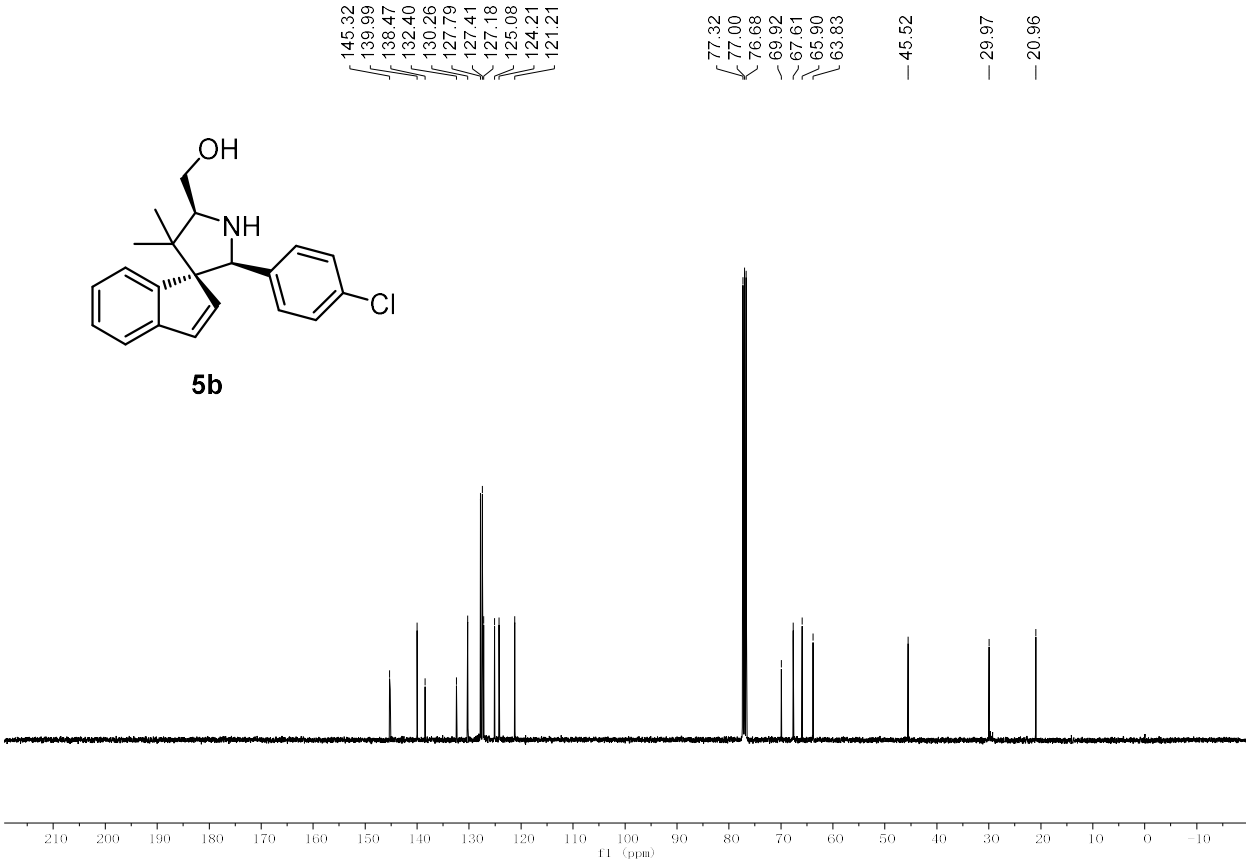
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.480	BB	0.2469	700.11383	43.70453	97.9019
2	9.107	MM	0.3121	15.00377	8.01317e-1	2.0981

Totals : 715.11760 44.50585



^{1}H NMR (400 MHz, Chloroform-*d*) of **5b**



^{13}C NMR (101 MHz, Chloroform-*d*) of **5b**

Data File E:\DATA\LXT\LXT-1-112-2-2-67 2021-07-21 12-21-51\LXT-1-112-2-2-673.D
Sample Name: LXT-2-67-RAC

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Acq. Operator : SYSTEM Seq. Line : 4
Acq. Instrument : 1260 Location : 42
Injection Date : 7/21/2021 1:36:40 PM Inj : 1
Inj Volume : 10.000 µl
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Analysis Method : E:\DATA\LXT\LXT-1-112-2-2-67 2021-07-21 12-21-51\1-ASH-92-8-1ML-10ul-40min-ALL-nml.M (Sequence Method)
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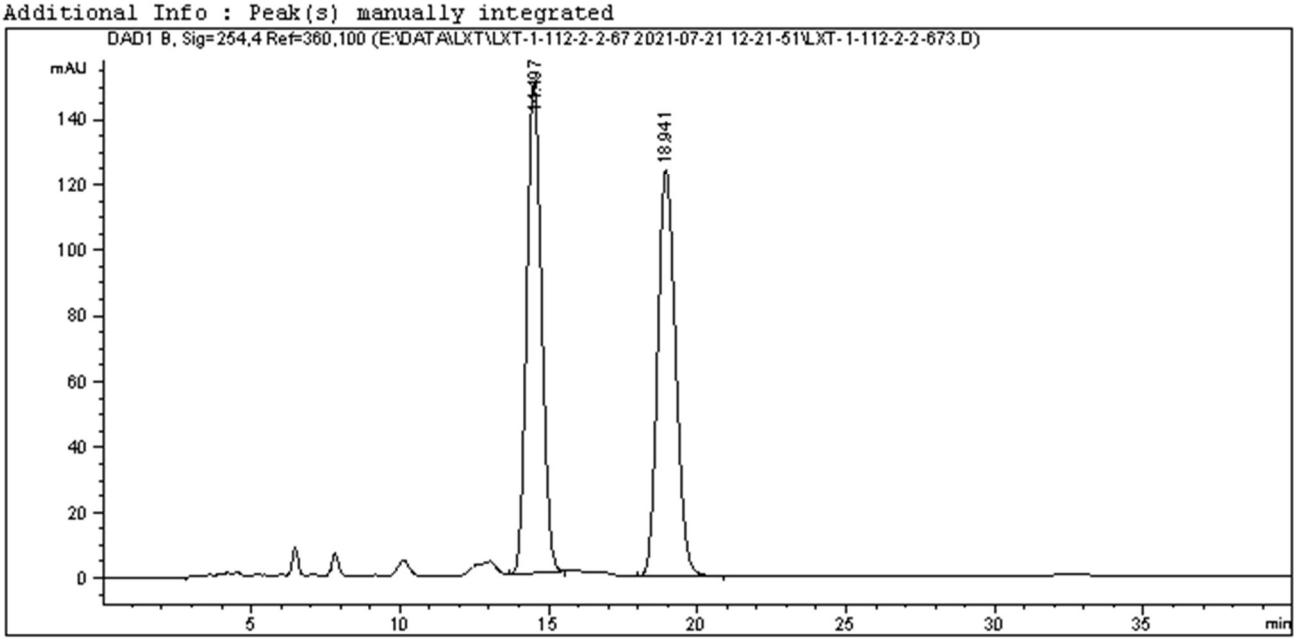

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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.497	BB	0.5323	5164.60791	149.39026	49.9310
2	18.941	BB	0.6366	5178.88672	124.17432	50.0690

Totals : 1.03435e4 273.56458

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*** End of Report ***

Data File E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\LXT-2-75-RAC15.D
Sample Name: LXT-2-68-OPT

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Acq. Operator : SYSTEM Seq. Line : 16
Acq. Instrument : 1260 Location : 6
Injection Date : 7/17/2021 6:37:33 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-ASH-92-8-1ML-10ul-40min-ALL-nml.M
Last changed : 7/17/2021 3:03:06 PM by SYSTEM
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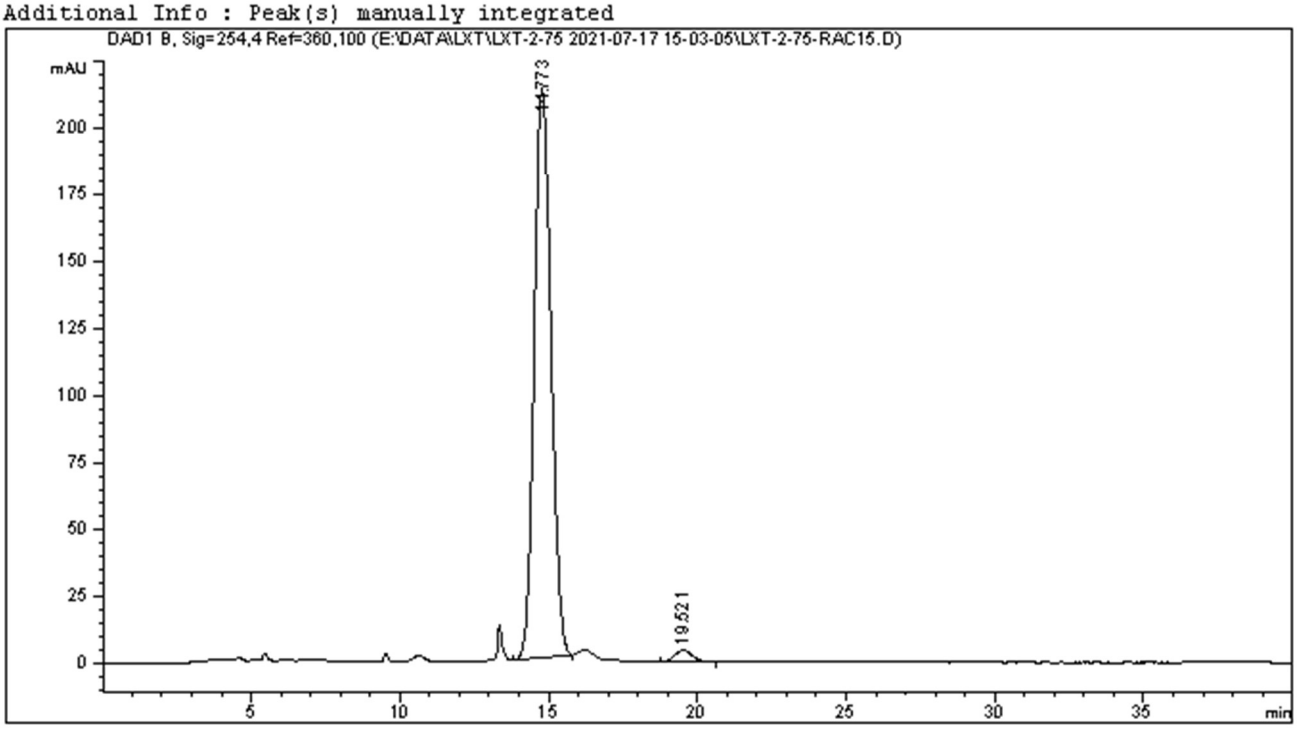
Additional Info : Peak(s) manually integrated



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Area Percent Report

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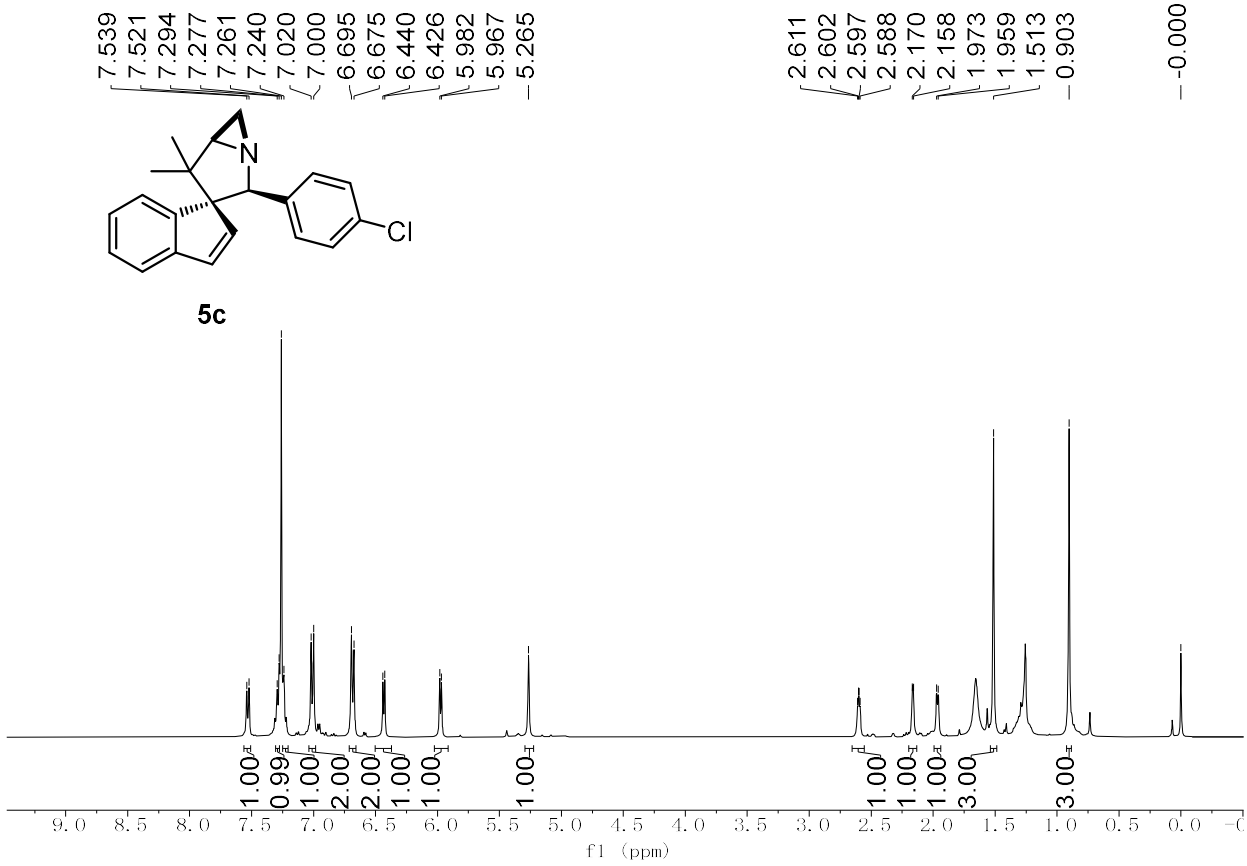
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

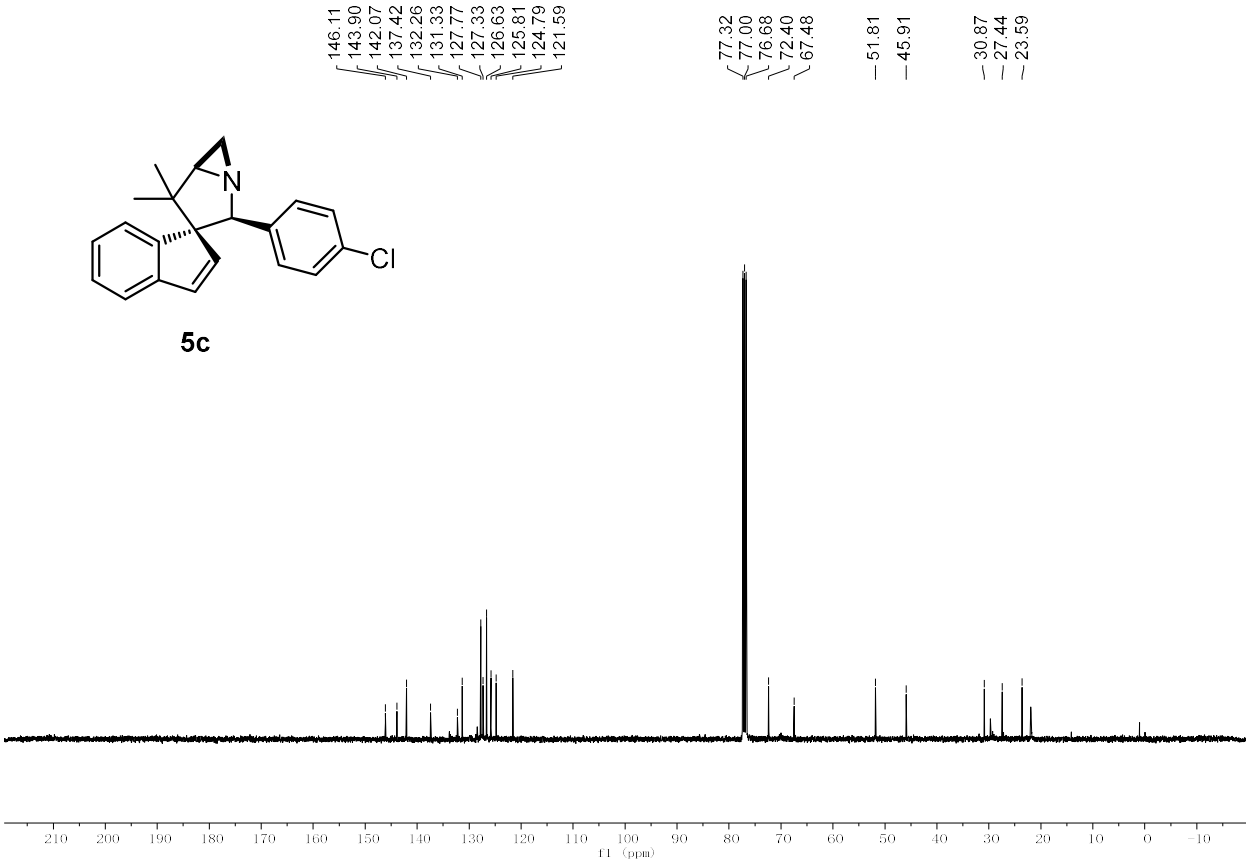
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.773	BB	0.6160	8356.45117	212.87859	97.9107
2	19.521	BB	0.4821	178.31964	4.37001	2.0893

Totals : 8534.77081 217.24860



^{1}H NMR (400 MHz, Chloroform-*d*) of **5c**



^{13}C NMR (101 MHz, Chloroform-*d*) of **5c**

Data File E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\LXT-2-75-RAC11.D
Sample Name: LXT-2-75-RAC

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==================================================================
Acq. Operator   : SYSTEM                          Seq. Line :  12
Acq. Instrument : 1260                             Location :   53
Injection Date  : 7/17/2021 5:32:28 PM                  Inj :   1
                                                 Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-0J-98-2-1ML-10ul-20min-ALL-nml.M
Last changed    : 7/17/2021 3:03:05 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-75 2021-07-17 15-03-05\1-0J-98-2-1ML-10ul-20min-ALL-nml.M
                  (Sequence Method)
Last changed    : 8/1/2021 4:35:20 PM by SYSTEM
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Additional Info : Peak(s) manually integrated
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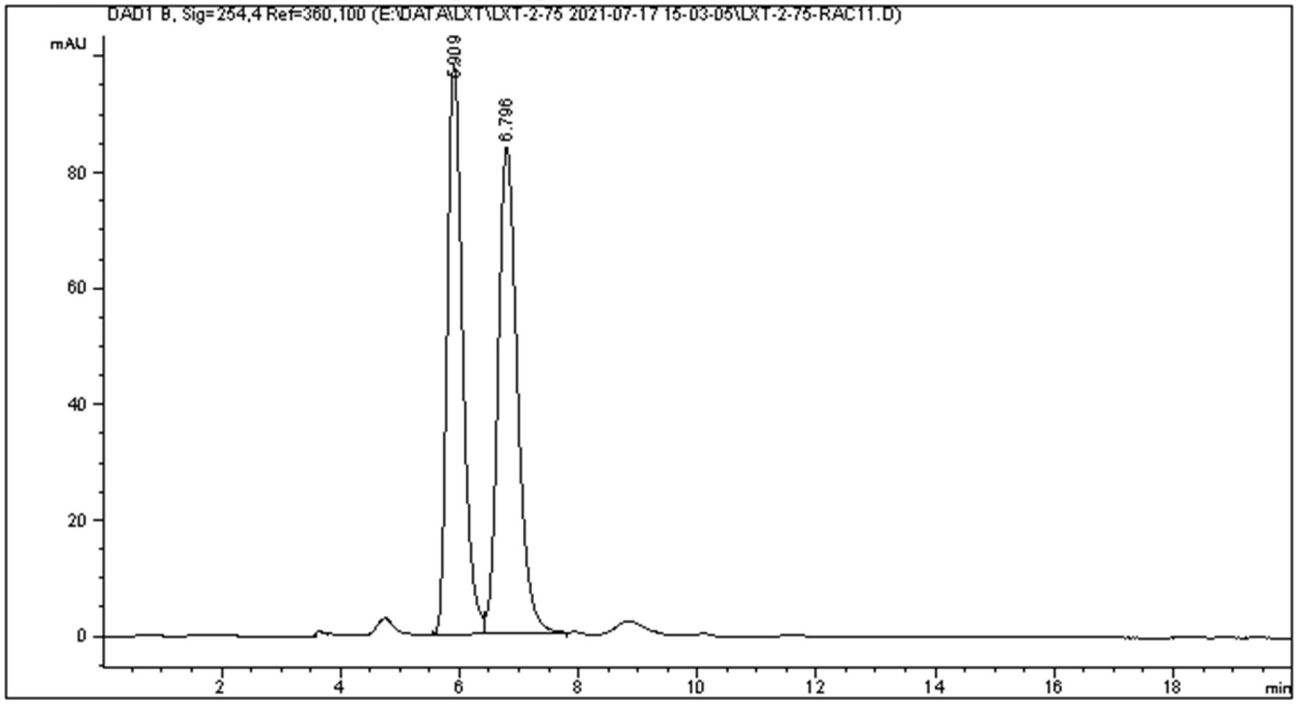


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==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100

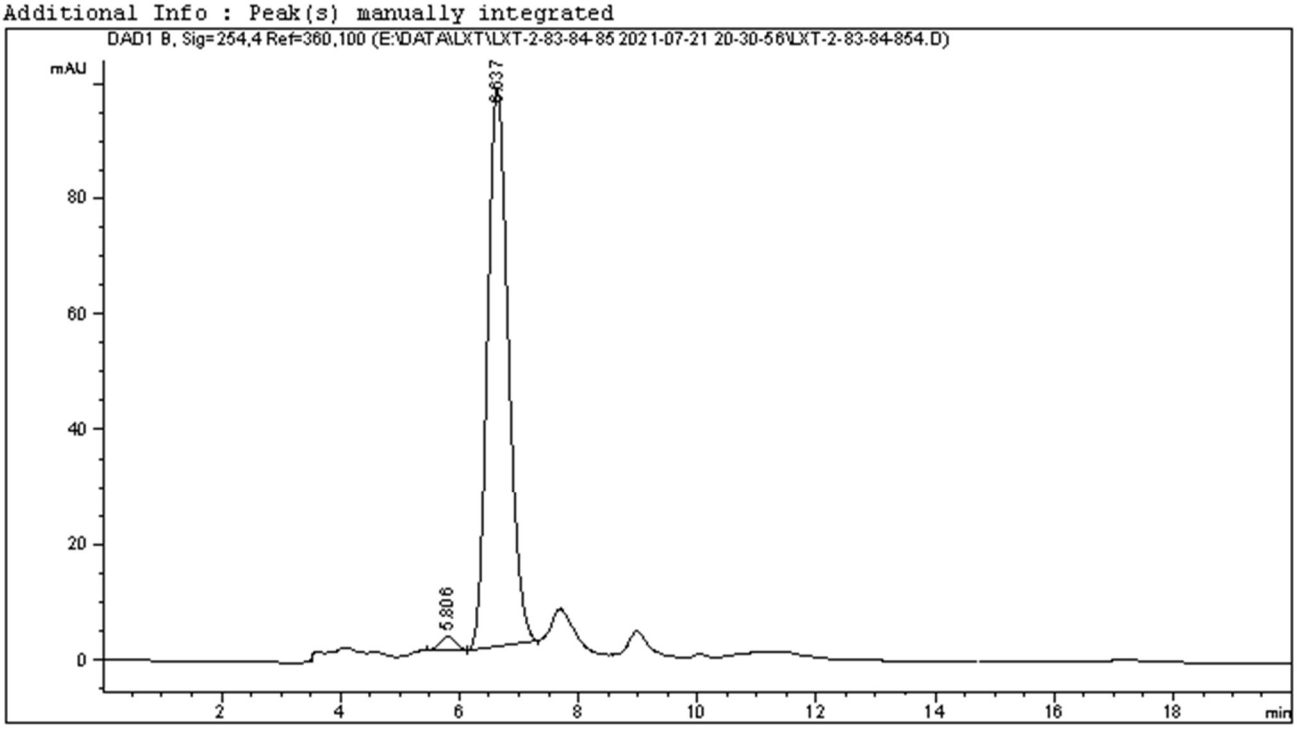
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.909 BV    0.2755 1774.58813   98.37280  48.4918
   2   6.796 VB    0.3443 1884.97168   83.84932  51.5082

