Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Synthesis of New Chiral Mn(III)-Salen Complexes as Recoverable and Reusable Homogeneous Catalysts for Asymmetric Epoxidation of Styrenes and Chromenes

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Table 1. Comparison of literature reported homogeneous Mn(III)-salen complexes with Mn(III)-salen complexes **1b** and **2b** for asymmetric epoxidation of styrene.

Entry	Homogeneous Catalyst	Styrene, Catalyst loading, reaction time, temp.	Solvent (mL)	Oxidant (mmol)/Axial base (mmol)	Yield (%)	*ee* (%)	TOF ($x10^{-3}$ s^{-1})	Ref.
1	C_2-Symmetrical diphenol-derived bi-Mn(III)-salen complex	0.5 mmol, 5 mol%, 1 h, 0 °C	CH_2Cl_2 (3 mL)	*m*-CPBA (1.6)/NMO (2.5)	99.4 (DACH)	27.5 (DACH)	5.52(DACH)	1
2	Polymeric Mn(III)-salen complex	0.5 mmol, 4 mol%, 2 h, 0 °C	CH_2Cl_2 (1 mL)	*m*-CPBA (1)/PyNO (1)	>99(DACH)	35(DACH)	3.44(DACH)	2
3	Macrocyclic Mn(III)-salen complex	0.625 mmol, 5 mol%, 6 h, 5 °C	DMC (1 mL)	NaOCl (1.5)/PyNO (0.12)	>99(DACH)	40(DACH)	0.92(DACH)	3
4	Macrocyclic Mn(III)-salen complexes	0.625 mmol, 5 mol%, 3 h, 0 °C	CH_2Cl_2 (1 mL)	NaOCl (1.5)/PyNO (0.12)	>99(DACH) >99(DPEN)	33(DACH) 59(DPEN)	1.83(DACH) 1.83(DPEN)	4
5	Dimeric homochiral Mn(III)-salen complex	0.4 mmol, 7 mol%, 5 h, 2 °C	CH_2Cl_2: CH_3CN (1.5:1.5 mL)	Oxone (0.6)/PyNO (0.4)	>99(DACH)	44(DACH)	0.79(DACH)	5
6	Macrocyclic Mn(III)-salen complex	0.625 mmol, 2.5 mol%, 4 h, 0 °C	CH_2Cl_2 (1 mL)	NaOCl (1.5)/PyNO (0.063)	>99(DPEN)	70(DPEN)	2.78(DPEN)	6
7	Polymeric ionic liquid-functionalized Mn(III)-salen complex	0.5 mmol, 4 mol%, 2 h, 0 °C	CH_2Cl_2 (1 mL)	*m*-CPBA (1)/PyNO (1)	99(DACH)	39(DACH)	3.44(DACH)	7
8	Ionic liquid-functionalized Mn(III)-salen complex	0.5 mmol, 4 mol%, 2 h, 0 °C	CH_2Cl_2 (1 mL)	*m*-CPBA (1)/PyNO (1)	99(DACH)	40(DACH)	3.44(DACH)	8
9	Dimeric Mn(III)-salen complex	1 mmol, 2.5 mol%, 10 min, 0 °C	CH_2Cl_2 (1 mL)	*m*-CPBA (2)/NMO (5)	73 (DPEN)	55 (DPEN)	48.67(DPEN)	9
10	Mn(III)-salen complexes	2.5 mmol, 1 mol%, 20 h, 2 °C	CH_2Cl_2: MeOH (1:1, 1.6 mL)	Urea-H_2O_2 adduct (3)/Ammonium acetate (0.2)	70(DACH) 75(DPEN)	32(DACH) 39(DPEN)	0.97(DACH) 1.04(DPEN)	10
11	Mn(III)-salen complexes	0.5 mmol, 2 mol%, 1 h (DPEN) or 2 h (DACH), 0 °C	Ethyl acetate (0.5 mL)	NaOCl (1.34)/PyNO (0.05)	98(DACH) 97(DPEN)	34(DACH) 53(DPEN)	6.8(DACH) 13.5(DPEN)	**This work**

DPEN = 1,2-Diphenyl-1,2-ethylenediamine
DACH = 1,2-Diaminocyclohexane
DMC = Dimethyl Carbonate
Turn over frequency = [product]/[catalyst][time]

Calibration of GC

The calibration curve of the conversion of styrene oxide was plotted between observed area% ratio of the styrene oxide with respect to styrene and known concentration of the styrene oxide and styrene. We have prepared the equal concentration (10 mM) solution of styrene and styrene oxide in ethyl acetate and mixed them in different ratios as given in Table 2 and calculated the area% for different known ratios of styrene and styrene oxide by gas chromatographic (GC) analysis. We obtained a straight line with slope 0.9798 as a response factor for styrene oxide.

Table 2. Area % for the known concentration ratios of styrene and styrene oxide using gas chromatographic (GC) analysis.

Entry	(Known conc.) Styrene : Styrene oxide	(Obtained Area %)	
		Styrene	Styrene oxide
1	10:90	11.5464	88.4536
2	30:70	31.4116	68.5884
3	50:50	49.7104	50.2896
4	70:30	70.4295	29.5705
5	90:10	89.5176	10.4824

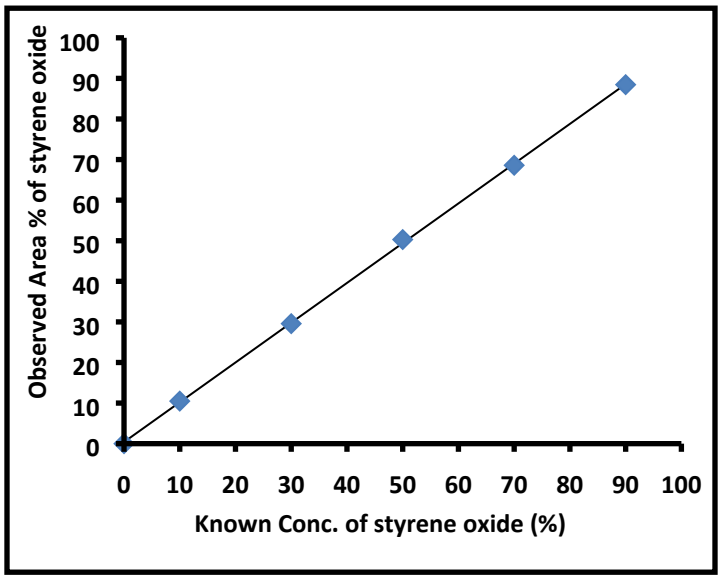
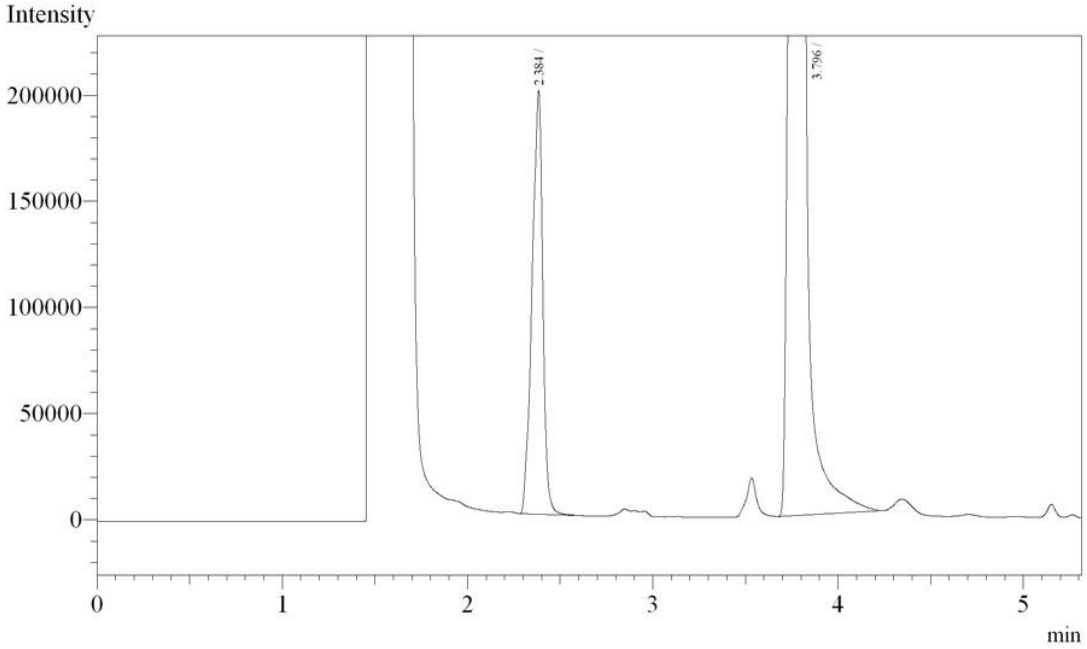


Figure 1. Calibration curve for the gas chromatographic (GC) studies using styrene and styrene oxide.

10% Styrene 90% styrene oxide

Analysis Date & Time : 11/7/2021 6:44:37 PM
User Name : Admin
Vial# : 0
Sample Name : 10 ST 90 STO
Sample ID : 10 ST 90 STO
Sample Type : Unknown
Injection Volume :
ISTD Amount :

Data Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\Mn complex paper calibration\NEW\
Method Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\condition\methanol Calibration.gcm

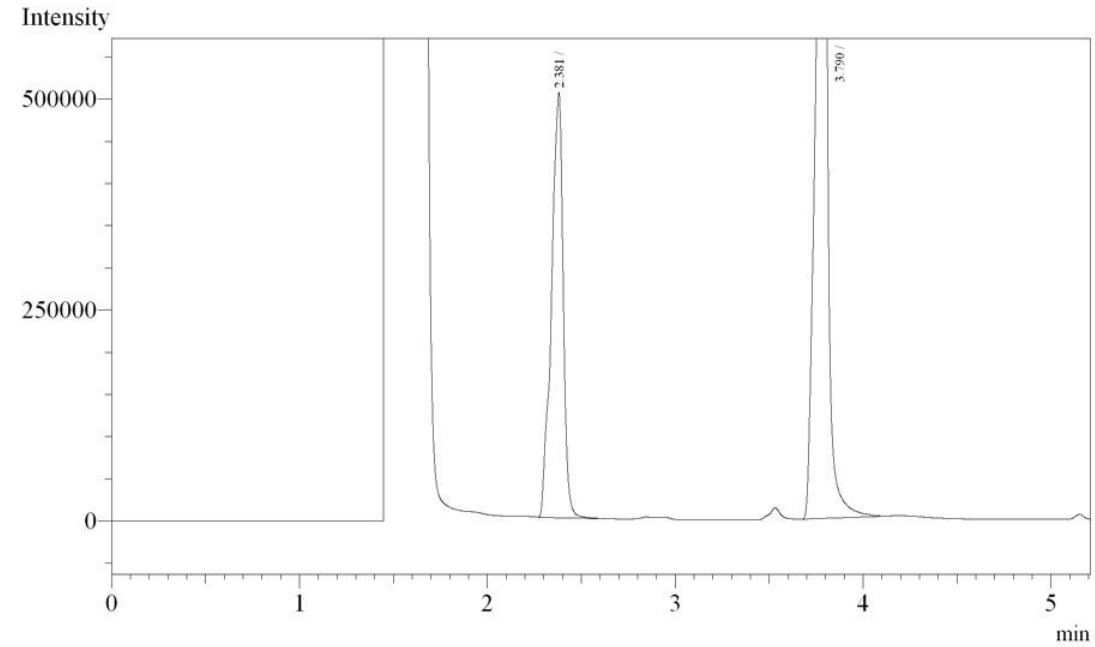


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name	Area%
1	2.384	800708	196423	11.546					11.5464
2	3.796	6133964	1703149	88.454					88.4536
Total		6934672	1899572						100.0000

30% Styrene 70% styrene oxide

Analysis Date & Time : 11/7/2021 7:11:15 PM
User Name : Admin
Vial# : 0
Sample Name : 30 ST 70 STO
Sample ID : 30 ST 70 STO
Sample Type : Unknown
Injection Volume :
ISTD Amount :

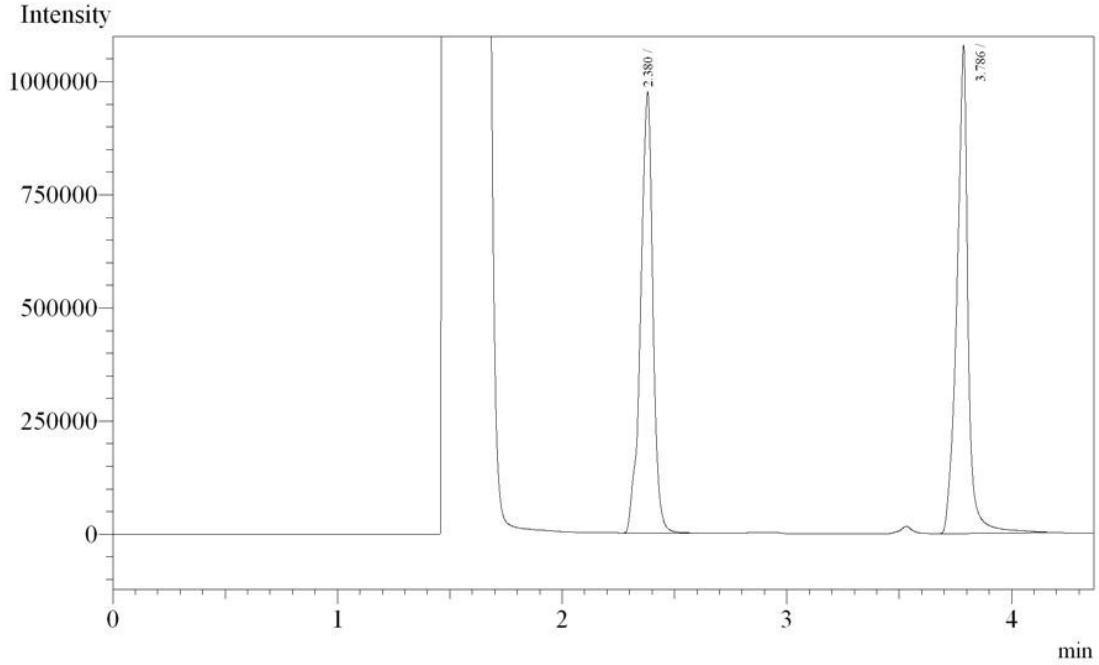
Data Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\Mn complex paper calibration\NEW\
Method Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\condition\methanol Calibration.gcm



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name	Area%
1	2.381	2180477	500863	31.412					31.4116
2	3.790	4761141	1277920	68.588					68.5884
Total		6941618	1778783						100.0000

50% Styrene 50% styrene oxide

Analysis Date & Time	: 11/7/2021 3:54:00 PM
User Name	: Admin
Vial#	: 0
Sample Name	: 50 ST 50 STO NEW 5
Sample ID	: 50 ST 50 STO NEW 5
Sample Type	: Unknown
Injection Volume	:
ISTD Amount	:
Data Name	: C:\GCsolution\Data\Project1\POOJA CHAUDHARY\Mn complex paper calibration\microl
Method Name	: C:\GCsolution\Data\Project1\POOJA CHAUDHARY\condition\methanol Calibration.gcm



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name	Area%
1	2.380	3714876	965730	49.710					49.7104
2	3.786	3758165	1072758	50.290					50.2896
Total		7473041	2038488						100.0000

70% Styrene 30% styrene oxide

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Vial# : 0
Sample Name : 70 ST 30 STO
Sample ID : 70 ST 30 STO
Sample Type : Unknown
Injection Volume :
ISTD Amount :

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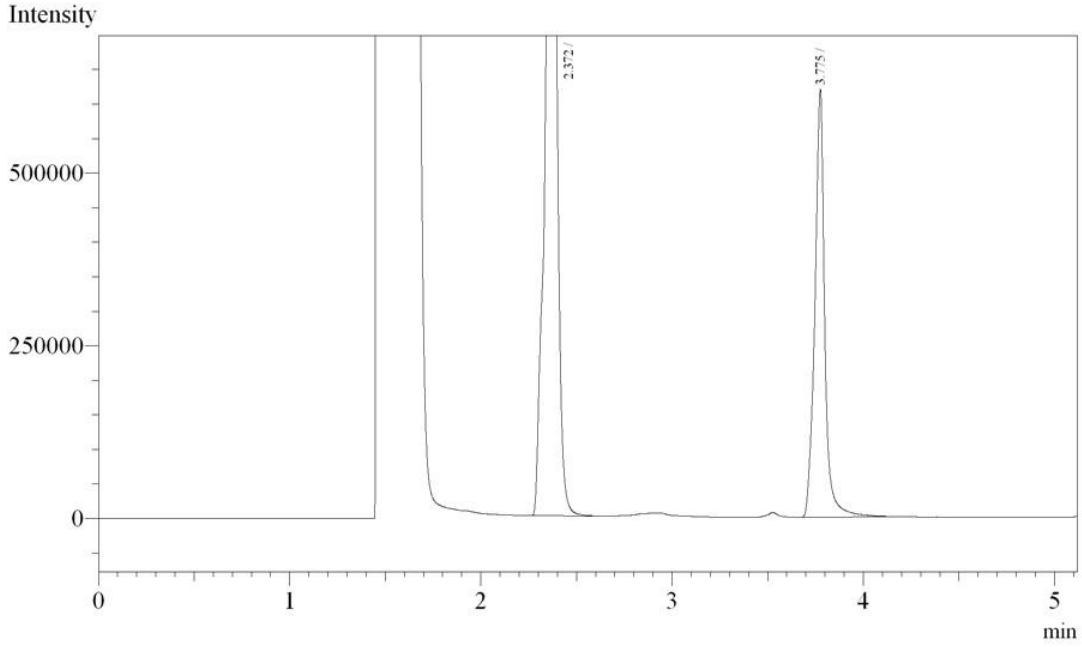

Peak#	Ret.Time	Area	Height	Conc.	Unit Mark	ID#	Cmpd Name	Area%
1	2.372	5325337	1310890	70.430				70.4295
2	3.775	2235893	607597	29.570				29.5705
Total		7561230	1918487					100.0000

90% Styrene 10% styrene oxide

Analysis Date & Time : 11/7/2021 7:39:16 PM
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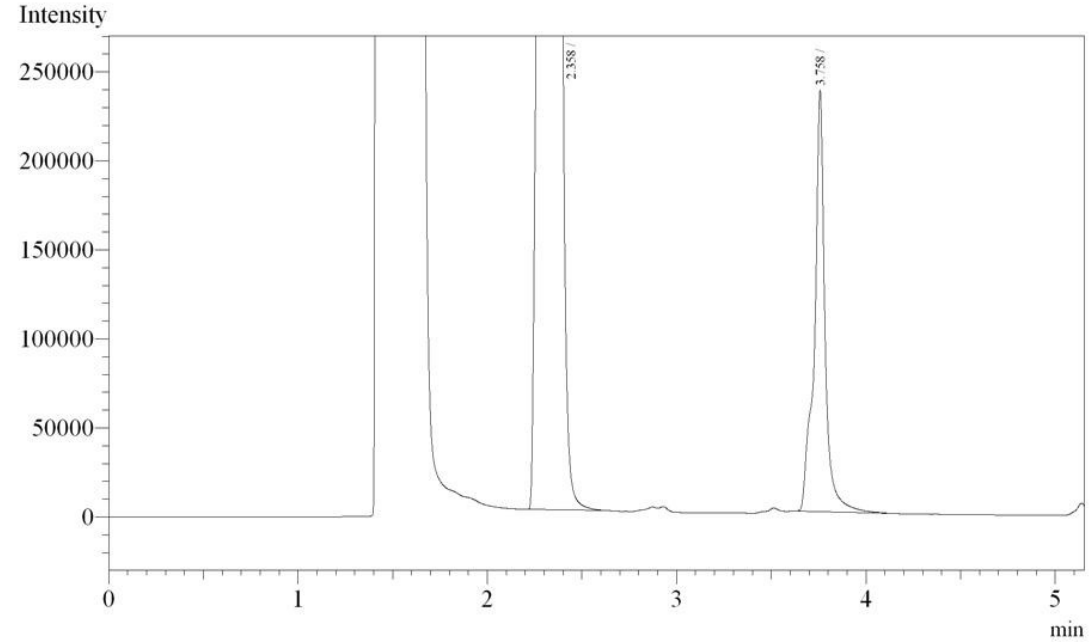
Vial# : 0
Sample Name : 90 ST 10 STO AG
Sample ID : 90 ST 10 STO AG
Sample Type : Unknown
Injection Volume :
ISTD Amount :

Data Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\Mn complex paper calibration\NEW\
Method Name : C:\GCsolution\Data\Project1\POOJA CHAUDHARY\condition\methanol Calibration.gcm



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name	Area%
1	2.358	7900130	1907881	89.518					89.5176
2	3.758	925093	235328	10.482					10.4824
Total		8825223	2143209						100.0000

Catalysts and ligands characterization

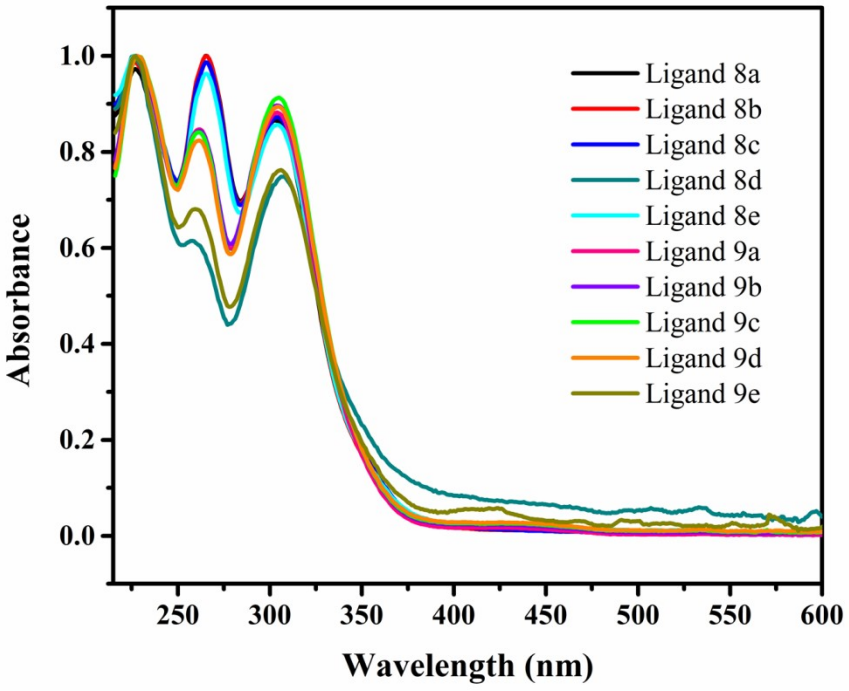


Figure 2. UV-visible spectra of ligands **8a-e** and **9a-e**.

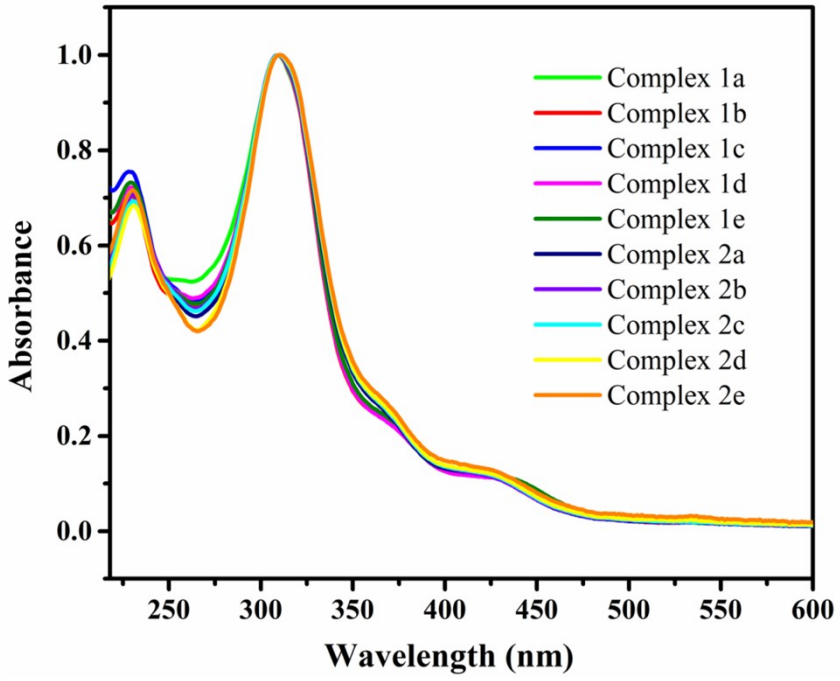


Figure 3. UV-visible spectra of Mn(III)-salen complexes **1a-e** and **2a-e**.

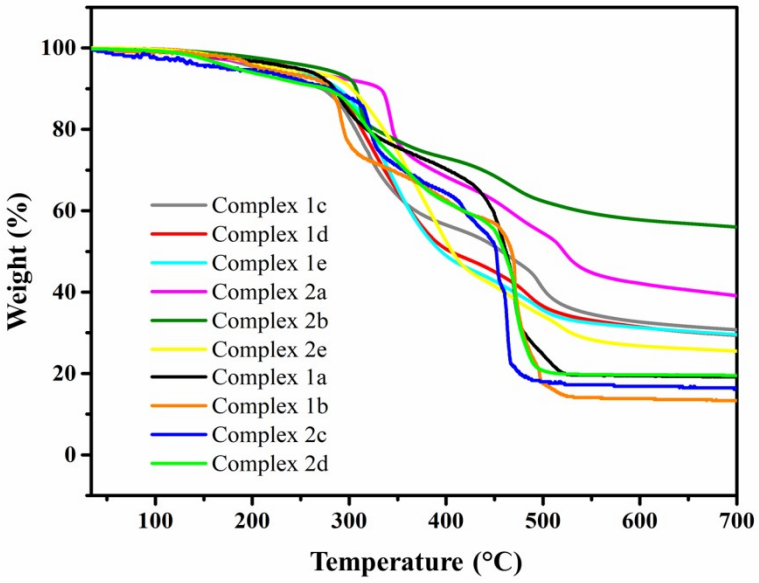


Figure 4. TGA thermograms of Mn(III)-salen complexes **1a-e** and **2a-e**.

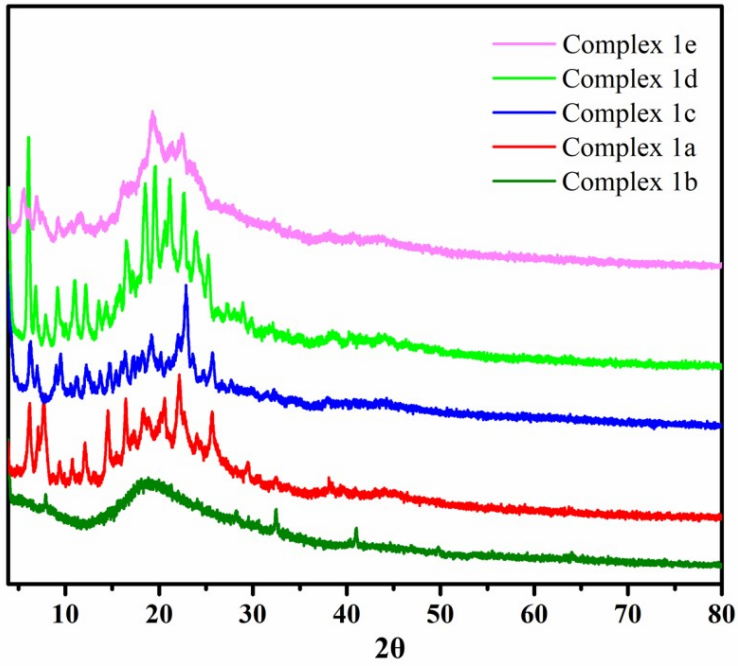


Figure 5. PXRD patterns of Mn(III)-salen complexes **1a-e**.

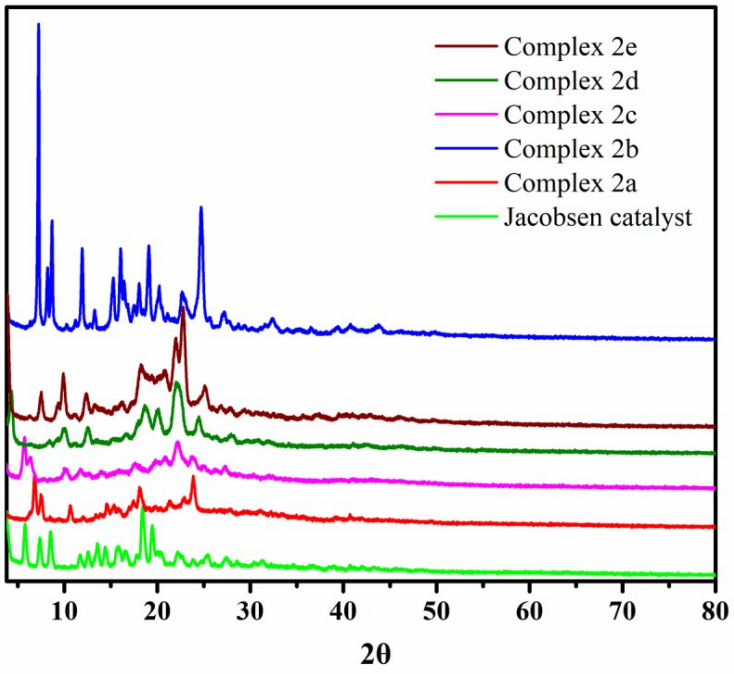


Figure 6. PXRD patterns of Mn(III)-salen complexes **2a-e** and Jacobsen catalyst.

Recovered catalysts 1b and 2b characterization

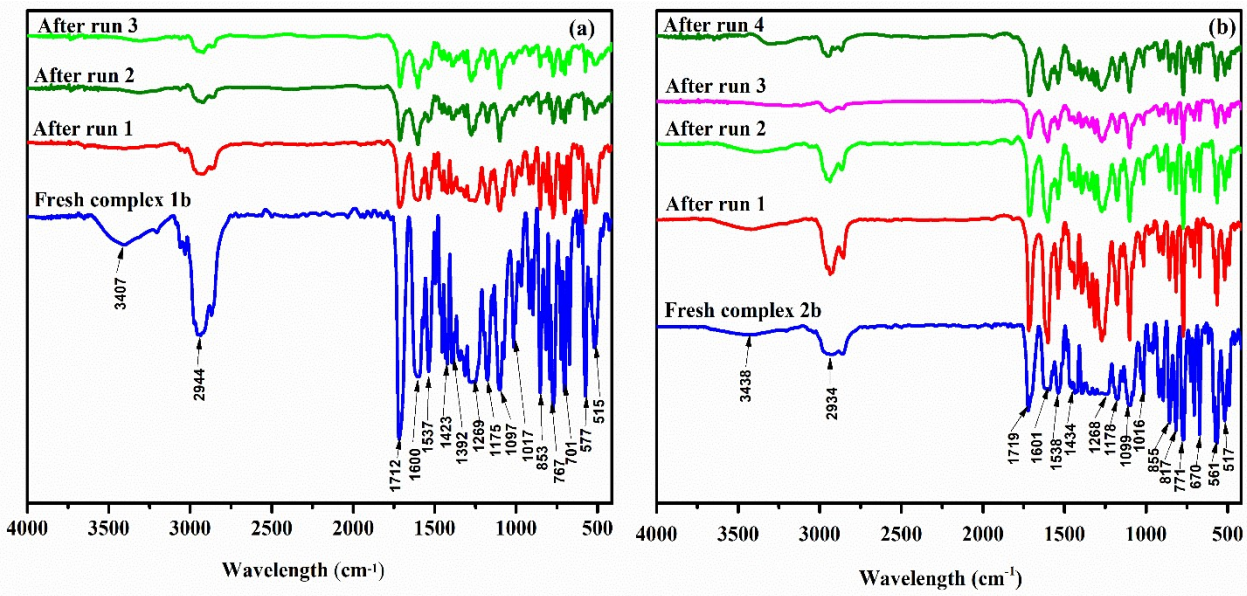


Figure 7. FT-IR spectra: (a) Fresh complex **1b** and recovered complex **1b** after each run; (b) Fresh complex **2b** and recovered complex **2b** after each run.

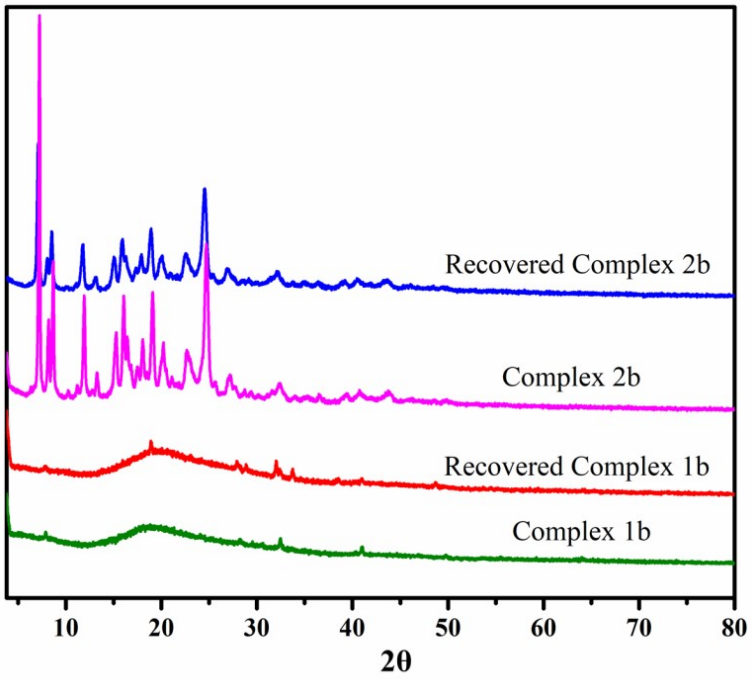


Figure 8. PXRD patterns of fresh and recovered complexes **1b** and **2b**.

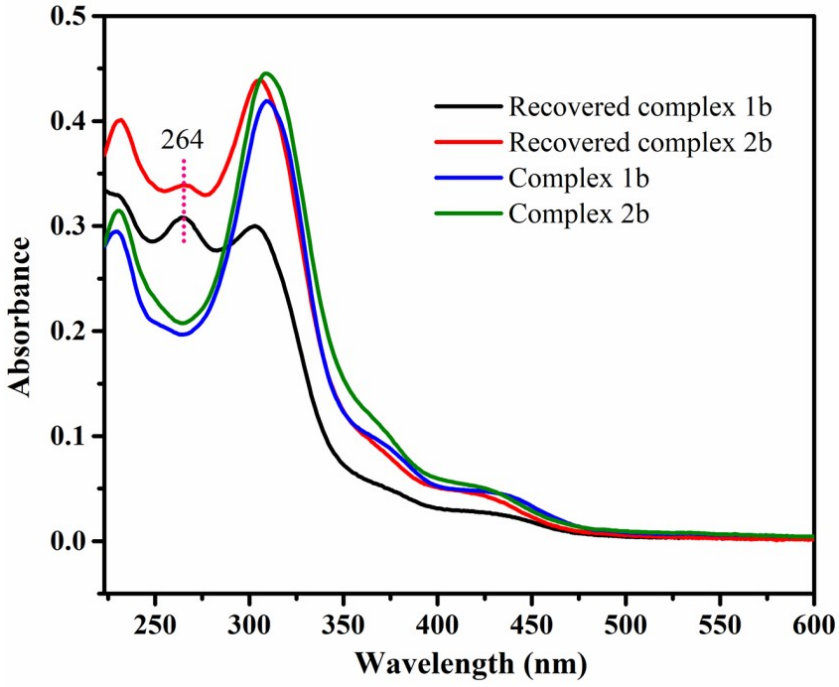


Figure 9. UV-visible spectra of fresh and recovered complexes **1b** and **2b**.

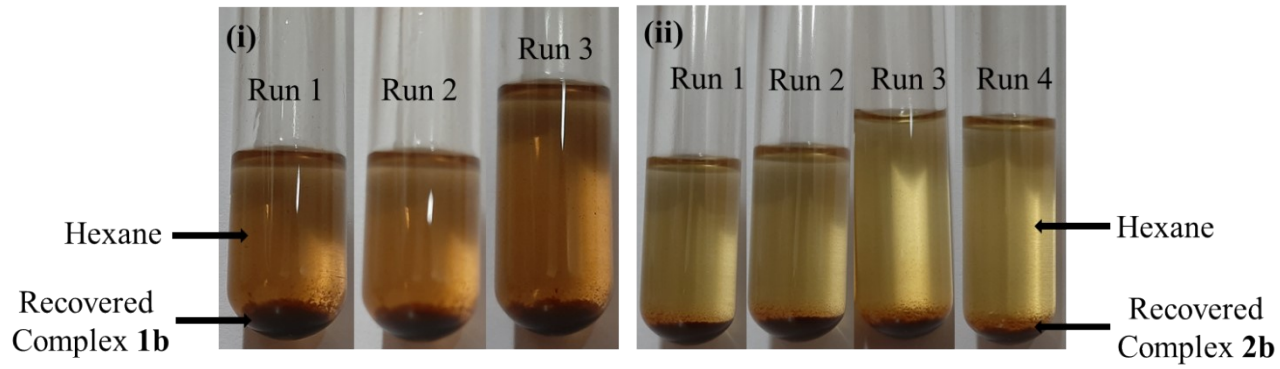
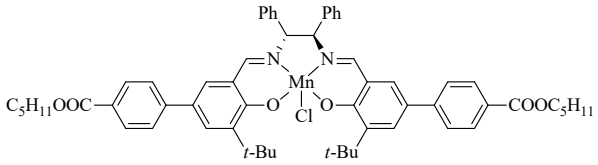


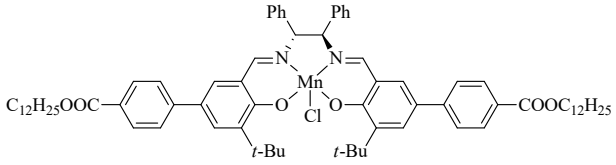
Figure 10. Recovered complex **1b** (i) and **2b** (ii) photos.

Complex 1c[11,12]



Synthesize by following the procedure of complex **1a**. Brown solid, Yield (317 mg, 94%); m.p. 248-250 °C; IR (KBr): 3411, 2925, 1719, 1601, 1537, 1454, 1426, 1390, 1310, 1272, 1182, 1110, 1079, 1013, 969, 894, 852, 769, 720, 701, 670, 575, 513 cm^{-1}. UV-vis (CH_3OH): λ_{max} 229, 309, 369, 432, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl]^+$ ($C_{60}H_{66}MnN_2O_6$): 965.4301, found: 965.4253. $[\alpha]_{589}^{25}$ = -1200 (*c* = 0.02, CH_2Cl_2). Anal. calcd. for $C_{60}H_{66}ClMnN_2O_6$: C, 71.95; H, 6.64; N, 2.80. Found: C, 72.12; H, 6.86; N, 2.95%.

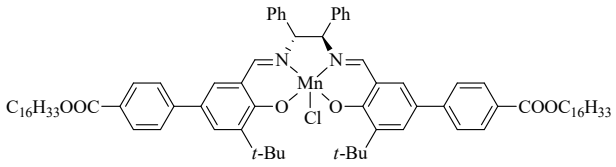
Complex 1d[11,12]



Synthesize by following the procedure of complex **1a**. Brown solid, Yield (428 mg, 92%); m.p. 228-230 °C; IR (KBr): 3417, 2921, 1716, 1600, 1535, 1455, 1421, 1387, 1315, 1269, 1179, 1112, 1076, 1020, 964, 897, 850, 771, 720, 701, 671, 574, 513 cm^{-1}. UV-vis (CH_3OH): λ_{max} 229, 309, 369, 431, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl]^+$ ($C_{74}H_{94}MnN_2O_6$): 1161.6492,

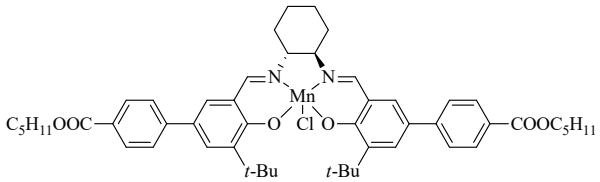
found: 1161.6444. $[\alpha]_{589}^{25}$ = -1064 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{74}H_{94}ClMnN_2O_6$: C, 74.19; H, 7.91; N, 2.34. Found: C, 74.52; H, 7.98; N, 2.61%.

Complex 1e[11,12]



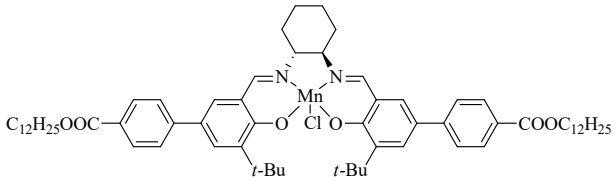
Synthesize by following the procedure of complex **1a**. Brown solid, Yield (374 mg, 94%); m.p. 198-200 °C; IR (KBr): 3416, 2922, 1717, 1601, 1537, 1456, 1428, 1389, 1314, 1269, 1179, 1104, 1076, 1016, 965, 892, 853, 812, 769, 721, 703, 671, 576, 513 cm^{-1}. UV-vis (CH_3OH): λ_{max} 229, 310, 370, 432, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl + H]^+$ ($C_{82}H_{111}MnN_2O_6$): 1274.7822, found: 1274.7801. $[\alpha]_{589}^{25}$ = -1149 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{82}H_{110}ClMnN_2O_6$: C, 75.17; H, 8.46; N, 2.14. Found: C, 75.00; H, 8.21; N, 2.39%.

Complex 2c[11,12]



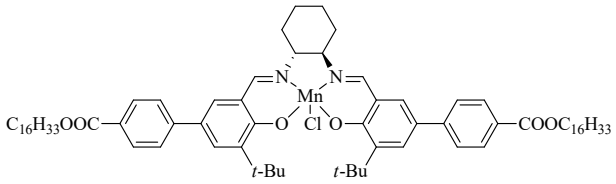
Synthesize by following the procedure of complex **1a**. Brown solid, Yield (317 mg, 95%); decomposed at 296-298 °C; IR (KBr): 3429, 2950, 1715, 1601, 1538, 1458, 1434, 1391, 1342, 1314, 1269, 1180, 1113, 1080, 1018, 970, 895, 854, 814, 772, 702, 677, 566, 519, 490 cm^{-1}. UV-vis (CH_3OH): λ_{max} 229, 309, 372, 429, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl]^+$ ($C_{52}H_{64}MnN_2O_6$): 867.4144, found: 867.4131. $[\alpha]_{589}^{25}$ = -1176 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{52}H_{64}ClMnN_2O_6$: C, 69.13; H, 7.14; N, 3.10. Found: C, 69.10; H, 7.20; N, 3.26%.

Complex 2d[11,12]



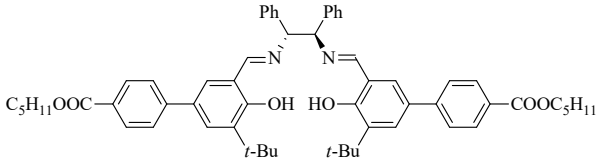
Synthesize by following the procedure of complex **1a**. Brown solid, Yield (402 mg, 92%); m.p. 278-280 °C; IR (KBr): 3430, 2924, 1712, 1602, 1537, 1466, 1436, 1392, 1341, 1312, 1268, 1177, 1106, 1013, 894, 860, 814, 771, 705, 673, 567, 518, 489 cm^{-1}. UV-vis (CH_3OH): λ_{max} 230, 310, 371, 429, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl]^+$ ($C_{66}H_{92}MnN_2O_6$): 1063.6335, found: 1063.6309. $[\alpha]_{589}^{25}$ = -1087 (*c* = 0.02, CH_2Cl_2). Anal. calcd. for $C_{66}H_{92}ClMnN_2O_6$: C, 72.07; H, 8.43; N, 2.55. Found: C, 72.44; H, 8.16; N, 2.71%.

Complex 2e[11,12]



Synthesize by following the procedure of complex **1a**. Brown solid, Yield (310 mg, 96%); m.p. 258-260 °C; IR (KBr): 3425, 2922, 1723, 1601, 1538, 1466, 1422, 1392, 1339, 1311, 1264, 1182, 1104, 861, 817, 773, 717, 673, 566, 515, 449 cm^{-1}. UV-vis (CH_3OH): λ_{max} 230, 310, 372, 429, 500 nm. HRMS(ESI): *m/z* calcd. for $[M - Cl + H]^+$ ($C_{74}H_{109}MnN_2O_6$): 1176.7666, found: 1176.7612. $[\alpha]_{589}^{25}$ = -1098 (*c* = 0.02, CH_2Cl_2). Anal. calcd. for $C_{74}H_{108}ClMnN_2O_6$: C, 73.33; H, 8.98; N, 2.31. Found: C, 73.63; H, 8.62; N, 2.34%.

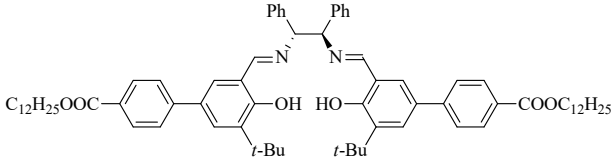
Ligand 8c[3,6]



Synthesize by following the procedure of ligand **8a**. Yellow solid, Yield (305 mg, 97%); m.p. 115-117 °C; ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 13.96 (s, 2H), 8.42 (s, 2H), 8.03 (d, *J* = 8.5 Hz, 4H), 7.49-7.46 (m, 6H), 7.26 (s, 2H), 7.24-7.21 (m, 10H), 4.77 (s, 2H), 4.33 (t, *J* = 6.7 Hz, 4H),

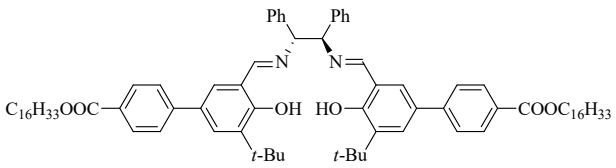
1.79 (pent, J = 7.2 Hz, 4H), 1.43-1.39 (m, 26H), 0.94 (t, J = 7.1 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 167.01 (2C), 166.66 (2C), 160.54 (2C), 145.22 (2C), 139.1 (2C), 137.98 (2C), 129.99 (4C), 129.74 (2C), 128.75 (2C), 128.64 (2C), 128.48 (6C), 128.01 (4C), 127.75 (2C), 126.29 (4C), 118.74 (2C), 80.15 (2C), 65.1 (2C), 35.01 (2C), 29.28 (6C), 28.48 (2C), 28.24 (2C), 22.40 (2C), 14.02 (2C) ppm. IR (KBr): 3401, 2959, 1716, 1624, 1467, 1446, 1389, 1355, 1275, 1176, 1112, 1058, 1012, 972, 885, 855, 769, 760, 702 cm^{-1}. UV-vis (CH_3OH): λ_{max} 226, 266, 305 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{60}H_{68}N_2O_6$): 913.5155, found: 913.5137. $[\alpha]_{589}^{25}$ = -110 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{60}H_{68}N_2O_6$: C, 78.91; H, 7.51; N, 3.07. Found: C, 79.00; H, 7.65; N, 3.12%.

Ligand 8d[3,6]



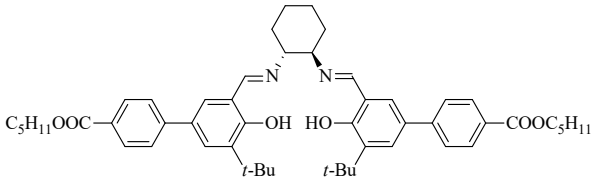
Synthesize by following the procedure of ligand **8a**. Viscous yellow liquid, Yield (470 mg, 97%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 13.96 (s, 2H), 8.42 (s, 2H), 8.03 (d, J = 8.4 Hz, 4H), 7.49-7.46 (m, 6H), 7.26 (s, 2H), 7.24-7.21 (m, 10H), 4.77 (s, 2H), 4.32 (t, J = 6.7 Hz, 4H), 1.77 (p, J = 7.8 Hz, 4H), 1.43 (s, 22H), 1.26 (s, 32H), 0.87 (t, J = 7 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 167.00 (2C), 166.66 (2C), 160.54 (2C), 145.22 (2C), 139.11 (2C), 137.98 (2C), 130.00 (4C), 129.74 (2C), 128.75 (2C), 128.64 (2C), 128.50 (2C), 128.48 (4C), 128.00 (4C), 127.75 (2C), 126.28 (4C), 118.74 (2C), 80.15 (2C), 65.12 (2C), 35.01 (2C), 31.93 (2C), 29.67 (2C), 29.65 (2C), 29.60 (2C), 29.57 (2C), 29.36 (2C), 29.32 (2C), 29.28 (6C), 28.78 (2C), 26.08 (2C), 22.7 (2C), 14.13 (2C) ppm. IR (KBr): 3400, 2956, 1714, 1626, 1467, 1442, 1394, 1359, 1278, 1172, 1109, 1052, 1012, 972, 917, 885, 854, 768, 756, 709, 692 cm^{-1}. UV-vis (CH_3OH): λ_{max} 227, 266, 303 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{74}H_{97}N_2O_6$): 1109.7346, found: 1109.7323. $[\alpha]_{589}^{25}$ = -168 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{74}H_{96}N_2O_6$: C, 80.10; H, 8.72; N, 2.52. Found: C, 80.41; H, 8.87; N, 2.64%.

Ligand 8e[3,6]



Synthesize by following the procedure of ligand **8a**. Viscous yellow liquid, Yield (382 mg, 96%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 13.96 (s, 2H), 8.42 (s, 2H), 8.03 (d, J = 8.4 Hz, 4H), 7.49-7.46 (m, 6H), 7.25 (s, 2H), 7.24-7.22 (m, 10H), 4.77 (s, 2H), 4.32 (t, J = 6.7 Hz, 4H), 1.78 (pent, J = 7.7 Hz, 4H), 1.43 (s, 22H), 1.25 (s, 48H), 0.87 (t, J = 7.0 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 167.00 (2C), 166.66 (2C), 160.54 (2C), 145.22 (2C), 139.11 (2C), 137.98 (2C), 130.00 (4C), 129.74 (2C), 128.75 (2C), 128.64 (2C), 128.50 (2C), 128.48 (4C), 128.00 (4C), 127.75 (2C), 126.28 (4C), 118.75 (2C), 80.16 (2C), 65.12 (2C), 35.01 (2C), 31.94 (2C), 29.71 (6C), 29.67 (6C), 29.62 (2C), 29.58 (2C), 29.37 (2C), 29.33 (2C), 29.28 (6C), 28.78 (2C), 26.08 (2C), 22.70 (2C), 14.14 (2C) ppm. IR (KBr): 3405, 2958, 1715, 1625, 1465, 1440, 1390, 1360, 1272, 1177, 1111, 1055, 1015, 979, 915, 889, 851, 771, 759, 711, 698 cm^{-1}. UV-vis (CH_3OH): λ_{max} 226, 266, 303 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{82}H_{113}N_2O_6$): 1221.8598, found: 1221.8583. $[\alpha]_{589}^{25}$ = -202 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{82}H_{112}N_2O_6$: C, 80.61; H, 9.24; N, 2.29. Found: C, 80.54; H, 9.45; N, 2.35%.

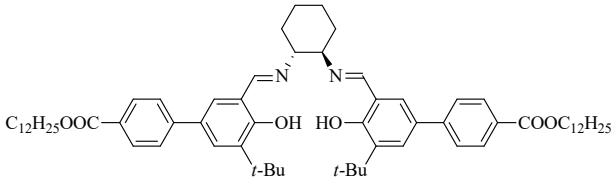
Ligand 9c[3,6]



Synthesize by following the procedure of ligand **9a**. Yellow solid, Yield (348 mg, 90%); mp; 78-80 °C; ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 14.06 (s, 2H), 8.35 (s, 2H), 8.03 (d, J = 8.4 Hz, 4H), 7.49-7.47 (m, 6H), 7.22 (d, J = 2.2 Hz, 2H), 4.32 (t, J = 6.7 Hz, 4H), 3.39-3.37 (m, 2H), 2.06-2.02 (m, 2H), 1.94-1.91 (m, 2H), 1.82-1.75 (m, 6H), 1.51-1.49 (m, 2H), 1.43-1.42 (m, 26H), 0.94 (t, J = 7.2 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.65 (2C), 165.63 (2C), 160.68 (2C), 145.28 (2C), 137.91 (2C), 129.98 (4C), 129.56 (2C), 128.44 (2C), 128.37 (4C), 126.26 (4C), 118.71 (2C), 72.40 (2C), 65.07 (2C), 34.96 (2C), 32.97 (2C), 29.29 (6C), 28.46 (2C), 28.23 (2C), 24.29 (2C), 22.38 (2C), 14.01 (2C) ppm. IR (KBr): 3414, 2959, 1717, 1626, 1470, 1440,

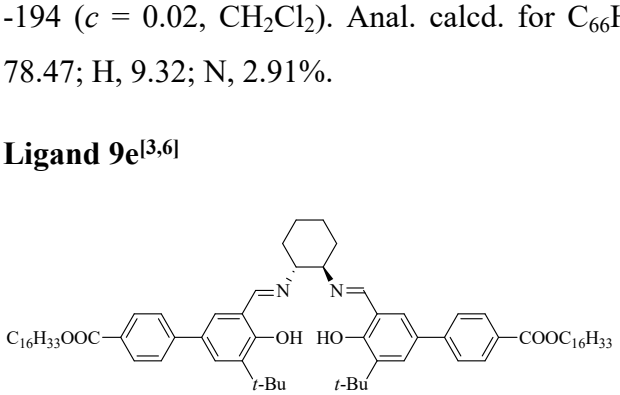
1390, 1360, 1289, 1179, 1107, 1069, 1038, 1018, 972, 936, 887, 851, 771, 757, 713 cm^{-1}. UV-vis (CH_3OH): λ_{max} 228, 261, 304 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{52}H_{67}N_2O_6$): 815.4999, found: 815.4986. $[\alpha]_{589}^{25}$ = -170 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{52}H_{66}N_2O_6$: C, 76.62; H, 8.16; N, 3.44. Found: C, 76.15; H, 8.12; N, 3.54%.

Ligand 9d[3,6]



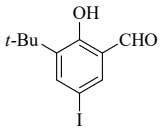
Synthesize by following the procedure of ligand **9a**. Viscous yellow liquid, Yield (400 mg, 92%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 14.06 (s, 2H), 8.35 (s, 2H), 8.03 (d, J = 8.5 Hz, 4H), 7.49-7.47 (m, 6H), 7.23 (d, J = 2.2 Hz, 2H), 4.32 (t, J = 6.7 Hz, 4H), 3.39-3.37 (m, 2H), 2.06-2.03 (m, 2H), 1.93-1.91 (m, 2H), 1.81-1.73 (m, 6H), 1.51-1.48 (m, 2H), 1.44 (s, 22H), 1.26 (s, 32H), 0.87 (t, J = 7.0 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.65 (2C), 165.62 (2C), 160.68 (2C), 145.27 (2C), 137.91 (2C), 129.99 (4C), 129.56 (2C), 128.45 (2C), 128.37 (4C), 126.26 (4C), 118.71 (2C), 72.4 (2C), 65.09 (2C), 34.96 (2C), 31.91 (2C), 29.65 (2C), 29.64 (2C), 29.59 (2C), 29.55 (2C), 29.35 (2C), 29.29 (10C), 28.76 (2C), 26.06 (2C), 24.29 (2C), 22.69 (2C), 14.12 (2C) ppm. IR (KBr): 3421, 2947, 1716, 1625, 1467, 1441, 1393, 1367, 1280, 1179, 1100, 1070, 1046, 1019, 975, 936, 887, 852, 773, 759, 713 cm^{-1}. UV-vis (CH_3OH): λ_{max} 228, 261, 304 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{66}H_{95}N_2O_6$): 1011.7190, found: 1011.7168. $[\alpha]_{589}^{25}$ = -194 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{66}H_{94}N_2O_6$: C, 78.37; H, 9.37; N, 2.77. Found: C, 78.47; H, 9.32; N, 2.91%.

Ligand 9e[3,6]



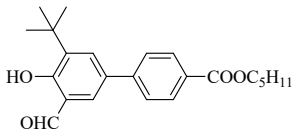
Synthesize by following the procedure of ligand **9a**. Viscous yellow liquid, Yield (342 mg, 91%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 14.06 (s, 2H), 8.36 (s, 2H), 8.03 (d, J = 8.4 Hz, 4H), 7.49-7.47 (m, 6H), 7.23 (d, J = 2.2 Hz, 2H), 4.32 (t, J = 6.7 Hz, 4H), 3.39-3.37 (m, 2H), 2.06-2.03 (m, 2H), 1.93-1.91 (m, 2H), 1.80-1.73 (m, 6H), 1.51-1.48 (m, 2H), 1.43 (s, 22H), 1.25 (s, 48H), 0.87 (t, J = 7.0 Hz, 6H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 166.66 (2C), 165.62 (2C), 160.69 (2C), 145.28 (2C), 137.92 (2C), 129.99 (4C), 129.57 (2C), 128.45 (2C), 128.37 (4C), 126.27 (4C), 118.72 (2C), 72.42 (2C), 65.10 (2C), 34.97 (2C), 32.99 (2C), 31.93 (2C), 29.71 (8C), 29.67 (6C), 29.61 (2C), 29.57 (2C), 29.37 (2C), 29.30 (6C), 28.78 (2C), 26.07 (2C), 24.30 (2C), 22.70 (2C), 14.13 (2C) ppm. IR (KBr): 3427, 2951, 1718, 1624, 1460, 1448, 1394, 1369, 1279, 1175, 1102, 1078, 1049, 1012, 978, 940, 882, 849, 778, 749, 714 cm^{-1}. UV-vis (CH_3OH): λ_{max} 228, 261, 305 nm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{74}H_{111}N_2O_6$): 1123.8442, found: 1123.8411. $[\alpha]_{589}^{25}$ = -187 (c = 0.02, CH_2Cl_2). Anal. calcd. for $C_{74}H_{110}N_2O_6$: C, 79.10; H, 9.87; N, 2.49. Found: C, 79.24; H, 9.89; N, 2.67%.

3-(*tert*-butyl)-2-hydroxy-5-iodobenzaldehyde (5)



Synthesize by following the reported procedure.[13] Yellow solid, Yield (2.75 g, 91%); m.p. 43-45 °C; ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 11.73 (s, 1H), 9.79 (s, 1H), 7.72-7.69 (m, 2H), 1.39 (s, 9H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 195.93, 160.86, 142.54, 141.35, 140.02, 122.49, 80.62, 35.05, 29.03 ppm.

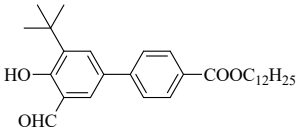
Pentyl 3'-(*tert*-butyl)-5'-formyl-4'-hydroxy-[1,1'-biphenyl]-4-carboxylate (6c)



Synthesize by following the procedure of compound **6b**. Viscous colorless liquid, Yield (391 mg, 83%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 11.86 (s, 1H), 9.98 (s, 1H), 8.12 (d, J = 8.3 Hz, 2H), 7.79 (d, J = 2.0 Hz, 1H), 7.65 (d, J = 2.2 Hz, 1H), 7.62 (d, J = 8.3 Hz, 2H), 4.35 (t, J = 6.7 Hz, 2H), 1.80 (pent, J = 7.2 Hz, 2H), 1.48-1.38 (m, 13H), 0.94 (t, J = 7.0 Hz, 3H) ppm. ^{13}C-NMR

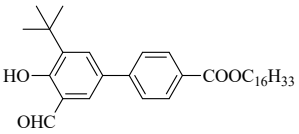
(100 MHz, $CDCl_3$): δ = 197.15, 166.47, 161.23, 144.36, 139.14, 133.04, 131.24, 130.32, 130.24 (2C), 129.19, 126.48 (2C), 120.78, 65.22, 35.09, 29.21 (3C), 28.46, 28.23, 22.38, 14.01 ppm. IR (KBr): 3413, 2972, 1713, 1657, 1608, 1566, 1515, 1446, 1391, 1360, 1331, 1273, 1218, 1165, 1108, 1072, 1014, 957, 855, 774, 715 cm^{-1}. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{23}H_{29}O_4$): 369.2065, found: 369.2061. Anal. calcd. for $C_{23}H_{28}O_4$: C, 74.97; H, 7.66. Found: C, 75.03; H, 7.39%.

Dodecyl 3'-(*tert*-butyl)-5'-formyl-4'-hydroxy-[1,1'-biphenyl]-4-carboxylate (6d)



Synthesize by following the procedure of compound **6b**. Viscous colorless liquid, Yield (490 mg, 82%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 11.85 (s, 1H), 9.95 (s, 1H), 8.09 (d, *J* = 8.8 Hz, 2H), 7.76 (s, 1H), 7.63-7.62 (m, 1H), 7.60 (d, *J* = 8.8 Hz, 2H), 4.32 (t, *J* = 7.2 Hz, 2H), 1.76 (pent, *J* = 6.8 Hz, 2H), 1.46 (s, 9H), 1.44-1.41 (m, 2H), 1.24 (s, 16H), 0.85 (t, *J* = 6.8 Hz, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 197.23, 166.54, 161.31, 144.42, 139.19, 133.11, 131.31, 130.39, 130.32 (2C), 129.27, 126.55 (2C), 120.85, 65.32, 35.17, 32.00, 29.73 (2C), 29.67, 29.63, 29.44, 29.38, 29.28 (3C), 28.83, 26.15, 22.77, 14.21 ppm. IR (KBr): 3410, 2973, 1712, 1606, 1568, 1509, 1441, 1394, 1324, 1278, 1215, 1168, 1071, 1014, 955, 894, 851, 761, 716 cm^{-1}. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{30}H_{43}O_4$): 467.3161, found: 467.3157. Anal. calcd. for $C_{30}H_{42}O_4$: C, 76.68; H, 8.73. Found: C, 76.88; H, 8.91%.

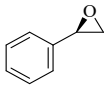
Hexadecyl 3'-(*tert*-butyl)-5'-formyl-4'-hydroxy-[1,1'-biphenyl]-4-carboxylate (6e)



Synthesize by following the procedure of compound **6b**. Viscous colorless liquid, Yield (521 mg, 78%); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 11.84 (s, 1H), 9.95 (s, 1H), 8.09 (d, *J* = 7.6 Hz, 2H), 7.76 (d, *J* = 2.0 Hz, 1H), 7.62 (d, *J* = 2.4 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 4.32 (t, *J* = 6.8 Hz, 2H), 1.76 (pent, *J* = 7.2 Hz, 2H), 1.46 (s, 9H), 1.43-1.39 (m, 2H), 1.23 (s, 24H), 0.85 (t, *J* = 6.8 Hz, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 197.12, 166.45, 161.20, 144.30, 139.07, 133.00,

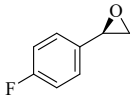
131.18, 130.28, 130.21 (2C), 129.13, 126.44 (2C), 120.73, 65.21, 35.05, 31.90, 29.68 (4C), 29.64 (3C), 29.57, 29.54, 29.35, 29.28, 29.17 (2C), 28.72, 26.04, 22.67, 14.11 ppm. IR (KBr): 3411, 2974, 1716, 1601, 1565, 1513, 1473, 1432, 1392, 1364, 1329, 1287, 1219, 1159, 1119, 1070, 1016, 957, 892, 852, 766, 717 cm^{-1}. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{34}H_{51}O_4$): 523.3787, found: 523.3785. Anal. calcd. for $C_{34}H_{50}O_4$: C, 78.12; H, 9.64. Found: C, 78.45; H, 9.47%.

Styrene oxide (11)[14]



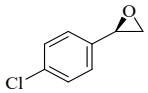
Colorless liquid, Yield (58.5 mg, 97%); $[\alpha]_{589}^{25}$ = +16 (*c* = 0.64, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.34-7.25 (m, 5H), 3.84-3.82 (m, 1H), 3.12-3.09 (m, 1H), 2.76 (dd, *J* = 5.5, 2.5 Hz, 1H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 137.53, 128.41(2C), 128.08, 125.40 (2C), 52.24, 51.09 ppm.

4-Fluorostyrene oxide (13)[14]



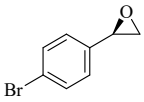
Colorless liquid, Yield (66.3 mg, 96%); $[\alpha]_{589}^{25}$ = -14 (*c* = 0.65, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.26-7.22 (m, 2H), 7.05-7.01 (m, 2H), 3.85-3.83 (m, 1H), 3.14-3.12 (m, 1H), 2.76 (dd, *J* = 5.4, 2.5 Hz, 1H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 163.93, 161.49, 133.34, 133.31, 127.23, 127.15, 115.60, 115.38, 51.85, 51.17 ppm.

4-Chlorostyrene oxide (15)[14]



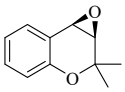
Colorless liquid, Yield (75.6 mg, 98%); $[\alpha]_{589}^{25}$ = -20 (*c* = 0.65, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.30 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 3.83-3.81 (m, 1H), 3.14-3.12 (m, 1H), 2.74 (dd, *J* = 5.4, 2.5 Hz, 1H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 136.22, 133.94, 128.72 (2C), 126.85 (2C), 51.78, 51.22 ppm.

4-Bromostyrene oxide (17)[14]



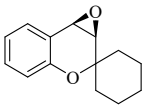
Colorless liquid, Yield (96.4 mg, 97%); $[\alpha]_{589}^{25}$ = -20 (c = 0.62, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.46 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 3.82-3.81 (m, 1H), 3.15-3.13 (m, 1H), 2.74 (dd, J = 5.4, 2.5 Hz, 1H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 136.75, 131.66 (2C), 127.18 (2C), 122.03, 51.83, 51.20 ppm.

2,2-dimethyl-2*H*-chromene oxide (19)[15]



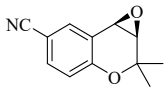
Colorless liquid, Yield (84.8 mg, 96%); $[\alpha]_{589}^{25}$ = 20 (c = 0.97, CH_2Cl_2); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.33 (dd, J = 7.4, 1.4 Hz, 1H), 7.23 (dt, J = 8.0, 1.6 Hz, 1H), 6.92 (dt, J = 7.4, 0.8 Hz, 1H), 6.80 (d, J = 8.1 Hz, 1H), 3.89 (d, J = 4.4 Hz, 1H), 3.49 (d, J = 4.4 Hz, 1H), 1.58 (s, 3H), 1.25 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 152.60, 130.32, 129.66, 121.07, 119.96, 118.03, 73.00, 62.89, 51.01, 25.71, 22.61 ppm.

spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (21)[16]



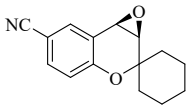
Colorless liquid, Yield (105.9 mg, 98%); $[\alpha]_{589}^{25}$ = 12 (c = 0.86, CH_2Cl_2); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.32 (dd, J = 1.5, 7.4 Hz, 1H), 7.26-7.21 (m, 1H), 6.92 (dt, J = 7.4, 1.0 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 3.86 (d, J = 4.4 Hz, 1H), 3.48 (d, J = 4.4 Hz, 1H), 2.11-2.05 (m, 1H), 1.93-1.84 (m, 1H), 1.72-1.64 (m, 3H), 1.61-1.56 (m, 2H), 1.52-1.46 (m, 1H), 1.43-1.32 (m, 2H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 152.29, 130.20, 129.60, 121.02, 120.76, 118.15, 73.55, 62.54, 50.55, 34.15, 30.26, 25.45, 21.18, 20.93 ppm.

6-cyano-2,2-dimethyl-2*H*-chromene oxide (23)[16]



Colorless liquid, Yield (95.8 mg, 95%); $[\alpha]_{589}^{25}$ = 85 (c = 0.27, CH_2Cl_2); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.65 (d, J = 2.0 Hz, 1H), 7.52 (dd, J = 8.5, 2.0 Hz, 1H), 6.86 (d, J = 8.5 Hz, 1H), 3.91 (d, J = 4.3 Hz, 1H), 3.54 (d, J = 4.4 Hz, 1H), 1.6 (s, 3H), 1.30 (s, 3H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 156.50, 134.42, 133.82, 121.12, 119.04, 118.74, 104.32, 74.69, 62.30, 49.88, 25.50, 23.03 ppm.

6-cyano-spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (25)[16]



Colorless liquid, Yield (116 mg, 96%); $[\alpha]_{589}^{25}$ = 35 (c = 0.97, CH_2Cl_2); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.64 (d, J = 1.9 Hz, 1H), 7.53 (dd, J = 8.4, 1.9 Hz, 1H), 6.91 (d, J = 8.4 Hz, 1H), 3.87 (d, J = 4.4 Hz, 1H), 3.54 (d, J = 4.4 Hz, 1H), 2.10-2.06 (m, 1H), 1.91-1.80 (m, 1H), 1.74-1.65 (m, 3H), 1.58-1.35 (m, 5H) ppm. ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 156.28, 134.39, 133.76, 121.89, 119.13, 118.78, 104.28, 75.31, 61.93, 49.44, 33.92, 30.85, 25.19, 21.16, 20.76 ppm.

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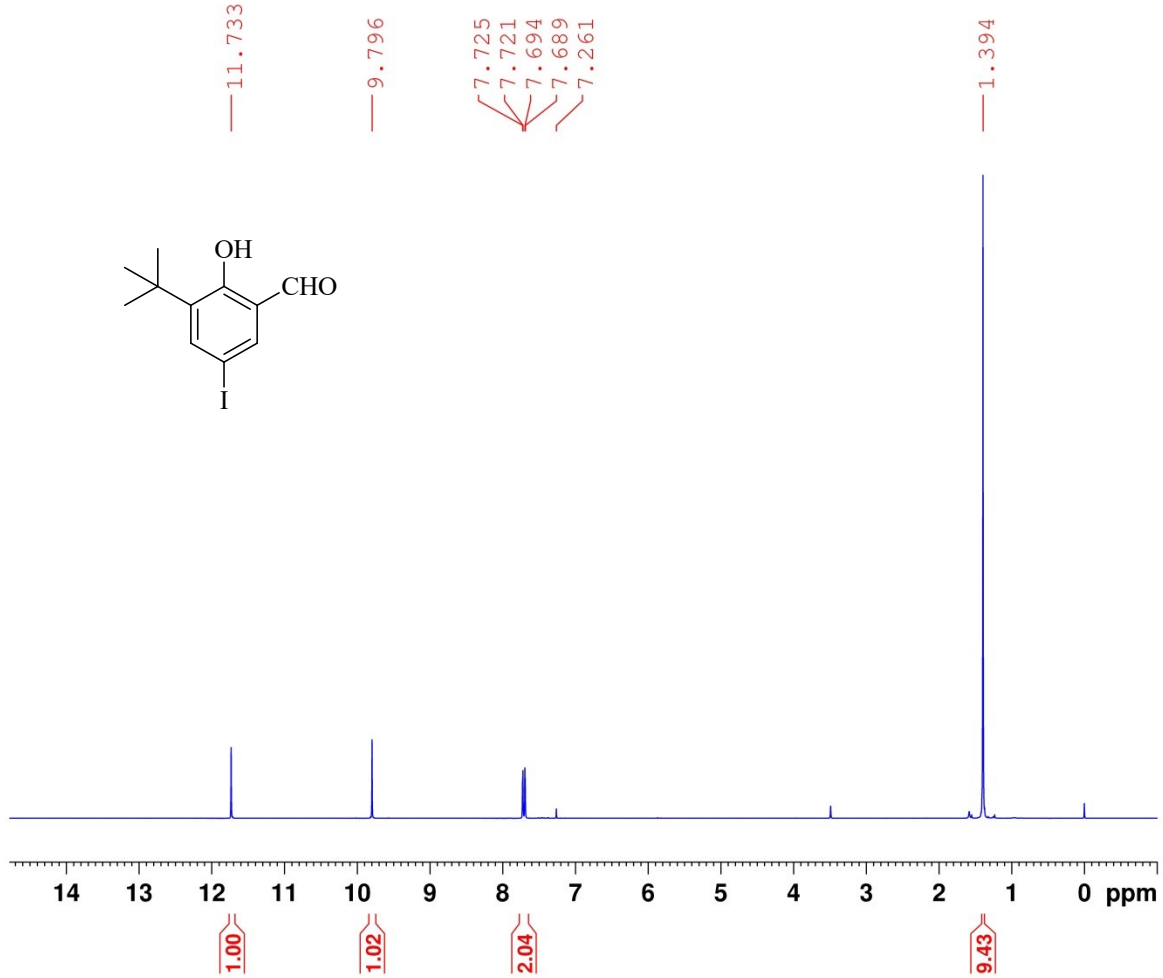


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PROCNO                 1

F2 - Acquisition Parameters
Date_           20201125
Time              13.39 h
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PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700093 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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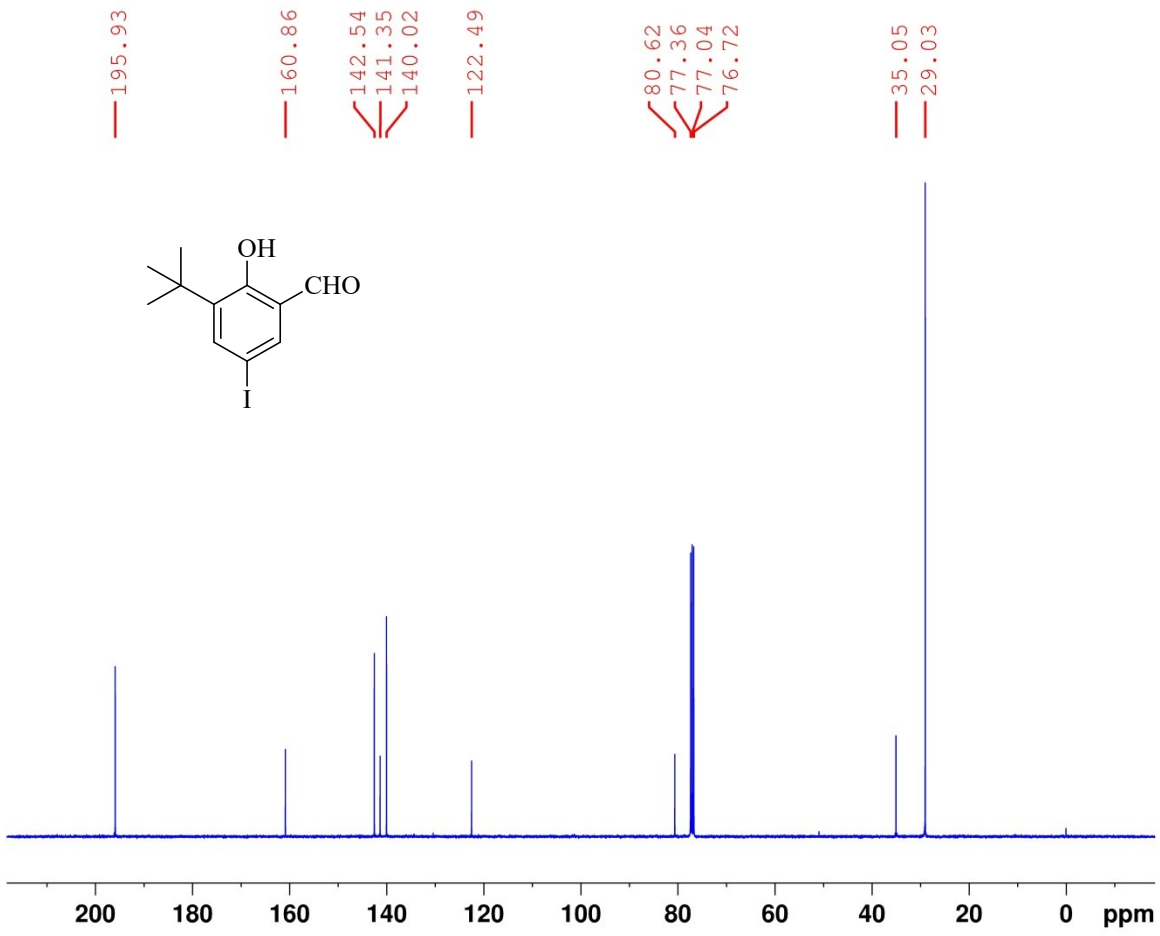


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Current Data Parameters
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EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201125
Time               15.34 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
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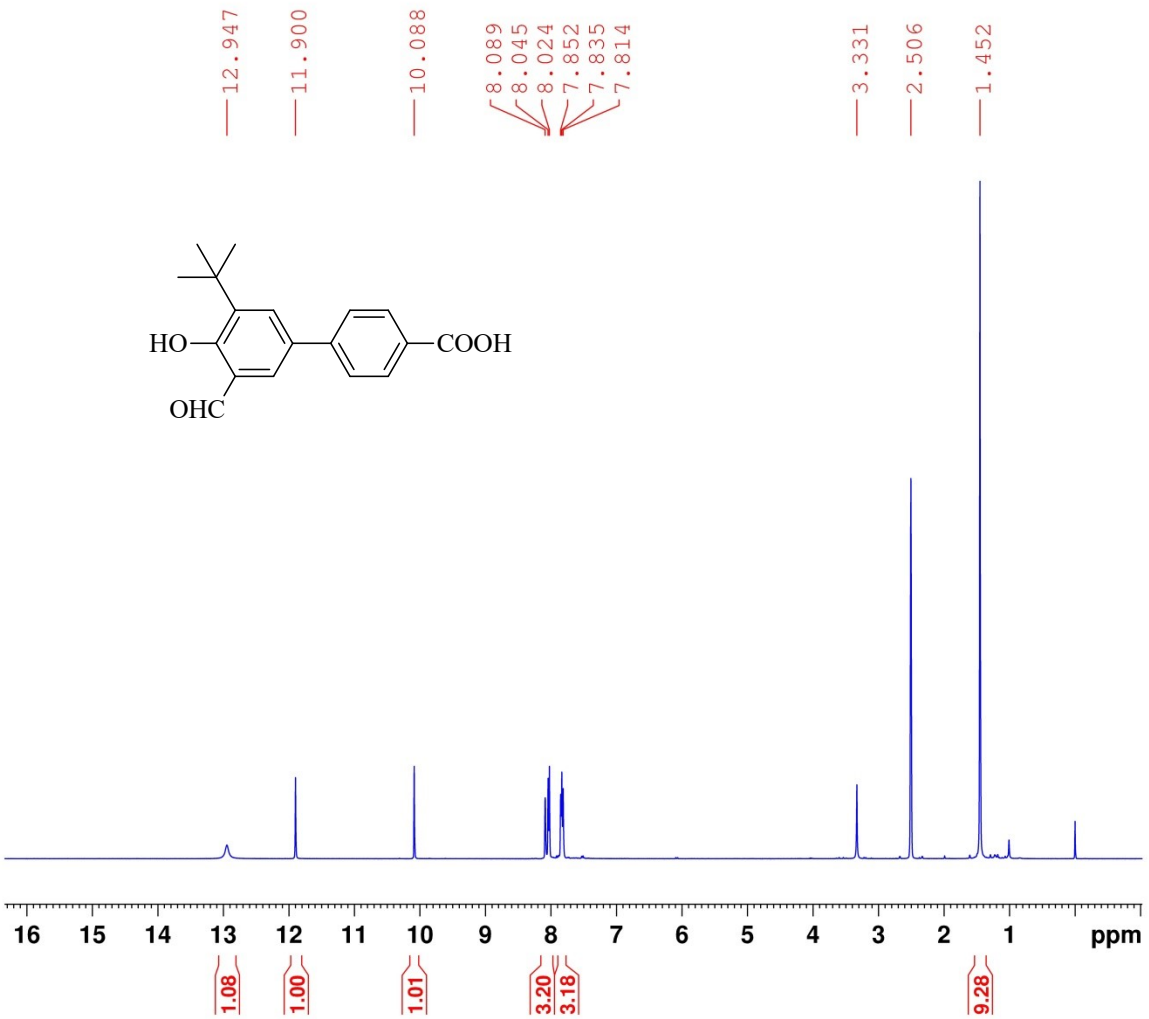

BRUKER

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Current Data Parameters
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EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201223
Time              14.48 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700002 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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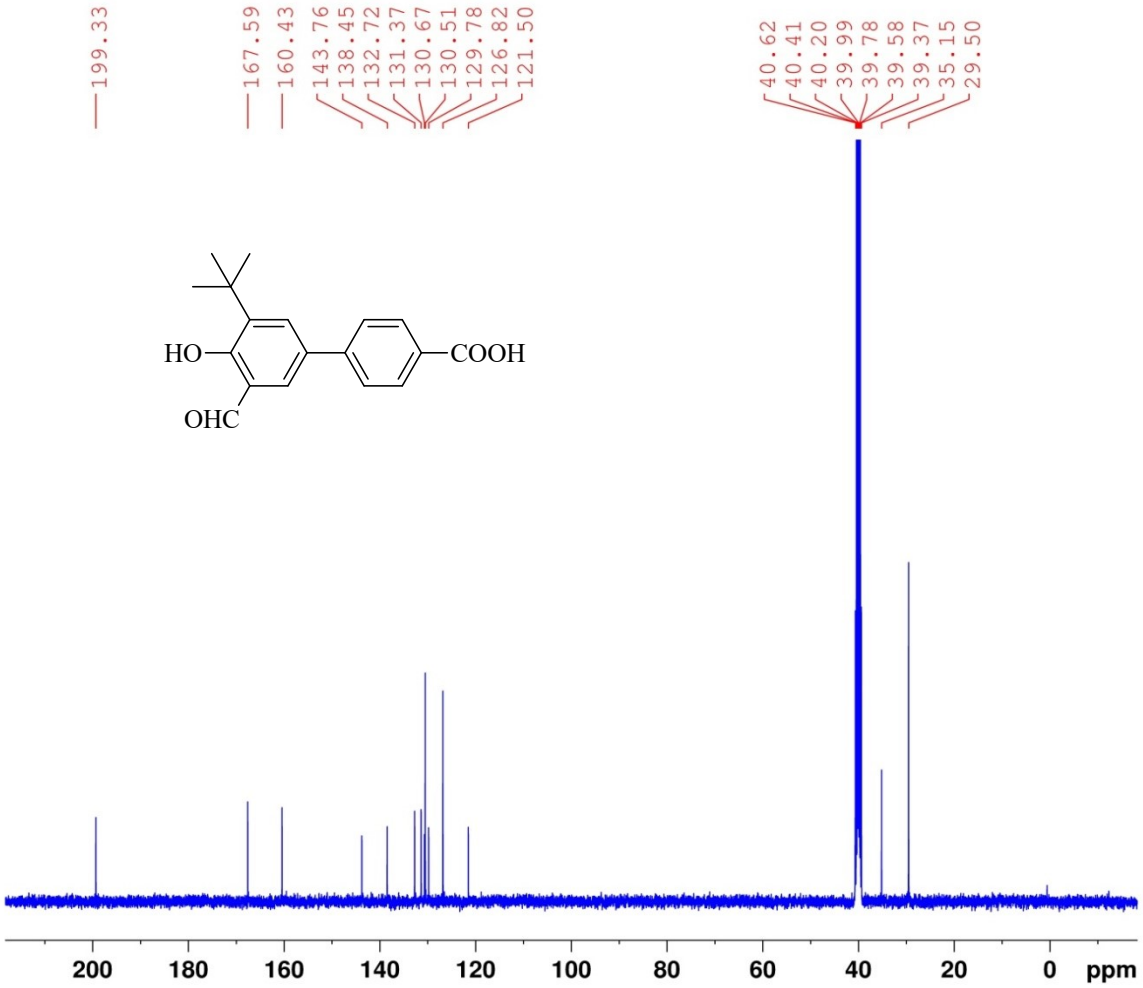