Totals :                  3659.55981  182.22211
```

Data File E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\LXT-2-83-84-854.D
Sample Name: LXT-2-83-OPT

==========

Acq. Operator : SYSTEM Seq. Line : 5
Acq. Instrument : 1260 Location : 33
Injection Date : 7/21/2021 9:47:47 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\1-OJ-98-2-1ML-10ul-20min-ALL -nml.M
Last changed : 7/21/2021 8:30:56 PM by SYSTEM
Analysis Method : E:\DATA\LXT\LXT-2-83-84-85 2021-07-21 20-30-56\1-OJ-98-2-1ML-10ul-20min-ALL -nml.M (Sequence Method)
Last changed : 8/1/2021 4:37:29 PM by SYSTEM
(modified after loading)
Additional Info : Peak(s) manually integrated



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Area Percent Report

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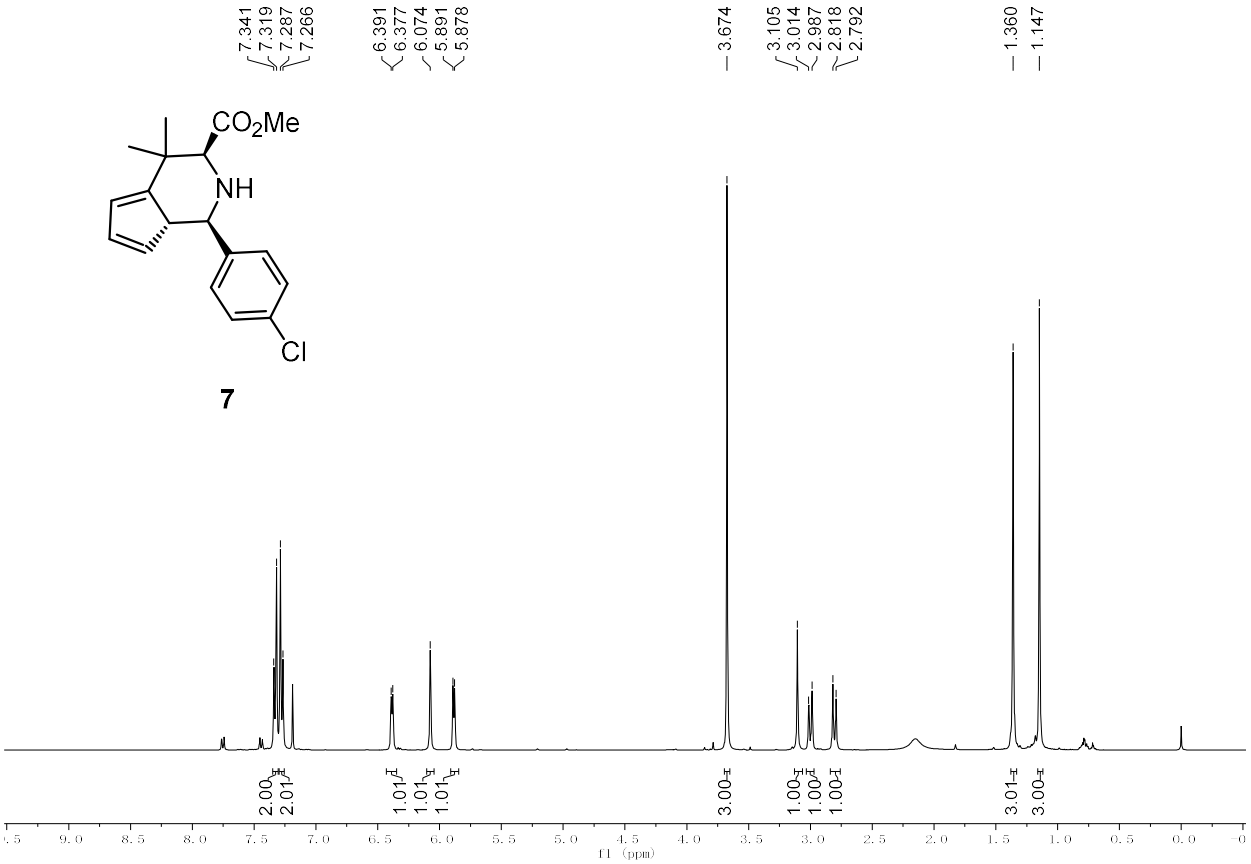
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

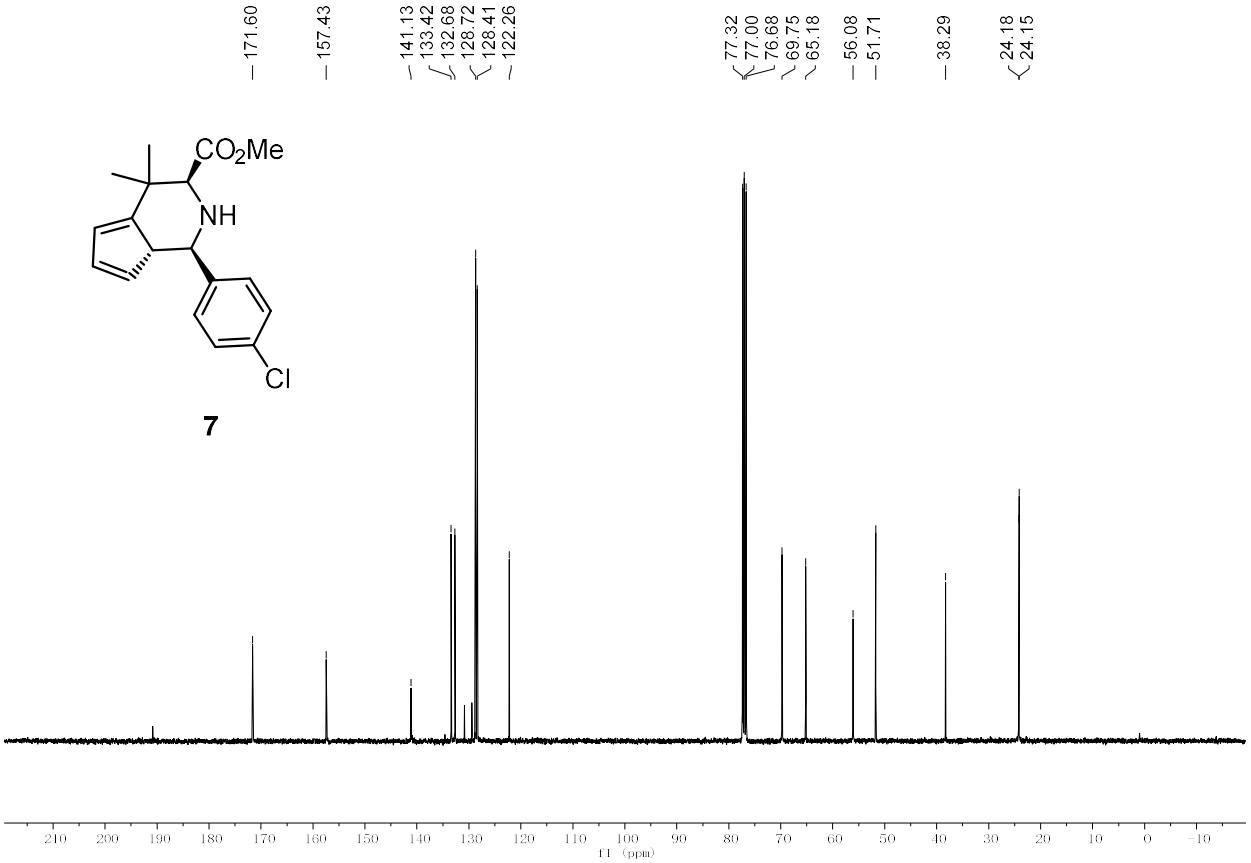
Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.806	BB	0.2223	43.61082	2.36343	1.8153
2	6.637	BB	0.3750	2358.80347	96.88718	98.1847

Totals : 2402.41429 99.25060



^{1}H NMR (400 MHz, Chloroform-*d*) of **7**



^{13}C NMR (400 MHz, Chloroform-*d*) of **7**

Data File D:\HPLC\DATA\20221014\A 2022-10-14 10-23-51\A28.D
Sample Name: LXT-DW-RAC

==========

Acq. Operator : SYSTEM Seq. Line : 29
Acq. Instrument : 1260 Location : 21
Injection Date : 10/14/2022 9:40:09 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20221014\A 2022-10-14 10-23-51\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M
Last changed : 10/14/2022 2:56:16 PM by SYSTEM
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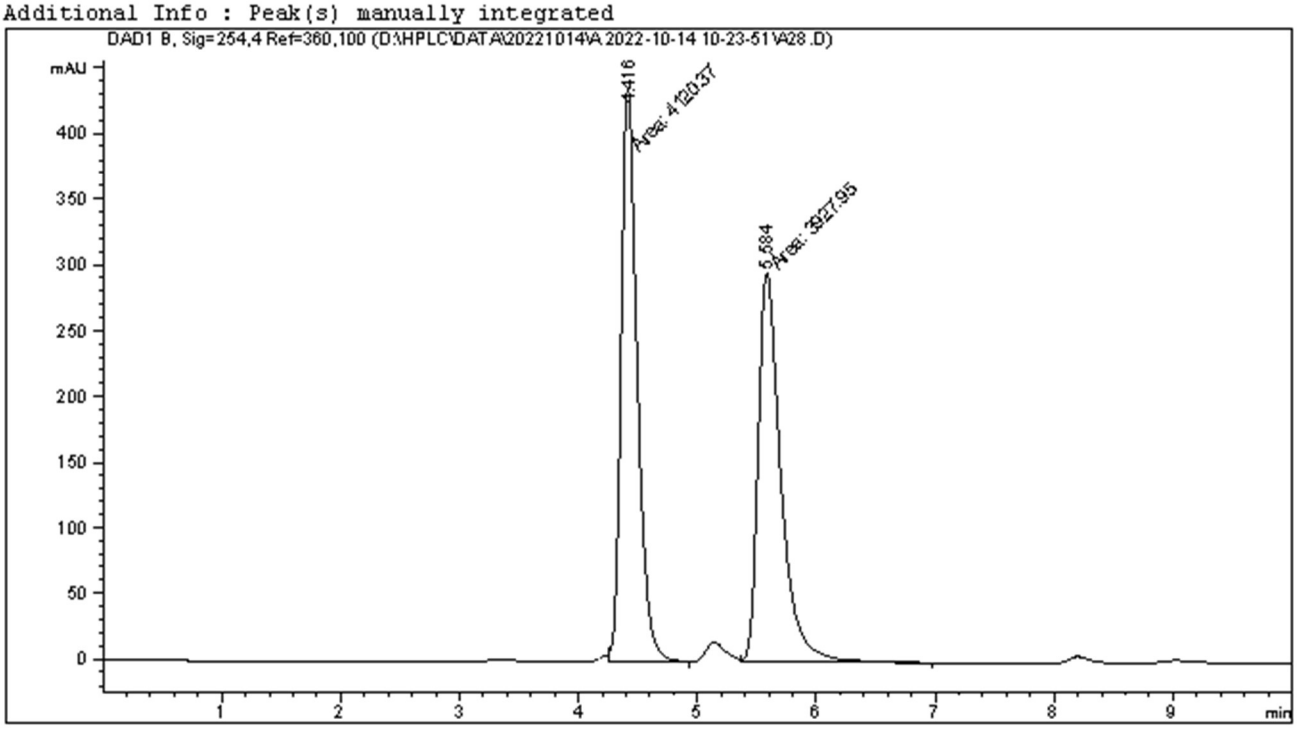
Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.416	FM	0.1573	4120.37012	436.61432	51.1954
2	5.584	FM	0.2218	3927.94629	295.22110	48.8046

Totals : 8048.31641 731.83542

Data File D:\HPLC\DATA\20221008\A 2022-10-08 09-10-07\A22.D
Sample Name: LXT-DW

==========

Acq. Operator : SYSTEM Seq. Line : 23
Acq. Instrument : 1260 Location : 1
Injection Date : 10/8/2022 6:00:11 PM Inj : 1
Inj Volume : 10.000 µl
Acq. Method : D:\HPLC\Data\20221008\A 2022-10-08 09-10-07\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M
Last changed : 10/8/2022 3:08:44 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20221008\A 2022-10-08 09-10-07\1-ASH-90-10-1ML-10ul-20min-ALL-nml.M (Sequence Method)
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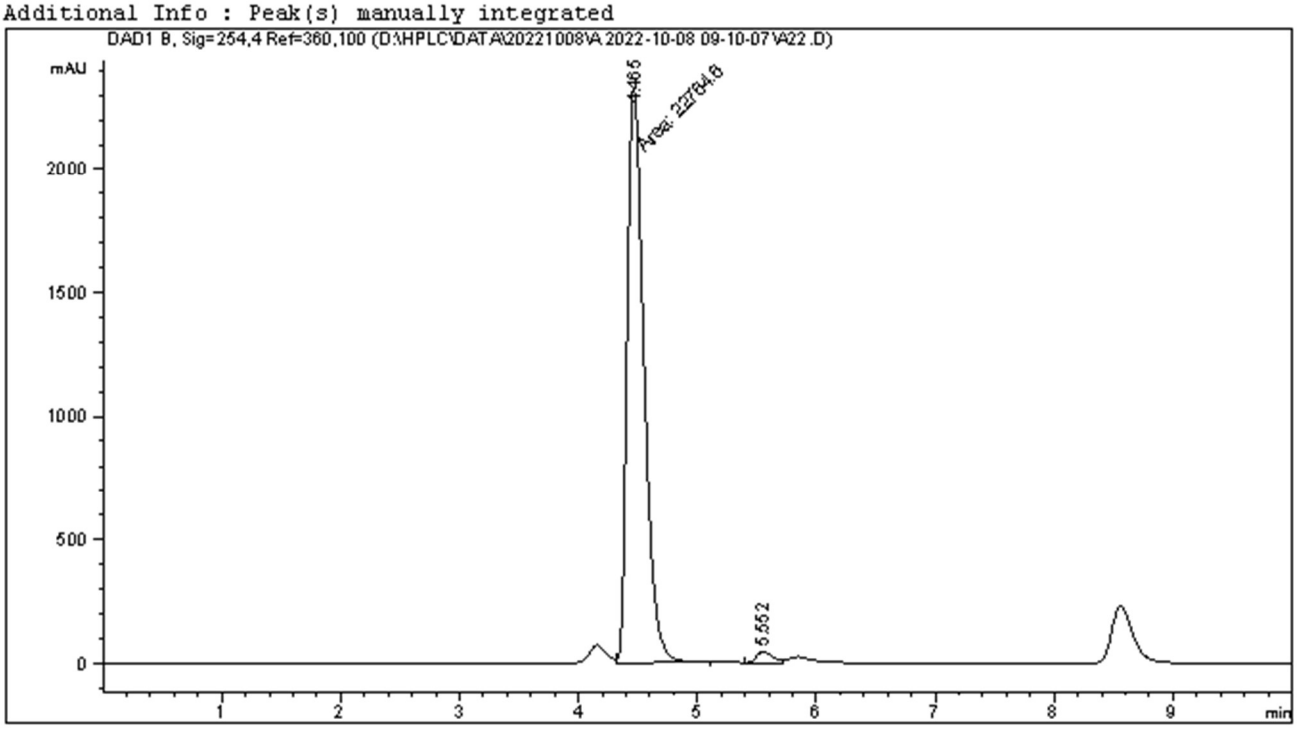

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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.465	FM	0.1631	2.27646e4	2325.98560	98.2347
2	5.552	BV	0.1421	409.08926	43.73790	1.7653

Totals : 2.31737e4 2369.72349

Computational Details

Density functional theory (DFT) calculations were carried out by Gaussian G09 (version D01) package.[S1] M06-L[S2] method combined with a mixed basis set of SDD[S3] for Cu and Fe (plus its effective core potential) and 6-31G*[S4] for the other atoms were used to optimize all intermediates and transition states in gas phase. Vibrational frequency calculations at the same level were carried out to ensure no imaginary frequency for all local minimum and one imaginary frequency relating to the appropriate reaction mode for all transition states. The solvation effect of diethylether was included by single-point energy calculation with implicit solvation models PCM[S5] and SMD[S6]. To test the effect of DFT functional, B3LYP[S7]-D3[S8], PBE0[S9]-D3 and ωB97X-D[S10] were used for single-point energy calculations in the solution. To test the effect of basis set, 6-311+G**[S11] valence triplet-zeta basis set was used for single-point energy calculations in the solution. Different solvent model, DFT methods and basis sets gave the same mechanistic conclusion. All entropy and free energy terms were further corrected under the Grimme's quasi-harmonic entropic correction[S12] evaluated by GoodVibes program.[S13] All 3D images of the optimized structures were generated by CYLview.[S14] The steric map of Cu-L was produced by SambVca 2.1.[S15]

Reference:

S1. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

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S4. (a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* 1971, **54**, 724-728; (b) P. C. Hariharan, J. A. Pople, *Theor. Chim. Acta.* 1973, **28**, 213-222.

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S6. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J Phys Chem B.* 2009, **113**, 6378-6396.
S7. (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B.* 1988, **37**, 785-789; (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; (c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* 1994, **98**, 11623-11627.
S8. (a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104/154101-154104/154119; (b) M. Bursch, E. Caldeweyher, A. Hansen, H. Neugebauer, S. Ehlert, S. Grimme, *Acc. Chem. Res.* 2019, **52**, 258-266.
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S10. J. D. Chai, M. Head-Gordon, *J. Chem. Phys.* 2008, **128**, 084106.
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S14. C. Y. Legault, CYL View, version 1.0 b; Universite de Sherbrooke, Sherbrooke, Quebec, Canada, 2009; http://www.cylview.org
S15. L. Falivene, Z. Cao, A. Petta, L. Serra, A. Poater, R. Oliva, V. Scarano, L. Cavallo, *Nat. Chem.* 2019, **11**, 872-879.

Supplementary discussion:

Bond length analysis shows a transformation from the aromatic substrate **2a** to the non-aromatic product **A9** after the [3+6] cycloaddition reaction. While, the [3+2] cycloaddition products **A1** and **A2** remain the aromatic phenyl rings (Figure S4). Bond angles around the reaction site of the [3+6] cycloaddition products (**A9**, **B2**) are larger than those for the [3+2] cycloaddition products (**A1**, **B1**), indicating less constraints of the new 6-membered rings than the 5-membered rings (Figure S5).

To future determine the origin of thermostability of different products. Different models were examined by using the PCM M06-L//M06-2X method (Figures S4 and S6). Without the formation of the new 5-membered and 6-membered rings, the free energy difference between **A1-s** and **A9-s** (ΔΔG -18.6 kcal/mol) is slightly larger than that between **A1** and **A9** (ΔΔG -17.2 kcal/mol) by 1.2 kcal/mol. These results indicate that the main factor influencing the thermostability difference between **A1** and **A9** is aromaticity. In addition, ΔΔG between **B1-s** and **B2-s** (4.0 kcal/mol) is smaller than ΔΔG between **B1** and **B2** (6.3 kcal/mol) by 2.3 kcal/mol, indicating that the new 6-

membered ring formed in the [3+6] cycloaddition has less ring strain than the 5-membered ring.

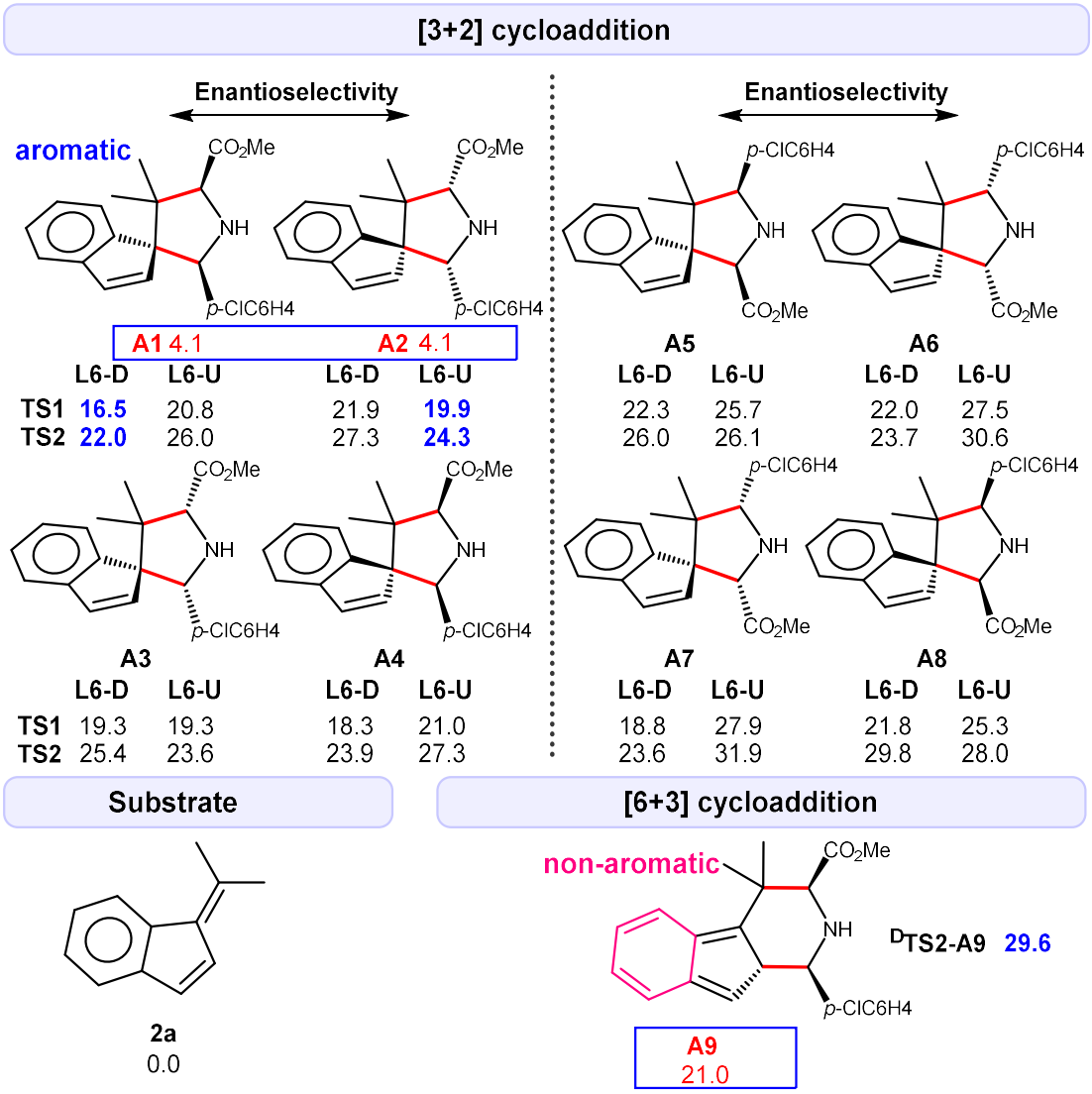

Figure S1. Calculated relative free energies (in kcal/mol) of transition states and key products to form different regio-, stereo- and chemoselective cycloaddition products from the reactions of **2a** catalyzed by **L6-D** and **L6-U**.

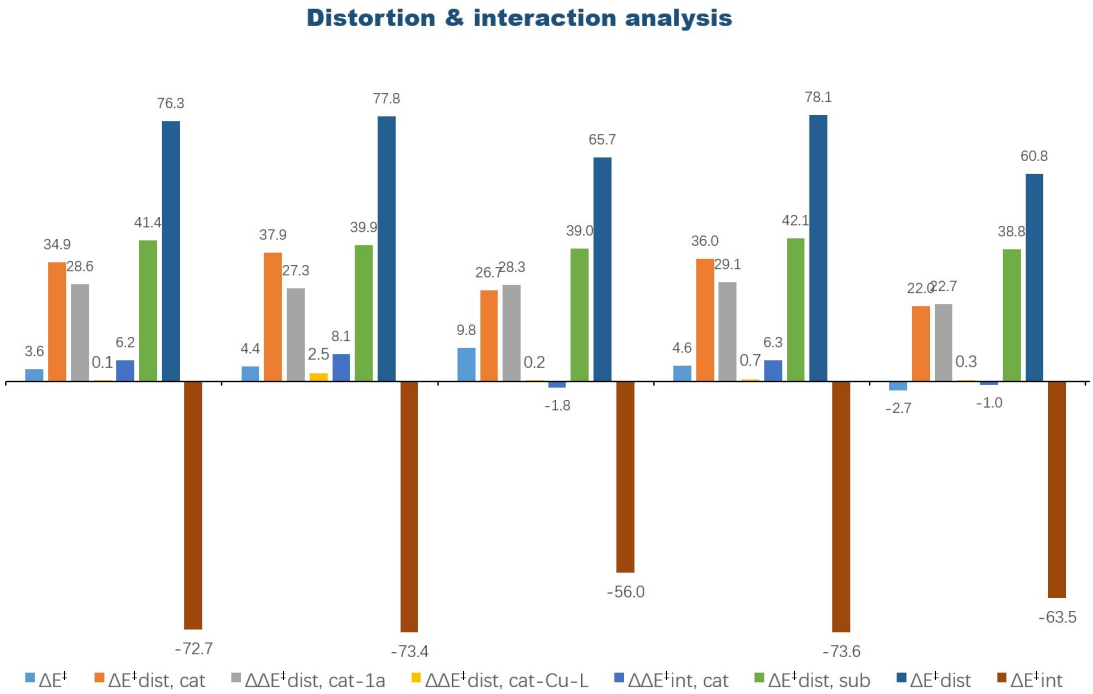

Figure S2. Distortion/interaction analysis for the key transition states. **Cat** contains Cu-**L** and **1a**; **cat-1a** means **1a** in **cat**; **cat**-Cu-**L** means Cu-**L** in cat.

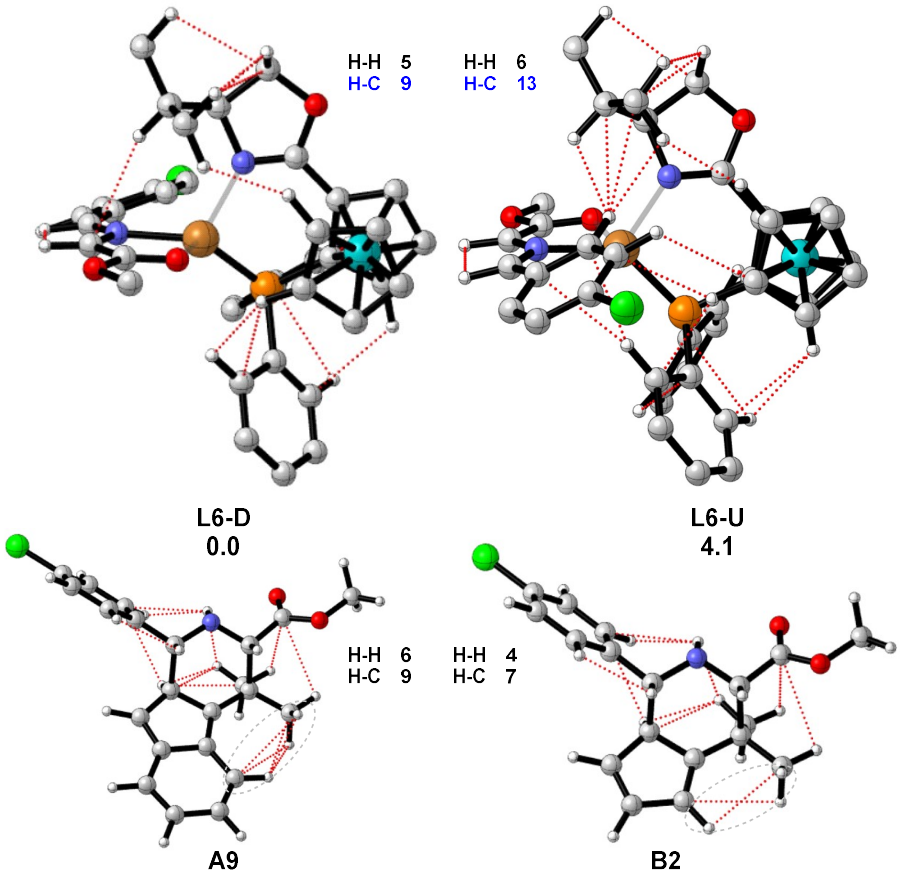

Figure S3. Some C--H and H--H steric interactions.

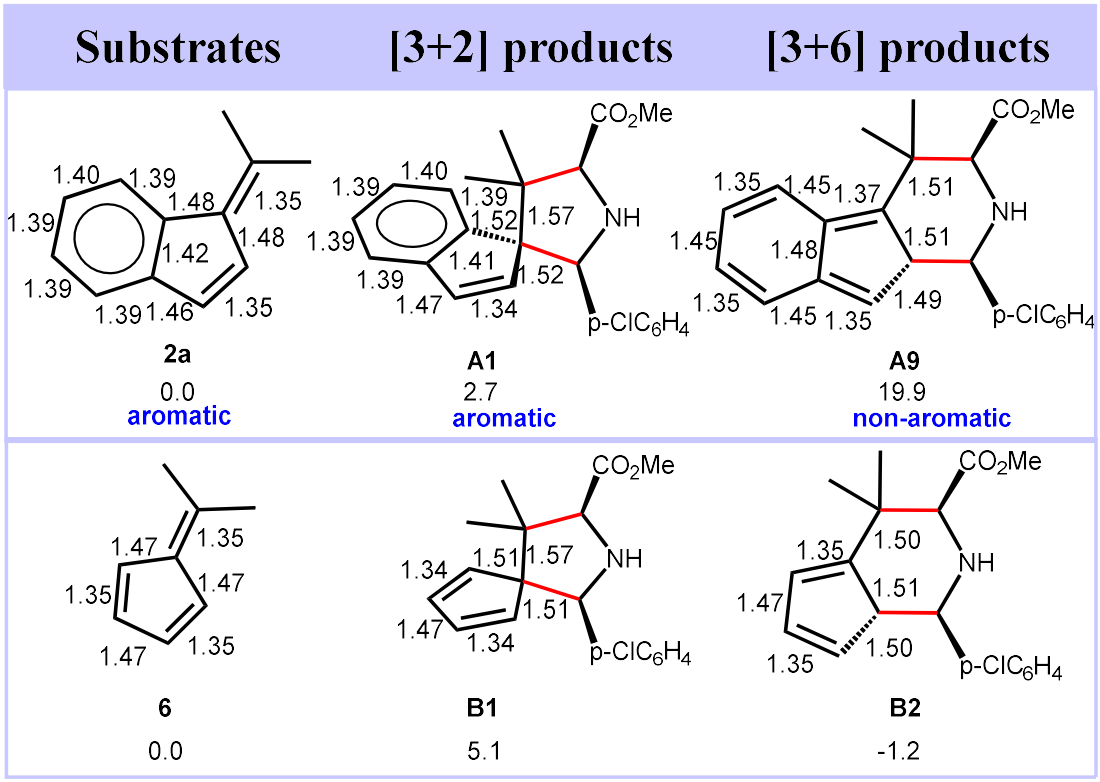

Figure S4. The substrates and products of the two different cycloaddition reactions with the key bond lengths (in angstrom) optimized by the M06-2X method in gas phase and relative free energies (kcal/mol) by the PCM M06-L//M06-2X method in solution.

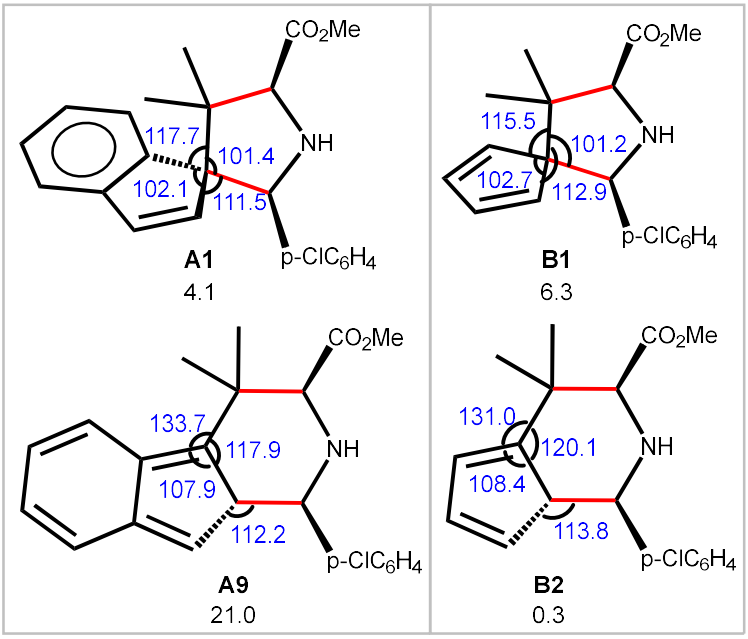

Figure S5. The products of the two different cycloaddition reactions with key angles (º) optimized by the M06-L method in gas phase and relative free energies (kcal/mol) by the PCM M06-L//M06-L method in solution.

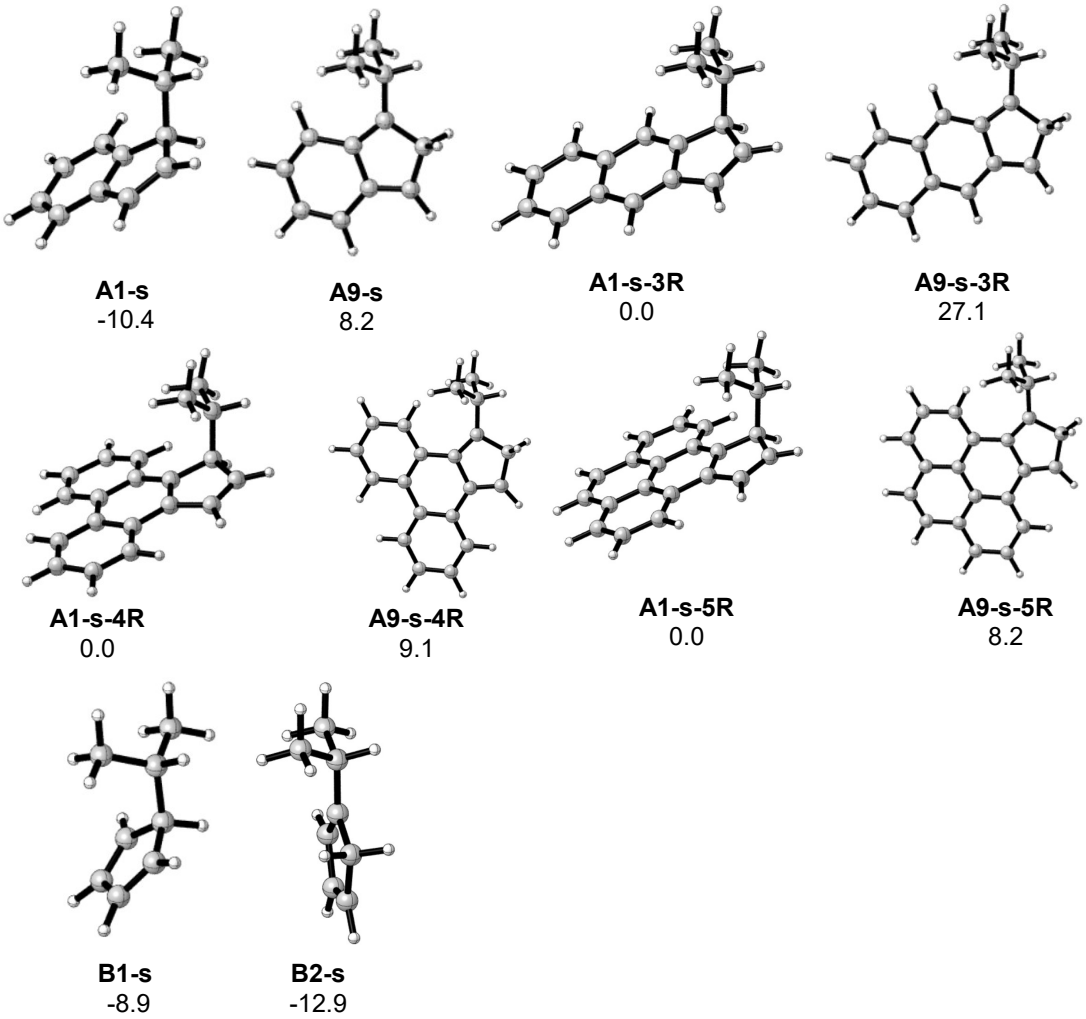

Figure S6. Simplified structures of the different cycloaddition products optimized by the M06-2X method in gas phase. The relative free energies (kcal/mol) by the PCM M06-L//M06-2X method in solution are given.

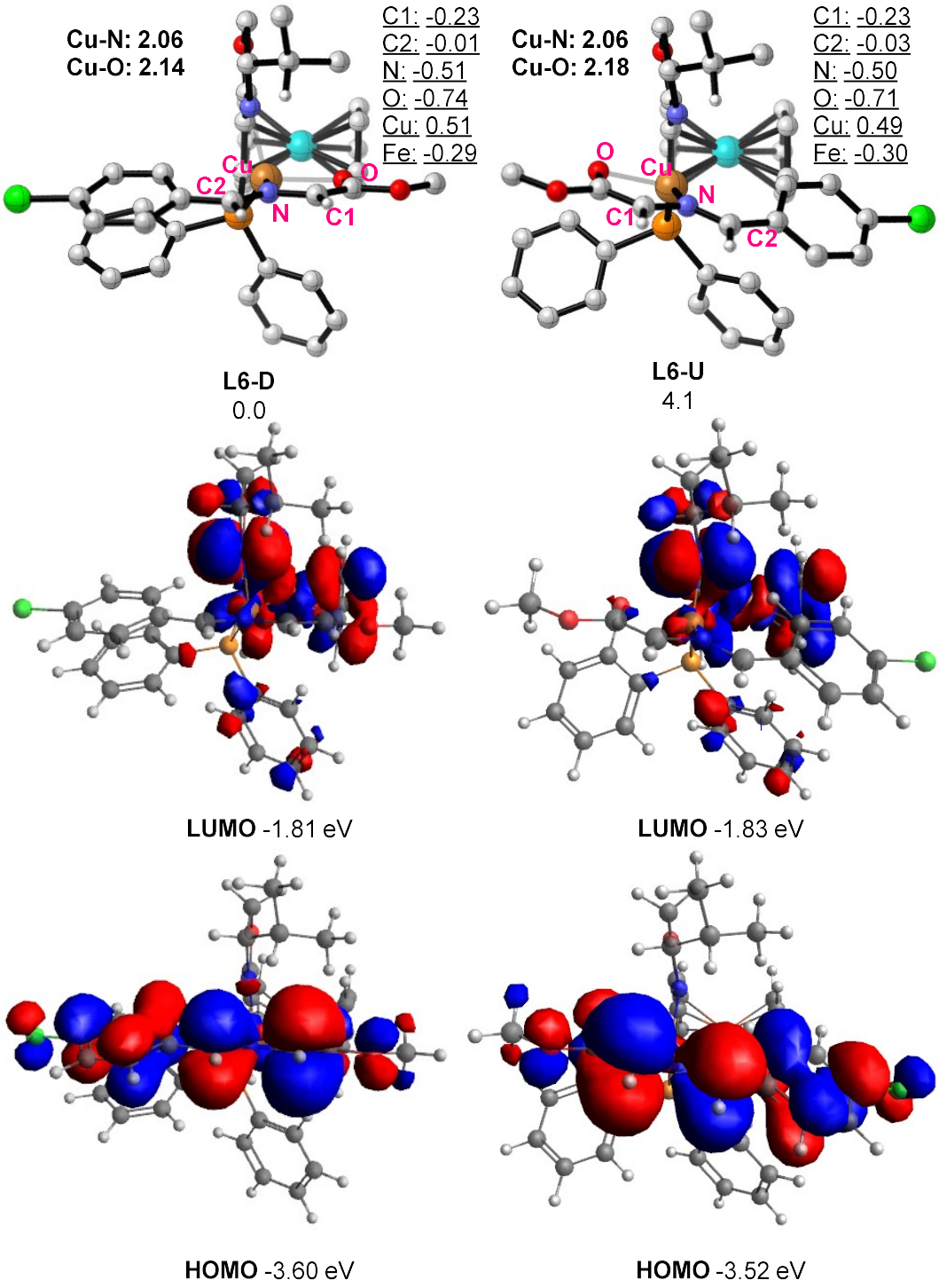

Figure S7. Two coordination modes in the Cu-azomethine ylide complex (**L6-U** and **L6-D**). The relative free energies (in kcal/mol) in diethylether solution, key bond lengths (in angstrom) and NPA charge (underlined) of key atoms are given by PCM M06-L//M06-L method. Unimportant hydrogen atoms are omitted for clarity. Their HOMOs and LUMOs were also given.

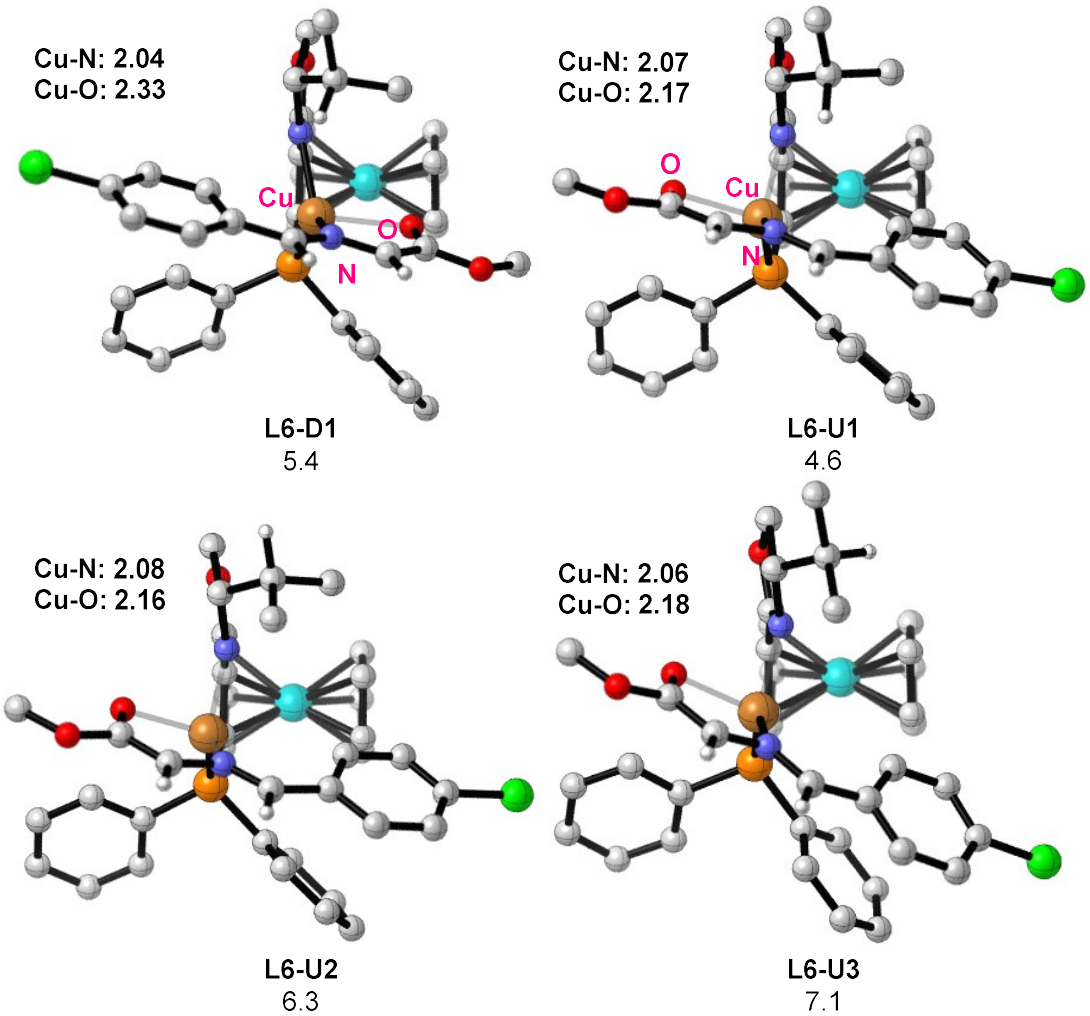

Figure S8. Other conformers of **L6-D** and **L6-U** with the key bond lengths (in angstrom) of key atoms optimized by the M06-L method, and relative free energies (in kcal/mol) in diethylether solution by the PCM M06-L//M06-L method. Unimportant hydrogen atoms are omitted for clarity.

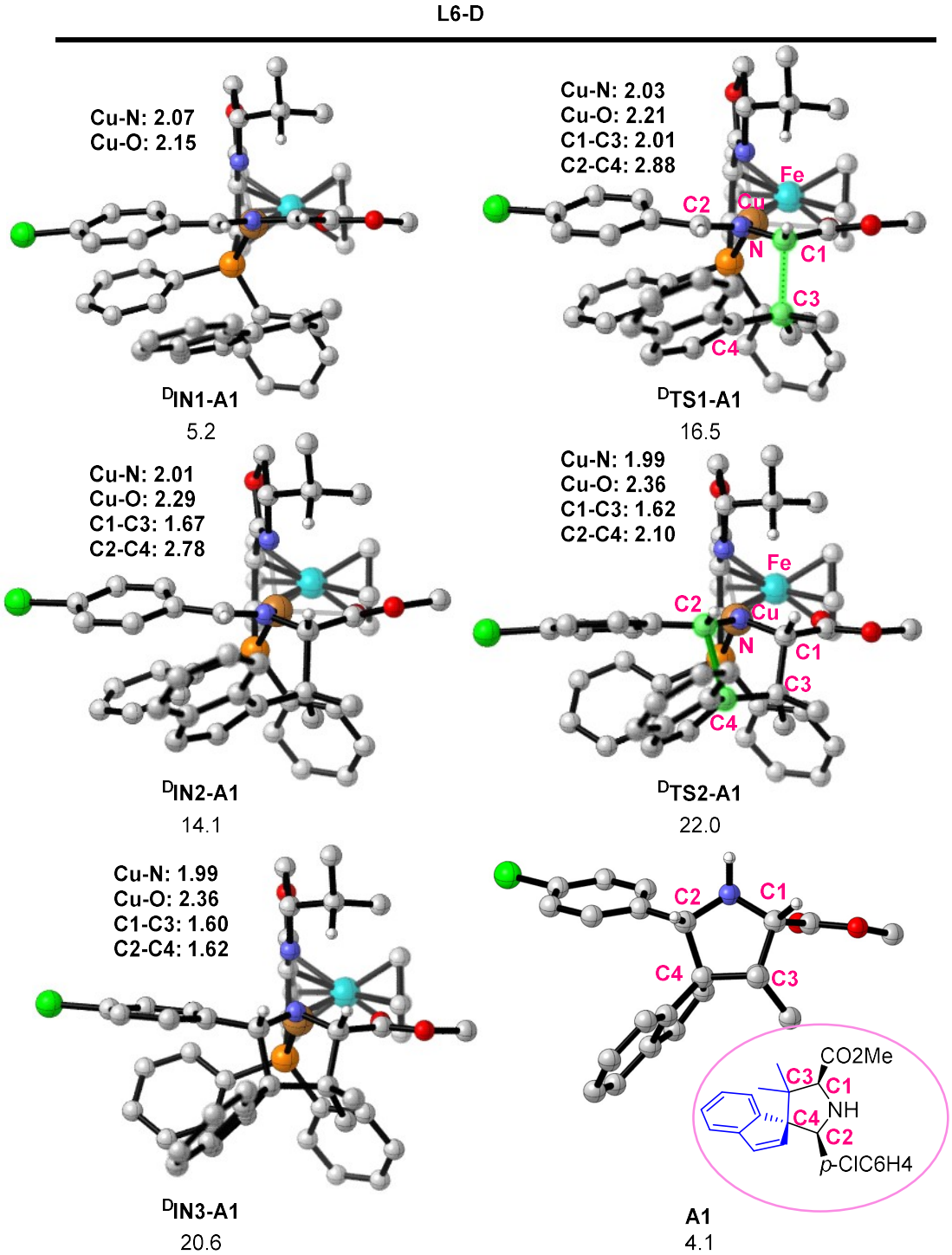

Figure S9. Optimized transition states and intermediates for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** to form the product **A1** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

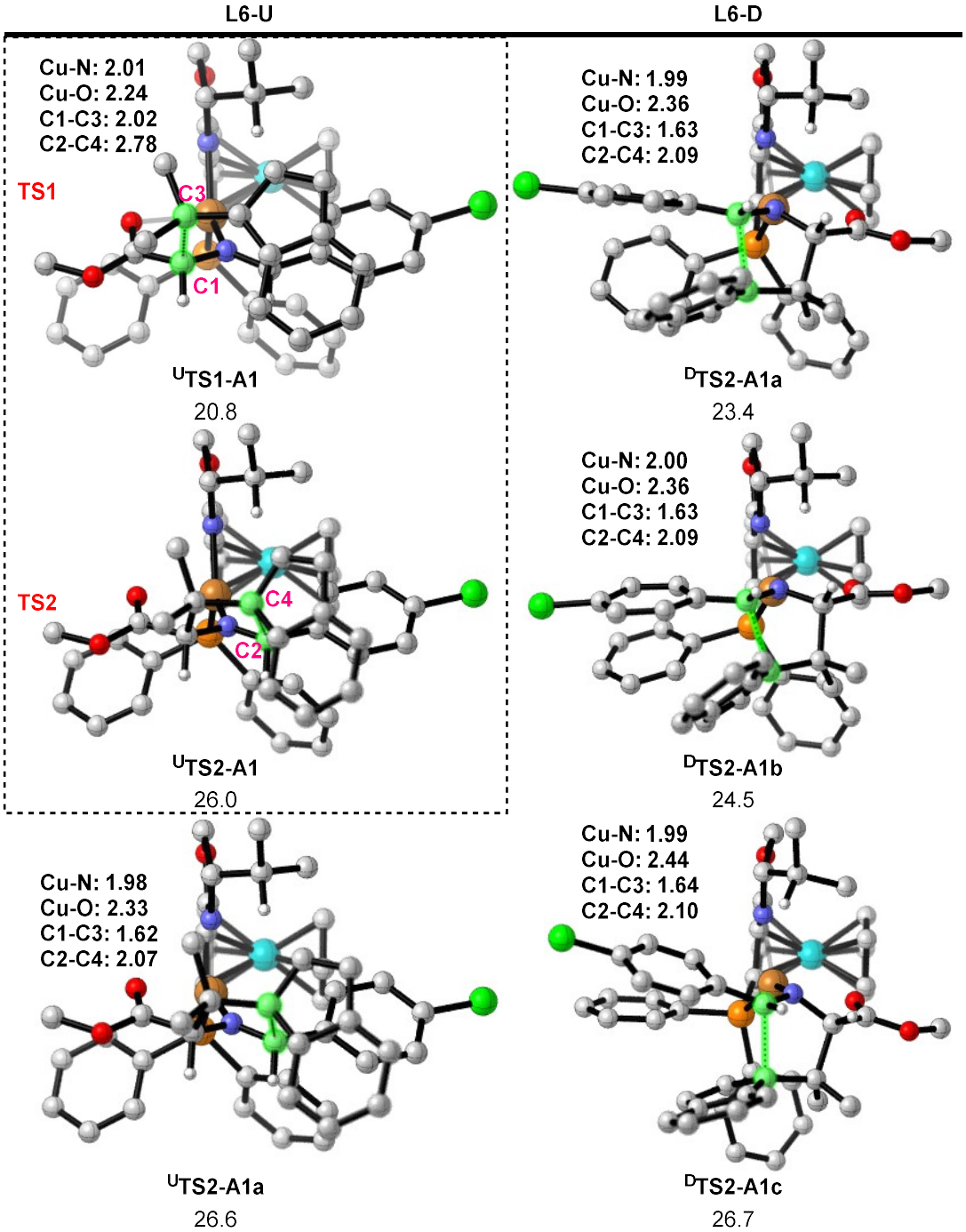

Figure S10. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** and **L6-U** to form the product **A1** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

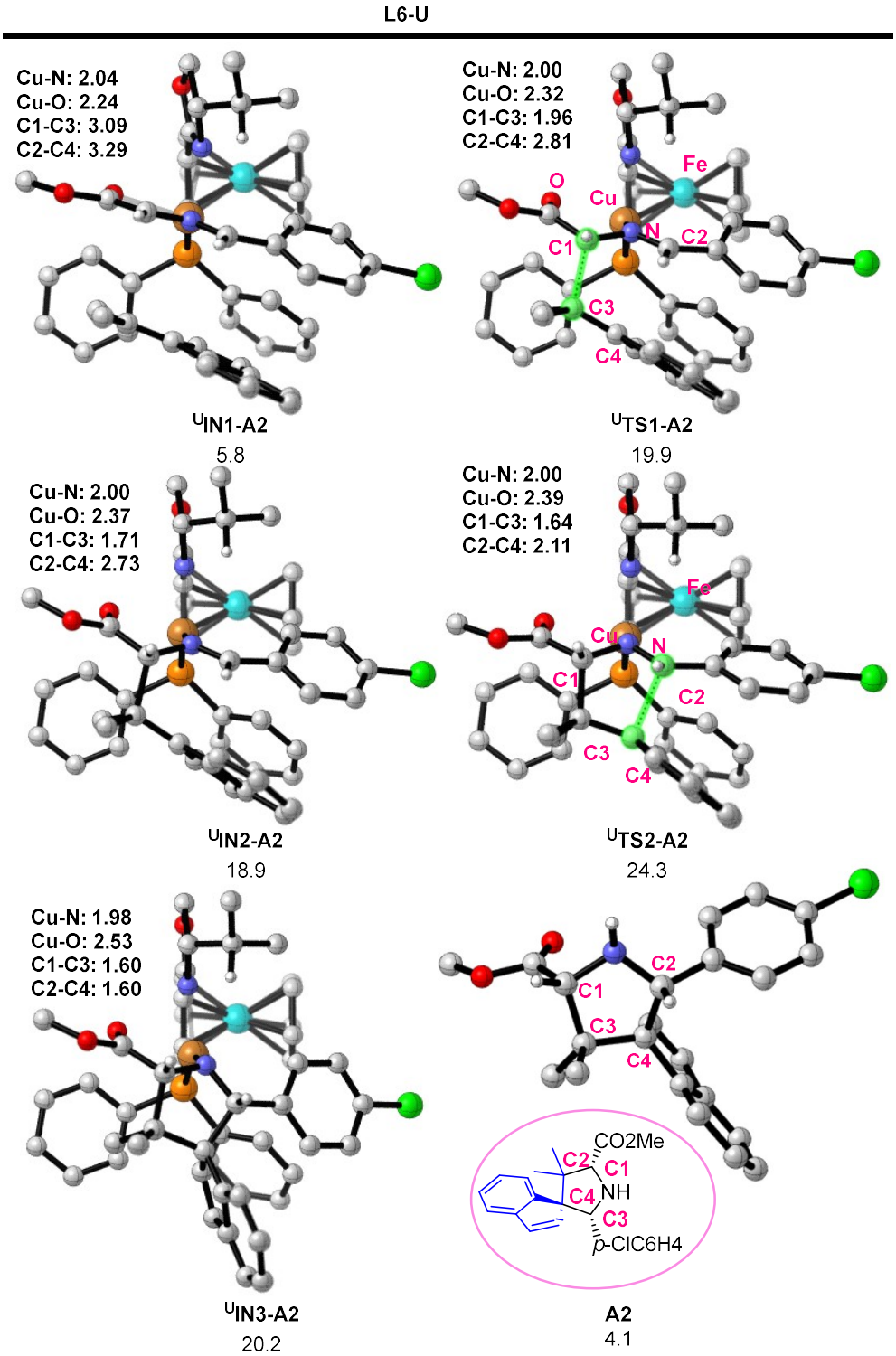

Figure S11. Optimized transition states and intermediates for the reaction catalyzed by the Cu-azomethine ylide inthermediate **L6-U** to form the product **A2** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

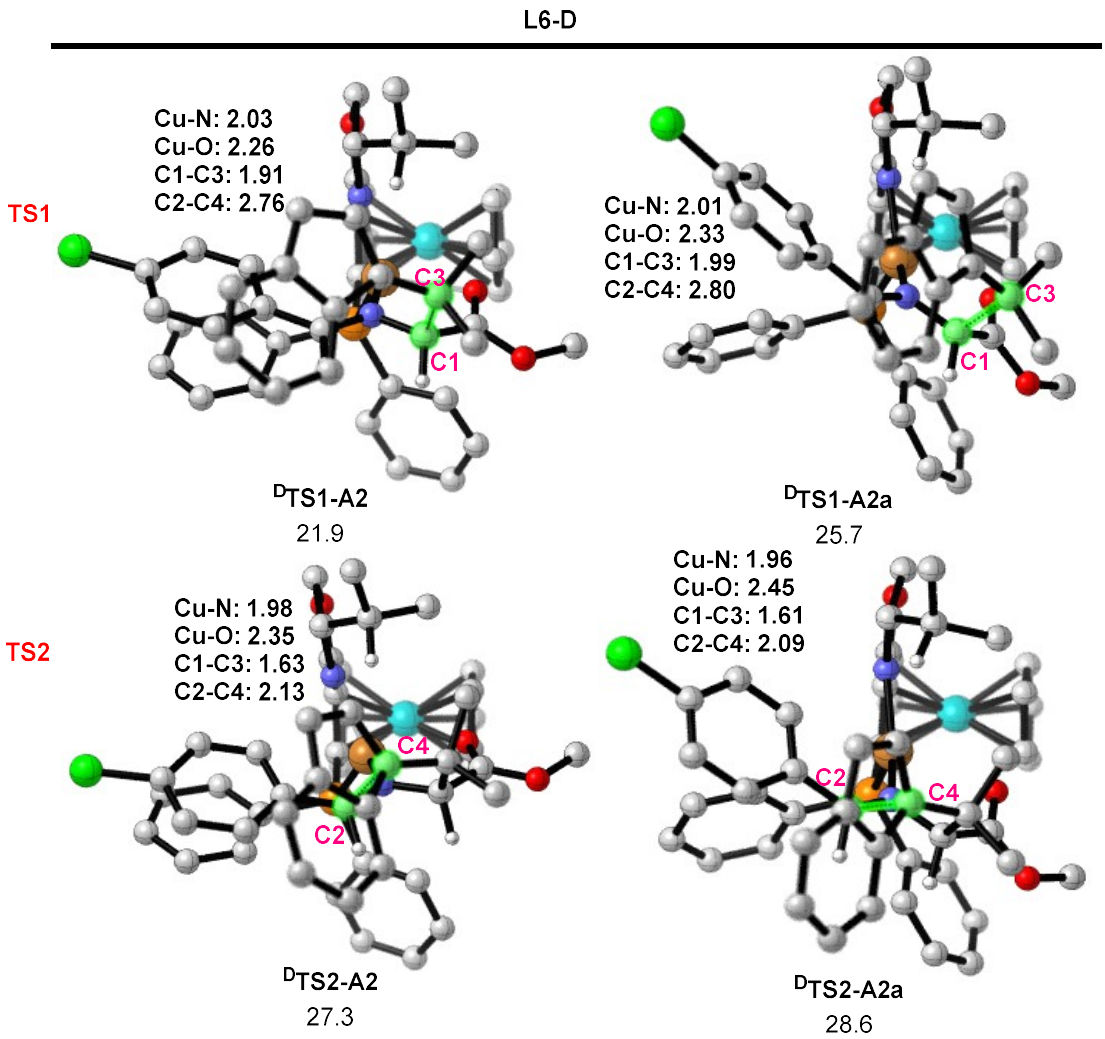

Figure S12. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** to form the product **A2** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

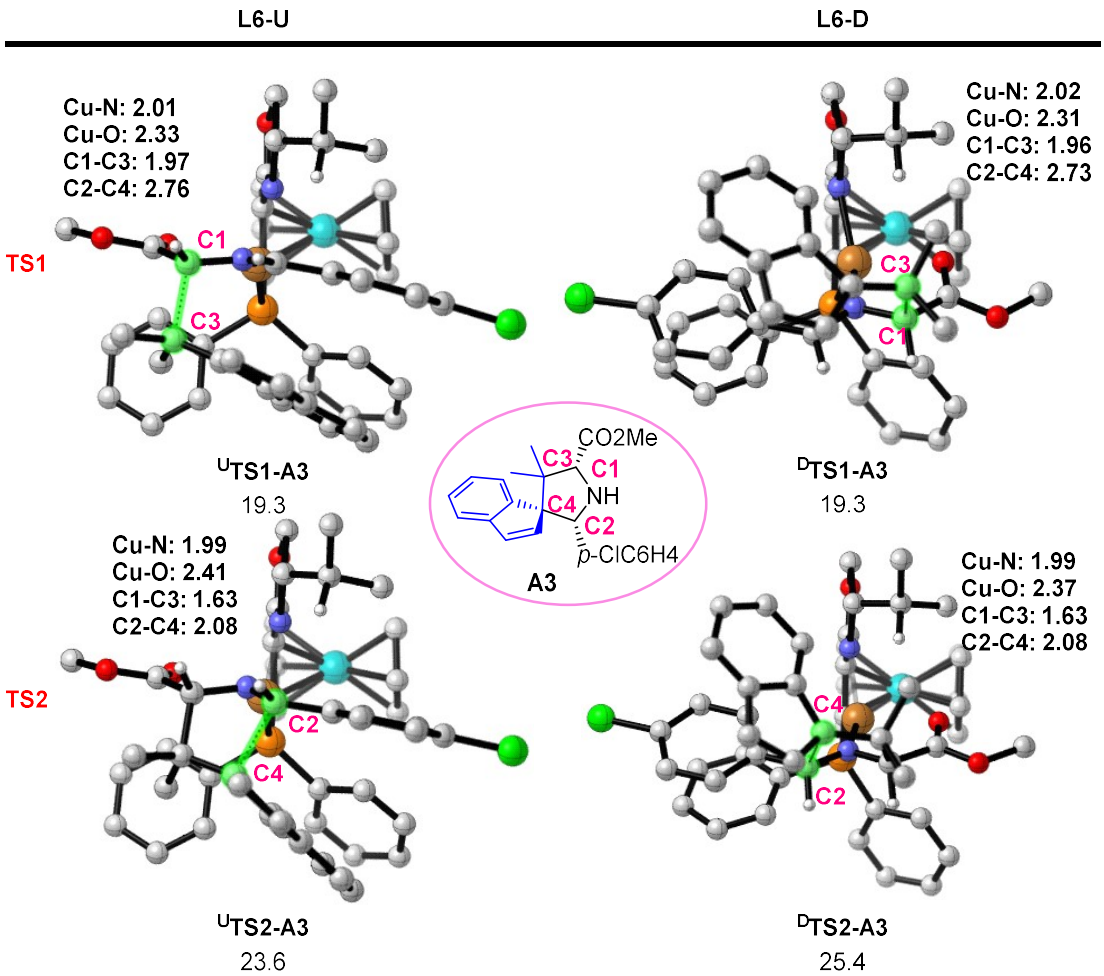

Figure S13. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** and **L6-U** to form the product **A3** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

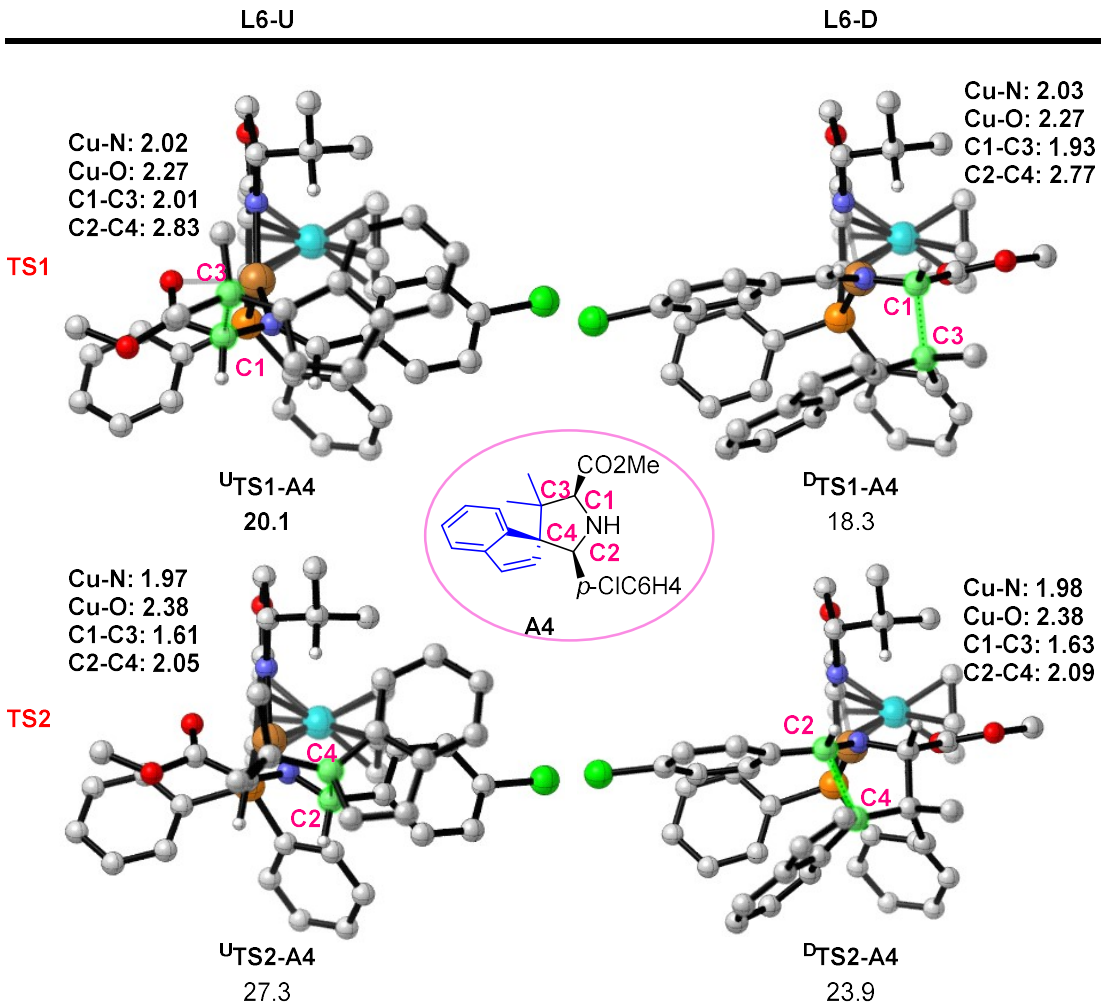

Figure S14. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** and **L6-U** to form the product **A4** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

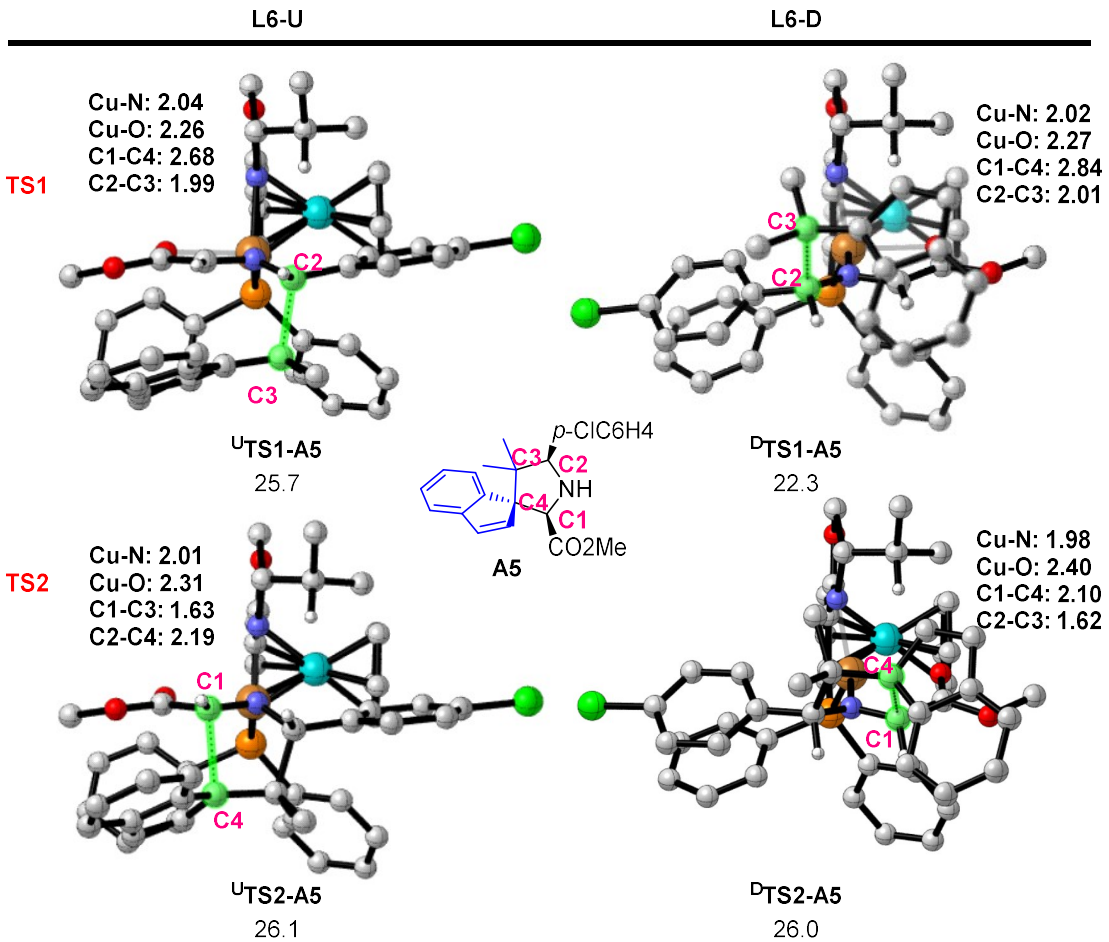

Figure S15. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-U** and **L6-D** to form the product **A5** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

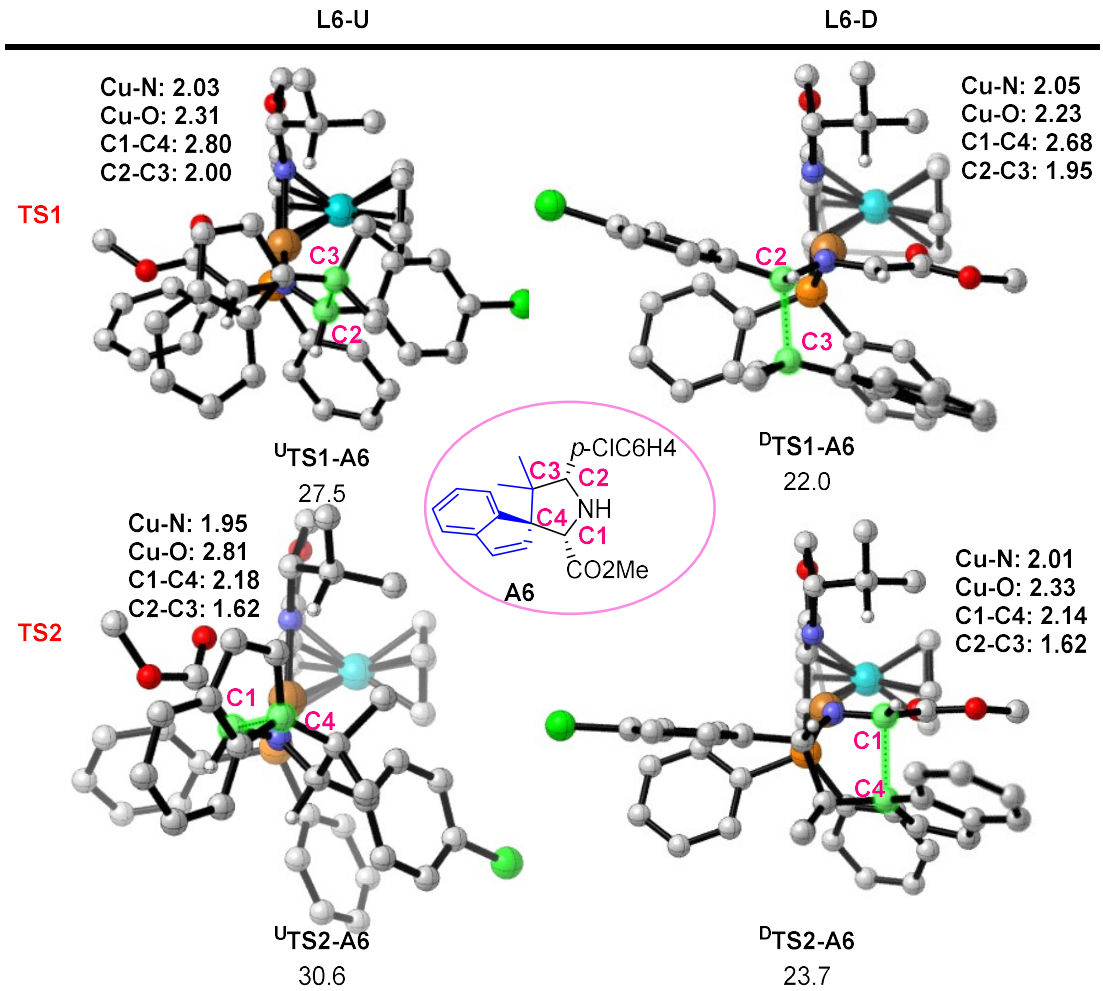

Figure S16. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-U** and **L6-D** to form the product **A6** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

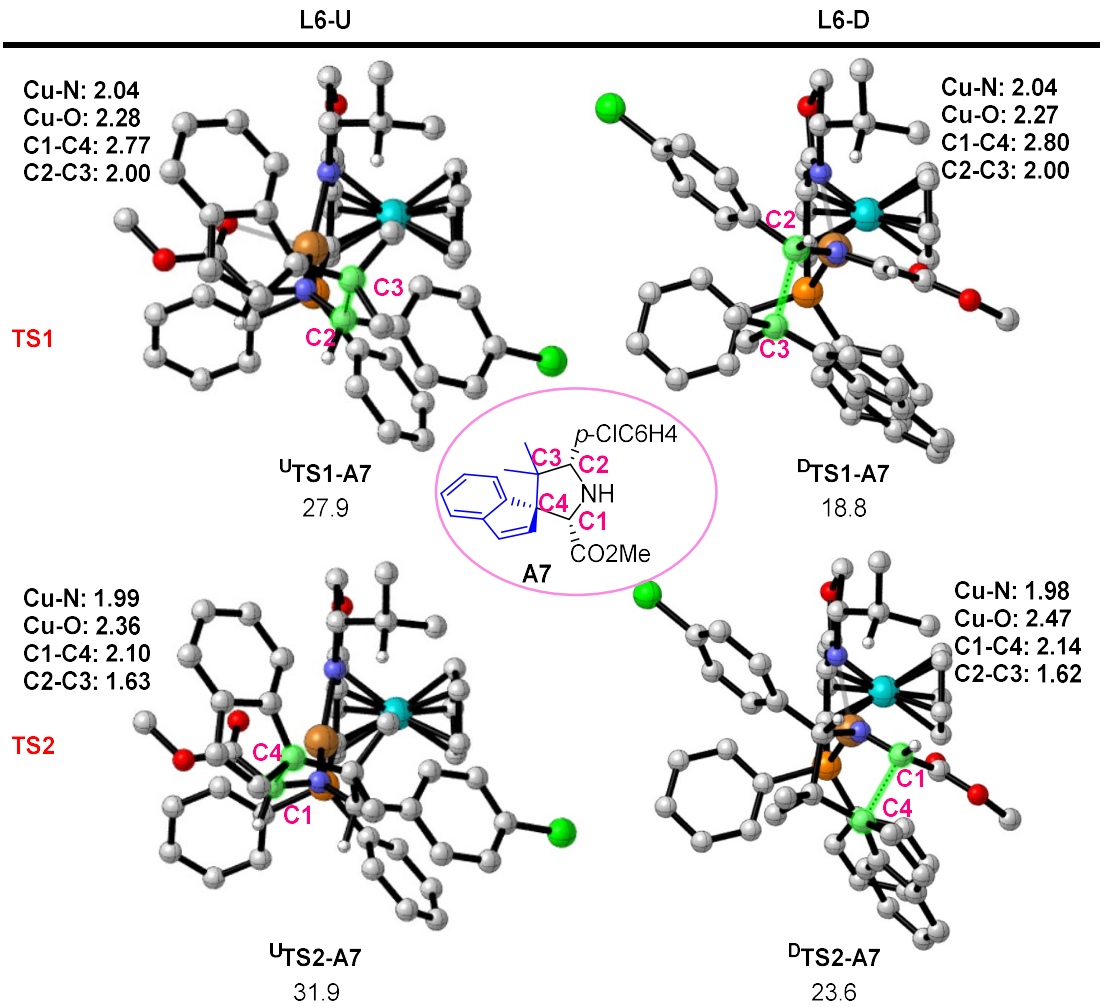

Figure S17. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-U** and **L6-D** to form the product **A7** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

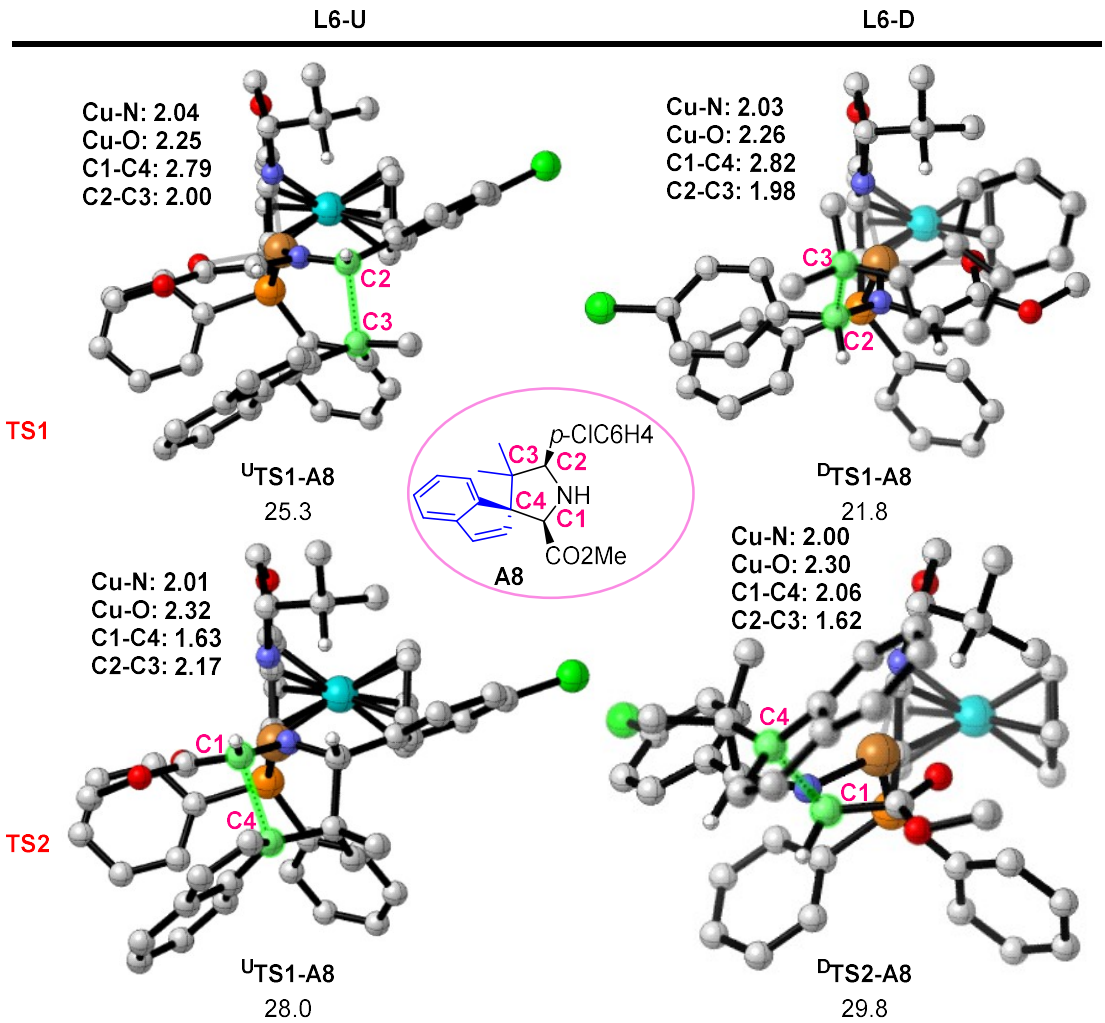

Figure S18. Optimized transition states for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-U** and **L6-D** to form the product **A8** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

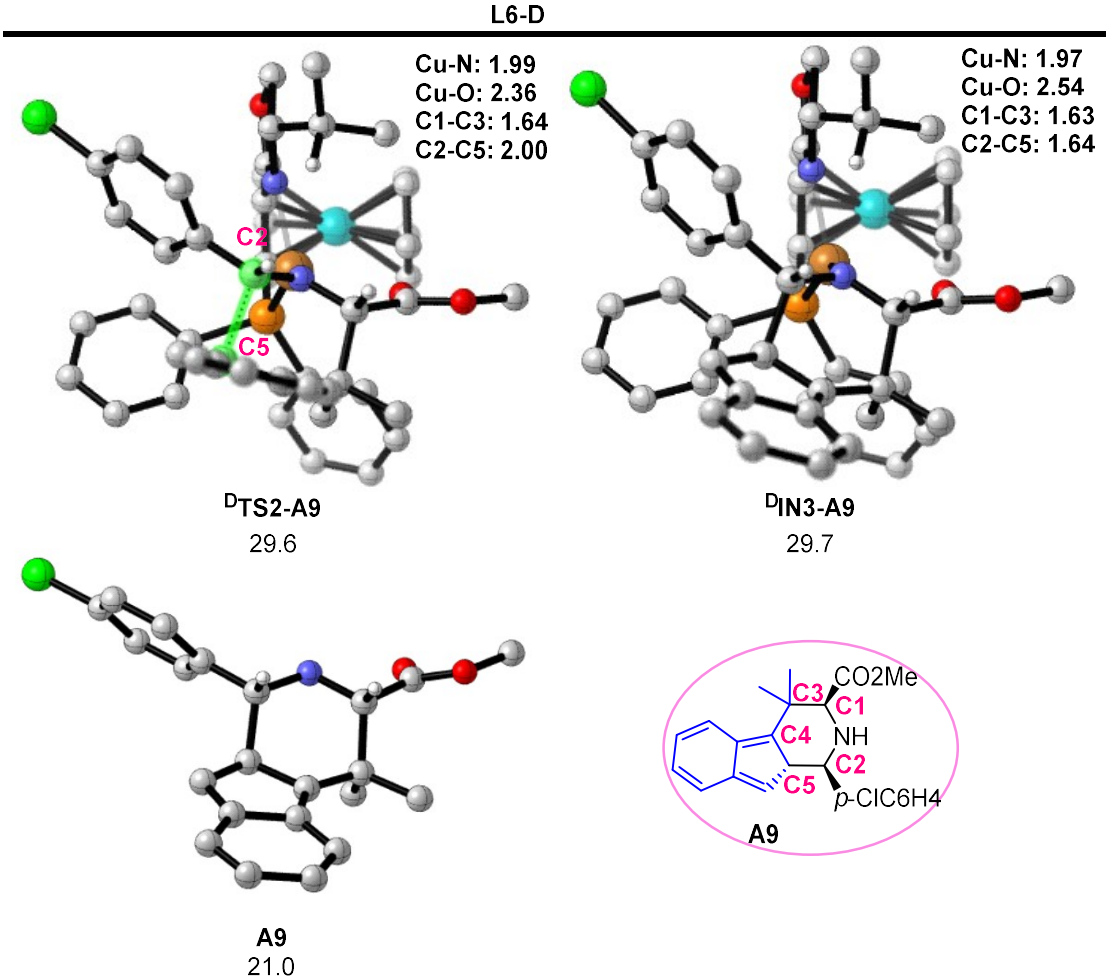

Figure S19. Optimized transition state and intermediate for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** to form the product **A9** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

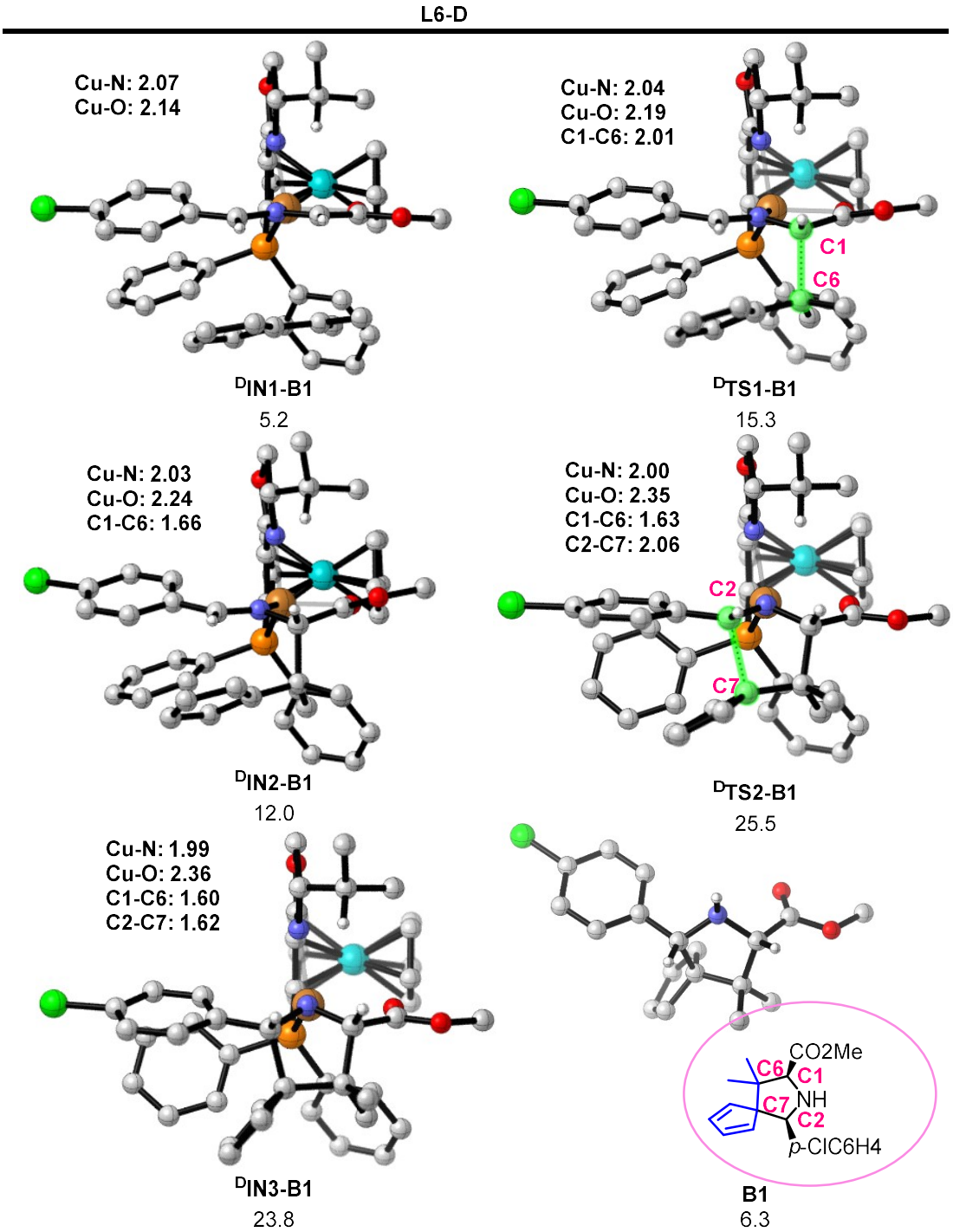

Figure S20. Optimized transition state and intermediate for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** to form the product **B1** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

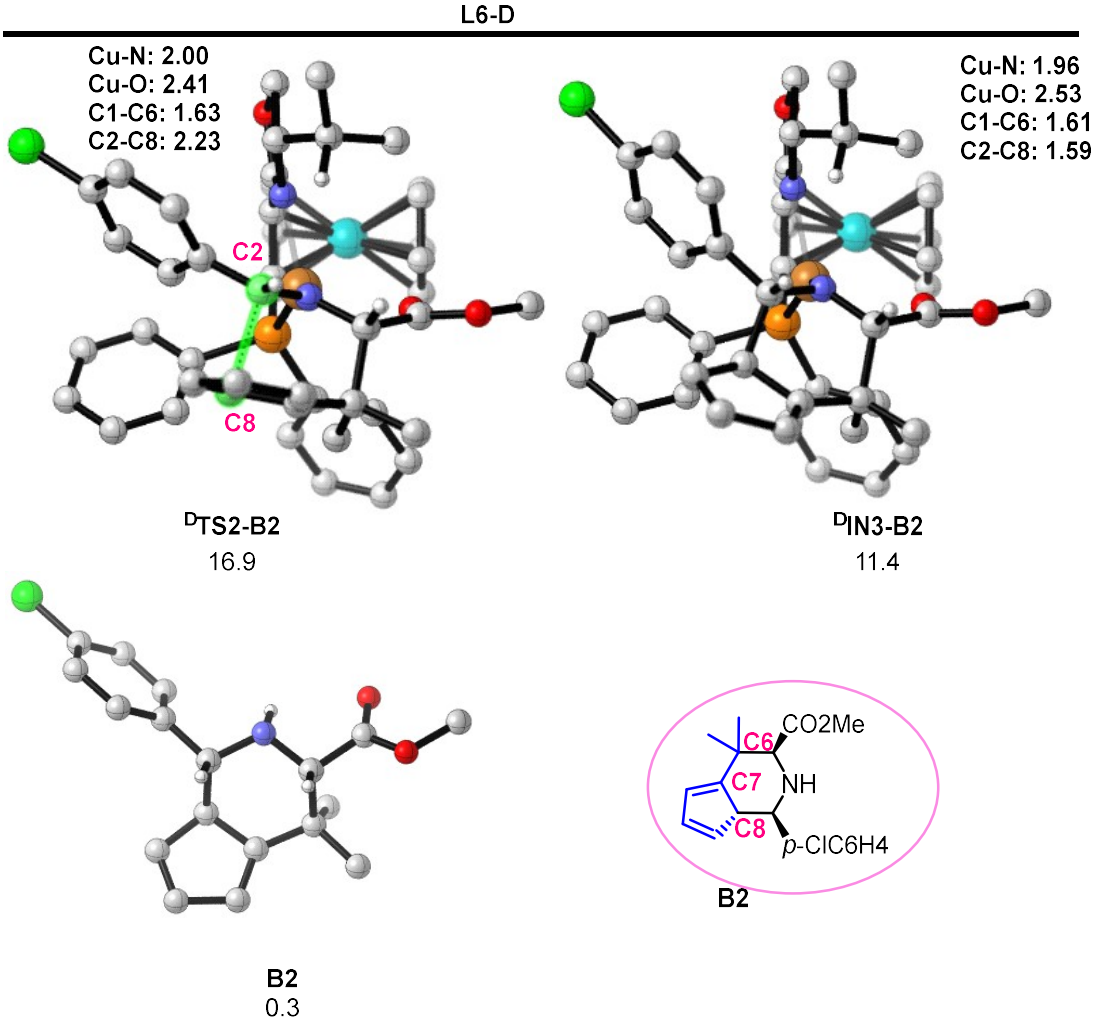

Figure S21. Optimized transition state and intermediate for the reaction catalyzed by the Cu-azomethine ylide intermediate **L6-D** to form the product **B2** by the M06-L method. Their relative free energies (in kcal/mol) in diethylether (by the PCM M06L//M06-L method) and key bond lengths (in angstrom) are given. Unimportant hydrogen atoms are omitted for clarity.

Table S1. The absolute electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in Hartree) for the substrates and Cu-L complexes by the M06-L (in gas phase) and PCM M06-L//M06-L methods (in solution).

	E	E+ZPE	G	E_{soln}	qh-G(T)
1a	-1052.381489	-1052.197069	-1052.239599	-1052.387804	-1052.237003
2a	-464.419788	-464.217152	-464.252536	-464.422863	-464.252143
6	-310.778372	-310.623868	-310.656390	-310.781147	-310.656116
L6-D	-2928.257438	-2927.591487	-2927.670374	-2928.266090	-2927.660570
L6-D1	-2928.249037	-2927.583186	-2927.661377	-2928.258015	-2927.652060
L6-U	-2928.248430	-2927.582610	-2927.662424	-2928.258993	-2927.652113
L6-U1	-2928.248852	-2927.582916	-2927.661520	-2928.258787	-2927.652013
L6-U2	-2928.248376	-2927.581142	-2927.657377	-2928.258436	-2927.649175
L6-U3	-2928.245843	-2927.579443	-2927.657255	-2928.255678	-2927.648143

Table S2. The relative electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in kcal/mol) for the substrates and Cu-L complexes by M06-L (in gas phase) and PCM M06-L//M06-L (in solution).

	ΔE	ΔE+ZPE	ΔG	ΔE_{soln}	ΔG_{soln}	Δqh-G(T)	$\Delta G_{soln\text{-}corr}$
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2a	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
L6-D	0.0	0.0	0.0	0.0	0.0	0.0	0.0
L6-D1	5.3	5.2	5.6	5.1	5.4	5.3	5.1
L6-U	5.7	5.6	5.0	4.5	3.8	5.3	4.1
L6-U1	5.4	5.4	5.6	4.6	4.8	5.4	4.6
L6-U2	5.7	6.5	8.2	4.8	7.3	7.2	6.3
L6-U3	7.3	7.6	8.2	6.5	7.5	7.8	7.1

Table S3. The absolute electronic energies (in Hartree) for the substrates and Cu-L complexes in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$E_{pcm\text{-}B3LYP\text{-}D3}$	$E_{pcm\text{-}PBE0\text{-}D3}$	$E_{pcm\text{-}\omega B97X\text{-}D}$	$E_{smd\text{-}M06\text{-}L}$
1a	-1052.498462	-1051.651145	-1052.268450	-1052.398113
2a	-464.508477	-463.944098	-464.332588	-464.433618
6	-310.843639	-310.458343	-310.725635	-310.788848
L6-D	-2928.552603	-2925.990513	-2927.827563	-2928.294401
L6-D1	-2928.543605	-2925.980912	-2927.816429	-2928.286326
L6-U	-2928.543594	-2925.982132	-2927.818923	-2928.287821
L6-U1	-2928.544852	-2925.982461	-2927.819029	-2928.286656
L6-U2	-2928.544816	-2925.982034	-2927.818629	-2928.285697
L6-U3	-2928.542091	-2925.979599	-2927.815643	-2928.284243

Table S4. The relative electronic energies (in kcal/mol) for the substrates and Cu-L complexes in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta E_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta E_{pcm\text{-}PBE0\text{-}D3}$	$\Delta E_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta E_{smd\text{-}M06\text{-}L}$
1a	0.0	0.0	0.0	0.0
2a	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0
L6-D	0.0	0.0	0.0	0.0
L6-D1	5.6	6.0	7.0	5.1
L6-U	5.7	5.3	5.4	4.1
L6-U1	4.9	5.1	5.4	4.9
L6-U2	4.9	5.3	5.6	5.5
L6-U3	6.6	6.8	7.5	6.4

Table S5. The relative Gibbs free energies (in kcal/mol) for the substrates and Cu-L complexes in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta G_{smd\text{-}M06\text{-}L}$
1a	0.0	0.0	0.0	0.0
2a	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0
L6-D	0.0	0.0	0.0	0.0
L6-D1	6.0	6.4	7.4	5.4
L6-U	5.0	4.6	4.8	3.5
L6-U1	5.0	5.2	5.5	5.0
L6-U2	7.4	7.8	8.1	7.9
L6-U3	7.6	7.8	8.4	7.3

Table S6. The relative Gibbs free energies with the quasi-harmonic entropic correction (in kcal/mol) for the substrates and Cu-L complexes in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D\text{-}corr}$	$\Delta G_{smd\text{-}M06\text{-}L\text{-}corr}$
1a	0.0	0.0	0.0	0.0
2a	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0
L6-D	0.0	0.0	0.0	0.0
L6-D1	5.7	6.1	7.1	5.1
L6-U	5.3	4.9	5.1	3.8
L6-U1	4.8	5.0	5.3	4.8
L6-U2	6.4	6.8	7.1	6.9
L6-U3	7.1	7.4	8.0	6.9

Table S7. The absolute electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in Hartree) for the intermediates and transition states for the products **A1**-**A4** by the M06-L (in gas phase) and PCM M06-L//M06-L methods (in solution).

	E	E+ZPE	G	E_{soln}	qh-G(T)
^{U}TS1-A1	-3392.670470	-3391.799803	-3391.888477	-3392.684454	-3391.877319
^{U}TS2-A1	-3392.666936	-3391.793823	-3391.880972	-3392.679757	-3391.870241
^{U}TS2-A1a	-3392.666632	-3391.793118	-3391.879975	-3392.679279	-3391.869373
^{D}IN1-A1	-3392.698949	-3391.827638	-3391.918790	-3392.708474	-3391.906679
^{D}TS1-A1	-3392.677843	-3391.807256	-3391.897235	-3392.690662	-3391.885403
^{D}IN2-A1	-3392.681082	-3391.809066	-3391.898188	-3392.696359	-3391.886707
^{D}TS2-A1	-3392.670469	-3391.798651	-3391.889277	-3392.683232	-3391.876598
^{D}IN3-A1	-3392.678805	-3391.803876	-3391.892641	-3392.689735	-3391.880757
A1	-1516.831309	-1516.436806	-1516.488124	-1516.838339	-1516.484928
^{D}TS2-A1a	-3392.671421	-3391.798097	-3391.885625	-3392.683971	-3391.874637
^{D}TS2-A1b	-3392.669877	-3391.797010	-3391.885579	-3392.681402	-3391.873832
^{D}TS2-A1c	-3392.667825	-3391.794073	-3391.881418	-3392.679284	-3391.870432
^{U}IN1-A2	-3392.695155	-3391.825527	-3391.916744	-3392.705469	-3391.904869
^{U}TS1-A2	-3392.674276	-3391.802418	-3391.890853	-3392.687375	-3391.879662
^{U}IN2-A2	-3392.675343	-3391.802440	-3391.891141	-3392.690020	-3391.879696
^{U}TS2-A2	-3392.669796	-3391.797299	-3391.884259	-3392.682015	-3391.873484
^{U}IN3-A2	-3392.681548	-3391.806034	-3391.892121	-3392.691975	-3391.881755
A2	-1516.831309	-1516.436805	-1516.488124	-1516.838339	-1516.484928
^{D}TS1-A2	-3392.668809	-3391.797630	-3391.887128	-3392.683059	-3391.875237
^{D}TS2-A2	-3392.663541	-3391.790835	-3391.879982	-3392.676209	-3391.868231
^{D}TS1-A2a	-3392.664478	-3391.792821	-3391.881382	-3392.677844	-3391.870050
^{D}TS2-A2a	-3392.661279	-3391.789014	-3391.877811	-3392.674102	-3391.866035
^{U}TS1-A3	-3392.674922	-3391.803873	-3391.890598	-3392.688198	-3391.880412
^{U}TS2-A3	-3392.670709	-3391.798440	-3391.885127	-3392.682975	-3391.874609
^{D}TS1-A3	-3392.673417	-3391.803092	-3391.892047	-3392.686364	-3391.880813
^{D}TS2-A3	-3392.668302	-3391.795627	-3391.881500	-3392.680662	-3391.871599
^{U}TS1-A4	-3392.672967	-3391.801574	-3391.889418	-3392.686839	-3391.878530
^{U}TS2-A4	-3392.665520	-3391.792081	-3391.879470	-3392.678070	-3391.868371
^{D}TS1-A4	-3392.677477	-3391.805915	-3391.891785	-3392.691185	-3391.881648
^{D}TS2-A4	-3392.671226	-3391.797419	-3391.884510	-3392.684077	-3391.873569

Table S8. The relative electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **A1**-**A4** by M06-L (in gas phase) and PCM M06-L//M06-L (in solution).

	ΔE	ΔE+ZPE	ΔG	ΔE_{soln}	ΔG_{soln}	Δqh-G(T)	$\Delta G_{soln\text{-}corr}$
^{U}TS1-A1	4.2	5.5	21.6	2.8	20.2	22.2	20.8
^{U}TS2-A1	6.5	9.3	26.3	5.8	25.6	26.7	26.0
^{U}TS2-A1a	6.6	9.7	26.9	6.1	26.4	27.2	26.6
^{D}IN1-A1	-13.6	-11.9	2.6	-12.2	4.0	3.8	5.2
^{D}TS1-A1	-0.4	0.9	16.1	-1.1	15.4	17.1	16.5
^{D}IN2-A1	-2.4	-0.3	15.5	-4.6	13.3	16.3	14.1
^{D}TS2-A1	4.2	6.3	21.1	3.6	20.5	22.7	22.0
^{D}IN3-A1	-1.0	3.0	19.0	-0.5	19.5	20.1	20.6
A1	-18.8	-14.2	2.5	-17.4	4.0	2.6	4.1
^{D}TS2-A1a	3.6	6.6	23.4	3.1	22.9	23.9	23.4
^{D}TS2-A1b	4.6	7.3	23.4	4.7	23.6	24.4	24.5
^{D}TS2-A1c	5.9	9.1	26.0	6.1	26.2	26.5	26.7
^{U}IN1-A2	-11.3	-10.6	3.9	-10.4	4.8	4.9	5.8
^{U}TS1-A2	1.9	3.9	20.1	1.0	19.3	20.7	19.9
^{U}IN2-A2	1.2	3.9	19.9	-0.7	18.1	20.7	18.9
^{U}TS2-A2	4.7	7.1	24.3	4.4	23.9	24.6	24.3
^{U}IN3-A2	-2.7	1.6	19.3	-1.9	20.1	19.4	20.2
A2	-18.8	-14.2	2.5	-17.4	4.0	2.6	4.1
^{D}TS1-A2	5.3	6.9	22.5	3.7	20.9	23.5	21.9
^{D}TS2-A2	8.6	11.2	26.9	8.0	26.3	27.9	27.3
^{D}TS1-A2a	8.0	9.9	26.1	7.0	25.0	26.8	25.7
^{D}TS2-A2a	10.0	12.3	28.3	9.3	27.6	29.3	28.6
^{U}TS1-A3	1.4	3.0	20.3	0.5	19.3	20.3	19.3
^{U}TS2-A3	4.1	6.4	23.7	3.8	23.4	23.9	23.6
^{D}TS1-A3	2.4	3.5	19.4	1.6	18.6	20.0	19.3
^{D}TS2-A3	5.6	8.2	26.0	5.2	25.6	25.8	25.4
^{U}TS1-A4	2.7	4.4	21.0	1.3	19.7	21.5	20.1
^{U}TS2-A4	7.3	10.4	27.3	6.8	26.7	27.8	27.3
^{D}TS1-A4	-0.2	1.7	19.5	-1.4	18.3	19.5	18.3
^{D}TS2-A4	3.8	7.0	24.1	3.1	23.4	24.6	23.9

Table S9. The absolute electronic energies (in Hartree) for the intermediates and transition states for the products **A1**-**A4** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$E_{pcm\text{-}B3LYP\text{-}D3}$	$E_{pcm\text{-}PBE0\text{-}D3}$	$E_{pcm\text{-}\omega B97X\text{-}D}$	$E_{smd\text{-}M06\text{-}L}$
^{U}TS1-A1	-3393.061103	-3389.938446	-3392.163505	-3392.720373
^{U}TS2-A1	-3393.057382	-3389.943448	-3392.171096	-3392.715211
^{U}TS2-A1a	-3393.056765	-3389.942459	-3392.170284	-3392.714530
^{D}IN1-A1	-3393.087482	-3389.957138	-3392.185305	-3392.742991
^{D}TS1-A1	-3393.070639	-3389.946967	-3392.171434	-3392.725898
^{D}IN2-A1	-3393.075795	-3389.956246	-3392.183320	-3392.732537
^{D}TS2-A1	-3393.063885	-3389.948994	-3392.175145	-3392.717999
^{D}IN3-A1	-3393.071281	-3389.960030	-3392.190719	-3392.723420
A1	-1517.041894	-1515.647741	-1516.655247	-1516.854832
^{D}TS2-A1a	-3393.064185	-3389.949119	-3392.175275	-3392.718602
^{D}TS2-A1b	-3393.062034	-3389.946922	-3392.173181	-3392.715854
^{D}TS2-A1c	-3393.057900	-3389.942403	-3392.167975	-3392.713778
^{U}IN1-A2	-3393.081240	-3389.950547	-3392.179927	-3392.740426
^{U}TS1-A2	-3393.064212	-3389.941014	-3392.167040	-3392.722995
^{U}IN2-A2	-3393.066975	-3389.946876	-3392.174517	-3392.726473
^{U}TS2-A2	-3393.059436	-3389.944124	-3392.170962	-3392.717010
^{U}IN3-A2	-3393.071114	-3389.959769	-3392.191569	-3392.725299
A2	-1517.041894	-1515.647741	-1516.655247	-1516.854832
^{D}TS1-A2	-3393.061641	-3389.940178	-3392.165734	-3392.719168
^{D}TS2-A2	-3393.054547	-3389.939721	-3392.166331	-3392.711649
^{D}TS1-A2a	-3393.055586	-3389.932828	-3392.156545	-3392.713532
^{D}TS2-A2a	-3393.052699	-3389.937831	-3392.162966	-3392.709645
^{U}TS1-A3	-3393.063483	-3389.940030	-3392.166019	-3392.724540
^{U}TS2-A3	-3393.060917	-3389.945109	-3392.172457	-3392.718159
^{D}TS1-A3	-3393.064173	-3389.940781	-3392.167222	-3392.722324
^{D}TS2-A3	-3393.058750	-3389.943622	-3392.172308	-3392.715393
^{U}TS1-A4	-3393.063321	-3389.940075	-3392.165795	-3392.723377
^{U}TS2-A4	-3393.056606	-3389.942139	-3392.169438	-3392.713169
^{D}TS1-A4	-3393.070327	-3389.946830	-3392.172227	-3392.726970
^{D}TS2-A4	-3393.065809	-3389.949521	-3392.176383	-3392.718477

Table S10. The relative electronic energies (in kcal/mol) for the intermediates and transition states for the products **A1**-**A4** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta E_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta E_{pcm\text{-}PBE0\text{-}D3}$	$\Delta E_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta E_{smd\text{-}M06\text{-}L}$
^{U}TS1-A1	0.0	-2.4	-2.1	4.8
^{U}TS2-A1	2.3	-5.5	-6.9	8.0
^{U}TS2-A1a	2.7	-4.9	-6.4	8.5
^{D}IN1-A1	-16.6	-14.1	-15.8	-9.4
^{D}TS1-A1	-6.0	-7.8	-7.1	1.3
^{D}IN2-A1	-9.2	-13.6	-14.5	-2.8
^{D}TS2-A1	-1.8	-9.0	-9.4	6.3
^{D}IN3-A1	-6.4	-16.0	-19.2	2.9
A1	-21.9	-32.9	-34.0	-14.5
^{D}TS2-A1a	-1.9	-9.1	-9.5	5.9
^{D}TS2-A1b	-0.6	-7.7	-8.2	7.6
^{D}TS2-A1c	2.0	-4.9	-4.9	8.9
^{U}IN1-A2	-12.7	-10.0	-12.4	-7.8
^{U}TS1-A2	-2.0	-4.0	-4.3	3.2
^{U}IN2-A2	-3.7	-7.7	-9.0	1.0
^{U}TS2-A2	1.0	-6.0	-6.8	6.9
^{U}IN3-A2	-6.3	-15.8	-19.7	1.7
A2	-21.9	-32.9	-34.0	-14.5
^{D}TS1-A2	-0.4	-3.5	-3.5	5.6
^{D}TS2-A2	4.1	-3.2	-3.9	10.3
^{D}TS1-A2a	3.4	1.1	2.3	9.1
^{D}TS2-A2a	5.3	-2.0	-1.8	11.5
^{U}TS1-A3	-1.5	-3.4	-3.7	2.2
^{U}TS2-A3	0.1	-6.6	-7.7	6.2
^{D}TS1-A3	-1.9	-3.9	-4.4	3.6
^{D}TS2-A3	1.5	-5.7	-7.6	7.9
^{U}TS1-A4	-1.4	-3.4	-3.5	2.9
^{U}TS2-A4	2.8	-4.7	-5.8	9.3
^{D}TS1-A4	-5.8	-7.7	-7.6	0.7
^{D}TS2-A4	-3.0	-9.4	-10.2	6.0

Table S11. The relative Gibbs free energies (in kcal/mol) for the intermediates and transition states for the products **A1**-**A4** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta G_{smd\text{-}M06\text{-}L}$
^{U}TS1-A1	17.4	15.0	15.3	22.2
^{U}TS2-A1	22.2	14.3	13.0	27.9
^{U}TS2-A1a	23.0	15.4	13.9	28.8
^{D}IN1-A1	-0.4	2.1	0.4	6.8
^{D}TS1-A1	10.5	8.7	9.4	17.8
^{D}IN2-A1	8.7	4.4	3.4	15.1
^{D}TS2-A1	15.1	7.8	7.5	23.2
^{D}IN3-A1	13.6	4.0	0.8	22.9
A1	-0.6	-11.6	-12.7	6.9
^{D}TS2-A1a	17.8	10.7	10.3	25.7
^{D}TS2-A1b	18.2	11.1	10.6	26.4
^{D}TS2-A1c	22.1	15.2	15.2	29.1
^{U}IN1-A2	2.5	5.1	2.7	7.3
^{U}TS1-A2	16.3	14.2	13.9	21.4
^{U}IN2-A2	15.1	11.1	9.7	19.7
^{U}TS2-A2	20.6	13.6	12.8	26.5
^{U}IN3-A2	15.7	6.2	2.3	23.7
A2	-0.6	-11.6	-12.7	6.9
^{D}TS1-A2	16.8	13.7	13.7	22.7
^{D}TS2-A2	22.4	15.1	14.5	28.6
^{D}TS1-A2a	21.5	19.2	20.3	27.2
^{D}TS2-A2a	23.6	16.3	16.5	29.8
^{U}TS1-A3	17.3	15.4	15.1	21.0
^{U}TS2-A3	19.7	13.0	11.9	25.8
^{D}TS1-A3	15.0	13.1	12.5	20.6
^{D}TS2-A3	21.8	14.7	12.8	28.3
^{U}TS1-A4	16.9	14.9	14.8	21.3
^{U}TS2-A4	22.7	15.2	14.1	29.2
^{D}TS1-A4	13.9	12.0	12.1	20.3
^{D}TS2-A4	17.4	11.0	10.1	26.3

Table S12. The relative Gibbs free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **A1**-**A4** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D\text{-}corr}$	$\Delta G_{smd\text{-}M06\text{-}L\text{-}corr}$
^{U}TS1-A1	18.0	15.6	15.9	22.8
^{U}TS2-A1	22.5	14.6	13.3	28.2
^{U}TS2-A1a	23.3	15.6	14.2	29.0
^{D}IN1-A1	0.9	3.3	1.6	8.0
^{D}TS1-A1	11.5	9.8	10.4	18.9
^{D}IN2-A1	9.5	5.2	4.2	15.9
^{D}TS2-A1	16.7	9.4	9.0	24.7
^{D}IN3-A1	14.6	5.1	1.9	23.9
A1	-0.4	-11.5	-12.5	7.0
^{D}TS2-A1a	18.3	11.1	10.8	26.2
^{D}TS2-A1b	19.2	12.1	11.6	27.4
^{D}TS2-A1c	22.6	15.7	15.7	29.6
^{U}IN1-A2	3.5	6.2	3.8	8.4
^{U}TS1-A2	16.9	14.9	14.6	22.0
^{U}IN2-A2	15.8	11.8	10.5	20.5
^{U}TS2-A2	21.0	14.0	13.2	26.9
^{U}IN3-A2	15.8	6.4	2.4	23.8
A2	-0.4	-11.5	-12.5	7.0
^{D}TS1-A2	17.9	14.7	14.7	23.8
^{D}TS2-A2	23.4	16.1	15.4	29.6
^{D}TS1-A2a	22.2	19.9	21.0	27.9
^{D}TS2-A2a	24.5	17.3	17.5	30.8
^{U}TS1-A3	17.3	15.4	15.1	21.0
^{U}TS2-A3	19.9	13.2	12.1	26.0
^{D}TS1-A3	15.7	13.8	13.2	21.2
^{D}TS2-A3	21.7	14.5	12.6	28.1
^{U}TS1-A4	17.4	15.3	15.2	21.7
^{U}TS2-A4	23.3	15.8	14.7	29.8
^{D}TS1-A4	13.8	12.0	12.1	20.3
^{D}TS2-A4	17.8	11.4	10.6	26.8

Table S13. The absolute electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in Hartree) for the intermediates and transition states for the products **A5**-**A9** by the M06-L (in gas phase) and PCM M06-L//M06-L methods (in solution).

	E	E+ZPE	G	E_{soln}	qh-G(T)
^{U}TS1-A5	-3392.663879	-3391.792541	-3391.880706	-3392.677717	-3391.869666
^{U}TS2-A5	-3392.666143	-3391.793502	-3391.881221	-3392.678859	-3391.870210
^{D}TS1-A5	-3392.669467	-3391.797801	-3391.887632	-3392.682490	-3391.875873
^{D}TS2-A5	-3392.667248	-3391.794658	-3391.882701	-3392.678787	-3391.871412
^{U}TS1-A6	-3392.659862	-3391.788581	-3391.877605	-3392.674354	-3391.866075
^{U}TS2-A6	-3392.658355	-3391.786109	-3391.874379	-3392.670961	-3391.863065
^{D}TS1-A6	-3392.669810	-3391.798863	-3391.888233	-3392.682612	-3391.876610
^{D}TS2-A6	-3392.670618	-3391.798160	-3391.886656	-3392.682159	-3391.875116
^{U}TS1-A7	-3392.660899	-3391.789418	-3391.878170	-3392.673984	-3391.866968
^{U}TS2-A7	-3392.658491	-3391.785523	-3391.872656	-3392.670126	-3391.861984
^{D}TS1-A7	-3392.675537	-3391.805062	-3391.894788	-3392.687012	-3391.883004
^{D}TS2-A7	-3392.673512	-3391.800476	-3391.888207	-3392.683286	-3391.877007
^{U}TS1-A8	-3392.666414	-3391.794455	-3391.881406	-3392.679579	-3391.870923
^{U}TS1-A8	-3392.666188	-3391.792510	-3391.878034	-3392.677897	-3391.868092
^{D}TS1-A8	-3392.672119	-3391.800912	-3391.888247	-3392.684094	-3391.877657
^{D}TS2-A8	-3392.663157	-3391.789812	-3391.875826	-3392.674437	-3391.865640
^{D}TS2-A9	-3392.659801	-3391.786997	-3391.875276	-3392.673403	-3391.863675
^{D}IN3-A9	-3392.664239	-3391.789838	-3391.878095	-3392.674813	-3391.866536
A9	-1516.803395	-1516.409543	-1516.462160	-1516.810229	-1516.458309

Table S14. The relative electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **A5-A9** by the M06-L (in gas phase) and PCM M06-L//M06-L methods(in solution).

	ΔE	ΔE+ZPE	ΔG	ΔE_{soln}	ΔG_{soln}	Δqh-G(T)	$\Delta G_{soln-corr}$
^{U}TS1-A5	8.4	10.1	26.5	7.1	25.2	27.0	25.7
^{U}TS2-A5	7.0	9.5	26.2	6.3	25.5	26.7	26.1
^{D}TS1-A5	4.9	6.8	22.1	4.1	21.3	23.1	22.3
^{D}TS2-A5	6.3	8.8	25.2	6.4	25.3	25.9	26.0
^{U}TS1-A6	10.9	12.6	28.4	9.2	26.7	29.3	27.5
^{U}TS2-A6	11.8	14.1	30.5	11.3	29.9	31.2	30.6
^{D}TS1-A6	4.7	6.1	21.8	4.0	21.1	22.7	22.0
^{D}TS2-A6	4.1	6.6	22.7	4.3	22.9	23.6	23.7
^{U}TS1-A7	10.2	12.1	28.1	9.4	27.2	28.7	27.9
^{U}TS2-A7	11.8	14.5	31.5	11.8	31.6	31.8	31.9
^{D}TS1-A7	1.1	2.2	17.6	1.2	17.8	18.6	18.8
^{D}TS2-A7	2.3	5.1	21.8	3.6	23.0	22.4	23.6
^{U}TS1-A8	6.8	8.9	26.0	5.9	25.1	26.2	25.3
^{U}TS1-A8	6.9	10.1	28.2	6.9	28.2	28.0	28.0
^{D}TS1-A8	3.2	4.8	21.8	3.0	21.6	22.0	21.8
^{D}TS2-A8	8.8	11.8	29.5	9.1	29.8	29.5	29.8
^{D}TS2-A9	10.9	13.6	29.9	9.8	28.7	30.8	29.6
^{D}IN3-A9	8.1	11.8	28.1	8.9	28.8	29.0	29.7
A9	-1.3	2.9	18.8	0.3	20.4	19.4	21.0

Table S15. The absolute electronic energies (in Hartree) for the intermediates and transition states for the products **A5-A9** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$E_{pcm\text{-}B3LYP\text{-}D3}$	$E_{pcm\text{-}PBE0\text{-}D3}$	$E_{pcm\text{-}\omega B97X\text{-}D}$	$E_{smd\text{-}M06\text{-}L}$
^{U}TS1-A5	-3393.052986	-3389.930682	-3392.154626	-3392.713712
^{U}TS2-A5	-3393.055843	-3389.940165	-3392.165957	-3392.713832
^{D}TS1-A5	-3393.058443	-3389.935156	-3392.158513	-3392.717337
^{D}TS2-A5	-3393.057597	-3389.942028	-3392.169127	-3392.713112
^{U}TS1-A6	-3393.048569	-3389.927040	-3392.149815	-3392.710889
^{U}TS2-A6	-3393.047252	-3389.931057	-3392.155780	-3392.707014
^{D}TS1-A6	-3393.059765	-3389.937308	-3392.160343	-3392.717747
^{D}TS2-A6	-3393.062927	-3389.947129	-3392.172241	-3392.716577
^{U}TS1-A7	-3393.050475	-3389.926985	-3392.151031	-3392.708825
^{U}TS2-A7	-3393.049069	-3389.932816	-3392.159816	-3392.704112
^{D}TS1-A7	-3393.065663	-3389.941592	-3392.165599	-3392.721299
^{D}TS2-A7	-3393.063661	-3389.946358	-3392.173444	-3392.716802
^{U}TS1-A8	-3393.054902	-3389.931459	-3392.155458	-3392.714980
^{U}TS1-A8	-3393.055413	-3389.938547	-3392.165150	-3392.712181
^{D}TS1-A8	-3393.060006	-3389.936816	-3392.161622	-3392.718722
^{D}TS2-A8	-3393.053228	-3389.937476	-3392.166140	-3392.708058
^{D}TS2-A9	-3393.055098	-3389.941066	-3392.164984	-3392.709100
^{D}IN3-A9	-3393.055347	-3389.942978	-3392.169392	-3392.709456
A9	-1517.012934	-1515.617785	-1516.620997	-1516.828491

Table S16. The relative electronic energies (in kcal/mol) for the intermediates and transition states for the products **A5-A9** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta E_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta E_{pcm\text{-}PBE0\text{-}D3}$	$\Delta E_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta E_{smd\text{-}M06\text{-}L}$
^{U}TS1-A5	5.1	2.5	3.5	9.0
^{U}TS2-A5	3.3	-3.5	-3.6	8.9
^{D}TS1-A5	1.7	-0.3	1.0	6.7
^{D}TS2-A5	2.2	-4.7	-5.6	9.4
^{U}TS1-A6	7.9	4.8	6.5	10.7
^{U}TS2-A6	8.7	2.2	2.7	13.2
^{D}TS1-A6	0.8	-1.7	-0.1	6.4
^{D}TS2-A6	-1.2	-7.9	-7.6	7.2
^{U}TS1-A7	6.7	4.8	5.7	12.0
^{U}TS2-A7	7.5	1.1	0.2	15.0
^{D}TS1-A7	-2.9	-4.4	-3.4	4.2
^{D}TS2-A7	-1.6	-7.4	-8.3	7.0
^{U}TS1-A8	3.9	2.0	2.9	8.2
^{U}TS1-A8	3.6	-2.5	-3.1	9.9
^{D}TS1-A8	0.7	-1.4	-0.9	5.8
^{D}TS2-A8	4.9	-1.8	-3.8	12.5
^{D}TS2-A9	3.8	-4.1	-3.0	11.9
^{D}IN3-A9	3.6	-5.3	-5.8	11.6
A9	-3.8	-14.1	-12.5	2.0

Table S17. The relative Gibbs free energies (in kcal/mol) for the intermediates and transition states for the products **A5-A9** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta G_{smd\text{-}M06\text{-}L}$
^{U}TS1-A5	23.2	20.6	21.6	27.1
^{U}TS2-A5	22.5	15.7	15.6	28.1
^{D}TS1-A5	18.9	16.9	18.3	24.0
^{D}TS2-A5	21.2	14.3	13.3	28.3
^{U}TS1-A6	25.4	22.3	24.0	28.3
^{U}TS2-A6	27.3	20.8	21.4	31.8
^{D}TS1-A6	17.9	15.4	17.0	23.6
^{D}TS2-A6	17.4	10.7	11.0	25.8
^{U}TS1-A7	24.5	22.6	23.6	29.9
^{U}TS2-A7	27.3	20.9	20.0	34.8
^{D}TS1-A7	13.7	12.2	13.2	20.8
^{D}TS2-A7	17.8	12.1	11.1	26.5
^{U}TS1-A8	23.1	21.2	22.2	27.4
^{U}TS1-A8	24.8	18.8	18.1	31.2
^{D}TS1-A8	19.2	17.2	17.6	24.4
^{D}TS2-A8	25.6	18.9	17.0	33.2
^{D}TS2-A9	22.7	14.9	15.9	30.8
^{D}IN3-A9	23.6	14.7	14.2	31.6
A9	16.4	6.0	7.6	22.2

Table S18. The relative Gibbs free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **A5-A9** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D\text{-}corr}$	$\Delta G_{smd\text{-}M06\text{-}L\text{-}corr}$
^{U}TS1-A5	23.7	21.1	22.1	27.6
^{U}TS2-A5	23.0	16.2	16.1	28.6
^{D}TS1-A5	19.9	17.9	19.3	25.0
^{D}TS2-A5	21.8	15.0	14.0	29.0
^{U}TS1-A6	26.2	23.1	24.9	29.1
^{U}TS2-A6	28.0	21.5	22.1	32.5
^{D}TS1-A6	18.8	16.3	17.9	24.4
^{D}TS2-A6	18.3	11.6	11.9	26.6
^{U}TS1-A7	25.1	23.2	24.2	30.5
^{U}TS2-A7	27.6	21.2	20.3	35.1
^{D}TS1-A7	14.7	13.2	14.2	21.8
^{D}TS2-A7	18.5	12.7	11.7	27.1
^{U}TS1-A8	23.3	21.4	22.4	27.6
^{U}TS1-A8	24.6	18.6	17.9	31.0
^{D}TS1-A8	19.5	17.4	17.9	24.6
^{D}TS2-A8	25.6	18.9	17.0	33.2
^{D}TS2-A9	23.6	15.8	16.8	31.7
^{D}IN3-A9	24.4	15.6	15.0	32.5
A9	16.9	6.5	8.2	22.7

Table S19. The absolute electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in Hartree) for the intermediates and transition states for the products **B1-B2** by the M06-L (in gas phase) and PCM M06-L//M06-L methods (in solution).

	E	E+ZPE	G	E_{soln}	qh-G(T)
^{D}IN1-B2	-3239.057223	-3238.234001	-3238.321341	-3239.066653	-3238.310474
^{D}TS1-B2	-3239.038432	-3238.215421	-3238.301619	-3239.050982	-3238.291127
^{D}IN2-B2	-3239.041586	-3238.217547	-3238.304868	-3239.057063	-3238.293542
^{D}TS2-B1	-3239.028238	-3238.201976	-3238.285516	-3239.039955	-3238.275728
^{D}IN3-B1	-3239.034186	-3238.206253	-3238.289626	-3239.044382	-3238.280037
B1	-1363.185536	-1362.839592	-1362.888711	-1363.192135	-1362.885633
^{D}TS2-B2	-3239.038050	-3238.212978	-3238.299140	-3239.051473	-3238.287805
^{D}IN3-B2	-3239.054054	-3238.226462	-3238.312069	-3239.062909	-3238.301074
B2	-1363.196295	-1362.849300	-1362.898476	-1363.202519	-1362.895460

Table S20. The relative electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **B1**-**B2** by the M06-L (in gas phase) and PCM M06-L//M06-L methods (in solution).

	ΔE	ΔE+ZPE	ΔG	ΔE_{soln}	ΔG_{soln}	Δqh-G(T)	$\Delta G_{soln-corr}$
^{D}IN1-B2	-13.4	-11.7	3.4	-12.2	4.7	3.9	5.2
^{D}TS1-B2	-1.6	0.0	15.8	-2.4	15.1	16.0	15.3
^{D}IN2-B2	-3.6	-1.4	13.7	-6.2	11.2	14.5	12.0
^{D}TS2-B1	4.8	8.4	25.9	4.6	25.7	25.7	25.5
^{D}IN3-B1	1.0	5.7	23.3	1.8	24.1	23.0	23.8
B1	-16.1	-11.7	4.6	-14.5	6.1	4.7	6.3
^{D}TS2-B2	-1.4	1.5	17.3	-2.7	16.1	18.1	16.9
^{D}IN3-B2	-11.4	-7.0	9.2	-9.8	10.8	9.8	11.4
B2	-22.9	-17.8	-1.6	-21.1	0.2	-1.5	0.3

Table S21. The absolute electronic energies (in Hartree) for the intermediates and transition states for the products **B1**-**B2** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$E_{pcm-B3LYP-D3}$	$E_{pcm-PBE0-D3}$	$E_{pcm-\omega B97X-D}$	$E_{smd-M06-L}$
^{D}IN1-B2	-3239.421441	-3236.470633	-3238.576738	-3239.098839
^{D}TS1-B2	-3239.405931	-3236.462144	-3238.566146	-3239.084084
^{D}IN2-B2	-3239.411240	-3236.472297	-3238.579924	-3239.091422
^{D}TS2-B1	-3239.395527	-3236.459803	-3238.565140	-3239.072241
^{D}IN3-B1	-3239.400821	-3236.468591	-3238.577686	-3239.075760
B1	-1363.371600	-1362.156594	-1363.042427	-1363.206140
^{D}TS2-B2	-3239.409864	-3236.473989	-3238.577825	-3239.084940
^{D}IN3-B2	-3239.422017	-3236.489609	-3238.598027	-3239.094444
B2	-1363.382764	-1362.167593	-1363.051383	-1363.217550

Table S22. The relative electronic energies (in kcal/mol) for the intermediates and transition states for the products **B1**-**B2** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta E_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta E_{pcm\text{-}PBE0\text{-}D3}$	$\Delta E_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta E_{smd\text{-}M06\text{-}L}$
^{D}IN1-B2	-15.8	-13.7	-14.8	-9.8
^{D}TS1-B2	-6.1	-8.3	-8.1	-0.5
^{D}IN2-B2	-9.4	-14.7	-16.8	-5.1
^{D}TS2-B1	0.4	-6.9	-7.5	6.9
^{D}IN3-B1	-2.9	-12.4	-15.4	4.7
B1	-18.5	-29.6	-30.3	-12.0
^{D}TS2-B2	-8.5	-15.8	-15.5	-1.1
^{D}IN3-B2	-16.2	-25.6	-28.1	-7.0
B2	-25.5	-36.5	-36.0	-19.2

Table S23. The relative Gibbs free energies (in kcal/mol) for the intermediates and transition states for the products **B1**-**B2** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D}$	$\Delta G_{smd\text{-}M06\text{-}L}$
^{D}IN1-B2	1.0	3.2	2.1	7.1
^{D}TS1-B2	11.3	9.1	9.3	16.9
^{D}IN2-B2	8.0	2.7	0.6	12.2
^{D}TS2-B1	21.6	14.3	13.6	28.0
^{D}IN3-B1	19.4	9.9	6.9	27.0
B1	2.2	-8.9	-9.7	8.6
^{D}TS2-B2	10.2	3.0	3.3	17.7
^{D}IN3-B2	4.5	-4.9	-7.5	13.6
B2	-4.2	-15.2	-14.7	2.1

Table S24. The relative Gibbs free energies with the quasi-harmonic entropic correction (in kcal/mol) for the intermediates and transition states for the products **B1**-**B2** in solution by different PCM DFT methods and SMD DFT method, based on the M06-L optimized structures.

	$\Delta G_{pcm\text{-}B3LYP\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}PBE0\text{-}D3\text{-}corr}$	$\Delta G_{pcm\text{-}\omega B97X\text{-}D\text{-}corr}$	$\Delta G_{smd\text{-}M06\text{-}L\text{-}corr}$
^{D}IN1-B2	1.5	3.7	2.6	7.6
^{D}TS1-B2	11.6	9.3	9.6	17.2
^{D}IN2-B2	8.7	3.4	1.4	13.0
^{D}TS2-B1	21.4	14.1	13.5	27.9
^{D}IN3-B1	19.1	9.6	6.6	26.7
B1	2.3	-8.8	-9.5	8.8
^{D}TS2-B2	11.0	3.8	4.1	18.5
^{D}IN3-B2	5.1	-4.3	-6.9	14.2
B2	-4.1	-15.1	-14.6	2.2

Table S25. The absolute electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in Hartree) for the substrates and Cu-L complexes as well as different cycloadducts (and their simpler model) by the M06-2X (in gas phase) and PCM M06-L//M06-2X methods (in solution).

	E	E+ZPE	G	E_{soln}	qh-G(T)
1a	-1052.193049	-1052.005747	-1052.047709	-1052.387008	-1052.045344
2a	-464.272777	-464.068316	-464.104474	-464.422239	-464.103568
6	-310.675635	-310.519057	-310.551300	-310.780601	-310.551152
H2	-1.163566	-1.153261	-1.164733	-1.167931	-1.164733
A1	-1516.517041	-1516.118879	-1516.171232	-1516.837612	-1516.167434
A1-s	-465.486038	-465.257672	-465.293522	-465.631976	-465.292773
A9	-1516.484576	-1516.086861	-1516.140330	-1516.809157	-1516.135991
A9-s	-465.449786	-465.223133	-465.259338	-465.600162	-465.258740
B1	-1362.915534	-1362.565514	-1362.614460	-1363.191384	-1362.611423
B1-s	-311.885744	-311.706036	-311.738588	-311.987008	-311.738110
B2	-1362.925150	-1362.574371	-1362.623811	-1363.201967	-1362.620525
B2-s	-311.890205	-311.710572	-311.743363	-311.993183	-311.742717
A1-s-3R	-619.069323	-618.793719	-618.833118	-619.260486	-618.831940
A9-s-3R	-619.015708	-618.742646	-618.782774	-619.213939	-618.781617