BRUKER

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Current Data Parameters
NAME      Dec23-2020-nmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201223
Time              16.17 h
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PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                    512
DS                      4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
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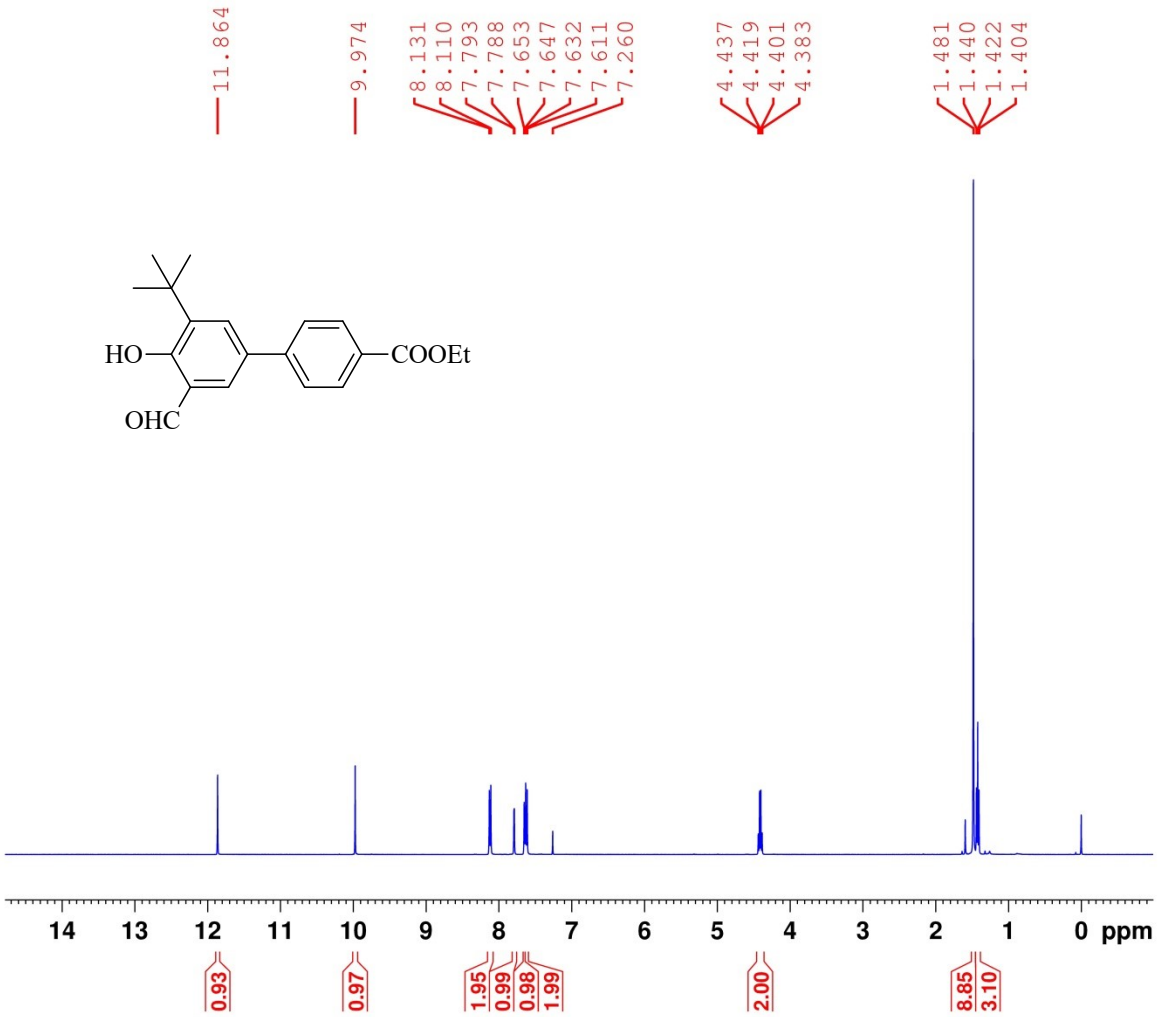


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EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
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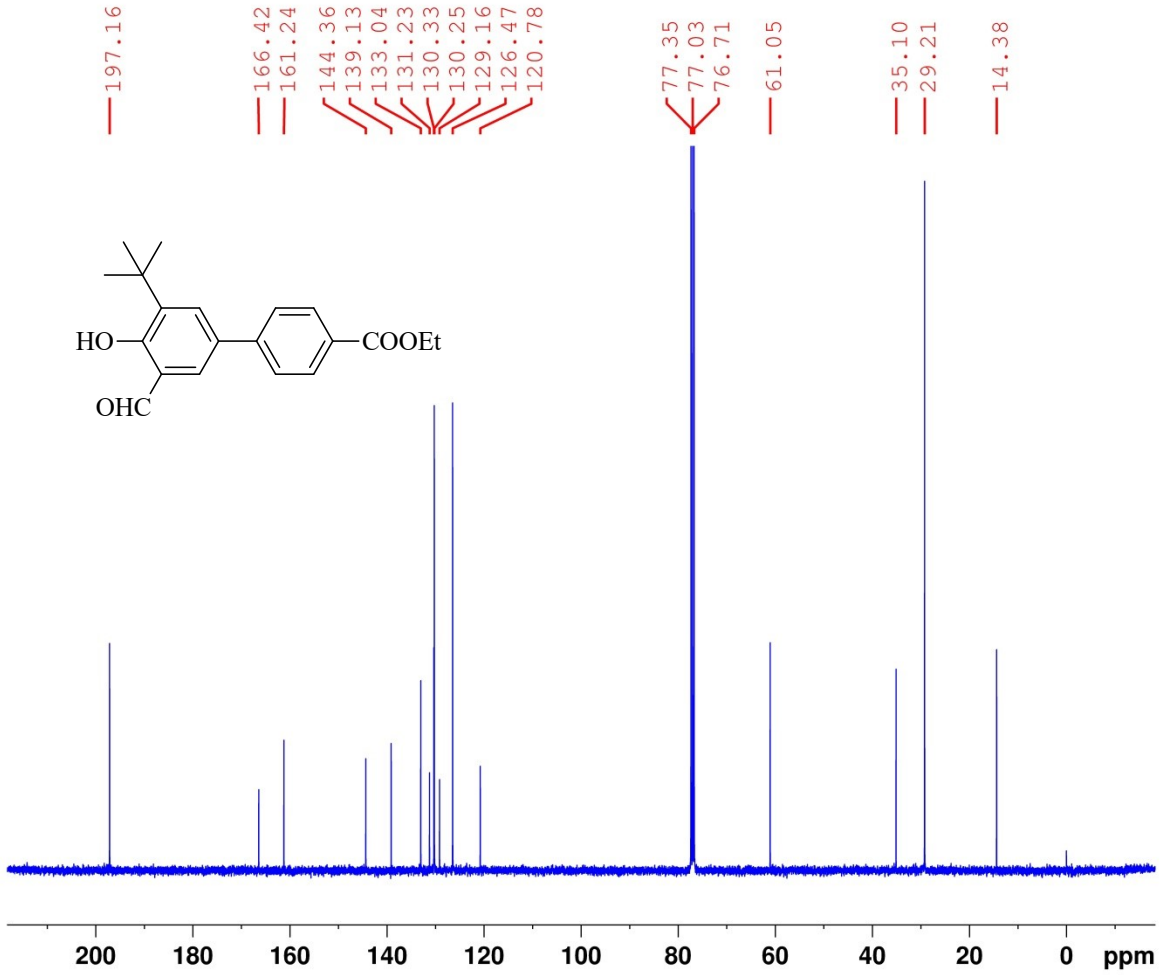
Time              12.31 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG                   101
DW                61.000 usec
DE                 12.86 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700097 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



BRUKER

```
Current Data Parameters
NAME      Oct22-2020-nmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201022
Time              20.16 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
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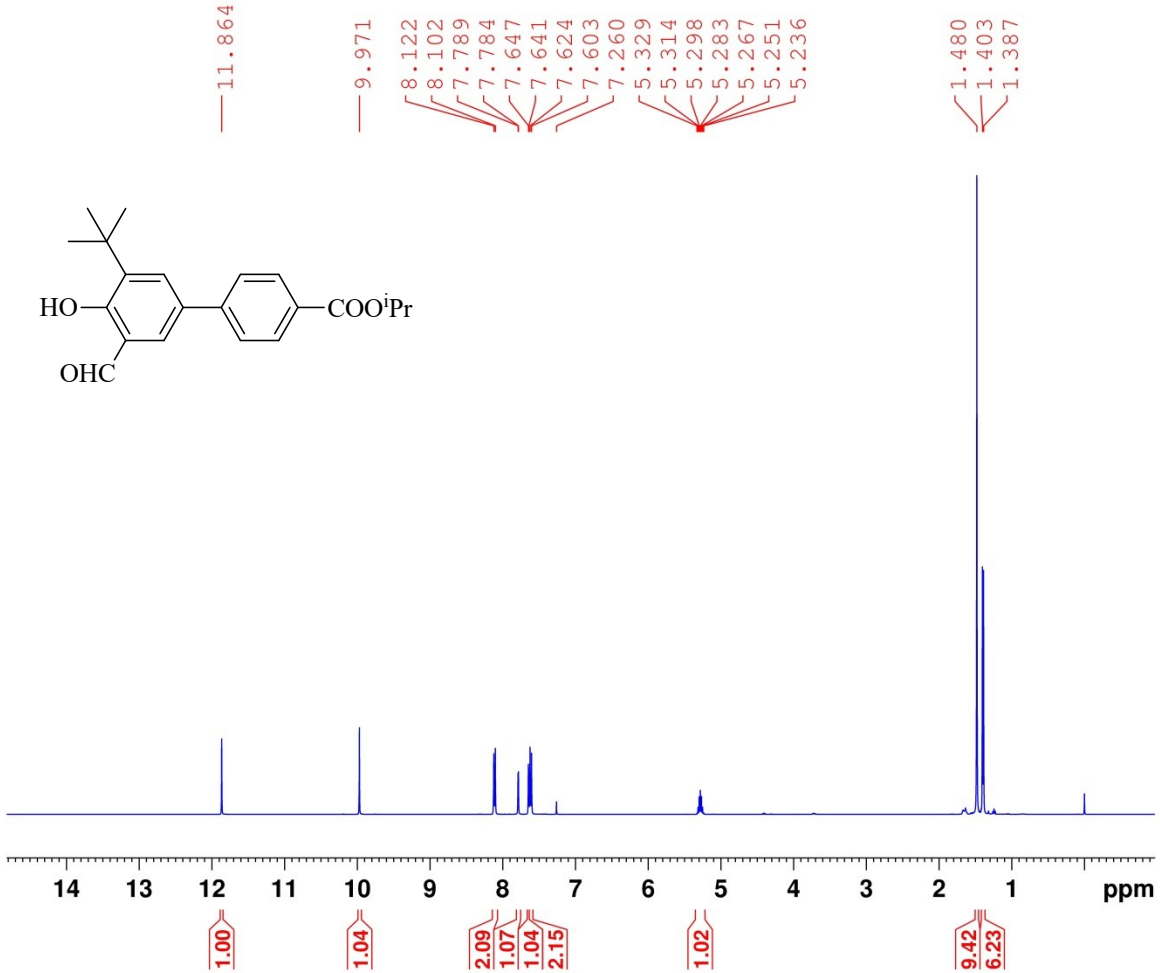


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Current Data Parameters
NAME      Sep26-2020-nmr
EXPNO                30
PROCNO                1

F2 - Acquisition Parameters
Date_          20200926
Time              21.32 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8196.722 Hz
FIDRES        0.250144 Hz
AQ            3.9976959 sec
RG                 101
DW              61.000 usec
DE               12.86 usec
TE               298.0 K
D1          1.00000000 sec
TD0                  1
SFO1        400.1724710 MHz
NUC1                1H
P0               4.67 usec
P1              14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI               65536
SF          400.1700097 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
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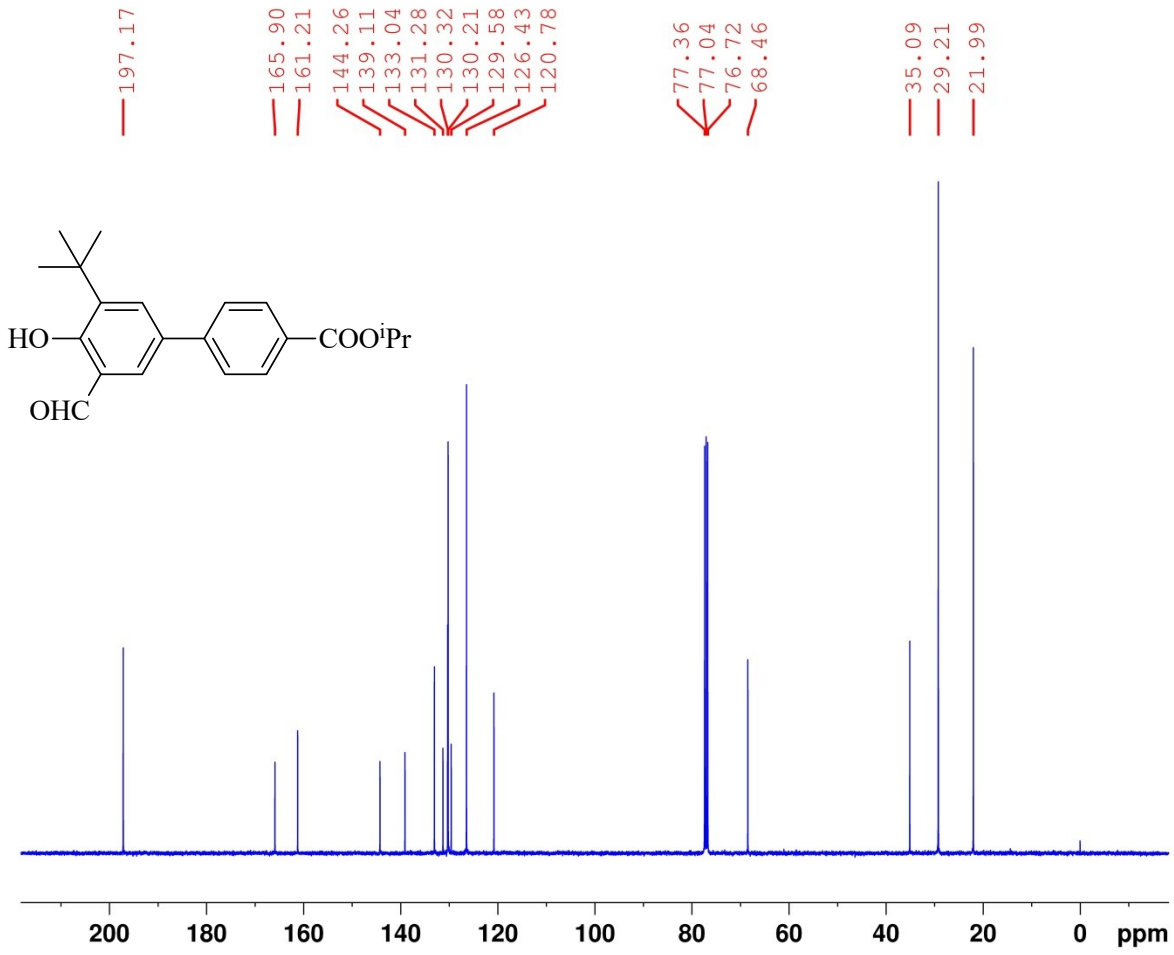


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Current Data Parameters
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EXPNO                 31
PROCNO                 1

F2 - Acquisition Parameters
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Time              22.33 h
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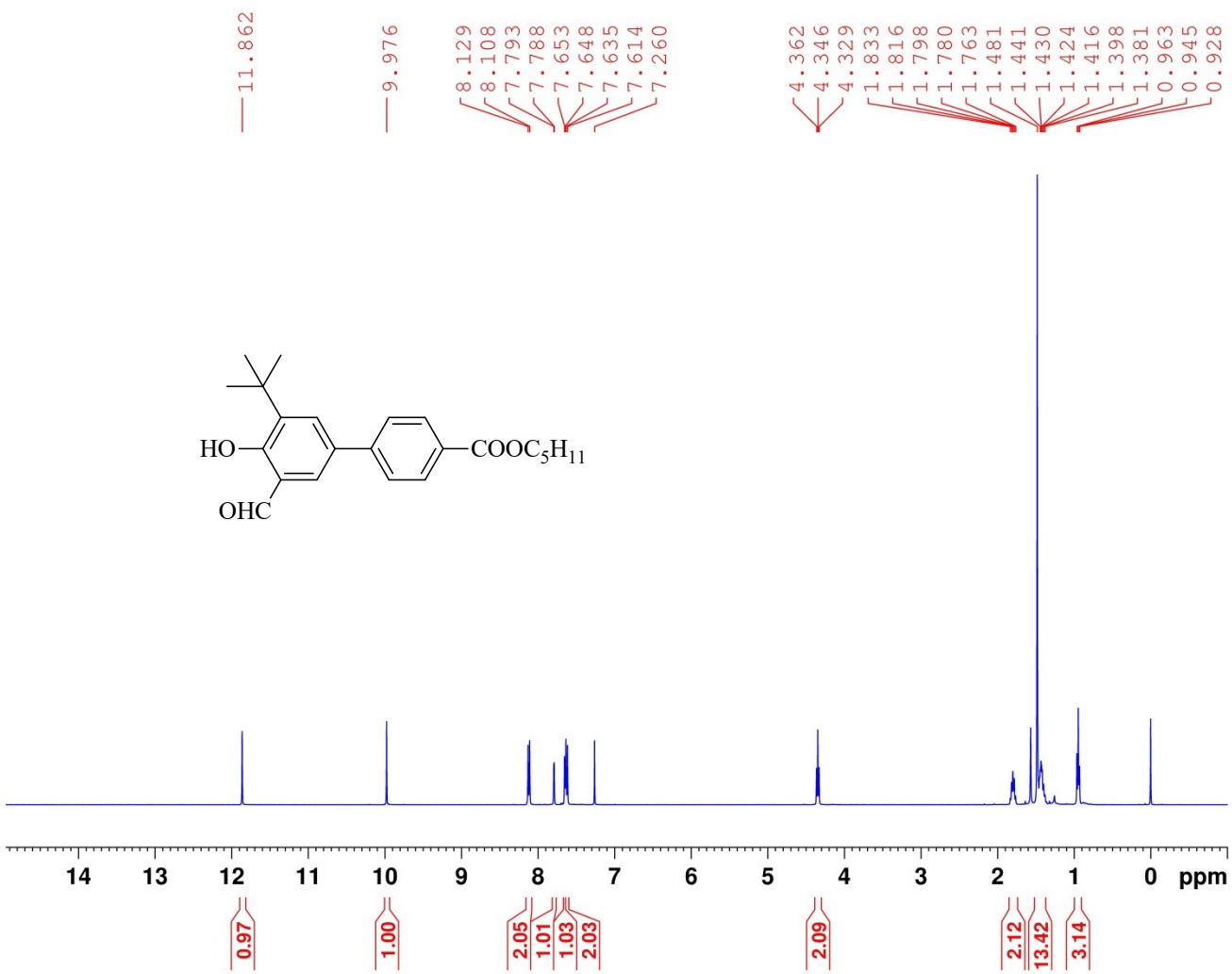
PULPROG           zgpg30
TD                65536
SOLVENT            CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

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Current Data Parameters
NAME      Nov28-2020-nmr
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
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Time              14.15 h
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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
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SF           400.1700098 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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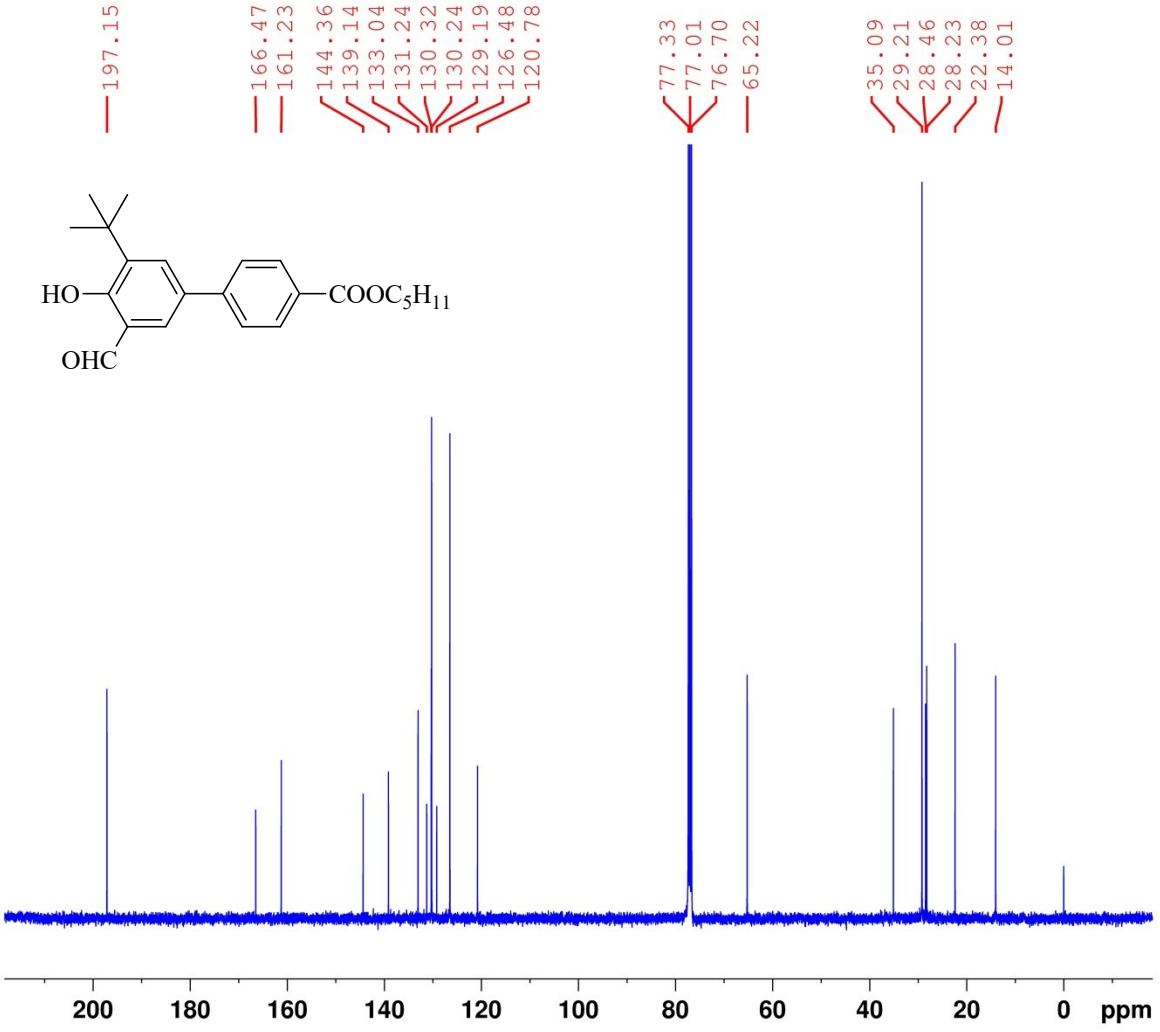

BRUKER

```
Current Data Parameters
NAME      Nov28-2020-nmr
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
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PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
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WDW                EM
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LB                 1.00 Hz
GB                    0
PC                 1.40
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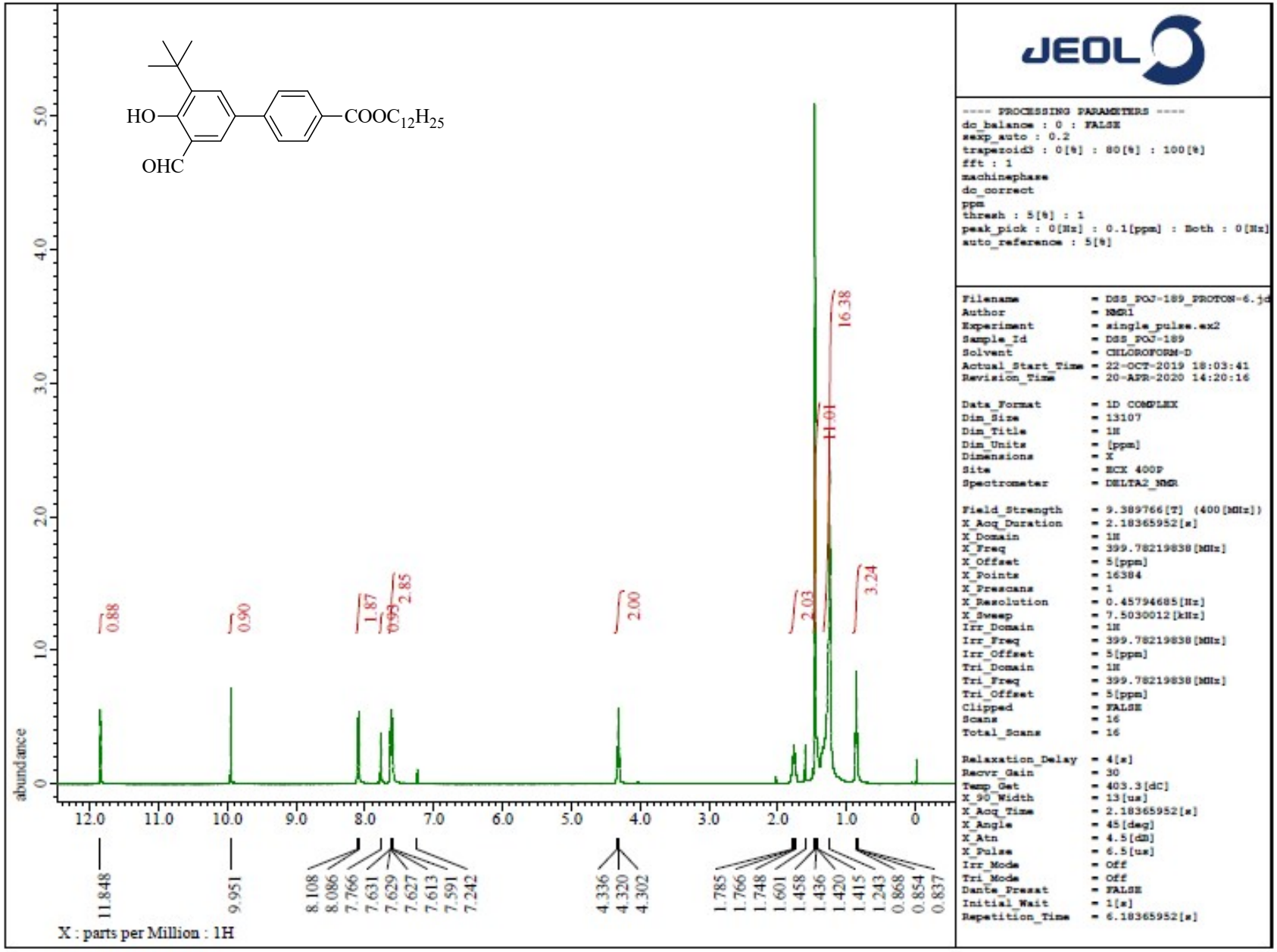
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OHC
COOC12H25
abundance
X : parts per Million : 1H
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0.90
1.87
0.93
2.85
2.00
2.03
16.38
11.01
3.24
11.848
9.951
8.108
8.086
7.766
7.631
7.629
7.627
7.613
7.591
7.242
4.336
4.320
4.302
1.785
1.766
1.748
1.601
1.458
1.436
1.420
1.415
1.243
0.868
0.854
0.837
==== PROCESSING PARAMETERS ====
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sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
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Experiment = single_pulse.ex2
Sample_Id = DSS_POJ-189
Solvent = CHLOROFORM-D
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Revision_Time = 20-APR-2020 14:20:16
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Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
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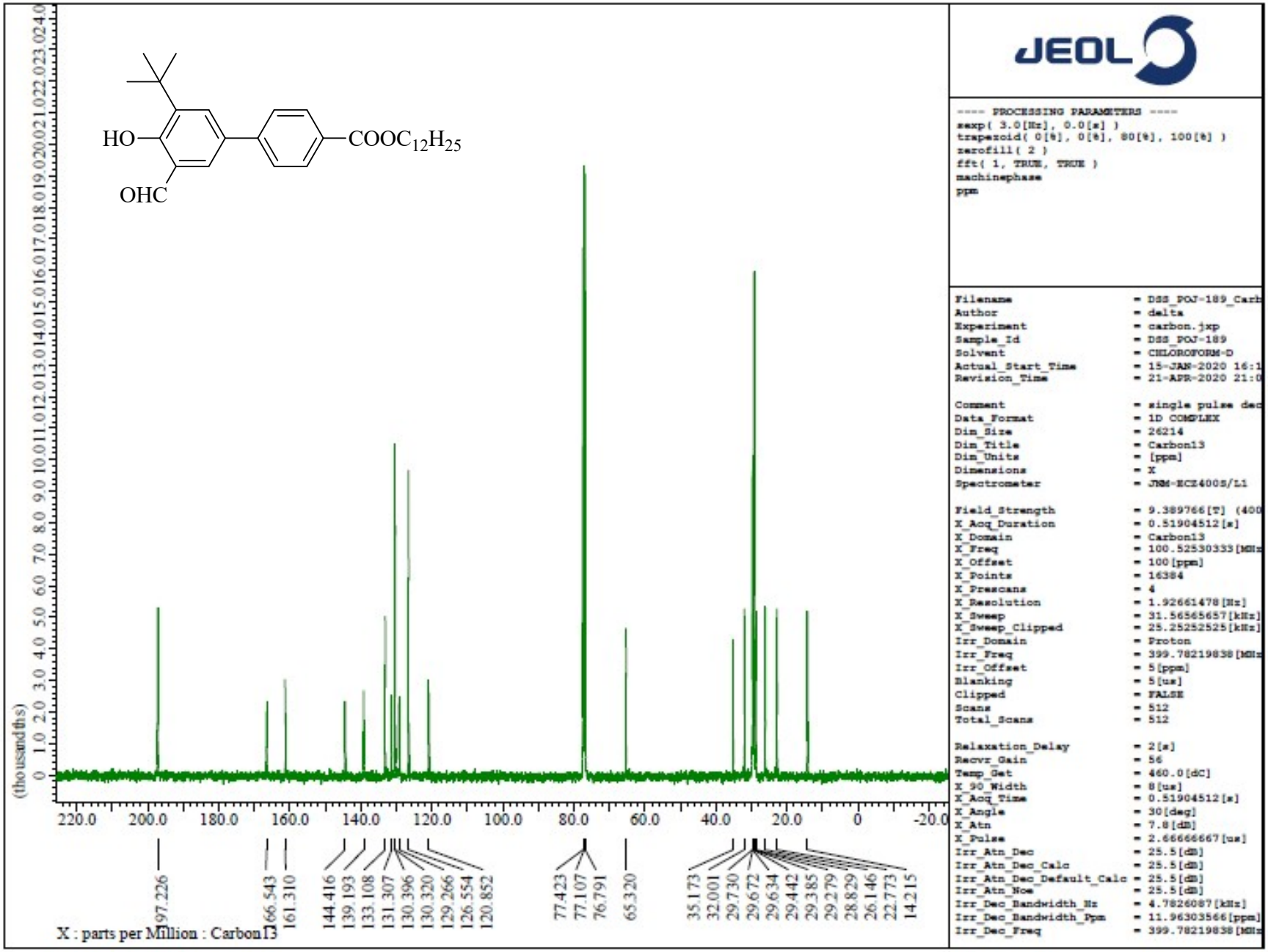
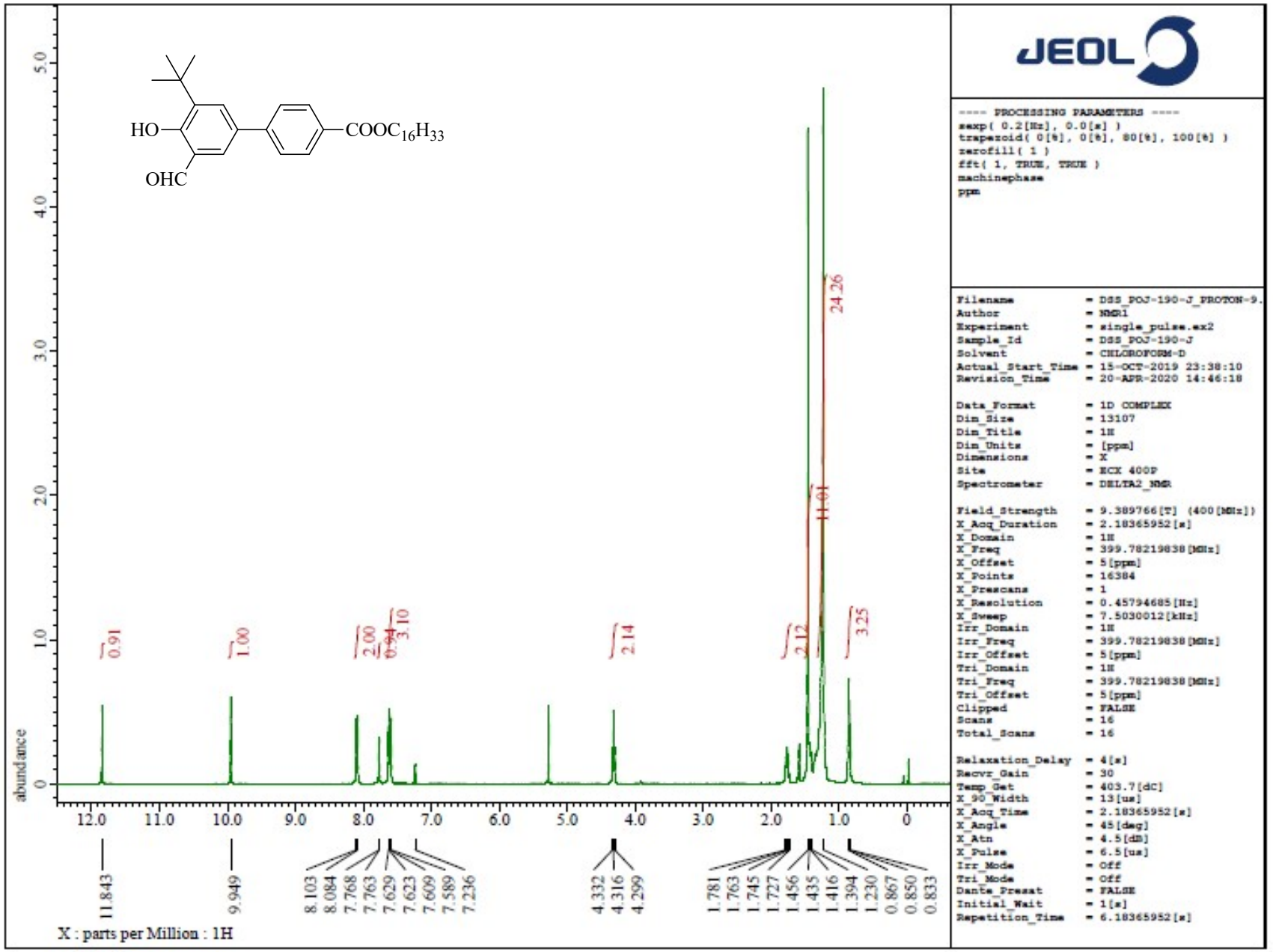
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 403.3[dC]
X_90_Width = 13[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 4.5[dB]
X_Pulse = 6.5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.18365952[s]