A1-s-4R	-772.649635	-772.326238	-772.368571	-772.884285	-772.367063
A9-s-4R	-772.631137	-772.308314	-772.352377	-772.868001	-772.350284
A1-s-5R	-848.858715	-848.522241	-848.564887	-849.114201	-848.563510
A9-s-5R	-848.841834	-848.506468	-848.550569	-849.098855	-848.548893

Table S26. The relative electronic energies, thermal corrections to energies, free energies and free energies with the quasi-harmonic entropic correction (in kcal/mol) for the substrates and Cu-L complexes as well as different cycloadducts (and their simplified (**-s**) models) by the M06-2X (in gas phase) and PCM M06-L//M06-2X methods (in solution).

	ΔE	**ΔE+ZPE**	**ΔG**	**ΔE_{soln}**	**ΔG_{soln}**	**Δqh-G(T)**	**$\Delta G_{soln-corr}$**
1a	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2a	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A1	-32.1	-28.1	-12.0	-17.8	2.4	-11.6	2.7
A1-s	-31.2	-22.6	-15.3	-26.2	-10.3	-15.4	-10.4
A9	-11.8	-8.0	7.4	0.1	19.3	8.1	19.9
A9-s	-8.4	-1.0	6.2	-6.3	8.4	6.0	8.2
B1	-29.4	-25.5	-9.7	-14.9	4.8	-9.4	5.1
B1-s	-29.2	-21.2	-14.2	-24.1	-9.1	-13.9	-8.9
B2	-35.4	-31.1	-15.6	-21.6	-1.7	-15.1	-1.2
B2-s	-32.0	-24.0	-17.1	-28.0	-13.2	-16.8	-12.9
A1-s-3R	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A9-s-3R	33.6	32.0	31.6	29.2	27.2	31.6	27.1
A1-s-4R	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A9-s-4R	11.6	11.2	10.2	10.2	8.8	10.5	9.1
A1-s-5R	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A9-s-5R	10.6	9.9	9.0	9.6	8.0	9.2	8.2

Table S27. Distortion/interaction analysis for key the transition states. The absolute electronic energies for the optimized transitions states, their catalytic active species (**$E_{dist,\ cat}$**) and substrates (**$E_{dist,\ sub}$**) (in Hartree) in solution are given.

	$E_{soln-pcm-M06L}$	**$E_{dist,\ cat}$**	**$E_{dist,\ sub}$**
$^{D}TS2_{A1}$	-3392.683232	-2928.210456	-464.356931
$^{U}TS2_{A2}$	-3392.682015	-2928.205758	-464.359243
$^{D}TS2_{A9}$	-3392.673403	-2928.223526	-464.360707
$^{D}TS2_{B1}$	-3239.039955	-2928.208645	-310.714093
$^{D}TS2_{B2}$	-3239.051473	-2928.231002	-310.719337

Table S28. (relative) Distortion/interaction analysis for the key transition states. The relative electronic energies for the optimized transitions states, their catalytic active species ($\Delta\Delta E^{\neq}_{dist,\ cat}$) and substrates ($\Delta\Delta E^{\neq}_{dist,\ sub}$) (in kcal/mol) in solution are given.

	$\Delta\Delta E^{\neq}$	$\Delta\Delta E^{\neq}_{dist,\ cat}$	$\Delta\Delta E^{\neq}_{dist,\ sub}$	$\Delta\Delta E^{\neq}_{dist}$	$\Delta\Delta E^{\neq}_{int}$
^{D}TS2$_{A1}$	0.0	0.0	0.0	0.0	0.0
^{U}TS2$_{A2}$	0.8	2.9	-1.5	1.5	-0.7
^{D}TS2$_{A9}$	6.2	-8.2	-2.4	-10.6	16.7
^{D}TS2$_{B1}$	7.2	14.0	3.3	17.3	-10.1
^{D}TS2$_{B2}$	0.0	0.0	0.0	0.0	0.0

Table S29. The absolute electronic energies (in Hartree), relative electronic energies and Gibbs free energies (in kcal/mol) by PCM M06-L//6-311+G**//M06-L method for the substrates and Cu-L complexes as well as different cycloadducts in solution.

	$E_{6\text{-}311+g(d,p)}$	$\Delta E_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)\text{-}corr}$
1a	-1052.571374	0.0	0.0	0.0
2a	-464.541752	0.0	0.0	0.0
1b	-310.867662	0.0	0.0	0.0
L6-D	-2928.780427	0.0	0.0	0.0
L6-D1	-2928.771073	5.9	6.2	5.9
L6-U	-2928.773471	4.4	3.7	4.0
L6-U1	-2928.772809	4.8	4.9	4.8
L6-U2	-2928.771834	5.4	7.9	6.9
L6-U3	-2928.769650	6.8	7.7	7.3

Table S30. The absolute electronic energies (in Hartree), relative electronic energies and Gibbs free energies (in kcal/mol) by PCM M06-L//6-311+G**//M06-L method for the intermediates and transition states for the products **A1-A4** in solution.

	$E_{6\text{-}311+g(d,p)}$	$\Delta E_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)\text{-}corr}$
^{U}TS1-A1	-3393.316238	3.7	21.1	21.7
^{U}TS2-A1	-3393.310035	7.6	27.5	27.8
^{U}TS2-A1a	-3393.309441	8.0	28.3	28.5
^{D}IN1-A1	-3393.341400	-12.1	4.2	5.4
^{D}TS1-A1	-3393.322158	0.0	16.5	17.5
^{D}IN2-A1	-3393.328151	-3.7	14.2	15.0
^{D}TS2-A1	-3393.313516	5.4	22.3	23.9
^{D}IN3-A1	-3393.318705	2.2	22.2	23.2
A1	-1517.138701	-16.0	5.3	5.4
^{D}TS2-A1a	-3393.314154	5.0	24.8	25.3
^{D}TS2-A1b	-3393.311373	6.8	25.6	26.6
^{D}TS2-A1c	-3393.309033	8.2	28.4	28.9
^{U}IN1-A2	-3393.338551	-10.3	4.8	5.9
^{U}TS1-A2	-3393.319151	1.9	20.2	20.8
^{U}IN2-A2	-3393.322178	0.0	18.8	19.5
^{U}TS2-A2	-3393.312285	6.2	25.8	26.2
^{U}IN3-A2	-3393.320996	0.7	22.8	22.9
A2	-1517.138701	-16.0	5.3	5.4
^{D}TS1-A2	-3393.315178	4.4	21.6	22.6
^{D}TS2-A2	-3393.307125	9.4	27.8	28.8
^{D}TS1-A2a	-3393.309309	8.1	26.1	26.8
^{D}TS2-A2a	-3393.303974	11.4	29.7	30.7
^{U}TS1-A3	-3393.320560	1.0	19.8	19.8
^{U}TS2-A3	-3393.313392	5.5	25.1	25.3
^{D}TS1-A3	-3393.319124	1.9	18.9	19.5
^{D}TS2-A3	-3393.311670	6.6	27.0	26.8
^{U}TS1-A4	-3393.318912	2.1	20.4	20.8
^{U}TS2-A4	-3393.308952	8.3	28.2	28.8
^{D}TS1-A4	-3393.323408	-0.8	18.9	18.9
^{D}TS2-A4	-3393.314313	4.9	25.3	25.7

Table S31. The absolute electronic energies (in Hartree), relative electronic energies and Gibbs free energies (in kcal/mol) by PCM M06-L//6-311+G**//M06-L method for the intermediates and transition states for the products **A5-A9** in solution.

	$E_{6\text{-}311+g(d,p)}$	$\Delta E_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)\text{-}corr}$
^{U}TS1-A5	-3393.308979	8.3	26.4	26.9
^{U}TS2-A5	-3393.308686	8.5	27.7	28.2
^{D}TS1-A5	-3393.314318	4.9	22.2	23.2
^{D}TS2-A5	-3393.308887	8.3	27.3	28.0
^{U}TS1-A6	-3393.306467	9.9	27.4	28.2
^{U}TS2-A6	-3393.302087	12.6	31.2	31.9
^{D}TS1-A6	-3393.313460	5.5	22.6	23.5
^{D}TS2-A6	-3393.311255	6.9	25.5	26.3
^{U}TS1-A7	-3393.305390	10.5	28.4	29.0
^{U}TS2-A7	-3393.299959	13.9	33.7	34.0
^{D}TS1-A7	-3393.318276	2.4	19.0	20.0
^{D}TS2-A7	-3393.312954	5.8	25.2	25.9
^{U}TS1-A8	-3393.311118	6.9	26.2	26.4
^{U}TS1-A8	-3393.307879	9.0	30.2	30.0
^{D}TS1-A8	-3393.315909	3.9	22.5	22.7
^{D}TS2-A8	-3393.304446	11.1	31.8	31.8
^{D}TS2-A9	-3393.302949	12.1	31.0	31.9
^{D}IN3-A9	-3393.303293	11.9	31.8	32.7
A9	-1517.110534	1.6	21.8	22.3

Table S32. The absolute electronic energies (in Hartree), relative electronic energies and Gibbs free energies (in kcal/mol) by PCM M06-L//6-311+G**//M06-L method for the intermediates and transition states for the products **B1-B2** in solution.

	$E_{6\text{-}311+g(d,p)}$	$\Delta E_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)}$	$\Delta G_{6\text{-}311+g(d,p)\text{-}corr}$
^{D}IN1-B2	-3239.666510	-11.6	5.3	5.8
^{D}TS1-B2	-3239.649697	-1.0	16.4	16.7
^{D}IN2-B2	-3239.656355	-5.2	12.2	13.0
^{D}TS2-B1	-3239.637224	6.8	27.9	27.8
^{D}IN3-B1	-3239.640288	4.9	27.2	26.9
B1	-1363.459540	-12.9	7.8	7.9
^{D}TS2-B2	-3239.649523	-0.9	17.8	18.6
^{D}IN3-B2	-3239.657883	-6.1	14.5	15.1
B2	-1363.469699	-19.2	2.1	2.2

Cartesian coordinates optimized by the M06-L method

1a

C	2.755465	0.724927	-0.746776
H	2.845459	1.752026	-0.338767
H	3.137406	0.765867	-1.775664
C	-0.884674	0.557757	-0.122567
C	-1.814493	1.435148	0.445270
C	-1.325092	-0.685607	-0.598736
C	-3.157243	1.092822	0.540600
H	-1.478254	2.402219	0.819927
C	-2.660521	-1.042847	-0.509428
H	-0.594570	-1.364686	-1.033095
C	-3.567146	-0.147390	0.060537
H	-3.881430	1.772484	0.981058
H	-3.009121	-2.005811	-0.873517
Cl	-5.246087	-0.593745	0.179667
C	0.519126	0.950101	-0.203606
H	0.763198	1.936799	0.241633
N	1.411909	0.220925	-0.748089
C	3.672947	-0.165266	0.066954
O	3.328983	-0.982540	0.885891
O	4.960144	0.120373	-0.231471
C	5.915667	-0.621475	0.531054
H	5.804288	-1.694214	0.345559
H	6.894020	-0.272715	0.198461
H	5.781890	-0.436465	1.601520

2a

C	0.387709	-0.158735	0.000059
C	1.254744	0.967724	-0.000041
C	2.635663	0.810277	-0.000114
C	3.169310	-0.478679	-0.000067
C	2.327744	-1.588887	0.000080
C	0.937492	-1.438278	0.000157
C	0.438556	2.167180	-0.000030
H	3.291377	1.680635	-0.000195
H	4.249231	-0.618400	-0.000130
H	2.754850	-2.590474	0.000153
H	0.314951	-2.328964	0.000321
H	0.830860	3.180863	-0.000096
C	-0.868940	1.812654	0.000096
H	-1.706992	2.501999	0.000144
C	-0.993590	0.355169	0.000096
C	-3.497930	0.319688	0.000014
H	-4.083747	0.005784	-0.876279
H	-4.083844	0.005495	0.876132
H	-3.451886	1.410908	0.000200
C	-2.160767	-0.343861	-0.000013
C	-2.207191	-1.842037	-0.000175
H	-1.705577	-2.266422	-0.879836
H	-1.706421	-2.266585	0.879892
H	-3.239592	-2.208129	-0.000682

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C	-0.964664	1.168465	-0.000008
C	-2.248361	0.728114	0.000139
C	-2.248373	-0.728144	-0.000228
H	-3.140302	-1.348551	-0.000378
C	-0.964685	-1.168484	0.000136
H	-0.638868	-2.202987	0.000824
C	-0.084340	-0.000007	0.000118
C	1.276114	-0.000029	0.000029
C	2.084791	1.254658	0.000030
H	2.748164	1.287975	0.876104
H	2.747254	1.288688	-0.876707
H	1.477221	2.162246	0.000704
C	2.084917	-1.254616	-0.000075
H	2.746719	-1.288664	-0.877332
H	2.748941	-1.287628	0.875492
H	1.477571	-2.162344	0.001044
H	-3.140272	1.348558	-0.000117
H	-0.638823	2.202967	-0.000482

L6-D

C	-3.637410	0.124951	0.415767
C	-3.917552	-0.726515	-0.691879
C	-4.774815	-0.023878	-1.590612
C	-5.028867	1.267500	-1.033925
C	-4.320649	1.360865	0.203947
H	-2.979938	-0.132124	1.239277
H	-3.493227	-1.714883	-0.846830
H	-5.135895	-0.387895	-2.546792
H	-5.615297	2.055276	-1.495660
H	-4.272554	2.232510	0.849998
Fe	-3.047688	1.000218	-1.328393
C	-2.176164	1.065262	-3.154301
C	-1.296606	0.501972	-2.168400
C	-2.528593	2.376612	-2.734200
H	-2.528950	0.547580	-4.039397
C	-1.106450	1.490157	-1.118754
C	-1.875644	2.640151	-1.495935
H	-3.218746	3.041480	-3.243384
P	-0.043453	1.279076	0.341151
C	1.463658	2.215005	-0.107419
C	1.682229	2.748664	-1.381893
C	2.486486	2.298499	0.849453
C	2.898553	3.356999	-1.690230
H	0.902579	2.685653	-2.140627
C	3.692331	2.914337	0.541834
H	2.340074	1.850003	1.833637
C	3.903021	3.443715	-0.731450
H	3.058677	3.764950	-2.687187
H	4.483046	2.959448	1.289269
H	4.856666	3.907062	-0.977840
C	-0.843376	2.329320	1.606772
C	-1.494641	1.695425	2.671660

C	-0.825510	3.728522	1.549644
C	-2.147414	2.448573	3.644187
H	-1.477352	0.604666	2.729735
C	-1.476031	4.478991	2.524003
H	-0.285966	4.229282	0.744350
C	-2.143123	3.839373	3.568364
H	-2.651089	1.947443	4.469085
H	-1.456601	5.566542	2.473673
H	-2.647866	4.428164	4.332620
C	-0.778156	-0.853101	-2.229669
N	-0.118348	-1.492963	-1.324491
O	-1.021607	-1.501629	-3.393535
C	-0.468160	-2.827837	-3.242379
H	-1.300195	-3.542463	-3.286264
H	0.193888	-3.008661	-4.094027
C	0.245148	-2.805149	-1.881091
C	0.459685	-2.807870	2.674494
H	0.855297	-3.503764	3.414921
C	3.537443	-1.475645	1.142144
C	4.873197	-1.356649	1.577532
C	3.211945	-0.893330	-0.100715
C	5.821765	-0.656137	0.847876
H	5.160236	-1.809853	2.526952
C	4.150031	-0.190881	-0.841111
H	2.195992	-0.984669	-0.486828
C	5.449827	-0.066369	-0.357941
H	6.842907	-0.559128	1.209287
H	3.873734	0.276497	-1.784277
Cl	6.627477	0.848159	-1.273724
C	2.593967	-2.175169	1.978350
H	3.014975	-2.787910	2.787818
N	1.289099	-2.096103	1.866615
C	-0.916784	-2.589604	2.543710
O	-1.454494	-1.771640	1.744836
O	-1.700039	-3.351261	3.360492
C	-3.092925	-3.111006	3.239255
H	-3.446848	-3.286149	2.215247
H	-3.573873	-3.808822	3.927926
H	-3.347241	-2.079338	3.514656
Cu	0.154194	-0.856005	0.668964
H	-1.977346	3.542259	-0.900802
H	1.338867	-2.807965	-2.020510
C	-0.098144	-3.965383	-0.940823
C	0.405609	-5.275504	-1.532254
C	-1.578867	-4.036008	-0.597670
H	0.450225	-3.763161	-0.007294
H	1.478331	-5.237003	-1.760531
H	0.242808	-6.108181	-0.838883
H	-0.124472	-5.525112	-2.463520
H	-1.922605	-3.096468	-0.151657
H	-2.199313	-4.265379	-1.476835
H	-1.760212	-4.829698	0.137764

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C	-3.637410	0.124951	0.415767
C	-3.917552	-0.726515	-0.691879
C	-4.774815	-0.023878	-1.590612
C	-5.028867	1.267500	-1.033925
C	-4.320649	1.360865	0.203947
H	-2.979938	-0.132124	1.239277
H	-3.493227	-1.714883	-0.846830
H	-5.135895	-0.387895	-2.546792
H	-5.615297	2.055276	-1.495660
H	-4.272554	2.232510	0.849998
Fe	-3.047688	1.000218	-1.328393
C	-2.176164	1.065262	-3.154301
C	-1.296606	0.501972	-2.168400
C	-2.528593	2.376612	-2.734200
H	-2.528950	0.547580	-4.039397
C	-1.106450	1.490157	-1.118754
C	-1.875644	2.640151	-1.495935
H	-3.218746	3.041480	-3.243384
P	-0.043453	1.279076	0.341151
C	1.463658	2.215005	-0.107419
C	1.682229	2.748664	-1.381893
C	2.486486	2.298499	0.849453
C	2.898553	3.356999	-1.690230
H	0.902579	2.685653	-2.140627
C	3.692331	2.914337	0.541834
H	2.340074	1.850003	1.833637
C	3.903021	3.443715	-0.731450
H	3.058677	3.764950	-2.687187
H	4.483046	2.959448	1.289269
H	4.856666	3.907062	-0.977840
C	-0.843376	2.329320	1.606772
C	-1.494641	1.695425	2.671660
C	-0.825510	3.728522	1.549644
C	-2.147414	2.448573	3.644187
H	-1.477352	0.604666	2.729735
C	-1.476031	4.478991	2.524003
H	-0.285966	4.229282	0.744350
C	-2.143123	3.839373	3.568364
H	-2.651089	1.947443	4.469085
H	-1.456601	5.566542	2.473673
H	-2.647866	4.428164	4.332620
C	-0.778156	-0.853101	-2.229669
N	-0.118348	-1.492963	-1.324491
O	-1.021607	-1.501629	-3.393535
C	-0.468160	-2.827837	-3.242379
H	-1.300195	-3.542463	-3.286264
H	0.193888	-3.008661	-4.094027
C	0.245148	-2.805149	-1.881091
C	0.459685	-2.807870	2.674494
H	0.855297	-3.503764	3.414921
C	3.537443	-1.475645	1.142144
C	4.873197	-1.356649	1.577532
C	3.211945	-0.893330	-0.100715
C	5.821765	-0.656137	0.847876
H	5.160236	-1.809853	2.526952
C	4.150031	-0.190881	-0.841111
H	2.195992	-0.984669	-0.486828
C	5.449827	-0.066369	-0.357941
H	6.842907	-0.559128	1.209287

H	3.873734	0.276497	-1.784277
Cl	6.627477	0.848159	-1.273724
C	2.593967	-2.175169	1.978350
H	3.014975	-2.787910	2.787818
N	1.289099	-2.096103	1.866615
C	-0.916784	-2.589604	2.543710
O	-1.454494	-1.771640	1.744836
O	-1.700039	-3.351261	3.360492
C	-3.092925	-3.111006	3.239255
H	-3.446848	-3.286149	2.215247
H	-3.573873	-3.808822	3.927926
H	-3.347241	-2.079338	3.514656
Cu	0.154194	-0.856005	0.668964
H	-1.977346	3.542259	-0.900802
H	1.338867	-2.807965	-2.020510
C	-0.098144	-3.965383	-0.940823
C	0.405609	-5.275504	-1.532254
C	-1.578867	-4.036008	-0.597670
H	0.450225	-3.763161	-0.007294
H	1.478331	-5.237003	-1.760531
H	0.242808	-6.108181	-0.838883
H	-0.124472	-5.525112	-2.463520
H	-1.922605	-3.096468	-0.151657
H	-2.199313	-4.265379	-1.476835
H	-1.760212	-4.829698	0.137764

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C	-2.839175	-1.007478	0.839618
C	-2.748410	-0.494564	2.166620
C	-3.046673	-1.553476	3.074618
C	-3.323947	-2.724863	2.305008
C	-3.191780	-2.387346	0.923246
H	-2.633612	-0.456434	-0.072323
H	-2.446443	0.513106	2.440624
H	-3.024066	-1.491002	4.157410
H	-3.548210	-3.709027	2.703277
H	-3.301009	-3.067548	0.084471
Fe	-1.459398	-2.043811	1.915643
C	0.075948	-2.322920	3.203151
C	0.398838	-1.338930	2.208186
C	-0.231821	-3.541117	2.539045
H	0.046316	-2.137907	4.271142
C	0.277774	-1.965392	0.900569
C	-0.108155	-3.326444	1.137249
H	-0.559868	-4.459141	3.015680
P	0.710563	-1.205316	-0.701789
C	2.185844	-2.183736	-1.168201
C	2.502365	-2.401430	-2.515155
C	3.088497	-2.605311	-0.184391
C	3.685181	-3.044385	-2.866480
H	1.815416	-2.068323	-3.293374
C	4.271446	-3.245468	-0.539073
H	2.865038	-2.426563	0.867742
C	4.572146	-3.469894	-1.880314
H	3.914392	-3.212951	-3.917560
H	4.960829	-3.572410	0.237823
H	5.496708	-3.973828	-2.156955
C	-0.583174	-1.801791	-1.852388
C	-1.490046	-0.867122	-2.364988
C	-0.711607	-3.146845	-2.224388
C	-2.534667	-1.271336	-3.192732
H	-1.374825	0.185636	-2.101719
C	-1.748358	-3.549344	-3.060235
H	0.019081	-3.877810	-1.876852
C	-2.667479	-2.614095	-3.536577
H	-3.238062	-0.530510	-3.570207
H	-1.837845	-4.596580	-3.345427
H	-3.480328	-2.933139	-4.186931
C	0.774303	0.029003	2.520314
N	0.927747	1.012942	1.703852
O	1.023583	0.269214	3.830601
C	1.420291	1.658414	3.921064
H	0.688323	2.170697	4.558421
H	2.396406	1.688644	4.414087
C	1.433883	2.159872	2.467201
C	2.572606	2.878691	-1.757700
H	2.860393	3.631875	-2.492287
C	-1.092818	2.899257	-1.977474
C	-2.045760	3.184044	-2.978868
C	-1.580832	2.396997	-0.750334
C	-3.396587	2.928601	-2.798584
H	-1.702331	3.589493	-3.930772
C	-2.933495	2.161952	-0.549661
H	-0.879653	2.204190	0.062283
C	-3.835327	2.404062	-1.583403
H	-4.112139	3.127779	-3.593052
H	-3.299222	1.798931	0.409050
Cl	-5.531909	2.048982	-1.350891
C	0.301748	3.135460	-2.229497
H	0.559225	3.808363	-3.057850
N	1.273950	2.575125	-1.539878
C	3.542121	2.161895	-1.031309
O	3.304065	1.259014	-0.191976
O	4.825669	2.527048	-1.310189
C	5.815630	1.779902	-0.620633
H	5.715579	0.707042	-0.823103
H	6.775136	2.148409	-0.990022
H	5.747173	1.932051	0.463320
Cu	1.162944	0.890688	-0.359641
H	-0.307336	-4.059003	0.361641
H	2.462957	2.338410	2.119228
C	0.614666	3.426335	2.195252
C	1.269446	4.635304	2.848666
C	-0.841567	3.283215	2.618057
H	0.645349	3.561562	1.101385
H	2.304563	4.766723	2.510065
H	0.722646	5.555919	2.615321
H	1.284614	4.538663	3.944388
H	-1.268324	2.338521	2.257651
H	-0.957127	3.308541	3.710568
H	-1.451491	4.096857	2.209514

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C	-2.900347	-1.192751	0.916214
C	-2.627808	-0.784750	2.255034
C	-2.847778	-1.901050	3.116941
C	-3.256708	-3.004231	2.307186
C	-3.288865	-2.565707	0.948810
H	-2.781204	-0.583910	0.024502
H	-2.259766	0.190199	2.563277
H	-2.684286	-1.919452	4.189350
H	-3.468160	-4.008921	2.658196
H	-3.542785	-3.175145	0.088455
Fe	-1.432647	-2.339436	1.739248
C	0.190834	-2.793689	2.848957
C	0.447582	-1.683339	1.975285
C	-0.173197	-3.910001	2.051513
H	0.238853	-2.754898	3.931202
C	0.227816	-2.122992	0.603613
C	-0.142937	-3.507238	0.687278
H	-0.464861	-4.888094	2.419632
P	0.609797	-1.149930	-0.903280
C	1.806072	-2.265629	-1.734672
C	1.429148	-3.312965	-2.581958
C	3.166159	-2.045534	-1.478576
C	2.395285	-4.136099	-3.153539
H	0.376247	-3.477213	-2.812680
C	4.127365	-2.877000	-2.046186
H	3.463504	-1.202970	-0.850730
C	3.744904	-3.923089	-2.882388
H	2.092124	-4.945168	-3.816526
H	5.182341	-2.697322	-1.843318
H	4.498848	-4.567548	-3.331719
C	-0.884829	-1.196045	-1.958979
C	-1.142626	-0.053540	-2.727340
C	-1.793587	-2.260157	-2.013137
C	-2.293312	0.033740	-3.507383
H	-0.445367	0.784641	-2.684597
C	-2.946144	-2.170994	-2.787295
H	-1.621700	-3.152608	-1.415143
C	-3.203318	-1.018751	-3.527953
H	-2.487394	0.939631	-4.079106
H	-3.650235	-3.002208	-2.806900
H	-4.113323	-0.943215	-4.120464
C	0.837957	-0.372442	2.464542
N	1.078574	0.690870	1.779869
O	1.003287	-0.290400	3.808129
C	1.484416	1.046251	4.079211
H	0.779849	1.517057	4.775601
H	2.456383	0.950906	4.573233
C	1.547514	1.730486	2.701683
C	2.867666	2.956037	-1.254686
H	3.187956	3.845947	-1.797881
C	-0.792755	3.227231	-1.483058
C	-1.681450	3.892985	-2.354062
C	-1.365092	2.407884	-0.484779
C	-3.054676	3.718773	-2.275563
H	-1.270957	4.547984	-3.123233
C	-2.738102	2.240691	-0.385283
H	-0.714032	1.899029	0.228345
C	-3.578634	2.880343	-1.293721
H	-3.720803	4.224003	-2.971194
H	-3.167662	1.622525	0.401248
Cl	-5.305051	2.619782	-1.205285
C	0.622307	3.424509	-1.644561
H	0.934378	4.274057	-2.267038
N	1.554000	2.662067	-1.112038
C	3.804624	2.062839	-0.710335
O	3.529164	1.005557	-0.085695
O	5.103614	2.429777	-0.905542
C	6.062842	1.511963	-0.407531
H	5.959834	0.529203	-0.884812
H	7.037287	1.942760	-0.647588
H	5.967116	1.379048	0.676320
Cu	1.382073	0.778934	-0.278199
H	-0.357699	-4.151095	-0.160006
H	2.587513	1.956198	2.422121
C	0.735118	3.024872	2.568803
C	1.379065	4.135346	3.387219
C	-0.730062	2.840214	2.936329
H	0.791043	3.296666	1.502105
H	2.422922	4.300676	3.092990
H	0.842890	5.082745	3.261543
H	1.367789	3.899107	4.461699
H	-1.170645	1.992239	2.398453
H	-0.866809	2.668033	4.013502
H	-1.314807	3.728955	2.673781

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C	-2.717802	-1.651817	0.477393
C	-2.583180	-1.433362	1.880158
C	-2.721065	-2.689805	2.543233
C	-2.940270	-3.689025	1.546367
C	-2.936817	-3.046647	0.271345
H	-2.616365	-0.901020	-0.301005
H	-2.359343	-0.484058	2.359349
H	-2.624894	-2.860541	3.610431
H	-3.048854	-4.753934	1.724016
H	-3.056247	-3.535489	-0.689774
Fe	-1.176441	-2.745457	1.234390
C	0.421112	-3.220670	2.377051
C	0.599425	-1.950591	1.730596
C	0.235746	-4.208263	1.375108
H	0.401807	-3.371490	3.450254
C	0.511024	-2.160319	0.292298
C	0.301764	-3.568436	0.106285
H	0.038428	-5.261077	1.547964
P	0.859359	-0.878430	-0.960052
C	2.283987	-1.625202	-1.841975
C	2.146135	-2.594894	-2.841179
C	3.565742	-1.206978	-1.462088
C	3.272393	-3.149751	-3.440654
H	1.151907	-2.905564	-3.164772
C	4.689595	-1.770295	-2.060213

H	3.671618	-0.422850	-0.709066
C	4.545609	-2.742362	-3.047002
H	3.155494	-3.900378	-4.220812
H	5.683149	-1.439525	-1.760542
H	5.425857	-3.176986	-3.518198
C	-0.506454	-0.918250	-2.176199
C	-0.801507	0.302254	-2.796647
C	-1.284734	-2.038519	-2.494027
C	-1.860241	0.408486	-3.693194
H	-0.208294	1.182745	-2.545912
C	-2.343770	-1.932885	-3.390743
H	-1.090350	-2.993139	-2.009171
C	-2.638078	-0.707867	-3.986676
H	-2.090813	1.373820	-4.140476
H	-2.947819	-2.810310	-3.618855
H	-3.478765	-0.624194	-4.673070
C	0.833265	-0.725693	2.480513
N	0.907371	0.493538	2.062964
O	1.044646	-0.942092	3.803156
C	1.395264	0.332761	4.374749
H	0.706304	0.528236	5.205868
H	2.412221	0.248416	4.772569
C	1.258920	1.337838	3.219977
C	2.354426	3.422646	-0.842714
H	2.541126	4.363900	-1.361685
C	-1.306359	3.176604	-1.093809
C	-2.287068	3.863476	-1.841588
C	-1.759375	2.148101	-0.237172
C	-3.632102	3.536765	-1.768656
H	-1.971103	4.670575	-2.503617
C	-3.104264	1.824052	-0.143325
H	-1.034795	1.595729	0.367626
C	-4.036947	2.510564	-0.918152
H	-4.368818	4.074590	-2.360879
H	-3.442909	1.048138	0.540700
Cl	-5.730204	2.090876	-0.806933
C	0.069496	3.567478	-1.237345
H	0.257946	4.486954	-1.808709
N	1.100464	2.929826	-0.722982
C	3.405270	2.703532	-0.250651
O	3.285477	1.623097	0.385039
O	4.630829	3.279488	-0.408620
C	5.712969	2.543014	0.135932
H	5.773578	1.539460	-0.303579
H	6.611467	3.113259	-0.109312
H	5.620920	2.437051	1.223206
Cu	1.241164	1.008738	0.062240
H	0.210089	-4.068470	-0.852879
H	2.224029	1.809625	2.987399
C	0.233635	2.443306	3.515965
C	-1.184126	1.895031	3.613247
C	0.309351	3.582612	2.512721
H	0.521865	2.837028	4.506334
H	-1.256987	1.018994	4.273670
H	-1.875777	2.654421	3.994499
H	-1.543232	1.598830	2.619132
H	1.328865	3.976676	2.415466
H	-0.003928	3.252694	1.516331
H	-0.348853	4.409084	2.806989

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C	2.418872	-1.731631	-1.401194
C	1.543953	-1.953164	-2.504977
C	1.556685	-3.348499	-2.806816
C	2.442053	-3.989530	-1.886549
C	2.976186	-2.989004	-1.020205
H	2.581523	-0.786078	-0.894370
H	0.925226	-1.197622	-2.982199
H	0.962481	-3.842060	-3.569012
H	2.643832	-5.054232	-1.832693
H	3.665489	-3.157483	-0.198814
Fe	0.949058	-3.037497	-0.901593
C	-0.866476	-3.924970	-0.808396
C	-0.955952	-2.507876	-0.595554
C	-0.013738	-4.470883	0.186180
H	-1.341321	-4.459102	-1.623086
C	-0.136989	-2.172233	0.561082
C	0.421819	-3.409600	1.028112
H	0.285438	-5.510682	0.266703
P	-0.133146	-0.522039	1.339239
C	-0.968101	-0.874018	2.933769
C	-0.293363	-1.391933	4.044809
C	-2.342129	-0.616631	3.019427
C	-0.984497	-1.655978	5.222859
H	0.781030	-1.573231	3.990502
C	-3.030111	-0.889650	4.198537
H	-2.859703	-0.181796	2.161090
C	-2.354093	-1.408436	5.299935
H	-0.451804	-2.052957	6.085860
H	-4.097884	-0.683584	4.260222
H	-2.892148	-1.612667	6.224375
C	1.575669	-0.118929	1.844113
C	1.784332	1.204966	2.259836
C	2.667463	-0.990873	1.806236
C	3.051488	1.641253	2.626471
H	0.945556	1.904029	2.262311
C	3.941469	-0.546493	2.155272
H	2.530515	-2.016712	1.471469
C	4.136585	0.768930	2.565426
H	3.196982	2.676547	2.930045
H	4.785250	-1.233651	2.102854
H	5.134188	1.117702	2.826391
C	-1.694940	-1.634346	-1.495978
N	-1.661995	-0.347973	-1.601265
O	-2.523037	-2.305071	-2.335856
C	-3.096794	-1.313635	-3.208983
H	-2.686273	-1.481191	-4.215930
H	-4.177807	-1.477692	-3.235427
C	-2.659948	0.033083	-2.617668
C	-2.352774	3.405609	0.439904
H	-2.515798	4.464616	0.644223
C	1.256580	3.391093	-0.281265
C	2.294431	4.297444	0.026034

C	1.625363	2.189634	-0.926198
C	3.624505	4.013382	-0.239260
H	2.038538	5.240986	0.509457
C	2.951845	1.904590	-1.216511
H	0.852708	1.468806	-1.205763
C	3.948698	2.807625	-0.855780
H	4.409494	4.717738	0.026285
H	3.224752	0.992131	-1.741567
Cl	5.623221	2.424438	-1.186740
C	-0.088124	3.754538	0.076439
H	-0.243732	4.803276	0.365558
N	-1.121141	2.942247	0.113469
C	-3.402576	2.481895	0.543719
O	-3.308898	1.240046	0.352897
O	-4.601721	3.039113	0.881765
C	-5.662592	2.115913	1.056694
H	-5.435621	1.391864	1.849484
H	-6.532512	2.714062	1.336294
H	-5.870428	1.560394	0.134279
Cu	-1.182589	0.879579	0.045107
H	1.077961	-3.514565	1.886732
H	-3.483004	0.526733	-2.074881
C	-2.138760	0.999337	-3.683300
C	-1.606289	2.287998	-3.081484
C	-3.254493	1.289511	-4.682417
H	-1.317558	0.485793	-4.215016
H	-0.716592	2.117886	-2.467667
H	-1.336727	3.004097	-3.867635
H	-2.356195	2.763861	-2.434009
H	-3.641328	0.380548	-5.161827
H	-4.098684	1.787449	-4.185877
H	-2.904143	1.955516	-5.478824

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C	2.426714	-2.773603	-0.132011
C	2.885866	-3.180444	1.157228
C	4.276392	-3.473339	1.060264
C	4.679664	-3.252026	-0.290661
C	3.537403	-2.820737	-1.029626
H	1.420731	-2.444191	-0.381200
H	2.296979	-3.209521	2.068814
H	4.923169	-3.765026	1.881060
H	5.688948	-3.348284	-0.677270
H	3.521397	-2.525903	-2.074679
Fe	3.913838	-1.549972	0.505589
C	4.653170	-0.358004	1.969772
C	3.335117	0.054001	1.573867
C	5.496111	-0.306294	0.826729
H	4.929547	-0.683709	2.966397
C	3.369930	0.356508	0.152965
C	4.717107	0.128867	-0.282471
H	6.538831	-0.604311	0.795068
P	1.978475	0.978341	-0.833523
C	2.516963	2.661915	-1.294830
C	1.822332	3.322754	-2.318885
C	3.505883	3.355905	-0.589466
C	2.132096	4.637382	-2.647076
H	1.035682	2.798120	-2.863666
C	3.807276	4.676533	-0.915225
H	4.046405	2.863054	0.218142
C	3.127014	5.318611	-1.945879
H	1.591597	5.134454	-3.450808
H	4.583605	5.202819	-0.362109
H	3.367938	6.348815	-2.201713
C	2.087169	0.046951	-2.402945
C	3.114383	0.216535	-3.340791
C	1.092750	-0.905117	-2.650756
C	3.161945	-0.583995	-4.478572
H	3.869259	0.988707	-3.186584
C	1.142902	-1.710443	-3.784784
H	0.271947	-1.016739	-1.941560
C	2.183593	-1.555500	-4.696650
H	3.963467	-0.447105	-5.202824
H	0.362814	-2.451646	-3.952582
H	2.226947	-2.179332	-5.587634
C	2.193580	0.085098	2.471575
N	0.964419	0.369789	2.194877
O	2.475312	-0.215354	3.760387
C	1.253511	-0.003916	4.505803
H	1.076898	-0.898779	5.113139
H	1.420452	0.848294	5.173223
C	0.182942	0.251951	3.434324
C	-2.268935	2.310528	-0.266951
H	-2.899369	2.621179	-1.108385
C	-2.271463	-1.270112	-0.983527
C	-3.186279	-2.040302	-1.723848
C	-1.311020	-1.949602	-0.212644
C	-3.136555	-3.426922	-1.718367
H	-3.965654	-1.532114	-2.291599
C	-1.241527	-3.334757	-0.205668
H	-0.606948	-1.368970	0.390558
C	-2.156997	-4.065751	-0.963750
H	-3.857115	-4.011269	-2.285145
H	-0.493430	-3.855743	0.389928
Cl	-2.081114	-5.810224	-0.949212
C	-2.438955	0.159669	-0.995605
H	-3.270822	0.523454	-1.606700
N	-1.709541	1.034561	-0.346640
C	-1.327224	3.313597	0.203754
O	-0.294855	3.071573	0.843609
O	-1.707619	4.581807	-0.063125
C	-0.846924	5.588720	0.469084
H	0.178862	5.452495	0.110836
H	-1.256087	6.537583	0.119436
H	-0.843811	5.554795	1.564235
Cu	0.153940	0.918957	0.409077
H	5.065864	0.232559	-1.305598
H	-0.321990	1.214535	3.603812
C	-0.890519	-0.836013	3.304043
C	-1.820159	-0.819739	4.508286
C	-0.295617	-2.215503	3.067543
H	-1.477060	-0.566852	2.407789
H	-2.289678	0.163277	4.643563

H	-2.622558	-1.557292	4.393746
H	-1.283854	-1.066122	5.436552
H	0.379523	-2.210129	2.202225
H	0.271745	-2.577119	3.937923
H	-1.085621	-2.947534	2.865191
C	-5.355437	0.552764	-0.244152
C	-5.742262	-0.815113	-0.030577
C	-6.616368	-1.452496	-0.918719
C	-7.086709	-0.768010	-2.032052
C	-6.682083	0.553793	-2.270522
C	-5.826719	1.210343	-1.390691
C	-5.049903	-1.295573	1.128186
H	-6.907501	-2.490078	-0.744719
H	-7.764848	-1.259611	-2.728959
H	-7.043331	1.077059	-3.155449
H	-5.521452	2.230818	-1.623606
H	-5.153042	-2.289496	1.556817
C	-4.253475	-0.278523	1.599292
H	-3.636394	-0.330610	2.493359
C	-4.416802	0.909714	0.804466
C	-3.771669	2.159282	1.068924
C	-4.548223	3.429362	0.801072
H	-3.902971	4.314230	0.824504
H	-5.071907	3.418473	-0.157614
H	-5.313863	3.556407	1.579443
C	-3.009765	2.229031	2.376888
H	-2.548777	3.214846	2.521277
H	-3.677746	2.047330	3.230650
H	-2.207219	1.479839	2.410818

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C	2.309785	-2.793922	-0.118792
C	2.816224	-3.221130	1.146288
C	4.182083	-3.589914	0.975175
C	4.521471	-3.397541	-0.397122
C	3.366135	-2.906015	-1.074796
H	1.312584	-2.404859	-0.313416
H	2.278625	-3.211129	2.089829
H	4.856470	-3.914149	1.760851
H	5.501235	-3.549344	-0.837583
H	3.311349	-2.618815	-2.120483
Fe	3.890986	-1.651455	0.427872
C	4.741659	-0.484875	1.850669
C	3.430371	-0.015313	1.498254
C	5.543379	-0.482483	0.677079
H	5.040535	-0.814419	2.839498
C	3.427259	0.273794	0.073890
C	4.745449	-0.020849	-0.407487
H	6.569281	-0.829775	0.610603
P	2.017664	0.940196	-0.854970
C	2.586502	2.608411	-1.330890
C	1.891660	3.283665	-2.346330
C	3.591496	3.287359	-0.632315
C	2.215215	4.595626	-2.671381
H	1.093384	2.770909	-2.885303
C	3.907003	4.605159	-0.955365
H	4.133843	2.782854	0.167166
C	3.225129	5.261440	-1.976495
H	1.675031	5.102458	-3.469405
H	4.696436	5.118362	-0.408412
H	3.477724	6.289304	-2.230596
C	2.032356	0.013610	-2.429778
C	3.037312	0.156482	-3.395254
C	0.997073	-0.901284	-2.653783
C	3.027170	-0.634160	-4.540207
H	3.821977	0.901017	-3.255010
C	0.990598	-1.697493	-3.796500
H	0.191120	-0.985344	-1.921587
C	2.010840	-1.570175	-4.736316
H	3.812386	-0.518248	-5.285687
H	0.182667	-2.411453	-3.949989
H	2.008020	-2.189086	-5.631840
C	2.322847	0.078158	2.434546
N	1.092303	0.386158	2.192241
O	2.646509	-0.183091	3.723404
C	1.457490	0.074650	4.504606
H	1.272923	-0.807341	5.128600
H	1.672039	0.928397	5.156021
C	0.359494	0.349035	3.465222
C	-2.264041	2.357627	-0.157635
H	-2.689968	2.710801	-1.120718
C	-2.429071	-1.200606	-0.795337
C	-3.306641	-1.949064	-1.591934
C	-1.480580	-1.891789	-0.030677
C	-3.243990	-3.336878	-1.629477
H	-4.062898	-1.428478	-2.180401
C	-1.390552	-3.278205	-0.067713
H	-0.791366	-1.320048	0.595928
C	-2.280507	-3.990820	-0.868178
H	-3.934967	-3.909878	-2.242759
H	-0.644178	-3.809180	0.521393
Cl	-2.187319	-5.736764	-0.910395
C	-2.583109	0.255171	-0.755127
H	-3.160465	0.630917	-1.617196
N	-1.630763	1.082687	-0.273209
C	-1.283356	3.383228	0.329626
O	-0.237643	3.129413	0.913964
O	-1.672798	4.642013	0.074039
C	-0.773832	5.653932	0.541841
H	0.224026	5.504521	0.116960
H	-1.201313	6.600534	0.210138
H	-0.701893	5.625181	1.633911
Cu	0.211157	0.892651	0.400698
H	5.058835	0.054268	-1.444260
H	-0.090996	1.341202	3.619828
C	-0.772574	-0.684877	3.418755
C	-1.647613	-0.581579	4.658838
C	-0.263015	-2.100421	3.198166
H	-1.376959	-0.410140	2.537638
H	-2.054057	0.430322	4.784067
H	-2.494577	-1.274917	4.601265
H	-1.086583	-0.832713	5.570993
H	0.376477	-2.152337	2.307632

H	0.316367	-2.472144	4.056081
H	-1.098978	-2.792527	3.044059
C	-5.263487	0.516268	-0.368927
C	-5.876530	-0.697568	0.067231
C	-6.906683	-1.280564	-0.673723
C	-7.330180	-0.672109	-1.850725
C	-6.717637	0.503914	-2.299008
C	-5.683661	1.092618	-1.571535
C	-5.195260	-1.136330	1.257179
H	-7.362858	-2.213234	-0.339341
H	-8.135001	-1.117854	-2.434103
H	-7.050967	0.964922	-3.228168
H	-5.201682	1.991275	-1.960286
H	-5.435572	-2.033354	1.822320
C	-4.193301	-0.249727	1.525698
H	-3.510785	-0.320318	2.369641
C	-4.118906	0.790724	0.505062
C	-3.538879	2.168403	0.821204
C	-4.541067	3.300414	0.610702
H	-4.089178	4.270926	0.851104
H	-4.902126	3.351156	-0.421271
H	-5.417564	3.165635	1.255682
C	-3.022054	2.239141	2.260808
H	-2.670307	3.254424	2.496814
H	-3.807153	1.982666	2.981671
H	-2.176826	1.554617	2.411823

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C	-2.194358	2.798703	0.129610
C	-2.756930	3.176880	1.387614
C	-4.101008	3.594463	1.162790
C	-4.369389	3.481324	-0.233953
C	-3.192479	2.992020	-0.873222
H	-1.199897	2.389044	-0.034444
H	-2.274058	3.098336	2.357101
H	-4.809377	3.897266	1.926926
H	-5.319608	3.683156	-0.717377
H	-3.088708	2.753788	-1.927729
Fe	-3.831956	1.677242	0.537618
C	-4.718372	0.466038	1.896502
C	-3.426471	-0.030115	1.511443
C	-5.524479	0.557417	0.728944
H	-4.999663	0.754959	2.903031
C	-3.438829	-0.240896	0.073111
C	-4.747277	0.128076	-0.383456
H	-6.537510	0.944147	0.687339
P	-2.080903	-0.939612	-0.912703
C	-2.829742	-2.467558	-1.576581
C	-2.267365	-3.053346	-2.720246
C	-3.866082	-3.136684	-0.913918
C	-2.747487	-4.266177	-3.200890
H	-1.453124	-2.546340	-3.239370
C	-4.340809	-4.353929	-1.395716
H	-4.308929	-2.700642	-0.018413
C	-3.786860	-4.920258	-2.540594
H	-2.308571	-4.702924	-4.096648
H	-5.152269	-4.859001	-0.874102
H	-4.162572	-5.869572	-2.918047
C	-1.963923	0.156022	-2.371738
C	-0.825299	0.964136	-2.449952
C	-2.945828	0.265404	-3.365397
C	-0.682326	1.902191	-3.467944
H	-0.045328	0.850180	-1.696887
C	-2.800813	1.197572	-4.389221
H	-3.817787	-0.389797	-3.344426
C	-1.676249	2.024302	-4.435625
H	0.208674	2.527625	-3.501920
H	-3.568119	1.280449	-5.157515
H	-1.572543	2.754177	-5.236689
C	-2.315695	-0.201139	2.431942
N	-1.098009	-0.533078	2.160835
O	-2.618883	0.008860	3.735606
C	-1.432271	-0.329079	4.489229
H	-1.217311	0.508387	5.162730
H	-1.665595	-1.214129	5.090747
C	-0.349997	-0.569921	3.425179
C	2.284079	-2.416943	-0.161704
H	2.683924	-2.753875	-1.142308
C	2.407376	1.147922	-0.761794
C	3.249368	1.900703	-1.592054
C	1.517509	1.836161	0.072765
C	3.207547	3.290080	-1.596533
H	3.965630	1.382289	-2.230596
C	1.449846	3.223895	0.072045
H	0.853236	1.259294	0.719523
C	2.302789	3.941389	-0.764774
H	3.872311	3.865682	-2.235906
H	0.750128	3.752194	0.717951
Cl	2.235136	5.688423	-0.765507
C	2.552084	-0.307362	-0.751448
H	3.112891	-0.672667	-1.629015
N	1.628624	-1.149692	-0.240645
C	1.337470	-3.464416	0.344806
O	0.268325	-3.235905	0.897491
O	1.790550	-4.712108	0.150226
C	0.939704	-5.749817	0.649023
H	-0.047458	-5.692359	0.180329
H	1.437986	-6.684908	0.391191
H	0.823985	-5.661132	1.733917
Cu	-0.265395	-1.043953	0.334824
H	-5.069492	0.112214	-1.420008
H	0.089645	-1.573903	3.524101
C	0.793862	0.452304	3.420085
C	1.680240	0.274263	4.643910
C	0.297510	1.883374	3.285508
H	1.385773	0.217310	2.519533
H	2.078046	-0.746608	4.710889
H	2.533686	0.961737	4.615889
H	1.130344	0.480954	5.573822
H	-0.371173	1.987807	2.421305
H	-0.248860	2.218564	4.179375
H	1.137991	2.571956	3.139000
C	5.251800	-0.526421	-0.437722

C	5.847874	0.697820	-0.006339
C	6.840457	1.314454	-0.771107
C	7.242364	0.730511	-1.967732
C	6.645339	-0.455495	-2.411220
C	5.649472	-1.078371	-1.659636
C	5.192507	1.106761	1.208487
H	7.283452	2.254364	-0.439289
H	8.017632	1.202636	-2.570102
H	6.961218	-0.897613	-3.355540
H	5.180149	-1.985209	-2.044414
H	5.427047	2.004492	1.774927
C	4.222118	0.191474	1.497955
H	3.562868	0.236055	2.362417
C	4.144011	-0.838482	0.468681
C	4.603393	-3.338736	0.510497
H	5.505199	-3.188735	1.115990
H	4.183037	-4.319426	0.763242
H	4.918311	-3.375289	-0.536936
C	3.590082	-2.227416	0.775489
C	3.124740	-2.333570	2.230359
H	3.931839	-2.083513	2.928884
H	2.280266	-1.660910	2.426050
H	2.792785	-3.357730	2.457024

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C	-4.017152	-1.573672	0.363211
C	-4.893406	-1.220110	-0.707112
C	-6.056963	-0.611063	-0.152524
C	-5.905466	-0.588286	1.266401
C	-4.647802	-1.182220	1.585213
H	-3.031724	-2.021021	0.249094
H	-4.682474	-1.334306	-1.766300
H	-6.884900	-0.188909	-0.712775
H	-6.602746	-0.152035	1.974125
H	-4.219865	-1.273489	2.578971
Fe	-4.393682	0.425681	0.370360
C	-4.480138	2.149641	-0.682677
C	-3.176826	1.551474	-0.762273
C	-4.768197	2.398909	0.687905
H	-5.136640	2.328021	-1.527297
C	-2.655730	1.432578	0.586786
C	-3.656796	1.962788	1.464672
H	-5.699176	2.798856	1.076106
P	-0.989954	0.864479	1.036573
C	-0.092435	2.438962	1.301019
C	1.282907	2.349469	1.556393
C	-0.682162	3.703759	1.194388
C	2.048229	3.497466	1.716345
H	1.762389	1.369615	1.581586
C	0.091827	4.853838	1.345054
H	-1.747704	3.795303	0.986083
C	1.455015	4.754086	1.607991
H	3.121248	3.412798	1.884347
H	-0.375915	5.832621	1.250337
H	2.060854	5.653148	1.706751
C	-1.238250	0.208019	2.725406
C	-1.463072	-1.167622	2.864409
C	-1.204922	1.014639	3.868745
C	-1.661605	-1.723791	4.124668
H	-1.463279	-1.801306	1.974042
C	-1.402389	0.455102	5.128484
H	-1.013712	2.083896	3.769886
C	-1.632337	-0.913143	5.258161
H	-1.825013	-2.796625	4.221605
H	-1.371222	1.089330	6.012815
H	-1.777163	-1.350058	6.244694
C	-2.561960	1.076234	-1.989200
N	-1.454913	0.426335	-2.116708
O	-3.248023	1.361014	-3.121084
C	-2.444668	0.867942	-4.217111
H	-3.078166	0.206927	-4.820469
H	-2.156864	1.730192	-4.827863
C	-1.257657	0.153438	-3.547255
C	1.206611	-2.718534	-1.298978
H	1.995569	-3.397060	-1.623199
C	2.896975	0.537968	-1.590543
C	4.250093	0.928782	-1.571082
C	1.924994	1.556829	-1.643154
C	4.620146	2.265275	-1.539688
H	5.023195	0.160607	-1.547584
C	2.281337	2.896556	-1.627284
H	0.868216	1.291803	-1.693481
C	3.628288	3.243637	-1.559718
H	5.669143	2.549774	-1.495924
H	1.519264	3.673168	-1.647112
Cl	4.076371	4.934443	-1.489257
C	2.584116	-0.869252	-1.561305
H	3.413626	-1.560550	-1.767849
N	1.408249	-1.371413	-1.274976
C	-0.032812	-3.196105	-0.864634
O	-0.987066	-2.478094	-0.454462
O	-0.162888	-4.557886	-0.878153
C	-1.408378	-5.040135	-0.398268
H	-2.244557	-4.673309	-1.006439
H	-1.348519	-6.128514	-0.462610
H	-1.583282	-4.734222	0.641810
Cu	-0.292688	-0.442074	-0.553674
H	-3.579287	1.986024	2.547842
H	-0.304525	0.614919	-3.849273
C	-1.155836	-1.349938	-3.837401
C	-0.839656	-1.577752	-5.309602
C	-2.393351	-2.118453	-3.398924
H	-0.307602	-1.713949	-3.237497
H	0.059737	-1.032221	-5.622136
H	-0.670503	-2.640956	-5.513825
H	-1.667678	-1.254910	-5.957852
H	-2.564251	-2.002391	-2.322954
H	-3.294894	-1.798345	-3.943456
H	-2.265870	-3.190382	-3.595038
C	4.858110	-1.899822	0.946184
C	5.247708	-0.571038	1.279022
C	6.510772	-0.088600	0.947628
C	7.401148	-0.923936	0.275608

C	7.032581	-2.231371	-0.045090
C	5.771876	-2.727123	0.294883
C	4.140806	0.068647	1.958708
H	6.793975	0.932679	1.204399
H	8.391310	-0.559046	0.006120
H	7.739715	-2.880978	-0.558708
H	5.536243	-3.760792	0.054543
H	4.153394	1.090449	2.331773
C	3.112768	-0.814290	2.050252
H	2.147700	-0.629023	2.517262