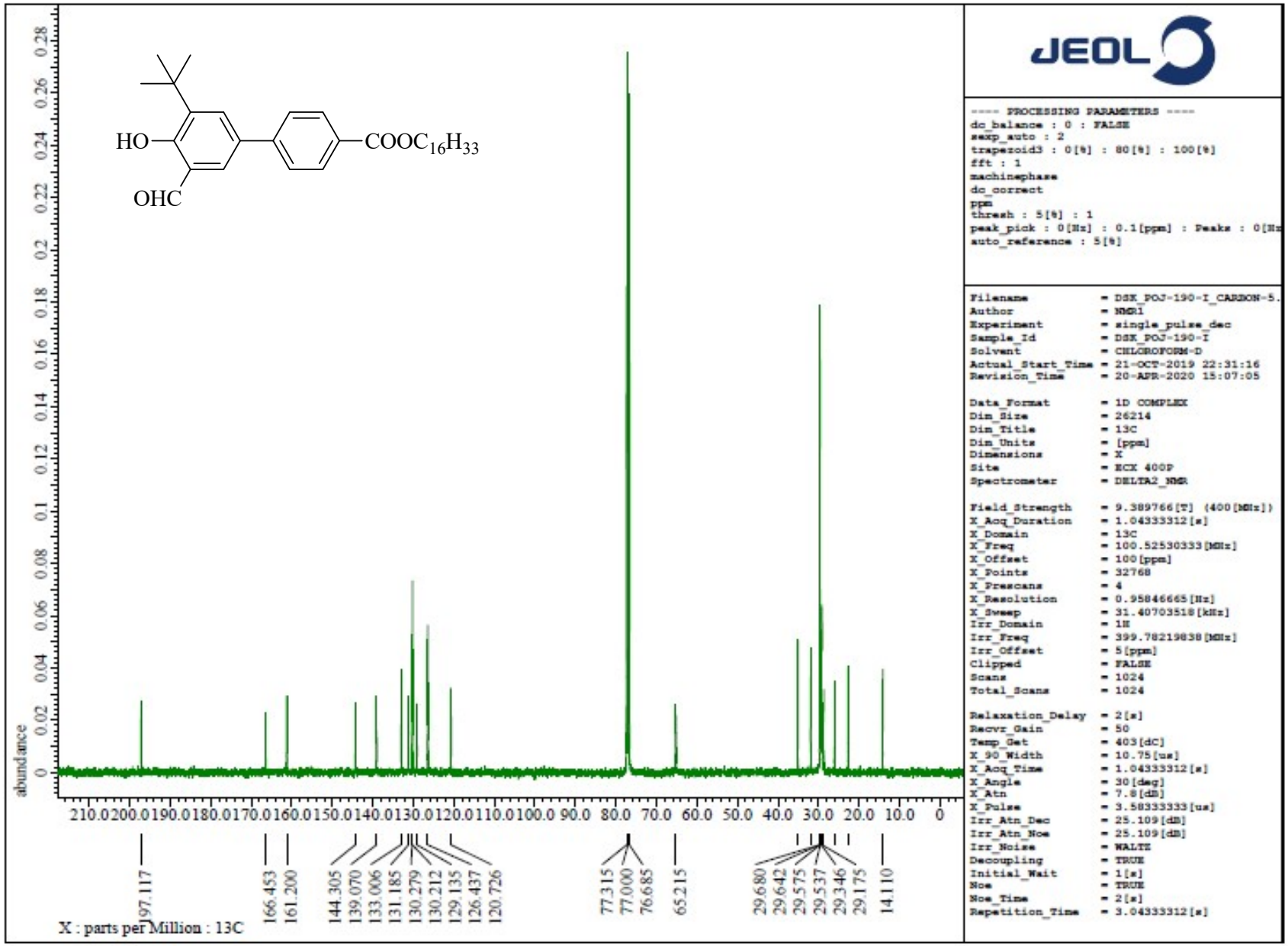


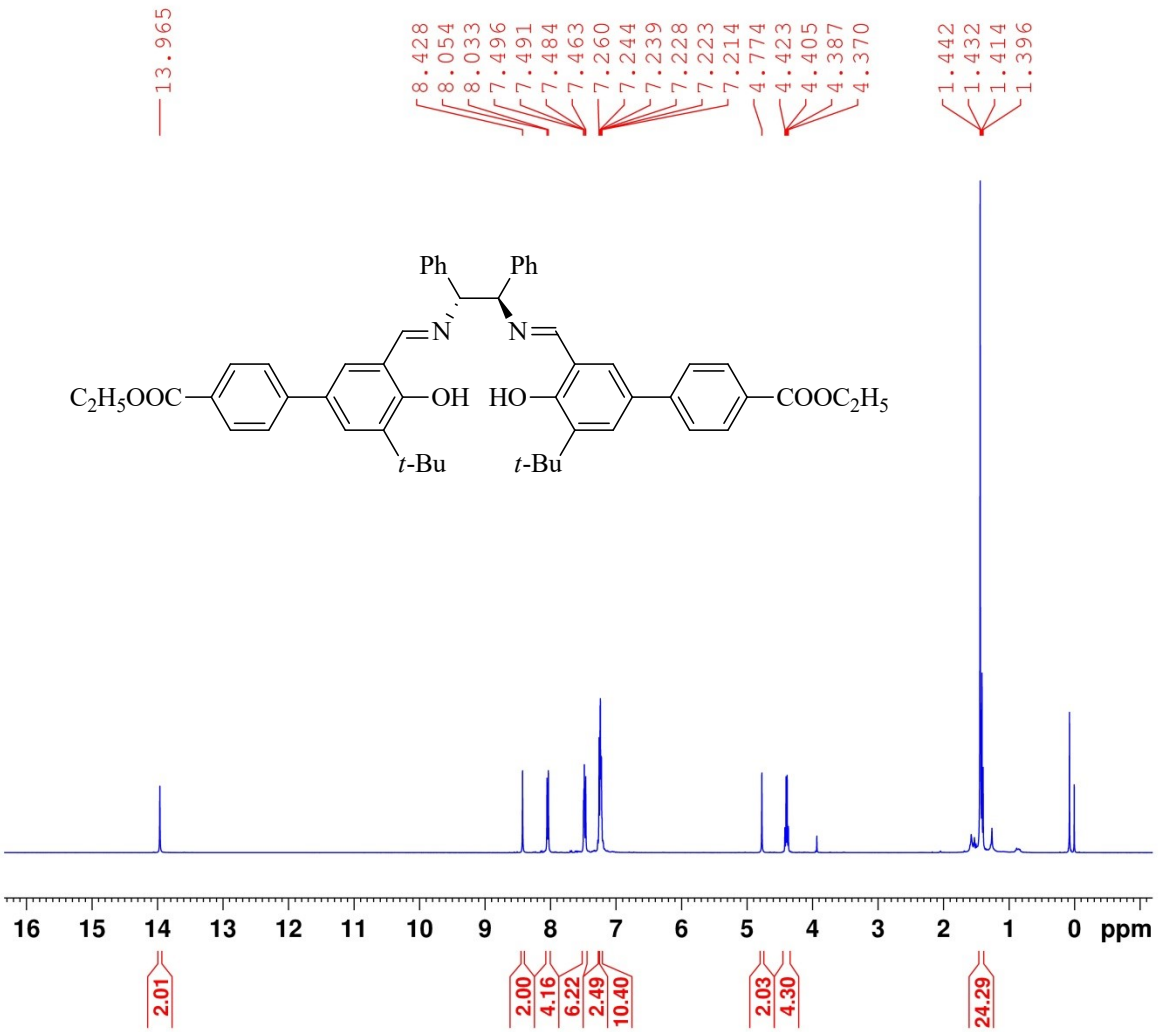
JEOL

```
==== PROCESSING PARAMETERS ====
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= DSS_POJ-189_Carb
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= DSS_POJ-189
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JAN-2020 16:1
Revision_Time	= 21-APR-2020 21:0
Comment	= single pulse dec
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 0.51904512[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 16384
X_Prescans	= 4
X_Resolution	= 1.92661478[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 460.0[dC]
X_90_Width	= 8[us]
X_Acq_Time	= 0.51904512[s]
X_Angle	= 30[deg]
X_Atn	= 7.8[dB]
X_Pulse	= 2.66666667[us]
Irr_Atn_Dec	= 25.5[dB]
Irr_Atn_Dec_Calc	= 25.5[dB]
Irr_Atn_Dec_Default_Calc	= 25.5[dB]
Irr_Atn_Noe	= 25.5[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz

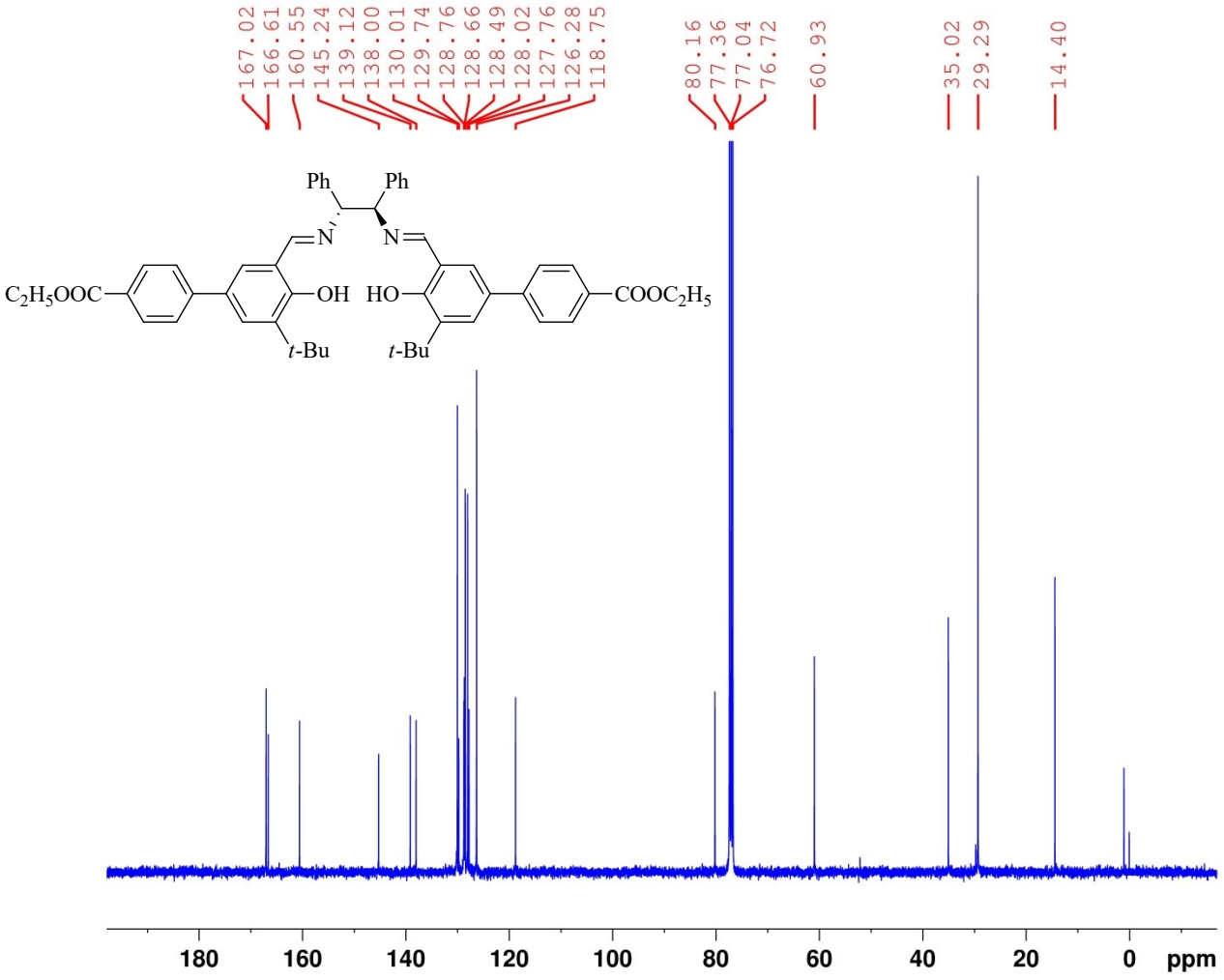

HO
OHC
$COOC_{16}H_{33}$
abundance
X : parts per Million : 1H
0.91
1.00
2.00
0.94
3.10
2.14
2.12
11.01
24.26
3.25
11.843
9.949
8.103
8.084
7.768
7.763
7.629
7.623
7.609
7.589
7.236
4.332
4.316
4.299
1.781
1.763
1.745
1.727
1.456
1.435
1.416
1.394
1.230
0.867
0.850
0.833
==== PROCESSING PARAMETERS ====
exp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = DSS_POJ-190-J_PROTON-9.
Author = NMR1
Experiment = single_pulse.ex2
Sample_Id = DSS_POJ-190-J
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-OCT-2019 23:38:10
Revision_Time = 20-APR-2020 14:46:18
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 4[s]
Recvr_Gain = 30
Temp_Get = 403.7[dC]
X_90_Width = 13[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 4.5[dB]
X_Pulse = 6.5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.18365952[s]


HO
COOC16H33
OHC
abundance
0 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16 0.18 0.2 0.22 0.24 0.26 0.28
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
197.117
166.453
161.200
144.305
139.070
133.006
131.185
130.279
130.212
129.135
126.437
120.726
77.315
77.000
76.685
65.215
29.680
29.642
29.575
29.537
29.346
29.175
14.110
X : parts per Million : 13C
JEOL
==== PROCESSING PARAMETERS ====
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz
auto_reference : 5[%]
Filename = DSK_POJ-190-I_CARBON-5.
Author = NMR1
Experiment = single_pulse_dec
Sample_Id = DSK_POJ-190-I
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-OCT-2019 22:31:16
Revision_Time = 20-APR-2020 15:07:05
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 403[dC]
X_90_Width = 10.75[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 7.0[dB]
X_Pulse = 3.58333333[us]
Irr_Atn_Dec = 25.109[dB]
Irr_Atn_Noe = 25.109[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]



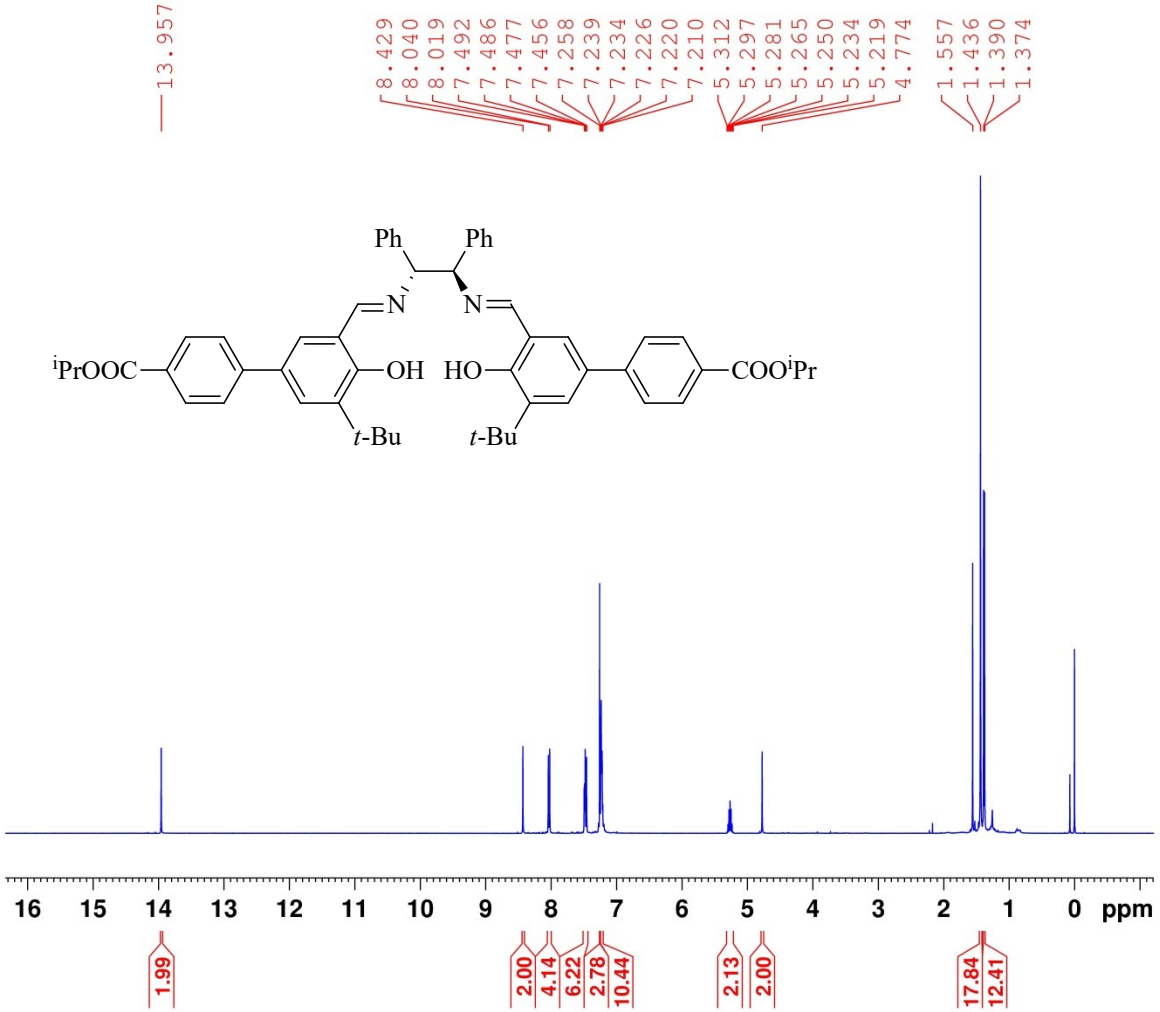
BRUKER

```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 36
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time               2.05 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700102 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



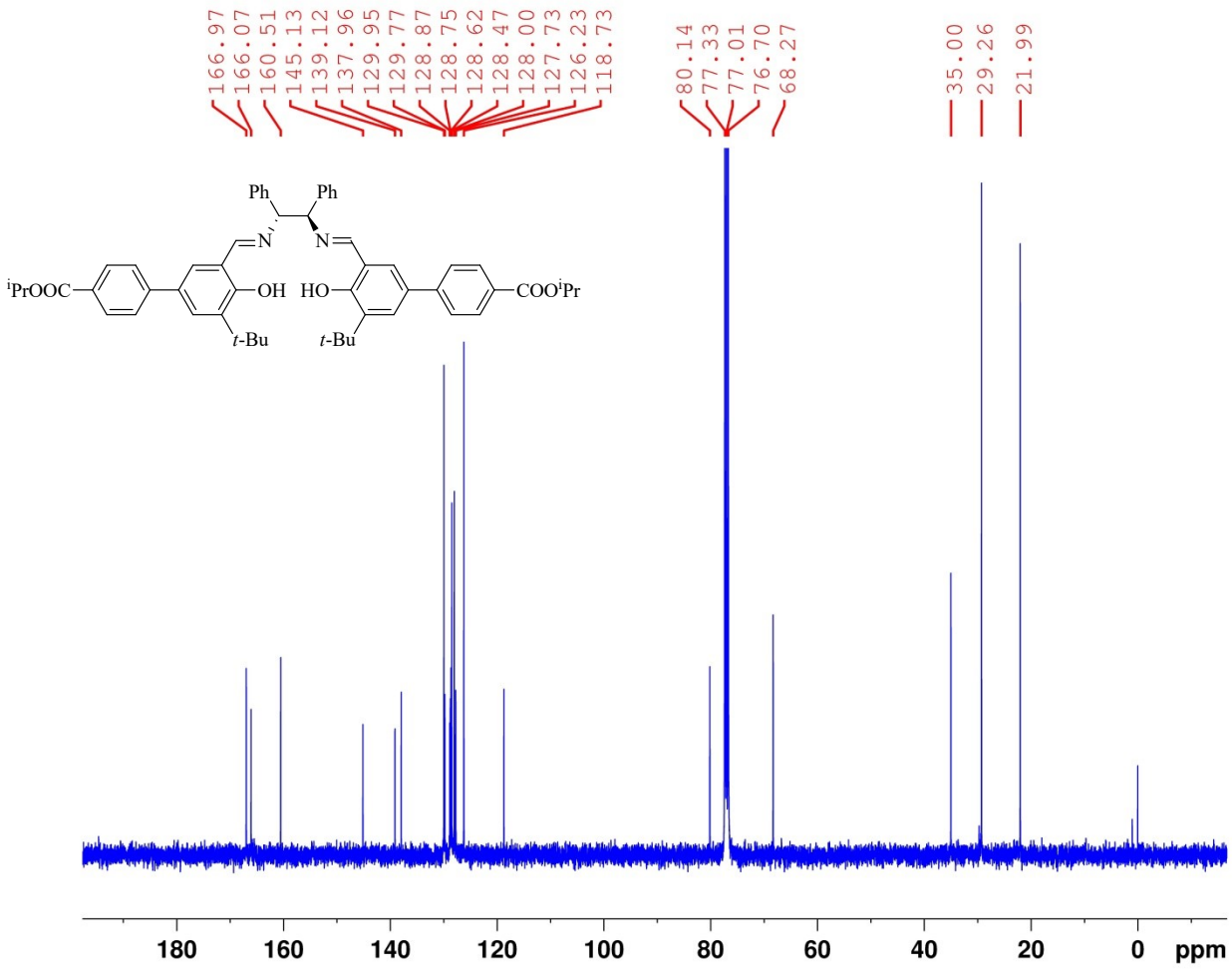
BRUKER

```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 37
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time                5.02 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3072
DS                     4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ              1.3762560 sec
RG                   101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1          60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2          16.77000046 W
PLW12          0.40580001 W
PLW13          0.20411000 W

F2 - Processing parameters
SI                 32768
SF           100.6228255 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



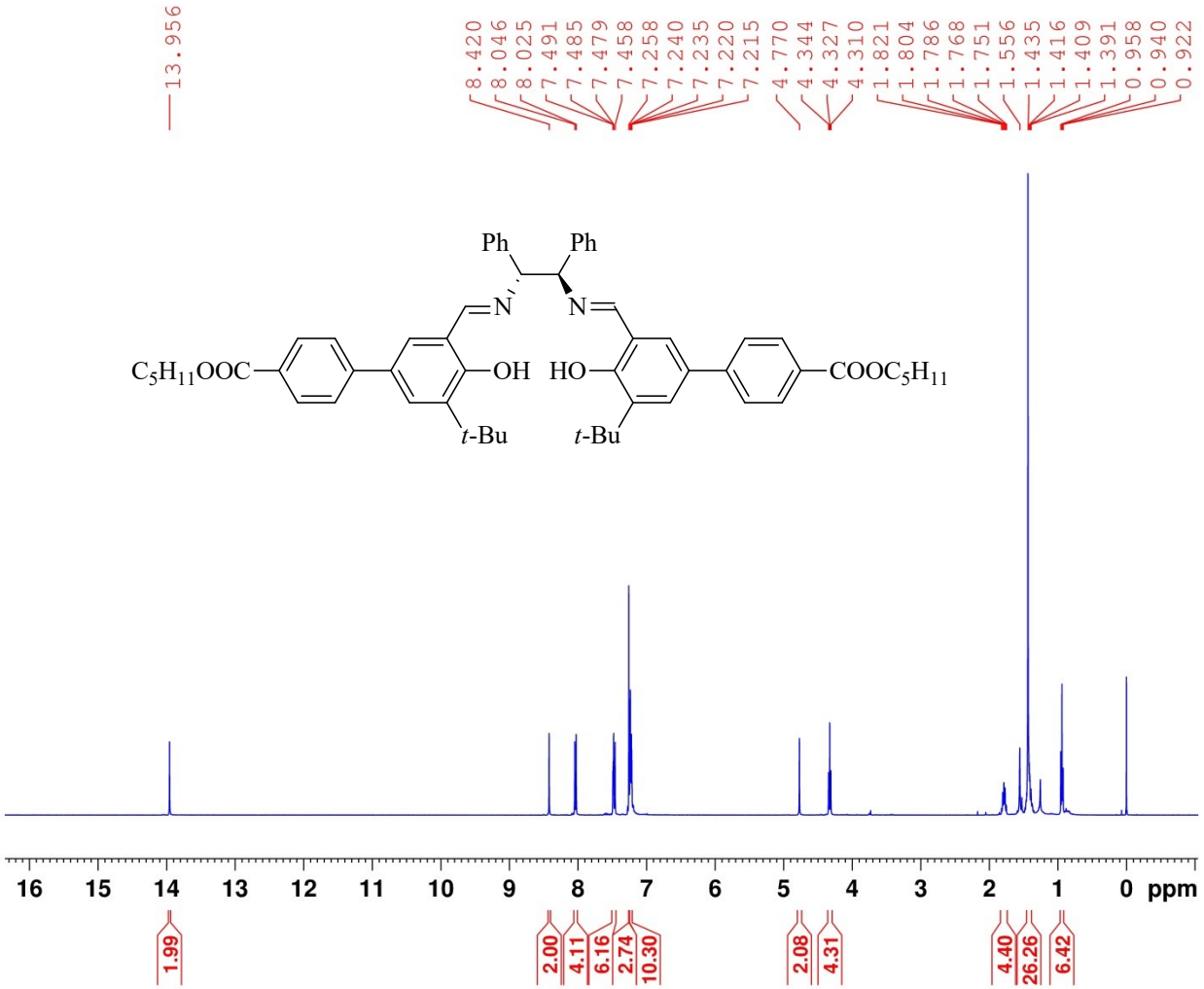
BRUKER

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time               10.35 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1          16.77000046 W

F2 - Processing parameters
SI                 65536
SF            400.1700107 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

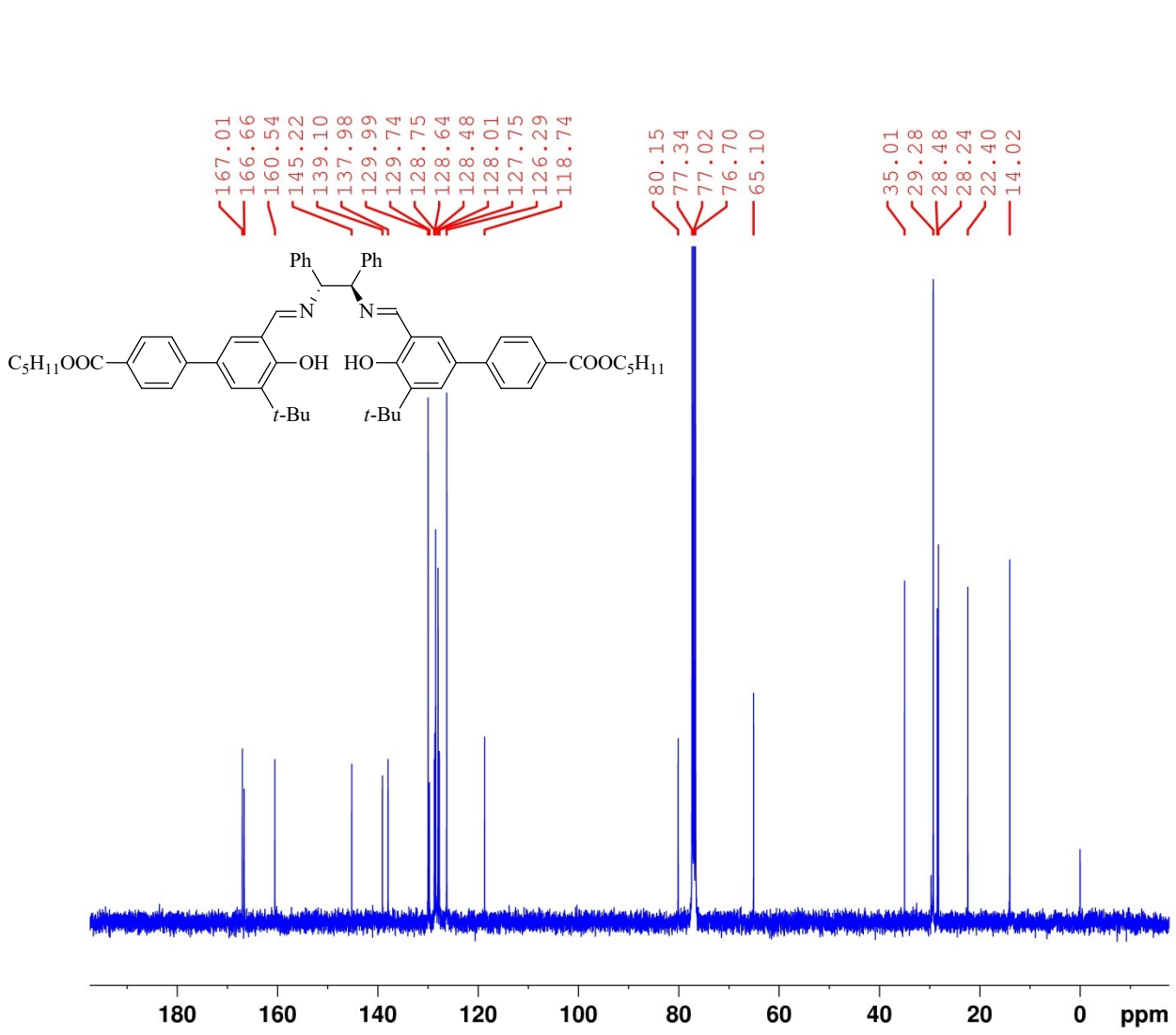


BRUKER

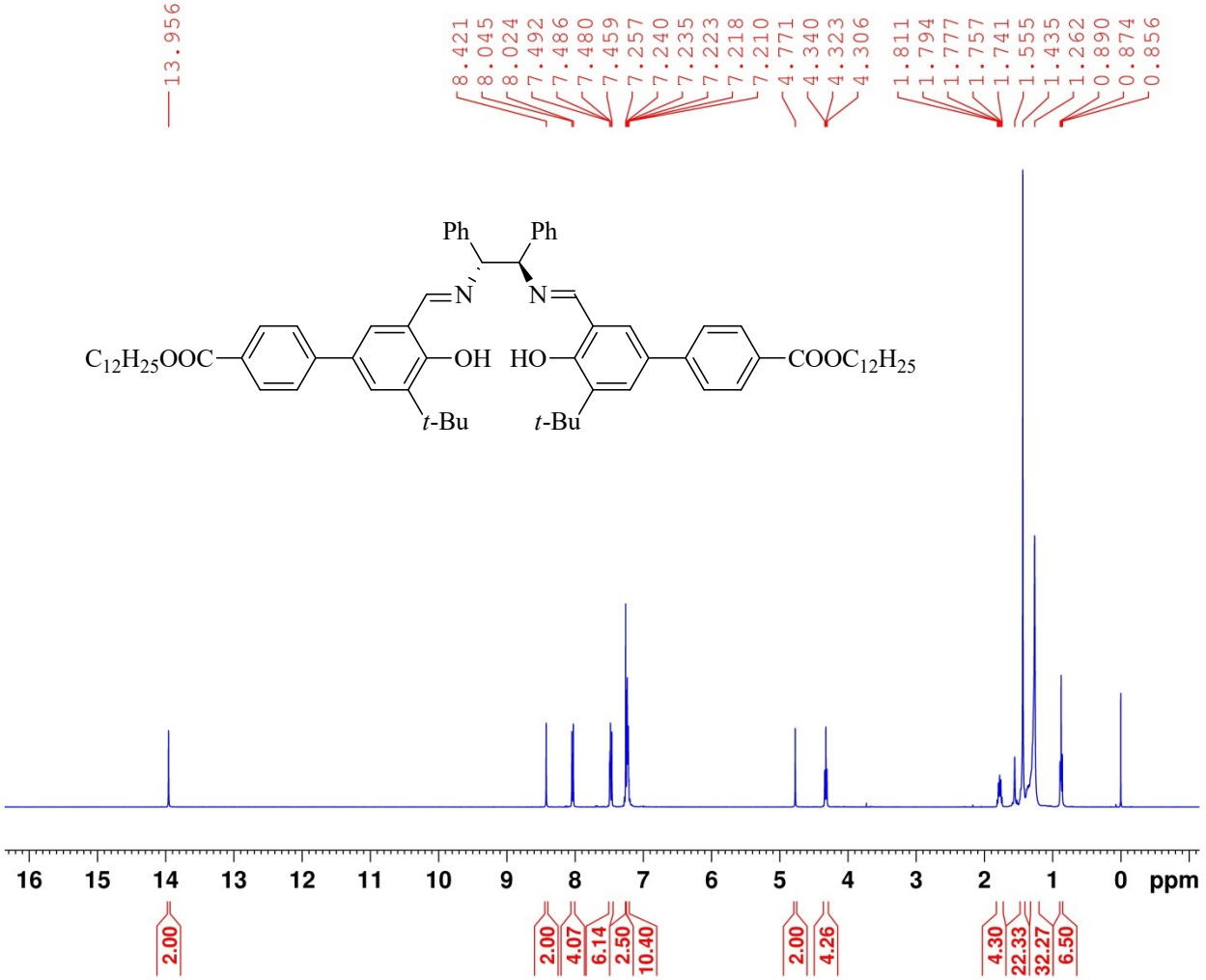
```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time                13.32 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3072
DS                     4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ              1.3762560 sec
RG                   101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1          60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2          16.77000046 W
PLW12          0.40580001 W
PLW13          0.20411000 W

F2 - Processing parameters
SI                 32768
SF           100.6228275 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



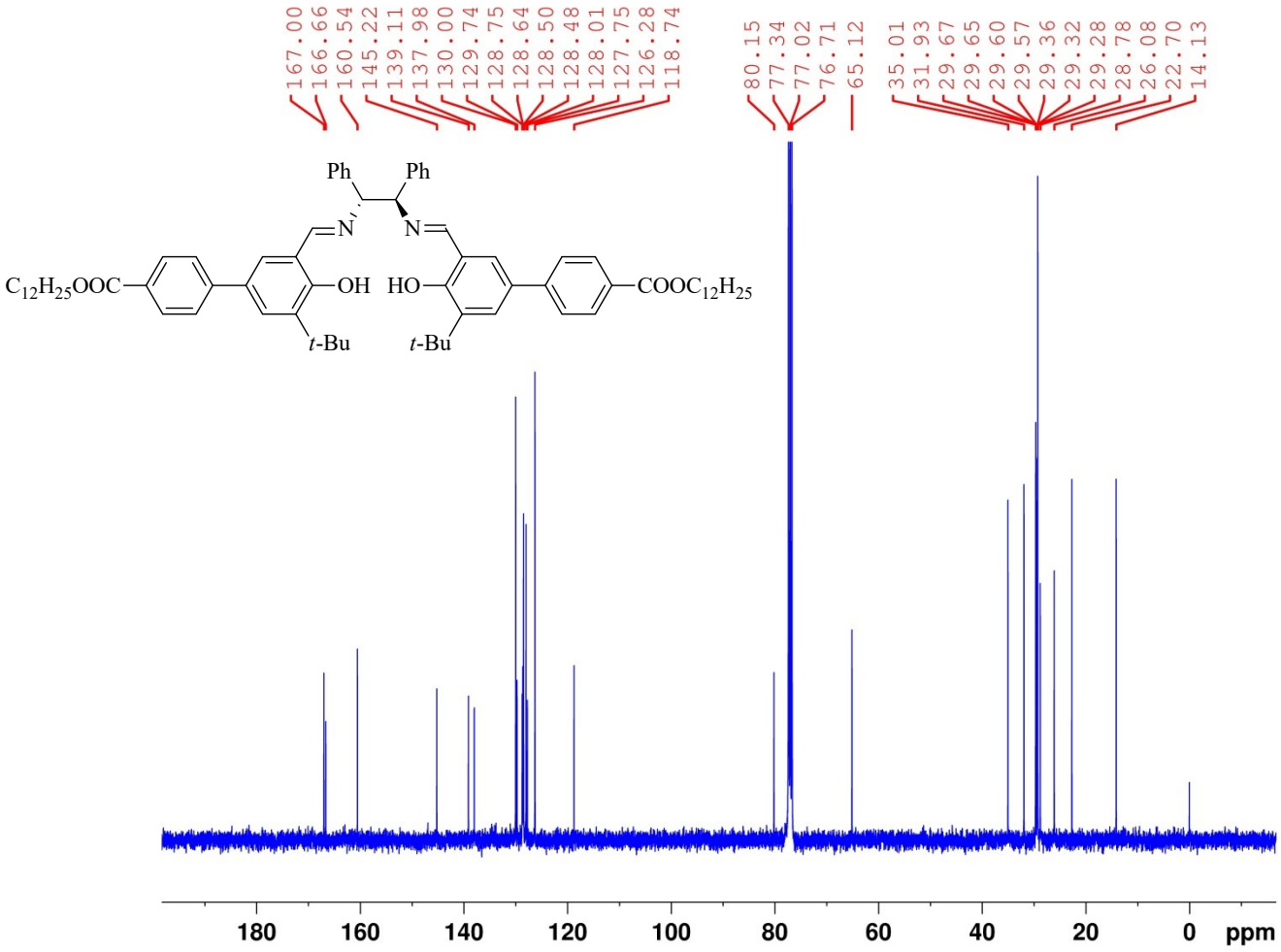

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time                2.30 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700110 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time                5.27 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

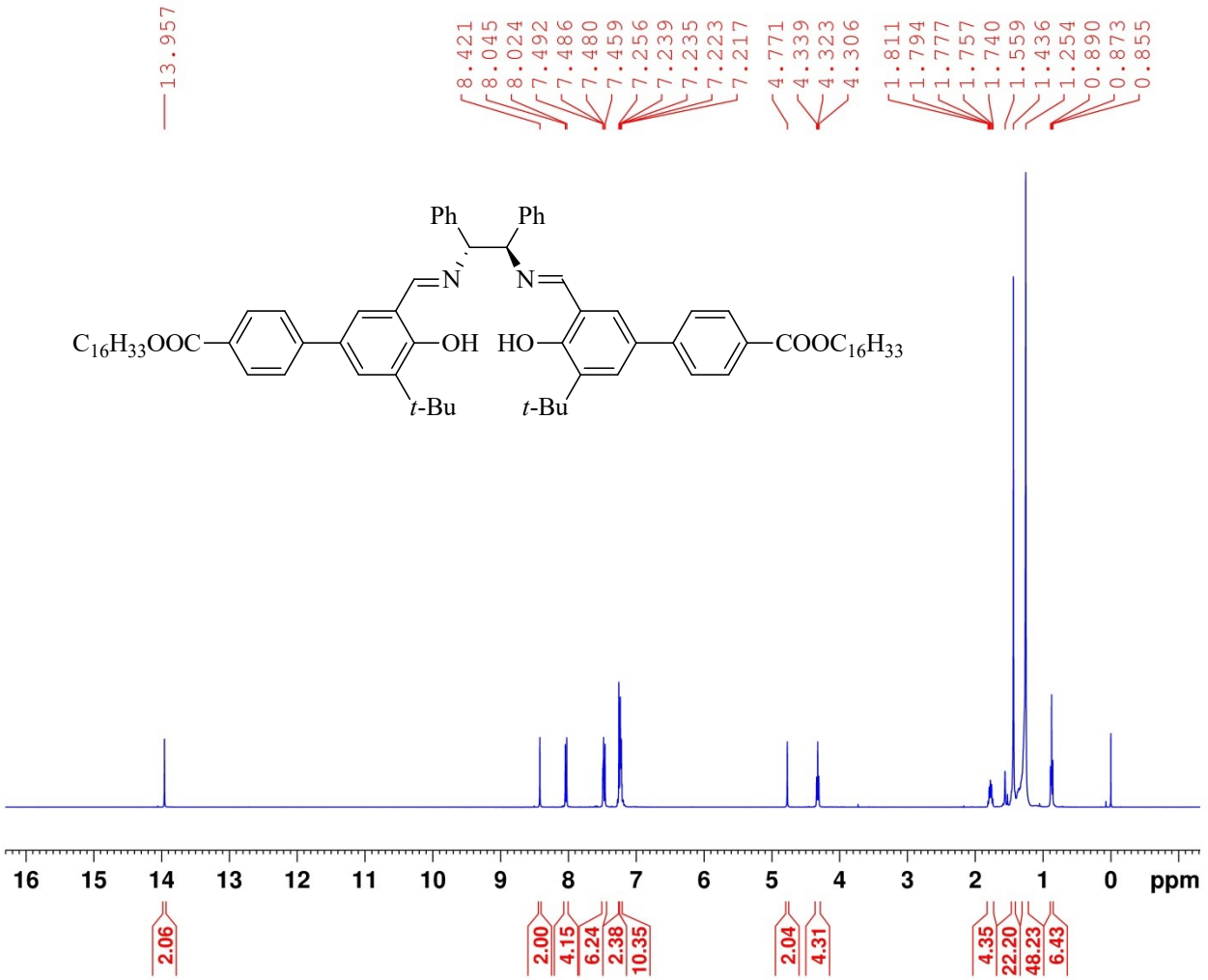


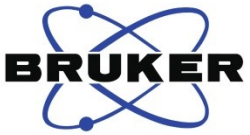

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time                7.34 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700111 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



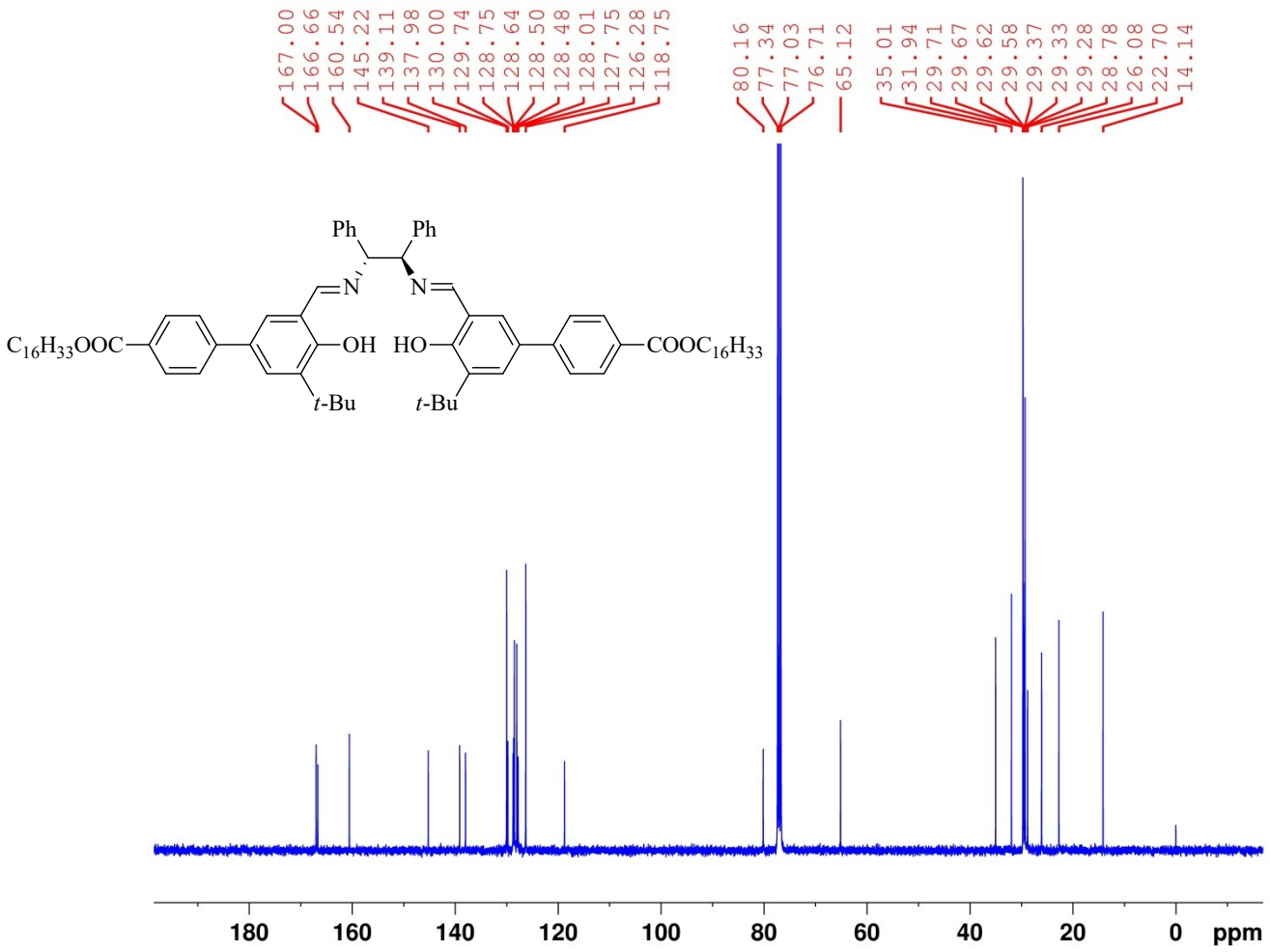
BRUKER

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time              10.31 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