C	3.480863	-2.083645	1.432580
C	2.648459	-3.162648	1.374344
C	3.017953	-4.470806	0.753606
H	2.122678	-5.006383	0.416769
H	3.677875	-4.354740	-0.111189
H	3.539086	-5.123355	1.471934
C	1.289526	-3.074999	2.005783
H	0.697036	-3.977362	1.815195
H	1.347005	-2.934626	3.094472
H	0.724588	-2.220395	1.605472

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C	3.921205	-1.691811	-0.344084
C	4.635085	-1.661575	0.891966
C	5.925309	-1.105850	0.649312
C	6.012736	-0.789678	-0.739483
C	4.776131	-1.150004	-1.354272
H	2.890790	-2.018479	-0.471182
H	4.242213	-1.955775	1.861157
H	6.686899	-0.913819	1.397792
H	6.854193	-0.314267	-1.232484
H	4.507728	-0.987108	-2.393366
Fe	4.464875	0.207372	0.116094
C	4.480021	1.702424	1.481451
C	3.152971	1.199436	1.253086
C	4.993772	2.172699	0.243251
H	5.001029	1.674271	2.431941
C	2.843738	1.372308	-0.157830
C	4.000251	1.973114	-0.757049
H	5.990178	2.569759	0.079787
P	1.298153	0.867300	-0.970990
C	0.397329	2.428568	-1.267790
C	-0.968126	2.305196	-1.559690
C	0.963292	3.703690	-1.172804
C	-1.749539	3.432815	-1.775793
H	-1.430902	1.315101	-1.572661
C	0.172912	4.834583	-1.372336
H	2.019919	3.815885	-0.927150
C	-1.179452	4.701345	-1.677536
H	-2.811803	3.315156	-1.985588
H	0.616729	5.824847	-1.282691
H	-1.795008	5.588348	-1.818299
C	1.837884	0.344382	-2.639230
C	1.769422	-1.017945	-2.951592
C	2.290882	1.246622	-3.609030
C	2.173255	-1.474935	-4.203449
H	1.383162	-1.714892	-2.205206
C	2.701799	0.788066	-4.856955
H	2.302669	2.315667	-3.390445
C	2.647053	-0.573470	-5.153965
H	2.109695	-2.536217	-4.438825
H	3.054615	1.495870	-5.605215
H	2.960654	-0.928813	-6.134102
C	2.368719	0.518390	2.268999
N	1.282466	-0.160546	2.114809
O	2.864097	0.611353	3.525695
C	2.003895	-0.195526	4.361206
H	2.598112	-1.044521	4.725263
H	1.705018	0.415935	5.216829
C	0.845252	-0.613811	3.441614
C	-1.891336	-2.444811	0.236076
H	-2.731078	-2.962429	0.713482
C	-2.753832	0.991336	1.237819
C	-3.994338	1.649856	1.149010
C	-1.619377	1.751207	1.573167
C	-4.094254	3.020333	1.347124
H	-4.883961	1.073067	0.895043
C	-1.709295	3.117326	1.789408
H	-0.648828	1.261156	1.659120
C	-2.948264	3.743984	1.663836
H	-5.051951	3.526712	1.256887
H	-0.826831	3.702849	2.037770
Cl	-3.058864	5.469983	1.911062
C	-2.729558	-0.426000	0.948540
H	-3.696161	-0.937022	1.001813
N	-1.668317	-1.118245	0.625987
C	-0.658667	-3.203383	0.161327
O	0.468457	-2.706079	-0.019405
O	-0.827006	-4.539796	0.238280
C	0.340182	-5.316671	-0.025182
H	1.160829	-5.036374	0.643053
H	0.045741	-6.353858	0.140373
H	0.668627	-5.177208	-1.062036
Cu	0.252925	-0.532631	0.310710
H	4.108528	2.189533	-1.815678
H	-0.070613	-0.053423	3.695108
C	0.489688	-2.104055	3.465902
C	-0.022820	-2.493130	4.846322
C	1.636300	-2.996695	3.015132
H	-0.332218	-2.221027	2.740905
H	-0.864972	-1.863950	5.160594
H	-0.362647	-3.534601	4.862114
H	0.764812	-2.401048	5.608390
H	1.966339	-2.736996	2.002502
H	2.499604	-2.937988	3.694246
H	1.316996	-4.046052	3.002613
C	-5.058034	-1.566452	-0.918230
C	-5.777450	-0.348313	-1.174695
C	-7.056571	-0.158216	-0.640407
C	-7.622076	-1.144703	0.159417
C	-6.913967	-2.320894	0.440184
C	-5.644186	-2.533576	-0.089568
C	-4.930080	0.511667	-1.945300

H	-7.601431	0.765574	-0.843140
H	-8.617090	-1.000355	0.578890
H	-7.361550	-3.080046	1.080734
H	-5.119049	-3.455215	0.163485
H	-5.210057	1.488274	-2.332899
C	-3.727325	-0.132507	-2.133278
H	-2.897544	0.249226	-2.724966
C	-3.754863	-1.441135	-1.540668
C	-2.694555	-2.398082	-1.602767
C	-3.074110	-3.850899	-1.800073
H	-2.198193	-4.507733	-1.764146
H	-3.793109	-4.217187	-1.063125
H	-3.539012	-3.970734	-2.787988
C	-1.513955	-2.003616	-2.463199
H	-0.732130	-2.774311	-2.442592
H	-1.816200	-1.870663	-3.511259
H	-1.057650	-1.061603	-2.126596

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C	-3.943676	-1.709993	0.345567
C	-4.629204	-1.735289	-0.906707
C	-5.925536	-1.174686	-0.716911
C	-6.045785	-0.801242	0.655070
C	-4.823560	-1.131528	1.313412
H	-2.914661	-2.024644	0.509035
H	-4.213210	-2.068734	-1.853195
H	-6.670202	-1.015589	-1.489624
H	-6.900495	-0.310660	1.108897
H	-4.581444	-0.925614	2.351103
Fe	-4.479599	0.164688	-0.206760
C	-4.452195	1.592301	-1.641453
C	-3.132740	1.104502	-1.345312
C	-5.007188	2.120877	-0.445379
H	-4.940187	1.517904	-2.606754
C	-2.870550	1.347070	0.065609
C	-4.047157	1.973622	0.595676
H	-6.008685	2.523027	-0.334214
P	-1.353100	0.881063	0.951738
C	-0.447785	2.448814	1.196315
C	0.919051	2.333115	1.486454
C	-1.014531	3.721029	1.069323
C	1.701671	3.466432	1.667483
H	1.384453	1.344996	1.527826
C	-0.223917	4.856772	1.236866
H	-2.071777	3.826224	0.822657
C	1.130082	4.731375	1.539590
H	2.765257	3.353760	1.874001
H	-0.668334	5.844321	1.123977
H	1.745626	5.622075	1.654454
C	-1.942912	0.438165	2.624629
C	-1.884479	-0.907816	3.003172
C	-2.420754	1.385288	3.537751
C	-2.325124	-1.306122	4.262426
H	-1.476618	-1.638591	2.302168
C	-2.865128	0.985927	4.794566
H	-2.423936	2.442738	3.269349
C	-2.822111	-0.360320	5.156186
H	-2.270890	-2.355024	4.548955
H	-3.235077	1.728050	5.499956
H	-3.161575	-0.668892	6.143461
C	-2.319664	0.370924	-2.300254
N	-1.252725	-0.319686	-2.074757
O	-2.759499	0.421674	-3.579878
C	-1.888241	-0.446675	-4.340379
H	-2.482392	-1.313929	-4.659526
H	-1.565557	0.104252	-5.227407
C	-0.757245	-0.809943	-3.367749
C	2.009408	-2.381868	0.060316
H	2.816497	-2.882445	-0.498820
C	2.713928	0.997052	-1.231256
C	3.946013	1.672566	-1.152715
C	1.571705	1.726726	-1.604254
C	4.029357	3.036126	-1.400143
H	4.837408	1.116837	-0.860414
C	1.647394	3.083619	-1.875991
H	0.607536	1.221803	-1.674498
C	2.877548	3.730054	-1.759646
H	4.978178	3.559716	-1.314818
H	0.760950	3.648743	-2.155169
Cl	2.968031	5.446706	-2.069729
C	2.713053	-0.402711	-0.864682
H	3.689421	-0.893204	-0.905675
N	1.670216	-1.099170	-0.492466
C	0.782190	-3.228077	0.060571
O	-0.364997	-2.795607	0.199476
O	1.038869	-4.537501	-0.065548
C	-0.085759	-5.403887	0.111826
H	-0.899679	-5.133043	-0.567308
H	0.281948	-6.407844	-0.101404
H	-0.448128	-5.342255	1.143932
Cu	-0.246878	-0.551465	-0.243728
H	-4.191303	2.239710	1.638814
H	0.154357	-0.235855	-3.607423
C	-0.367184	-2.290264	-3.329964
C	0.191979	-2.713910	-4.681903
C	-1.504859	-3.195129	-2.880787
H	0.437503	-2.360138	-2.579676
H	1.028065	-2.076277	-4.994992
H	0.555289	-3.747198	-4.654025
H	-0.577246	-2.664912	-5.466384
H	-1.878023	-2.907094	-1.890892
H	-2.346808	-3.184417	-3.588409
H	-1.159799	-4.234628	-2.819898
C	5.049104	-1.454752	0.936137
C	5.823589	-0.259300	1.176797
C	7.106406	-0.134521	0.627486
C	7.622421	-1.152405	-0.164559
C	6.864726	-2.305329	-0.424573
C	5.593005	-2.460100	0.117943
C	5.023124	0.632977	1.948067
H	7.694858	0.765408	0.816942
H	8.619658	-1.055107	-0.592782
H	7.279262	-3.091763	-1.054929

H	5.031930	-3.370323	-0.104808
H	5.338272	1.601911	2.327736
C	3.795714	0.022151	2.160493
H	2.983042	0.444640	2.749829
C	3.767746	-1.270781	1.561408
C	2.632991	-2.223417	1.596504
C	3.066264	-3.622601	2.048251
H	2.209758	-4.300649	2.158910
H	3.773936	-4.088910	1.355704
H	3.562521	-3.548734	3.022130
C	1.517283	-1.741430	2.520199
H	0.711691	-2.484094	2.595779
H	1.909245	-1.570564	3.529817
H	1.070138	-0.801193	2.170113

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C	4.097898	-1.589058	-0.205819
C	4.782486	-1.577888	1.047714
C	6.048887	-0.952664	0.858254
C	6.152397	-0.576355	-0.514293
C	4.949435	-0.969701	-1.173313
H	3.088309	-1.957657	-0.374235
H	4.384338	-1.929573	1.994562
H	6.784222	-0.756558	1.631597
H	6.980465	-0.041436	-0.967619
H	4.697924	-0.778085	-2.211630
Fe	4.541726	0.312483	0.343416
C	4.443209	1.742018	1.773833
C	3.141001	1.226049	1.455625
C	5.008585	2.281034	0.586489
H	4.911559	1.685128	2.750013
C	2.907246	1.444866	0.038540
C	4.074367	2.104316	-0.472646
H	6.002765	2.705546	0.492939
P	1.405604	0.985907	-0.879972
C	0.646351	2.609169	-1.239503
C	-0.354919	2.675305	-2.219406
C	0.931078	3.751076	-0.482631
C	-1.046690	3.858807	-2.443782
H	-0.593412	1.787200	-2.807122
C	0.235049	4.936942	-0.710409
H	1.700773	3.715075	0.288174
C	-0.754017	4.993952	-1.688061
H	-1.824159	3.893084	-3.204929
H	0.468051	5.819649	-0.117114
H	-1.302602	5.918556	-1.857346
C	2.035184	0.447966	-2.511495
C	1.972878	-0.915261	-2.821475
C	2.570327	1.336903	-3.452709
C	2.461991	-1.386733	-4.036918
H	1.531515	-1.603261	-2.099728
C	3.061761	0.864123	-4.665958
H	2.584489	2.406471	-3.240031
C	3.012694	-0.498779	-4.958081
H	2.404266	-2.449822	-4.267362
H	3.475884	1.562711	-5.391033
H	3.391468	-0.865015	-5.910655
C	2.280432	0.550965	2.411294
N	1.132249	0.007900	2.193987
O	2.758030	0.505937	3.678486
C	1.718838	-0.103903	4.478221
H	2.176303	-0.923919	5.044291
H	1.359452	0.652945	5.183847
C	0.657648	-0.561251	3.462052
C	-1.669322	-2.575419	-0.026751
H	-2.315078	-3.273382	0.546492
C	-3.127100	0.546537	1.088320
C	-4.441150	0.848687	1.474673
C	-2.228142	1.608519	0.926624
C	-4.851867	2.160911	1.677656
H	-5.161379	0.037990	1.589372
C	-2.612404	2.923827	1.144233
H	-1.204950	1.399526	0.606498
C	-3.929483	3.188378	1.510283
H	-5.878323	2.387010	1.955879
H	-1.905545	3.740325	1.014236
Cl	-4.431151	4.848374	1.749580
C	-2.795760	-0.842371	0.765782
H	-3.517694	-1.558008	1.192284
N	-1.533490	-1.303394	0.609613
C	-0.325481	-3.210387	-0.206037
O	0.744374	-2.611605	-0.149991
O	-0.388988	-4.521192	-0.481306
C	0.866729	-5.136871	-0.785747
H	1.560765	-5.042023	0.055115
H	0.639417	-6.184629	-0.983284
H	1.316298	-4.667987	-1.668921
Cu	0.197414	-0.361618	0.329776
H	4.230052	2.375256	-1.512557
H	-0.322779	-0.116074	3.686704
C	0.470254	-2.081547	3.362610
C	-0.108546	-2.624051	4.661614
C	1.755182	-2.795911	2.971545
H	-0.266452	-2.226275	2.557328
H	-1.044896	-2.118951	4.929613
H	-0.320300	-3.696417	4.581912
H	0.590466	-2.498018	5.501489
H	2.126621	-2.437685	2.004396
H	2.547349	-2.657456	3.723399
H	1.586529	-3.876242	2.880695
C	-4.919789	-1.554035	-0.838759
C	-5.688704	-0.426660	-1.259313
C	-7.052958	-0.352155	-0.968085
C	-7.657791	-1.384014	-0.256566
C	-6.904105	-2.478775	0.182329
C	-5.540974	-2.562889	-0.097083
C	-4.794419	0.502703	-1.900866
H	-7.634814	0.515263	-1.282342
H	-8.721736	-1.335106	-0.027496
H	-7.387268	-3.273607	0.749502
H	-4.970118	-3.411908	0.283250
H	-5.082489	1.468128	-2.309886
C	-3.534482	-0.020338	-1.863601

H	-2.644136	0.467389	-2.254225
C	-3.514455	-1.291307	-1.152765
C	-2.453488	-2.346581	-1.430113
C	-3.041725	-3.665053	-1.930311
H	-2.248685	-4.385187	-2.167119
H	-3.704553	-4.134007	-1.196607
H	-3.629761	-3.500289	-2.840921
C	-1.435944	-1.855899	-2.463527
H	-0.700415	-2.643892	-2.689775
H	-1.927463	-1.586594	-3.405698
H	-0.882428	-0.976637	-2.104246

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C	4.155754	-1.438413	-0.172403
C	4.837683	-1.174027	1.053473
C	6.058615	-0.503526	0.750002
C	6.135600	-0.351133	-0.667077
C	4.960092	-0.926629	-1.238568
H	3.173794	-1.898002	-0.261790
H	4.461456	-1.387560	2.049160
H	6.775712	-0.128376	1.472489
H	6.926302	0.155547	-1.210463
H	4.697944	-0.930455	-2.292324
Fe	4.471825	0.556470	0.053628
C	4.329317	2.209324	1.216672
C	3.061510	1.550668	1.075553
C	4.789834	2.565605	-0.080498
H	4.847972	2.362268	2.156595
C	2.737874	1.501975	-0.339124
C	3.820644	2.136877	-1.031232
H	5.741179	3.035554	-0.308206
P	1.213324	0.818055	-1.062460
C	0.317102	2.339372	-1.543557
C	-0.648122	2.287260	-2.559130
C	0.459482	3.522515	-0.807741
C	-1.447856	3.391357	-2.831483
H	-0.771709	1.373404	-3.142610
C	-0.341954	4.627268	-1.085362
H	1.201693	3.580140	-0.010545
C	-1.300397	4.563796	-2.093106
H	-2.193411	3.333305	-3.622999
H	-0.220551	5.540473	-0.504348
H	-1.934128	5.424009	-2.299524
C	1.778705	0.122843	-2.657768
C	1.855625	-1.270015	-2.778425
C	2.143657	0.921145	-3.749553
C	2.311569	-1.852694	-3.958193
H	1.546815	-1.894645	-1.938814
C	2.597942	0.337606	-4.928339
H	2.051927	2.005435	-3.679389
C	2.687240	-1.050055	-5.032761
H	2.363329	-2.937361	-4.040759
H	2.876785	0.967059	-5.771840
H	3.037923	-1.503990	-5.958119
C	2.315250	0.970698	2.179872
N	1.234577	0.275081	2.117447
O	2.840807	1.201437	3.408114
C	1.934657	0.586899	4.353355
H	2.519292	-0.111209	4.965233
H	1.547040	1.379944	5.001155
C	0.860326	-0.097715	3.487503
C	-1.509553	-2.717651	0.599774
H	-2.048410	-3.385329	1.311112
C	-3.132832	0.468735	1.248108
C	-4.451100	0.813292	1.568820
C	-2.198606	1.501794	1.147588
C	-4.836557	2.137509	1.751797
H	-5.200648	0.026545	1.660029
C	-2.555898	2.831761	1.338761
H	-1.159885	1.266392	0.904998
C	-3.879604	3.138914	1.627100
H	-5.867299	2.391514	1.986823
H	-1.816929	3.624523	1.250895
Cl	-4.342751	4.815898	1.833945
C	-2.797299	-0.967485	0.949549
H	-3.445648	-1.597825	1.604874
N	-1.435813	-1.369242	1.066186
C	-0.151863	-3.309812	0.381228
O	0.880683	-2.666872	0.228357
O	-0.166938	-4.651880	0.318954
C	1.091845	-5.252369	0.000463
H	1.843966	-4.993213	0.752242
H	0.910826	-6.327536	-0.011429
H	1.441476	-4.910258	-0.980498
Cu	0.169169	-0.417127	0.382748
H	3.900716	2.225355	-2.110093
H	-0.136447	0.324305	3.685449
C	0.756706	-1.619445	3.658948
C	0.302745	-1.955780	5.072506
C	2.045846	-2.339328	3.294323
H	-0.029239	-1.923321	2.950187
H	-0.639358	-1.453277	5.325470
H	0.144471	-3.034275	5.188897
H	1.050523	-1.660461	5.823814
H	2.326012	-2.141210	2.253605
H	2.884680	-2.047548	3.945819
H	1.925262	-3.424927	3.402180
C	-4.740762	-1.487428	-0.692246
C	-5.167078	-0.513410	-1.624979
C	-6.522085	-0.309251	-1.875163
C	-7.460112	-1.075243	-1.184442
C	-7.047148	-2.020283	-0.245574
C	-5.687839	-2.224982	0.008306
C	-3.989559	0.184152	-2.115469
H	-6.846114	0.450713	-2.586248
H	-8.523124	-0.925263	-1.368588
H	-7.789885	-2.599851	0.300798
H	-5.387230	-2.944271	0.770200
H	-4.010716	1.016735	-2.816118
C	-2.898370	-0.316490	-1.505967
H	-1.878215	0.048363	-1.608720
C	-3.245035	-1.415322	-0.541935
C	-2.397580	-2.733808	-0.731647

C	-3.218847	-4.014079	-0.803801
H	-2.550679	-4.878573	-0.909940
H	-3.811375	-4.176155	0.103689
H	-3.908774	-4.011044	-1.656319
C	-1.512069	-2.657168	-1.977201
H	-0.962321	-3.600047	-2.122044
H	-2.109223	-2.482158	-2.880382
H	-0.774968	-1.845414	-1.902393

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C	2.436230	-0.859579	-0.958281
H	3.069196	-0.859137	-1.859665
C	-1.266285	-0.794875	-0.814119
C	-2.385520	-0.047893	-1.186514
C	-1.452861	-1.968660	-0.080589
C	-3.668855	-0.449859	-0.831095
H	-2.252807	0.871768	-1.758015
C	-2.728278	-2.391008	0.276074
H	-0.575999	-2.547243	0.206869
C	-3.825997	-1.623308	-0.101590
H	-4.539101	0.134635	-1.117574
H	-2.875781	-3.305377	0.845407
Cl	-5.432501	-2.147195	0.346185
C	0.116273	-0.299113	-1.149602
H	0.048801	0.283145	-2.092777
N	1.098252	-1.368078	-1.201555
C	3.162032	-1.705321	0.076764
O	2.664469	-2.332914	0.984396
O	4.496933	-1.628085	-0.134233
C	5.290328	-2.287402	0.855150
H	5.025235	-3.346951	0.917473
H	6.326207	-2.165186	0.536204
H	5.133142	-1.828760	1.837365
C	0.040490	1.985479	-0.005666
C	-0.472378	2.163085	1.296372
C	-1.205389	3.301381	1.621979
C	-1.435511	4.259236	0.634904
C	-0.951531	4.075785	-0.658959
C	-0.215149	2.932455	-0.987399
C	-0.135577	0.983810	2.082556
H	-1.606214	3.434890	2.626173
H	-2.009794	5.152858	0.873973
H	-1.151061	4.824965	-1.423078
H	0.137231	2.792275	-2.009400
H	-0.412913	0.842591	3.124740
C	0.532427	0.104746	1.316152
H	0.901831	-0.873837	1.612186
C	0.733096	0.644605	-0.082016
C	2.249095	0.628901	-0.494415
C	2.533498	1.534793	-1.692046
H	3.577250	1.411555	-2.007533
H	1.901366	1.303285	-2.558669
H	2.383354	2.589168	-1.434666
C	3.162988	1.055079	0.650551
H	4.212778	1.065426	0.333450
H	2.899876	2.068870	0.977256
H	3.074061	0.398524	1.523677
H	1.028130	-1.934644	-2.038221

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C	-4.145685	-1.482417	-0.128221
C	-4.764854	-1.174383	-1.377586
C	-6.019078	-0.551021	-1.113022
C	-6.180622	-0.472726	0.302741
C	-5.024624	-1.047120	0.912500
H	-3.157697	-1.920498	-0.003311
H	-4.327277	-1.328338	-2.359247
H	-6.706097	-0.160647	-1.856405
H	-7.013512	-0.012317	0.823821
H	-4.823282	-1.095566	1.978381
Fe	-4.503591	0.510156	-0.272859
C	-4.325692	2.224569	-1.337222
C	-3.052409	1.591130	-1.138132
C	-4.886205	2.502157	-0.060523
H	-4.782274	2.410586	-2.302816
C	-2.830742	1.472559	0.292528
C	-3.976729	2.046239	0.935308
H	-5.864169	2.935766	0.120752
P	-1.349563	0.774394	1.084660
C	-0.479709	2.266470	1.681703
C	0.501563	2.123089	2.672408
C	-0.647047	3.512637	1.066690
C	1.301754	3.199344	3.035814
H	0.638177	1.156078	3.158946
C	0.152467	4.591786	1.438384
H	-1.404798	3.640256	0.292922
C	1.131148	4.436940	2.416513
H	2.066476	3.067985	3.799365
H	0.012281	5.557631	0.955316
H	1.763908	5.277985	2.693109
C	-1.995851	0.006657	2.613032
C	-2.056739	-1.390791	2.671661
C	-2.435503	0.755222	3.712421
C	-2.571475	-2.028029	3.797498
H	-1.686861	-1.974801	1.827510
C	-2.950682	0.116678	4.836354
H	-2.357278	1.842826	3.692262
C	-3.024101	-1.275193	4.878479
H	-2.609378	-3.115943	3.833619
H	-3.287866	0.706634	5.687001
H	-3.421878	-1.771938	5.761929
C	-2.221586	1.078899	-2.214929
N	-1.132023	0.398534	-2.115501
O	-2.666662	1.359296	-3.462563
C	-1.697389	0.794936	-4.375383
H	-2.233526	0.107300	-5.040971
H	-1.290669	1.616366	-4.973556
C	-0.659871	0.100645	-3.473821
C	1.572616	-2.660466	-0.400122
H	2.204084	-3.287508	-1.063293
C	3.095084	0.551221	-1.101357
C	4.423991	0.861263	-1.424969

C	2.214346	1.612431	-0.851993
C	4.865966	2.177432	-1.491339
H	5.131116	0.048917	-1.597145
C	2.631023	2.933680	-0.932174
H	1.179320	1.400270	-0.575373
C	3.960385	3.203526	-1.245742
H	5.902945	2.406009	-1.724397
H	1.938419	3.748897	-0.736208
Cl	4.499252	4.868151	-1.324657
C	2.733037	-0.857266	-0.937024
H	3.459645	-1.533496	-1.418143
N	1.463604	-1.314076	-0.859456
C	0.217357	-3.286456	-0.301429
O	-0.840767	-2.665264	-0.267734
O	0.257540	-4.623761	-0.205613
C	-1.009971	-5.252032	0.009041
H	-1.696232	-5.028609	-0.813649
H	-0.802718	-6.321019	0.061286
H	-1.455043	-4.899726	0.946781
Cu	-0.229296	-0.383139	-0.373639
H	-4.136588	2.072995	2.008829
H	0.333785	0.559983	-3.588312
C	-0.504914	-1.408625	-3.706396
C	0.044916	-1.669023	-5.101969
C	-1.796437	-2.171514	-3.453659
H	0.237746	-1.737917	-2.963535
H	0.988886	-1.136302	-5.272747
H	0.234304	-2.737250	-5.257847
H	-0.662219	-1.353173	-5.883350
H	-2.149304	-2.017500	-2.427122
H	-2.597408	-1.872486	-4.147499
H	-1.642952	-3.248957	-3.591809
C	4.813082	-1.631087	0.713502
C	5.451232	-0.493890	1.299826
C	6.819508	-0.277313	1.120737
C	7.559827	-1.173236	0.356897
C	6.936886	-2.273368	-0.244543
C	5.571780	-2.500169	-0.076929
C	4.439505	0.294912	1.954754
H	7.297438	0.598818	1.561374
H	8.627784	-1.012646	0.213219
H	7.524762	-2.959191	-0.853684
H	5.107238	-3.346944	-0.583560
H	4.609763	1.243507	2.459376
C	3.236147	-0.320833	1.772080
H	2.277477	0.060894	2.114998
C	3.373506	-1.512052	0.946334
C	2.365053	-2.649687	1.025810
C	3.009002	-4.014222	1.265663
H	2.244166	-4.790163	1.393361
H	3.651006	-4.326080	0.435677
H	3.628430	-3.998286	2.169966
C	1.339047	-2.401996	2.136523
H	0.645860	-3.253235	2.225899
H	1.829348	-2.273627	3.108569
H	0.737914	-1.503476	1.940520

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C	4.007027	-1.615817	-0.436487
C	4.759556	-1.594545	0.776350
C	6.012880	-0.968139	0.513655
C	6.040203	-0.601712	-0.865040
C	4.802311	-1.000553	-1.453167
H	2.992217	-1.991909	-0.540574
H	4.413423	-1.938239	1.746595
H	6.788275	-0.764147	1.244712
H	6.840579	-0.067992	-1.366592
H	4.493639	-0.814895	-2.477476
Fe	4.481674	0.290892	0.074721
C	4.501285	1.737659	1.492332
C	3.176323	1.225515	1.281247
C	4.975723	2.256292	0.256197
H	5.046674	1.688624	2.428351
C	2.830658	1.434610	-0.111784
C	3.959335	2.072301	-0.724776
H	5.963504	2.669555	0.080163
P	1.220796	1.066607	-0.871419
C	0.434731	2.722516	-0.926898
C	-0.904727	2.791386	-1.335237
C	1.078972	3.900373	-0.527495
C	-1.578396	4.006136	-1.362047
H	-1.440464	1.876718	-1.588837
C	0.397904	5.116058	-0.546967
H	2.114230	3.872817	-0.190965
C	-0.928386	5.173461	-0.966830
H	-2.625535	4.031325	-1.659460
H	0.909486	6.022722	-0.227381
H	-1.462078	6.122347	-0.967523
C	1.669623	0.721412	-2.610096
C	1.774860	-0.618449	-3.003264
C	1.914098	1.729875	-3.549337
C	2.138146	-0.945172	-4.306190
H	1.561594	-1.404978	-2.276870
C	2.277020	1.401296	-4.852635
H	1.808525	2.775796	-3.257912
C	2.392702	0.065068	-5.231767
H	2.210992	-1.990727	-4.602052
H	2.461976	2.191590	-5.578304
H	2.668502	-0.188489	-6.253829
C	2.391337	0.541121	2.294316
N	1.261755	-0.061400	2.144408
O	2.931589	0.553879	3.535814
C	1.981405	-0.112186	4.397326
H	2.511906	-0.925948	4.906794
H	1.650823	0.614025	5.147092
C	0.861962	-0.592883	3.454911
C	-1.570200	-2.748790	0.130329
H	-2.172297	-3.461311	0.729063
C	-3.068544	0.369890	1.225548
C	-4.415955	0.746942	1.337436
C	-2.094832	1.353885	1.436282
C	-4.780971	2.067580	1.567265
H	-5.192653	-0.006055	1.212340

C	-2.438975	2.674214	1.694207
H	-1.037528	1.084693	1.401068
C	-3.784067	3.025337	1.728960
H	-5.829297	2.352807	1.613069
H	-1.671328	3.430347	1.843285
Cl	-4.220925	4.701886	1.978901
C	-2.744847	-1.011682	0.849103
H	-3.488282	-1.736114	1.222218
N	-1.474486	-1.461800	0.739228
C	-0.204795	-3.323109	-0.075703
O	0.825034	-2.659885	-0.139812
O	-0.206621	-4.653713	-0.243343
C	1.063274	-5.222692	-0.580143
H	1.806685	-4.998185	0.190930
H	0.893342	-6.297046	-0.653201
H	1.416823	-4.823548	-1.537328
Cu	0.184086	-0.432544	0.315799
H	4.028507	2.329645	-1.777841
H	-0.101609	-0.132898	3.722692
C	0.654087	-2.112650	3.418072
C	0.153854	-2.607055	4.768238
C	1.901752	-2.857201	2.968742
H	-0.135045	-2.273524	2.667642
H	-0.754388	-2.077522	5.081942
H	-0.081250	-3.676958	4.734013
H	0.908453	-2.471341	5.557044
H	2.223932	-2.520360	1.976723
H	2.737554	-2.723534	3.672568
H	1.707403	-3.935399	2.907170
C	-4.808948	-1.551109	-0.931251
C	-5.407997	-0.367450	-1.463918
C	-6.777694	-0.136651	-1.318775
C	-7.559612	-1.067621	-0.643043
C	-6.976579	-2.216844	-0.096055
C	-5.609974	-2.456895	-0.228962
C	-4.361618	0.442202	-2.032060
H	-7.225356	0.774411	-1.718267
H	-8.629429	-0.897944	-0.527154
H	-7.597131	-2.931608	0.443368
H	-5.179104	-3.344538	0.235621
H	-4.505402	1.408381	-2.510538
C	-3.175408	-0.205627	-1.846455
H	-2.206705	0.143575	-2.196477
C	-3.357876	-1.444172	-1.101548
C	-2.380386	-2.599288	-1.278270
C	-3.053320	-3.929690	-1.607569
H	-2.300524	-4.709853	-1.778884
H	-3.703778	-4.281196	-0.800305
H	-3.667105	-3.845772	-2.512015
C	-1.364252	-2.288921	-2.382599
H	-0.701649	-3.149596	-2.563165
H	-1.865169	-2.054806	-3.328897
H	-0.731077	-1.432750	-2.115187

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C	-4.109146	-1.730446	-0.507147
C	-4.255899	-0.871923	-1.633953
C	-5.544565	-0.262025	-1.561901
C	-6.192918	-0.742925	-0.382468
C	-5.302223	-1.648151	0.271081
H	-3.211703	-2.292987	-0.277112
H	-3.488064	-0.680674	-2.378969
H	-5.943251	0.473627	-2.252988
H	-7.170150	-0.437535	-0.022965
H	-5.489336	-2.156227	1.212350
Fe	-4.465774	0.193802	0.086000
C	-4.555522	2.205681	0.150886
C	-3.207658	1.746646	-0.038478
C	-5.037424	1.660136	1.372088
H	-5.108917	2.820430	-0.550110
C	-2.850395	0.915372	1.095663
C	-4.000464	0.871546	1.949484
H	-6.039314	1.784014	1.770021
P	-1.157874	0.323836	1.396098
C	-0.419309	1.744562	2.291912
C	-1.188572	2.663000	3.017665
C	0.971016	1.907052	2.246816
C	-0.575749	3.721484	3.681183
H	-2.271936	2.554744	3.059775
C	1.581808	2.962695	2.919186
H	1.582107	1.208639	1.673715
C	0.809190	3.873076	3.634317
H	-1.184059	4.432856	4.237796
H	2.664103	3.076127	2.864761
H	1.284461	4.704886	4.151465
C	-1.333222	-0.952621	2.691684
C	-0.368028	-1.079743	3.699646
C	-2.336761	-1.925536	2.593071
C	-0.411572	-2.153028	4.584865
H	0.424475	-0.336052	3.789359
C	-2.381434	-2.991997	3.483720
H	-3.092102	-1.835279	1.815755
C	-1.415302	-3.112932	4.479927
H	0.347274	-2.238697	5.360476
H	-3.173361	-3.734892	3.395529
H	-1.444143	-3.952204	5.172443
C	-2.416867	2.015138	-1.225687
N	-1.244327	1.563912	-1.520549
O	-3.003105	2.851116	-2.116549
C	-2.125742	2.880151	-3.265840
H	-2.617176	2.318377	-4.073370
H	-2.017793	3.922920	-3.574890
C	-0.832846	2.219362	-2.775636
C	1.185880	-2.342664	-1.648486
H	1.749616	-2.736864	-2.515774
C	3.106290	0.686537	-1.112158
C	4.496152	0.879092	-1.083648
C	2.288088	1.784187	-0.816432
C	5.051036	2.101503	-0.728115
H	5.154635	0.045278	-1.325380
C	2.823381	3.021709	-0.481385
H	1.202172	1.671468	-0.838048
C	4.206416	3.164213	-0.423550

H	6.129822	2.227613	-0.682632
H	2.175495	3.863245	-0.244004
Cl	4.888757	4.705770	0.045181
C	2.585957	-0.649678	-1.414321
H	3.278221	-1.233436	-2.044982
N	1.270170	-0.921203	-1.558015
C	-0.236949	-2.782591	-1.769007
O	-1.206726	-2.129595	-1.404280
O	-0.356088	-4.015534	-2.288882
C	-1.691230	-4.526988	-2.331096
H	-2.346942	-3.850579	-2.888811
H	-1.619741	-5.494633	-2.828542
H	-2.085657	-4.647273	-1.315899
Cu	-0.219246	-0.066177	-0.556439
H	-4.061167	0.305240	2.874337
H	-0.092223	2.991966	-2.506401
C	-0.161375	1.265621	-3.765005
C	0.244606	2.024824	-5.021348
C	-1.017104	0.049799	-4.083508
H	0.745203	0.899411	-3.260653
H	0.876885	2.890991	-4.787327
H	0.807655	1.380219	-5.705493
H	-0.632778	2.391670	-5.574680
H	-1.289541	-0.488234	-3.167537
H	-1.940115	0.316823	-4.619817
H	-0.463548	-0.648599	-4.723146
C	4.396585	-2.083993	0.133974
C	4.910879	-1.262023	1.187473
C	6.285275	-1.049352	1.320236
C	7.159967	-1.639571	0.415038
C	6.665097	-2.430903	-0.628907
C	5.296851	-2.648711	-0.777356
C	3.793647	-0.724457	1.918216
H	6.664349	-0.407133	2.116482
H	8.233296	-1.480227	0.511094
H	7.358652	-2.881626	-1.337959
H	4.948306	-3.246667	-1.618077
H	3.862669	-0.058327	2.776396
C	2.647213	-1.180286	1.333318
H	1.634956	-0.956814	1.664466
C	2.937385	-1.989307	0.158910
C	1.925336	-3.009060	-0.342871
C	2.545221	-4.333830	-0.779192
H	1.760520	-5.041570	-1.076541
H	3.212225	-4.216789	-1.639975
H	3.125220	-4.788913	0.032367
C	0.865814	-3.304840	0.727110
H	0.189749	-4.108201	0.397607
H	1.332022	-3.629276	1.664973
H	0.247981	-2.425894	0.949890

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C	-2.696044	2.504849	0.020664
C	-3.732798	2.429518	0.999761
C	-4.980975	2.619945	0.338436
C	-4.718461	2.812828	-1.050729
C	-3.307240	2.744025	-1.249615
H	-1.636601	2.330377	0.196240
H	-3.600324	2.200662	2.053381
H	-5.960625	2.572315	0.802486
H	-5.465475	2.945128	-1.826245
H	-2.790067	2.807325	-2.202397
Fe	-3.989348	1.018367	-0.428136
C	-4.927950	-0.644402	0.249891
C	-3.504779	-0.720558	0.425678
C	-5.194771	-0.471099	-1.134478
H	-5.653867	-0.666278	1.055106
C	-2.882161	-0.595477	-0.884486
C	-3.952504	-0.447425	-1.827550
H	-6.174267	-0.336441	-1.581075
P	-1.091534	-0.672023	-1.255778
C	-0.985215	-2.176874	-2.290310
C	-0.236375	-2.222562	-3.472192
C	-1.554417	-3.361042	-1.800396
C	-0.076189	-3.423380	-4.159634
H	0.226516	-1.314939	-3.858958
C	-1.393913	-4.556394	-2.490802
H	-2.111037	-3.344402	-0.862981
C	-0.655048	-4.591541	-3.672820
H	0.507180	-3.442223	-5.078784
H	-1.843321	-5.468229	-2.100321
H	-0.528517	-5.529993	-4.210054
C	-0.828597	0.710191	-2.423982
C	-0.026543	1.769858	-1.991188
C	-1.428380	0.786616	-3.689377
C	0.136126	2.908495	-2.777096
H	0.481405	1.691829	-1.029288
C	-1.256752	1.917845	-4.480950
H	-2.013360	-0.052461	-4.066184
C	-0.485428	2.986381	-4.020415
H	0.757086	3.727000	-2.413961
H	-1.724577	1.966734	-5.463018
H	-0.359740	3.872496	-4.640295
C	-2.860891	-0.762062	1.728873
N	-1.627585	-0.517817	2.003873
O	-3.676534	-1.082475	2.762288
C	-2.862485	-0.996015	3.955637
H	-3.247344	-0.163455	4.560828
H	-2.996688	-1.926676	4.513466
C	-1.433425	-0.767633	3.436890
C	1.957702	-2.186104	2.079862
H	2.898827	-2.441712	2.567717
C	2.393857	1.421317	1.525806
C	3.514106	2.258810	1.353386
C	1.119080	2.007556	1.387499
C	3.378932	3.593947	1.006835
H	4.513150	1.830785	1.447060
C	0.969284	3.348101	1.057380
H	0.229248	1.398315	1.560600
C	2.102449	4.131507	0.851998
H	4.257615	4.212896	0.839882
H	-0.020661	3.792543	0.961726
Cl	1.915731	5.811539	0.401013

C	2.600465	0.034329	1.850583
H	3.592979	-0.244234	2.230901
N	1.699801	-0.910203	1.697784
C	0.997646	-3.175113	1.803684
O	-0.111377	-2.990198	1.247408
O	1.383788	-4.433185	2.182354
C	0.441618	-5.452194	1.886931
H	0.239623	-5.508130	0.809819
H	0.894093	-6.383789	2.233703
H	-0.509286	-5.280052	2.404948
Cu	-0.051083	-0.835379	0.647284
H	-3.829224	-0.303795	-2.895572
H	-0.837493	-1.690858	3.520491
C	-0.651254	0.357305	4.121955
C	-0.408634	0.011193	5.584715
C	-1.311544	1.719478	3.964740
H	0.322846	0.391238	3.609533
H	0.094748	-0.958147	5.690748
H	0.217759	0.767085	6.071532
H	-1.351593	-0.037277	6.149200
H	-1.505090	1.947424	2.909050
H	-2.267628	1.780781	4.505170
H	-0.666045	2.512545	4.359462
C	4.829900	-0.341999	-0.732690
C	4.548991	0.874400	-1.417800
C	5.451555	1.933633	-1.404581
C	6.644178	1.800143	-0.696735
C	6.930459	0.612397	-0.021672
C	6.037496	-0.462669	-0.044196
C	3.252998	0.751924	-2.049298
H	5.220594	2.859173	-1.932921
H	7.358620	2.622052	-0.673800
H	7.869111	0.513271	0.521762
H	6.311506	-1.379784	0.471787
H	2.771011	1.535746	-2.629248
C	2.755606	-0.485849	-1.790432
H	1.803033	-0.879423	-2.137390
C	3.693757	-1.246512	-0.971589
C	3.499228	-2.536673	-0.573374
C	4.483796	-3.274087	0.278835
H	4.026372	-4.158289	0.736163
H	5.353977	-3.614394	-0.303784
H	4.873138	-2.648374	1.089674
C	2.296989	-3.300443	-1.043944
H	2.183311	-4.244020	-0.499056
H	1.364838	-2.733225	-0.906443
H	2.361091	-3.542365	-2.115187

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C	2.765038	-2.362686	0.067917
C	3.827899	-2.223921	1.012047
C	5.061122	-2.393391	0.318670
C	4.763416	-2.642155	-1.054700
C	3.345129	-2.626231	-1.211275
H	1.704333	-2.224545	0.265839
H	3.725951	-1.970321	2.063184
H	6.051664	-2.299674	0.751129
H	5.490943	-2.774227	-1.848619
H	2.799710	-2.737507	-2.143972
Fe	3.993205	-0.852570	-0.473242
C	4.908753	0.871639	0.069860
C	3.491181	0.926866	0.296571
C	5.125667	0.625705	-1.311739
H	5.665157	0.968343	0.840435
C	2.821887	0.700617	-0.974915
C	3.858366	0.525953	-1.950552
H	6.090524	0.487813	-1.788295
P	1.018488	0.713694	-1.278907
C	0.852773	2.170232	-2.371533
C	0.044297	2.166762	-3.514191
C	1.434634	3.375397	-1.953185
C	-0.165798	3.343279	-4.229389
H	-0.432006	1.242950	-3.841899
C	1.221170	4.546848	-2.668616
H	2.050889	3.394276	-1.052977
C	0.419345	4.534165	-3.809478
H	-0.797172	3.326379	-5.115966
H	1.679827	5.475531	-2.332766
H	0.248956	5.453109	-4.367691
C	0.738679	-0.729466	-2.362477
C	-0.025126	-1.782146	-1.848648
C	1.282753	-0.849535	-3.649999
C	-0.199994	-2.955439	-2.577924
H	-0.498582	-1.671756	-0.873184
C	1.098044	-2.016726	-4.383700
H	1.832943	-0.016969	-4.088985
C	0.367952	-3.076776	-3.842709
H	-0.798449	-3.763749	-2.159781
H	1.521156	-2.099786	-5.383517
H	0.228655	-3.990127	-4.418662
C	2.898280	1.089736	1.611780
N	1.656188	0.996866	1.941590
O	3.778812	1.379408	2.599236
C	3.001061	1.548810	3.805011
H	3.384930	0.839331	4.548581
H	3.176068	2.565818	4.169979
C	1.547322	1.278395	3.378129
C	-2.509262	2.021840	1.462425
H	-3.387195	2.078380	2.115083
C	-2.170774	-1.626710	1.441727
C	-3.137687	-2.600821	1.135146
C	-0.836584	-2.037802	1.601600
C	-2.781573	-3.929072	0.949701
H	-4.178018	-2.298311	1.009894
C	-0.475161	-3.371389	1.462947
H	-0.075085	-1.296582	1.850405
C	-1.452110	-4.305850	1.121514
H	-3.530642	-4.668901	0.678062
H	0.552824	-3.694342	1.617690
Cl	-0.996010	-5.976923	0.904175
C	-2.604344	-0.254307	1.563908
H	-3.669198	-0.112033	1.777003
N	-1.831985	0.795633	1.466531

C	-1.600320	3.153490	1.579039
O	-0.402162	3.130860	1.277148
O	-2.214687	4.290781	1.977062
C	-1.397572	5.458915	1.931190
H	-1.017043	5.624723	0.916914
H	-2.043907	6.282710	2.237250
H	-0.546227	5.366884	2.613515
Cu	0.008595	0.935202	0.654586
H	3.696790	0.309397	-3.001081
H	0.931705	2.183433	3.486165
C	0.847833	0.138493	4.129507
C	0.634348	0.517052	5.588673
C	1.585602	-1.186240	3.996963
H	-0.138864	0.032931	3.649195
H	0.076412	1.456560	5.686556
H	0.074525	-0.260243	6.120404
H	1.591416	0.641090	6.116273
H	1.781783	-1.429097	2.945116
H	2.550477	-1.173535	4.524452
H	0.996859	-2.007817	4.420836
C	-4.775795	-0.058295	-0.566575
C	-4.547322	-1.187720	-1.430968
C	-5.434897	-2.269549	-1.448595
C	-6.531163	-2.274145	-0.597297
C	-6.748659	-1.193608	0.272697
C	-5.891789	-0.097199	0.286789
C	-3.322601	-0.969692	-2.133566
H	-5.248163	-3.113718	-2.115023
H	-7.222604	-3.116237	-0.598413
H	-7.606619	-1.207730	0.944344
H	-6.099512	0.713383	0.984881
H	-2.887841	-1.639372	-2.871917
C	-2.810755	0.242069	-1.725831
H	-1.899409	0.697639	-2.110515
C	-3.681304	0.874039	-0.774748
C	-3.453077	2.193811	-0.250149
C	-4.661270	3.002350	0.179771
H	-4.355219	3.945083	0.649457
H	-5.281224	3.247153	-0.693309
H	-5.299450	2.473023	0.892075
C	-2.497745	3.039812	-1.075677
H	-2.399339	4.050746	-0.658773
H	-1.491674	2.606722	-1.124887
H	-2.863144	3.143102	-2.105874

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C	2.777720	-2.389574	0.103671
C	3.805902	-2.217841	1.079754
C	5.064116	-2.372457	0.428696
C	4.815666	-2.644805	-0.950096
C	3.403119	-2.657049	-1.152410
H	1.707945	-2.285372	0.265766
H	3.663951	-1.955027	2.123953
H	6.038349	-2.254367	0.891082
H	5.570562	-2.772399	-1.718695
H	2.888399	-2.791498	-2.099622
Fe	3.998879	-0.862318	-0.420175
C	4.909164	0.874139	0.088515
C	3.489648	0.939654	0.300863
C	5.137381	0.593481	-1.284524
H	5.659543	0.991373	0.862088
C	2.831196	0.680524	-0.969471
C	3.875347	0.479311	-1.931394
H	6.105891	0.441192	-1.749148
P	1.031647	0.684411	-1.290925
C	0.874347	2.122547	-2.408060
C	0.089920	2.096177	-3.566753
C	1.430991	3.339517	-1.989397
C	-0.118218	3.262259	-4.299426
H	-0.371104	1.163624	-3.891402
C	1.219226	4.500493	-2.722139
H	2.026556	3.375112	-1.075468
C	0.443435	4.464785	-3.880491
H	-0.731214	3.228620	-5.198327
H	1.658485	5.438577	-2.386576
H	0.273979	5.375174	-4.452773
C	0.766254	-0.780774	-2.346885
C	-0.001614	-1.824264	-1.820010
C	1.322282	-0.924220	-3.627061
C	-0.167691	-3.011464	-2.528355
H	-0.485222	-1.695462	-0.851826
C	1.146191	-2.105502	-4.339758
H	1.874470	-0.098977	-4.077189
C	0.412679	-3.156129	-3.784982
H	-0.771232	-3.811397	-2.101661
H	1.578010	-2.206816	-5.334119
H	0.279670	-4.080545	-4.344553
C	2.884926	1.173479	1.598947
N	1.632714	1.176628	1.905213
O	3.762678	1.441917	2.595084
C	2.970839	1.758827	3.761615
H	3.318623	1.121391	4.583155
H	3.171721	2.803628	4.020829
C	1.517314	1.494328	3.333755
C	-2.626254	2.019719	1.254090
H	-3.466040	2.053332	1.963932
C	-2.141737	-1.608940	1.454585
C	-3.087239	-2.609581	1.169507
C	-0.803790	-1.986900	1.654993
C	-2.704494	-3.936711	1.038840
H	-4.130390	-2.330609	1.017464
C	-0.418204	-3.318619	1.579978
H	-0.061195	-1.220734	1.885013
C	-1.372145	-4.282070	1.252104
H	-3.435130	-4.699147	0.779824
H	0.610698	-3.617770	1.771626
Cl	-0.879388	-5.949655	1.102990
C	-2.605213	-0.241044	1.502571
H	-3.676426	-0.121728	1.692111
N	-1.855405	0.822884	1.386112
C	-1.736341	3.194954	1.444245
O	-0.529280	3.200543	1.217298
O	-2.402144	4.297668	1.833268

C	-1.613436	5.488687	1.884267
H	-1.167246	5.694096	0.905425
H	-2.301888	6.284712	2.169697
H	-0.812351	5.389335	2.623458
Cu	-0.005729	0.965153	0.625707
H	3.721966	0.232452	-2.976425
H	0.910067	2.406469	3.420191
C	0.803530	0.374098	4.101931
C	0.542441	0.796461	5.540873
C	1.557271	-0.946465	4.033168
H	-0.166812	0.246128	3.593784
H	-0.035121	1.727815	5.591458
H	-0.018129	0.026749	6.082770
H	1.481541	0.956752	6.090639
H	1.801552	-1.209683	2.996153
H	2.497757	-0.912482	4.601976
H	0.957481	-1.764437	4.448446
C	-4.756238	-0.154759	-0.580447
C	-4.550730	-1.303739	-1.433565
C	-5.443262	-2.383574	-1.403503
C	-6.514971	-2.371000	-0.523317
C	-6.707658	-1.273387	0.335048
C	-5.849524	-0.180195	0.307335
C	-3.343651	-1.103460	-2.160055
H	-5.274873	-3.242831	-2.055965
H	-7.207437	-3.211707	-0.490203
H	-7.546779	-1.275586	1.030616
H	-6.030568	0.640387	1.003092
H	-2.927299	-1.780501	-2.902098
C	-2.818144	0.118250	-1.773082
H	-1.907249	0.560554	-2.176483
C	-3.660128	0.755839	-0.813324
C	-3.401514	2.108359	-0.270597
C	-4.665854	2.930057	-0.022883
H	-4.419046	3.914452	0.394191
H	-5.202188	3.083746	-0.966829
H	-5.357092	2.441932	0.669816
C	-2.479679	2.911802	-1.191081
H	-2.386233	3.952838	-0.850234
H	-1.469224	2.490523	-1.237797
H	-2.879776	2.929976	-2.211271

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C	-2.689004	2.579114	-0.205473
C	-3.625564	2.700233	0.865618
C	-4.926755	2.836465	0.301340
C	-4.796744	2.798207	-1.119692
C	-3.414021	2.641981	-1.435085
H	-1.619321	2.406316	-0.108156
H	-3.398007	2.639422	1.925412
H	-5.856635	2.901111	0.856615
H	-5.612628	2.838370	-1.833870
H	-2.989742	2.540784	-2.429646
Fe	-4.061894	1.093611	-0.294676
C	-5.016675	-0.401764	0.676709
C	-3.589691	-0.548608	0.751136
C	-5.391395	-0.401209	-0.693754
H	-5.672397	-0.273194	1.530648
C	-3.075402	-0.632221	-0.606450
C	-4.211584	-0.542717	-1.476902
H	-6.396814	-0.263383	-1.077759
P	-1.329083	-0.857083	-1.095507
C	-1.363275	-2.500341	-1.894691
C	-0.632343	-2.767926	-3.058637
C	-1.993073	-3.560331	-1.228822
C	-0.548787	-4.066122	-3.553934
H	-0.112610	-1.958806	-3.571898
C	-1.907301	-4.855255	-1.726689
H	-2.541652	-3.368043	-0.305668
C	-1.185600	-5.112030	-2.891381
H	0.023257	-4.260284	-4.459738
H	-2.405340	-5.668709	-1.201362
H	-1.117050	-6.126746	-3.279635
C	-1.103704	0.321370	-2.477396
C	-0.233148	1.396843	-2.274416
C	-1.783651	0.221695	-3.699791
C	-0.074689	2.379853	-3.248047
H	0.341213	1.454052	-1.349232
C	-1.619730	1.199071	-4.677012
H	-2.424252	-0.638307	-3.897082
C	-0.774379	2.285742	-4.447792
H	0.607348	3.209722	-3.066066
H	-2.149068	1.110385	-5.624512
H	-0.650212	3.048673	-5.214286
C	-2.843084	-0.504296	1.996259
N	-1.565292	-0.526464	2.151554
O	-3.600994	-0.428242	3.117314
C	-2.678061	-0.444603	4.231280
H	-2.877837	0.446530	4.838696
H	-2.901346	-1.333650	4.829699
C	-1.279650	-0.457870	3.587689
C	2.378420	-2.106056	1.428874
H	3.166262	-2.215390	2.199082
C	2.519170	1.492847	1.013505
C	3.627792	2.338832	0.855255
C	1.242982	2.059807	0.901970
C	3.475325	3.683777	0.544583
H	4.629965	1.924003	0.957332
C	1.069339	3.409948	0.620031
H	0.363315	1.425818	1.048587
C	2.192371	4.208610	0.424297
H	4.344541	4.319159	0.393271
H	0.074213	3.847126	0.550989
Cl	1.980923	5.900024	0.032490
C	2.749822	0.066573	1.249738
H	3.708554	-0.124794	1.760562
N	1.757795	-0.820215	1.473114
C	1.364617	-3.190224	1.626602
O	0.159873	-3.065808	1.454139
O	1.927395	-4.362148	1.970625
C	1.023389	-5.468917	2.031647
H	0.535763	-5.616457	1.061742