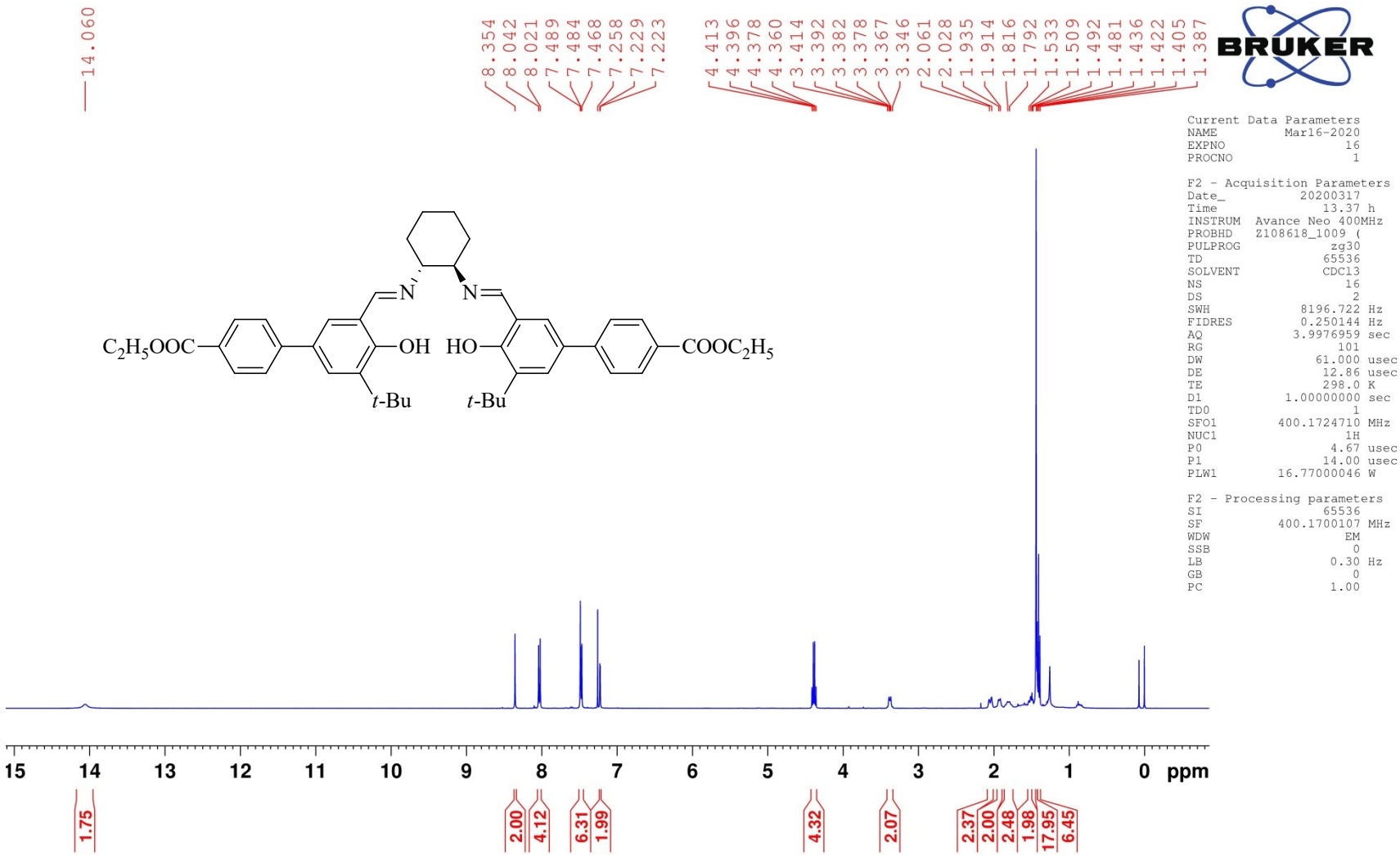


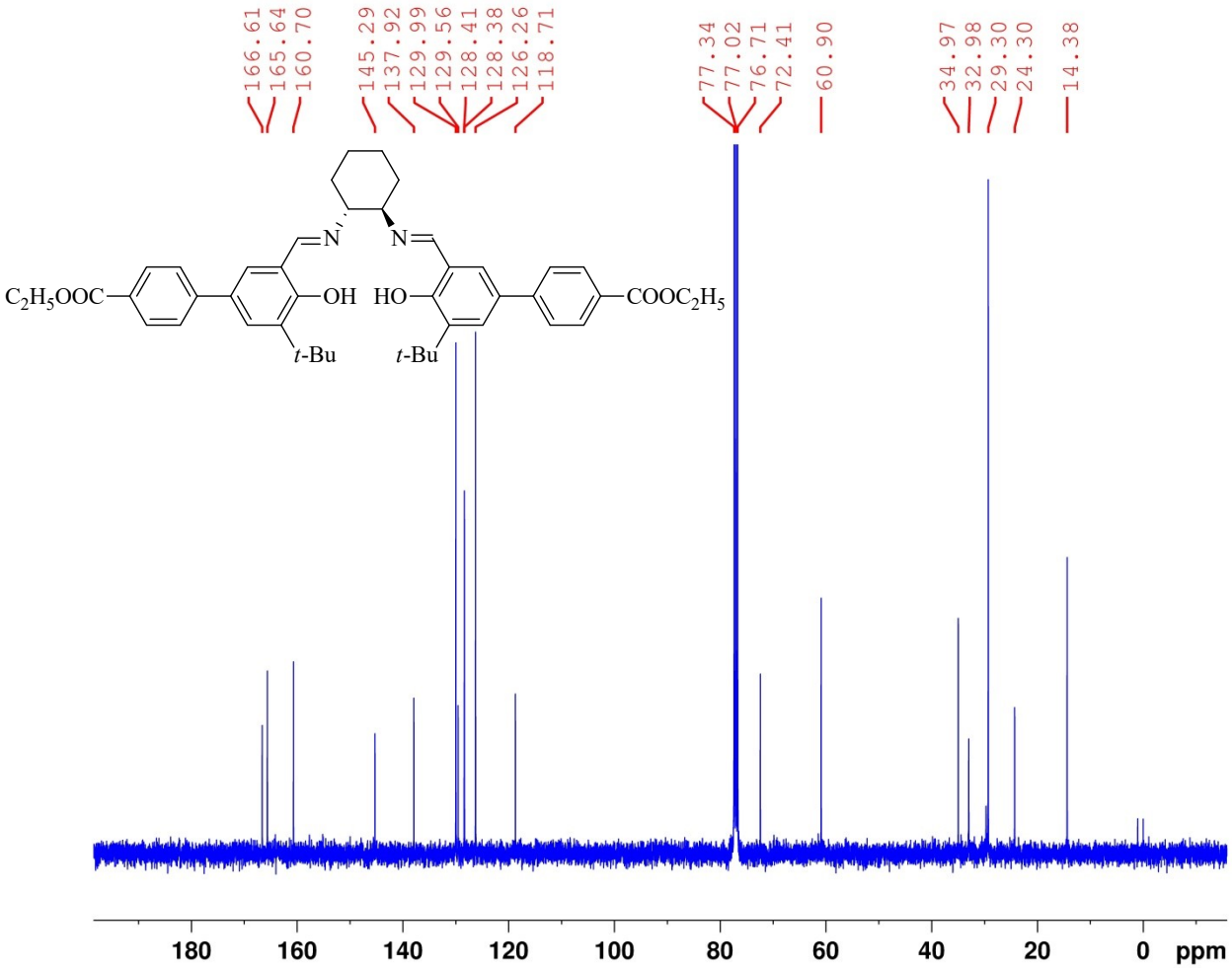

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200316
Time               18.25 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700117 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



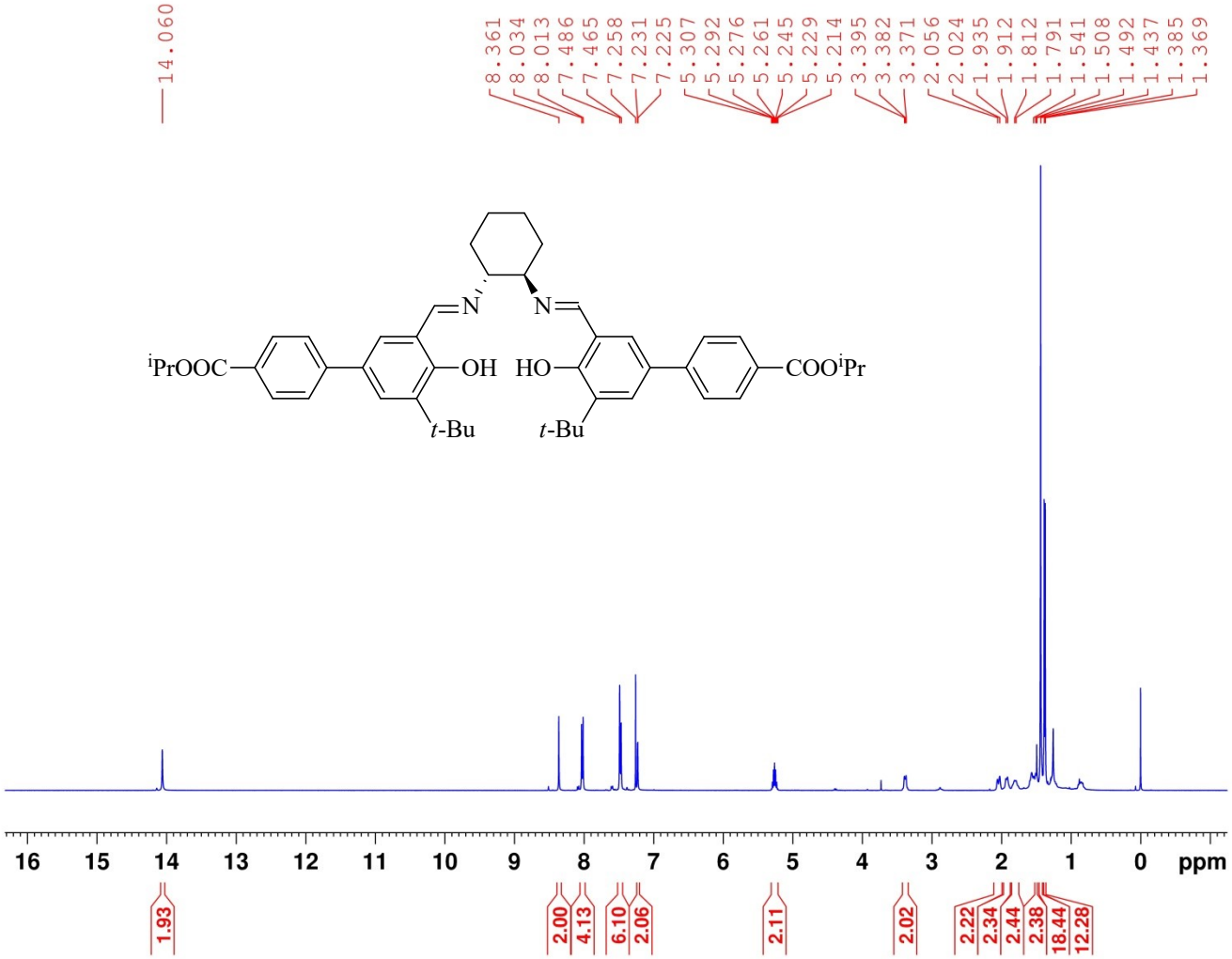
BRUKER

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 15
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200316
Time                21.22 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  3072
DS                     4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             1.3762560 sec
RG                   101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                 32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

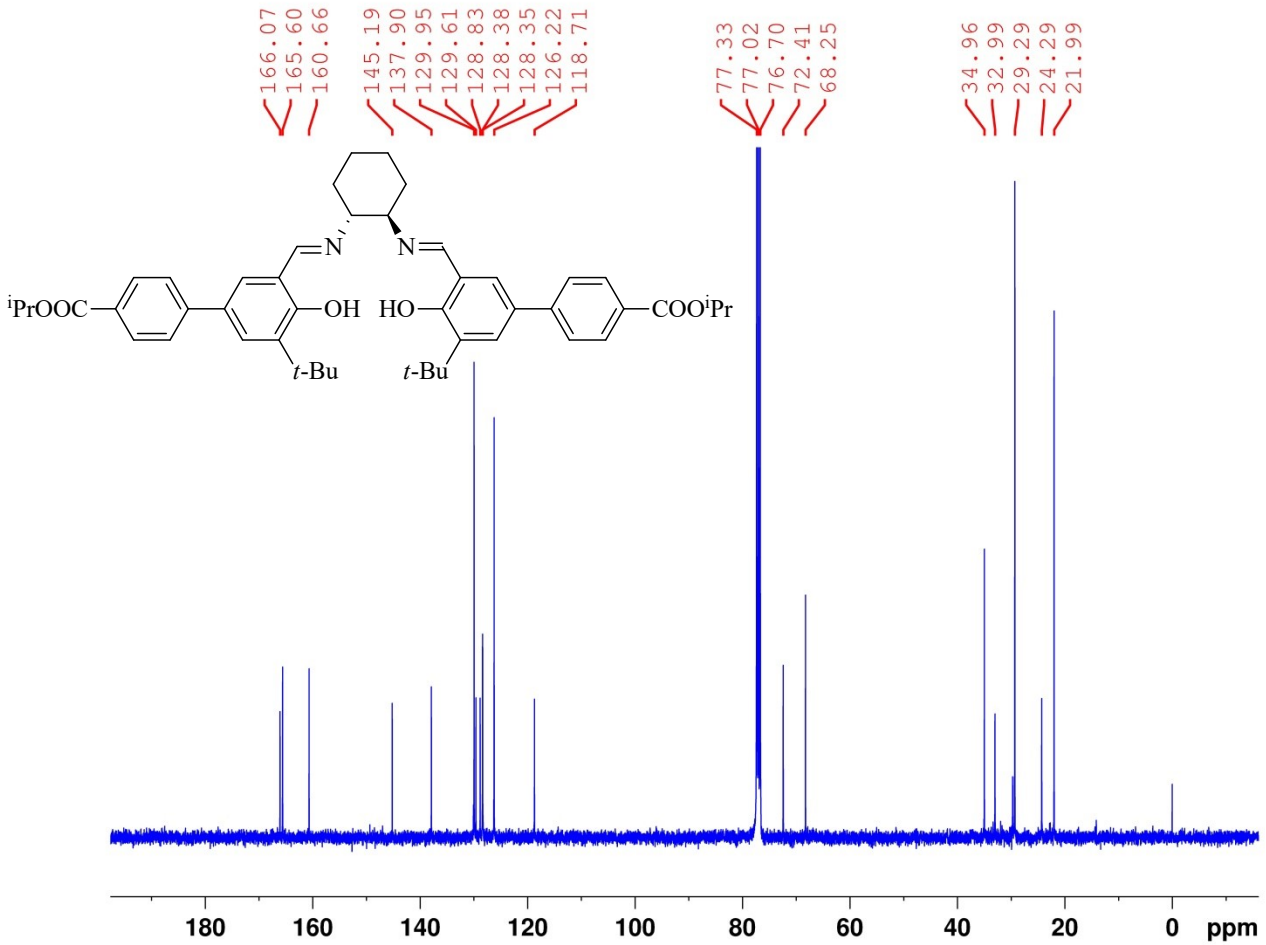

14.060
8.354
8.042
8.021
7.489
7.484
7.468
7.258
7.229
7.223
4.413
4.396
4.378
4.360
3.414
3.392
3.382
3.378
3.367
3.346
2.061
2.028
1.935
1.914
1.816
1.792
1.533
1.509
1.492
1.481
1.436
1.422
1.405
1.387
BRUKER
Current Data Parameters
NAME Mar16-2020
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200317
Time 13.37 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W
F2 - Processing parameters
SI 65536
SF 400.1700107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
C2H5OOC
OH
HO
COOC2H5
t-Bu
t-Bu
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.75
2.00
4.12
6.31
1.99
4.32
2.07
2.37
2.00
2.48
1.98
17.95
6.45




```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 17
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time               14.20 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  726
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 42
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time              11.09 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI                 65536
SF          400.1700108 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



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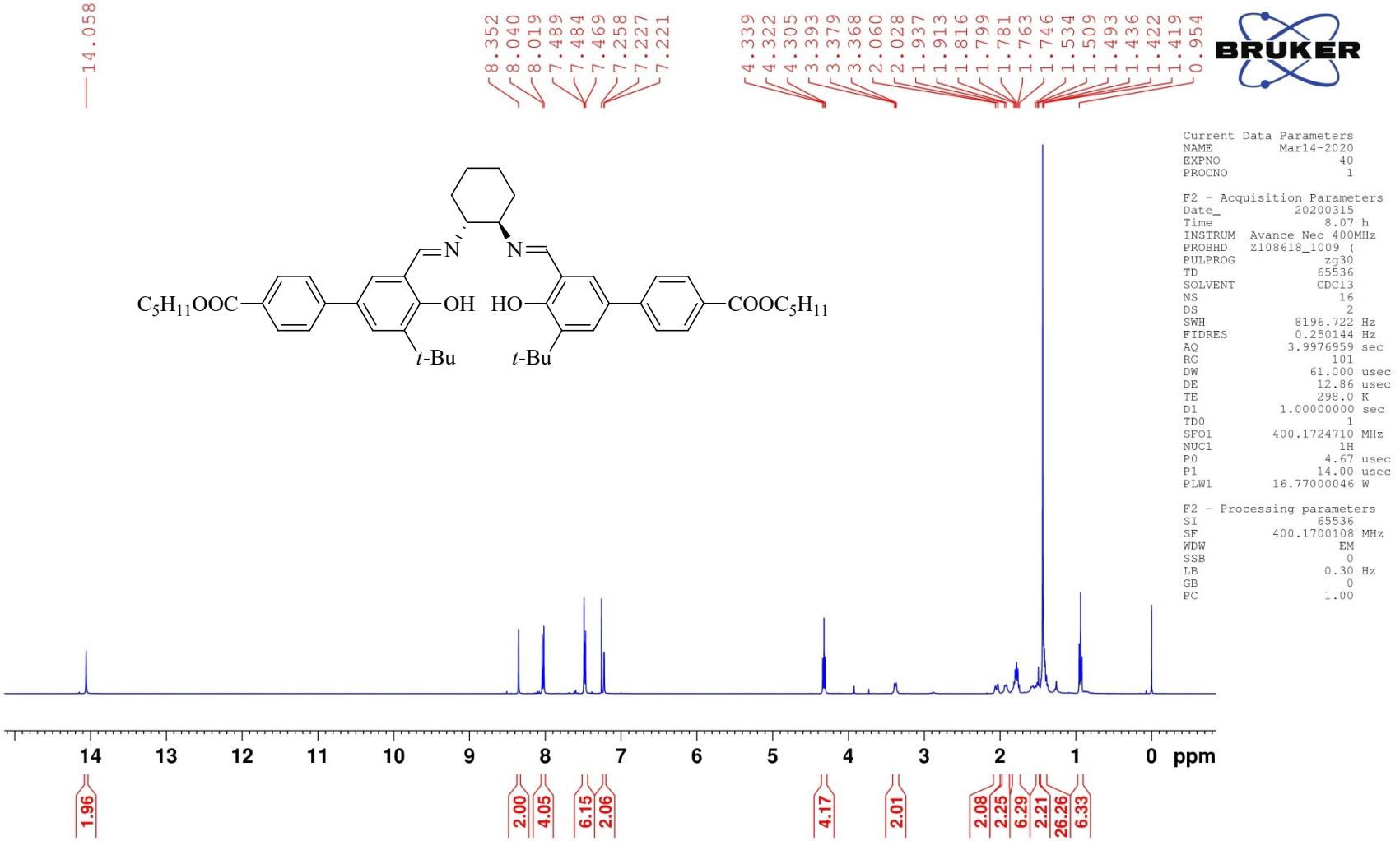
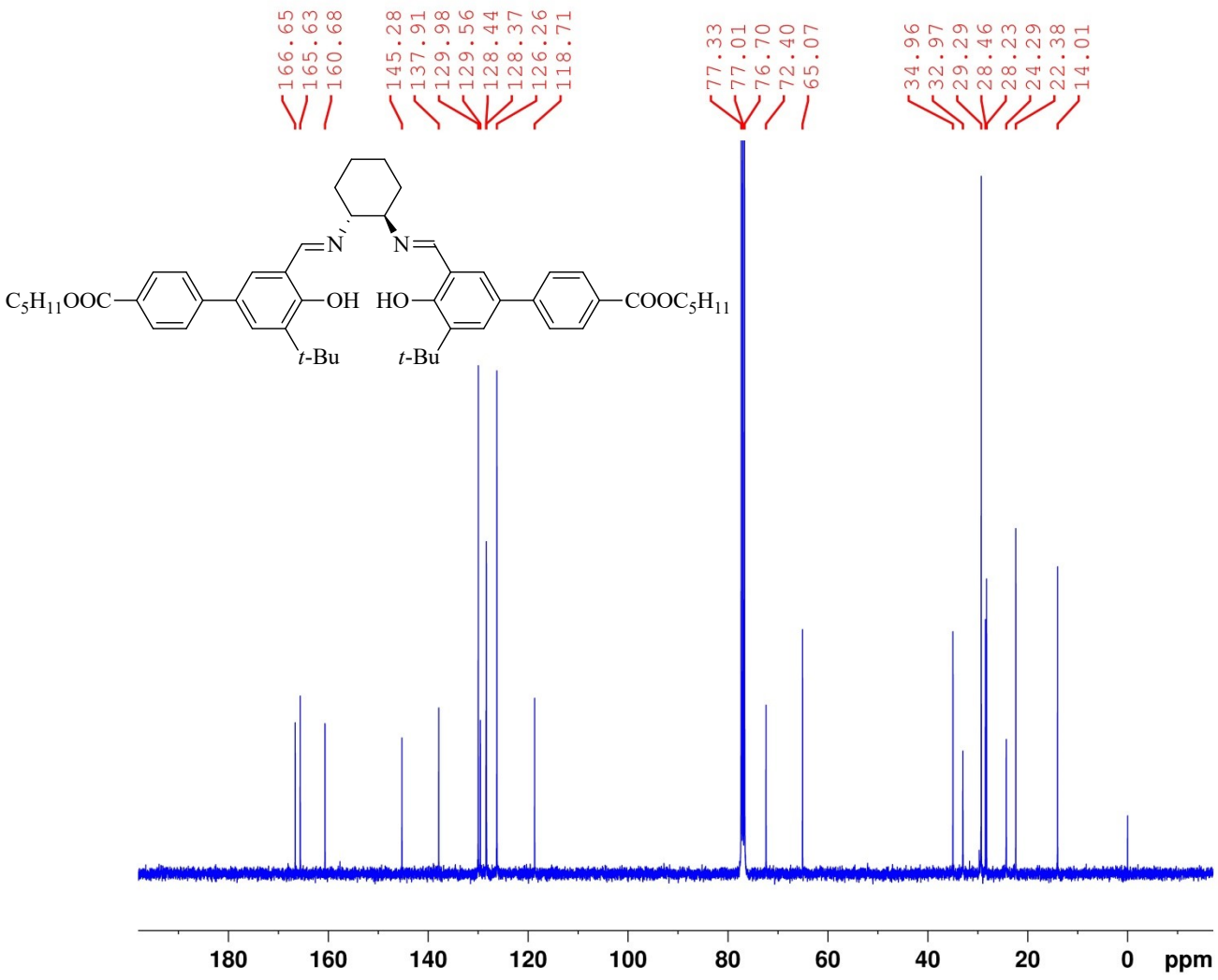
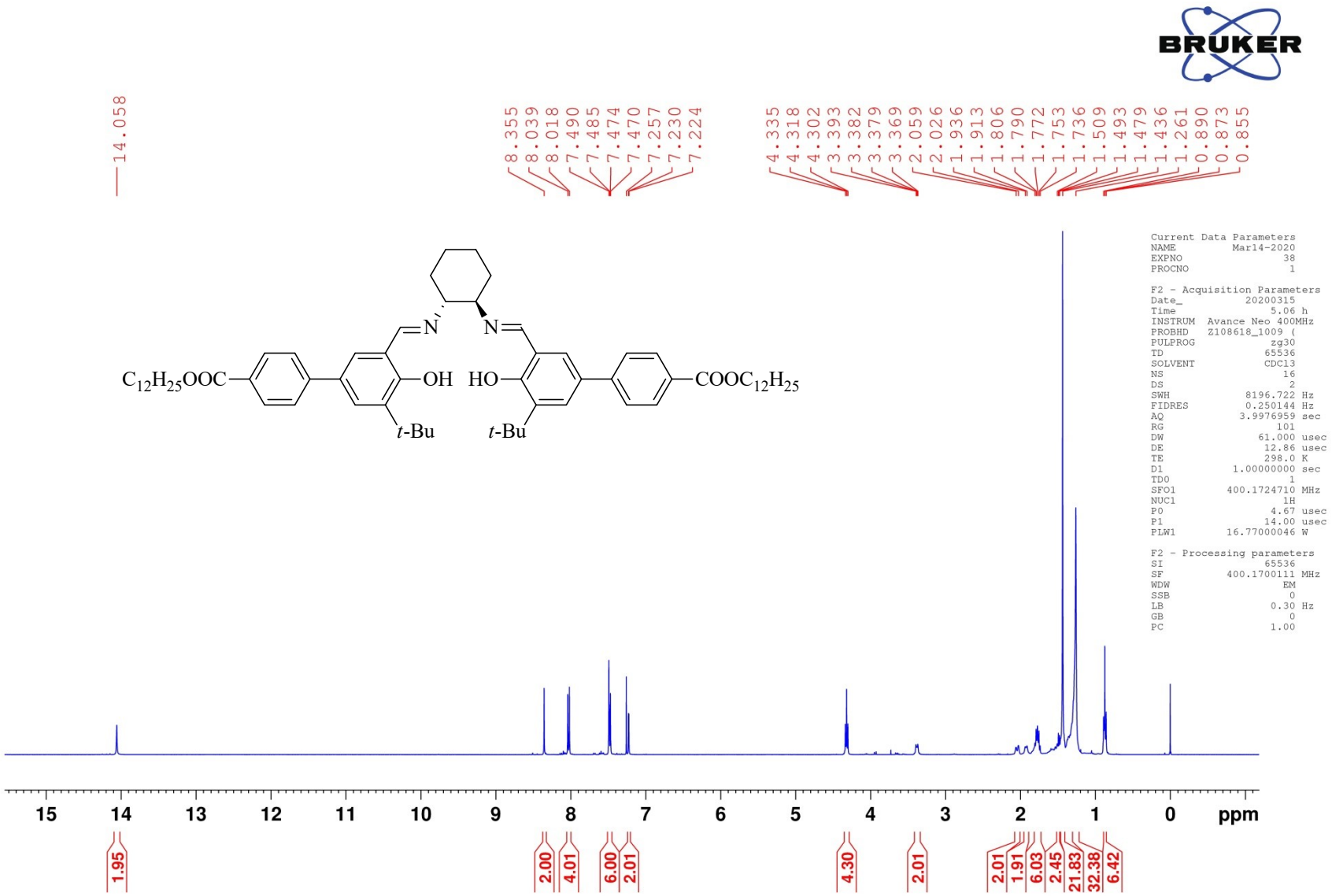
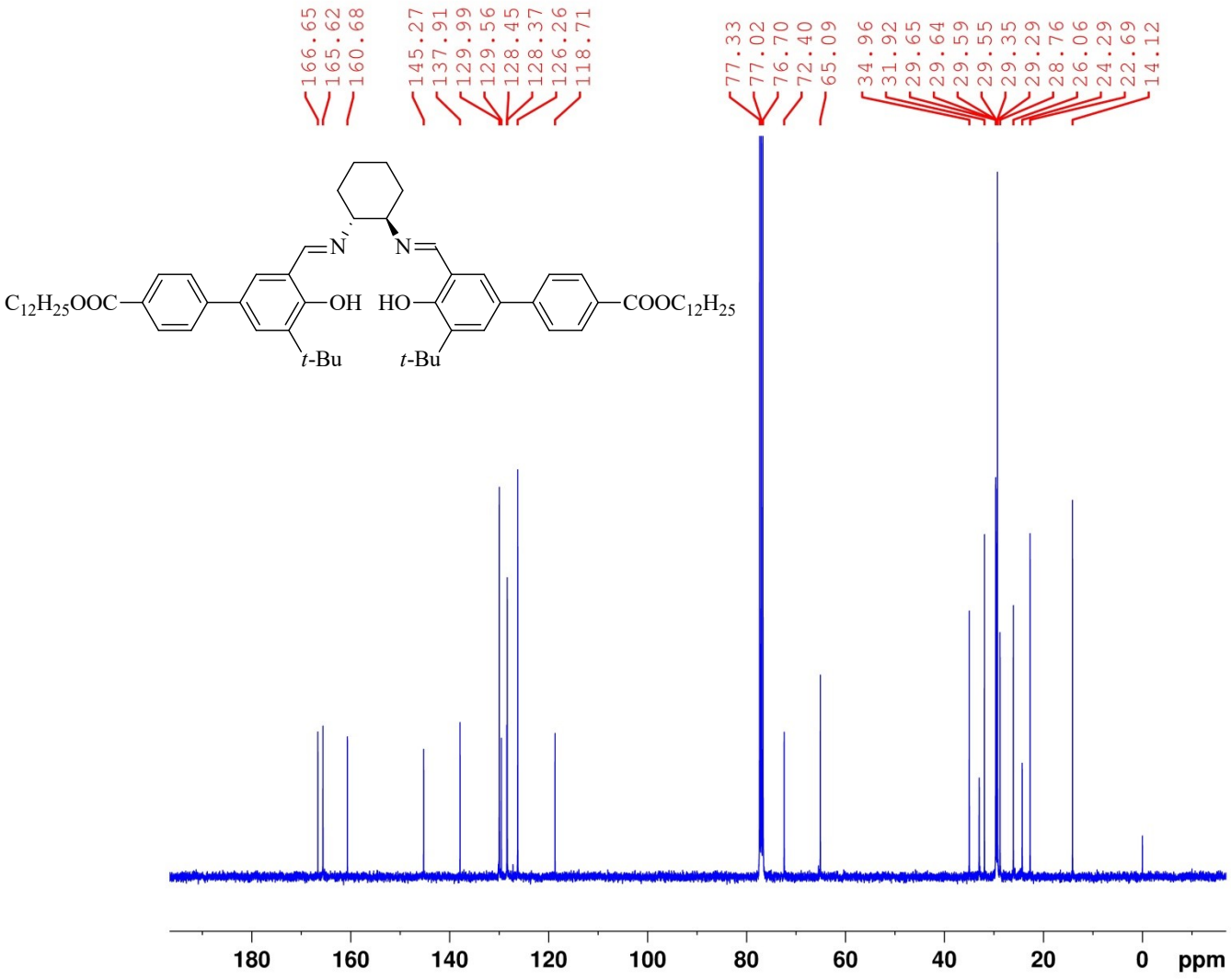
```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 43
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time              14.06 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228276 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


14.058
8.352
8.040
8.019
7.489
7.484
7.469
7.258
7.227
7.221
4.339
4.322
4.305
3.393
3.379
3.368
2.060
2.028
1.937
1.913
1.816
1.799
1.781
1.763
1.746
1.534
1.509
1.493
1.436
1.422
1.419
0.954
BRUKER
C5H11OOC
OH
HO
COOC5H11
t-Bu
t-Bu
Current Data Parameters
NAME Mar14-2020
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200315
Time 8.07 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W
F2 - Processing parameters
SI 65536
SF 400.1700108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.96
2.00
4.05
6.15
2.06
4.17
2.01
2.08
2.25
6.29
2.21
26.26
6.33



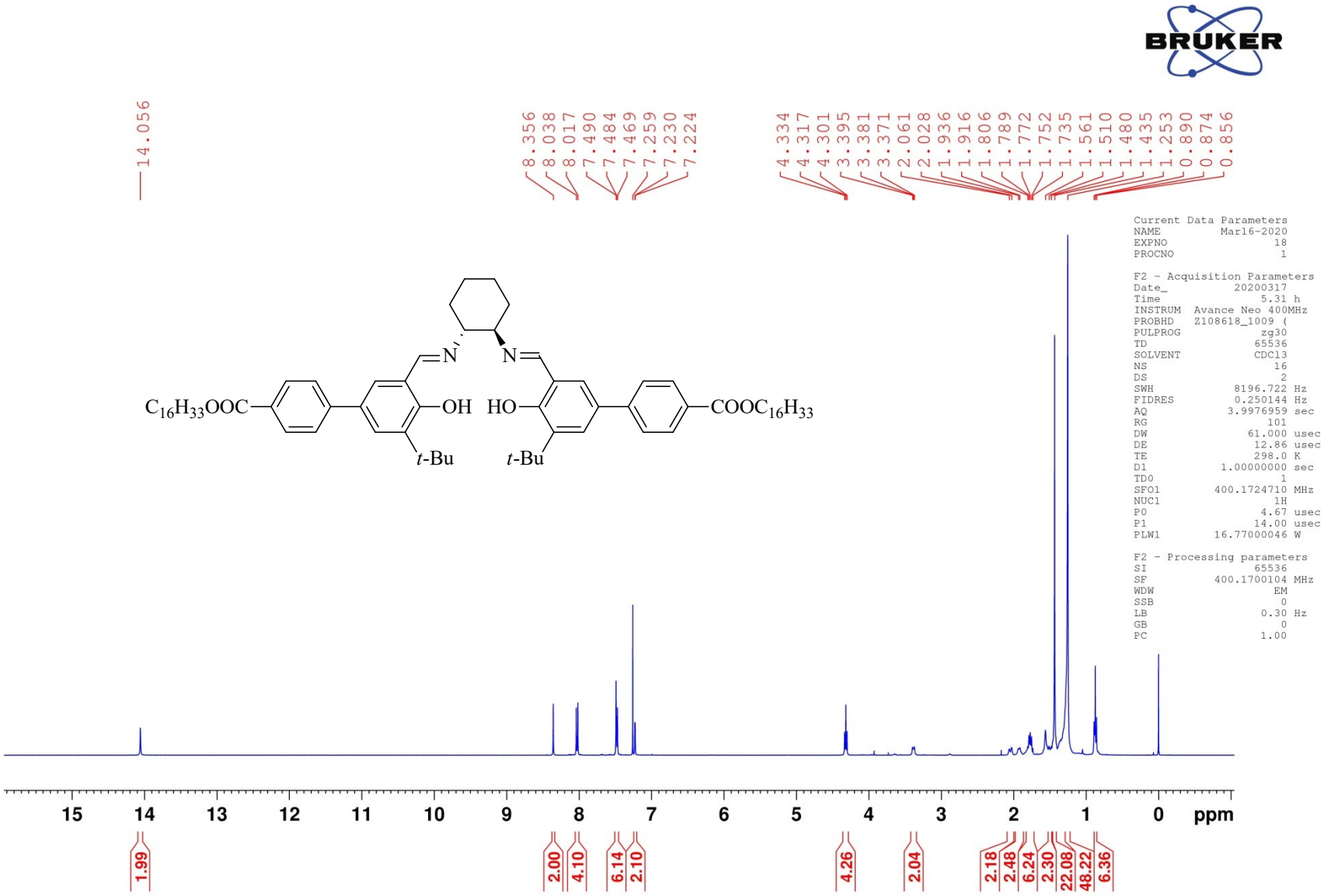

```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 41
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time              11.04 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228275 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

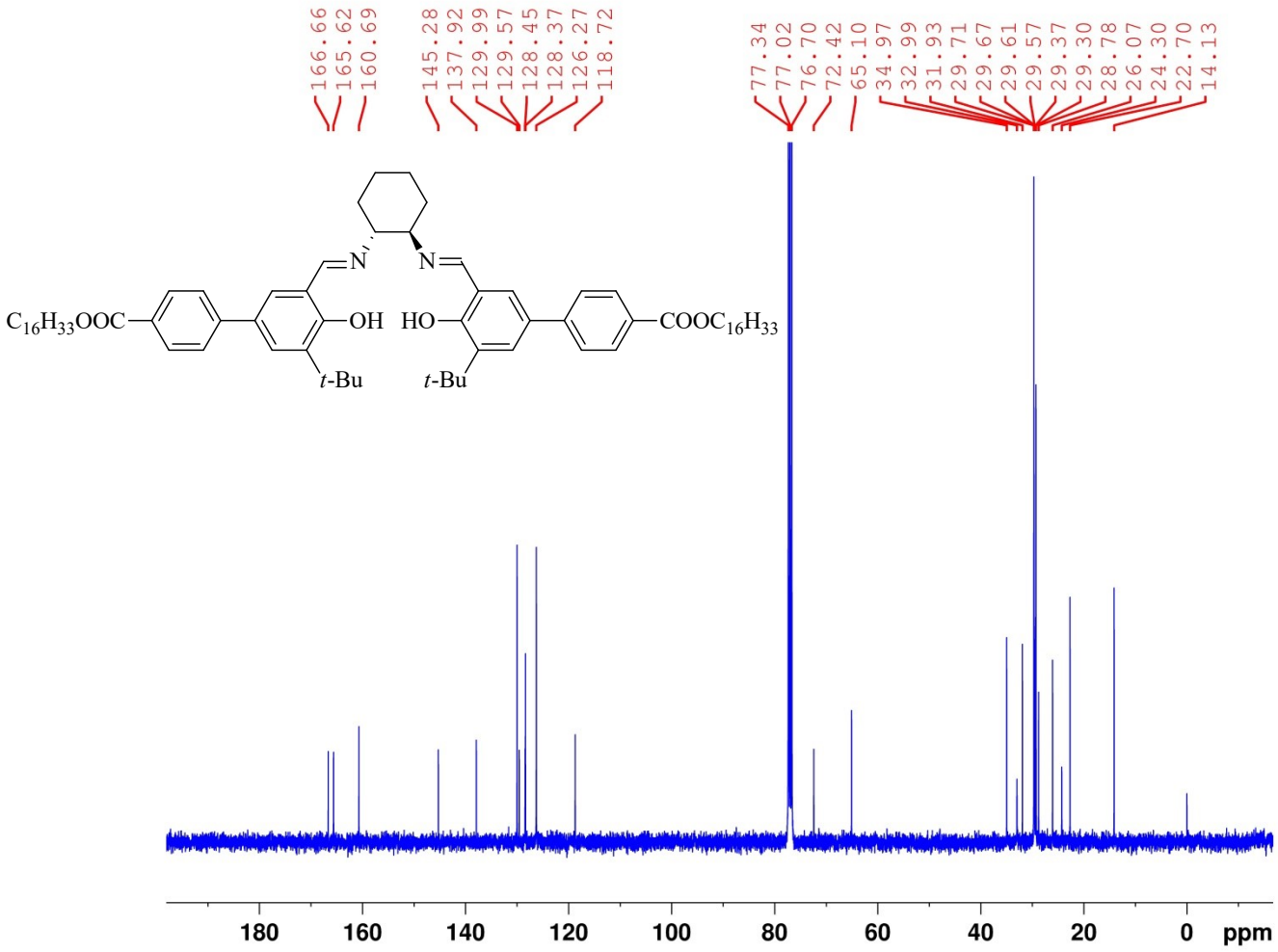

14.058
8.355
8.039
8.018
7.490
7.485
7.474
7.470
7.257
7.230
7.224
4.335
4.318
4.302
3.393
3.382
3.379
3.369
2.059
2.026
1.936
1.913
1.806
1.790
1.772
1.753
1.736
1.509
1.493
1.479
1.436
1.261
0.890
0.873
0.855
C12H25OOC
OH
HO
COOC12H25
t-Bu
t-Bu
Current Data Parameters
NAME Mar14-2020
EXPNO 38
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200315
Time 5.06 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W
F2 - Processing parameters
SI 65536
SF 400.1700111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.95
2.00
4.01
6.00
2.01
4.30
2.01
2.01
1.91
6.03
2.45
21.83
32.38
6.42



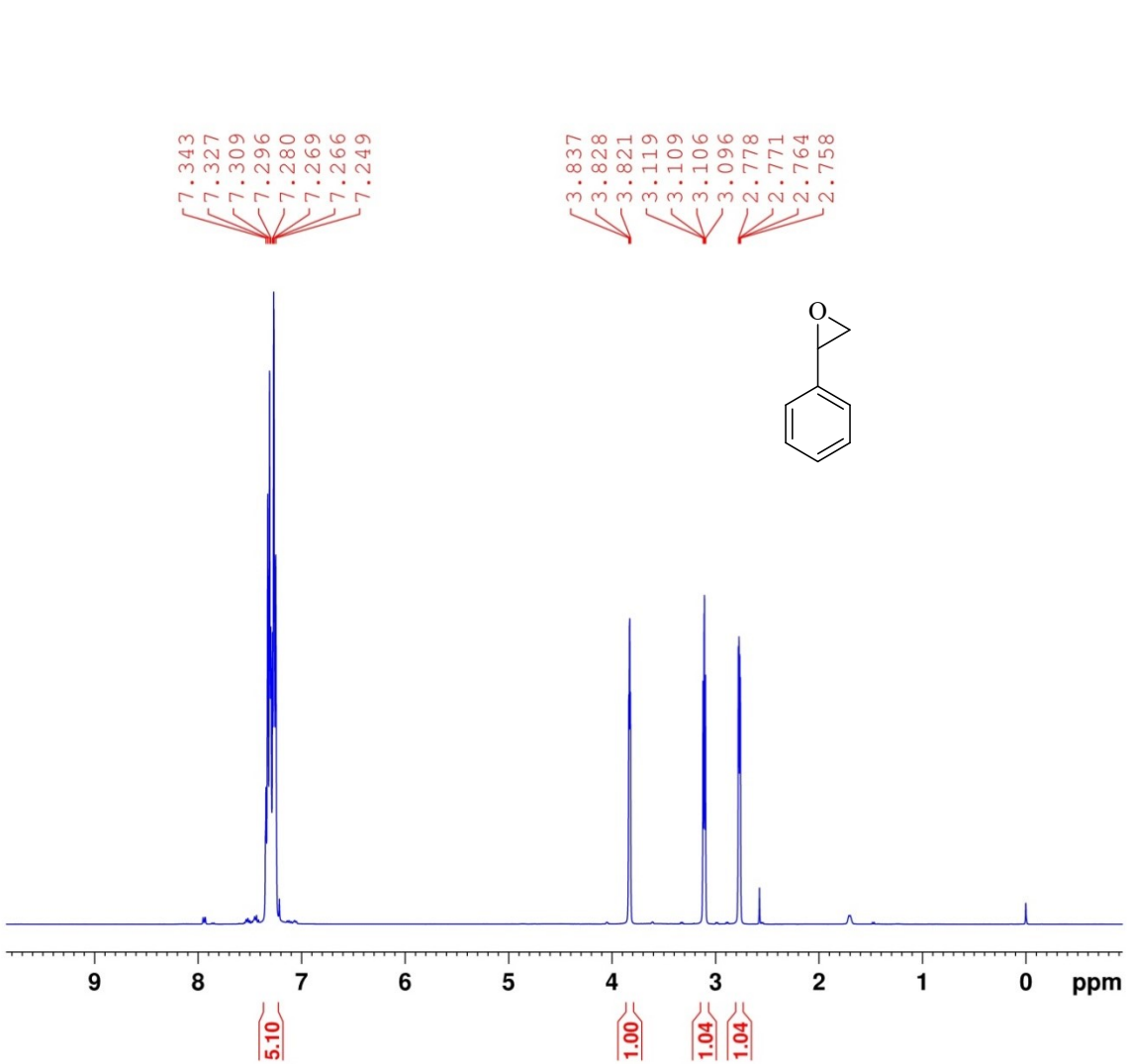
BRUKER