H	1.635049	-6.333565	2.291067

H	0.254724	-5.298578	2.791405
Cu	-0.083472	-0.815784	0.694989
H	-4.168701	-0.538699	-2.560788
H	-0.727249	-1.370223	3.859284
C	-0.390935	0.746413	3.927227
C	-0.013812	0.726457	5.401774
C	-1.028519	2.068484	3.528523
H	0.523207	0.609238	3.328226
H	0.474314	-0.215301	5.682805
H	0.676303	1.542762	5.642527
H	-0.895543	0.850926	6.047969
H	-1.309610	2.067066	2.468179
H	-1.931813	2.287400	4.118172
H	-0.332073	2.900847	3.680851
C	4.858564	-0.265149	-0.560295
C	4.819916	0.744322	-1.575172
C	5.918513	1.578390	-1.795293
C	7.058636	1.428571	-1.014367
C	7.099031	0.458119	-0.005313
C	6.009265	-0.378749	0.229225
C	3.509737	0.729810	-2.169116
H	5.870961	2.353148	-2.561886
H	7.921464	2.072745	-1.179930
H	7.993960	0.355553	0.607632
H	6.067350	-1.104995	1.039398
H	3.174248	1.387161	-2.968381
C	2.771623	-0.233240	-1.543692
H	1.739297	-0.485643	-1.778627
C	3.528865	-0.867166	-0.474235
C	3.172737	-2.267766	0.003858
C	4.384413	-3.167708	0.233444
H	4.059685	-4.180269	0.504352
H	5.004637	-3.236617	-0.667956
H	5.021870	-2.807784	1.048109
C	2.239526	-2.964108	-0.993013
H	2.039855	-4.003075	-0.690662
H	1.271696	-2.453497	-1.064936
H	2.678766	-2.989249	-1.997400

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C	3.050778	-1.964209	0.695033
C	4.107847	-1.359201	1.439694
C	5.337521	-1.647656	0.778621
C	5.041813	-2.432131	-0.376352
C	3.629205	-2.629199	-0.428979
H	1.988646	-1.887572	0.914717
H	3.993743	-0.736098	2.321838
H	6.318371	-1.291192	1.075648
H	5.761522	-2.780740	-1.109737
H	3.081221	-3.147835	-1.209620
Fe	4.071745	-0.650680	-0.460822
C	4.832887	1.207273	-0.715207
C	3.437692	1.250649	-0.378248
C	4.974650	0.455574	-1.913150
H	5.628339	1.650056	-0.126390
C	2.708088	0.505002	-1.388406
C	3.681597	0.027664	-2.326968
H	5.912115	0.210369	-2.401808
P	0.905384	0.248790	-1.411614
C	0.366488	1.290591	-2.816056
C	-0.651537	0.881883	-3.687812
C	0.850898	2.602603	-2.909263
C	-1.163158	1.763026	-4.636375
H	-1.053486	-0.129080	-3.618517
C	0.338315	3.478978	-3.858556
H	1.623628	2.943007	-2.218475
C	-0.671138	3.062178	-4.724895
H	-1.956039	1.430932	-5.304897
H	0.727308	4.494190	-3.920441
H	-1.074661	3.750523	-5.465393
C	0.715020	-1.462740	-2.031403
C	0.212635	-2.426369	-1.149561
C	1.056914	-1.849024	-3.335624
C	0.091832	-3.756069	-1.546031
H	-0.097703	-2.125084	-0.147268
C	0.927391	-3.175429	-3.734427
H	1.403186	-1.101138	-4.049790
C	0.453468	-4.132437	-2.836753
H	-0.294251	-4.492618	-0.843085
H	1.193115	-3.463286	-4.750497
H	0.355368	-5.170510	-3.150366
C	2.910129	1.882456	0.819087
N	1.691406	1.906975	1.231953
O	3.836754	2.528235	1.572328
C	3.115970	3.133052	2.668272
H	3.571781	2.779229	3.601605
H	3.258953	4.216717	2.600174
C	1.656612	2.681200	2.477422
C	-2.628380	2.091961	1.183524
H	-3.270716	2.361833	2.051331
C	-1.886053	-1.403615	1.745344
C	-2.406779	-2.648795	1.378143
C	-0.638984	-1.382098	2.382658
C	-1.682844	-3.822017	1.572152
H	-3.389369	-2.715275	0.916927
C	0.093304	-2.545763	2.604003
H	-0.244849	-0.422211	2.706450
C	-0.424943	-3.758272	2.162968
H	-2.086532	-4.780615	1.253916
H	1.064217	-2.511947	3.095912
Cl	0.525422	-5.218158	2.326921
C	-2.609841	-0.103020	1.506730
H	-3.367039	0.009968	2.322796
N	-1.728185	1.027233	1.489378
C	-1.911450	3.337851	0.754784
O	-0.778227	3.388497	0.306550
O	-2.695173	4.432165	0.864219
C	-2.121610	5.630805	0.339813
H	-1.882918	5.508039	-0.722423
H	-2.877012	6.405449	0.477789
H	-1.203722	5.887948	0.877916
Cu	-0.061828	0.969384	0.419942
H	3.465359	-0.601599	-3.183890

H	0.995986	3.543431	2.310058
C	1.070539	1.856077	3.630115
C	0.949256	2.706888	4.886010
C	1.868586	0.585258	3.886163
H	0.058474	1.572293	3.293303
H	0.358561	3.613758	4.704387
H	0.462056	2.150623	5.694754
H	1.934650	3.021279	5.261025
H	1.952479	-0.017486	2.972055
H	2.886561	0.800910	4.244367
H	1.384458	-0.035311	4.650035
C	-4.774080	-0.789856	0.179122
C	-4.790989	-1.660798	-0.937372
C	-5.848166	-2.542692	-1.143461
C	-6.893697	-2.570457	-0.221337
C	-6.868358	-1.739181	0.897765
C	-5.808896	-0.849310	1.103830
C	-3.534808	-1.500867	-1.651421
H	-5.849827	-3.213405	-2.002757
H	-7.726532	-3.257225	-0.366114
H	-7.678719	-1.785881	1.623712
H	-5.797657	-0.225773	1.997621
H	-3.238998	-2.074175	-2.529014
C	-2.782586	-0.587918	-1.008838
H	-1.781316	-0.273531	-1.286588
C	-3.489104	0.006536	0.176682
C	-3.644158	1.587328	0.055395
C	-5.042638	2.106778	0.362421
H	-5.036274	3.204326	0.338307
H	-5.784508	1.752831	-0.363760
H	-5.383989	1.808100	1.360835
C	-3.231421	2.090423	-1.329330
H	-3.418079	3.170093	-1.420841
H	-2.164181	1.917911	-1.526275
H	-3.799293	1.590053	-2.123591

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C	-2.436230	-0.859579	-0.958281
H	-3.069196	-0.859137	-1.859665
C	1.266285	-0.794875	-0.814119
C	2.385520	-0.047893	-1.186514
C	1.452861	-1.968660	-0.080589
C	3.668855	-0.449859	-0.831095
H	2.252807	0.871768	-1.758015
C	2.728278	-2.391008	0.276074
H	0.575999	-2.547243	0.206869
C	3.825997	-1.623308	-0.101590
H	4.539101	0.134635	-1.117574
H	2.875781	-3.305377	0.845407
Cl	5.432501	-2.147195	0.346185
C	-0.116273	-0.299113	-1.149602
H	-0.048801	0.283145	-2.092777
N	-1.098252	-1.368078	-1.201555
C	-3.162032	-1.705321	0.076764
O	-2.664469	-2.332914	0.984396
O	-4.496933	-1.628085	-0.134233
C	-5.290328	-2.287402	0.855150
H	-5.025235	-3.346951	0.917473
H	-6.326207	-2.165186	0.536204
H	-5.133142	-1.828760	1.837365
C	-0.040490	1.985479	-0.005666
C	0.472378	2.163085	1.296372
C	1.205389	3.301381	1.621979
C	1.435511	4.259236	0.634904
C	0.951531	4.075785	-0.658959
C	0.215149	2.932455	-0.987399
C	0.135577	0.983810	2.082556
H	1.606214	3.434890	2.626173
H	2.009794	5.152858	0.873973
H	1.151061	4.824965	-1.423078
H	-0.137231	2.792275	-2.009400
H	0.412913	0.842591	3.124740
C	-0.532427	0.104746	1.316152
H	-0.901831	-0.873837	1.612186
C	-0.733096	0.644605	-0.082016
C	-2.249095	0.628901	-0.494415
C	-2.533498	1.534793	-1.692046
H	-3.577250	1.411555	-2.007533
H	-1.901366	1.303285	-2.558669
H	-2.383354	2.589168	-1.434666
C	-3.162988	1.055079	0.650551
H	-4.212778	1.065426	0.333450
H	-2.899876	2.068870	0.977256
H	-3.074061	0.398524	1.523677
H	-1.028130	-1.934644	-2.038221

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C	-3.863154	-1.840571	-0.265780
C	-4.207833	-1.794615	-1.650239
C	-5.563711	-1.368178	-1.760217
C	-6.062783	-1.148773	-0.440798
C	-5.013282	-1.438664	0.482946
H	-2.881344	-2.093323	0.130442
H	-3.532852	-1.990798	-2.478480
H	-6.103685	-1.192333	-2.684777
H	-7.052198	-0.782540	-0.187030
H	-5.063442	-1.324598	1.561563
Fe	-4.451583	0.030921	-0.796759
C	-4.317652	1.613380	-2.053460
C	-3.029835	1.216420	-1.554848
C	-5.137578	1.944717	-0.940163
H	-4.608595	1.612595	-3.097643
C	-3.063164	1.308728	-0.105380
C	-4.374631	1.764152	0.248998
H	-6.181184	2.237617	-0.987009
P	-1.674477	0.906624	0.986788
C	-0.910027	2.532984	1.314395
C	0.145575	2.588944	2.237128
C	-1.218339	3.674434	0.565995
C	0.866569	3.763124	2.413802
H	0.415623	1.695113	2.801957

C	-0.483513	4.846228	0.736629
H	-2.030601	3.648478	-0.160371
C	0.558389	4.893740	1.657781
H	1.691643	3.788427	3.123685
H	-0.727141	5.725696	0.142704
H	1.140643	5.805630	1.777465
C	-2.484853	0.439878	2.555456
C	-2.491069	-0.915973	2.904815
C	-3.095625	1.368941	3.406708
C	-3.127410	-1.341322	4.067832
H	-1.988801	-1.632467	2.251539
C	-3.728546	0.942541	4.570298
H	-3.063893	2.430505	3.157754
C	-3.750844	-0.412751	4.898214
H	-3.127061	-2.397786	4.332003
H	-4.200775	1.670179	5.228309
H	-4.243683	-0.742630	5.811152
C	-1.953896	0.701391	-2.382145
N	-0.845350	0.159820	-1.998327
O	-2.159166	0.805078	-3.714183
C	-1.033525	0.155803	-4.352118
H	-1.414184	-0.739397	-4.861892
H	-0.636257	0.845616	-5.101199
C	-0.065425	-0.159886	-3.204691
C	1.603562	-2.244269	1.240603
H	2.052408	-2.305810	2.240304
C	2.804705	1.108721	0.364276
C	3.998059	1.759617	0.721306
C	1.952408	1.742528	-0.554332
C	4.307372	3.017506	0.223132
H	4.698479	1.254760	1.388878
C	2.239008	3.003991	-1.049132
H	1.029871	1.251094	-0.863496
C	3.411787	3.638801	-0.642992
H	5.233703	3.514181	0.501071
H	1.552218	3.505685	-1.727978
Cl	3.753672	5.251208	-1.224065
C	2.544825	-0.186880	0.945639
H	3.284467	-0.518181	1.680494
N	1.507085	-0.944970	0.707195
C	0.327307	-2.945153	1.142470
O	-0.599785	-2.634522	0.376953
O	0.243686	-4.036795	1.931359
C	-0.936595	-4.820646	1.761061
H	-1.014742	-5.184314	0.730657
H	-0.835985	-5.655796	2.455344
H	-1.834471	-4.236307	1.994260
Cu	-0.293600	-0.443559	-0.077311
H	-4.732659	1.894563	1.265805
H	0.801532	0.521391	-3.227744
C	0.474037	-1.588770	-3.149499
C	1.376510	-1.874348	-4.340603
C	-0.623667	-2.631878	-2.998144
H	1.090574	-1.606680	-2.234721
H	2.180677	-1.132536	-4.427972
H	1.847211	-2.860405	-4.245176
H	0.812459	-1.875977	-5.285119
H	-1.236857	-2.439944	-2.109457
H	-1.281350	-2.670685	-3.879001
H	-0.189419	-3.631802	-2.880454
C	5.069378	-1.663861	0.439893
C	5.724226	-0.843105	-0.546123
C	6.855885	-0.090824	-0.210465
C	7.337723	-0.111024	1.091276
C	6.686781	-0.879524	2.069101
C	5.569803	-1.647018	1.752638
C	4.994871	-0.956666	-1.770510
H	7.341918	0.524977	-0.969296
H	8.216580	0.474665	1.358914
H	7.063249	-0.882384	3.091926
H	5.089698	-2.214444	2.549647
H	5.257662	-0.474338	-2.708946
C	3.928115	-1.799934	-1.551796
H	3.218551	-2.113813	-2.313809
C	3.926141	-2.287441	-0.202094
C	2.953501	-3.223356	0.315750
C	3.427116	-4.187760	1.389529
H	2.589700	-4.769944	1.792336
H	4.153412	-4.892134	0.962940
H	3.917053	-3.688181	2.228484
C	2.184927	-3.983780	-0.755402
H	1.486459	-4.701101	-0.303822
H	1.602015	-3.320431	-1.401069
H	2.873908	-4.552339	-1.393730

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C	-3.804060	-1.954299	0.581749
C	-3.929523	-2.279985	-0.799324
C	-5.292398	-2.091999	-1.177932
C	-6.011729	-1.650374	-0.024314
C	-5.088566	-1.558954	1.063263
H	-2.873295	-1.955721	1.139034
H	-3.110397	-2.570597	-1.450445
H	-5.703870	-2.224290	-2.172970
H	-7.063026	-1.383809	0.006776
H	-5.308578	-1.204196	2.065756
Fe	-4.519446	-0.360176	-0.461391
C	-4.675994	1.005179	-1.953040
C	-3.315964	0.853849	-1.519216
C	-5.452105	1.408765	-0.832482
H	-5.034663	0.814089	-2.958285
C	-3.256894	1.166555	-0.103299
C	-4.589330	1.511714	0.297470
H	-6.526318	1.562069	-0.827001
P	-1.738478	1.062188	0.881823
C	-1.048632	2.752745	0.789927
C	0.133736	3.017422	1.497890
C	-1.569096	3.736901	-0.057199
C	0.770214	4.245615	1.370749
H	0.568453	2.242258	2.131476
C	-0.919861	4.962602	-0.191993
H	-2.482227	3.543616	-0.620229
C	0.247891	5.219593	0.520037

H	1.695793	4.433150	1.912950
H	-1.330831	5.719104	-0.858862
H	0.761223	6.172363	0.403872
C	-2.359247	0.912321	2.594319
C	-2.154776	-0.295575	3.270092
C	-3.033311	1.953005	3.245850
C	-2.651638	-0.477477	4.558169
H	-1.588885	-1.088941	2.775992
C	-3.526802	1.772698	4.533779
H	-3.161332	2.911136	2.739768
C	-3.344100	0.554247	5.187158
H	-2.487874	-1.421326	5.075520
H	-4.050154	2.586128	5.033373
H	-3.729641	0.415509	6.195795
C	-2.211603	0.464139	-2.376184
N	-1.000511	0.186265	-2.025402
O	-2.500618	0.433479	-3.697269
C	-1.269566	0.100820	-4.378709
H	-1.446947	-0.812718	-4.958758
H	-1.048188	0.917916	-5.071988
C	-0.232144	-0.062680	-3.255557
C	1.579195	-2.345847	1.041930
H	1.814919	-2.402541	2.127824
C	2.883186	0.937671	0.251093
C	3.967008	1.673053	0.750270
C	2.144336	1.481675	-0.808478
C	4.284140	2.924822	0.234886
H	4.575012	1.248083	1.550225
C	2.429102	2.739179	-1.318850
H	1.309204	0.911704	-1.215921
C	3.497896	3.454057	-0.783715
H	5.126885	3.491258	0.623686
H	1.821800	3.175659	-2.109697
Cl	3.844345	5.059121	-1.391125
C	2.581099	-0.371345	0.821503
H	3.059228	-0.539673	1.801262
N	1.424341	-1.011277	0.577521
C	0.302409	-3.096338	0.809801
O	-0.662507	-2.661451	0.189205
O	0.301246	-4.324118	1.351524
C	-0.864246	-5.107459	1.074765
H	-0.993195	-5.229323	-0.006271
H	-0.689575	-6.071777	1.552535
H	-1.759584	-4.629906	1.485587
Cu	-0.333298	-0.343782	-0.041998
H	-4.891136	1.755617	1.310997
H	0.538978	0.720699	-3.330360
C	0.486852	-1.410823	-3.191848
C	1.466680	-1.561546	-4.345375
C	-0.478863	-2.583688	-3.105862
H	1.055002	-1.367473	-2.246160
H	2.185303	-0.732475	-4.376339
H	2.039081	-2.492903	-4.255229
H	0.947587	-1.593955	-5.314745
H	-1.182426	-2.454572	-2.275566
H	-1.050948	-2.715055	-4.035415
H	0.062700	-3.521177	-2.929758
C	5.079527	-1.533890	0.772018
C	5.954329	-0.826276	-0.112258
C	7.142169	-0.265023	0.362782
C	7.467617	-0.386545	1.709612
C	6.601107	-1.048030	2.588071
C	5.410959	-1.609943	2.129437
C	5.335110	-0.787199	-1.409953
H	7.799447	0.280022	-0.316169
H	8.393999	0.044972	2.087012
H	6.857791	-1.123217	3.644349
H	4.743127	-2.089451	2.845379
H	5.756595	-0.311789	-2.292154
C	4.128403	-1.421818	-1.325690
H	3.429288	-1.542799	-2.151118
C	3.865351	-1.872862	0.031225
C	2.891351	-3.005772	0.325022
C	3.473999	-4.075188	1.248028
H	2.760356	-4.897362	1.382875
H	4.398336	-4.490617	0.829726
H	3.712014	-3.683738	2.241732
C	2.445105	-3.695765	-0.967396
H	1.791258	-4.552010	-0.748051
H	1.895076	-3.013170	-1.621867
H	3.307459	-4.072170	-1.530078

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C	3.866451	1.419265	-1.558450
C	3.538047	0.559062	-2.646118
C	4.736793	-0.073689	-3.095444
C	5.811896	0.397394	-2.280155
C	5.272312	1.317669	-1.331824
H	3.143797	1.991510	-0.983837
H	2.531811	0.374273	-3.012813
H	4.813641	-0.814082	-3.885049
H	6.847649	0.080939	-2.345054
H	5.832861	1.831662	-0.557313
Fe	4.395360	-0.508037	-1.150035
C	4.328953	-2.526719	-1.099942
C	3.075639	-1.942669	-0.713297
C	5.330309	-2.060083	-0.209156
H	4.470798	-3.178765	-1.953884
C	3.312986	-1.087787	0.445931
C	4.715873	-1.193498	0.737792
H	6.388845	-2.291344	-0.265055
P	1.968463	-0.226695	1.307934
C	1.711015	-1.240901	2.812573
C	2.758144	-1.639609	3.651906
C	0.401685	-1.619261	3.128404
C	2.498036	-2.409036	4.780097
H	3.782231	-1.344563	3.421798
C	0.141227	-2.388292	4.260042
H	-0.416702	-1.307575	2.476286
C	1.189686	-2.785044	5.084502
H	3.318493	-2.717101	5.426233
H	-0.882175	-2.678389	4.491058
H	0.989434	-3.388808	5.967946

C	2.598934	1.349797	1.981028
C	1.635034	2.122698	2.648725
C	3.889819	1.867774	1.838120
C	1.959719	3.365066	3.178404
H	0.613758	1.745030	2.736540
C	4.212958	3.117488	2.365691
H	4.643994	1.303444	1.295900
C	3.253695	3.866396	3.041115
H	1.195270	3.950007	3.686651
H	5.223912	3.505522	2.245977
H	3.509050	4.842167	3.450513
C	1.846936	-2.169655	-1.456956
N	0.692468	-1.604677	-1.315918
O	1.941526	-3.121989	-2.413931
C	0.671549	-3.124609	-3.109973
H	0.836863	-2.683042	-4.102069
H	0.365787	-4.166499	-3.231692
C	-0.250592	-2.291046	-2.218805
C	-1.318339	2.362508	0.229355
H	-1.759696	2.959703	1.035739
C	-3.063080	-0.787331	0.908884
C	-4.414451	-0.973543	1.253890
C	-2.309387	-1.921500	0.559424
C	-5.001015	-2.230148	1.221783
H	-5.018883	-0.106398	1.520259
C	-2.877304	-3.186637	0.543047
H	-1.250451	-1.807972	0.316442
C	-4.227232	-3.330279	0.864398
H	-6.053101	-2.355460	1.465681
H	-2.283919	-4.062991	0.289758
Cl	-4.949200	-4.919223	0.820036
C	-2.572724	0.568578	0.874493
H	-3.246679	1.313923	1.306710
N	-1.434961	0.972346	0.363652
C	0.017551	2.778754	-0.168150
O	0.835399	2.066201	-0.766627
O	0.280538	4.074732	0.112048
C	1.570305	4.523632	-0.298018
H	1.694461	4.421459	-1.382038
H	1.624235	5.572755	-0.003288
H	2.354218	3.947533	0.208765
Cu	0.223609	-0.068241	-0.074528
H	5.232208	-0.678795	1.541355
H	-0.867206	-2.956748	-1.591920
C	-1.200010	-1.318397	-2.915060
C	-2.278370	-2.078695	-3.673438
C	-0.473149	-0.313672	-3.796955
H	-1.690944	-0.757922	-2.098819
H	-2.835931	-2.750229	-3.007554
H	-3.001162	-1.386986	-4.120918
H	-1.854646	-2.680991	-4.490692
H	0.237437	0.287895	-3.214168
H	0.074622	-0.795852	-4.619434
H	-1.186800	0.379584	-4.257880
C	-4.908448	2.110719	-0.362921
C	-5.773136	1.060687	-0.830349
C	-7.000968	0.818540	-0.203845
C	-7.370096	1.573210	0.902656
C	-6.514883	2.572019	1.391675
C	-5.300100	2.842364	0.768851
C	-5.109972	0.387372	-1.906672
H	-7.650140	0.020633	-0.569193
H	-8.321802	1.385450	1.398854
H	-6.805275	3.148250	2.269541
H	-4.658811	3.613814	1.194642
H	-5.518629	-0.443878	-2.476495
C	-3.887829	0.989504	-2.094359
H	-3.173135	0.728923	-2.872538
C	-3.709624	2.086435	-1.182385
C	-2.574723	2.963322	-1.195239
C	-2.788035	4.407828	-0.793540
H	-1.832885	4.934843	-0.687707
H	-3.371140	4.924097	-1.568533
H	-3.335190	4.518608	0.145352
C	-1.704797	2.857374	-2.432532
H	-0.881811	3.583267	-2.403907
H	-1.259345	1.861789	-2.528122
H	-2.289446	3.057128	-3.340693

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C	-4.133951	1.253978	1.350393
C	-4.054320	0.183315	2.287911
C	-5.337149	-0.437916	2.369951
C	-6.216919	0.254595	1.482216
C	-5.472665	1.298062	0.854071
H	-3.300278	1.879083	1.042648
H	-3.151633	-0.139927	2.799455
H	-5.585586	-1.312135	2.962808
H	-7.255369	0.006400	1.289465
H	-5.856459	1.990868	0.112040
Fe	-4.636326	-0.516752	0.475856
C	-4.612641	-2.489677	0.062853
C	-3.291590	-1.923196	0.028582
C	-5.410128	-1.814166	-0.898112
H	-4.936586	-3.270986	0.740279
C	-3.282349	-0.869371	-0.980168
C	-4.602683	-0.833399	-1.539846
H	-6.464563	-1.990536	-1.083391
P	-1.779274	0.063128	-1.368244
C	-1.183997	-0.686046	-2.928480
C	-1.822409	-0.498419	-4.160322
C	-0.023551	-1.466658	-2.872257
C	-1.308735	-1.087230	-5.310638
H	-2.715885	0.124880	-4.218286
C	0.489572	-2.056849	-4.023902
H	0.489251	-1.596536	-1.916305
C	-0.154237	-1.867537	-5.243648
H	-1.807179	-0.934194	-6.266632
H	1.399279	-2.652716	-3.962961
H	0.247161	-2.320607	-6.148680
C	-2.216725	1.761457	-1.853412
C	-1.111847	2.569115	-2.178073
C	-3.485110	2.350550	-1.807488

C	-1.275146	3.919470	-2.456763
H	-0.112900	2.127115	-2.192687
C	-3.645595	3.707499	-2.085143
H	-4.350653	1.750618	-1.537749
C	-2.545218	4.495571	-2.411104
H	-0.404577	4.528107	-2.695349
H	-4.641185	4.148814	-2.046795
H	-2.674239	5.555422	-2.623523
C	-2.254007	-2.312756	0.970271
N	-1.044471	-1.867781	1.095837
O	-2.633998	-3.285217	1.835219
C	-1.540879	-3.463985	2.761411
H	-1.872072	-3.095072	3.742026
H	-1.343047	-4.536414	2.837516
C	-0.391474	-2.648361	2.162549
C	1.435087	2.201655	0.508432
H	1.790393	2.881702	-0.296330
C	3.127157	-0.802140	-0.597759
C	4.325891	-0.975549	-1.303392
C	2.487306	-1.943446	-0.095940
C	4.870582	-2.238591	-1.504963
H	4.847737	-0.098117	-1.686404
C	3.004274	-3.214833	-0.304534
H	1.555692	-1.822456	0.458732
C	4.199899	-3.350439	-1.006060
H	5.807606	-2.362071	-2.042401
H	2.496669	-4.099428	0.075414
Cl	4.868309	-4.948718	-1.254288
C	2.645918	0.556770	-0.349854
H	3.091639	1.293093	-1.039702
N	1.400035	0.833768	0.094111
C	0.071607	2.659043	0.935794
O	-0.830620	1.924238	1.318776
O	-0.064993	3.993127	0.867213
C	-1.350310	4.490150	1.250190
H	-1.592559	4.188633	2.274475
H	-1.279732	5.575604	1.172742
H	-2.119957	4.109018	0.569480
Cu	-0.253429	-0.202726	0.248745
H	-4.934354	-0.153526	-2.318102
H	0.333276	-3.321016	1.674157
C	0.387161	-1.767036	3.142297
C	1.123770	-2.630966	4.155958
C	-0.480900	-0.706331	3.803895
H	1.138966	-1.242086	2.527681
H	1.768628	-3.370252	3.662661
H	1.759840	-2.016681	4.803335
H	0.426290	-3.175322	4.809222
H	-0.884211	-0.004584	3.061491
H	-1.319038	-1.143303	4.366230
H	0.107705	-0.118269	4.517421
C	4.900580	1.878883	0.507820
C	5.973830	0.989735	0.815866
C	7.204381	1.115959	0.167661
C	7.374814	2.113689	-0.788090
C	6.317945	2.971027	-1.114219
C	5.082572	2.851550	-0.478660
C	5.491398	0.033317	1.779462
H	8.020360	0.430290	0.399867
H	8.333553	2.222352	-1.293958
H	6.460587	3.739077	-1.873427
H	4.264417	3.512709	-0.770300
H	6.073840	-0.783265	2.198649
C	4.179741	0.310024	2.037572
H	3.544821	-0.254831	2.717989
C	3.708380	1.424244	1.225370
C	2.550890	2.310902	1.669198
C	2.958241	3.767623	1.879802
H	2.104188	4.365189	2.223530
H	3.747452	3.841463	2.637310
H	3.340218	4.232121	0.965266
C	1.920597	1.787435	2.960028
H	1.120669	2.456334	3.309410
H	1.475643	0.798850	2.800502
H	2.663580	1.709070	3.762194

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C	2.976749	-2.616025	-0.120333
C	3.792384	-2.656742	1.049413
C	5.155662	-2.577968	0.639928
C	5.183078	-2.489042	-0.784554
C	3.836635	-2.511480	-1.256761
H	1.890251	-2.621654	-0.142614
H	3.436222	-2.678951	2.075265
H	6.017002	-2.538921	1.298410
H	6.071437	-2.377390	-1.397438
H	3.515620	-2.421248	-2.290705
Fe	4.123582	-0.946065	0.005872
C	4.760868	0.592626	1.149091
C	3.327122	0.554924	1.067034
C	5.275703	0.728276	-0.167675
H	5.333634	0.490951	2.063957
C	2.952641	0.663467	-0.334035
C	4.178003	0.768852	-1.071442
H	6.325466	0.743187	-0.440868
P	1.260548	0.726918	-1.025823
C	1.245651	2.358674	-1.849738
C	0.522028	2.557695	-3.032932
C	1.829647	3.462683	-1.216309
C	0.396716	3.833170	-3.575374
H	0.046994	1.711708	-3.531206
C	1.702730	4.735254	-1.763059
H	2.372714	3.324317	-0.281522
C	0.986414	4.924635	-2.943092
H	-0.169259	3.972163	-4.494928
H	2.166776	5.584145	-1.262637
H	0.885971	5.921715	-3.368160
C	1.334953	-0.457583	-2.417036
C	0.604759	-1.645551	-2.328587
C	2.130767	-0.233370	-3.549236
C	0.704017	-2.616444	-3.323569
H	-0.080969	-1.787123	-1.493271
C	2.227674	-1.198999	-4.545100

H	2.660023	0.712895	-3.661380
C	1.523875	-2.398821	-4.426782
H	0.114593	-3.529083	-3.245140
H	2.846881	-1.012877	-5.421088
H	1.600012	-3.153257	-5.207781
C	2.472763	0.291324	2.210169
N	1.195411	0.137478	2.223552
O	3.121608	0.179267	3.395177
C	2.115903	-0.164608	4.374875
H	2.353233	-1.168007	4.754334
H	2.198948	0.549523	5.199270
C	0.783106	-0.098729	3.610385
C	-2.323651	2.220461	1.615511
H	-3.123643	2.413690	2.340241
C	-2.940803	-1.351688	1.217831
C	-4.135654	-2.078717	1.375317
C	-1.855198	-1.993622	0.594535
C	-4.259832	-3.374068	0.896306
H	-4.991335	-1.589786	1.838905
C	-1.959841	-3.290076	0.121993
H	-0.911351	-1.449757	0.478902
C	-3.173635	-3.964873	0.258589
H	-5.196011	-3.918239	0.991689
H	-1.117188	-3.781729	-0.362623
Cl	-3.328699	-5.581576	-0.384458
C	-2.936193	0.029636	1.614107
H	-3.864856	0.387969	2.073413
N	-1.953052	0.884639	1.456495
C	-1.181647	3.122065	1.732343
O	-0.027270	2.859447	1.384151
O	-1.517322	4.344613	2.204219
C	-0.463213	5.305574	2.175708
H	-0.088201	5.436901	1.154140
H	-0.901740	6.233535	2.545572
H	0.367769	4.992722	2.816325
Cu	-0.112668	0.641501	0.673202
H	4.251660	0.838995	-2.151282
H	0.192210	0.774732	3.931791
C	-0.110954	-1.337462	3.733697
C	-0.562692	-1.524751	5.175196
C	0.543595	-2.592837	3.177853
H	-0.995411	-1.120509	3.116573
H	-1.054930	-0.625329	5.566576
H	-1.271619	-2.355764	5.260931
H	0.285244	-1.755426	5.836692
H	0.892205	-2.432622	2.149703
H	1.403556	-2.914771	3.783832
H	-0.168446	-3.425728	3.160420
C	-3.709308	0.496882	-1.319660
C	-4.810647	-0.424462	-1.403039
C	-4.739505	-1.555890	-2.219908
C	-3.600909	-1.783655	-2.982384
C	-2.529842	-0.883733	-2.924974
C	-2.568798	0.237484	-2.096228
C	-5.840105	0.035823	-0.521288
H	-5.575023	-2.257817	-2.252988
H	-3.540870	-2.660450	-3.627236
H	-1.653275	-1.049648	-3.550437
H	-1.705980	0.903550	-2.076797
H	-6.804425	-0.444784	-0.374626
C	-5.403216	1.194968	0.078465
H	-5.981559	1.782245	0.788827
C	-4.085699	1.541563	-0.384515
C	-2.255820	3.187698	-0.927774
H	-2.621363	3.274486	-1.959671
H	-1.875482	4.173054	-0.623074
H	-1.396592	2.507484	-0.940219
C	-3.349563	2.712186	0.008171
C	-4.184256	3.863465	0.535141
H	-4.742550	4.332789	-0.286333
H	-4.915677	3.542144	1.284780
H	-3.554189	4.632597	0.994763

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C	-3.045434	2.576918	-0.141617
C	-3.891714	2.596738	1.006209
C	-5.242049	2.497018	0.560100
C	-5.230700	2.417712	-0.865143
C	-3.872598	2.465280	-1.301426
H	-1.959401	2.603329	-0.132990
H	-3.562015	2.619591	2.040734
H	-6.119598	2.440278	1.195498
H	-6.100437	2.294055	-1.502020
H	-3.522356	2.385783	-2.326572
Fe	-4.167515	0.887282	-0.057451
C	-4.809854	-0.670168	1.058217
C	-3.376029	-0.612321	1.012472
C	-5.290675	-0.800357	-0.272864
H	-5.406449	-0.584258	1.959470
C	-2.966448	-0.704329	-0.379827
C	-4.170667	-0.817810	-1.150281
H	-6.333501	-0.825251	-0.571063
P	-1.255446	-0.736995	-1.017670
C	-1.167229	-2.365195	-1.843096
C	-0.358985	-2.548512	-2.973930
C	-1.763217	-3.483580	-1.247041
C	-0.163362	-3.821120	-3.501134
H	0.131933	-1.693076	-3.439532
C	-1.565209	-4.753844	-1.778262
H	-2.373096	-3.358240	-0.352262
C	-0.764744	-4.927070	-2.905555
H	0.468864	-3.946820	-4.378457
H	-2.039853	-5.613671	-1.307114
H	-0.609774	-5.922082	-3.318984
C	-1.295846	0.449472	-2.409661
C	-0.613750	1.662768	-2.278867
C	-2.007293	0.197211	-3.590856
C	-0.677299	2.626958	-3.282283
H	-0.000826	1.837912	-1.394956
C	-2.064139	1.154761	-4.598017
H	-2.499343	-0.765387	-3.731489
C	-1.408782	2.376828	-4.439687
H	-0.130765	3.561788	-3.166459

H	-2.616722	0.945822	-5.512631
H	-1.454429	3.125004	-5.229139
C	-2.544855	-0.351093	2.174250
N	-1.270291	-0.189750	2.206238
O	-3.213099	-0.251538	3.350998
C	-2.221584	0.098864	4.344625
H	-2.470567	1.100867	4.720843
H	-2.311975	-0.615823	5.167868
C	-0.877631	0.042510	3.598061
C	2.364639	-2.188858	1.624377
H	3.020849	-2.341252	2.504809
C	2.980703	1.345153	1.134290
C	4.142493	2.107367	1.328368
C	1.866585	1.982623	0.572343
C	4.205106	3.442505	0.949115
H	5.018458	1.631707	1.767203
C	1.902077	3.319772	0.202922
H	0.942478	1.409997	0.440263
C	3.082657	4.036266	0.381618
H	5.114244	4.021741	1.089700
H	1.025661	3.810797	-0.218863
Cl	3.146501	5.718650	-0.094551
C	3.000597	-0.077803	1.468448
H	3.798960	-0.327183	2.185745
N	1.887800	-0.846614	1.537918
C	1.228095	-3.162704	1.718265
O	0.065430	-2.921544	1.429148
O	1.629059	-4.380262	2.127460
C	0.611660	-5.385255	2.102386
H	0.215767	-5.499821	1.087291
H	1.098102	-6.303678	2.432809
H	-0.210083	-5.119709	2.774387
Cu	0.110508	-0.631771	0.675670
H	-4.213223	-0.877416	-2.232994
H	-0.284078	-0.828373	3.920585
C	0.012001	1.283498	3.734279
C	0.439204	1.472269	5.182971
C	-0.638434	2.536282	3.168143
H	0.904883	1.062017	3.129976
H	0.927624	0.573861	5.581535
H	1.144504	2.305118	5.280986
H	-0.420015	1.700192	5.831064
H	-0.968064	2.374288	2.133825
H	-1.511353	2.853303	3.758282
H	0.069310	3.373092	3.163668
C	3.653546	-0.351012	-1.228545
C	4.799941	0.437583	-1.553142
C	4.765110	1.356514	-2.603017
C	3.605574	1.485298	-3.360843
C	2.480320	0.714455	-3.055834
C	2.492474	-0.184955	-1.988769
C	5.849350	0.092247	-0.630236
H	5.643955	1.960648	-2.831764
H	3.573942	2.185464	-4.195100
H	1.579790	0.809847	-3.663029
H	1.590742	-0.752825	-1.762811
H	6.843367	0.533505	-0.618017
C	5.377484	-0.867630	0.217850
H	5.947496	-1.317946	1.028019
C	3.970334	-1.145289	-0.033919
C	2.461916	-3.064526	-0.778809
H	2.979700	-3.050806	-1.744839
H	2.194243	-4.108174	-0.555445
H	1.521939	-2.512566	-0.897613
C	3.325850	-2.478011	0.341208
C	4.371138	-3.516652	0.749135
H	5.052567	-3.740057	-0.080537
H	4.979172	-3.173622	1.595540
H	3.885581	-4.451435	1.054397

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C	-4.031886	-1.458609	0.072440
C	-4.550535	-1.701738	-1.237299
C	-5.794020	-1.017508	-1.359368
C	-6.052030	-0.351375	-0.124995
C	-4.968058	-0.624535	0.760976
H	-3.071196	-1.807274	0.449843
H	-4.055043	-2.254765	-2.028815
H	-6.409534	-0.971230	-2.251594
H	-6.900471	0.290569	0.087814
H	-4.846153	-0.218928	1.760406
Fe	-4.295420	0.287994	-0.922145
C	-3.867775	1.322896	-2.608934
C	-2.671195	0.904248	-1.932921
C	-4.619338	2.135758	-1.717454
H	-4.148297	1.029370	-3.614219
C	-2.697783	1.465629	-0.593497
C	-3.907537	2.226590	-0.487590
H	-5.594575	2.565672	-1.921231
P	-1.399401	1.234642	0.648127
C	-0.568892	2.860271	0.691506
C	-0.688562	3.790984	-0.346353
C	0.343821	3.109218	1.727293
C	0.090332	4.946620	-0.346758
H	-1.388187	3.610661	-1.162496
C	1.112152	4.266355	1.726924
H	0.464180	2.378586	2.528784
C	0.991256	5.186519	0.686255
H	-0.006553	5.660989	-1.162881
H	1.827927	4.438648	2.528995
H	1.612006	6.080427	0.673566
C	-2.292491	1.148775	2.239927
C	-2.904939	2.256419	2.839325
C	-2.357950	-0.095603	2.878833
C	-3.599209	2.111479	4.036441
H	-2.822345	3.238243	2.371294
C	-3.053102	-0.239835	4.076435
H	-1.863803	-0.952456	2.416953
C	-3.679650	0.862733	4.652708
H	-4.074691	2.976803	4.495548
H	-3.099375	-1.213086	4.562934
H	-4.219653	0.754111	5.591759
C	-1.682290	0.011940	-2.514296

N	-0.615545	-0.477771	-1.970788
O	-1.930193	-0.339046	-3.796977
C	-0.787238	-1.109280	-4.237415
H	-1.166034	-2.015688	-4.722765
H	-0.251125	-0.507194	-4.979368
C	0.014970	-1.371699	-2.957216
C	1.361476	-2.076328	1.959960
H	1.633319	-2.007871	3.020080
C	2.931810	1.028021	0.835114
C	3.997005	1.758518	1.390347
C	2.436498	1.423296	-0.421195
C	4.527592	2.865969	0.746766
H	4.419440	1.430466	2.339881
C	2.953348	2.529551	-1.073542
H	1.648397	0.840465	-0.901829
C	3.989517	3.247581	-0.478596
H	5.350466	3.428245	1.180675
H	2.566283	2.838071	-2.041820
Cl	4.614550	4.667876	-1.283695
C	2.461181	-0.119628	1.564977
H	3.021405	-0.355835	2.477796
N	1.449945	-0.882416	1.235289
C	0.091707	-2.754774	1.741291
O	-0.695025	-2.529118	0.809830
O	-0.160780	-3.722329	2.651849
C	-1.351502	-4.472816	2.421160
H	-1.301866	-4.994064	1.458344
H	-1.409687	-5.190923	3.240241
H	-2.232802	-3.820643	2.420062
Cu	-0.093331	-0.447092	0.009780
H	-4.241063	2.743502	0.407174
H	1.063719	-1.059977	-3.070507
C	-0.000234	-2.823575	-2.464800
C	0.844673	-3.704317	-3.373138
C	-1.404798	-3.368568	-2.268644
H	0.463981	-2.788663	-1.468368
H	1.872062	-3.327110	-3.461364
H	0.900686	-4.728151	-2.985012
H	0.420350	-3.765982	-4.386040
H	-1.969590	-2.740232	-1.571310
H	-1.962537	-3.438962	-3.214999
H	-1.367006	-4.375696	-1.836579
C	4.147077	-1.734992	-0.263043
C	5.373628	-0.988802	-0.198121
C	5.819111	-0.255772	-1.303730
C	5.069052	-0.244248	-2.473188
C	3.859394	-0.948589	-2.536321
C	3.397146	-1.681304	-1.444798
C	5.905995	-1.138005	1.121030
H	6.747752	0.314069	-1.242102
H	5.410930	0.326382	-3.335942
H	3.274513	-0.931300	-3.458938
H	2.442629	-2.196630	-1.523210
H	6.840877	-0.711365	1.475858
C	5.046333	-1.935787	1.844239
H	5.206874	-2.244271	2.875043
C	3.937643	-2.356952	1.032162
C	2.871807	-3.222200	1.463209
C	2.282224	-4.172330	0.436655
H	1.492476	-4.791021	0.884952
H	1.851646	-3.659591	-0.425285
H	3.057192	-4.851930	0.057130
C	3.115819	-3.947592	2.774414
H	2.200827	-4.439135	3.125814
H	3.886110	-4.720911	2.649857
H	3.454599	-3.270494	3.566760

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C	-4.190415	-1.578554	0.014650
C	-4.453639	-1.887149	-1.354231
C	-5.679802	-1.261657	-1.722861
C	-6.179564	-0.565232	-0.581354
C	-5.259571	-0.758144	0.493006
H	-3.304120	-1.870689	0.572146
H	-3.806329	-2.450874	-2.018480
H	-6.128200	-1.273154	-2.710887
H	-7.074938	0.046715	-0.551478
H	-5.329921	-0.316382	1.482296
Fe	-4.340194	0.122906	-1.079483
C	-3.792469	1.205816	-2.699287
C	-2.647644	0.781108	-1.941323
C	-4.621216	1.986141	-1.848000
H	-3.991348	0.937108	-3.730558
C	-2.784270	1.305414	-0.595138
C	-4.009339	2.048677	-0.563319
H	-5.581918	2.412947	-2.117494
P	-1.571737	1.071816	0.732768
C	-0.760957	2.707507	0.825103
C	-0.924127	3.691106	-0.156715
C	0.170175	2.920380	1.852715
C	-0.174663	4.865013	-0.108004
H	-1.633047	3.538883	-0.970021
C	0.902577	4.099472	1.906624
H	0.331181	2.145780	2.604272
C	0.736123	5.073237	0.922650
H	-0.302663	5.618706	-0.883404
H	1.629348	4.246387	2.703759
H	1.328949	5.985663	0.951880
C	-2.600059	1.007695	2.244930
C	-3.250186	2.132145	2.768927
C	-2.738085	-0.223400	2.897477
C	-4.054872	2.017418	3.898136
H	-3.109474	3.104760	2.295378
C	-3.544464	-0.338072	4.027201
H	-2.199119	-1.091571	2.511780
C	-4.209972	0.780456	4.523179
H	-4.557678	2.896938	4.297507
H	-3.647026	-1.300694	4.525599
H	-4.837681	0.693807	5.408392
C	-1.613422	-0.099063	-2.456723
N	-0.579168	-0.572222	-1.843357
O	-1.779151	-0.454727	-3.752589
C	-0.631781	-1.257974	-4.108295

H	-1.003247	-2.198151	-4.533184
H	-0.077157	-0.717180	-4.882242
C	0.144433	-1.431228	-2.794015
C	1.664422	-2.040110	2.012233
H	1.746432	-1.864867	3.107537
C	2.944623	1.118960	0.797042
C	3.929402	1.986817	1.288296
C	2.331829	1.436484	-0.423731
C	4.280691	3.144306	0.602267
H	4.435907	1.737526	2.221002
C	2.656355	2.594523	-1.113603
H	1.589390	0.756049	-0.842832
C	3.629647	3.441007	-0.589995
H	5.045263	3.814505	0.987851
H	2.161558	2.844696	-2.049391
Cl	4.019388	4.922141	-1.438634
C	2.623806	-0.099378	1.537838
H	2.959562	-0.061887	2.589219
N	1.517600	-0.831272	1.282087
C	0.465094	-2.915037	1.808049
O	-0.439641	-2.703359	1.007227
O	0.462246	-3.986456	2.617844
C	-0.625733	-4.893263	2.422503
H	-0.588681	-5.321014	1.414877
H	-0.496713	-5.673193	3.173301
H	-1.584780	-4.382498	2.555174
Cu	-0.121597	-0.498737	0.203964
H	-4.419175	2.531694	0.318464
H	1.166451	-1.034403	-2.888862
C	0.240360	-2.870849	-2.276052
C	1.151327	-3.699571	-3.169775
C	-1.120840	-3.516995	-2.074291
H	0.701700	-2.786385	-1.279572
H	2.148468	-3.248304	-3.260382
H	1.282320	-4.710719	-2.766816
H	0.735724	-3.807101	-4.182469
H	-1.735317	-2.921831	-1.389368
H	-1.667738	-3.644587	-3.020971
H	-1.010932	-4.512961	-1.629714
C	4.278227	-1.298957	-0.274139
C	5.547877	-0.651486	-0.352953
C	6.016249	-0.151014	-1.569610
C	5.238611	-0.292236	-2.714770
C	3.984620	-0.907888	-2.640278
C	3.501387	-1.400043	-1.427837
C	6.101258	-0.611553	0.974106
H	6.981443	0.354468	-1.619597
H	5.600884	0.088352	-3.668720
H	3.375930	-1.002146	-3.542568
H	2.503007	-1.827658	-1.375791
H	7.058701	-0.170834	1.241682
C	5.216029	-1.208349	1.828371
H	5.365439	-1.322374	2.900015
C	4.000673	-1.599870	1.132522
C	3.094476	-2.722634	1.630802
C	2.892702	-3.820505	0.581744
H	2.378153	-4.686491	1.020504
H	2.300665	-3.477076	-0.272523
H	3.854674	-4.168332	0.188323
C	3.648461	-3.374154	2.898819
H	2.954717	-4.138716	3.270999
H	4.617009	-3.852908	2.710721
H	3.789427	-2.640954	3.703211

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C	2.199099	-2.820236	0.051213
C	2.575911	-3.228835	1.366365
C	3.955962	-3.580964	1.343711
C	4.435696	-3.393235	0.012844
C	3.351126	-2.925301	-0.787647
H	1.221256	-2.449349	-0.249036
H	1.940472	-3.219992	2.246627
H	4.549149	-3.886090	2.199184
H	5.458132	-3.536263	-0.321218
H	3.402648	-2.642501	-1.834681
Fe	3.702394	-1.651206	0.750691
C	4.389464	-0.469535	2.246652
C	3.117308	-0.015031	1.758483
C	5.308175	-0.467682	1.162057
H	4.585028	-0.793414	3.262644
C	3.260607	0.267816	0.338633
C	4.623381	-0.018271	-0.002289
H	6.338631	-0.804873	1.203937
P	1.949222	0.904411	-0.740149
C	2.520778	2.583566	-1.175991
C	1.826772	3.264808	-2.187902
C	3.523195	3.257231	-0.470398
C	2.144190	4.581507	-2.498835
H	1.030044	2.755874	-2.733580
C	3.835888	4.579109	-0.782173
H	4.063146	2.748602	0.327788
C	3.151885	5.242957	-1.796704
H	1.599074	5.095588	-3.288638
H	4.622413	5.090113	-0.229096
H	3.399145	6.275096	-2.038463
C	2.130236	-0.030366	-2.300744
C	1.131877	-0.963053	-2.600701
C	3.200663	0.130385	-3.190943
C	1.214053	-1.754462	-3.742342
H	0.281085	-1.067203	-1.927427
C	3.281314	-0.657852	-4.335611
H	3.962161	0.886864	-2.995677
C	2.294301	-1.606624	-4.608167
H	0.427203	-2.477517	-3.951999
H	4.115368	-0.527820	-5.023610
H	2.363091	-2.218732	-5.505749
C	1.920567	0.054860	2.580014
N	0.709400	0.324267	2.221382
O	2.128098	-0.194649	3.893148
C	0.859299	0.005465	4.557061
H	0.643677	-0.898810	5.138726
H	0.978711	0.846972	5.247223
C	-0.140454	0.270291	3.420039

C	-2.120589	2.542210	-0.559478
H	-2.580558	2.919132	-1.478880
C	-2.264672	-1.034480	-1.367724
C	-2.882873	-1.751970	-2.407406
C	-1.585389	-1.765872	-0.376948
C	-2.798623	-3.133315	-2.483937
H	-3.452439	-1.203288	-3.157477
C	-1.487031	-3.148970	-0.441944
H	-1.127949	-1.231654	0.457718
C	-2.092826	-3.823134	-1.499585
H	-3.285433	-3.679803	-3.287470
H	-0.962730	-3.709153	0.330237
Cl	-1.981495	-5.563999	-1.581714
C	-2.393157	0.402130	-1.347046
H	-3.111006	0.829200	-2.057139
N	-1.705649	1.207270	-0.575176
C	-1.141074	3.431700	0.044333
O	-0.291084	3.089335	0.877479
O	-1.274948	4.720178	-0.341646
C	-0.410973	5.636201	0.329863
H	0.635093	5.328832	0.233694
H	-0.575998	6.601722	-0.151254
H	-0.666105	5.694172	1.394552
Cu	0.043418	0.896294	0.389280
H	5.041790	0.058380	-1.001338
H	-0.617630	1.255391	3.534129
C	-1.246287	-0.779691	3.267973
C	-2.207007	-0.722211	4.446279
C	-0.699028	-2.180744	3.043807
H	-1.801259	-0.495670	2.359068
H	-2.626666	0.283621	4.577222
H	-3.045284	-1.413591	4.303705
H	-1.711721	-1.003416	5.387276
H	-0.016071	-2.202400	2.184472
H	-0.152682	-2.559813	3.920351
H	-1.513753	-2.885143	2.838826
C	-4.810791	0.181665	0.268784
C	-5.644941	-0.411295	-0.740166
C	-5.963997	-1.772634	-0.690159
C	-5.471502	-2.560307	0.341690
C	-4.692207	-1.980204	1.353168
C	-4.377123	-0.624548	1.331604
C	-5.986531	0.609227	-1.683634
H	-6.589354	-2.214024	-1.468602
H	-5.700507	-3.624857	0.375458
H	-4.337412	-2.599290	2.179219
H	-3.809902	-0.204847	2.158156
H	-6.618735	0.471786	-2.557797
C	-5.388241	1.784385	-1.284057
H	-5.463242	2.733600	-1.810869
C	-4.635052	1.582829	-0.078409
C	-3.804607	2.576223	0.529791
C	-3.263603	2.307764	1.916613
H	-2.718055	3.179126	2.302993
H	-4.073837	2.075961	2.621737
H	-2.564175	1.461703	1.916325
C	-4.245921	4.012819	0.344270
H	-3.503755	4.719381	0.731152
H	-4.426063	4.267167	-0.705815
H	-5.185540	4.186204	0.886562

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C	1.649535	-2.920704	0.159222
C	1.974491	-3.343367	1.484197
C	3.242181	-3.994285	1.444753
C	3.701999	-3.978811	0.094144
C	2.720054	-3.315864	-0.700664
H	0.766141	-2.356229	-0.132975
H	1.391632	-3.148578	2.379670
H	3.782526	-4.387956	2.299348
H	4.654656	-4.360019	-0.258205
H	2.793454	-3.102625	-1.762470
Fe	3.395184	-2.084643	0.762130
C	4.377434	-1.024525	2.177888
C	3.207552	-0.332167	1.714259
C	5.228459	-1.250934	1.061220
H	4.545186	-1.347423	3.199329
C	3.343407	-0.133524	0.280480
C	4.602281	-0.706895	-0.096085
H	6.166728	-1.795796	1.080392
P	2.133529	0.721801	-0.768089
C	2.962527	2.307430	-1.126880
C	2.552841	3.068322	-2.232625
C	3.883941	2.861809	-0.229335
C	3.074844	4.339460	-2.446112
H	1.825269	2.654759	-2.932561
C	4.398868	4.137104	-0.443039
H	4.202757	2.289070	0.641552
C	4.000033	4.878591	-1.552370
H	2.757160	4.913207	-3.315337
H	5.121056	4.550228	0.259390
H	4.407898	5.873635	-1.721215
C	2.174860	-0.190123	-2.348436
C	1.058737	-0.973352	-2.668322
C	3.262836	-0.158213	-3.230042
C	1.043064	-1.741865	-3.829458
H	0.196526	-0.974450	-1.997913
C	3.245052	-0.923698	-4.392060
H	4.120337	0.478426	-3.007997
C	2.139418	-1.721758	-4.688577
H	0.168748	-2.348335	-4.060383
H	4.095346	-0.896419	-5.071874
H	2.130389	-2.319570	-5.598409