```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 39
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200315
Time                8.03 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                 32768
SF           100.6228276 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


14.056
8.356
8.038
8.017
7.490
7.484
7.469
7.259
7.230
7.224
4.334
4.317
4.301
3.395
3.381
3.371
2.061
2.028
1.936
1.916
1.806
1.789
1.772
1.752
1.735
1.561
1.510
1.480
1.435
1.253
0.890
0.874
0.856
C16H33OOC
OH
HO
COOC16H33
t-Bu
t-Bu
N
N
Current Data Parameters
NAME Mar16-2020
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200317
Time 5.31 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W
F2 - Processing parameters
SI 65536
SF 400.1700104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.00
4.10
6.14
2.10
4.26
2.04
2.18
2.48
6.24
2.30
22.08
48.22
6.36



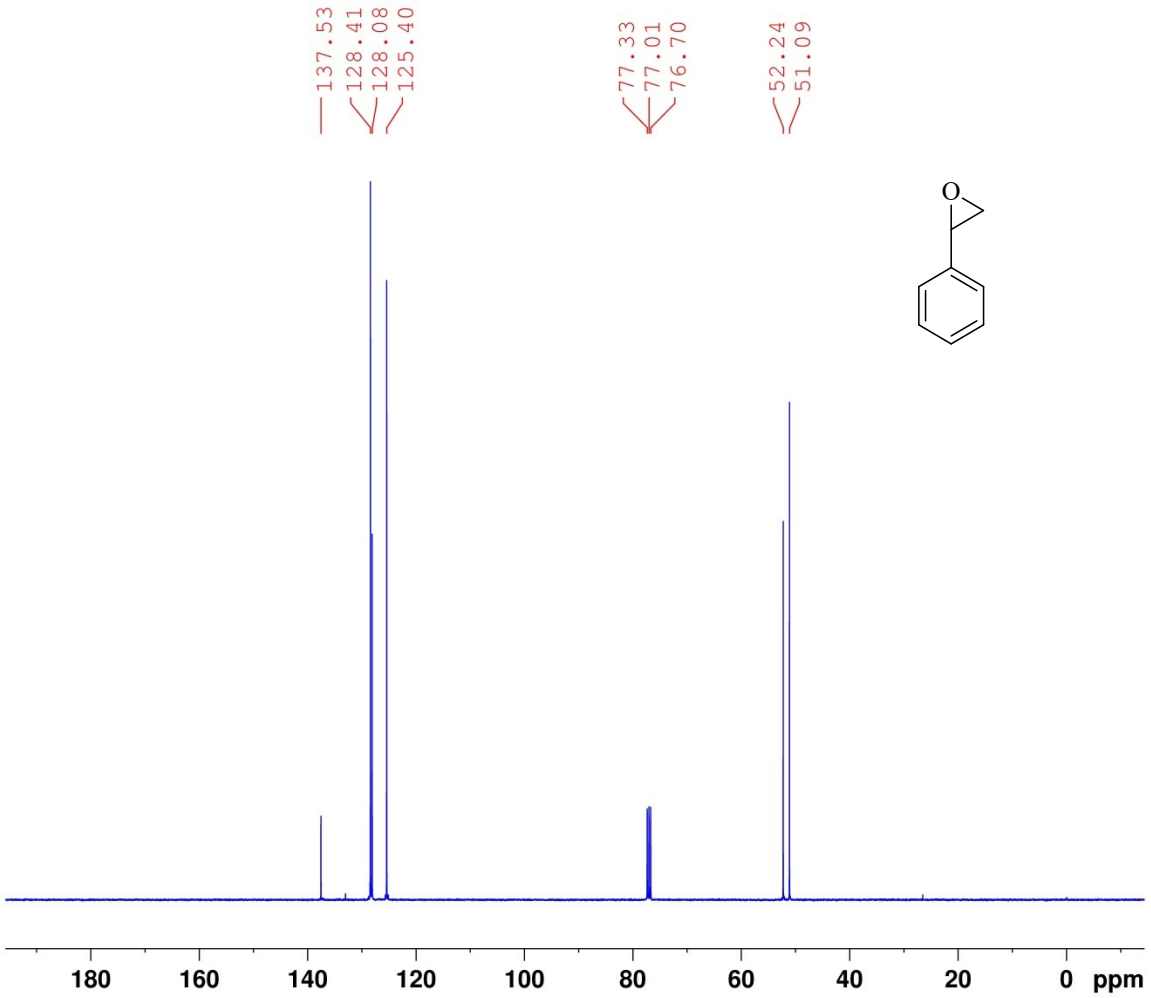

```
Current Data Parameters
NAME          Mar16-2020
EXPNO                 19
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200317
Time                7.30 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



Current Data Parameters
NAME Dec23-2020-nmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201223
Time 14.44 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 80
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W

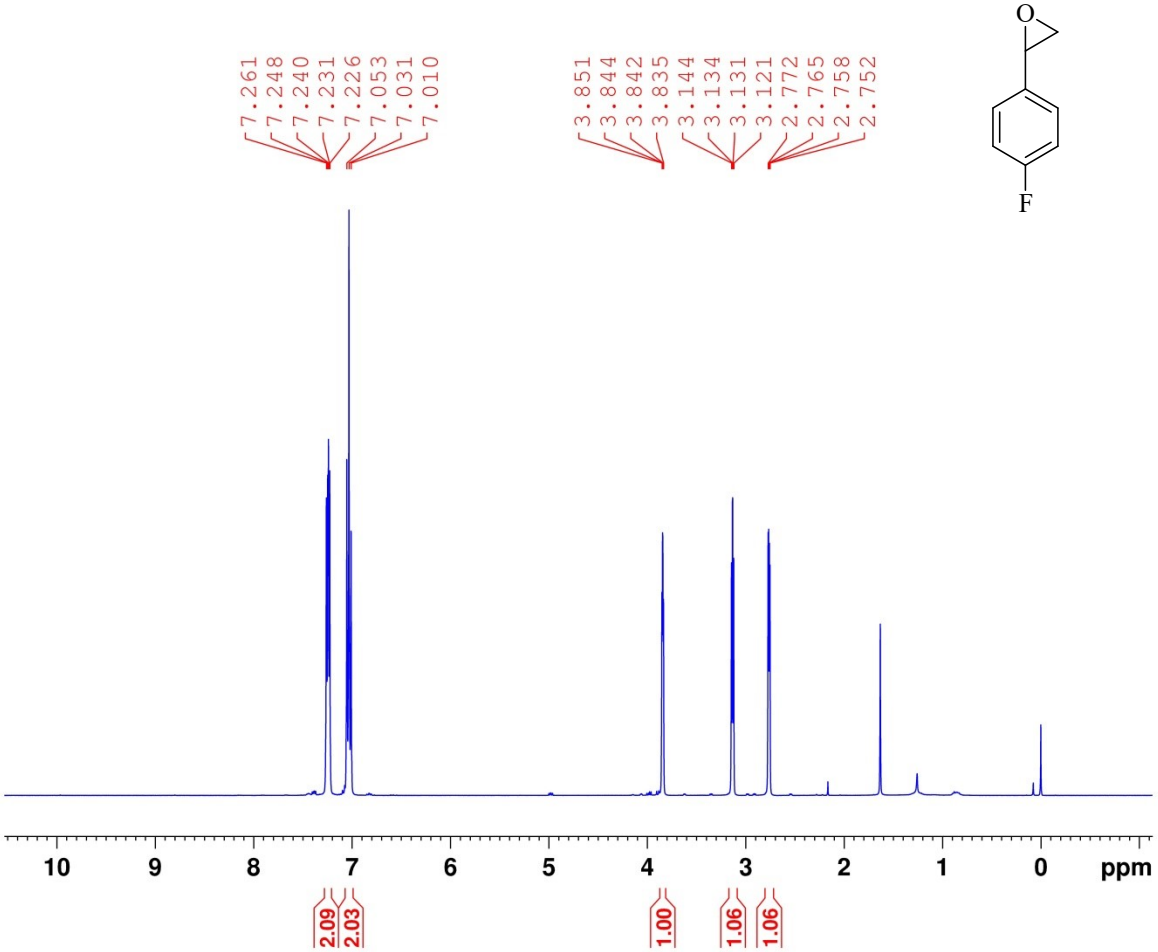
F2 - Processing parameters
SI 65536
SF 400.1700282 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



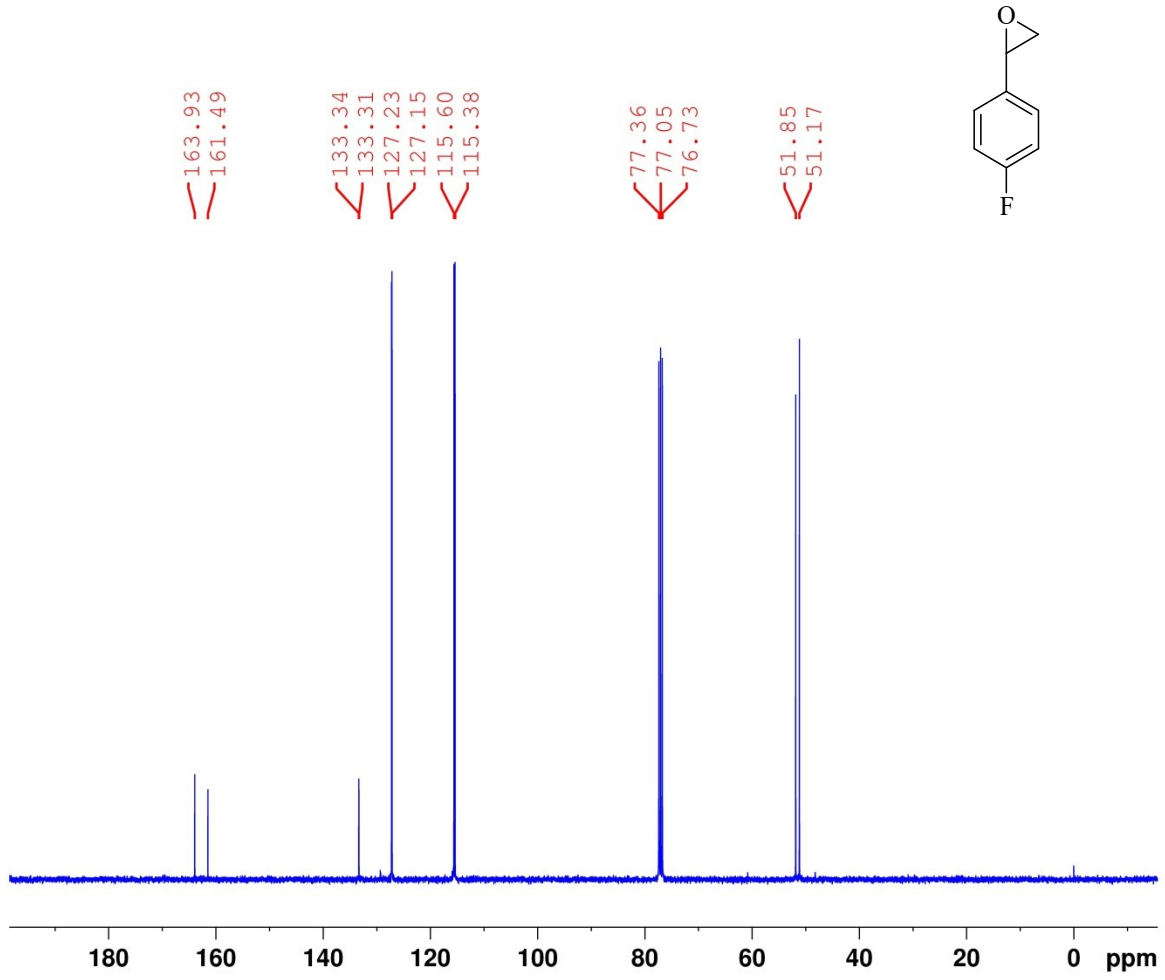
Current Data Parameters
NAME Dec23-2020-nmr
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201223
Time 15.44 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 60.89300156 W
SFO2 400.1716007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 16.77000046 W
PLW12 0.40580001 W
PLW13 0.20411000 W

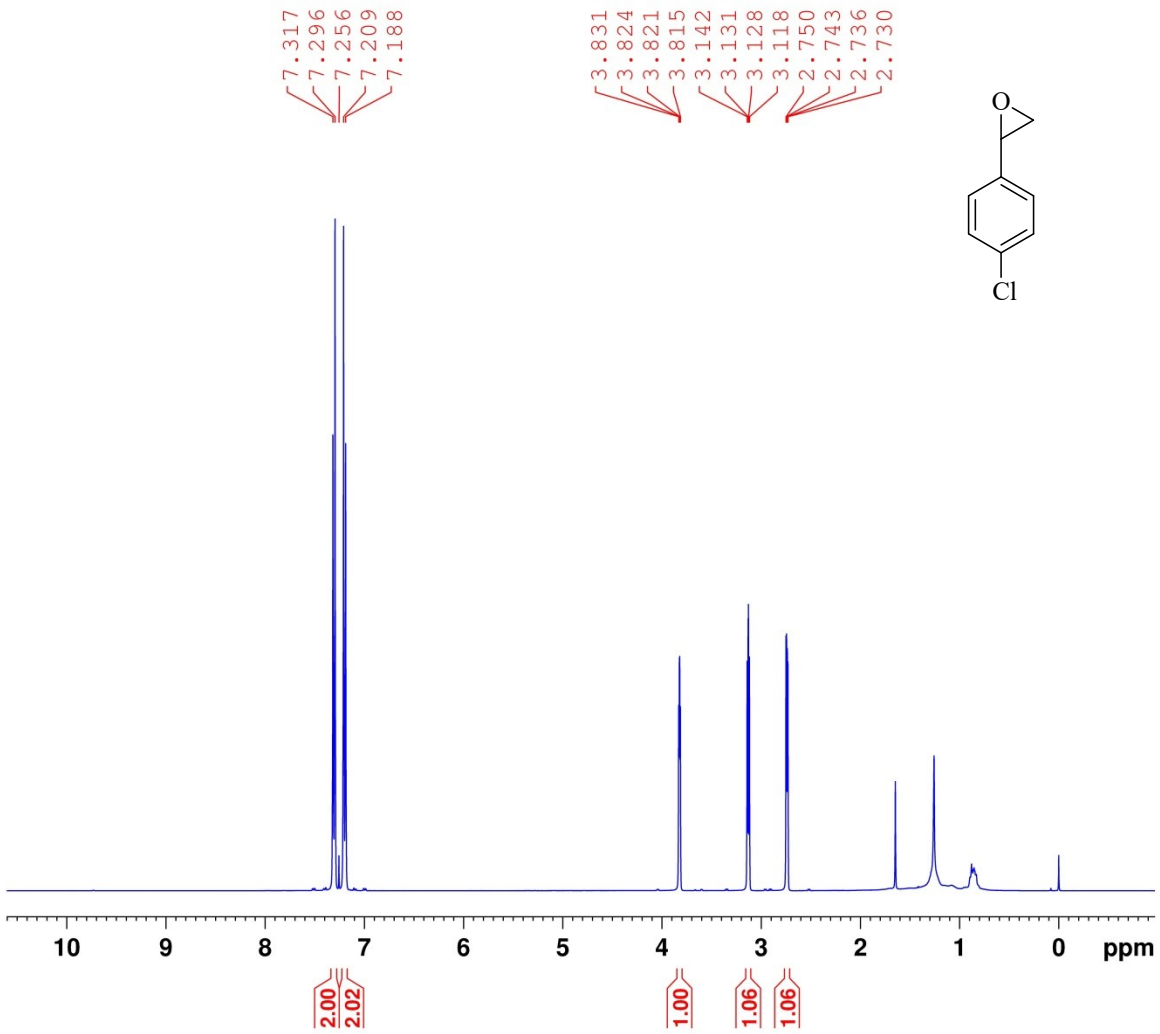
F2 - Processing parameters
SI 32768
SF 100.6228404 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME      Oct09-2020-nmr
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201009
Time              18.07 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                 12.86 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700102 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

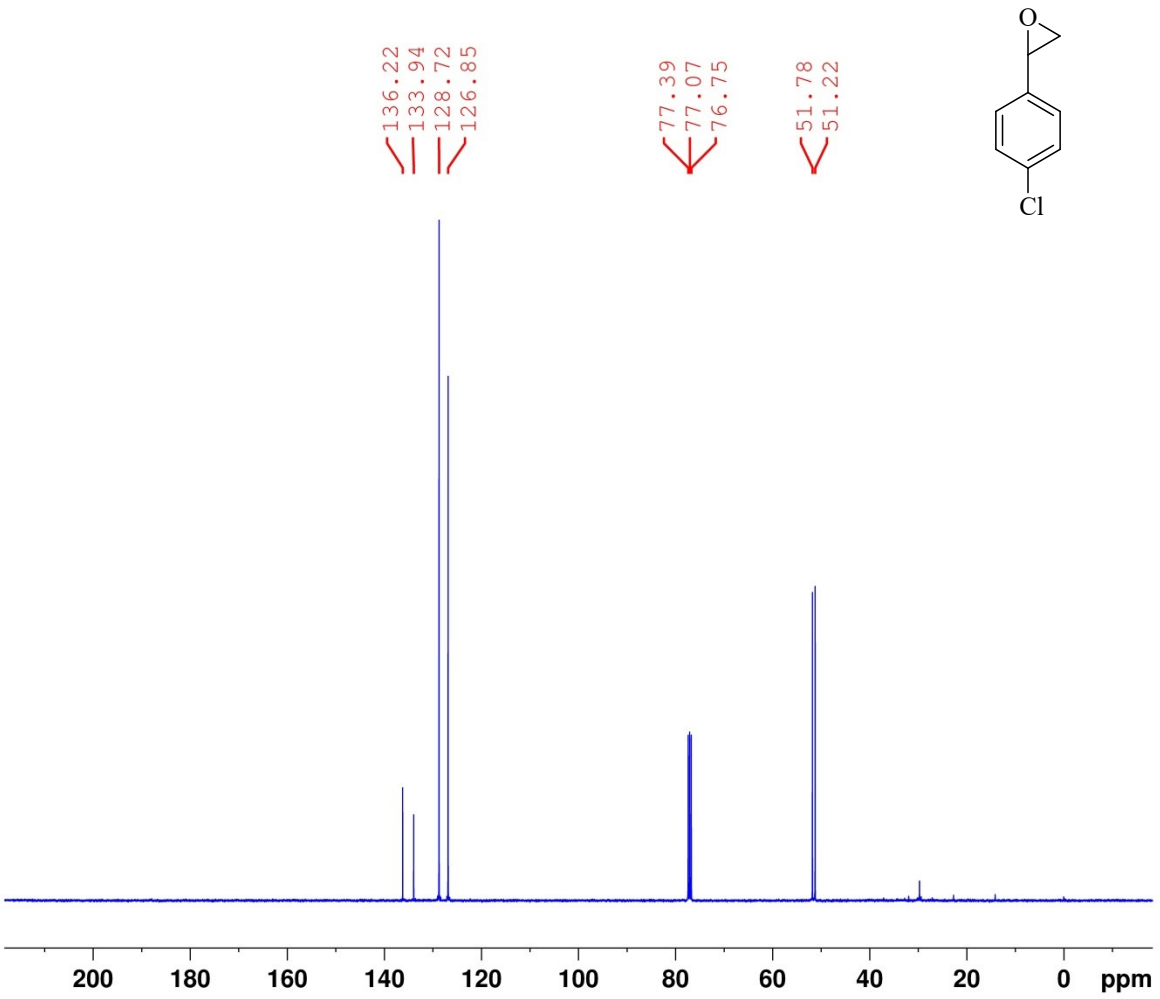



```
Current Data Parameters
NAME      Oct09-2020-nmr
EXPNO                 51
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201010
Time                12.08 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                 EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

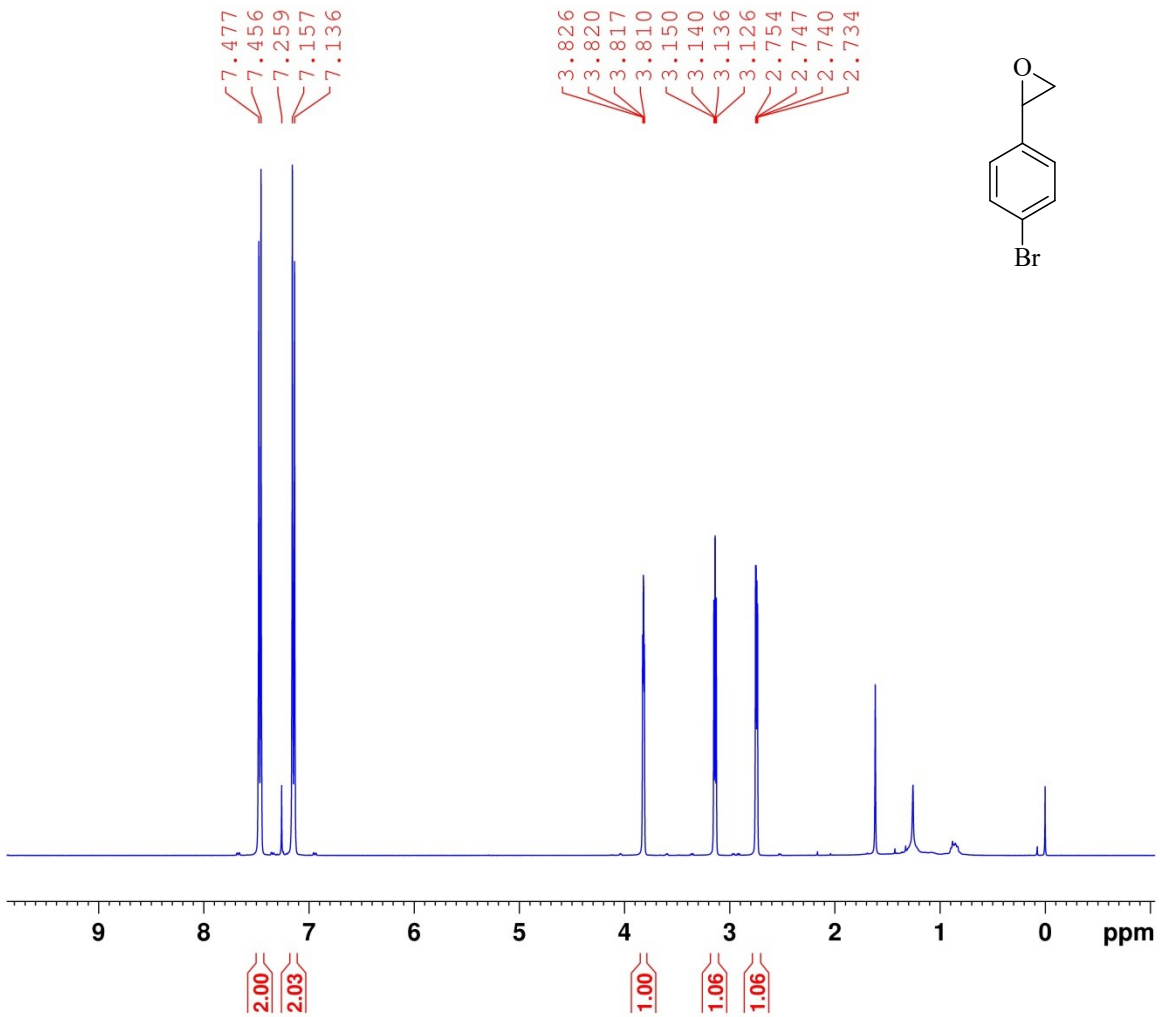


BRUKER

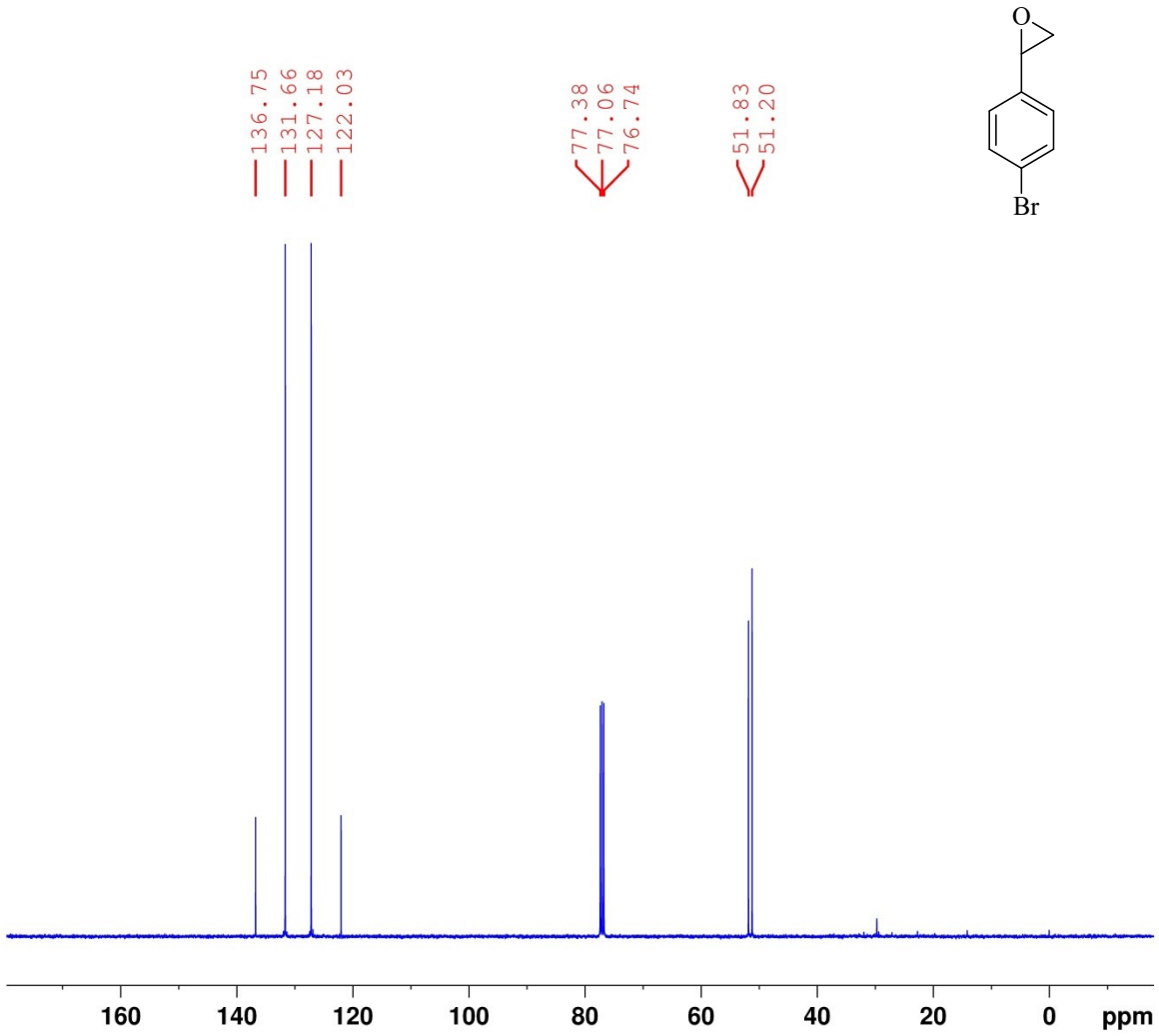
```
Current Data Parameters
NAME      Jul27-2020-nmr
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200727
Time                14.00 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700114 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      Jul27-2020-nmr
EXPNO                17
PROCNO                1

F2 - Acquisition Parameters
Date_          20200727
Time              15.12 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

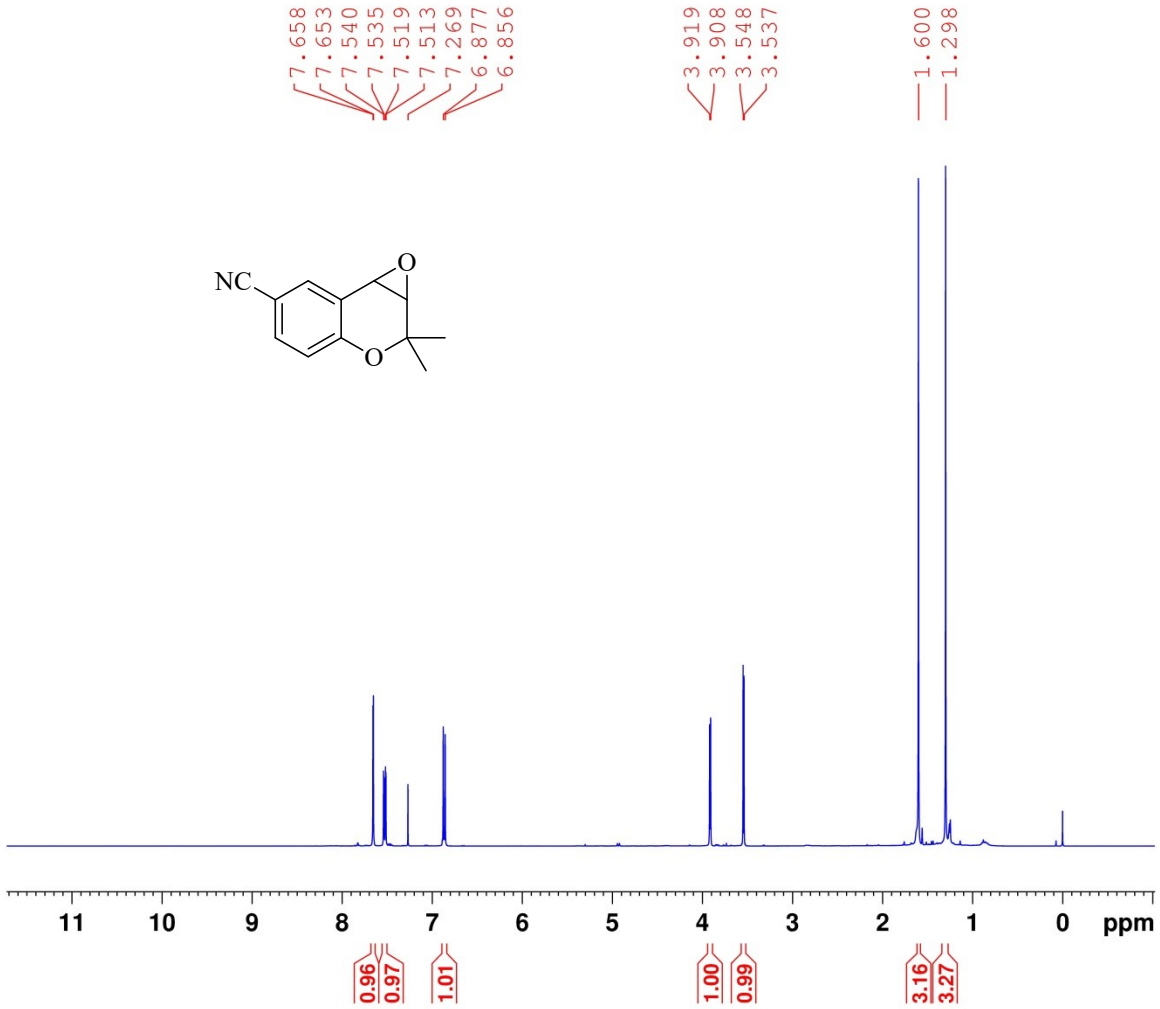



```
Current Data Parameters
NAME      Jul23-2020-nmr
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200723
Time              12.49 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI                 65536
SF          400.1700101 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



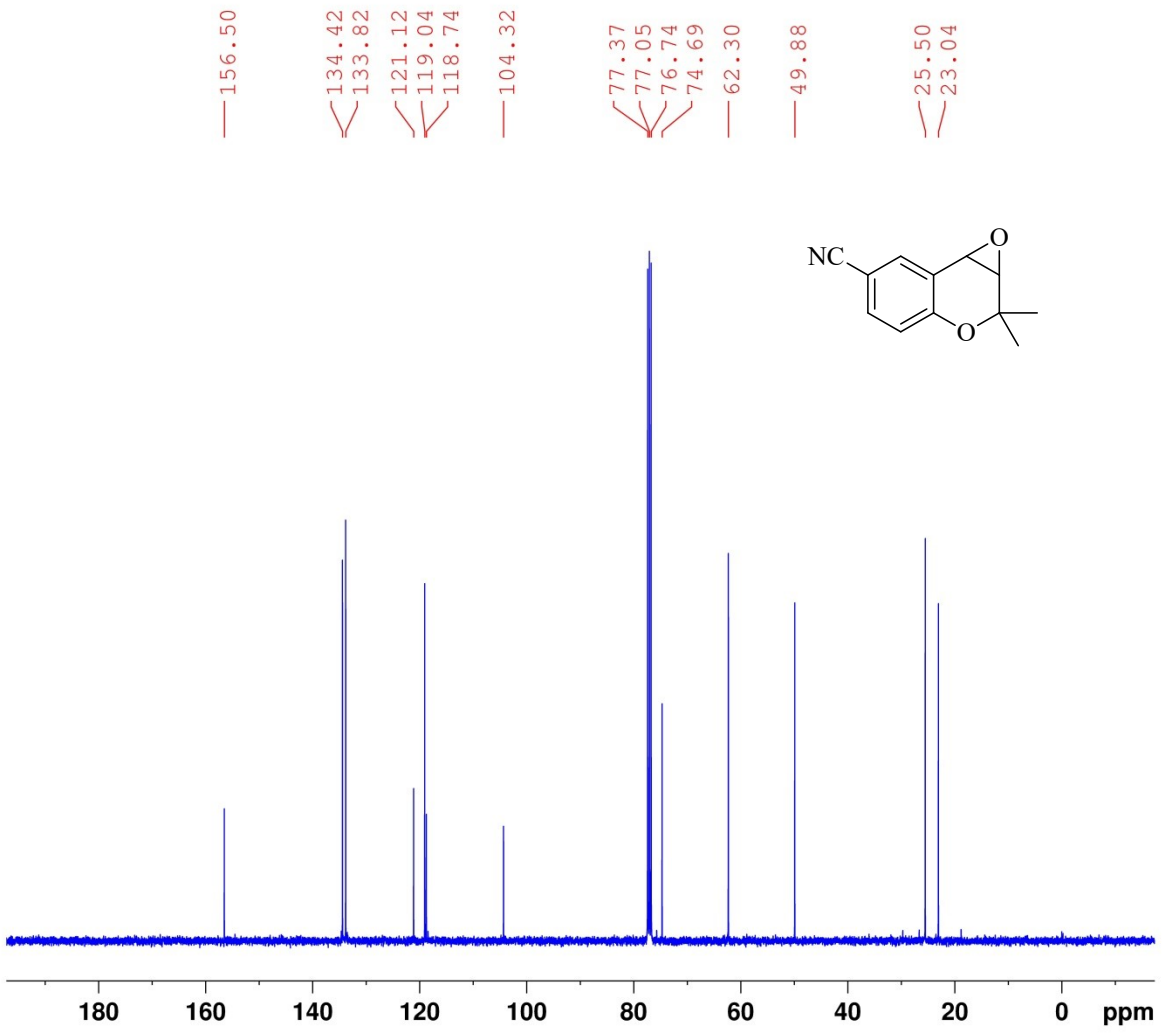
BRUKER

```
Current Data Parameters
NAME      Jul27-2020-nmr
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20200727
Time               15.45 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

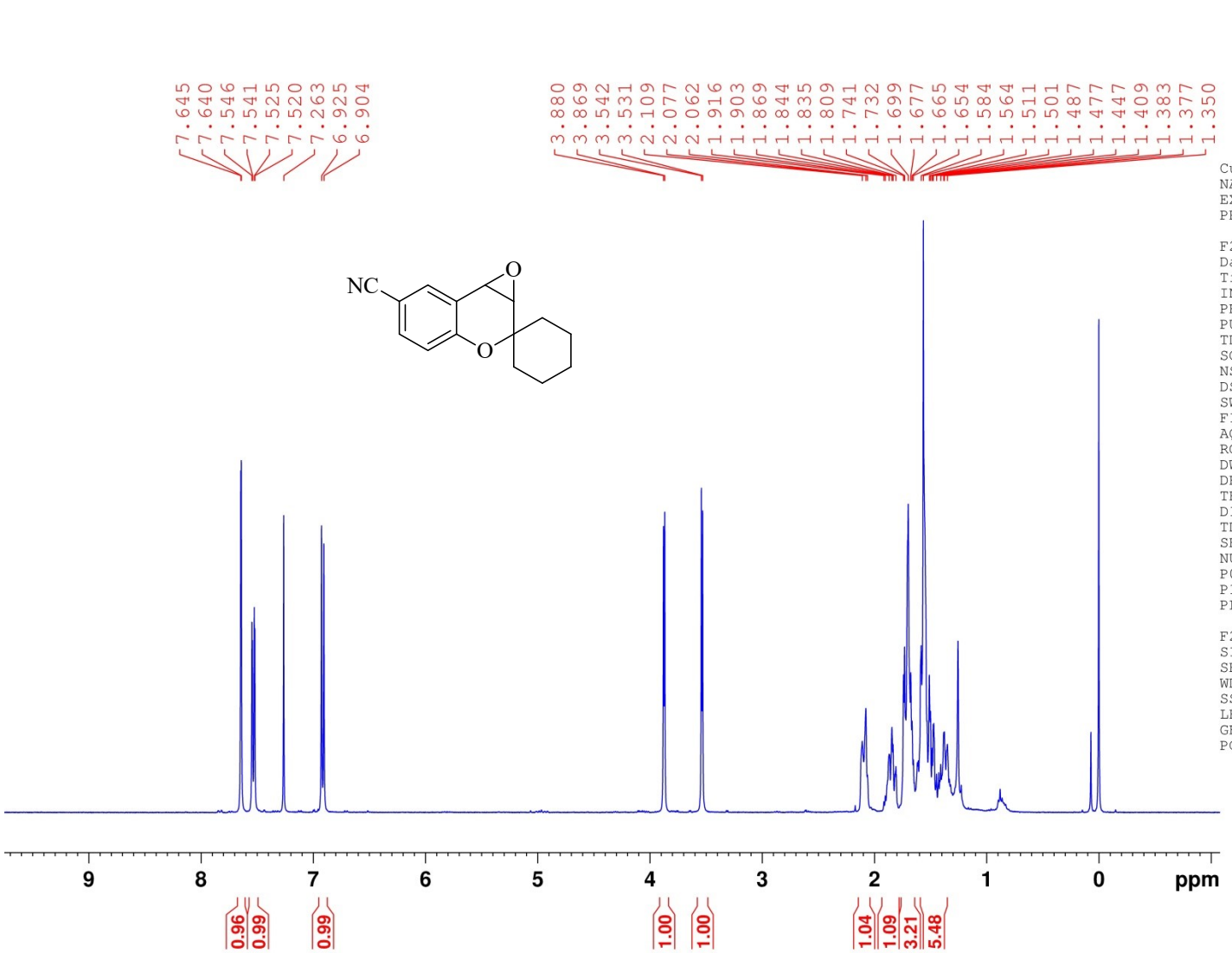


BRUKER

```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200314
Time              18.04 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700065 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