C	2.079045	0.020370	2.558470
N	0.935898	0.499172	2.200226
O	2.274224	-0.179446	3.882978
C	1.068716	0.265339	4.548335
H	0.681022	-0.579245	5.130667
H	1.351627	1.066878	5.237726
C	0.136236	0.717569	3.412929
C	-1.927342	2.676967	-0.674224
H	-1.980635	3.024310	-1.729505
C	-2.390264	-0.843579	-1.320943

C	-2.934908	-1.541040	-2.407721
C	-1.921367	-1.582454	-0.225466
C	-3.000980	-2.929313	-2.414632
H	-3.316433	-0.976920	-3.258585
C	-1.970160	-2.970028	-0.218203
H	-1.517255	-1.042988	0.631669
C	-2.512240	-3.632125	-1.317482
H	-3.426890	-3.466534	-3.258481
H	-1.602060	-3.541107	0.632447
Cl	-2.565841	-5.379850	-1.322424
C	-2.352796	0.616930	-1.345254
H	-2.528507	1.017715	-2.358902
N	-1.500075	1.322822	-0.563490
C	-0.977663	3.585206	0.051662
O	-0.142371	3.218620	0.867383
O	-1.120812	4.874102	-0.298016
C	-0.205961	5.772707	0.338677
H	0.826847	5.473889	0.130378
H	-0.419319	6.754843	-0.084606
H	-0.363580	5.778332	1.421903
Cu	0.223238	0.935716	0.312976
H	4.980183	-0.761062	-1.112538
H	-0.074979	1.795364	3.477381
C	-1.202851	-0.017951	3.317290
C	-2.122993	0.377629	4.462281
C	-1.044347	-1.526910	3.211051
H	-1.642951	0.333962	2.368784
H	-2.276041	1.463852	4.502440
H	-3.108399	-0.091776	4.358783
H	-1.715374	0.060638	5.433625
H	-0.348181	-1.790741	2.403996
H	-0.670508	-1.973142	4.144256
H	-2.008704	-1.998762	2.985053
C	-4.652153	0.356403	0.188304
C	-5.619107	-0.354012	-0.588284
C	-6.211401	-1.520709	-0.103967
C	-5.876849	-1.984962	1.164390
C	-4.951435	-1.284274	1.941482
C	-4.337808	-0.126761	1.461019
C	-5.762287	0.327658	-1.849083
H	-6.932332	-2.063304	-0.716990
H	-6.336431	-2.893119	1.552064
H	-4.705012	-1.644609	2.941478
H	-3.624168	0.387710	2.096966
H	-6.422548	0.019329	-2.656368
C	-4.921671	1.400597	-1.855439
H	-4.791824	2.086985	-2.690275
C	-4.100345	1.432551	-0.648235
C	-3.452798	2.728774	-0.150387
C	-3.407267	2.846260	1.373486
H	-3.101456	3.862092	1.665059
H	-4.382539	2.644636	1.830470
H	-2.675169	2.150052	1.801353
C	-4.150473	3.965118	-0.718018
H	-3.669706	4.882936	-0.357905
H	-4.116622	3.987632	-1.813710
H	-5.204956	3.993891	-0.419211

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C	4.110043	0.999224	0.665905
C	4.883022	1.140924	-0.527279
C	6.022848	0.291710	-0.425470
C	5.960054	-0.378132	0.832884
C	4.781282	0.058689	1.508006
H	3.158780	1.487432	0.864340
H	4.616635	1.739531	-1.393055
H	6.775862	0.141452	-1.191923
H	6.658936	-1.126564	1.191555
H	4.425029	-0.304522	2.467099
Fe	4.309395	-0.791031	-0.272268
C	4.120905	-1.846168	-1.992620
C	2.879622	-1.230144	-1.615488
C	4.526899	-2.705045	-0.935207
H	4.659048	-1.648513	-2.912911
C	2.521025	-1.716659	-0.295221
C	3.551222	-2.632154	0.098745
H	5.449246	-3.275520	-0.900739
P	0.996238	-1.317999	0.614530
C	0.049227	-2.869577	0.421311
C	-0.916640	-3.225221	1.371101
C	0.168551	-3.638185	-0.744705
C	-1.727727	-4.337316	1.169896
H	-1.034233	-2.625616	2.273944
C	-0.648108	-4.747490	-0.944524
H	0.907588	-3.370107	-1.500210
C	-1.596284	-5.101941	0.012839
H	-2.475467	-4.599011	1.916846
H	-0.543257	-5.336395	-1.854192
H	-2.238134	-5.966228	-0.146939
C	1.523691	-1.304835	2.361837
C	1.634341	-0.057601	2.987939
C	1.828368	-2.463771	3.086873
C	2.054673	0.032423	4.312112
H	1.383835	0.842694	2.425074
C	2.249384	-2.371108	4.410382
H	1.716284	-3.442338	2.618882
C	2.364832	-1.123956	5.023616
H	2.129168	1.008199	4.789910
H	2.480681	-3.276408	4.969212
H	2.685964	-1.057299	6.061670
C	2.169437	-0.262781	-2.432764
N	1.105478	0.401238	-2.131558
O	2.695546	-0.061129	-3.664350
C	1.775902	0.813587	-4.356324
H	2.361166	1.632715	-4.789607
H	1.320689	0.237053	-5.168995
C	0.776492	1.261644	-3.276761
C	-1.158421	3.042721	0.237422
H	-1.666570	3.912858	-0.197382
C	-3.186757	0.476852	-1.400432
C	-4.470497	0.558884	-1.972273
C	-2.634291	-0.799434	-1.190604
C	-5.178890	-0.581167	-2.319943

H	-4.926829	1.539463	-2.105041
C	-3.328918	-1.946611	-1.531904
H	-1.657707	-0.892275	-0.712832
C	-4.600996	-1.826610	-2.088805
H	-6.178160	-0.513241	-2.742486
H	-2.905752	-2.930093	-1.339583
Cl	-5.491353	-3.275972	-2.491721
C	-2.568874	1.696367	-0.948768
H	-3.183536	2.598353	-1.056418
N	-1.380775	1.817313	-0.408309
C	0.252835	3.264307	0.519191
O	1.103893	2.365910	0.602986
O	0.574444	4.553089	0.759456
C	1.913939	4.765341	1.205610
H	2.637353	4.391207	0.472896
H	2.014844	5.844315	1.328158
H	2.086629	4.255321	2.160703
Cu	0.143734	0.493318	-0.253701
H	3.597752	-3.140424	1.057225
H	-0.258854	1.043972	-3.576796
C	0.858452	2.751344	-2.913251
C	0.393194	3.604617	-4.084884
C	2.240703	3.157289	-2.424722
H	0.152276	2.890309	-2.082248
H	-0.619117	3.330606	-4.407863
H	0.381099	4.667042	-3.816884
H	1.059468	3.500541	-4.953520
H	2.533096	2.568384	-1.547221
H	3.008296	3.030931	-3.202971
H	2.250511	4.215183	-2.134314
C	-3.795074	0.969515	1.727898
C	-5.173603	0.872397	1.328932
C	-5.839021	-0.356411	1.345477
C	-5.165416	-1.498613	1.757849
C	-3.824973	-1.413693	2.154011
C	-3.137425	-0.202504	2.134971
C	-5.616035	2.178302	0.945060
H	-6.881347	-0.415183	1.026956
H	-5.676200	-2.461280	1.769783
H	-3.309927	-2.313209	2.489854
H	-2.093910	-0.190970	2.448985
H	-6.618129	2.428551	0.604998
C	-4.566336	3.053161	1.111636
H	-4.609657	4.121892	0.910624
C	-3.405224	2.362302	1.603452
C	-2.140842	2.983850	1.899904
C	-2.214017	4.453127	2.273884
H	-1.217381	4.904813	2.332150
H	-2.799718	5.038793	1.557229
H	-2.692218	4.567259	3.255716
C	-1.198128	2.218256	2.808029
H	-0.334476	2.837962	3.092820
H	-1.701612	1.901695	3.730740
H	-0.805797	1.317687	2.319741

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C	4.118276	1.021330	0.700838
C	4.890506	1.182713	-0.490480
C	6.040486	0.346043	-0.393904
C	5.983618	-0.336003	0.858415
C	4.798736	0.080854	1.535625
H	3.161069	1.494891	0.904009
H	4.616137	1.783498	-1.352351
H	6.795488	0.209955	-1.161052
H	6.690856	-1.079254	1.211422
H	4.445707	-0.295125	2.491045
Fe	4.340174	-0.756165	-0.253847
C	4.173180	-1.793899	-1.986033
C	2.926043	-1.187247	-1.613732
C	4.573305	-2.661943	-0.933639
H	4.719590	-1.583047	-2.898452
C	2.556600	-1.689778	-0.303283
C	3.587262	-2.604398	0.091554
H	5.497820	-3.228828	-0.896421
P	1.012435	-1.310820	0.584272
C	0.076296	-2.858479	0.319055
C	-0.873793	-3.292422	1.251632
C	0.187229	-3.538045	-0.901511
C	-1.681170	-4.391856	0.976073
H	-0.979915	-2.765464	2.200130
C	-0.620141	-4.637864	-1.173254
H	0.911687	-3.203420	-1.644277
C	-1.555847	-5.069114	-0.234812
H	-2.419421	-4.713353	1.709078
H	-0.520306	-5.157336	-2.124811
H	-2.192808	-5.924540	-0.451250
C	1.511881	-1.346198	2.339566
C	1.607432	-0.116333	3.001934
C	1.824700	-2.521685	3.034139
C	2.024992	-0.059017	4.328804
H	1.351218	0.796994	2.462465
C	2.240868	-2.462303	4.360969
H	1.724852	-3.487860	2.538391
C	2.344884	-1.231776	5.008597
H	2.091339	0.903472	4.833838
H	2.478702	-3.380797	4.895168
H	2.664817	-1.190666	6.048283
C	2.219100	-0.210986	-2.424503
N	1.148671	0.440551	-2.124872
O	2.760337	0.009446	-3.647680
C	1.849603	0.896601	-4.335033
H	2.437391	1.734355	-4.727965
H	1.421604	0.342364	-5.177411
C	0.818102	1.303074	-3.267621
C	-1.194478	3.044053	0.340079
H	-1.570797	3.931913	-0.209433
C	-3.268134	0.540856	-1.258993
C	-4.516274	0.651857	-1.889394
C	-2.715612	-0.739516	-1.111435
C	-5.186992	-0.466124	-2.370062
H	-4.970453	1.637243	-1.991125
C	-3.364009	-1.867244	-1.592219
H	-1.766124	-0.854861	-0.586488

C	-4.598536	-1.717864	-2.218361
H	-6.155836	-0.373365	-2.854610
H	-2.927228	-2.855643	-1.465918
Cl	-5.420909	-3.136432	-2.832057
C	-2.644379	1.745314	-0.716509
H	-3.110575	2.666745	-1.102078
N	-1.328041	1.839795	-0.411708
C	0.238808	3.285227	0.692381
O	1.104429	2.417170	0.718922
O	0.503298	4.561115	1.011388
C	1.848376	4.809416	1.435963
H	2.560296	4.503559	0.662094
H	1.906085	5.883414	1.613826
H	2.066319	4.254826	2.355264
Cu	0.111454	0.486494	-0.245134
H	3.627173	-3.123243	1.044466
H	-0.204813	1.057131	-3.588752
C	0.841412	2.791305	-2.890564
C	0.402810	3.638855	-4.076774
C	2.190383	3.235429	-2.345205
H	0.093353	2.892499	-2.091103
H	-0.583575	3.334449	-4.448610
H	0.342886	4.698425	-3.803093
H	1.111699	3.564381	-4.914500
H	2.466880	2.654622	-1.457194
H	2.992823	3.133722	-3.091638
H	2.159966	4.293774	-2.056166
C	-3.751771	0.798471	1.669181
C	-5.169615	0.665625	1.535842
C	-5.809946	-0.540967	1.818049
C	-5.057414	-1.627017	2.251490
C	-3.671158	-1.510302	2.377548
C	-3.012537	-0.317509	2.075713
C	-5.692244	1.919959	1.063289
H	-6.890227	-0.629111	1.697167
H	-5.546600	-2.571763	2.486265
H	-3.094269	-2.368053	2.720506
H	-1.923863	-0.282106	2.143009
H	-6.739547	2.121689	0.851645
C	-4.652509	2.791588	0.919937
H	-4.740497	3.816777	0.565214
C	-3.381337	2.141054	1.203456
C	-2.156456	2.932243	1.645526
C	-2.518971	4.344699	2.105323
H	-1.618349	4.904251	2.388267
H	-3.022925	4.915649	1.316410
H	-3.188467	4.317173	2.973078
C	-1.365431	2.242845	2.758157
H	-0.606684	2.926786	3.170549
H	-2.016956	1.926273	3.580036
H	-0.838991	1.355211	2.386966

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C	5.345957	0.248318	-0.574539
C	5.781508	-1.114636	-0.463104
C	7.044445	-1.415786	0.050649
C	7.878547	-0.385128	0.468836
C	7.453575	0.946439	0.384938
C	6.200522	1.265952	-0.131730
C	4.710947	-1.961781	-0.905216
H	7.368829	-2.454843	0.130447
H	8.864587	-0.612483	0.872870
H	8.110936	1.744897	0.727457
H	5.899845	2.312811	-0.166146
H	4.742921	-3.048618	-0.943281
C	3.647772	-1.164324	-1.244875
H	2.688853	-1.518603	-1.614628
C	3.989833	0.231229	-1.099157
C	3.161264	1.317731	-1.533931
C	3.848612	2.545896	-2.097557
H	3.114160	3.306821	-2.388374
H	4.548896	3.012157	-1.398353
H	4.421272	2.281357	-2.996396
C	1.964075	0.919952	-2.372811
H	1.350907	1.794087	-2.628273
H	2.278516	0.451077	-3.316081
H	1.319019	0.201456	-1.847307
C	-3.915366	0.945398	-0.594203
C	-4.679090	1.085498	0.603934
C	-5.878193	0.330218	0.453033
C	-5.857186	-0.276862	-0.838443
C	-4.644721	0.101419	-1.487670
H	-2.927575	1.361682	-0.774786
H	-4.376488	1.625359	1.496022
H	-6.645112	0.197789	1.208649
H	-6.609500	-0.948916	-1.237797
H	-4.311185	-0.232592	-2.465605
Fe	-4.247578	-0.868089	0.246842
C	-4.160116	-2.028931	1.902544
C	-2.878344	-1.460501	1.590638
C	-4.584957	-2.802899	0.789389
H	-4.710147	-1.853426	2.820332
C	-2.513022	-1.889127	0.249775
C	-3.583395	-2.721129	-0.218140
H	-5.534813	-3.320077	0.701595
P	-0.960193	-1.513571	-0.629441
C	-0.171375	-3.155933	-0.752191
C	0.758252	-3.395681	-1.771679
C	-0.344592	-4.116209	0.249766
C	1.500002	-4.571691	-1.788480
H	0.906199	-2.651972	-2.556350
C	0.393753	-5.295580	0.226982
H	-1.049452	-3.931708	1.060829
C	1.319029	-5.525322	-0.788651
H	2.227009	-4.737557	-2.581746
H	0.248317	-6.036797	1.011152
H	1.901379	-6.444997	-0.799654
C	-1.506913	-1.171608	-2.342751
C	-1.447045	0.145214	-2.811797
C	-1.999227	-2.171087	-3.192685
C	-1.905777	0.468991	-4.085588
H	-1.022726	0.920783	-2.173525

C	-2.456555	-1.849181	-4.466652
H	-2.002820	-3.209595	-2.860616
C	-2.418999	-0.527657	-4.911708
H	-1.851431	1.499396	-4.432959
H	-2.836822	-2.633286	-5.119451
H	-2.774454	-0.279507	-5.910295
C	-2.163413	-0.555871	2.473495
N	-1.043479	0.039379	2.250966
O	-2.754632	-0.325992	3.669549
C	-1.848343	0.522990	4.413432
H	-2.416875	1.398914	4.747321
H	-1.520819	-0.039493	5.293642
C	-0.715249	0.852118	3.426480
C	2.895538	0.277830	1.350582
H	3.881355	0.717133	1.504423
C	1.305440	3.089776	-0.268971
C	1.703469	4.421282	-0.469502
C	-0.049817	2.790184	-0.479805
C	0.809819	5.401819	-0.882742
H	2.745529	4.691812	-0.296829
C	-0.958925	3.753640	-0.895621
H	-0.401452	1.768603	-0.300301
C	-0.521080	5.058860	-1.101584
H	1.139313	6.426982	-1.032184
H	-2.007675	3.504235	-1.051372
Cl	-1.654006	6.279245	-1.630927
C	2.307184	2.076115	0.100884
H	3.238047	2.527908	0.477134
N	1.901209	0.958798	0.797896
C	2.675784	-1.092053	1.728092
O	1.585183	-1.678417	1.656865
O	3.804843	-1.702700	2.120556
C	3.704581	-3.118467	2.258035
H	3.254405	-3.556017	1.360124
H	4.730314	-3.469981	2.383976
H	3.096374	-3.383968	3.130207
Cu	0.225015	-0.192985	0.641309
H	-3.633302	-3.172529	-1.204079
H	0.256058	0.505093	3.810540
C	-0.575305	2.336494	3.061971
C	-0.115244	3.136421	4.272525
C	-1.848037	2.908141	2.456784
H	0.212678	2.377728	2.293570
H	0.821105	2.742395	4.687009
H	0.053232	4.186601	4.009246
H	-0.866981	3.122635	5.075385
H	-2.164138	2.324768	1.582810
H	-2.678207	2.923154	3.179001
H	-1.690475	3.939368	2.120486

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C	5.281281	0.204691	-0.390354
C	5.804744	-1.118144	-0.525379
C	7.106685	-1.408169	-0.114714
C	7.892610	-0.397053	0.429935
C	7.379021	0.895287	0.584880
C	6.078262	1.197093	0.186287
C	4.761417	-1.951920	-1.063502
H	7.502404	-2.420193	-0.214076
H	8.911794	-0.613831	0.748084
H	8.001471	1.673488	1.025049
H	5.690602	2.204925	0.345136
H	4.850630	-3.016388	-1.271668
C	3.643080	-1.183710	-1.233544
H	2.692128	-1.537198	-1.622838
C	3.877746	0.180843	-0.793569
C	3.064779	1.354840	-1.301052
C	3.932544	2.389684	-2.021050
H	3.311774	3.198795	-2.428898
H	4.684637	2.839921	-1.364447
H	4.468118	1.928539	-2.859066
C	1.977858	0.898441	-2.275969
H	1.418806	1.759650	-2.665871
H	2.415432	0.367528	-3.130408
H	1.257739	0.222291	-1.794270
C	-3.959641	0.927368	-0.566927
C	-4.717051	1.061484	0.635926
C	-5.909257	0.293780	0.494018
C	-5.890371	-0.315134	-0.796635
C	-4.686131	0.074674	-1.454314
H	-2.978231	1.354626	-0.756242
H	-4.414473	1.605514	1.525213
H	-6.670112	0.155175	1.254682
H	-6.637993	-0.995884	-1.190025
H	-4.355412	-0.257810	-2.433757
Fe	-4.268273	-0.888585	0.278736
C	-4.156762	-2.050348	1.932964
C	-2.881239	-1.473901	1.610821
C	-4.586561	-2.825450	0.822228
H	-4.698935	-1.881126	2.856637
C	-2.525839	-1.896963	0.266062
C	-3.594465	-2.735452	-0.194088
H	-5.533697	-3.348949	0.742274
P	-0.984278	-1.499655	-0.622968
C	-0.178203	-3.133346	-0.753845
C	0.743523	-3.368107	-1.781770
C	-0.328883	-4.091017	0.254562
C	1.500448	-4.534699	-1.799010
H	0.873666	-2.627055	-2.572333
C	0.424377	-5.260681	0.231638
H	-1.027990	-3.911396	1.071673
C	1.342460	-5.484684	-0.791727
H	2.219424	-4.697724	-2.600406
H	0.295685	-5.999295	1.021236
H	1.936133	-6.397084	-0.803695
C	-1.546455	-1.161100	-2.332098
C	-1.496202	0.156619	-2.800461
C	-2.040706	-2.161904	-3.179262
C	-1.968508	0.479450	-4.069616
H	-1.070122	0.933443	-2.164136
C	-2.510775	-1.841143	-4.448867
H	-2.036427	-3.200729	-2.848042
C	-2.484299	-0.518788	-4.892248

H	-1.923214	1.510415	-4.416458
H	-2.892968	-2.626334	-5.099302
H	-2.850693	-0.271002	-5.886991
C	-2.158778	-0.571469	2.490247
N	-1.022468	-0.006276	2.275425
O	-2.763631	-0.309262	3.674462
C	-1.839137	0.514669	4.423900
H	-2.391259	1.394573	4.774015
H	-1.513750	-0.065362	5.294054
C	-0.708079	0.837359	3.433114
C	2.932029	0.287898	1.175598
H	3.829279	0.792776	1.550315
C	1.345065	3.120380	-0.375773
C	1.767025	4.431358	-0.621308
C	-0.019822	2.847080	-0.507442
C	0.876661	5.428902	-1.005923
H	2.823196	4.678104	-0.507222
C	-0.930456	3.825726	-0.890148
H	-0.380032	1.836059	-0.287273
C	-0.470993	5.114014	-1.143503
H	1.220791	6.443133	-1.192163
H	-1.992225	3.601054	-0.979795
Cl	-1.601547	6.356362	-1.625415
C	2.350752	2.062160	-0.016329
H	3.197222	2.570104	0.492800
N	1.854247	0.997288	0.804722
C	2.743228	-1.096509	1.601056
O	1.664475	-1.692675	1.568097
O	3.889870	-1.678272	1.971513
C	3.821032	-3.095988	2.129347
H	3.360272	-3.551084	1.245645
H	4.855929	-3.425040	2.237842
H	3.235872	-3.359968	3.017058
Cu	0.222014	-0.170556	0.609056
H	-3.651028	-3.184082	-1.180919
H	0.267841	0.517035	3.827258
C	-0.594142	2.314906	3.031459
C	-0.145414	3.153016	4.220069
C	-1.881188	2.847223	2.420751
H	0.191352	2.347838	2.260169
H	0.800316	2.787155	4.638887
H	0.001864	4.199377	3.929796
H	-0.892755	3.145439	5.027324
H	-2.191535	2.237110	1.562521
H	-2.708105	2.860111	3.147083
H	-1.748037	3.874365	2.062157

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C	3.023524	-2.845482	-0.639819
C	3.509299	-3.373031	0.595262
C	4.933454	-3.337925	0.567730
C	5.334850	-2.792011	-0.687772
C	4.157218	-2.486653	-1.433491
H	1.976072	-2.700116	-0.898833
H	2.901779	-3.687579	1.437840
H	5.592875	-3.627101	1.379449
H	6.355328	-2.593824	-0.998889
H	4.124424	-2.015209	-2.411052
Fe	4.171358	-1.470094	0.324987
C	4.538325	-0.464373	2.042794
C	3.186426	-0.265101	1.597475
C	5.413188	-0.012645	1.017924
H	4.821032	-0.921180	2.984545
C	3.235583	0.313913	0.266459
C	4.622315	0.460923	-0.067448
H	6.496400	-0.073180	1.037514
P	1.796386	0.798236	-0.726999
C	1.883173	2.623046	-0.709130
C	1.002634	3.329490	-1.541702
C	2.716011	3.336550	0.158953
C	0.977567	4.717684	-1.523747
H	0.326044	2.782639	-2.200491
C	2.679057	4.729897	0.181685
H	3.397921	2.804567	0.821971
C	1.818043	5.422882	-0.662537
H	0.282935	5.253832	-2.168707
H	3.330930	5.274544	0.863092
H	1.784762	6.510074	-0.637465
C	2.286765	0.368232	-2.435682
C	1.669392	-0.731284	-3.043497
C	3.260502	1.084344	-3.143299
C	2.045443	-1.129151	-4.324174
H	0.895568	-1.274933	-2.498701
C	3.636011	0.683650	-4.421664
H	3.711882	1.970332	-2.694192
C	3.033553	-0.427508	-5.010940
H	1.559026	-1.985124	-4.789595
H	4.395630	1.244154	-4.964239
H	3.325258	-0.736331	-6.013369
C	2.021877	-0.695801	2.350856
N	0.774476	-0.623185	2.020088
O	2.307450	-1.245027	3.554710
C	1.039698	-1.523876	4.187933
H	1.062944	-2.563852	4.532338
H	0.955650	-0.866749	5.060173
C	-0.008642	-1.244725	3.100629
C	-2.378962	-1.036223	-1.046894
H	-3.338275	-1.044022	-1.563378
C	-2.280282	2.392137	0.119518
C	-2.873641	3.550213	-0.406131
C	-1.224886	2.561841	1.031178
C	-2.444823	4.821378	-0.046536
H	-3.698341	3.445035	-1.112375
C	-0.777328	3.824728	1.398583
H	-0.744689	1.684171	1.470318
C	-1.397125	4.947993	0.860494
H	-2.915177	5.708621	-0.463751
H	0.048015	3.941510	2.097410
Cl	-0.852898	6.542669	1.328353
C	-2.813930	1.074938	-0.264723
H	-3.574527	1.139681	-1.057000
N	-1.922540	0.041023	-0.416397

C	-1.520776	-2.176236	-1.128266
O	-0.353831	-2.215989	-0.686081
O	-2.078724	-3.229167	-1.757301
C	-1.241928	-4.373887	-1.873354
H	-0.943358	-4.745300	-0.886580
H	-1.838300	-5.122644	-2.396143
H	-0.335578	-4.140022	-2.445818
Cu	0.015243	-0.136358	0.143649
H	4.995695	0.834529	-1.015875
H	-0.741670	-0.505827	3.455575
C	-0.779866	-2.478442	2.609541
C	-1.713026	-2.975679	3.704683
C	0.135751	-3.579250	2.097600
H	-1.390024	-2.137204	1.755530
H	-2.394603	-2.184802	4.045302
H	-2.326522	-3.811579	3.349525
H	-1.154097	-3.334945	4.581193
H	0.730974	-3.230787	1.246947
H	0.811211	-3.954808	2.881359
H	-0.456161	-4.434858	1.751404
C	-5.607285	-0.948985	-0.497657
C	-5.891091	-2.353642	-0.588667
C	-6.748599	-2.835605	-1.579387
C	-7.302909	-1.949627	-2.498100
C	-6.996104	-0.584767	-2.443523
C	-6.154050	-0.083415	-1.453427
C	-5.142038	-3.025196	0.434890
H	-6.972448	-3.901545	-1.639587
H	-7.972495	-2.320876	-3.273315
H	-7.422843	0.095144	-3.179689
H	-5.930092	0.983780	-1.444280
H	-5.168600	-4.093120	0.634887
C	-4.398404	-2.085991	1.105543
H	-3.752105	-2.282620	1.958956
C	-4.674807	-0.764280	0.597172
C	-4.136003	0.451304	1.112813
C	-5.047897	1.657461	1.195431
H	-4.501824	2.551920	1.517694
H	-5.550109	1.890907	0.252705
H	-5.835729	1.467584	1.937032
C	-3.280525	0.307590	2.348900
H	-2.830339	1.265960	2.636388
H	-3.875607	-0.047022	3.202856
H	-2.473870	-0.413702	2.177483

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C	-2.823094	-3.029728	0.298244
C	-3.412464	-3.406013	-0.948443
C	-4.825827	-3.458611	-0.775356
C	-5.115380	-3.114340	0.578467
C	-3.880748	-2.853368	1.243325
H	-1.762463	-2.861403	0.477310
H	-2.883418	-3.569961	-1.882026
H	-5.555061	-3.665597	-1.551624
H	-6.104680	-3.019020	1.013703
H	-3.768144	-2.518381	2.269847
Fe	-4.118084	-1.602226	-0.338211
C	-4.647263	-0.379224	-1.859890
C	-3.281754	-0.164092	-1.466287
C	-5.476788	-0.139025	-0.730916
H	-4.966710	-0.705639	-2.843233
C	-3.276078	0.207453	-0.062099
C	-4.643794	0.218491	0.367595
H	-6.554555	-0.261248	-0.699433
P	-1.783454	0.572406	0.896364
C	-1.852763	2.379736	1.142470
C	-0.794701	2.962955	1.857288
C	-2.828999	3.205609	0.576287
C	-0.736392	4.339794	2.028090
H	-0.005178	2.326562	2.261892
C	-2.754980	4.588754	0.734298
H	-3.647530	2.769417	0.003911
C	-1.716180	5.157110	1.464809
H	0.091434	4.780829	2.581001
H	-3.514924	5.224531	0.282382
H	-1.656046	6.237803	1.577853
C	-2.126827	-0.114462	2.555722
C	-1.382566	-1.232199	2.951876
C	-3.074609	0.422251	3.435661
C	-1.607131	-1.826745	4.190982
H	-0.625672	-1.630805	2.273098
C	-3.299636	-0.174180	4.672986
H	-3.625376	1.321484	3.155309
C	-2.570640	-1.302433	5.049129
H	-1.022865	-2.695717	4.489119
H	-4.038883	0.247911	5.351898
H	-2.744541	-1.762481	6.020370
C	-2.145074	-0.396992	-2.341310
N	-0.884132	-0.279847	-2.078338
O	-2.476431	-0.789512	-3.595194
C	-1.240673	-0.863675	-4.339354
H	-1.220809	-1.831253	-4.853456
H	-1.259552	-0.065774	-5.089957
C	-0.142267	-0.690593	-3.281378
C	2.560674	-0.729677	0.923643
H	3.231826	-0.584030	1.779762
C	2.185635	2.667506	-0.188378
C	2.679105	3.864357	0.337768
C	1.092699	2.741939	-1.060823
C	2.100833	5.093072	0.030955
H	3.532793	3.832699	1.016442
C	0.491635	3.955014	-1.374837
H	0.694147	1.825208	-1.499911
C	1.000545	5.123729	-0.817902
H	2.489111	6.016307	0.454407
H	-0.372933	3.995247	-2.033648
Cl	0.231419	6.652984	-1.177267
C	2.807395	1.356223	0.206358
H	3.405743	1.539609	1.125799
N	1.860317	0.308838	0.430878
C	1.907017	-2.037141	0.869524
O	0.821719	-2.255210	0.321601
O	2.624730	-2.994624	1.468525

C	2.103562	-4.315934	1.348276
H	2.008473	-4.596256	0.293941
H	2.825026	-4.961595	1.850379
H	1.119460	-4.391502	1.824989
Cu	0.013473	-0.060019	-0.195169
H	-4.974121	0.419761	1.382157
H	0.540132	0.127591	-3.557385
C	0.703517	-1.940757	-3.006265
C	1.616987	-2.235645	-4.186701
C	-0.140461	-3.142802	-2.616142
H	1.324042	-1.688295	-2.131796
H	2.253573	-1.375238	-4.431764
H	2.275662	-3.084639	-3.969531
H	1.044731	-2.495660	-5.089343
H	-0.741564	-2.921405	-1.727599
H	-0.810552	-3.461765	-3.428946
H	0.499530	-3.997296	-2.368583
C	5.302373	-1.015094	0.561429
C	5.719138	-2.349929	0.282426
C	6.680623	-2.972752	1.078640
C	7.230882	-2.278594	2.152460
C	6.809952	-0.977695	2.446013
C	5.842860	-0.348514	1.662811
C	4.966004	-2.819354	-0.852544
H	6.995542	-3.994842	0.863953
H	7.988030	-2.753688	2.775205
H	7.242146	-0.449529	3.295088
H	5.514032	0.659084	1.923840
H	5.066685	-3.801475	-1.308826
C	4.112438	-1.827038	-1.241552
H	3.435111	-1.881031	-2.090059
C	4.218902	-0.665559	-0.362074
C	3.888839	0.745270	-0.831985
C	5.111489	1.661261	-0.871798
H	4.823597	2.664949	-1.214710
H	5.590137	1.766192	0.107645
H	5.869342	1.276646	-1.564706
C	3.263013	0.722158	-2.226402
H	3.061989	1.740437	-2.582441
H	3.931497	0.239570	-2.949604
H	2.311342	0.174043	-2.219058

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C	5.750219	0.727794	-0.315205
C	6.487871	-0.325224	0.324877
C	7.526920	-0.973103	-0.346245
C	7.834218	-0.608531	-1.652580
C	7.100664	0.394310	-2.297079
C	6.066829	1.058438	-1.639691
C	5.930202	-0.532577	1.629245
H	8.085102	-1.768383	0.149772
H	8.642888	-1.111538	-2.181736
H	7.339320	0.661965	-3.325727
H	5.514108	1.825069	-2.181303
H	6.285581	-1.258294	2.355959
C	4.872064	0.327777	1.782243
H	4.252506	0.411515	2.673571
C	4.732237	1.172924	0.619105
C	3.796826	2.245611	0.498000
C	4.192469	3.465695	-0.310168
H	3.356028	4.172805	-0.384174
H	5.023054	3.988998	0.182212
H	4.518508	3.232310	-1.327036
C	3.112730	2.652513	1.786408
H	2.382765	3.453088	1.618713
H	2.590607	1.812384	2.256956
H	3.849982	3.025650	2.510469
C	-3.670455	1.518803	0.342379
C	-4.081766	1.310362	1.692164
C	-5.447695	0.900435	1.679875
C	-5.882813	0.861948	0.320128
C	-4.784026	1.242868	-0.507488
H	-2.671175	1.790386	0.017172
H	-3.448032	1.387985	2.571786
H	-6.038673	0.626002	2.547077
H	-6.863411	0.550387	-0.024399
H	-4.774818	1.272796	-1.592712
Fe	-4.310544	-0.386216	0.597836
C	-4.333755	-2.145499	1.598149
C	-2.993528	-1.724946	1.298986
C	-5.041697	-2.270040	0.371602
H	-4.730229	-2.296586	2.595879
C	-2.876537	-1.588313	-0.143406
C	-4.156326	-1.933584	-0.692470
H	-6.090265	-2.529436	0.268673
P	-1.364688	-1.119593	-1.033368
C	-0.766574	-2.698583	-1.732749
C	0.433583	-2.656798	-2.459308
C	-1.375294	-3.934757	-1.496626
C	0.998135	-3.824520	-2.957550
H	0.930501	-1.698517	-2.623208
C	-0.802991	-5.104768	-1.993019
H	-2.296971	-3.987326	-0.917864
C	0.378882	-5.052865	-2.725867
H	1.930996	-3.777265	-3.516740
H	-1.286729	-6.062124	-1.805101
H	0.823249	-5.969336	-3.110347
C	-1.988222	-0.197040	-2.483067
C	-2.665169	-0.820197	-3.539618
C	-1.796439	1.188967	-2.517875
C	-3.174664	-0.062285	-4.589273
H	-2.779920	-1.905237	-3.543471
C	-2.312784	1.947341	-3.565314
H	-1.231433	1.673014	-1.719607
C	-3.008375	1.322641	-4.597757
H	-3.698723	-0.553939	-5.407244
H	-2.163183	3.026165	-3.573500
H	-3.409268	1.912579	-5.420341
C	-1.993750	-1.417832	2.306518
N	-0.840115	-0.864614	2.143452
O	-2.325369	-1.778115	3.569843
C	-1.261088	-1.277806	4.416022
H	-1.656475	-0.411792	4.965864

H	-1.008388	-2.066607	5.128458
C	-0.142121	-0.915536	3.437640
C	2.846531	-0.648435	-0.367027
H	3.734792	-0.528304	-0.986914
C	1.198333	2.544051	-0.676289
C	1.040356	3.463203	-1.723320
C	0.262261	2.587348	0.372298
C	-0.032382	4.349583	-1.757348
H	1.759020	3.463496	-2.543480
C	-0.803283	3.476094	0.365949
H	0.395704	1.914026	1.219460
C	-0.958682	4.338456	-0.717977
H	-0.158537	5.038928	-2.589243
H	-1.514318	3.503343	1.189783
Cl	-2.343473	5.402496	-0.776594
C	2.301224	1.572597	-0.653445
H	2.912609	1.576716	-1.567513
N	1.961096	0.320218	-0.188879
C	2.556859	-1.928934	0.223213
O	1.541011	-2.185329	0.887405
O	3.506513	-2.849405	-0.030840
C	3.245957	-4.138704	0.514880
H	2.298091	-4.536455	0.133350
H	4.082089	-4.764950	0.200812
H	3.193313	-4.094499	1.607822
Cu	0.152739	-0.404428	0.392119
H	-4.411312	-1.891759	-1.746892
H	0.592675	-1.732555	3.363013
C	0.624098	0.377995	3.704440
C	1.522610	0.254481	4.925603
C	-0.282248	1.599062	3.788158
H	1.267207	0.487285	2.813298
H	2.195634	-0.608290	4.847237
H	2.143847	1.149999	5.047161
H	0.934634	0.140432	5.847942
H	-0.999546	1.620357	2.956559
H	-0.854672	1.623028	4.725935
H	0.304748	2.525051	3.747057

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C	5.534526	0.801693	0.180661
C	6.466910	-0.264778	0.359561
C	7.656214	-0.288586	-0.370913
C	7.923050	0.733831	-1.277713
C	7.001601	1.767986	-1.474064
C	5.808031	1.801177	-0.755916
C	5.900274	-1.188030	1.308284
H	8.368505	-1.104309	-0.237339
H	8.851018	0.723320	-1.848391
H	7.217601	2.553578	-2.197196
H	5.091236	2.602406	-0.945495
H	6.372179	-2.106429	1.650301
C	4.668491	-0.722735	1.678307
H	4.001079	-1.206030	2.389063
C	4.346116	0.510819	0.976827
C	3.352565	1.529026	1.500461
C	3.992794	2.887958	1.788174
H	3.238754	3.595724	2.160187
H	4.771653	2.797788	2.554574
H	4.459615	3.329360	0.901586
C	2.701152	1.030218	2.789993
H	2.027327	1.785420	3.213328
H	2.117509	0.119008	2.613663
H	3.462326	0.800331	3.545088
C	-4.103104	0.603299	1.495749
C	-3.713178	-0.520336	2.281176
C	-4.835031	-1.399152	2.385325
C	-5.918689	-0.815559	1.660019
C	-5.463825	0.419519	1.108323
H	-3.463828	1.426789	1.190809
H	-2.715820	-0.707968	2.671648
H	-4.845007	-2.363649	2.883053
H	-6.900786	-1.254120	1.519032
H	-6.043101	1.090138	0.481171
Fe	-4.323980	-1.132154	0.449308
C	-4.135662	-3.004664	-0.274685
C	-2.870272	-2.326676	-0.224895
C	-5.003873	-2.257482	-1.113275
H	-4.377021	-3.908669	0.272287
C	-2.966772	-1.128932	-1.045859
C	-4.294438	-1.120678	-1.591690
H	-6.042986	-2.490835	-1.320446
P	-1.544205	-0.043838	-1.363520
C	-1.033273	-0.583958	-3.041487
C	-1.611519	-0.078262	-4.211239
C	-0.023989	-1.551316	-3.138922
C	-1.185369	-0.530409	-5.455982
H	-2.388255	0.684115	-4.144657
C	0.394317	-2.006337	-4.386217
H	0.445266	-1.939075	-2.230359
C	-0.183580	-1.495309	-5.545483
H	-1.636022	-0.126268	-6.361219
H	1.184168	-2.752805	-4.451443
H	0.151258	-1.843788	-6.521007
C	-2.159248	1.645786	-1.647545
C	-1.196213	2.576598	-2.069569
C	-3.462904	2.091456	-1.404109
C	-1.536800	3.910152	-2.255943
H	-0.170038	2.246669	-2.243319
C	-3.795876	3.433059	-1.575646
H	-4.219379	1.387757	-1.065889
C	-2.836859	4.345232	-2.004411
H	-0.776188	4.618063	-2.582253
H	-4.812669	3.765082	-1.369430
H	-3.097345	5.394634	-2.130695
C	-1.766864	-2.788408	0.599670
N	-0.581774	-2.290998	0.722021
O	-2.033573	-3.909311	1.311850
C	-0.869077	-4.151277	2.136959
H	-1.153421	-3.941082	3.177740
H	-0.617099	-5.211216	2.047088
C	0.194543	-3.196621	1.588593
C	2.990479	-0.100258	-0.610917

H	3.608644	0.500154	-1.287723
C	1.010239	2.538966	0.804794
C	0.892676	3.887018	0.458996
C	-0.023489	1.969099	1.559050
C	-0.218869	4.643291	0.821957
H	1.686824	4.354480	-0.125490
C	-1.138035	2.704922	1.942183
H	0.060909	0.927965	1.876680
C	-1.233055	4.038560	1.555078
H	-0.306642	5.686613	0.527964
H	-1.918122	2.257769	2.554415
Cl	-2.650869	4.960593	1.999644
C	2.203849	1.735972	0.371668
H	2.725757	2.309140	-0.425331
N	1.867523	0.422781	-0.095545
C	3.104909	-1.547999	-0.787353
O	2.283703	-2.387254	-0.430830
O	4.280482	-1.859899	-1.363921
C	4.584614	-3.249429	-1.410878
H	3.923898	-3.769670	-2.114081
H	5.622082	-3.311065	-1.743974
H	4.472396	-3.700862	-0.419399
Cu	0.186807	-0.556816	-0.015408
H	-4.696049	-0.356260	-2.249176
H	0.900255	-3.726038	0.935407
C	1.014861	-2.423099	2.619078
C	1.926795	-3.357521	3.399091
C	0.154819	-1.565239	3.536081
H	1.646291	-1.752961	2.011376
H	2.583762	-3.924531	2.726802
H	2.565639	-2.794324	4.090039
H	1.354962	-4.077995	4.002609
H	-0.482257	-0.884182	2.954276
H	-0.500955	-2.167613	4.181592
H	0.777091	-0.949695	4.196017

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C	3.253449	-2.271720	0.857334
C	4.031970	-1.761557	1.940987
C	5.397285	-1.725086	1.532660
C	5.467941	-2.213784	0.193746
C	4.145706	-2.551834	-0.224168
H	2.169963	-2.375872	0.847404
H	3.645226	-1.400484	2.888760
H	6.227664	-1.345651	2.119084
H	6.362907	-2.268925	-0.417097
H	3.858886	-2.906038	-1.209705
Fe	4.251917	-0.594907	0.291249
C	4.722082	1.339399	0.657366
C	3.299827	1.137919	0.620990
C	5.257585	0.937747	-0.596226
H	5.277777	1.698959	1.516119
C	2.958516	0.592720	-0.682891
C	4.185700	0.486564	-1.416384
H	6.309485	0.925804	-0.861597
P	1.286972	0.179178	-1.276591
C	0.980660	1.520074	-2.481728
C	0.165189	1.304484	-3.600004
C	1.421520	2.821259	-2.205963
C	-0.200115	2.365903	-4.421467
H	-0.196770	0.300140	-3.822071
C	1.056590	3.880165	-3.031779
H	2.051723	3.006526	-1.334507
C	0.241566	3.656163	-4.138872
H	-0.838903	2.182238	-5.283836
H	1.408295	4.886038	-2.806698
H	-0.049718	4.486682	-4.778984
C	1.537366	-1.310236	-2.305225
C	1.048485	-2.529543	-1.820128
C	2.202454	-1.281247	-3.538629
C	1.245032	-3.702988	-2.544274
H	0.500343	-2.547261	-0.876497
C	2.396144	-2.455137	-4.259489
H	2.549740	-0.330818	-3.945069
C	1.922285	-3.668348	-3.760381
H	0.855959	-4.644968	-2.160824
H	2.911006	-2.423034	-5.218425
H	2.069707	-4.584631	-4.329656
C	2.421558	1.377445	1.752146
N	1.151683	1.164085	1.828883
O	3.027207	1.894103	2.846186
C	1.982082	2.129862	3.816937
H	2.281478	1.637615	4.749640
H	1.930834	3.209918	3.990252
C	0.712039	1.538552	3.180487
C	-2.347068	-1.139381	1.455448
H	-3.366929	-1.377642	1.760326
C	-2.856007	2.300366	0.489894
C	-3.910477	3.180615	0.771450
C	-1.649336	2.859699	0.041245
C	-3.776422	4.557395	0.627560
H	-4.859850	2.773142	1.120640
C	-1.492965	4.231134	-0.105183
H	-0.812079	2.206603	-0.213212
C	-2.561265	5.073936	0.191728
H	-4.602957	5.225298	0.856959
H	-0.552246	4.644636	-0.461507
Cl	-2.367550	6.802692	0.014657
C	-3.068190	0.845329	0.640342
H	-3.995165	0.627067	1.194069
N	-1.998911	0.066574	1.026263
C	-1.344448	-2.158450	1.522150
O	-0.140952	-1.979768	1.250467
O	-1.829781	-3.357307	1.876118
C	-0.895908	-4.431735	1.828993
H	-0.103407	-4.292564	2.573968
H	-1.474613	-5.330136	2.047913
H	-0.440498	-4.504360	0.835061
Cu	-0.023542	0.107246	0.475559
H	4.279287	0.070579	-2.414296
H	-0.071999	2.303611	3.078658
C	0.111756	0.344633	3.936784
C	-0.409454	0.793515	5.295248

C	1.084009	-0.819093	4.056532
H	-0.742324	0.008332	3.330831
H	-1.128409	1.617243	5.203270
H	-0.912510	-0.029900	5.814295
H	0.405236	1.134333	5.950786
H	1.404079	-1.164944	3.067384
H	1.974853	-0.553570	4.646221
H	0.607618	-1.668802	4.560595
C	-4.503111	-2.351450	-0.386644
C	-3.959509	-3.656414	-0.641778
C	-4.637782	-4.802827	-0.221828
C	-5.844858	-4.677404	0.456002
C	-6.373900	-3.408967	0.725257
C	-5.714097	-2.254909	0.311546
C	-2.700392	-3.491088	-1.308972
H	-4.217089	-5.790123	-0.421136
H	-6.380594	-5.567447	0.784347
H	-7.316145	-3.321267	1.265215
H	-6.154347	-1.287534	0.550269
H	-2.058547	-4.300354	-1.651619
C	-2.463185	-2.144941	-1.445452
H	-1.593292	-1.703822	-1.929841
C	-3.564995	-1.376008	-0.915579
C	-3.674431	0.054310	-1.037589
C	-2.726829	0.670141	-2.048322
H	-2.861823	1.755962	-2.120553
H	-1.679411	0.487713	-1.774063
H	-2.885812	0.246637	-3.049586
C	-5.064648	0.651132	-1.150952
H	-5.008689	1.744590	-1.223173
H	-5.567434	0.285088	-2.055788
H	-5.711500	0.410699	-0.302047

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C	3.008597	-2.654314	0.114763
C	3.800008	-2.675358	1.303474
C	5.174632	-2.666066	0.926471
C	5.238155	-2.640302	-0.499022
C	3.902343	-2.634545	-1.000642
H	1.922380	-2.613386	0.076754
H	3.422591	-2.637793	2.320961
H	6.021930	-2.629939	1.603292
H	6.143161	-2.587277	-1.095178
H	3.613653	-2.570972	-2.045340
Fe	4.220874	-1.025611	0.197749
C	4.863303	0.554872	1.285750
C	3.434940	0.569398	1.128598
C	5.451394	0.585766	-0.008274
H	5.383980	0.493540	2.234848
C	3.143019	0.601174	-0.293630
C	4.405298	0.616137	-0.972971
H	6.513950	0.537025	-0.222966
P	1.485448	0.671596	-1.037975
C	1.428712	2.381815	-1.679914
C	0.583453	2.699967	-2.752426
C	2.098274	3.417362	-1.014492
C	0.420414	4.021712	-3.152923
H	0.050141	1.905499	-3.275484
C	1.933332	4.739084	-1.420028
H	2.755032	3.186685	-0.175017
C	1.092858	5.045356	-2.487666
H	-0.238568	4.253819	-3.987799
H	2.463368	5.533380	-0.896858
H	0.958898	6.079806	-2.798559
C	1.619021	-0.365246	-2.536044
C	0.944068	-1.591206	-2.523555
C	2.349859	0.001259	-3.673614
C	1.009906	-2.445293	-3.621288
H	0.365226	-1.868195	-1.641270
C	2.419305	-0.856518	-4.767803
H	2.847263	0.971378	-3.710423
C	1.752288	-2.081499	-4.742174
H	0.467429	-3.390260	-3.600882
H	2.988144	-0.564186	-5.648929
H	1.800413	-2.744016	-5.604705
C	2.495117	0.496621	2.234306
N	1.207993	0.431609	2.180722
O	3.062437	0.512677	3.464179
C	1.972187	0.547749	4.412067
H	2.142241	-0.253260	5.141006
H	2.018757	1.511047	4.931738
C	0.705379	0.361226	3.559876
C	-2.420345	-1.279759	0.896369
H	-3.350907	-1.529081	1.420316
C	-2.871688	2.279638	0.613871
C	-3.953742	3.099687	0.949032
C	-1.640704	2.895692	0.369188
C	-3.827810	4.483310	1.030325
H	-4.922803	2.641523	1.151803
C	-1.486528	4.274686	0.449206
H	-0.777461	2.282164	0.103379
C	-2.587809	5.058841	0.776397
H	-4.677887	5.108238	1.292451
H	-0.522123	4.737656	0.252936
Cl	-2.404872	6.796931	0.867604
C	-3.073595	0.794305	0.499166
H	-3.962940	0.537431	1.114088
N	-1.957757	-0.015444	0.894569
C	-1.448835	-2.357747	0.767568
O	-0.256947	-2.181839	0.489171
O	-1.981928	-3.573478	0.924797
C	-1.118148	-4.661983	0.598130
H	-0.282865	-4.722687	1.305594
H	-1.740747	-5.555517	0.657478
H	-0.719351	-4.540525	-0.415185
Cu	0.004280	0.135378	0.478430
H	4.531785	0.600220	-2.051081
H	0.004481	1.196283	3.704704
C	-0.062449	-0.942073	3.822781
C	-0.654743	-0.928097	5.225537
C	0.785016	-2.182233	3.582393
H	-0.889050	-0.943100	3.096490
H	-1.282789	-0.044368	5.393538

H	-1.275036	-1.814713	5.398488
H	0.129511	-0.931461	5.996718
H	1.165639	-2.207413	2.555088
H	1.637324	-2.240937	4.276550
H	0.188486	-3.090482	3.734618
C	-4.625719	-2.092873	-0.602983
C	-4.454126	-3.357354	-1.241184
C	-5.352487	-4.397612	-0.998956
C	-6.416040	-4.190828	-0.124931
C	-6.575729	-2.960746	0.521534
C	-5.681364	-1.916083	0.293110
C	-3.258358	-3.284866	-2.043689
H	-5.219974	-5.364981	-1.485428
H	-7.125915	-4.995169	0.064556
H	-7.406091	-2.817812	1.211896
H	-5.811961	-0.971775	0.825119
H	-2.865488	-4.091664	-2.659463
C	-2.711190	-2.041863	-1.891202
H	-1.814169	-1.683676	-2.390520
C	-3.488622	-1.240792	-0.954083
C	-3.488425	0.277644	-0.983721
C	-2.471058	0.808289	-1.995129
H	-2.470030	1.905910	-2.005867
H	-1.451360	0.474265	-1.754170
H	-2.709377	0.461694	-3.008546
C	-4.859302	0.852818	-1.344634
H	-4.815826	1.949390	-1.385726
H	-5.186762	0.495022	-2.328034
H	-5.634531	0.573873	-0.622405

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C	-5.021310	0.243419	-0.548434
C	-6.190528	-0.257729	0.117868
C	-6.694756	-1.525264	-0.188558
C	-6.052214	-2.311631	-1.138562
C	-4.905143	-1.831609	-1.787318
C	-4.397213	-0.566108	-1.507076
C	-6.614910	0.732016	1.061255
H	-7.585471	-1.895870	0.321524
H	-6.441468	-3.299440	-1.384093
H	-4.403945	-2.458463	-2.527845
H	-3.499755	-0.233281	-2.023639
H	-7.476879	0.645848	1.717842
C	-5.752298	1.801373	0.986940
H	-5.839331	2.710807	1.576708
C	-4.747859	1.572196	-0.013615
C	-3.742869	2.515550	-0.399459
C	-3.167613	2.393902	-1.793428
H	-2.537876	3.257443	-2.040452
H	-2.541855	1.502935	-1.885272
H	-3.959852	2.318769	-2.550338
C	-4.007650	3.959505	-0.022490
H	-3.123586	4.581817	-0.210396
H	-4.830083	4.369178	-0.624528
H	-4.283545	4.079755	1.031531
C	4.120511	0.762407	-1.444348
C	3.685545	0.084456	-2.620054
C	4.668686	-0.890463	-2.963972
C	5.717119	-0.814361	-1.997770
C	5.377232	0.206624	-1.059087
H	3.575315	1.532832	-0.907317
H	2.748590	0.246683	-3.142281
H	4.606360	-1.595365	-3.786466
H	6.596339	-1.448604	-1.959506
H	5.963106	0.491961	-0.191054
Fe	3.957456	-1.246516	-1.104117
C	3.339041	-3.164205	-1.212612
C	2.246415	-2.291757	-0.886144
C	4.329049	-3.031906	-0.203643
H	3.391112	-3.786346	-2.098632
C	2.576518	-1.596580	0.348736
C	3.866586	-2.082250	0.749560
H	5.291521	-3.532645	-0.187949
P	1.374376	-0.623747	1.317074
C	1.298357	-1.609625	2.863841
C	2.210760	-1.426899	3.909677
C	0.302726	-2.587354	2.985133
C	2.135948	-2.215040	5.053240
H	2.976665	-0.654282	3.832910
C	0.235354	-3.377176	4.130147
H	-0.427000	-2.714956	2.183060
C	1.150503	-3.193798	5.163972
H	2.848683	-2.062619	5.862326
H	-0.544024	-4.132624	4.218832
H	1.091374	-3.808080	6.060837
C	2.191267	0.909338	1.872506
C	1.355153	1.868158	2.460531
C	3.557801	1.180260	1.761391
C	1.877907	3.069483	2.925287
H	0.283625	1.671365	2.532986
C	4.075473	2.395433	2.204178
H	4.216626	0.442596	1.308384
C	3.237568	3.341244	2.788570
H	1.213159	3.808687	3.369122
H	5.139217	2.602317	2.091341
H	3.641558	4.293240	3.128256
C	1.057502	-2.191878	-1.715170
N	-0.014790	-1.499566	-1.523462
O	1.092941	-2.972159	-2.821743
C	-0.218156	-2.885840	-3.423675
H	-0.077839	-2.668636	-4.488843
H	-0.693130	-3.867540	-3.321977
C	-0.930118	-1.772008	-2.643183
C	-2.920655	0.153098	1.506908
H	-3.639998	0.671284	2.141850
C	-0.967398	2.917128	0.256740
C	-0.677308	4.176646	0.800637
C	-0.092559	2.419842	-0.725578
C	0.461025	4.887872	0.440228
H	-1.345953	4.590137	1.557168
C	1.050859	3.115106	-1.097615
H	-0.305654	1.460376	-1.202889

C	1.333205	4.337848	-0.493579
H	0.687972	5.847954	0.898193
H	1.722262	2.717214	-1.856593
Cl	2.811927	5.176507	-0.898357
C	-2.136949	2.164715	0.739540
H	-2.589475	2.618615	1.633321
N	-2.001982	0.795305	0.804188
C	-2.959757	-1.279170	1.403604
O	-2.153464	-1.952816	0.741208
O	-3.976768	-1.827957	2.087742
C	-4.141355	-3.230448	1.901926
H	-3.253319	-3.775432	2.243496
H	-5.012469	-3.504263	2.498831
H	-4.320704	-3.451088	0.844427
Cu	-0.520488	-0.462739	0.182900
H	4.399599	-1.768102	1.642234
H	-1.881966	-2.122318	-2.217067
C	-1.204474	-0.498363	-3.449447
C	-2.244366	-0.747831	-4.531152
C	0.064469	0.132187	-3.999219
H	-1.626241	0.209598	-2.722827
H	-3.167601	-1.173410	-4.117344
H	-2.512270	0.186920	-5.037504
H	-1.870179	-1.437392	-5.301461
H	0.748416	0.386498	-3.180493
H	0.597334	-0.536126	-4.691865
H	-0.160442	1.056684	-4.543723

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C	-4.844948	0.146218	-0.543655
C	-6.119293	-0.335979	-0.113995
C	-6.706350	-1.445620	-0.724612
C	-6.038346	-2.089666	-1.762898
C	-4.779617	-1.636535	-2.174360
C	-4.183639	-0.529559	-1.570679
C	-6.542250	0.471902	0.997243
H	-7.677065	-1.808862	-0.384212
H	-6.491136	-2.952154	-2.250822
H	-4.254274	-2.161152	-2.974559
H	-3.183252	-0.225583	-1.869913
H	-7.470209	0.341396	1.548748
C	-5.576387	1.404055	1.247045
H	-5.621880	2.150884	2.036553
C	-4.441602	1.241732	0.352913
C	-3.530360	2.413802	-0.002941
C	-3.231912	2.489978	-1.499105
H	-2.741798	3.440517	-1.748124
H	-2.555980	1.688064	-1.810071
H	-4.146073	2.405998	-2.098075
C	-4.124937	3.756575	0.427995
H	-3.433280	4.571644	0.172797
H	-5.077450	3.958997	-0.076017
H	-4.302450	3.805802	1.509439
C	4.156624	0.745518	-1.222730
C	3.807262	0.145017	-2.467377
C	4.822337	-0.795355	-2.812968
C	5.806806	-0.775634	-1.779096
C	5.394547	0.175346	-0.797722
H	3.567417	1.474952	-0.673328
H	2.903397	0.331295	-3.036945
H	4.820805	-1.444324	-3.682318
H	6.689956	-1.403514	-1.727575
H	5.921404	0.407728	0.122384
Fe	3.996252	-1.280948	-1.028538
C	3.346128	-3.167666	-1.319949
C	2.260761	-2.298559	-0.960662
C	4.300310	-3.143553	-0.267882
H	3.423056	-3.711605	-2.254190
C	2.560560	-1.715190	0.338572
C	3.822209	-2.265353	0.744751
H	5.250200	-3.668011	-0.260202
P	1.351249	-0.758503	1.310135
C	1.134830	-1.834631	2.778213
C	1.845776	-1.669616	3.971805
C	0.180102	-2.857146	2.685423
C	1.606987	-2.515238	5.052221
H	2.580647	-0.868887	4.060115
C	-0.047452	-3.705560	3.763811
H	-0.401483	-2.968397	1.768528
C	0.663006	-3.534327	4.950037
H	2.159773	-2.374264	5.979991
H	-0.793714	-4.494431	3.681411
H	0.474712	-4.189583	5.798879
C	2.180055	0.722207	1.976454
C	1.327948	1.721221	2.469631
C	3.561725	0.936279	2.006331
C	1.849999	2.908714	2.970671
H	0.247601	1.565536	2.431940
C	4.080438	2.137096	2.484663
H	4.235515	0.171032	1.626792
C	3.226005	3.126310	2.965206
H	1.175022	3.678391	3.340874
H	5.157826	2.299530	2.481348
H	3.631876	4.068569	3.329018
C	1.108755	-2.091097	-1.821979
N	0.037202	-1.404000	-1.602777
O	1.183187	-2.746539	-3.006812
C	-0.093834	-2.561504	-3.656737
H	0.102447	-2.231916	-4.683556
H	-0.593540	-3.535871	-3.687815
C	-0.821544	-1.523903	-2.792170
C	-2.943698	0.255784	1.451346
H	-3.340407	0.664606	2.389152
C	-0.960365	3.027403	0.318623
C	-0.671085	4.266361	0.895021
C	-0.086352	2.547787	-0.665161
C	0.468378	4.988199	0.550014
H	-1.338006	4.661044	1.663545
C	1.059962	3.247903	-1.024235
H	-0.292827	1.587615	-1.142753
C	1.338638	4.457762	-0.395244
H	0.696134	5.937890	1.028499
H	1.737194	2.859947	-1.783435

Cl	2.817800	5.304934	-0.781097
C	-2.133401	2.223956	0.809136
H	-2.383918	2.605603	1.824002
N	-1.877738	0.823682	0.857121
C	-3.070357	-1.194935	1.285401
O	-2.314658	-1.875110	0.589868
O	-4.127670	-1.700407	1.932372
C	-4.429495	-3.060452	1.618068
H	-3.600142	-3.716818	1.904373
H	-5.326322	-3.299854	2.191194
H	-4.625191	-3.160945	0.544222
Cu	-0.508987	-0.427105	0.123625
H	4.328853	-2.037844	1.678289
H	-1.800814	-1.896923	-2.457054
C	-1.028024	-0.158583	-3.459435
C	-2.033202	-0.253728	-4.597374
C	0.276816	0.491173	-3.889312
H	-1.458676	0.479696	-2.674160
H	-2.990887	-0.668521	-4.257088
H	-2.236600	0.736014	-5.022112
H	-1.661740	-0.886766	-5.416393
H	0.937584	0.626351	-3.024588
H	0.815196	-0.103904	-4.642000
H	0.095038	1.480619	-4.325008

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C	3.329033	-1.114579	1.706331
C	3.819005	0.007925	2.438318
C	5.203753	0.168562	2.139690
C	5.576018	-0.859164	1.220694
C	4.418719	-1.650870	0.950633
H	2.296416	-1.456490	1.696495
H	3.220775	0.665284	3.063147
H	5.848451	0.959608	2.508482
H	6.555454	-0.987464	0.772007
H	4.362399	-2.483015	0.255562
Fe	4.092035	0.283234	0.445471
C	4.214583	2.203035	-0.179707
C	2.852578	1.751452	-0.093452
C	4.902228	1.356176	-1.089728
H	4.633846	3.022798	0.392577
C	2.703094	0.603071	-0.972244
C	3.984589	0.383887	-1.576808
H	5.958066	1.411196	-1.333508
P	1.179733	-0.361664	-1.237813
C	0.607021	0.246324	-2.862949
C	-0.145650	-0.582449	-3.705866
C	0.755665	1.598570	-3.197386
C	-0.730101	-0.068627	-4.858644
H	-0.283349	-1.634841	-3.451690
C	0.163911	2.110484	-4.348102
H	1.336628	2.254753	-2.546752
C	-0.581769	1.278879	-5.180370
H	-1.314880	-0.723485	-5.502435
H	0.287145	3.163945	-4.595751
H	-1.046615	1.680529	-6.078850
C	1.814238	-2.040050	-1.578749
C	1.636981	-3.025101	-0.601348
C	2.509947	-2.357707	-2.754533
C	2.183905	-4.294973	-0.778641
H	1.050902	-2.797884	0.289750
C	3.052306	-3.626547	-2.927951
H	2.616269	-1.608667	-3.540183
C	2.898105	-4.594663	-1.934543
H	2.029603	-5.056429	-0.014920
H	3.592082	-3.864575	-3.843113
H	3.321446	-5.587928	-2.073978
C	1.887455	2.300200	0.840689
N	0.715540	1.849014	1.137233
O	2.298651	3.420733	1.480723
C	1.287175	3.699351	2.475300
H	1.708773	3.443765	3.458881
H	1.077731	4.771301	2.445956
C	0.106662	2.806179	2.078408
C	-2.343102	-1.037800	1.880874
H	-3.332908	-1.222701	2.299742
C	-2.964902	2.033350	0.097937
C	-3.827675	3.071777	0.481272
C	-1.910021	2.357854	-0.771457
C	-3.636147	4.380704	0.053785
H	-4.664036	2.845486	1.144058
C	-1.698305	3.659845	-1.205055
H	-1.235130	1.576109	-1.119632
C	-2.561377	4.667734	-0.782688
H	-4.308173	5.174957	0.369550
H	-0.872751	3.892652	-1.874706
Cl	-2.300196	6.311140	-1.318081
C	-3.192619	0.671963	0.619455
H	-4.061465	0.628247	1.292981
N	-2.096029	-0.019931	1.070989
C	-1.256806	-1.912748	2.202286
O	-0.080608	-1.726774	1.836725
O	-1.625826	-2.973732	2.935688
C	-0.619868	-3.965640	3.122907
H	0.268438	-3.538347	3.600771
H	-1.074058	-4.725182	3.760548
H	-0.343688	-4.407556	2.157670
Cu	-0.151280	0.073369	0.453313
H	4.223367	-0.431373	-2.251786
H	-0.635730	3.389673	1.509466
C	-0.624015	2.130787	3.239578
C	-1.191960	3.188199	4.177540
C	0.238971	1.114690	3.973987
H	-1.463129	1.586462	2.784388
H	-1.824846	3.906442	3.639250
H	-1.803075	2.729982	4.963402
H	-0.395320	3.755337	4.681290
H	0.622450	0.346112	3.289990
H	1.096119	1.585593	4.478291
H	-0.345158	0.603585	4.748647
C	-3.238526	-2.954454	-0.210351
C	-3.845730	-4.012282	0.548405
C	-3.233492	-5.263635	0.652753

C	-2.026825	-5.493386	0.001270
C	-1.430726	-4.471184	-0.750494
C	-2.020221	-3.213554	-0.857674
C	-5.069625	-3.514261	1.100250
H	-3.707715	-6.055792	1.234360
H	-1.548730	-6.471110	0.062609
H	-0.494464	-4.662454	-1.273742
H	-1.511983	-2.446274	-1.442229
H	-5.751732	-4.084066	1.726081
C	-5.229325	-2.210122	0.697085
H	-6.078240	-1.580186	0.951725
C	-4.132168	-1.801820	-0.136451
C	-4.012658	-0.521893	-0.760068
C	-3.049866	-0.394522	-1.919752
H	-3.145371	0.579357	-2.416299
H	-2.005805	-0.494776	-1.596124
H	-3.231473	-1.172655	-2.673919
C	-5.301748	0.238903	-0.994562
H	-5.098076	1.271255	-1.305172
H	-5.885248	-0.237672	-1.793868
H	-5.940274	0.277651	-0.104646

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C	3.281901	0.840544	-1.845392
C	3.725164	-0.335193	-2.521780
C	5.117003	-0.504125	-2.261392
C	5.539362	0.570827	-1.421544
C	4.406732	1.401125	-1.162428
H	2.256094	1.202900	-1.818711
H	3.094168	-1.016145	-3.086292
H	5.733659	-1.330132	-2.599939
H	6.535619	0.706157	-1.013617
H	4.387467	2.272686	-0.514805
Fe	4.062742	-0.490687	-0.526428
C	4.165278	-2.366623	0.222144
C	2.810700	-1.890765	0.152934
C	4.902883	-1.476539	1.048434
H	4.545371	-3.232630	-0.307844
C	2.717521	-0.683704	0.954136
C	4.024356	-0.450269	1.497366
H	5.965489	-1.539941	1.258902
P	1.228392	0.336944	1.174853
C	0.607993	-0.200750	2.808590
C	-0.175764	0.665015	3.584405
C	0.740214	-1.537036	3.208830
C	-0.812506	0.201445	4.730567
H	-0.298091	1.706967	3.282609
C	0.101165	-1.996713	4.356612
H	1.341815	-2.223369	2.610929
C	-0.680931	-1.130739	5.117172
H	-1.422436	0.884200	5.319703
H	0.213867	-3.037770	4.656647
H	-1.186109	-1.492760	6.010659
C	1.918829	2.002123	1.469462
C	1.810306	2.955174	0.451121
C	2.585421	2.339646	2.656215
C	2.395710	4.211074	0.599865
H	1.239257	2.718432	-0.446209
C	3.162798	3.596804	2.803415
H	2.645623	1.614014	3.468629
C	3.077447	4.530862	1.770005
H	2.290442	4.949356	-0.194231
H	3.679157	3.850766	3.727850
H	3.527766	5.514914	1.889441
C	1.799685	-2.477050	-0.708106
N	0.612598	-2.041713	-0.960914
O	2.188706	-3.621214	-1.323046
C	1.137233	-3.936536	-2.261631
H	1.515859	-3.715617	-3.271286
H	0.932154	-5.007423	-2.186769
C	-0.028834	-3.028797	-1.849588
C	-2.361649	1.092006	-1.860238
H	-3.195581	1.059646	-2.570907
C	-3.122706	-1.890402	-0.015646
C	-3.972825	-2.920094	-0.431473
C	-2.137192	-2.206642	0.929304
C	-3.848974	-4.219724	0.052551
H	-4.747784	-2.699971	-1.167307
C	-1.991762	-3.496672	1.426439
H	-1.454515	-1.435569	1.286112
C	-2.849671	-4.496674	0.979018
H	-4.513823	-5.010147	-0.287026
H	-1.219782	-3.722235	2.159173
Cl	-2.666490	-6.125622	1.588669
C	-3.258591	-0.521018	-0.627857
H	-4.008855	-0.611145	-1.442676
N	-2.034067	-0.008367	-1.159736
C	-1.276005	2.006971	-2.207930
O	-0.097637	1.833352	-1.893477
O	-1.706991	3.083010	-2.878177
C	-0.760372	4.145934	-2.993438
H	0.126708	3.822792	-3.547917
H	-1.281228	4.942224	-3.526633
H	-0.468731	4.493456	-1.994524
Cu	-0.207684	-0.136003	-0.405319
H	4.302087	0.404810	2.104936
H	-0.752964	-3.593065	-1.238136
C	-0.796727	-2.396429	-3.013040
C	-1.339329	-3.487292	-3.927312
C	0.023798	-1.362923	-3.769568
H	-1.643653	-1.864930	-2.558483
H	-1.938885	-4.219686	-3.369832
H	-1.978572	-3.062207	-4.709602
H	-0.532638	-4.035247	-4.436576
H	0.359322	-0.555993	-3.102939
H	0.910613	-1.802306	-4.251361
H	-0.577006	-0.903427	-4.563917
C	-2.820699	3.096140	0.086907
C	-3.346845	4.304847	-0.469554
C	-2.733579	5.534288	-0.225620
C	-1.607157	5.587398	0.591909
C	-1.082515	4.411516	1.137555
C	-1.667950	3.172507	0.875226

C	-4.498104	3.962662	-1.260682
H	-3.141974	6.446359	-0.663489
H	-1.133596	6.544753	0.808087
H	-0.202659	4.457159	1.779056
H	-1.204507	2.274208	1.282091
H	-5.101789	4.669081	-1.825249
C	-4.685807	2.613475	-1.189350
H	-5.480050	2.067595	-1.694029
C	-3.643895	1.976958	-0.400308
C	-3.878678	0.648611	0.310182
C	-3.224413	0.602973	1.689828
H	-3.547795	-0.285046	2.248180
H	-2.131318	0.563141	1.620131
H	-3.483419	1.489034	2.281865
C	-5.368226	0.337295	0.482215
H	-5.492731	-0.640858	0.967913
H	-5.867936	1.087578	1.106149
H	-5.899240	0.295038	-0.476567

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C	-4.487373	0.606782	1.018198
C	-5.802531	0.652106	0.440574
C	-6.568722	-0.508652	0.308912
C	-6.063721	-1.720559	0.765655
C	-4.794733	-1.769456	1.357281
C	-4.007501	-0.627320	1.482994
C	-6.094254	2.014232	0.107950
H	-7.564592	-0.456506	-0.133947
H	-6.660297	-2.628938	0.683832
H	-4.422157	-2.716646	1.747287
H	-3.029518	-0.716834	1.954199
H	-7.015715	2.364246	-0.350383
C	-5.022411	2.789051	0.480088
H	-4.958703	3.868408	0.358786
C	-3.985317	1.974840	1.054440
C	-2.752845	2.486790	1.566279
C	-1.886524	1.555962	2.380300
H	-0.994812	2.076689	2.754131
H	-2.428167	1.159342	3.250291
H	-1.550206	0.698827	1.781731
C	-2.801752	3.885306	2.147403
H	-1.797107	4.252845	2.389439
H	-3.269056	4.610538	1.471201
H	-3.387604	3.886454	3.076377
C	-2.733177	1.335768	-1.360549
H	-3.531132	2.068242	-1.487063
C	-0.330688	3.423358	0.353143
C	-0.183002	4.819434	0.307657
C	0.762585	2.674752	0.819013
C	0.992574	5.447657	0.697375
H	-1.018263	5.425339	-0.045372
C	1.945207	3.284794	1.218759
H	0.678922	1.583192	0.850893
C	2.054465	4.671375	1.151873
H	1.091069	6.529026	0.645275
H	2.790318	2.696127	1.571148
Cl	3.551824	5.443096	1.615401
C	-1.615191	2.827110	-0.044845
H	-2.301205	3.575642	-0.466868
N	-1.605623	1.630001	-0.728619
C	-2.900782	0.003142	-1.876385
O	-2.026410	-0.874343	-1.837607
O	-4.119551	-0.213123	-2.396662
C	-4.407228	-1.580886	-2.687860
H	-4.358767	-2.175812	-1.768514
H	-5.422081	-1.585270	-3.088251
H	-3.697135	-1.984520	-3.417356
C	3.538716	0.006372	1.360949
C	4.457488	0.323578	0.315965
C	5.546682	-0.592008	0.393788
C	5.303295	-1.474634	1.489417
C	4.061529	-1.105785	2.089541
H	2.577492	0.481762	1.531877
H	4.328615	1.095794	-0.436066
H	6.390770	-0.635493	-0.286131
H	5.928996	-2.310678	1.783605
H	3.568741	-1.612669	2.913653
Fe	3.792264	-1.591175	0.145536
C	3.842174	-2.464262	-1.684913
C	2.623311	-1.729350	-1.487651
C	3.932075	-3.452271	-0.666999
H	4.569508	-2.268814	-2.464777
C	1.961000	-2.269493	-0.313812
C	2.784322	-3.339634	0.166661
H	4.759475	-4.139115	-0.521712
P	0.335392	-1.774117	0.340582
C	-0.703817	-3.176918	-0.201359
C	-1.881262	-3.477006	0.491350
C	-0.427050	-3.850623	-1.395919
C	-2.755804	-4.444287	0.008011
H	-2.117519	-2.943427	1.412061
C	-1.306347	-4.814091	-1.880059
H	0.477035	-3.615991	-1.958136
C	-2.471111	-5.115264	-1.178758
H	-3.670775	-4.664991	0.555988
H	-1.077689	-5.333261	-2.809621
H	-3.158920	-5.868713	-1.558858
C	0.521722	-2.023371	2.143535
C	0.625426	-0.893436	2.962573
C	0.579647	-3.293896	2.732574
C	0.814005	-1.023919	4.335612
H	0.543668	0.098966	2.516636
C	0.766853	-3.425404	4.105044
H	0.460386	-4.182567	2.111908
C	0.890502	-2.291499	4.907443
H	0.886544	-0.134087	4.958400
H	0.810375	-4.417137	4.552381
H	1.030293	-2.397757	5.981706
C	2.166216	-0.645555	-2.340253
N	1.123006	0.096528	-2.185358
O	2.920035	-0.426825	-3.442327
C	2.207302	0.554677	-4.230924
H	2.919829	1.340648	-4.504928

H	1.864501	0.054264	-5.143180
C	1.063122	1.030849	-3.319645
Cu	-0.319095	0.045509	-0.692670
H	2.582367	-3.923817	1.058878
H	0.087002	0.897513	-3.809333
C	1.166651	2.487907	-2.850817
C	0.906885	3.444363	-4.005265
C	2.490317	2.778884	-2.161906
H	0.365270	2.613390	-2.107245
H	-0.063814	3.254636	-4.480601
H	0.909757	4.483764	-3.656905
H	1.681220	3.363043	-4.782162
H	2.660664	2.071937	-1.341717
H	3.341847	2.718295	-2.855386
H	2.493744	3.785589	-1.728227

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C	4.381602	0.505746	-0.869939
C	5.766766	0.496325	-0.506686
C	6.548601	-0.645489	-0.681123
C	5.976762	-1.786766	-1.236410
C	4.623749	-1.789427	-1.588765
C	3.821152	-0.664846	-1.394315
C	6.094566	1.791261	0.028571
H	7.600914	-0.637429	-0.394235
H	6.581562	-2.678504	-1.398548
H	4.188375	-2.685611	-2.030599
H	2.762461	-0.718394	-1.648102
H	7.070734	2.082156	0.408735
C	4.975579	2.569355	-0.014618
H	4.914682	3.599936	0.330654
C	3.835876	1.822764	-0.519826
C	2.659874	2.534561	-1.162397
C	1.948723	1.689843	-2.216053
H	1.199970	2.290196	-2.749814
H	2.655057	1.295776	-2.955626
H	1.427786	0.838347	-1.758072
C	3.089793	3.851742	-1.815831
H	2.229961	4.350595	-2.283819
H	3.525999	4.552015	-1.092835
H	3.839154	3.677702	-2.596705
C	2.717271	1.440803	1.303156
H	3.284873	2.236634	1.795478
C	0.317204	3.490998	-0.432388
C	0.162571	4.880748	-0.408588
C	-0.751319	2.727263	-0.913922
C	-1.001734	5.498692	-0.854060
H	0.981010	5.496419	-0.032814
C	-1.924896	3.320642	-1.366526
H	-0.660632	1.635788	-0.909994
C	-2.038414	4.707380	-1.335369
H	-1.107275	6.580248	-0.827705
H	-2.755526	2.720205	-1.733362
Cl	-3.511795	5.462004	-1.895472
C	1.611310	2.882797	0.029314
H	2.143602	3.663002	0.613703
N	1.489207	1.687875	0.807874
C	3.010379	0.077602	1.738963
O	2.226118	-0.863601	1.620788
O	4.246839	-0.060173	2.233159
C	4.668112	-1.418015	2.398225
H	4.581648	-1.953023	1.445752
H	5.711095	-1.362441	2.712747
H	4.058430	-1.925711	3.153095
C	-3.600846	0.005461	-1.206616
C	-4.515212	0.283258	-0.146199
C	-5.584473	-0.654506	-0.229329
C	-5.335103	-1.510936	-1.343944
C	-4.108708	-1.103847	-1.951086
H	-2.649299	0.503221	-1.372527
H	-4.395629	1.041932	0.620500
H	-6.418651	-0.730020	0.460009
H	-5.945672	-2.355050	-1.646728
H	-3.613190	-1.586552	-2.788023
Fe	-3.804461	-1.619642	-0.021195
C	-3.783508	-2.498491	1.807587
C	-2.576501	-1.756764	1.568888
C	-3.904815	-3.483890	0.790661
H	-4.483233	-2.306853	2.613306
C	-1.954025	-2.289195	0.370212
C	-2.788537	-3.362314	-0.083739
H	-4.733424	-4.174503	0.672597
P	-0.358833	-1.771614	-0.342218
C	0.713011	-3.159496	0.175115
C	1.838723	-3.508054	-0.577350
C	0.520213	-3.757490	1.426106
C	2.749383	-4.441246	-0.092563
H	2.006689	-3.039973	-1.547193
C	1.432032	-4.689560	1.909115
H	-0.343481	-3.483655	2.032554
C	2.550338	-5.032384	1.152477
H	3.626554	-4.695311	-0.685942
H	1.269116	-5.148425	2.883067
H	3.266531	-5.758515	1.533187
C	-0.602171	-2.024095	-2.138209
C	-0.726289	-0.895026	-2.955864
C	-0.686289	-3.295203	-2.722791
C	-0.962137	-1.027663	-4.321542
H	-0.627838	0.097818	-2.513229
C	-0.918137	-3.428923	-4.088015
H	-0.550224	-4.182988	-2.104173
C	-1.063507	-2.295911	-4.887889
H	-1.053238	-0.139180	-4.943619
H	-0.980974	-4.421209	-4.531768
H	-1.240291	-2.403308	-5.956661
C	-2.103901	-0.664191	2.401329
N	-1.046594	0.054444	2.236904
O	-2.869146	-0.404407	3.488707
C	-2.141713	0.579981	4.258924
H	-2.847494	1.370728	4.536410
H	-1.786132	0.086564	5.170860
C	-1.011609	1.044155	3.325473
Cu	0.340873	0.052125	0.625051

H	-2.618575	-3.941383	-0.985926
H	-0.031577	0.970004	3.819040
C	-1.168072	2.473990	2.788566
C	-0.987979	3.491203	3.905735
C	-2.482541	2.669900	2.050976
H	-0.349520	2.602296	2.065477
H	-0.028888	3.360152	4.422969
H	-1.013643	4.511992	3.506220
H	-1.785985	3.421403	4.659682
H	-2.565553	1.963616	1.216067
H	-3.354439	2.531649	2.708686
H	-2.547851	3.679635	1.628786

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C	-2.385823	3.225646	-0.322644
C	-2.711474	3.733997	0.972330
C	-4.118934	3.948892	1.027729
C	-4.669729	3.575745	-0.234444
C	-3.601618	3.130820	-1.068949
H	-1.394465	2.918894	-0.653633
H	-2.016824	3.878434	1.793622
H	-4.678523	4.284472	1.894542
H	-5.722339	3.581085	-0.497169
H	-3.701432	2.733916	-2.074159
Fe	-3.709611	2.001691	0.613943
C	-4.161078	0.937497	2.275673
C	-2.888938	0.546169	1.732818
C	-5.151365	0.726271	1.278673
H	-4.312345	1.356218	3.264104
C	-3.106698	0.094781	0.369513
C	-4.512947	0.211095	0.115020
H	-6.204938	0.969415	1.370809
P	-1.816426	-0.524647	-0.741515
C	-2.142823	-2.320206	-0.813406
C	-1.346969	-3.075469	-1.687344
C	-3.070694	-2.975557	0.001306
C	-1.500513	-4.453338	-1.765591
H	-0.592648	-2.575310	-2.298004
C	-3.207757	-4.361422	-0.067342
H	-3.686864	-2.404222	0.695411
C	-2.431110	-5.100480	-0.953891
H	-0.875332	-5.028443	-2.446669
H	-3.926319	-4.864242	0.578131
H	-2.534731	-6.182956	-0.997736
C	-2.352932	0.046729	-2.394112
C	-1.658773	1.095900	-3.008180
C	-3.436340	-0.539583	-3.060290
C	-2.064980	1.572411	-4.252957
H	-0.800713	1.538974	-2.498396
C	-3.841120	-0.061632	-4.302078
H	-3.952562	-1.386350	-2.605858
C	-3.158957	0.998642	-4.897304
H	-1.519549	2.388598	-4.723883
H	-4.684799	-0.523493	-4.812413
H	-3.472570	1.368556	-5.872013
C	-1.630767	0.697181	2.442846
N	-0.432918	0.439824	2.029042
O	-1.754960	1.174786	3.702364
C	-0.428178	1.168307	4.275803
H	-0.248638	2.160579	4.705018
H	-0.421514	0.426971	5.082273
C	0.499582	0.820308	3.102338
C	2.410450	0.356983	-1.549252
H	3.207934	0.146926	-2.262427
C	1.854344	-2.919101	-0.117442
C	2.048775	-4.199871	-0.655557
C	0.987929	-2.802111	0.981540
C	1.397361	-5.314974	-0.144391
H	2.726308	-4.319624	-1.502060
C	0.317227	-3.903118	1.499503
H	0.833626	-1.824583	1.441636
C	0.526161	-5.155324	0.928956
H	1.550068	-6.299991	-0.579209
H	-0.368365	-3.793699	2.337259
Cl	-0.316987	-6.547404	1.566021
C	2.574729	-1.770086	-0.695080
H	3.117708	-2.035398	-1.613729
N	1.895335	-0.572570	-0.758451
C	1.865154	1.679573	-1.454842
O	0.924673	1.999169	-0.701138
O	2.464168	2.563667	-2.268355
C	2.053654	3.917932	-2.105115
H	2.257330	4.258814	-1.084269
H	2.649875	4.490881	-2.816451
H	0.983359	4.031583	-2.317286
Cu	0.144131	0.024777	0.084165
H	-4.993063	-0.010338	-0.833615
H	1.121423	-0.056488	3.341150
C	1.433838	1.953244	2.661409
C	2.478215	2.210940	3.738316
C	0.686769	3.217145	2.271765
H	1.940846	1.592627	1.752578
H	3.049382	1.303359	3.976512
H	3.193445	2.976924	3.417744
H	2.019138	2.569999	4.671390
H	-0.000881	3.018108	1.443458
H	0.121200	3.642772	3.115035
H	1.392072	3.983144	1.928410
C	4.949076	1.090568	-0.189188
C	5.670343	1.668703	-1.288315
C	5.897736	3.047259	-1.346825
C	5.433563	3.865874	-0.324808
C	4.767847	3.303763	0.774673
C	4.541790	1.932971	0.855537
C	6.048115	0.607608	-2.171417
H	6.444659	3.473864	-2.189156
H	5.607809	4.940869	-0.362790
H	4.442667	3.948433	1.593325
H	4.068536	1.531196	1.746753
H	6.605055	0.729095	-3.097220
C	5.590592	-0.579716	-1.644696
H	5.724248	-1.557150	-2.103345
C	4.889385	-0.349419	-0.414332

C	4.223115	-1.375794	0.331363
C	4.882412	-2.741046	0.310657
H	4.252524	-3.498764	0.792016
H	5.107467	-3.088290	-0.704519
H	5.834347	-2.704346	0.857001
C	3.687481	-1.025124	1.700185
H	3.222736	-1.899520	2.173785
H	4.490712	-0.675574	2.363898
H	2.931503	-0.232104	1.641163

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C	-3.401225	3.091323	-0.074385
C	-3.674499	3.315123	1.307381
C	-5.030731	2.952241	1.553698
C	-5.595254	2.500172	0.322781
C	-4.588698	2.585029	-0.684372
H	-2.447215	3.238947	-0.568682
H	-2.959382	3.641031	2.056233
H	-5.527435	2.961638	2.518425
H	-6.599631	2.111669	0.189632
H	-4.686039	2.275462	-1.720685
Fe	-3.991787	1.364658	0.826968
C	-3.735035	0.115755	2.389710
C	-2.516088	0.263230	1.641855
C	-4.731255	-0.398205	1.515848
H	-3.865390	0.396507	3.428857
C	-2.776426	-0.161473	0.275585
C	-4.152882	-0.559213	0.224788
H	-5.767728	-0.584115	1.777387
P	-1.541667	-0.246761	-1.056849
C	-1.685764	-1.963011	-1.668368
C	-1.062683	-2.264559	-2.889324
C	-2.263797	-3.001904	-0.931614
C	-1.045744	-3.567025	-3.371527
H	-0.583511	-1.468425	-3.460555
C	-2.235169	-4.309047	-1.412763
H	-2.728616	-2.797731	0.032134
C	-1.633607	-4.594400	-2.634290
H	-0.564240	-3.782601	-4.324142
H	-2.682311	-5.106346	-0.820105
H	-1.612812	-5.616864	-3.008013
C	-2.242590	0.729793	-2.439274
C	-1.630511	1.955602	-2.725365
C	-3.327783	0.312547	-3.220949
C	-2.116002	2.770069	-3.744930
H	-0.758390	2.259828	-2.141113
C	-3.808776	1.123655	-4.244583
H	-3.785831	-0.660000	-3.036406
C	-3.209114	2.356927	-4.502326
H	-1.632686	3.722662	-3.955682
H	-4.652828	0.792005	-4.847503
H	-3.586936	2.988075	-5.304997
C	-1.328989	0.912731	2.171533
N	-0.154657	1.001312	1.639429
O	-1.509613	1.524241	3.368325
C	-0.271855	2.198795	3.676622
H	-0.491938	3.272570	3.749800
H	0.069671	1.844190	4.653808
C	0.670494	1.848989	2.512852
C	2.921868	-0.408429	-1.443842
H	3.398228	-0.952593	-2.269794
C	1.365776	-3.046550	0.453331
C	1.263564	-4.407588	0.156806
C	0.453736	-2.510633	1.373180
C	0.287815	-5.214438	0.734564
H	1.955749	-4.844260	-0.564283
C	-0.532125	-3.295187	1.961051
H	0.509160	-1.453719	1.630314
C	-0.608189	-4.643907	1.629759
H	0.208206	-6.268318	0.478379
H	-1.246133	-2.863792	2.660323
Cl	-1.882669	-5.626800	2.319234
C	2.410578	-2.205965	-0.230483
H	2.845401	-2.825932	-1.045473
N	1.915688	-0.971972	-0.743039
C	2.782604	1.037354	-1.666510
O	1.877315	1.725211	-1.183254
O	3.761124	1.549410	-2.416267
C	3.811074	2.976930	-2.471143
H	3.890157	3.388302	-1.458742
H	4.707214	3.214299	-3.045633
H	2.918042	3.377191	-2.962468
Cu	0.425612	0.237197	-0.196939
H	-4.665028	-0.910249	-0.666289
H	1.519280	1.244117	2.870740
C	1.240632	3.057903	1.757562
C	2.057175	3.924597	2.706070
C	0.164805	3.853743	1.035657
H	1.913292	2.650549	0.990184
H	2.832566	3.341327	3.220834
H	2.557896	4.734874	2.163956
H	1.427047	4.393649	3.475546
H	-0.384192	3.215057	0.330969
H	-0.561622	4.304507	1.729452
H	0.613757	4.672635	0.461802
C	4.990683	0.507731	0.236656
C	6.194587	0.781422	-0.483874
C	6.839361	2.012692	-0.366542
C	6.305012	2.987933	0.470887
C	5.125658	2.732976	1.177680
C	4.467402	1.507832	1.062167
C	6.501908	-0.372283	-1.289377
H	7.753872	2.207825	-0.928286
H	6.804152	3.950368	0.577443
H	4.717139	3.499631	1.835516
H	3.543682	1.349973	1.616364
H	7.354639	-0.456489	-1.958626
C	5.538614	-1.310652	-1.083026
H	5.493674	-2.281103	-1.574228
C	4.500699	-0.819585	-0.179302
C	3.699770	-1.805138	0.664404
C	4.483572	-3.081924	0.973420
H	3.863119	-3.772845	1.561317

H	4.791915	-3.609740	0.062915
H	5.389024	-2.867832	1.553773
C	3.229539	-1.201494	1.984415
H	2.764233	-1.968149	2.616518
H	4.066817	-0.767888	2.543559
H	2.485397	-0.411904	1.813638

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C	3.487741	-1.481032	1.727167
C	3.983987	-0.460106	2.592458
C	5.386393	-0.327791	2.370518
C	5.761696	-1.269110	1.364616
C	4.590448	-1.981316	0.965763
H	2.446146	-1.783075	1.640179
H	3.383096	0.153135	3.257990
H	6.041901	0.395243	2.844469
H	6.754577	-1.388783	0.943994
H	4.534040	-2.732617	0.183737
Fe	4.357413	0.007588	0.651833
C	4.530559	1.984150	0.252308
C	3.165499	1.542345	0.182019
C	5.287043	1.232630	-0.686782
H	4.905443	2.732442	0.941423
C	3.084782	0.496095	-0.822711
C	4.408845	0.326031	-1.346572
H	6.359379	1.301687	-0.837372
P	1.574733	-0.402441	-1.280631
C	1.071717	0.403323	-2.841636
C	0.166134	-0.263191	-3.680921
C	1.421246	1.726408	-3.135117
C	-0.376532	0.380687	-4.786337
H	-0.118810	-1.292946	-3.459952
C	0.875782	2.367819	-4.245682
H	2.117426	2.260894	-2.487713
C	-0.026919	1.700946	-5.068910
H	-1.081608	-0.147797	-5.425414
H	1.156133	3.397288	-4.464161
H	-0.459716	2.207916	-5.929211
C	2.196358	-2.031947	-1.826878
C	1.959398	-3.142460	-1.008846
C	2.898742	-2.203010	-3.027219
C	2.441747	-4.397962	-1.371462
H	1.385606	-3.013065	-0.090547
C	3.380426	-3.457798	-3.386143
H	3.053992	-1.349749	-3.688834
C	3.156912	-4.555601	-2.555756
H	2.249082	-5.257079	-0.730805
H	3.924898	-3.582363	-4.320840
H	3.529212	-5.537873	-2.842025
C	2.119737	2.015500	1.071140
N	0.916058	1.569426	1.195768
O	2.480610	3.054776	1.861165
C	1.364329	3.283465	2.750435
H	1.672560	2.964254	3.756537
H	1.167011	4.358385	2.765798
C	0.227271	2.434752	2.168787
C	-2.238307	-1.720455	1.209673
H	-3.086791	-1.676504	1.916598
C	-2.610395	1.728970	-0.006083
C	-3.292324	2.761563	0.645619
C	-1.653835	2.068597	-0.969885
C	-3.005880	4.097859	0.381919
H	-4.057882	2.511241	1.380576
C	-1.355232	3.397347	-1.251969
H	-1.145309	1.277959	-1.524777
C	-2.029286	4.401734	-0.562152
H	-3.532583	4.896630	0.898206
H	-0.616927	3.651808	-2.008960
Cl	-1.651014	6.076985	-0.897653
C	-2.890862	0.321886	0.365401
H	-3.826621	0.200718	0.936275
N	-1.837152	-0.425219	0.761083
C	-1.081486	-2.376810	1.894680
O	0.101440	-2.187483	1.625519
O	-1.468139	-3.230025	2.856800
C	-0.410020	-3.947065	3.497206
H	0.331871	-3.256097	3.909770
H	-0.885263	-4.524721	4.290288
H	0.085534	-4.614467	2.783794
Cu	0.067584	-0.126508	0.279372
H	4.695302	-0.416228	-2.084958
H	-0.469784	3.070367	1.598209
C	-0.595948	1.650436	3.194342
C	-1.246181	2.612721	4.178990
C	0.210343	0.567582	3.897925
H	-1.385993	1.147959	2.617914
H	-1.834226	3.382511	3.661855
H	-1.919869	2.083449	4.862474
H	-0.497521	3.126569	4.799979
H	0.657017	-0.128680	3.175467
H	1.018571	0.985152	4.516917
H	-0.434783	-0.017174	4.565880
C	-5.300469	-1.733920	-0.226635
C	-5.881501	-0.527874	-0.819633
C	-7.260101	-0.243503	-0.639742
C	-8.041986	-1.095729	0.098058
C	-7.483755	-2.261652	0.689965
C	-6.153842	-2.575962	0.539612
C	-4.884969	0.161832	-1.501682
H	-7.688055	0.650494	-1.095675
H	-9.102287	-0.884692	0.235588
H	-8.127448	-2.920242	1.272387
H	-5.776581	-3.488596	0.994718
H	-4.995042	1.096321	-2.044852
C	-3.658854	-0.528953	-1.273101
H	-2.782598	-0.387187	-1.908498
C	-3.938257	-1.782766	-0.581902
C	-2.833133	-2.611546	-0.027549
C	-3.280415	-3.964693	0.521928
H	-2.416832	-4.617102	0.707051
H	-3.821432	-3.870635	1.469668
H	-3.935929	-4.472568	-0.195414

C	-1.719826	-2.838108	-1.052410
H	-0.907264	-3.448379	-0.632752
H	-2.115037	-3.364731	-1.930300
H	-1.277636	-1.893304	-1.391290

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C	-3.474697	-1.572014	-1.616111
C	-4.038736	-0.502226	-2.372967
C	-5.435496	-0.442071	-2.091255
C	-5.739080	-1.478273	-1.156674
C	-4.528125	-2.175728	-0.861062
H	-2.421565	-1.841183	-1.596353
H	-3.484143	0.185850	-3.004883
H	-6.133827	0.291044	-2.480919
H	-6.710698	-1.670092	-0.713443
H	-4.414812	-2.986697	-0.148118
Fe	-4.357802	-0.213809	-0.387793
C	-4.654467	1.694473	0.216176
C	-3.257171	1.369493	0.151071
C	-5.274613	0.795516	1.126488
H	-5.140893	2.470189	-0.364208
C	-3.016801	0.247059	1.039567
C	-4.278856	-0.087938	1.631991
H	-6.334143	0.758093	1.357633
P	-1.412897	-0.561017	1.295729
C	-0.834778	0.149302	2.877487
C	0.240652	-0.474045	3.529053
C	-1.313331	1.368026	3.369917
C	0.820142	0.108638	4.649341
H	0.627982	-1.420409	3.146281
C	-0.728947	1.949998	4.493760
H	-2.141128	1.868760	2.867254
C	0.338650	1.325841	5.132471
H	1.656163	-0.383901	5.142653
H	-1.110355	2.898647	4.868685
H	0.798351	1.786706	6.004819
C	-1.870914	-2.271995	1.748736
C	-1.641556	-3.287157	0.813380
C	-2.439854	-2.596917	2.987152
C	-1.998991	-4.602189	1.101510
H	-1.166424	-3.036399	-0.135748
C	-2.796994	-3.911166	3.272031
H	-2.588033	-1.816655	3.735093
C	-2.581944	-4.914267	2.327065
H	-1.813648	-5.385911	0.368571
H	-3.238542	-4.155522	4.236961
H	-2.856861	-5.942807	2.554686
C	-2.313936	2.002486	-0.754069
N	-1.085607	1.680635	-0.971290
O	-2.816143	3.053556	-1.447280
C	-1.775718	3.458625	-2.365134
H	-2.121166	3.222341	-3.382045
H	-1.656194	4.541891	-2.274981
C	-0.543066	2.645877	-1.939473
C	2.250201	-1.418570	-1.609589
H	3.050859	-1.264158	-2.361574
C	2.501348	1.907708	-0.066738
C	2.948824	3.005441	-0.805237
C	1.648267	2.143916	1.015698
C	2.553537	4.304240	-0.493009
H	3.620742	2.838684	-1.648224
C	1.232806	3.431341	1.343025
H	1.299324	1.307492	1.624045
C	1.688434	4.501443	0.578896
H	2.906652	5.153400	-1.073585
H	0.565638	3.602482	2.184645
Cl	1.163756	6.123275	0.974998
C	2.898368	0.513934	-0.471934
H	3.750658	0.584162	-1.178278
N	1.808418	-0.193098	-1.034760
C	1.084103	-2.065763	-2.300144
O	-0.074128	-2.036258	-1.904074
O	1.433872	-2.701942	-3.432096
C	0.357790	-3.362120	-4.104764
H	-0.453961	-2.657939	-4.313035
H	0.782896	-3.752010	-5.030038
H	-0.033713	-4.178943	-3.488994
Cu	-0.013211	-0.058155	-0.307342
H	-4.444733	-0.916361	2.313508
H	0.169416	3.284513	-1.393976
C	0.224021	1.972416	-3.080486
C	0.748849	3.026604	-4.045511
C	-0.590244	0.900329	-3.790389
H	1.075745	1.466082	-2.601060
H	1.336946	3.792626	-3.522180
H	1.393591	2.576870	-4.809643
H	-0.067074	3.539838	-4.576435
H	-0.935124	0.131086	-3.085437
H	-1.469998	1.314060	-4.307253
H	0.020002	0.399422	-4.553123
C	5.346991	-1.599769	0.114548
C	5.830233	-0.404546	0.830957
C	7.233974	-0.172196	0.963267
C	8.118642	-1.059964	0.424920
C	7.659422	-2.218734	-0.280020
C	6.328123	-2.485839	-0.438381
C	4.756656	0.318852	1.280192
H	7.581281	0.711046	1.499660
H	9.190819	-0.895333	0.526040
H	8.396148	-2.903593	-0.698144
H	6.029989	-3.381410	-0.976125
H	4.784933	1.255864	1.829632
C	3.531878	-0.322819	0.787417
H	2.702956	-0.388420	1.506425
C	3.959694	-1.603004	0.152345
C	2.937287	-2.438261	-0.537584
C	3.509588	-3.633586	-1.288574
H	2.706502	-4.232826	-1.735993
H	4.178888	-3.324658	-2.100760
H	4.070552	-4.290662	-0.612646
C	1.870226	-2.931242	0.445225
H	1.174623	-3.629899	-0.040134
H	2.334449	-3.455640	1.290057

H	1.275664	-2.095147	0.837818

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C	1.479034	-1.461797	-0.423494
H	1.816110	-1.058250	-1.389166
C	-2.025142	-0.119675	-0.300359
C	-2.829602	0.461384	-1.280538
C	-2.645697	-0.713026	0.802523
C	-4.216862	0.448380	-1.177820
H	-2.361052	0.936923	-2.142106
C	-4.029881	-0.743663	0.923069
H	-2.041802	-1.159867	1.594730
C	-4.805471	-0.158948	-0.073766
H	-4.838824	0.901557	-1.945439
H	-4.507107	-1.210068	1.780991
Cl	-6.544104	-0.181916	0.069085
C	-0.524152	-0.076772	-0.408009
H	-0.243636	0.369605	-1.374255
N	0.037006	-1.411682	-0.381744
C	1.872182	-2.917200	-0.328990
O	1.311606	-3.728695	0.378240
O	2.939038	-3.200639	-1.099560
C	3.392347	-4.555659	-1.002457
H	2.599458	-5.246002	-1.304439
H	4.246745	-4.628708	-1.675651
H	3.688146	-4.787833	0.025541
C	2.070131	1.999906	0.196124
C	0.936760	2.948109	0.128855
C	1.172343	4.316803	-0.223837
C	2.439139	4.728343	-0.498492
C	3.545112	3.811597	-0.445307
C	3.381259	2.499631	-0.115570
C	-0.220857	2.298426	0.442286
H	0.333402	5.010733	-0.263310
H	2.632792	5.766459	-0.763946
H	4.541687	4.185486	-0.675601
H	4.247590	1.845552	-0.084863
H	-1.221123	2.720432	0.478899
C	0.096358	0.874208	0.691471
H	-0.285440	0.520602	1.662050
C	1.586273	0.767267	0.575916
C	2.201869	-0.591296	0.699336
C	3.707615	-0.614415	0.466253
H	4.109456	-1.624278	0.609491
H	3.969304	-0.298512	-0.550985
H	4.220465	0.045999	1.175371
C	1.902543	-1.184536	2.084505
H	2.371032	-2.167645	2.210889
H	2.281482	-0.520353	2.869890
H	0.826111	-1.313557	2.253724
H	-0.311018	-1.981651	0.386319

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C	3.781679	1.138158	0.269907
C	4.590331	0.685237	-0.816346
C	5.696810	-0.036744	-0.281530
C	5.579373	-0.028810	1.140722
C	4.397928	0.694993	1.482727
H	2.840379	1.677021	0.173659
H	4.366179	0.812385	-1.871669
H	6.464917	-0.544044	-0.855961
H	6.244663	-0.528451	1.837334
H	4.003722	0.835021	2.484620
Fe	3.943622	-0.886119	0.297387
C	3.771585	-2.619198	-0.728652
C	2.557397	-1.852110	-0.777162
C	4.069858	-2.890146	0.634341
H	4.368174	-2.891773	-1.591712
C	2.100176	-1.648552	0.587862
C	3.055039	-2.297640	1.439228
H	4.949550	-3.410345	0.999341
P	0.595395	-0.754552	1.085285
C	-0.563689	-2.085697	1.563692
C	-1.910548	-1.721120	1.695618
C	-0.202356	-3.426079	1.734289
C	-2.873913	-2.671726	2.008076
H	-2.209991	-0.689431	1.499023
C	-1.173508	-4.380779	2.032406
H	0.837256	-3.732401	1.618378
C	-2.506574	-4.006218	2.173474
H	-3.918676	-2.373780	2.084417
H	-0.885088	-5.424423	2.148918
H	-3.264332	-4.757498	2.388183
C	1.076445	0.016383	2.673671
C	1.303808	1.398031	2.677154
C	1.224210	-0.704751	3.864088
C	1.700647	2.042815	3.845684
H	1.155550	1.962709	1.753264
C	1.625294	-0.058691	5.030334
H	1.007985	-1.774265	3.878862
C	1.869101	1.314314	5.021083
H	1.870740	3.119015	3.838160
H	1.737864	-0.625959	5.953006
H	2.175651	1.818032	5.936480
C	2.016449	-1.275594	-1.996252
N	1.057963	-0.420908	-2.109395
O	2.616606	-1.686122	-3.139239
C	1.976644	-0.964526	-4.216249
H	2.742983	-0.347153	-4.702520
H	1.612104	-1.702083	-4.937304
C	0.866985	-0.142813	-3.537721
C	-1.518276	2.802621	-1.248201
H	-2.325349	3.486338	-1.514579
C	-3.240230	-0.447899	-1.391209
C	-4.585313	-0.843323	-1.251533
C	-2.275861	-1.463604	-1.544131
C	-4.948761	-2.181416	-1.205722
H	-5.348451	-0.072405	-1.144470
C	-2.625244	-2.804633	-1.502014
H	-1.229604	-1.192077	-1.685372
C	-3.960158	-3.156857	-1.320486
H	-5.988844	-2.472739	-1.076137

H	-1.867660	-3.579431	-1.599819
Cl	-4.398616	-4.848060	-1.228090
C	-2.928411	0.960179	-1.374380
H	-3.772754	1.653350	-1.493694
N	-1.728168	1.457477	-1.196458
C	-0.244321	3.270897	-0.911023
O	0.727004	2.554032	-0.540541
O	-0.093279	4.629868	-0.986331
C	1.171002	5.113864	-0.560230
H	1.988472	4.660817	-1.132574
H	1.145811	6.192935	-0.725776
H	1.342043	4.903875	0.504551
Cu	0.008825	0.535180	-0.552132
H	3.023635	-2.288682	2.524888
H	-0.127015	-0.527457	-3.820038
C	0.879707	1.359401	-3.843686
C	0.582100	1.589504	-5.319900
C	2.170318	2.043423	-3.418395
H	0.059166	1.790724	-3.248028
H	-0.359222	1.115223	-5.625026
H	0.503156	2.659276	-5.543472
H	1.380936	1.186127	-5.960034
H	2.358750	1.906766	-2.347751
H	3.039713	1.677598	-3.985515
H	2.104319	3.122942	-3.601556
C	-5.216180	2.997687	0.614554
C	-6.021846	1.909491	0.765577
C	-5.307223	0.896740	1.523219
H	-5.716331	-0.069135	1.809899
C	-4.058615	1.362380	1.804176
H	-3.296131	0.864614	2.395335
C	-3.942930	2.710814	1.264629
C	-2.863399	3.535740	1.393369
C	-2.879907	4.963645	0.967575
H	-2.018522	5.193241	0.326024
H	-3.796475	5.245187	0.441076
H	-2.788088	5.618090	1.848247
C	-1.608861	3.065748	2.063612
H	-0.753016	3.699735	1.799859
H	-1.700479	3.086079	3.160047
H	-1.356715	2.035454	1.775775
H	-5.461507	3.914205	0.086924
H	-7.035804	1.803850	0.387130

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C	-3.817918	1.158194	-0.211637
C	-4.457783	0.925435	1.042529
C	-5.634141	0.155201	0.808374
C	-5.726207	-0.088943	-0.595059
C	-4.605167	0.528905	-1.226649
H	-2.870287	1.674617	-0.351356
H	-4.080943	1.232196	2.014043
H	-6.312174	-0.220027	1.567705
H	-6.489153	-0.681258	-1.089377
H	-4.361996	0.484493	-2.283861
Fe	-3.986203	-0.831498	0.142116
C	-3.680886	-2.387409	1.399861
C	-2.476923	-1.633945	1.179610
C	-4.140608	-2.864011	0.142759
H	-4.162818	-2.521428	2.361886
C	-2.188988	-1.654113	-0.246365
C	-3.234719	-2.418633	-0.861795
H	-5.053104	-3.425779	-0.027747
P	-0.771637	-0.849829	-1.051780
C	0.383973	-2.218885	-1.406344
C	1.723316	-1.857333	-1.600881
C	0.030147	-3.571782	-1.437829
C	2.691964	-2.824976	-1.836783
H	2.016898	-0.808248	-1.517769
C	1.004649	-4.542306	-1.664353
H	-1.004496	-3.870043	-1.264656
C	2.332548	-4.171283	-1.866254
H	3.730928	-2.520741	-1.960915
H	0.725301	-5.594591	-1.674721
H	3.091349	-4.935481	-2.025782
C	-1.428394	-0.373134	-2.690641
C	-1.635207	0.989120	-2.938458
C	-1.711510	-1.302215	-3.698652
C	-2.148191	1.412742	-4.161652
H	-1.375580	1.715363	-2.164929
C	-2.228027	-0.877756	-4.919247
H	-1.505713	-2.361192	-3.533945
C	-2.452429	0.479057	-5.149535
H	-2.300369	2.474941	-4.346742
H	-2.443274	-1.606665	-5.698854
H	-2.847366	0.809777	-6.108600