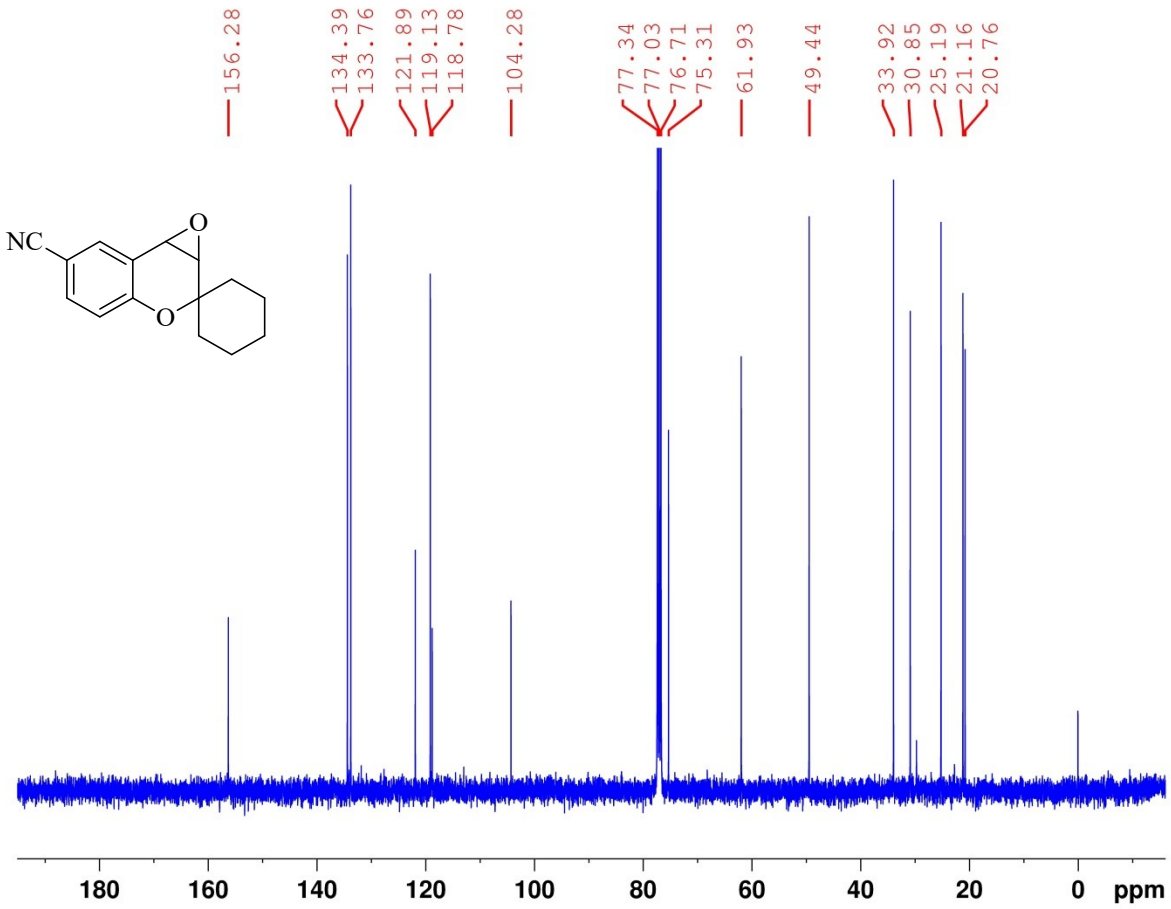



```
Current Data Parameters
NAME          Mar14-2020
EXPNO                 23
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200314
Time                18.35 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             1.3762560 sec
RG                    101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         100.6328888 MHz
NUC1                 13C
P0                  3.33 usec
P1                 10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                 1H
CPDPRG[2          waltz65
PCPD2              90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                  32768
SF           100.6228265 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

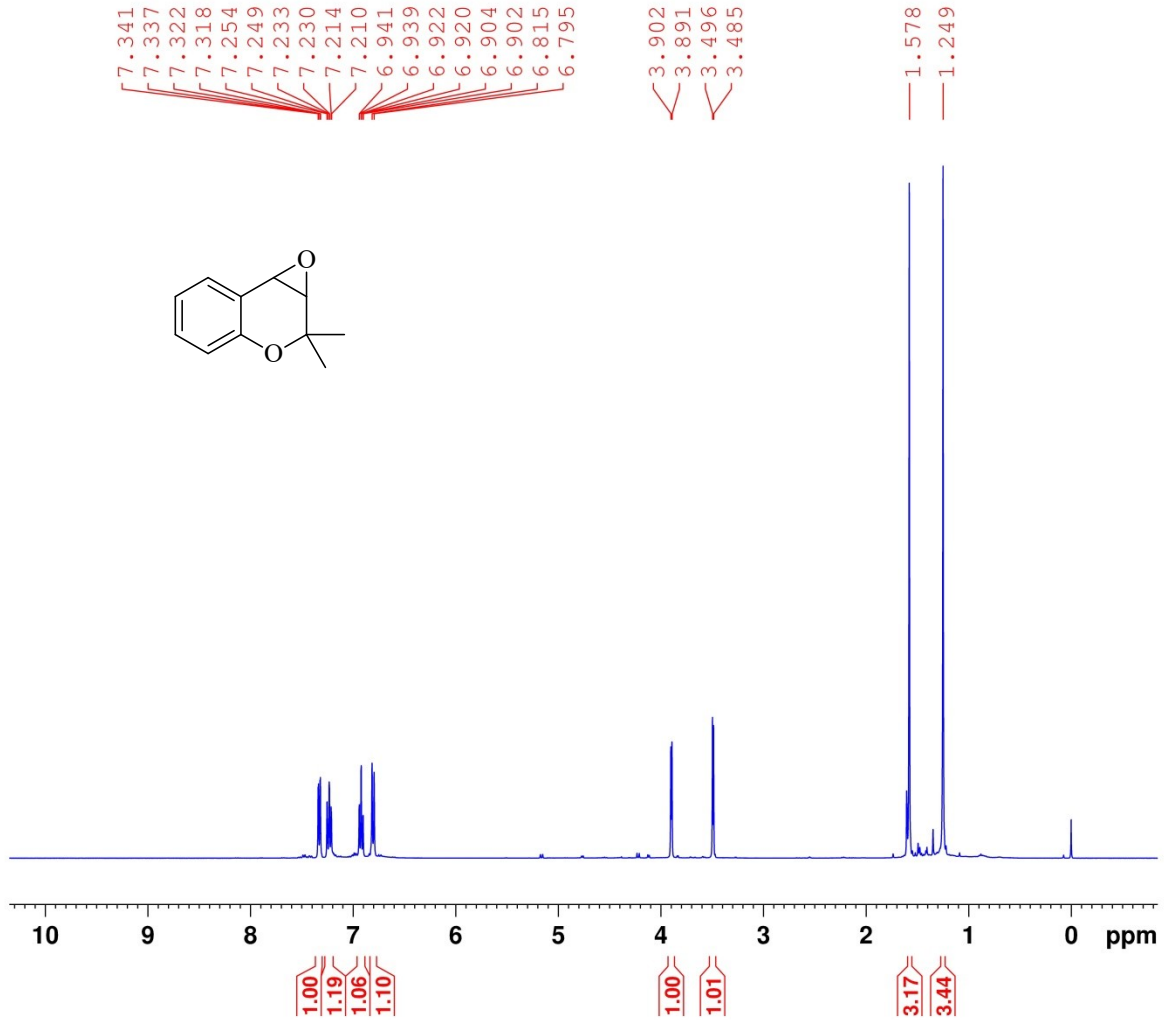


BRUKER

```
Current Data Parameters
NAME      Oct28-2020-nmr
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201028
Time              17.41 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1          16.77000046 W

F2 - Processing parameters
SI                 65536
SF            400.1700088 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



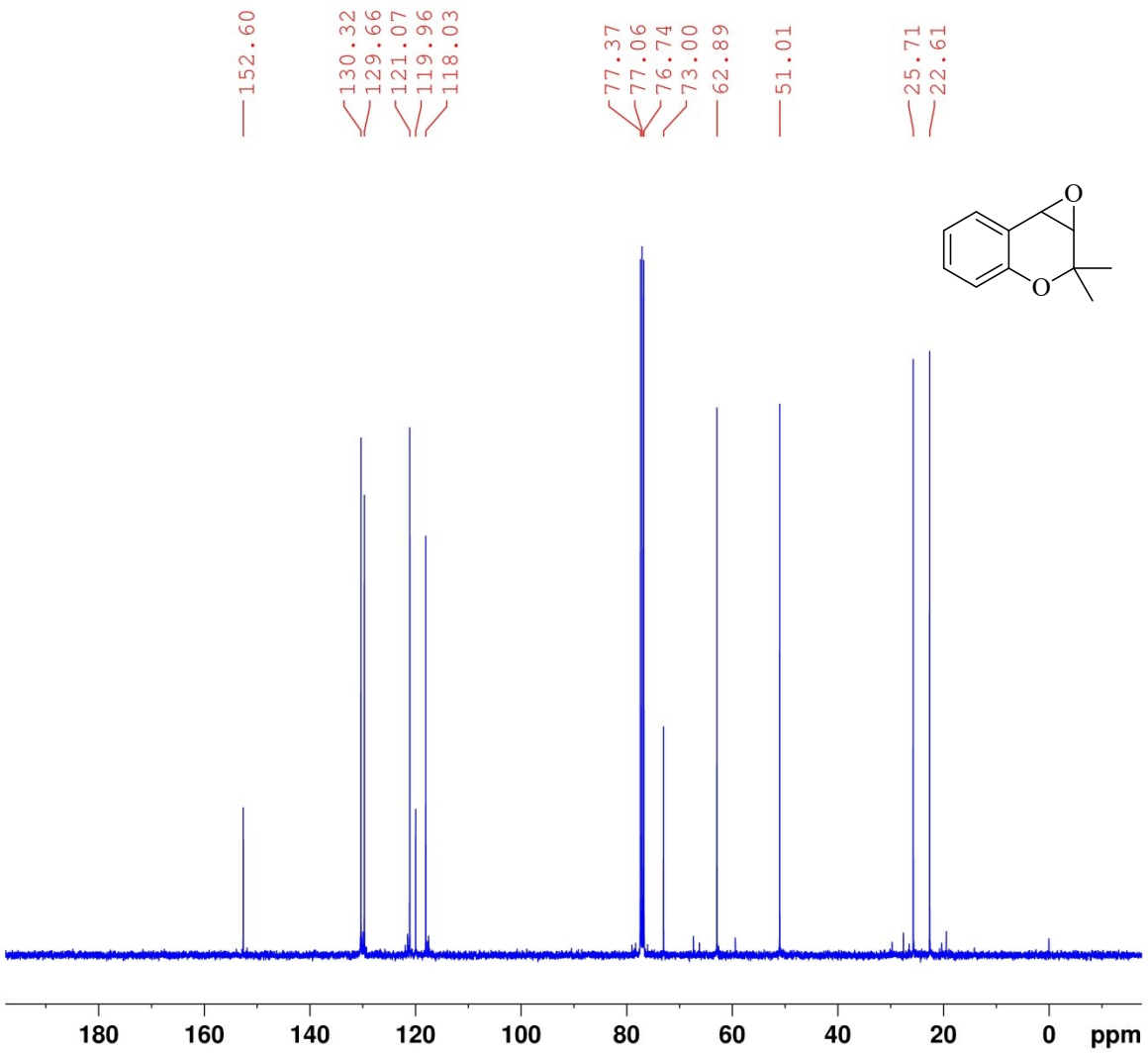

```
Current Data Parameters
NAME      Oct28-2020-nmr
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201028
Time               18.49 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW             21.000 usec
DE              6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2        waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



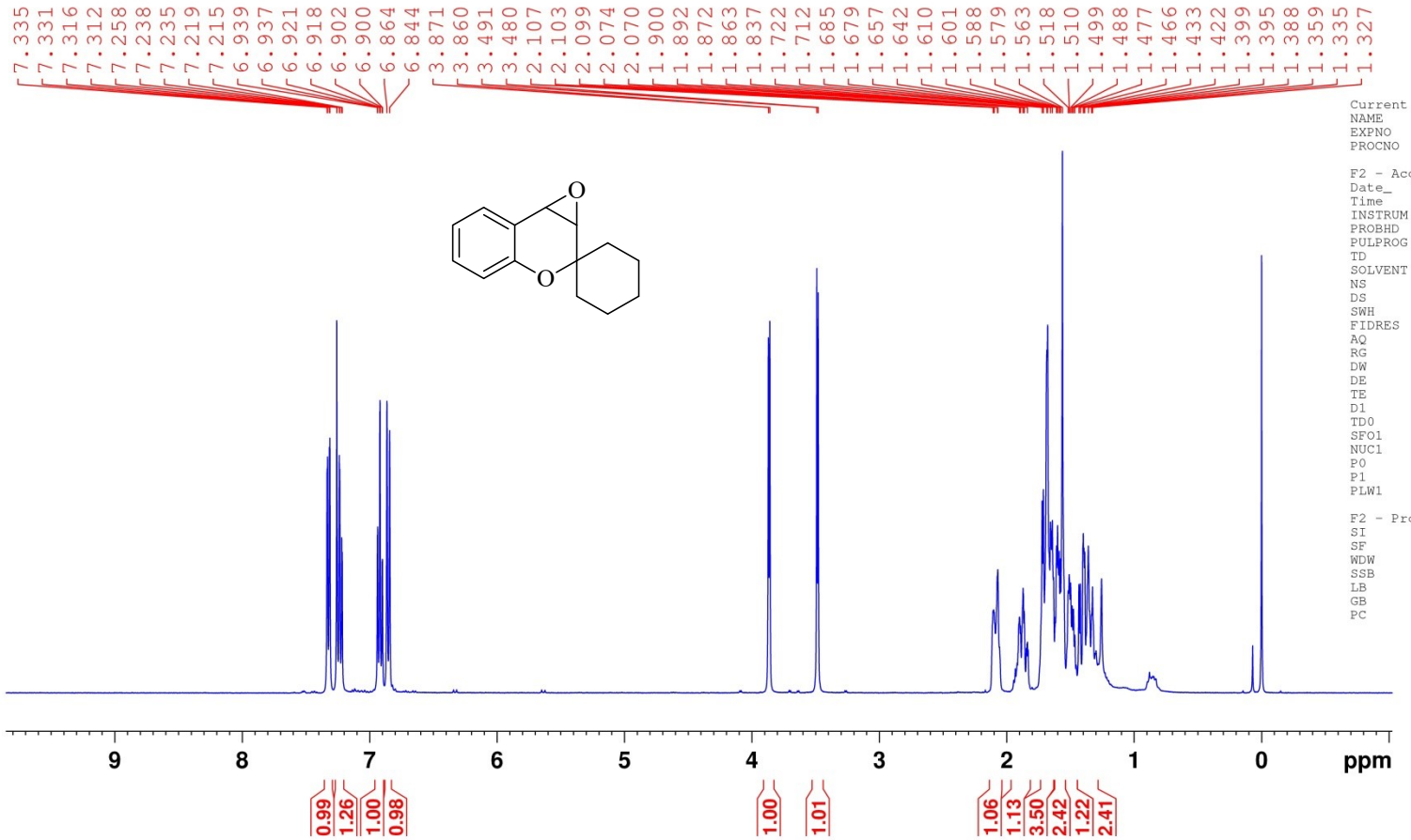
Current Data Parameters
NAME Oct31-2020-nmr
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201031
Time 11.47 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W

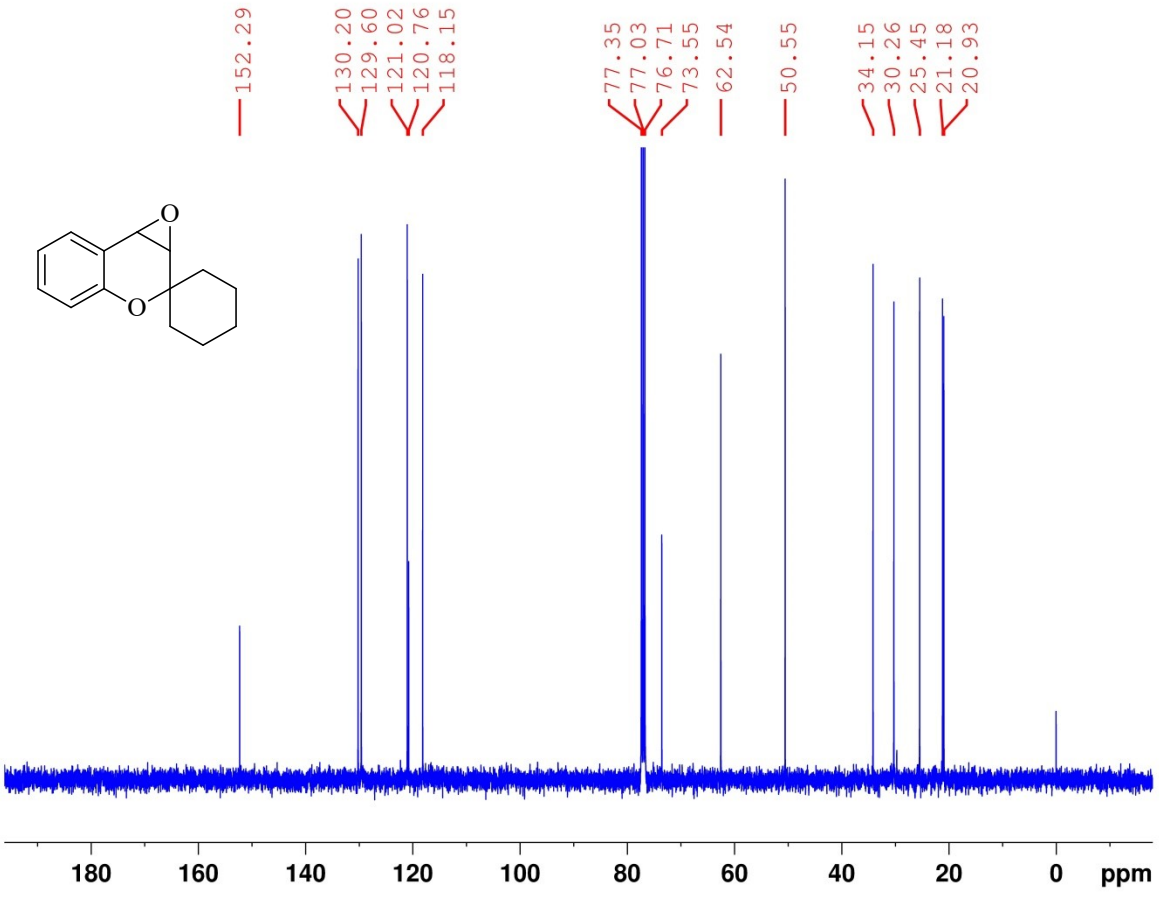
F2 - Processing parameters
SI 65536
SF 400.1700120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME      Oct31-2020-nmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201031
Time                13.15 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                 32768
SF          100.6228265 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME      Sep15-2020-nmr
EXPNO                 18
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200915
Time               13.01 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI                 65536
SF          400.1700107 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

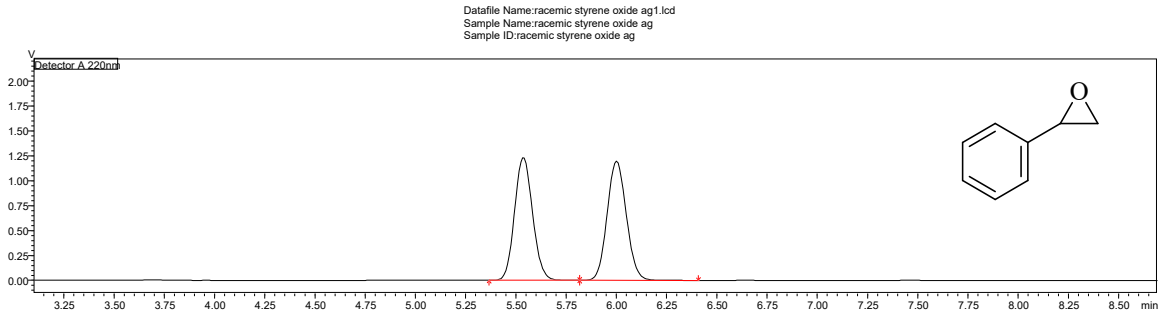



```
Current Data Parameters
NAME      Sep15-2020-nmr
EXPNO                19
PROCNO                1

F2 - Acquisition Parameters
Date_          20200915
Time               13.38 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

HPLC Chromatograms

Racemic-styrene oxide (11)

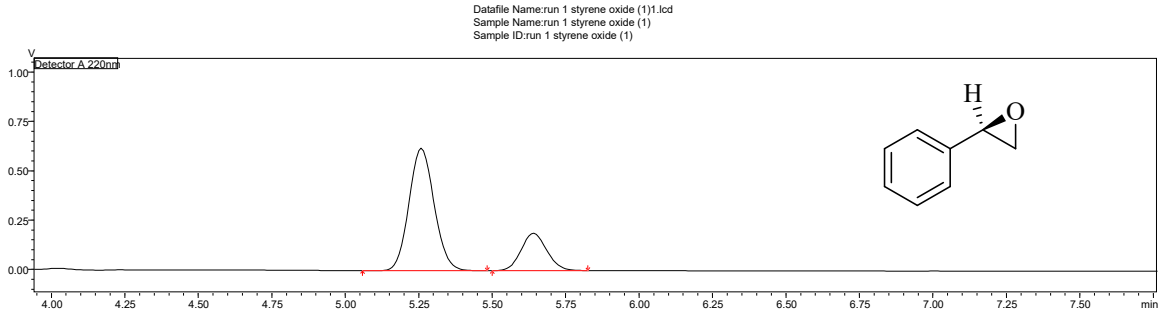
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.537	7722037	1231486	49.230	49.230
2	6.000	7963750	1197046	50.770	50.770
Total		15685787	2428532	100.000	100.000

Styrene oxide (11) with catalyst 1b after first run

HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.

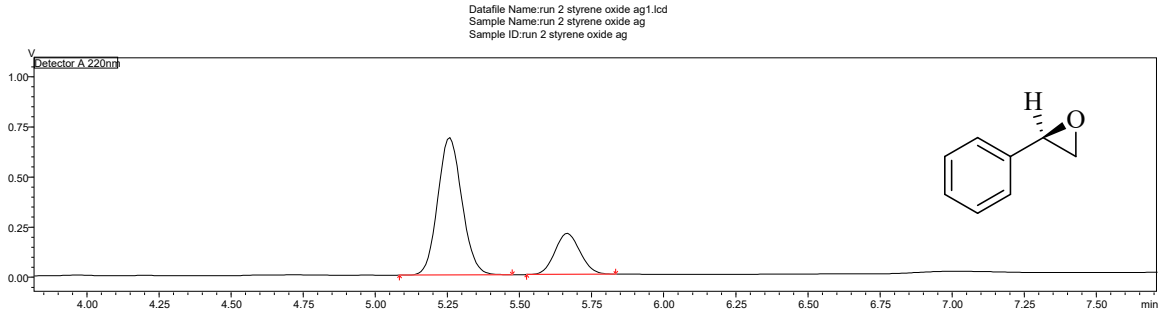


Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.258	3701242	621343	76.343	76.343

2	5.640	1146940	188724	23.657	23.657
Total		4848183	810067	100.000	100.000

Styrene oxide (11) with catalyst 1b after second run

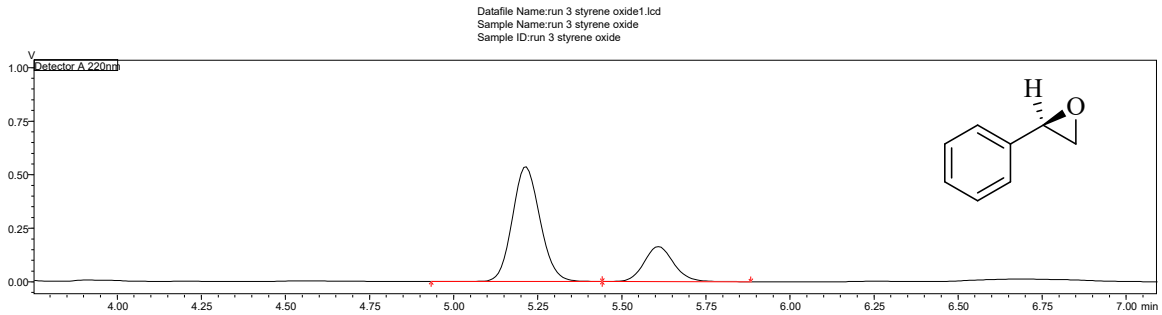
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.257	3990759	685240	76.308	76.308
2	5.664	1239077	203894	23.692	23.692
Total		5229837	889134	100.000	100.000

Styrene oxide (11) with catalyst 1b after third run

HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.

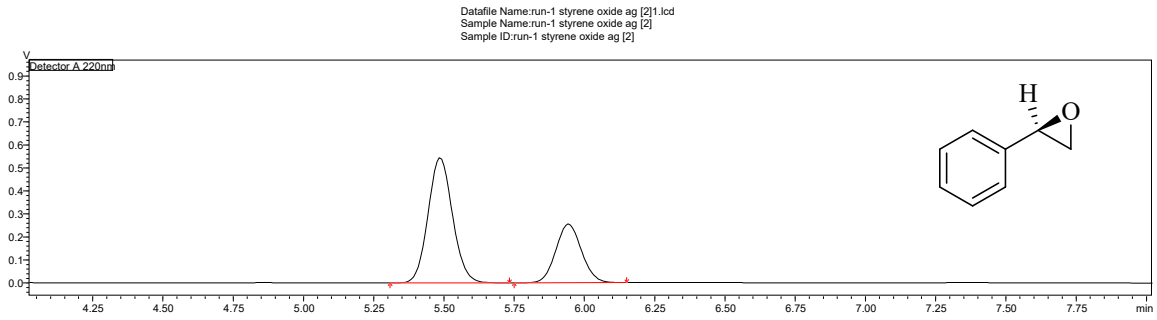


Peak	Ret. Time	Area	Height	Conc.	Area%

1	5.214	3087745	536158	75.451	75.451
2	5.608	1004633	163903	24.549	24.549
Total		4092378	700061	100.000	100.000

Styrene oxide (11) with catalyst 2b after first run

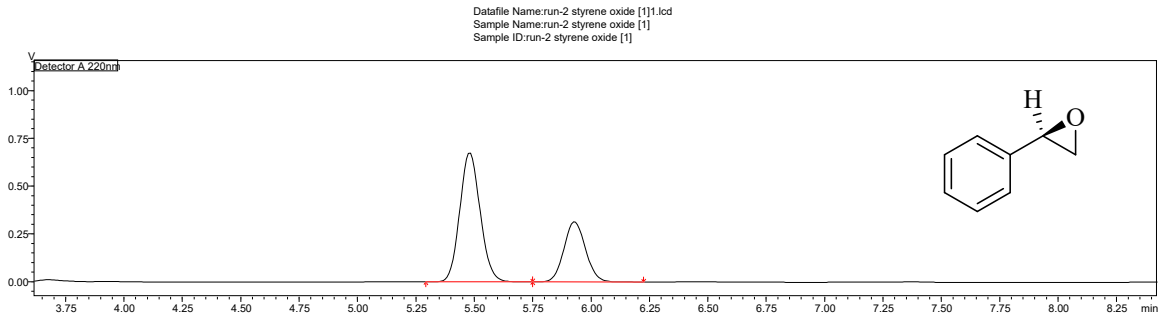
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.485	3302957	544350	67.047	67.047
2	5.942	1623391	255306	32.953	32.953
Total		4926348	799656	100.000	100.000

Styrene oxide (11) with catalyst 2b after second run

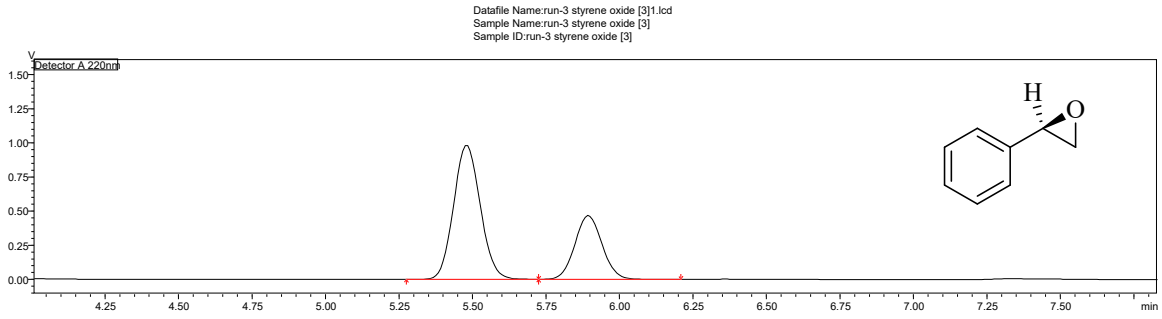
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.479	4120163	672948	67.019	67.019
2	5.929	2027631	314070	32.981	32.981
Total		6147794	987018	100.000	100.000

Styrene oxide (11) with catalyst 2b after third run

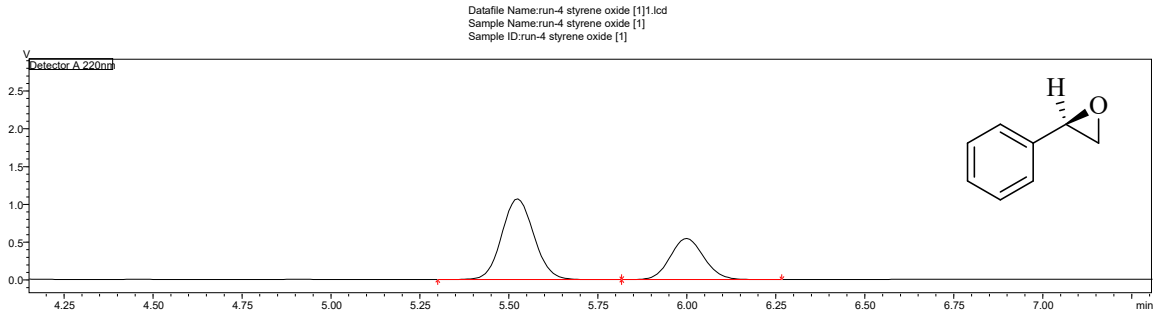
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.479	6222633	979815	67.286	67.286
2	5.893	3025373	468013	32.714	32.714
Total		9248007	1447829	100.000	100.000

Styrene oxide (11) with catalyst 2b after fourth run

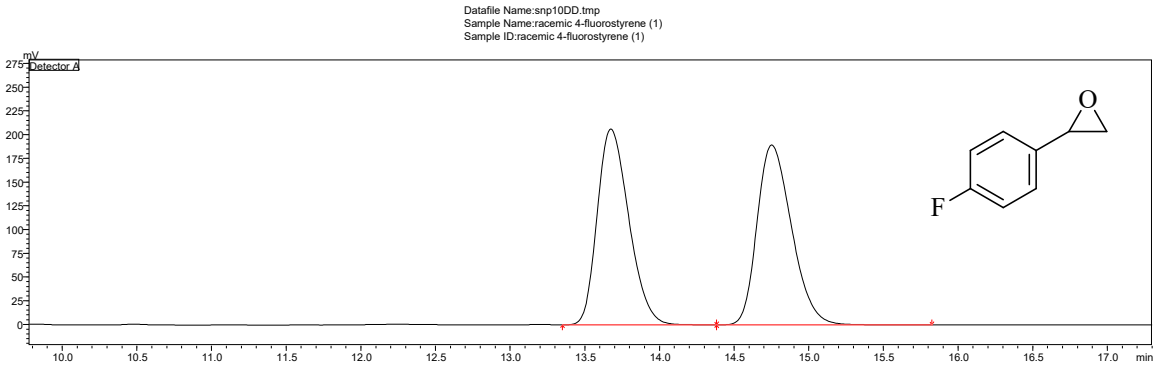
HPLC condition: Chiralpak IC column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.523	6737151	1069381	65.251	65.251
2	5.999	3587904	544713	34.749	34.749
Total		10325055	1614093	100.000	100.000

Racemic-4-fluorostyrene oxide (13)

HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.8/0.2, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.

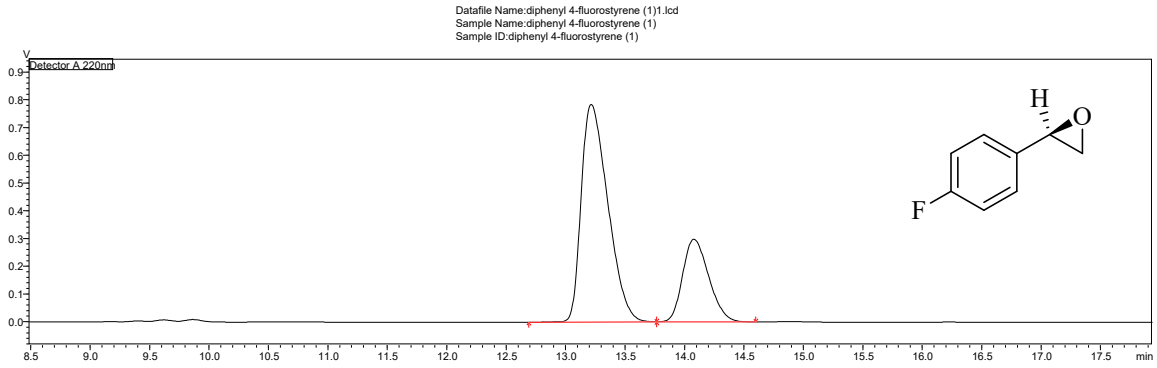


Peak	Ret. Time	Area	Height	Conc.	Area%
1	13.674	3029568	206408	49.872	49.872
2	14.752	3045171	189420	50.128	50.128

Total		6074740	395828	100.000	100.000

4-Fluorostyrene oxide (13) with catalyst 1b

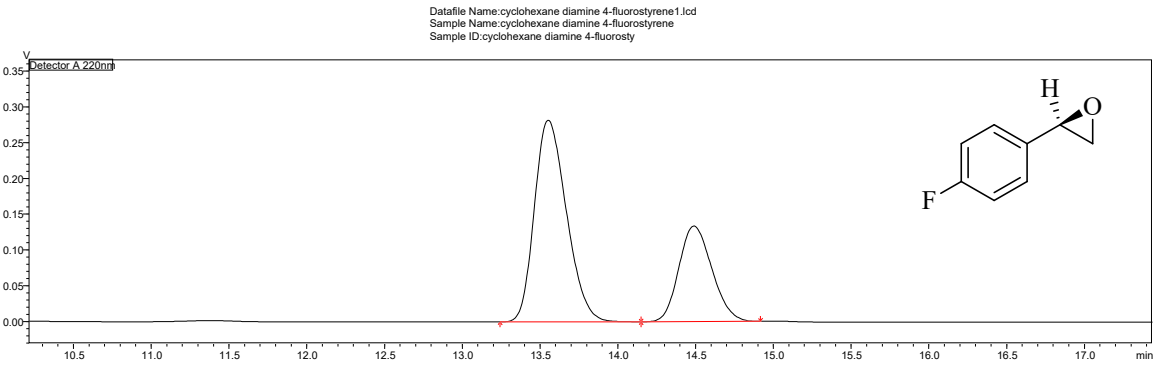
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.8/0.2, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	13.215	12223688	784645	72.770	72.770
2	14.079	4574128	298127	27.230	27.230
Total		16797816	1082772	100.000	100.000

4-fluorostyrene oxide (13) with catalyst 2b

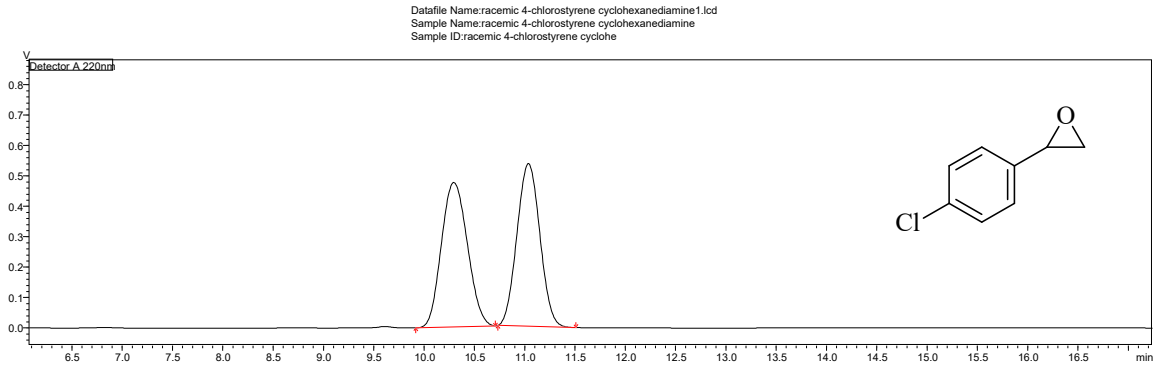
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.8/0.2, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	13.552	4037433	281933	67.145	67.145
2	14.489	1975608	133647	32.855	32.855
Total		6013041	415580	100.000	100.000

Racemic-4-chlorostyrene oxide (15)

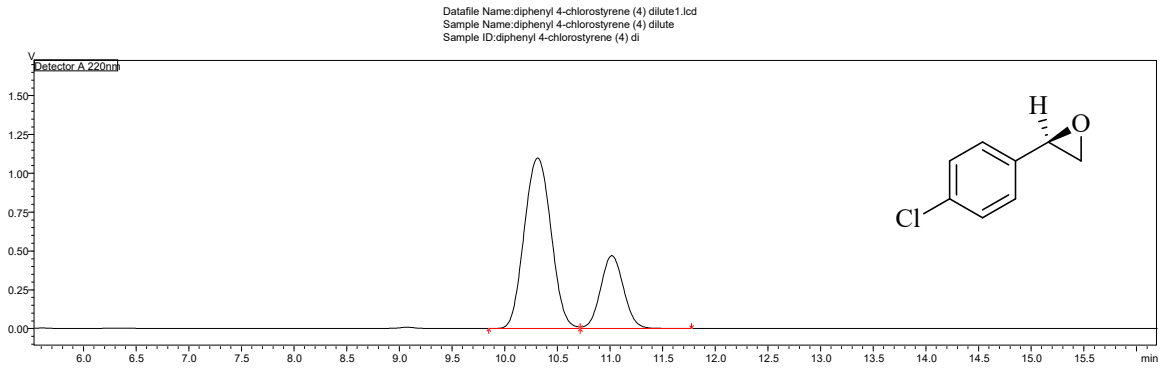
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.296	8534087	474768	50.131	50.131
2	11.037	8489510	534524	49.869	49.869
Total		17023597	1009292	100.000	100.000

4-Chlorostyrene oxide (15) with catalyst 1b

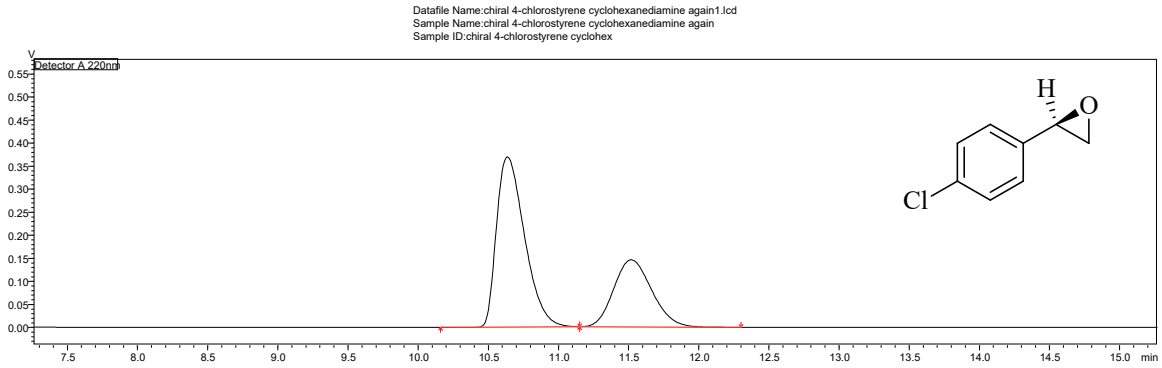
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.313	19425864	1097747	73.216	73.216
2	11.018	7106403	469357	26.784	26.784
Total		26532267	1567104	100.000	100.000

4-Chlorostyrene oxide (15) with catalyst 2b

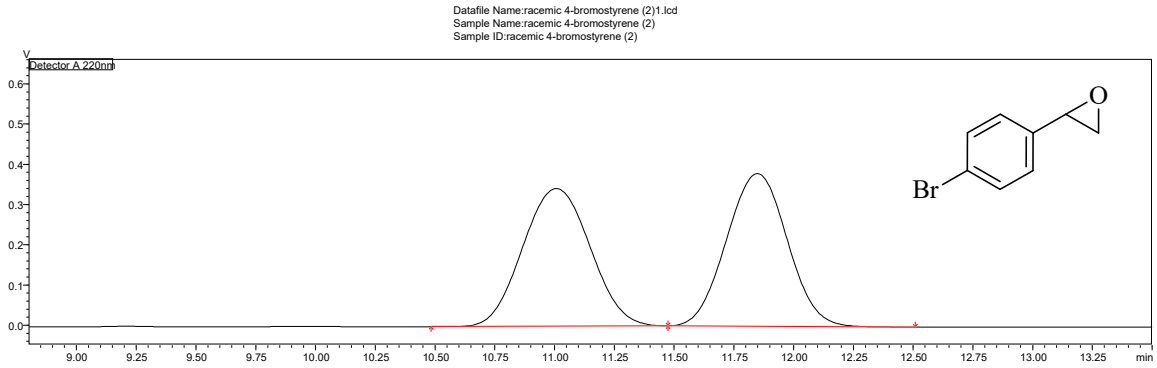
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.636	5120333	369184	65.136	65.136
2	11.518	2740671	145580	34.864	34.864
Total		7861004	514765	100.000	100.000

Racemic-4-bromostyrene oxide (17)

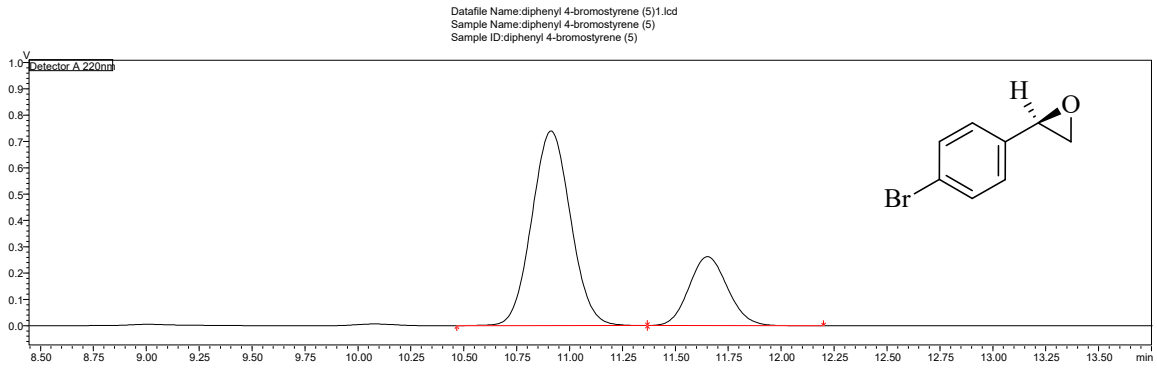
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	11.007	6713146	342403	49.962	49.962
2	11.848	6723443	379871	50.038	50.038
Total		13436589	722274	100.000	100.000

4-bromostyrene oxide (17) with catalyst 1b

HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.