C	-1.807319	-0.868893	2.217974
N	-0.892735	0.029888	2.075911
O	-2.214645	-1.137078	3.481314
C	-1.509581	-0.209079	4.338330
H	-2.250413	0.485637	4.757923
H	-1.067464	-0.785020	5.155484
C	-0.488390	0.472967	3.415452
C	1.853994	2.867990	0.326843
H	2.602503	3.487821	0.829401
C	3.243606	-0.443409	1.172080
C	4.573134	-0.896487	1.100587
C	2.236946	-1.378703	1.466762
C	4.884090	-2.239348	1.265102
H	5.357895	-0.178145	0.863619
C	2.535886	-2.720468	1.650109
H	1.198974	-1.050416	1.525750
C	3.858311	-3.141807	1.534900
H	5.910385	-2.589144	1.184187
H	1.750308	-3.444993	1.853477
Cl	4.230198	-4.838230	1.730657
C	3.007328	0.961857	0.910733
H	3.895401	1.604873	0.939419
N	1.848065	1.500849	0.644074
C	0.515421	3.422243	0.305464
O	-0.521391	2.764341	0.096038
O	0.468708	4.761162	0.466755
C	-0.806073	5.356901	0.232753

H	-1.568144	4.933330	0.894387
H	-0.673096	6.421347	0.431294
H	-1.117906	5.201075	-0.806738
Cu	0.021161	0.655328	0.288695
H	-3.337646	-2.578565	-1.930939
H	0.523410	0.072819	3.599843
C	-0.402415	1.998209	3.528662
C	0.082357	2.388657	4.918732
C	-1.703920	2.699261	3.168830
H	0.358427	2.302392	2.791090
H	1.029845	1.897145	5.172950
H	0.238347	3.470573	4.994131
H	-0.652601	2.115438	5.690162
H	-2.021832	2.451645	2.149618
H	-2.517879	2.444469	3.863568
H	-1.574408	3.787327	3.221899
C	5.114478	2.773946	-0.894526
C	6.051774	1.766561	-1.051251
C	5.427646	0.662284	-1.709817
H	5.920320	-0.263706	-2.000027
C	4.101638	0.985370	-1.931061
H	3.378527	0.386249	-2.479016
C	3.872833	2.323117	-1.453710
C	2.645959	3.053441	-1.506429
C	2.775515	4.555373	-1.622923
H	1.811520	5.066626	-1.527651
H	3.455787	4.972051	-0.871936
H	3.190632	4.807467	-2.608049
C	1.559964	2.479448	-2.386285
H	0.636049	3.070664	-2.328340
H	1.878527	2.465396	-3.437490
H	1.311360	1.447128	-2.102084
H	5.285423	3.742921	-0.430661
H	7.094577	1.810735	-0.743868

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C	3.805830	1.299732	0.218061
C	4.430815	1.092059	-1.048025
C	5.626249	0.344347	-0.838302
C	5.744588	0.089812	0.561129
C	4.621184	0.678524	1.215807
H	2.849406	1.793509	0.375844
H	4.033079	1.399836	-2.010833
H	6.299627	-0.010984	-1.611229
H	6.527306	-0.490365	1.038522
H	4.395530	0.619532	2.276300
Fe	4.008526	-0.681338	-0.156150
C	3.717438	-2.232051	-1.424097
C	2.501846	-1.504306	-1.180381
C	4.203318	-2.710944	-0.177998
H	4.189060	-2.347502	-2.393530
C	2.233529	-1.544344	0.248986
C	3.302478	-2.293208	0.842659
H	5.129359	-3.255409	-0.025363
P	0.806204	-0.783421	1.079384
C	-0.310177	-2.187912	1.426597
C	-1.657796	-1.869408	1.642888
C	0.083110	-3.530540	1.431664
C	-2.592648	-2.869488	1.881077
H	-1.990202	-0.830789	1.573756
C	-0.859232	-4.533302	1.653401
H	1.123135	-3.795952	1.239523
C	-2.194035	-4.204739	1.880971
H	-3.637823	-2.600104	2.029551
H	-0.549587	-5.577019	1.640135
H	-2.928282	-4.993247	2.037448
C	1.475581	-0.319849	2.716739
C	1.679327	1.038890	2.983599
C	1.777244	-1.262979	3.706245
C	2.208850	1.446218	4.205272
H	1.407394	1.776122	2.225404
C	2.309651	-0.855247	4.925599
H	1.574263	-2.320137	3.527336
C	2.531862	0.498617	5.173711
H	2.359412	2.505919	4.404637
H	2.539447	-1.595218	5.690457
H	2.939488	0.816381	6.131814
C	1.803473	-0.746192	-2.204689
N	0.888452	0.151718	-2.049231
O	2.179443	-1.026209	-3.475017
C	1.462486	-0.098134	-4.320725
H	2.193759	0.612160	-4.732110
H	1.026917	-0.669683	-5.144119
C	0.436328	0.557924	-3.387065
C	-2.121905	2.756626	-0.118973
H	-2.881589	3.284926	-0.712419
C	-3.185740	-0.666729	-1.073843
C	-4.454414	-1.268807	-1.008440
C	-2.090746	-1.460566	-1.446882
C	-4.614166	-2.625178	-1.256944
H	-5.305561	-0.658539	-0.704076
C	-2.237048	-2.813337	-1.715080
H	-1.100191	-1.011850	-1.506828
C	-3.500894	-3.387889	-1.604400
H	-5.591794	-3.094414	-1.180453
H	-1.378898	-3.426689	-1.981872
Cl	-3.691699	-5.097510	-1.908270
C	-3.084470	0.744016	-0.734700
H	-4.029779	1.299974	-0.721875
N	-1.962733	1.379940	-0.522712
C	-0.803356	3.435819	-0.266027
O	0.291687	2.891632	-0.091313
O	-0.908352	4.737842	-0.563456
C	0.313785	5.479286	-0.518419
H	1.050621	5.058461	-1.208798
H	0.049246	6.497137	-0.805865
H	0.727548	5.463620	0.495709
Cu	-0.067846	0.691251	-0.252300
H	3.422212	-2.462317	1.908648
H	-0.561386	0.111370	-3.542107
C	0.284097	2.074639	-3.526598
C	-0.211003	2.420898	-4.924791
C	1.554336	2.832281	-3.171399

H	-0.493439	2.358171	-2.798079
H	-1.132002	1.880660	-5.177162
H	-0.418953	3.492735	-5.016981
H	0.540867	2.172783	-5.688126
H	1.862764	2.623148	-2.140665
H	2.387659	2.581383	-3.843852
H	1.392693	3.913437	-3.263461
C	-5.203162	2.672697	0.886070
C	-6.174263	1.668120	0.995798
C	-5.595223	0.551433	1.642765
H	-6.110423	-0.367500	1.916445
C	-4.259423	0.856772	1.912588
H	-3.562414	0.237549	2.474628
C	-4.004973	2.194151	1.468191
C	-2.693078	2.880006	1.432722
C	-2.831583	4.372440	1.739907
H	-1.858257	4.879773	1.790362
H	-3.440235	4.891464	0.990084
H	-3.327373	4.495262	2.708913
C	-1.676779	2.261385	2.386385
H	-0.719947	2.801120	2.363856
H	-2.058696	2.295813	3.413681
H	-1.469104	1.210777	2.145554
H	-5.344448	3.649968	0.427190
H	-7.208729	1.745231	0.666015

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C	-3.930082	0.923435	-0.088368
C	-4.516870	0.725951	1.198148
C	-5.640678	-0.137827	1.048872
C	-5.753883	-0.476480	-0.332961
C	-4.698339	0.177549	-1.036690
H	-3.027562	1.496448	-0.289405
H	-4.134404	1.111899	2.138125
H	-6.269405	-0.509552	1.851334
H	-6.484707	-1.152234	-0.764698
H	-4.481744	0.082520	-2.096443
Fe	-3.947306	-1.047738	0.390332
C	-3.499794	-2.502132	1.727649
C	-2.350639	-1.699869	1.412491
C	-3.978034	-3.081848	0.521275
H	-3.935910	-2.605277	2.714931
C	-2.121678	-1.788760	-0.019057
C	-3.138787	-2.650974	-0.544664
H	-4.862045	-3.703706	0.424405
P	-0.760406	-1.001352	-0.938499
C	0.340452	-2.421850	-1.276127
C	1.238547	-2.360098	-2.350358
C	0.419959	-3.501035	-0.387051
C	2.198306	-3.350613	-2.525353
H	1.191443	-1.525135	-3.050333
C	1.379446	-4.494140	-0.569366
H	-0.270333	-3.562927	0.455472
C	2.275353	-4.417783	-1.632461
H	2.894813	-3.281816	-3.359185
H	1.431417	-5.327976	0.129502
H	3.035430	-5.185750	-1.762049
C	-1.510439	-0.624091	-2.562824
C	-1.814630	0.711496	-2.852592
C	-1.800940	-1.611184	-3.513570
C	-2.417926	1.051935	-4.060400
H	-1.569621	1.484241	-2.121901
C	-2.406660	-1.269671	-4.718781
H	-1.533946	-2.649574	-3.313724
C	-2.719205	0.061536	-4.992286
H	-2.644509	2.094884	-4.276713
H	-2.626530	-2.043596	-5.452399
H	-3.185913	0.326757	-5.939547
C	-1.641659	-0.877139	2.377732
N	-0.689727	-0.039806	2.150209
O	-2.048343	-1.023256	3.661203
C	-1.205879	-0.156605	4.453995
H	-1.862326	0.526069	5.007631
H	-0.668714	-0.785258	5.171285
C	-0.294076	0.552132	3.434749
C	1.478599	3.098849	0.021849
H	1.989658	3.904982	0.585763
C	3.559452	0.291125	0.990682
C	4.943551	0.217939	1.197980
C	2.824412	-0.900126	1.056443
C	5.580490	-0.996018	1.434222
H	5.534584	1.130908	1.145479
C	3.437471	-2.118372	1.307029
H	1.744014	-0.877819	0.896919
C	4.818256	-2.156470	1.480710
H	6.656937	-1.043705	1.577700
H	2.854690	-3.035248	1.345719
Cl	5.602948	-3.697752	1.761964
C	2.967469	1.586450	0.643176
H	3.594308	2.430891	0.974272
N	1.630650	1.821044	0.634750
C	0.033644	3.459147	-0.105745
O	-0.893495	2.655089	-0.095278
O	-0.167683	4.773052	-0.291280
C	-1.525776	5.145597	-0.546049
H	-2.171818	4.844040	0.284265
H	-1.517029	6.230214	-0.655946
H	-1.885643	4.669059	-1.465084
Cu	0.120514	0.564207	0.281942
H	-3.268599	-2.886246	-1.596498
H	0.763213	0.297850	3.605855
C	-0.404394	2.082809	3.420793
C	0.074173	2.654563	4.748147
C	-1.803962	2.564840	3.070604
H	0.283133	2.410100	2.626015
H	1.092314	2.324028	4.989088
H	0.077492	3.750380	4.726572
H	-0.579926	2.353926	5.580064
H	-2.126154	2.169691	2.100259
H	-2.545076	2.274213	3.831226
H	-1.829884	3.659952	3.006273
C	4.743942	2.293654	-1.427199
C	5.383956	1.173598	-1.892298

C	4.397018	0.165561	-2.182972
H	4.608398	-0.847914	-2.518848
C	3.164400	0.679153	-1.892957
H	2.212776	0.153363	-1.934988
C	3.320424	2.017808	-1.335777
C	2.230585	3.073817	-1.428674
C	2.781793	4.469765	-1.699775
H	1.974511	5.213985	-1.692159
H	3.511111	4.768875	-0.935865
H	3.282258	4.517701	-2.674200
C	1.214642	2.705878	-2.512816
H	0.451547	3.491362	-2.637845
H	1.710037	2.565622	-3.480252
H	0.699110	1.767454	-2.266011
H	5.218398	3.225100	-1.125855
H	6.458878	1.051698	-2.007167

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C	3.907952	0.918591	0.219489
C	4.526266	0.723088	-1.052331
C	5.647910	-0.138731	-0.876272
C	5.727808	-0.478435	0.507824
C	4.653426	0.172852	1.185610
H	3.000915	1.491522	0.399016
H	4.165219	1.107252	-2.001256
H	6.296531	-0.509252	-1.663287
H	6.449722	-1.152544	0.956938
H	4.412554	0.078401	2.240329
Fe	3.942795	-1.053786	-0.262499
C	3.554518	-2.516291	-1.607804
C	2.389797	-1.717421	-1.346095
C	3.984450	-3.087079	-0.379012
H	4.030572	-2.623613	-2.576012
C	2.101955	-1.798695	0.074216
C	3.099745	-2.652596	0.648455
H	4.866231	-3.704385	-0.240491
P	0.704717	-1.001513	0.925877
C	-0.414362	-2.416555	1.227896
C	-1.316243	-2.376043	2.299803
C	-0.510382	-3.464275	0.303158
C	-2.288099	-3.359732	2.442575
H	-1.258823	-1.565605	3.027670
C	-1.485270	-4.447567	0.449878
H	0.178962	-3.503981	-0.541924
C	-2.378843	-4.396368	1.516458
H	-2.981985	-3.313249	3.280483
H	-1.553909	-5.253093	-0.280238
H	-3.146423	-5.160140	1.623642
C	1.384129	-0.611950	2.579375
C	1.654841	0.729329	2.876370
C	1.650614	-1.589963	3.546496
C	2.202924	1.084171	4.106434
H	1.429233	1.494839	2.131693
C	2.199345	-1.234214	4.774868
H	1.406734	-2.632975	3.341323
C	2.480380	0.102621	5.054861
H	2.404364	2.131518	4.326713
H	2.399661	-2.001654	5.520827
H	2.902587	0.379279	6.019600
C	1.712168	-0.906944	-2.344880
N	0.731777	-0.092889	-2.164505
O	2.190081	-1.042345	-3.607003
C	1.358264	-0.206227	-4.442727
H	2.018710	0.481121	-4.985526
H	0.859585	-0.857785	-5.167903
C	0.396585	0.497654	-3.466954
C	-1.455812	3.114503	-0.205578
H	-1.889099	3.922377	-0.837855
C	-3.589382	0.270150	-0.966258
C	-4.976758	0.087176	-0.982383
C	-2.785575	-0.824840	-1.290361
C	-5.546583	-1.153639	-1.242592
H	-5.625825	0.932057	-0.755632
C	-3.333588	-2.074266	-1.566190
H	-1.701504	-0.706053	-1.325054
C	-4.712082	-2.231520	-1.517940
H	-6.625335	-1.287826	-1.230748
H	-2.695236	-2.920561	-1.807688
Cl	-5.410472	-3.813671	-1.811622
C	-3.029935	1.607405	-0.567627
H	-3.623937	2.389425	-1.097781
N	-1.634330	1.817427	-0.777465
C	-0.013063	3.452045	0.007128
O	0.900835	2.638443	0.077329
O	0.195580	4.769489	0.172236
C	1.538030	5.127633	0.513022
H	2.237429	4.790731	-0.258525
H	1.541914	6.215112	0.591477
H	1.822377	4.672831	1.469046
Cu	-0.173014	0.565090	-0.286076
H	3.188100	-2.880981	1.705960
H	-0.650125	0.240509	-3.689050
C	0.495405	2.028910	-3.447533
C	0.061000	2.596851	-4.791503
C	1.878685	2.520452	-3.050567
H	-0.226519	2.343956	-2.678281
H	-0.947458	2.262704	-5.066074
H	0.053026	3.692832	-4.771965
H	0.743960	2.297169	-5.600662
H	2.170970	2.124527	-2.071365
H	2.647280	2.236957	-3.786614
H	1.895118	3.615757	-2.982398
C	-4.686904	2.226026	1.379952
C	-5.119075	1.288447	2.252649
C	-4.033005	0.354513	2.517046
H	-4.109387	-0.525950	3.151765
C	-2.950973	0.738576	1.809318
H	-1.994998	0.224942	1.739771
C	-3.266808	1.958959	0.997029
C	-2.284875	3.174690	1.166258
C	-2.997439	4.519233	1.258924
H	-2.261460	5.334198	1.236556

H	-3.680174	4.673162	0.412489
H	-3.580684	4.609007	2.183482
C	-1.389820	2.993539	2.389450
H	-0.742147	3.870509	2.541715
H	-1.991976	2.862713	3.297020
H	-0.753771	2.103478	2.287200
H	-5.272089	3.050897	0.980561
H	-6.118900	1.214961	2.675340

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C	2.218888	-0.444512	-1.001111
H	2.826949	-0.441666	-1.919915
C	-1.453959	-0.008031	-0.745940
C	-2.493544	0.866006	-1.064919
C	-1.755603	-1.204888	-0.092333
C	-3.811915	0.567599	-0.736106
H	-2.268505	1.801079	-1.580034
C	-3.067518	-1.524987	0.237801
H	-0.939455	-1.884906	0.150075
C	-4.084233	-0.630912	-0.085771
H	-4.621510	1.248910	-0.985176
H	-3.305347	-2.457175	0.744453
Cl	-5.737796	-1.026455	0.325192
C	-0.032581	0.366598	-1.074471
H	-0.058609	1.018194	-1.972350
N	0.828961	-0.792910	-1.235472
C	2.873975	-1.433039	-0.049109
O	2.333361	-2.066141	0.829178
O	4.205093	-1.478619	-0.293256
C	4.947096	-2.279554	0.628620
H	4.592651	-3.314519	0.613255
H	5.986545	-2.222878	0.303056
H	4.839833	-1.887920	1.645910
C	0.214541	2.564767	0.203497
C	-0.244330	2.738176	1.458437
C	-0.092348	1.489925	2.203751
H	-0.390604	1.350141	3.239840
C	0.454604	0.559088	1.400251
H	0.690183	-0.474055	1.638176
C	0.706852	1.157309	0.040022
C	2.198448	1.013584	-0.422918
C	2.521569	1.985595	-1.559714
H	3.527558	1.784684	-1.949205
H	1.822011	1.901117	-2.400840
H	2.502471	3.023510	-1.207270
C	3.183589	1.257961	0.715226
H	4.219277	1.207739	0.357296
H	3.018104	2.255853	1.139545
H	3.065554	0.533164	1.528516
H	0.218220	3.300524	-0.596631
H	-0.672608	3.652013	1.863749
H	0.678265	-1.279749	-2.111077

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C	3.339218	-0.980031	1.617147
C	3.617384	0.007019	2.610129
C	4.952649	0.470104	2.418512
C	5.504842	-0.232096	1.304751
C	4.509836	-1.126881	0.808400
H	2.386400	-1.484841	1.476195
H	2.910308	0.386721	3.342063
H	5.443635	1.254015	2.985494
H	6.490599	-0.075914	0.879220
H	4.598987	-1.760850	-0.068807
Fe	3.839966	0.783310	0.749041
C	3.531390	2.780654	0.613264
C	2.312854	2.040914	0.438758
C	4.449847	2.362021	-0.386748
H	3.711281	3.501711	1.402666
C	2.488930	1.146896	-0.692989
C	3.817587	1.367523	-1.186890
H	5.475143	2.702358	-0.488712
P	1.236245	-0.010681	-1.315557
C	0.588063	0.837986	-2.801219
C	-0.343030	0.144848	-3.590442
C	0.875928	2.172544	-3.106635
C	-0.971687	0.773569	-4.657709
H	-0.586707	-0.892645	-3.352366
C	0.243166	2.800346	-4.179205
H	1.592677	2.728230	-2.502310
C	-0.682800	2.106438	-4.951911
H	-1.698875	0.225420	-5.254011
H	0.473759	3.840050	-4.405904
H	-1.184541	2.603109	-5.780166
C	2.228259	-1.381502	-2.008048
C	2.229450	-2.604405	-1.327817
C	2.982101	-1.250032	-3.181609
C	2.994012	-3.669509	-1.797495
H	1.621421	-2.713194	-0.429157
C	3.747386	-2.314732	-3.647006
H	2.957254	-0.312385	-3.738975
C	3.758054	-3.524092	-2.952499
H	2.986036	-4.618209	-1.262921
H	4.330764	-2.204645	-4.559743
H	4.352833	-4.357752	-3.322061
C	1.172089	2.145673	1.331873
N	0.128328	1.390222	1.384363
O	1.235224	3.175329	2.209340
C	0.081773	3.036673	3.069270
H	0.445243	2.735384	4.062407
H	-0.392454	4.018206	3.149075
C	-0.779861	1.964230	2.391458
C	-2.120585	-2.503691	1.045525
H	-2.926634	-2.698716	1.775155
C	-3.356270	0.825322	0.080529
C	-4.322273	1.622719	0.707249
C	-2.477712	1.436513	-0.824093
C	-4.378659	2.994906	0.486447
H	-5.033598	1.156085	1.388942
C	-2.521055	2.804175	-1.063916
H	-1.764382	0.820295	-1.372243
C	-3.465737	3.575460	-0.390374

H	-5.122043	3.611866	0.985420
H	-1.841505	3.266304	-1.776588
Cl	-3.518774	5.301643	-0.666727
C	-3.257846	-0.599345	0.419915
H	-4.139084	-1.030462	0.920673
N	-2.058291	-1.119010	0.674365
C	-0.813277	-2.883028	1.666597
O	0.271277	-2.372840	1.396595
O	-0.928845	-3.865659	2.571973
C	0.303467	-4.300882	3.153489
H	0.807947	-3.468567	3.655396
H	0.031700	-5.076731	3.869519
H	0.968734	-4.704910	2.383113
Cu	-0.271262	-0.332852	0.237182
H	4.276681	0.821866	-2.005219
H	-1.617335	2.430074	1.843931
C	-1.369780	0.911577	3.334709
C	-2.271108	1.583470	4.361766
C	-0.305769	0.038802	3.985579
H	-1.987815	0.260204	2.701247
H	-3.045170	2.193525	3.877855
H	-2.776952	0.840685	4.989178
H	-1.701812	2.239528	5.036499
H	0.318880	-0.455846	3.229847
H	0.354408	0.613604	4.652325
H	-0.772689	-0.744359	4.596332
C	-5.099238	-3.208738	-0.148833
C	-6.049234	-2.255965	-0.610154
C	-5.399050	-1.322681	-1.405978
H	-5.851217	-0.479364	-1.921410
C	-4.014785	-1.643128	-1.398861
H	-3.271183	-1.210572	-2.069081
C	-3.848764	-2.882337	-0.670183
C	-2.536397	-3.428250	-0.224942
C	-2.655721	-4.876355	0.241428
H	-1.677151	-5.310260	0.485074
H	-3.287696	-4.966299	1.133300
H	-3.109156	-5.485234	-0.549444
C	-1.454422	-3.313271	-1.296305
H	-0.499611	-3.739063	-0.954564
H	-1.756037	-3.848988	-2.204608
H	-1.268297	-2.264772	-1.563341
H	-5.317081	-4.042812	0.515430
H	-7.113581	-2.272606	-0.384306

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C	3.394477	0.527431	-1.702236
C	3.545257	-0.693217	-2.424992
C	4.844756	-1.215206	-2.154907
C	5.503227	-0.314034	-1.263433
C	4.606965	0.761942	-0.981445
H	2.497293	1.140755	-1.682413
H	2.777724	-1.173270	-3.025202
H	5.243524	-2.154200	-2.524138
H	6.491884	-0.449187	-0.837328
H	4.788333	1.584939	-0.296207
Fe	3.794350	-1.009297	-0.433128
C	3.461941	-2.886865	0.248786
C	2.246951	-2.124263	0.182372
C	4.363530	-2.207019	1.113103
H	3.655439	-3.798774	-0.304646
C	2.407961	-0.953240	1.023749
C	3.724322	-1.026516	1.588465
H	5.383055	-2.508977	1.329912
P	1.158355	0.340291	1.258969
C	0.409709	-0.090440	2.870596
C	-0.430135	0.854426	3.481192
C	0.517157	-1.366329	3.433666
C	-1.141088	0.529447	4.629857
H	-0.532479	1.848871	3.041490
C	-0.199868	-1.689746	4.584862
H	1.159568	-2.113548	2.967174
C	-1.031078	-0.747035	5.182668
H	-1.792625	1.270891	5.089107
H	-0.107611	-2.686472	5.013934
H	-1.595971	-1.005117	6.076452
C	2.167426	1.812700	1.654507
C	2.296073	2.816339	0.687672
C	2.825028	1.956997	2.883019
C	3.094642	3.930679	0.934621
H	1.750171	2.720625	-0.252341
C	3.622641	3.069982	3.127247
H	2.699522	1.195016	3.653505
C	3.763966	4.054759	2.149920
H	3.188000	4.707963	0.177668
H	4.130933	3.173895	4.084649
H	4.385189	4.927572	2.344092
C	1.121880	-2.450414	-0.677184
N	0.058863	-1.756296	-0.890953
O	1.234203	-3.639120	-1.320097
C	0.078246	-3.737689	-2.181266
H	0.434694	-3.695717	-3.220367
H	-0.385060	-4.713139	-2.006699
C	-0.801200	-2.537480	-1.792617
C	-2.066381	2.255756	-1.631610
H	-2.897151	2.357614	-2.361991
C	-3.392130	-0.751123	0.034079
C	-4.183089	-1.648269	-0.686985
C	-2.661908	-1.244426	1.120253
C	-4.243097	-3.000130	-0.355244
H	-4.760396	-1.280370	-1.536363
C	-2.696207	-2.592957	1.466528
H	-2.049021	-0.565412	1.715082
C	-3.486722	-3.459861	0.718558
H	-4.860787	-3.690936	-0.924708
H	-2.117726	-2.965482	2.308860
Cl	-3.518961	-5.163522	1.123671
C	-3.303964	0.693156	-0.389447
H	-4.148062	0.891080	-1.086295
N	-2.050311	0.961720	-1.026409
C	-0.774695	2.431121	-2.382798
O	0.312777	1.998621	-2.024851
O	-0.921845	3.130184	-3.522451

C	0.286847	3.341075	-4.257953
H	0.750536	2.383509	-4.515911
H	-0.006470	3.884546	-5.156720
H	0.997719	3.929029	-3.667842
Cu	-0.363004	0.280844	-0.295714
H	4.169290	-0.272662	2.230428
H	-1.668134	-2.871294	-1.201133
C	-1.338458	-1.716198	-2.968716
C	-2.210994	-2.596723	-3.852571
C	-0.237565	-1.021828	-3.756193
H	-1.958049	-0.926064	-2.517935
H	-3.002002	-3.088988	-3.270706
H	-2.694564	-2.009556	-4.642114
H	-1.626542	-3.384780	-4.351428
H	0.351135	-0.359997	-3.107220
H	0.449268	-1.734306	-4.239152
H	-0.669613	-0.403613	-4.553871
C	-4.724732	3.626344	0.292155
C	-5.598125	2.746987	1.049650
C	-4.920470	1.626517	1.393650
H	-5.298431	0.777379	1.956997
C	-3.552859	1.698782	0.815250
H	-2.748290	1.502554	1.542880
C	-3.493782	3.059922	0.188724
C	-2.309616	3.483776	-0.614038
C	-2.594470	4.765593	-1.387356
H	-1.717650	5.097083	-1.956409
H	-3.421743	4.628699	-2.096103
H	-2.871236	5.578018	-0.702641
C	-1.082370	3.681161	0.279500
H	-0.237482	4.099858	-0.286075
H	-1.305983	4.372989	1.101944
H	-0.750474	2.725654	0.710541
H	-5.031652	4.576774	-0.140279
H	-6.635992	2.970552	1.288390

B2

C	2.029247	-0.433889	-0.469434
H	2.241292	-0.111673	-1.499732
C	-1.697581	0.050877	-0.343747
C	-2.628241	0.255357	-1.362142
C	-2.142342	-0.502678	0.860589
C	-3.966972	-0.086075	-1.197621
H	-2.299002	0.691071	-2.305344
C	-3.473134	-0.857596	1.045218
H	-1.438933	-0.660665	1.680486
C	-4.376891	-0.644339	0.008367
H	-4.687722	0.073745	-1.995310
H	-3.812703	-1.290829	1.982402
Cl	-6.050887	-1.082939	0.227463
C	-0.254433	0.444503	-0.519828
H	-0.106686	0.811973	-1.548078
N	0.613635	-0.709327	-0.358190
C	2.750708	-1.732481	-0.194652
O	2.375876	-2.563714	0.605615
O	3.885878	-1.837554	-0.912084
C	4.651282	-3.016173	-0.637861
H	4.064475	-3.912287	-0.858835
H	5.525925	-2.956867	-1.286135
H	4.950262	-3.042252	0.414732
C	1.809173	3.100810	-0.230622
C	0.524016	3.773384	-0.367602
C	-0.466439	2.939550	0.017737
H	-1.532790	3.146136	0.031889
C	0.136545	1.634731	0.417974
H	-0.141951	1.350617	1.446001
C	1.611796	1.855405	0.264217
C	2.563958	0.724130	0.477816
C	3.986159	1.114611	0.094364
H	4.692847	0.298254	0.278333
H	4.055434	1.383748	-0.967278
H	4.314887	1.981152	0.681532
C	2.526850	0.262079	1.940274
H	3.267847	-0.523691	2.131929
H	2.740096	1.102302	2.611135
H	1.545342	-0.144147	2.217567
H	2.767033	3.539052	-0.503266
H	0.401809	4.791338	-0.730957
H	0.425940	-1.234822	0.492878

Cartesian coordinates optimized by M06-2X method

1a

C	-2.798774	-0.724415	1.018754
H	-2.925156	-0.141774	1.945468
H	-3.280801	-1.692743	1.164333
C	0.783060	0.060594	0.492366
C	1.588433	1.166344	0.767319
C	1.346686	-1.065209	-0.117724
C	2.941781	1.159188	0.446278
H	1.153364	2.044985	1.236916
C	2.694137	-1.086589	-0.443155
H	0.708225	-1.916558	-0.330391
C	3.480425	0.028648	-0.156014
H	3.573353	2.014726	0.658572
H	3.142573	-1.953167	-0.916373
Cl	5.174927	0.002615	-0.562942
C	-0.644919	0.090142	0.854160
H	-1.001717	1.024713	1.313839
N	-1.410550	-0.902982	0.657930
C	-3.546377	0.045359	-0.063698
O	-3.064741	0.899879	-0.760039
O	-4.835992	-0.316940	-0.100389
C	-5.635363	0.407794	-1.036871
H	-5.245020	0.276197	-2.048050
H	-6.638383	-0.006893	-0.952785
H	-5.635016	1.472293	-0.792096

2a

C	-0.391182	-0.161521	-0.000016
C	-1.252608	0.962103	0.000041
C	-2.632918	0.813287	0.000056
C	-3.171020	-0.473618	-0.000003
C	-2.332127	-1.585567	-0.000094
C	-0.941826	-1.440299	-0.000110
C	-0.430375	2.172659	0.000042
H	-3.281401	1.685047	0.000101
H	-4.248192	-0.610166	0.000007
H	-2.761033	-2.583091	-0.000165
H	-0.324541	-2.330175	-0.000218
H	-0.826743	3.181374	0.000088
C	0.870297	1.823303	-0.000023
H	1.704000	2.512909	-0.000024
C	1.000673	0.353282	-0.000026
C	3.508287	0.314245	-0.000071
H	4.080265	-0.007586	0.879042
H	4.080283	-0.007911	-0.879053
H	3.464188	1.402767	-0.000280
C	2.157520	-0.343864	0.000022
C	2.197225	-1.851526	0.000168
H	1.696116	-2.262337	0.883412
H	1.696759	-2.262488	-0.883379
H	3.228635	-2.213243	0.000564

6

C	0.970359	1.173373	0.000056
C	2.247359	0.733602	-0.000223
C	2.247357	-0.733602	0.000045
H	3.137995	-1.350615	0.000094
C	0.970355	-1.173370	-0.000227
H	0.647790	-2.205948	-0.000345
C	0.079882	0.000003	-0.000023
C	-1.271931	0.000001	0.000042
C	-2.090290	1.259760	0.000148
H	-2.745737	1.281639	-0.879008
H	-2.745535	1.281593	0.879457
H	-1.482981	2.164367	0.000106
C	-2.090279	-1.259764	0.000092
H	-2.745292	-1.281796	0.879572
H	-2.745956	-1.281454	-0.878893
H	-1.482961	-2.164366	-0.000307
H	3.137999	1.350613	-0.000303
H	0.647798	2.205953	0.000168

H2

H	0.000000	0.000000	0.368263
H	0.000000	0.000000	-0.368263

A1

C	2.403174	-0.907253	-0.990466
H	3.068025	-0.934920	-1.862890
C	-1.293075	-0.752180	-0.820565
C	-2.404131	0.035172	-1.123372
C	-1.478557	-1.958949	-0.144503
C	-3.684970	-0.366161	-0.757121
H	-2.267986	0.979438	-1.645405
C	-2.753466	-2.376895	0.221740
H	-0.606886	-2.562859	0.090624
C	-3.845372	-1.573680	-0.088480
H	-4.550671	0.243702	-0.990834
H	-2.904497	-3.315775	0.743404
Cl	-5.451125	-2.095515	0.364758
C	0.093727	-0.269517	-1.184085
H	0.012526	0.320863	-2.113354
N	1.054991	-1.357744	-1.285339
C	3.055984	-1.791888	0.066916
O	2.494406	-2.435185	0.917217
O	4.394791	-1.734678	-0.049398
C	5.117146	-2.440025	0.958847
H	4.841093	-3.496422	0.956137
H	6.170784	-2.314846	0.714216
H	4.898718	-2.019890	1.944076
C	0.104984	2.010921	-0.016357
C	-0.378753	2.202213	1.290757
C	-1.045742	3.370738	1.641654
C	-1.242197	4.349643	0.667614
C	-0.789599	4.153691	-0.635641

C	-0.117302	2.979059	-0.986912
C	-0.089404	0.991513	2.069537
H	-1.420683	3.512239	2.651248
H	-1.764457	5.266651	0.923147
H	-0.962879	4.917114	-1.387749
H	0.211703	2.834191	-2.012233
H	-0.365513	0.856392	3.109362
C	0.525549	0.093289	1.289639
H	0.844093	-0.904519	1.571161
C	0.745924	0.640095	-0.110127
C	2.262395	0.581449	-0.514866
C	2.580813	1.484735	-1.712720
H	3.619619	1.323610	-2.019772
H	1.942895	1.270680	-2.577495
H	2.465303	2.539122	-1.448256
C	3.185791	0.976450	0.638912
H	4.231353	0.978153	0.315456
H	2.925700	1.984969	0.978561
H	3.088714	0.303953	1.496227
H	0.976144	-1.889509	-2.144105

A1-s

C	0.317457	-0.143002	-0.428445
C	1.152589	0.915097	-0.022956
C	2.464829	0.681366	0.373615
C	2.945363	-0.627550	0.356728
C	2.129370	-1.676095	-0.064822
C	0.811450	-1.439663	-0.466274
C	0.395031	2.167943	-0.139643
H	3.105466	1.502372	0.683310
H	3.967261	-0.831199	0.662437
H	2.523188	-2.687654	-0.088811
H	0.197874	-2.264449	-0.816185
H	0.796174	3.147282	0.098092
C	-0.838622	1.898920	-0.590613
H	-1.627000	2.623786	-0.766304
C	-1.046171	0.413748	-0.787479
C	-2.233089	-0.114891	0.059775
C	-2.577685	-1.567803	-0.267116
H	-3.519101	-1.853236	0.213499
H	-2.685673	-1.727076	-1.345595
H	-1.803425	-2.245893	0.105587
C	-1.988290	0.052410	1.559385
H	-2.872409	-0.253635	2.127667
H	-1.146885	-0.570816	1.881191
H	-1.757179	1.090407	1.815742
H	-3.097389	0.504172	-0.220010
H	-1.274288	0.203065	-1.843541

A9

C	1.473985	-1.472373	-0.439056
H	1.806075	-1.107573	-1.418670
C	-2.031243	-0.111734	-0.301272
C	-2.836996	0.445224	-1.293016
C	-2.645330	-0.681288	0.816704
C	-4.224468	0.432209	-1.184390
H	-2.373729	0.897600	-2.165649
C	-4.029467	-0.709295	0.941109
H	-2.040434	-1.110302	1.613427
C	-4.808431	-0.149262	-0.065791
H	-4.849439	0.864679	-1.958231
H	-4.503688	-1.155723	1.808299
Cl	-6.546892	-0.172897	0.081328
C	-0.524371	-0.072285	-0.416424
H	-0.254014	0.367455	-1.385683
N	0.029561	-1.414422	-0.386518
C	1.854686	-2.935181	-0.310623
O	1.281772	-3.717977	0.408823
O	2.916621	-3.257626	-1.059408
C	3.343223	-4.616666	-0.940703
H	2.543405	-5.291204	-1.252988
H	4.207787	-4.712877	-1.595084
H	3.612642	-4.841131	0.093810
C	2.077920	1.999596	0.187207
C	0.941139	2.950859	0.134162
C	1.175927	4.337803	-0.199622
C	2.434241	4.749474	-0.467435
C	3.553074	3.824273	-0.428177
C	3.399538	2.515289	-0.120534
C	-0.211820	2.303595	0.430149
H	0.336015	5.026163	-0.226918
H	2.630999	5.787684	-0.717574
H	4.543608	4.208618	-0.653249
H	4.265696	1.866405	-0.100968
H	-1.208647	2.726842	0.472257
C	0.102159	0.868161	0.670816
H	-0.255418	0.527873	1.652879
C	1.598585	0.767675	0.537622
C	2.220564	-0.598473	0.650895
C	3.723906	-0.610506	0.375138
H	4.127294	-1.621339	0.483848
H	3.948503	-0.269027	-0.640536
H	4.245256	0.035561	1.088278
C	1.967017	-1.174381	2.056549
H	2.469042	-2.138413	2.183157
H	2.346415	-0.481522	2.813641
H	0.901091	-1.333090	2.247670
H	-0.318400	-1.977953	0.386157

A9-s

C	0.278531	-0.075637	-0.000061
C	1.387413	0.903426	-0.000084
C	2.753125	0.426016	-0.000016
C	2.986750	-0.905106	0.000053
C	1.899095	-1.871709	-0.000077
C	0.602308	-1.487693	-0.000148
C	0.879940	2.159651	-0.000008
H	3.570304	1.141944	0.000032

H	4.006000	-1.279988	0.000216
H	2.152048	-2.927836	-0.000174
H	-0.191114	-2.229252	-0.000363
H	1.439224	3.087103	0.000035
C	-0.612160	2.064427	0.000104
H	-1.059925	2.555825	0.877935
C	-0.909600	0.590693	0.000029
C	-2.316435	0.053472	0.000098
C	-2.617344	-0.761787	-1.265241
H	-3.663019	-1.087378	-1.275663
H	-2.429527	-0.171244	-2.166674
H	-1.984323	-1.653500	-1.314485
C	-2.617019	-0.762196	1.265263
H	-3.662705	-1.087746	1.275906
H	-1.984022	-1.653949	1.314022
H	-2.428885	-0.171959	2.166825
H	-1.060247	2.556084	-0.877408
H	-2.991431	0.920564	0.000316

B1

C	2.228677	-0.417581	-1.040665
H	2.887497	-0.419934	-1.918235
C	-1.434353	0.044269	-0.775123
C	-2.472949	0.953322	-0.971996
C	-1.722004	-1.207174	-0.227993
C	-3.781549	0.632289	-0.624650
H	-2.258667	1.929505	-1.401028
C	-3.025535	-1.546027	0.117987
H	-0.906812	-1.908859	-0.075940
C	-4.043855	-0.619789	-0.082615
H	-4.590596	1.338169	-0.777583
H	-3.254782	-2.517782	0.542278
Cl	-5.684485	-1.039943	0.347549
C	-0.015758	0.440779	-1.117483
H	-0.060390	1.131333	-1.976801
N	0.843580	-0.708587	-1.364039
C	2.790806	-1.460252	-0.079900
O	2.165955	-2.119928	0.711390
O	4.128918	-1.528402	-0.202415
C	4.774450	-2.390062	0.733527
H	4.384513	-3.406191	0.646990
H	5.834394	-2.360128	0.485980
H	4.607293	-2.032623	1.753009
C	0.261680	2.586391	0.241798
C	-0.210334	2.726606	1.490801
C	-0.090709	1.441471	2.200358
H	-0.406709	1.273127	3.223397
C	0.447942	0.532125	1.374613
H	0.655148	-0.511361	1.582831
C	0.732751	1.171175	0.032482
C	2.226917	1.017598	-0.410772
C	2.585638	2.023081	-1.513451
H	3.595723	1.818625	-1.883988
H	1.900815	1.968779	-2.366489
H	2.570677	3.045317	-1.124294
C	3.200061	1.207497	0.753474
H	4.236699	1.163009	0.404743
H	3.026548	2.188306	1.209255
H	3.062053	0.451914	1.532302
H	0.290737	3.348241	-0.529377
H	-0.626420	3.631407	1.919775
H	0.713204	-1.119365	-2.281037

B1-s

C	-0.672998	-1.192274	-0.220309
C	-1.905231	-0.798531	-0.582940
C	-2.205613	0.494261	0.053722
H	-3.136501	1.036920	-0.067387
C	-1.152361	0.869564	0.797787
H	-1.059784	1.776911	1.384916
C	-0.065380	-0.168430	0.704652
C	1.307570	0.387500	0.261233
C	2.385721	-0.694247	0.320928
H	3.368995	-0.274302	0.085216
H	2.442579	-1.152702	1.313917
H	2.183599	-1.487576	-0.407617
C	1.245257	1.015877	-1.130692
H	2.205806	1.472959	-1.389850
H	1.017347	0.256063	-1.885900
H	0.470815	1.786364	-1.186162
H	-0.173641	-2.106010	-0.521841
H	-2.587013	-1.336198	-1.232561
H	1.574806	1.172742	0.982488
H	0.071206	-0.627499	1.698494

B2

C	2.032705	-0.428628	-0.472253
H	2.240925	-0.125449	-1.506027
C	-1.703041	0.045540	-0.338700
C	-2.630757	0.259971	-1.356734
C	-2.145804	-0.519253	0.860243
C	-3.970060	-0.082685	-1.194257
H	-2.301914	0.701223	-2.293800
C	-3.477447	-0.873912	1.039827
H	-1.445145	-0.685692	1.676247
C	-4.380159	-0.650076	0.005549
H	-4.690128	0.083555	-1.988064
H	-3.818726	-1.314670	1.970240
Cl	-6.056673	-1.084428	0.223351
C	-0.254691	0.442962	-0.512816
H	-0.110897	0.811308	-1.537927
N	0.617080	-0.710756	-0.350084
C	2.763608	-1.726891	-0.189264
O	2.391103	-2.547606	0.614422
O	3.892839	-1.843837	-0.899720
C	4.650156	-3.025925	-0.632383
H	4.057883	-3.913496	-0.863491
H	5.526194	-2.968140	-1.276018
H	4.943545	-3.059000	0.419270
C	1.797861	3.104053	-0.225188

C	0.496872	3.775035	-0.352949
C	-0.481917	2.934661	0.029251
H	-1.547078	3.133138	0.048984
C	0.130906	1.625394	0.427492
H	-0.134363	1.347228	1.457600
C	1.608925	1.859801	0.258785
C	2.573116	0.726626	0.460878
C	3.990518	1.128141	0.054270
H	4.696251	0.308726	0.214541
H	4.031875	1.411137	-1.003003
H	4.320257	1.985403	0.650851
C	2.561509	0.276567	1.931371
H	3.315381	-0.496162	2.112888
H	2.775973	1.129574	2.582274
H	1.590435	-0.137223	2.223019
H	2.747114	3.549827	-0.501916
H	0.367664	4.791248	-0.708656
H	0.433301	-1.238723	0.500248

B2-s

C	0.786080	1.121619	-0.193102
C	2.217805	0.799667	-0.273323
C	2.399691	-0.495066	0.033639
H	3.339114	-1.033485	0.060648
C	1.064785	-1.119166	0.328565
H	0.848927	-1.943744	-0.365373
C	0.090186	0.022572	0.159745
C	-1.391423	-0.124589	0.374628
C	-2.132452	1.197661	0.186337
H	-3.201689	1.071486	0.381218
H	-1.748848	1.968226	0.861786
H	-2.016366	1.557904	-0.842224
C	-1.978526	-1.204141	-0.545939
H	-3.054908	-1.311296	-0.376758
H	-1.821742	-0.932171	-1.595582
H	-1.513047	-2.179355	-0.374761
H	0.370440	2.104832	-0.384926
H	2.991376	1.511410	-0.539642
H	-1.547008	-0.458415	1.412219
H	1.016864	-1.546732	1.340090

A1-s-3R

C	-0.767742	0.123988	-0.490499
C	-0.371785	1.454436	-0.139423
C	0.930828	1.754483	0.158463
C	1.913350	0.728103	0.112259
C	1.529365	-0.593346	-0.260123
C	0.164439	-0.871913	-0.566367
C	-1.562512	2.308041	-0.211568
H	1.231310	2.766522	0.419634
H	-1.559456	3.373162	-0.007445
C	-2.620693	1.570829	-0.576209
H	-3.634990	1.935823	-0.704140
C	-2.262816	0.110446	-0.750448
C	-3.099761	-0.797467	0.188385
C	-2.874877	-2.282747	-0.093077
H	-3.599980	-2.889642	0.458726
H	-2.979592	-2.514467	-1.158731
H	-1.876304	-2.593729	0.230456
C	-2.847874	-0.487599	1.663725
H	-3.493578	-1.102130	2.299034
H	-1.807324	-0.706090	1.928034
H	-3.041118	0.564262	1.893370
H	-4.151221	-0.568940	-0.037691
H	-2.465639	-0.208503	-1.783922
C	4.213927	-0.014694	0.349919
C	3.833080	-1.325158	-0.022681
C	2.522696	-1.603485	-0.320148
C	3.276369	0.984659	0.413632
H	5.252792	0.197412	0.583499
H	4.582097	-2.109415	-0.073928
H	2.224372	-2.608920	-0.606920
H	3.564124	1.994117	0.696582
H	-0.101460	-1.880917	-0.871594

A9-s-3R

C	0.800132	0.276355	-0.000012
C	0.230401	1.642183	-0.000047
C	-1.194467	1.808533	-0.000008
C	-2.014320	0.714946	0.000018
C	-1.450654	-0.645440	0.000028
C	-0.097011	-0.844257	0.000038
C	1.240999	2.551883	-0.000044
H	-1.620288	2.809313	-0.000028
H	0.290107	-1.859992	0.000032
H	1.146027	3.630429	-0.000056
C	2.536817	1.811075	0.000011
H	3.155937	2.058340	-0.876865
C	2.165166	0.356699	-0.000042
C	3.191205	-0.743824	-0.000012
C	3.101575	-1.609384	1.265130
H	3.893050	-2.366407	1.271703
H	3.199844	-0.998180	2.167009
H	2.137947	-2.126031	1.317842
C	3.101578	-1.609471	-1.265091
H	3.893049	-2.366498	-1.271589
H	2.137949	-2.126118	-1.317787
H	3.199872	-0.998334	-2.167014
H	3.155692	2.058243	0.877102
H	4.179360	-0.263113	-0.000026
C	-3.712958	-1.569264	-0.000012
C	-4.267028	-0.231725	0.000027
C	-3.457395	0.849758	0.000001
C	-2.375435	-1.760674	-0.000041
H	-4.388295	-2.419114	-0.000036
H	-5.345644	-0.108586	0.000077
H	-3.869688	1.855602	0.000043
H	-1.956548	-2.763924	-0.000064

A1-s-4R

C	0.793266	-0.363194	-0.502441
C	-0.190239	-1.317624	-0.486845
C	-1.556399	-0.998449	-0.178808
C	-1.889423	0.353259	0.093438
C	-0.867228	1.387714	-0.034887
C	0.470915	1.026794	-0.358051
C	0.403685	-2.620677	-0.817318
H	-0.143635	-3.552334	-0.903338
C	1.721567	-2.459593	-1.003361
H	2.439602	-3.240199	-1.231055
C	2.134738	-1.033116	-0.727264
C	3.105036	-1.030394	0.500588
C	3.868978	0.278081	0.699958
H	4.653581	0.134102	1.450244
H	4.349511	0.616731	-0.225078
H	3.210968	1.073730	1.060770
C	2.394023	-1.420952	1.796675
H	3.124783	-1.557923	2.600172
H	1.697667	-0.633928	2.104975
H	1.828632	-2.350345	1.684843
H	3.851436	-1.804453	0.273236
H	2.669647	-0.601106	-1.585637
C	-1.167376	2.758901	0.113345
C	-3.223714	0.643898	0.452027
C	1.093807	3.375937	-0.449384
C	-0.211620	3.733949	-0.076211
C	1.421615	2.046528	-0.590273
H	1.838212	4.143725	-0.636208
H	-0.476665	4.780098	0.040768
H	2.419906	1.767176	-0.909249
C	-4.182072	-0.344619	0.521802
C	-3.847734	-1.677905	0.233490
C	-2.552683	-1.994588	-0.109818
H	-5.199567	-0.089043	0.801025
H	-4.605037	-2.453794	0.288510
H	-2.284302	-3.024917	-0.322911
H	-3.513665	1.662195	0.684433
H	-2.175920	3.066606	0.364530

A9-s-4R

C	-0.747220	-0.522724	-0.001113
C	0.388167	-1.475577	-0.003280
C	1.774601	-1.010723	-0.002076
C	2.035966	0.372467	0.001080
C	0.912672	1.345515	0.000079
C	-0.440267	0.918439	-0.001596
C	-0.072510	-2.742591	-0.004066
H	0.510822	-3.654580	-0.005107
C	-1.558039	-2.702214	-0.001359
H	-1.995577	-3.203263	-0.879064
C	-1.911111	-1.237269	0.000801
C	-3.390458	-0.910342	0.005047
C	-3.867818	-0.224401	1.294778
H	-4.954915	-0.093054	1.269241
H	-3.620846	-0.845882	2.160909
H	-3.413075	0.753986	1.461095
C	-3.876682	-0.232702	-1.285859
H	-4.963583	-0.101102	-1.253853
H	-3.422978	0.744553	-1.461514
H	-3.635520	-0.859697	-2.149678
H	-1.991600	-3.205098	0.877247
H	-3.888132	-1.890418	0.009838
C	3.378327	0.786178	0.004568
C	1.174951	2.723780	-0.000403
C	-1.163995	3.250108	-0.005049
C	0.162394	3.669397	-0.002470
C	-1.446488	1.893560	-0.004864
H	-1.974746	3.972041	-0.007680
H	0.409278	4.726464	-0.002821
H	-2.478522	1.579757	-0.007506
C	4.420948	-0.126332	0.004319
C	4.151437	-1.495192	0.000487
C	2.836169	-1.924354	-0.002587
H	5.446211	0.230476	0.007122
H	4.962768	-2.216375	0.000226
H	2.617750	-2.987744	-0.005381
H	3.628832	1.839891	0.007733
H	2.197563	3.079904	0.000558

A1-s-5R

C	1.201970	-0.264474	-0.502345
C	0.548688	-1.469820	-0.459946
C	-0.861909	-1.570023	-0.195392
C	-1.582373	-0.357200	-0.009939
C	-0.922010	0.905904	-0.136008
C	0.477371	0.974035	-0.413894
C	1.510532	-2.546177	-0.731363
H	1.265365	-3.600792	-0.784176
C	2.723081	-2.005071	-0.915090
H	3.645611	-2.541906	-1.108285
C	2.685871	-0.511508	-0.692076
C	3.594305	-0.176463	0.537119
C	3.929766	1.306457	0.689171
H	4.713600	1.430695	1.443699
H	4.296220	1.740739	-0.248075
H	3.059369	1.879250	1.021359
C	3.015139	-0.717263	1.844941
H	3.743927	-0.605003	2.654065
H	2.113811	-0.161474	2.124132
H	2.751052	-1.775549	1.764949
H	4.540225	-0.699877	0.339443
H	3.079279	0.029921	-1.564950
C	-3.698852	0.826726	0.429724
C	-3.080091	2.022031	0.291623
C	-1.674429	2.106179	-0.010879
C	-2.975699	-0.407756	0.268819

H	-4.761218	0.774449	0.653240
H	-3.635190	2.950218	0.399998
C	0.306964	3.395801	-0.530260
C	-1.041072	3.339090	-0.199154
C	1.056471	2.229874	-0.640431
H	0.780020	4.356613	-0.708848
H	-1.622208	4.252621	-0.105060
H	2.101171	2.288026	-0.925491
C	-3.611739	-1.649984	0.365638
C	-2.898296	-2.828376	0.182388
C	-1.536771	-2.790848	-0.098931
H	-4.676538	-1.681563	0.581123
H	-3.406158	-3.784857	0.259155
H	-0.989831	-3.718309	-0.238546

A9-s-5R

C	-1.159801	-0.523872	-0.000005
C	-0.259814	-1.703696	0.000112
C	1.194682	-1.553755	0.000008
C	1.736353	-0.244783	0.000032
C	0.876295	0.923164	0.000060
C	-0.548668	0.818016	-0.000025
C	-0.986717	-2.838426	0.000304
H	-0.614919	-3.855415	0.000484
C	-2.428311	-2.474527	0.000315
H	-2.962964	-2.869324	-0.877807
C	-2.450847	-0.968346	0.000096
C	-3.814716	-0.312464	-0.000092
C	-4.117155	0.463294	1.292230
H	-5.127365	0.884563	1.251901
H	-4.064887	-0.212080	2.151659
H	-3.415511	1.277412	1.481973
C	-4.116738	0.463030	-1.292669
H	-5.126785	0.884714	-1.252608
H	-3.414710	1.276794	-1.482550
H	-4.064615	-0.212615	-2.151895
H	-2.962902	-2.869061	0.878591
H	-4.528625	-1.148213	-0.000080
C	2.912993	2.326678	0.000157
C	3.709513	1.234471	0.000098
C	3.144694	-0.086116	-0.000002
C	1.480315	2.206072	0.000108
H	3.339474	3.326364	0.000218
H	4.791817	1.332835	0.000125
C	-0.691590	3.255074	-0.000050
C	0.680306	3.363586	0.000061
C	-1.293053	1.991746	-0.000068
H	-1.314768	4.143895	-0.000079
H	1.163051	4.337239	0.000115
H	-2.370631	1.938939	-0.000126
C	3.976190	-1.221318	-0.000148
C	3.432363	-2.489515	-0.000236
C	2.043804	-2.651740	-0.000149
H	5.053850	-1.080869	-0.000211
H	4.077678	-3.362367	-0.000390
H	1.622224	-3.652247	-0.000148