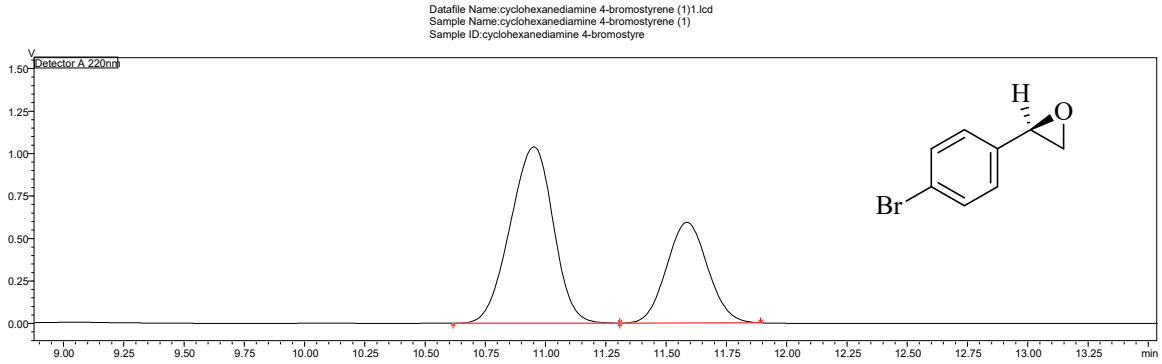


Peak	Ret. Time	Area	Height	Conc.	Area%

1	10.912	9448307	738859	73.951	73.951
2	11.651	3328170	262260	26.049	26.049
Total		12776476	1001119	100.000	100.000

4-bromostyrene oxide (17) with catalyst 2b

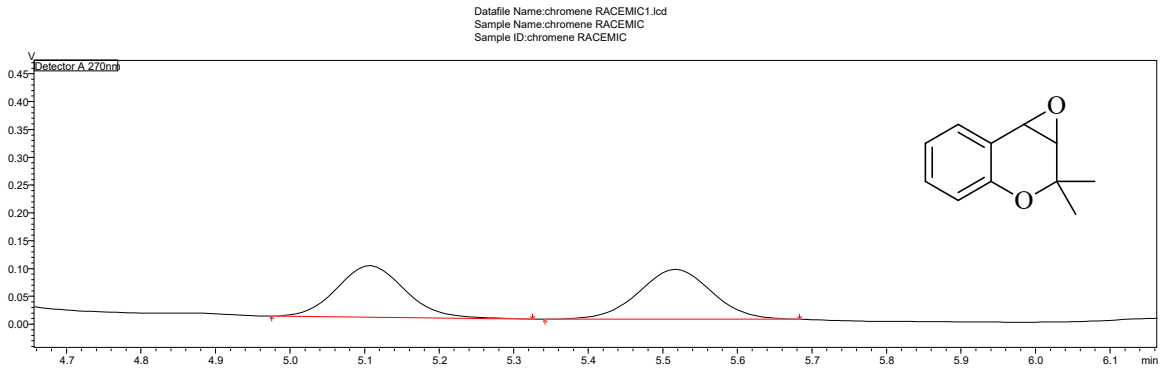
HPLC condition: Chiralpak AD-H column, hexane/isopropyl alcohol = 99.5/0.5, flow rate = 0.8 mL/min, wavelength = 220 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.951	12906694	1037333	64.733	64.733
2	11.586	7031693	592333	35.267	35.267
Total		19938387	1629666	100.000	100.000

Racemic-2,2-dimethyl-2*H*-chromene oxide (19)

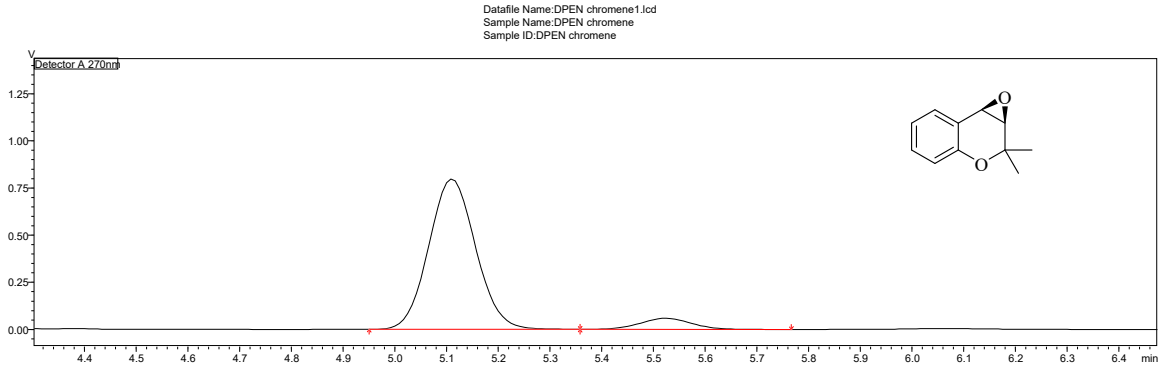
HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 270 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.107	586834	92616	49.005	49.005
2	5.517	610661	89517	50.995	50.995
Total		1197495	182133	100.000	100.000

2,2-dimethyl-2*H*-chromene oxide (19) with catalyst 1b

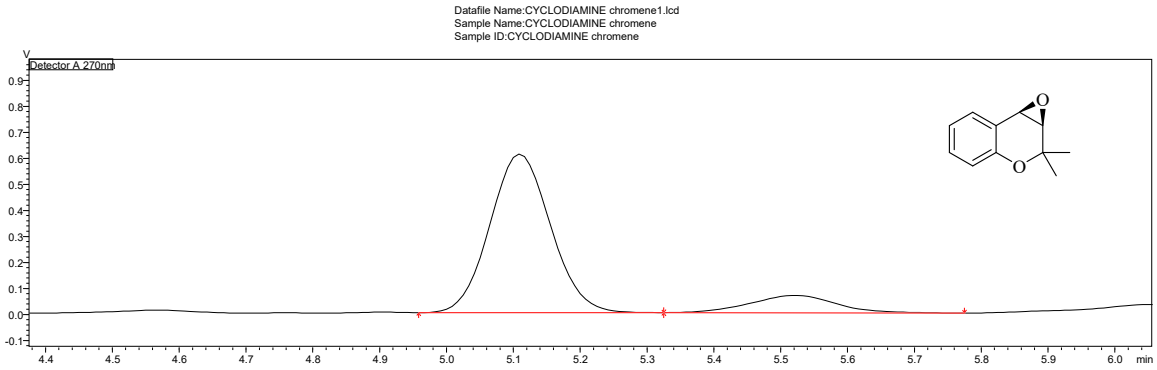
HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 270 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.110	5020335	797210	92.440	92.440
2	5.523	410595	58829	7.560	7.560
Total		5430930	856039	100.000	100.000

2,2-dimethyl-2*H*-chromene oxide (19) with catalyst 2b

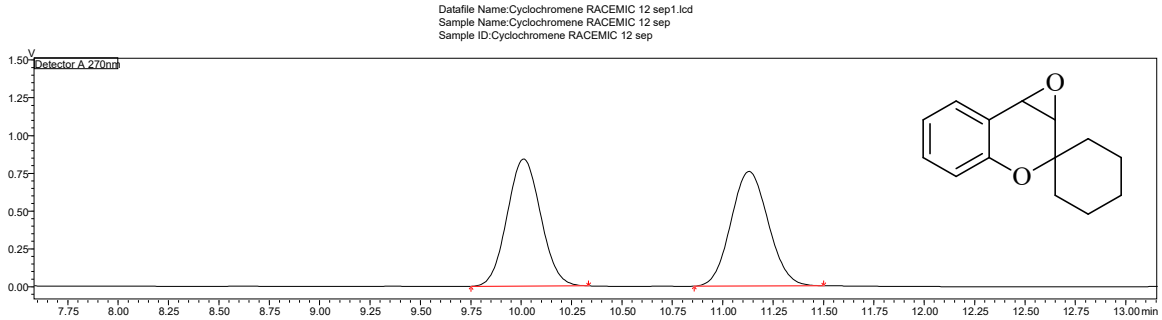
HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 1 mL/min, wavelength = 270 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	5.109	3855471	610207	86.347	86.347
2	5.522	609612	67645	13.653	13.653
Total		4465083	677852	100.000	100.000

Racemic-spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (21)

HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 270 nm, temperature = 25 °C.

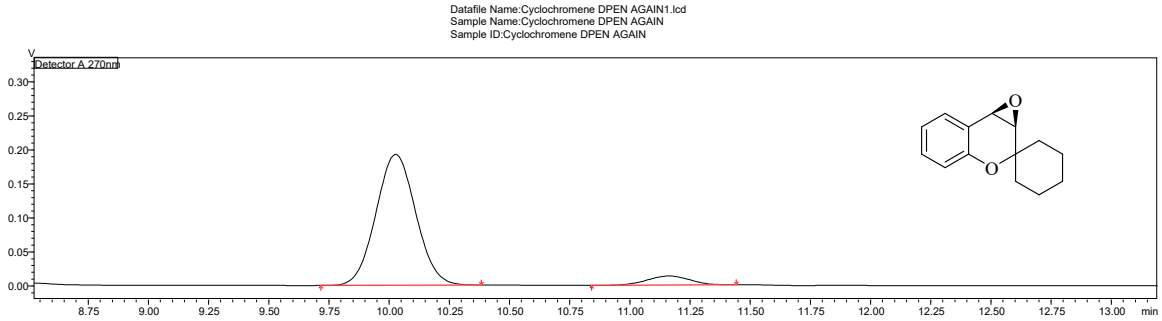


Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.012	9778018	841651	49.991	49.991

2	11.130	9781562	758281	50.009	50.009
Total		19559579	1599932	100.000	100.000

Spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (21) with catalyst 1b

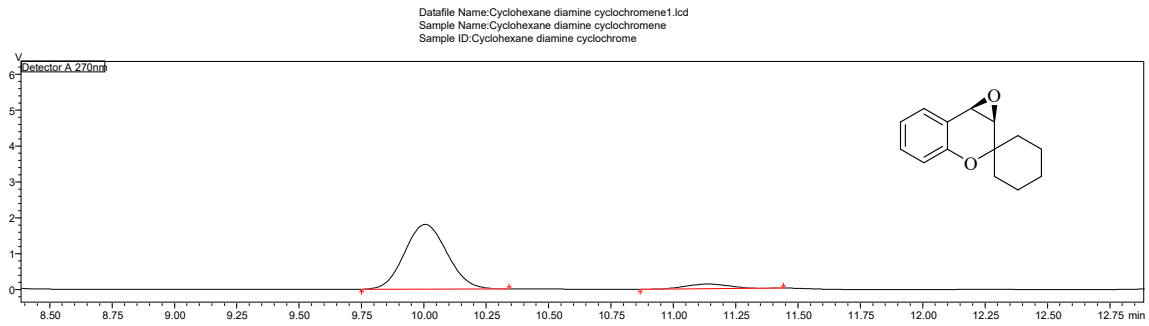
HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 270 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.027	2218764	192499	93.116	93.116
2	11.162	164020	13355	6.884	6.884
Total		2382784	205853	100.000	100.000

Spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (21) with catalyst 2b

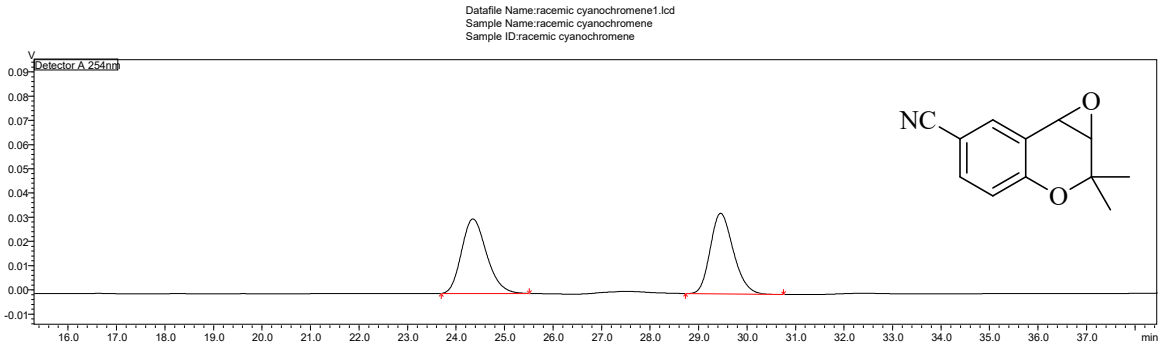
HPLC condition: Chiralpak IA column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 270 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	10.005	21433810	1803986	93.286	93.286
2	11.140	1542552	129259	6.714	6.714
Total		22976362	1933244	100.000	100.000

Racemic-6-cyano-2,2-dimethyl-2*H*-chromene oxide (23)

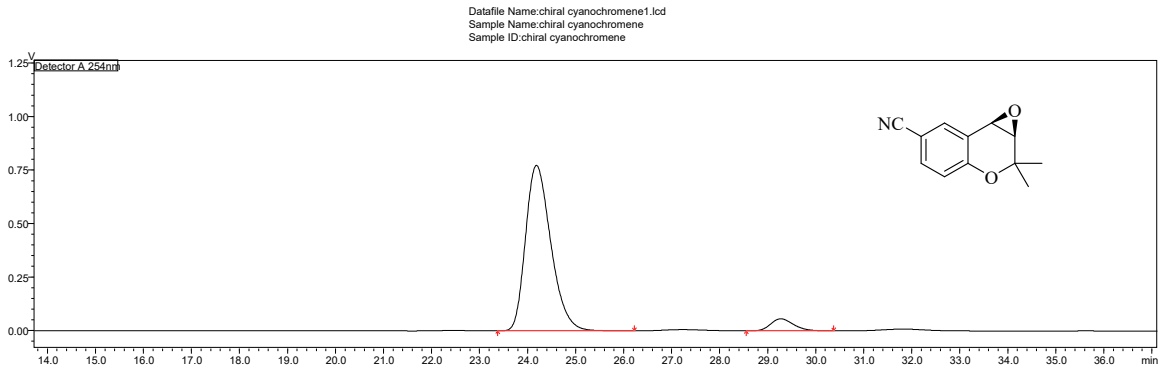
HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	24.348	1108309	30774	50.115	50.115
2	29.454	1103225	33290	49.885	49.885
Total		2211534	64065	100.000	100.000

6-cyano-2,2-dimethyl-2*H*-chromene oxide (23) with catalyst 1b

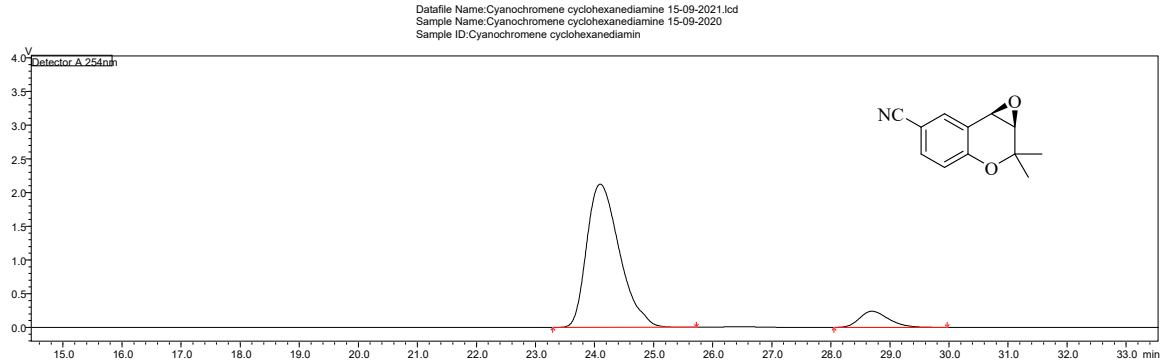
HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	24.184	28358064	773635	93.821	93.821
2	29.273	1867798	56431	6.179	6.179
Total		30225862	830067	100.000	100.000

6-cyano-2,2-dimethyl-2*H*-chromene oxide (23) with catalyst 2b

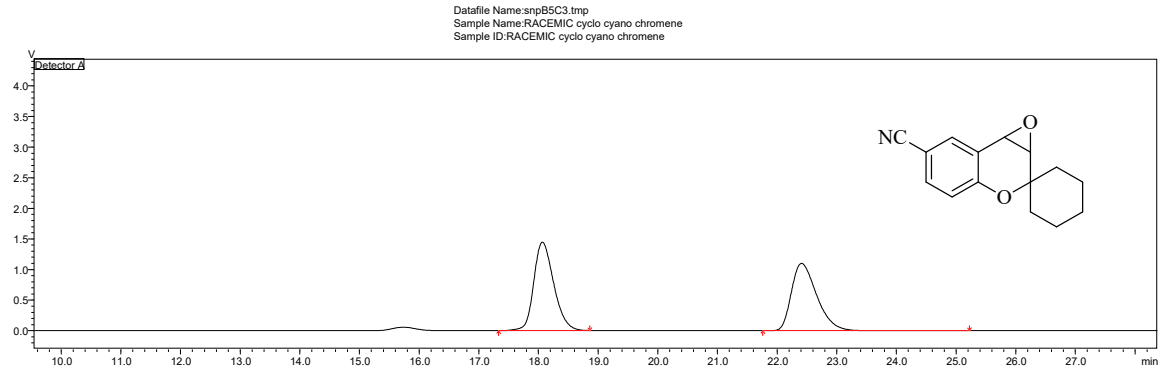
HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 95/5, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	24.094	81878164	2124876	90.944	90.944
2	28.697	8153522	239097	9.056	9.056
Total		90031686	2363973	100.000	100.000

Racemic-6-cyano-spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (25)

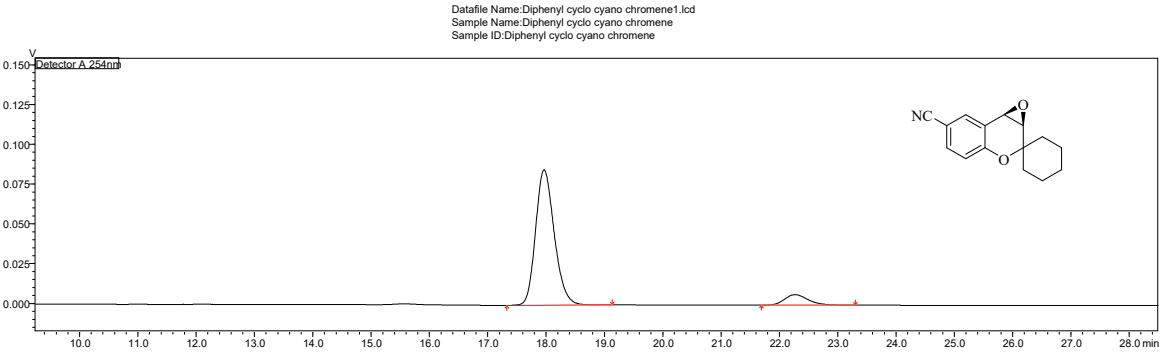
HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 90/10, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.



Peak	Ret. Time	Area	Height	Conc.	Area%
1	18.066	33782517	1445375	50.975	50.975
2	22.411	32489881	1101197	49.025	49.025
Total		66272398	2546572	100.000	100.000

6-cyano-spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (25) with catalyst 1b

HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 90/10, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.

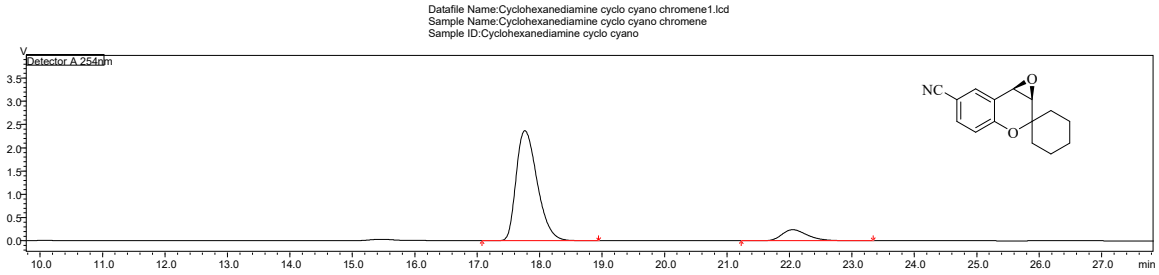


Peak	Ret. Time	Area	Height	Conc.	Area%

1	17.965	1900271	85176	91.086	91.086
2	22.269	185956	6601	8.914	8.914
Total		2086227	91778	100.000	100.000

6-cyano-spiro[cyclohexane-1,2'-[2*H*][1]chromene oxide (25) with catalyst 2b

HPLC condition: Chiralcel OD-H column, hexane/isopropyl alcohol = 90/10, flow rate = 0.5 mL/min, wavelength = 254 nm, temperature = 25 °C.

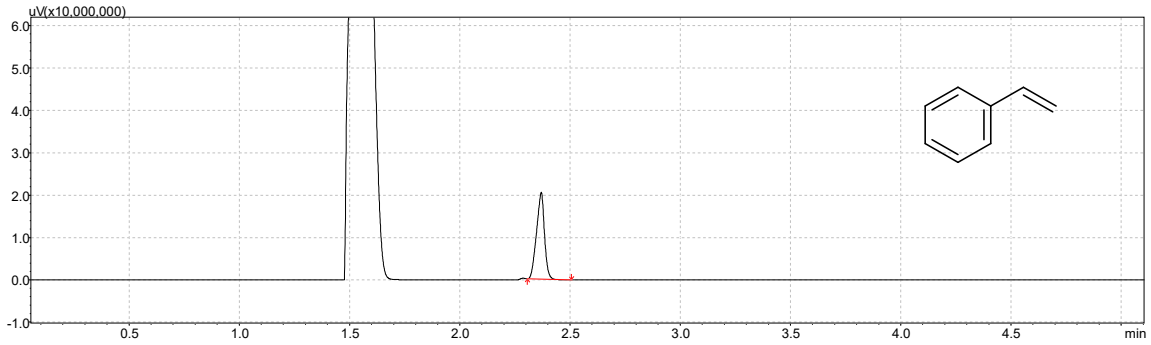


Peak	Ret. Time	Area	Height	Conc.	Area%
1	17.762	55507426	2369040	89.015	89.015
2	22.052	6850286	239861	10.985	10.985
Total		62357712	2608901	100.000	100.000

GC Chromatograms

GC chromatogram of styrene (10)

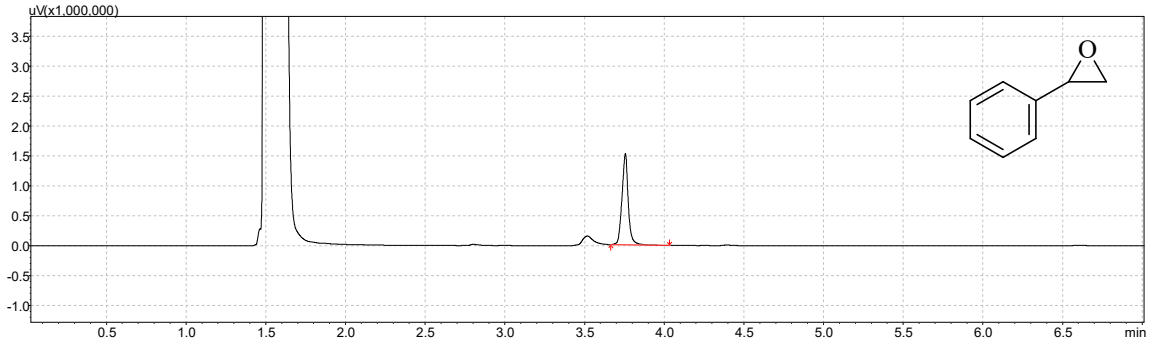
GC conditions of styrene (**10**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.369	51027387.6	20425079.2	100.00000

GC chromatogram of styrene oxide (11) synthesized in first run with catalyst 1b

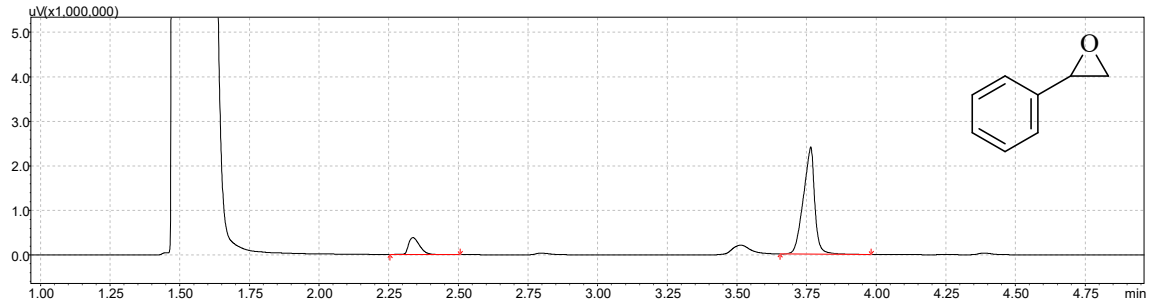
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	3.756	4131901.6	1477936.2	100.00000

GC chromatogram of styrene oxide (11) synthesized in second run with catalyst 1b

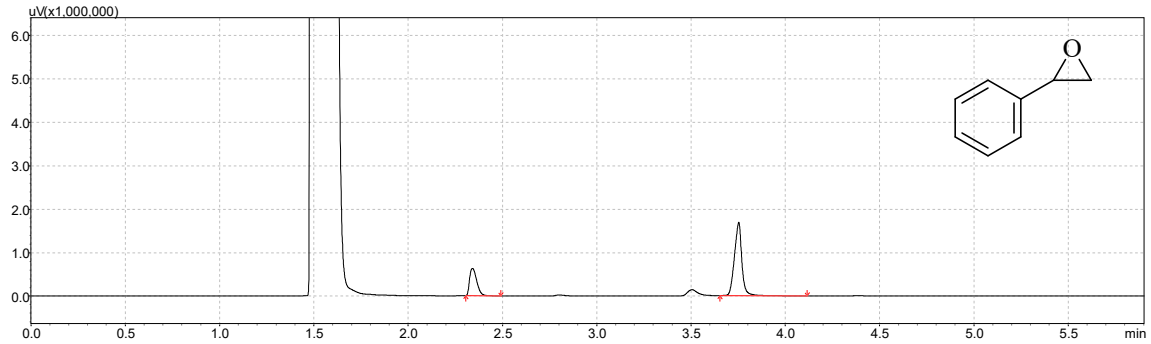
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.337	1068325.8	379837.4	13.54397
2	3.764	6819509.7	2394947.8	86.45603

GC chromatogram of styrene oxide (11) synthesized in third run with catalyst 1b

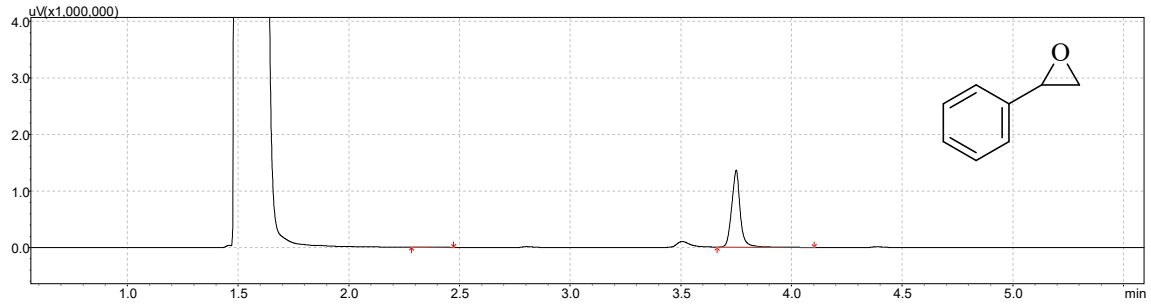
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.341	1658975.5	613936.6	26.37926
2	3.753	4629963.9	1675308.5	73.62074

GC chromatogram of styrene oxide (11) synthesized in first run with catalyst 2b

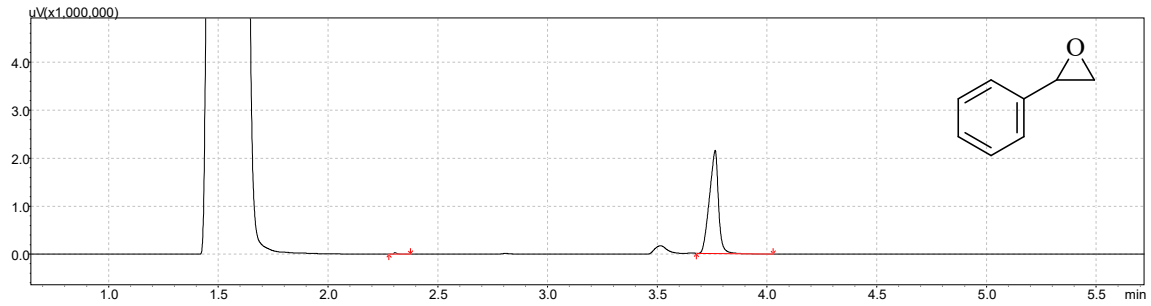
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.310	2438.4	235.4	0.06734
2	3.750	3618516.4	1356621.7	99.93266

GC chromatogram of styrene oxide (11) synthesized in second run with catalyst 2b

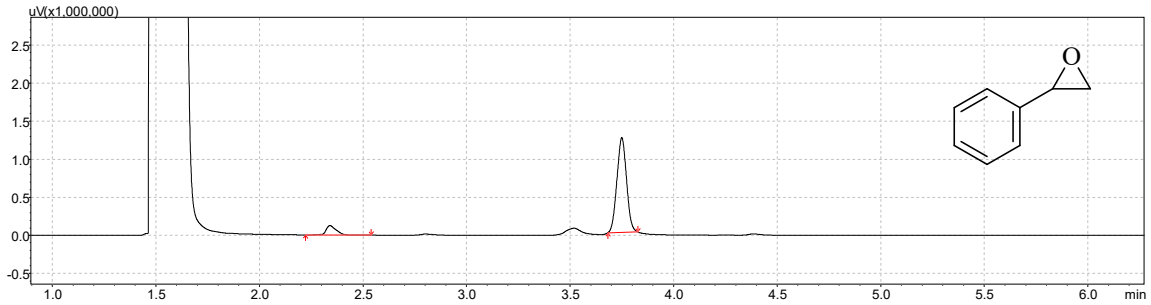
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.305	38511.6	26936.1	0.62502
2	3.763	6123176.3	2135993.4	99.37498

GC chromatogram of styrene oxide (11) synthesized in third run with catalyst 2b

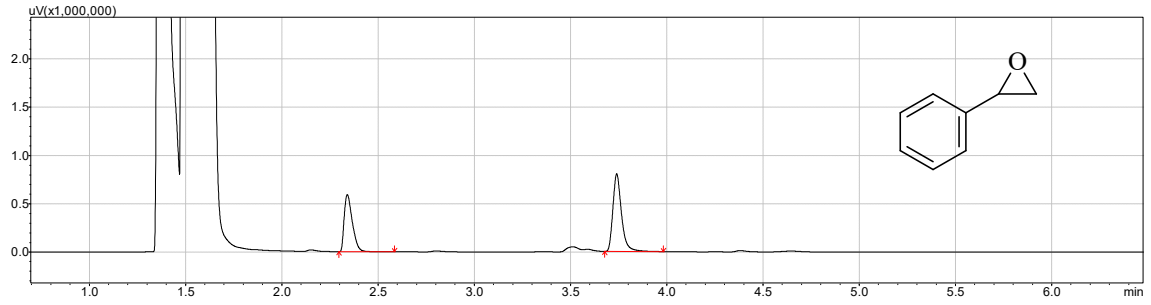
GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.341	420592.2	124089.1	9.47374
2	3.750	4018967.9	1240984.4	90.52626

GC chromatogram of styrene oxide (11) synthesized in fourth run with catalyst 2b

GC conditions of styrene oxide (**11**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.

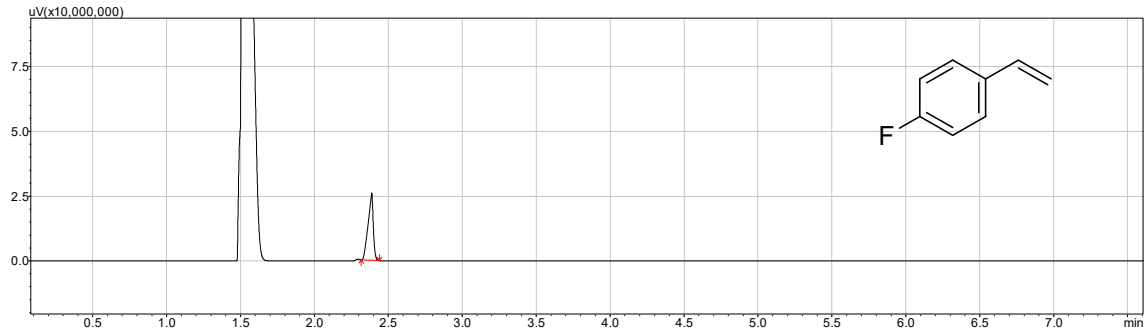


Peak	Ret.Time	Area	Height	Conc.
1	2.341	1737486.6	588534.4	40.98633

2	3.740	2501698.7	798493.7	59.01367

GC chromatogram of 4-fluorostyrene (12)

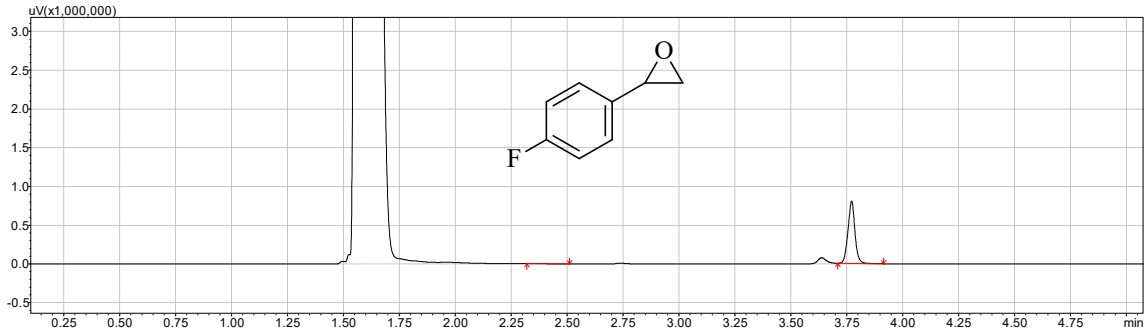
GC conditions of 4-fluorostyrene (**12**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.387	62514346.9	25662949.4	100.00000

GC chromatogram of 4-fluorostyrene oxide (13) with catalyst 1b

GC conditions of 4-fluorostyrene oxide (**13**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.

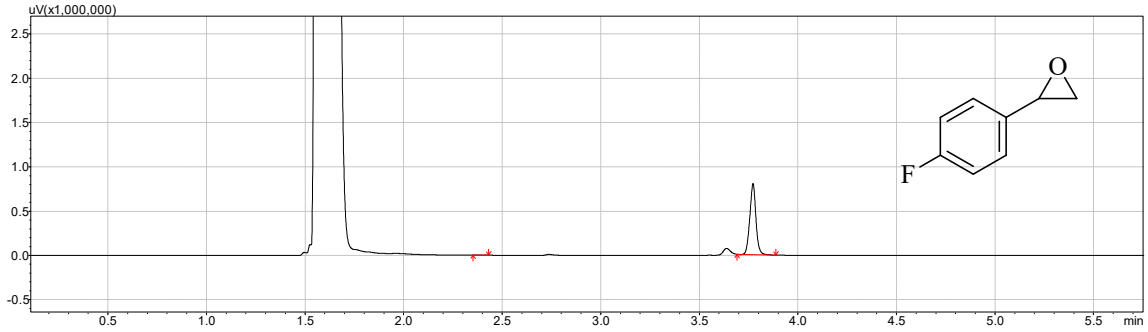


Peak	Ret.Time	Area	Height	Conc.
1	2.378	1320.4	1006.8	0.07596

2	3.773	1736943.1	797015.2	99.92404

GC chromatogram of 4-fluorostyrene oxide (13) with catalyst 2b

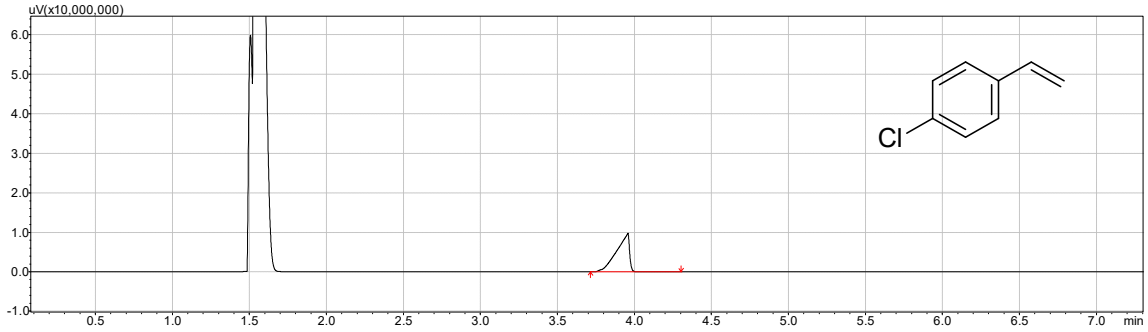
GC conditions of 4-fluorostyrene oxide (**13**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	2.378	2233.3	1058.2	0.12982
2	3.773	1718046.9	795122.7	99.87018

GC chromatogram of 4-chlorostyrene (14)

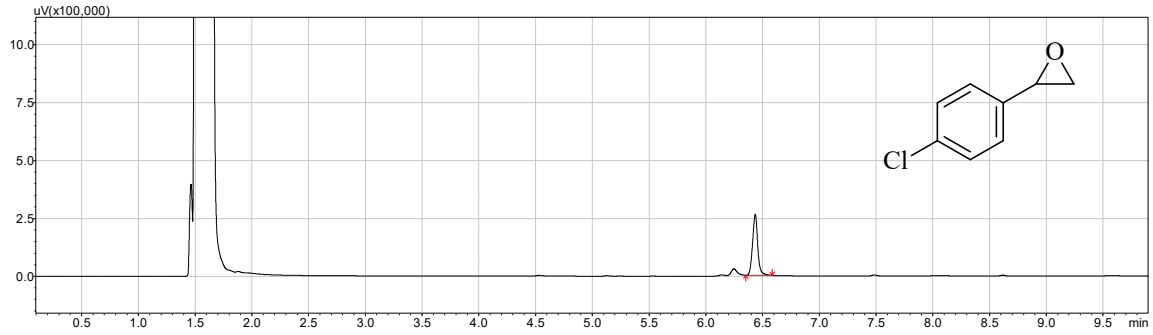
GC conditions of 4-chlorostyrene (**14**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	3.956	56967231.2	9436832.9	100.00000

GC chromatogram of 4-chlorostyrene oxide (15) with catalyst 1b

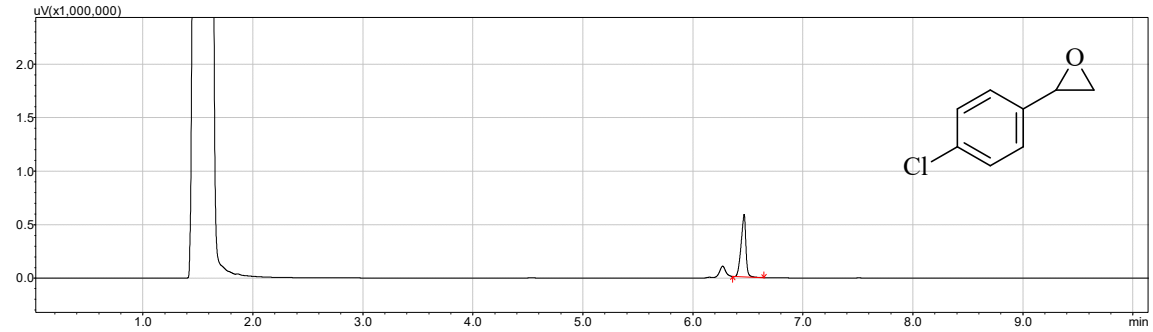
GC conditions of 4-chlorostyrene oxide (**15**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	6.436	827152.2	260663.6	100.00000

GC chromatogram of 4-chlorostyrene oxide (15) with catalyst 2b

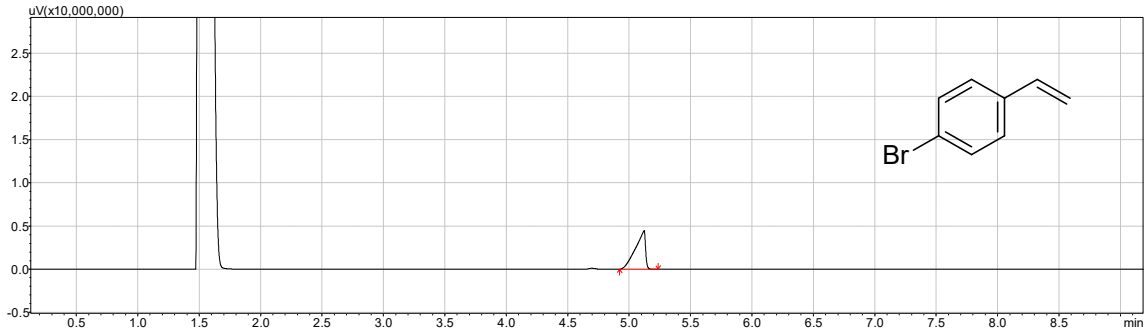
GC conditions of 4-chlorostyrene oxide (**15**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	6.466	1745448.4	579706.5	100.00000

GC chromatogram of 4-bromostyrene (16)

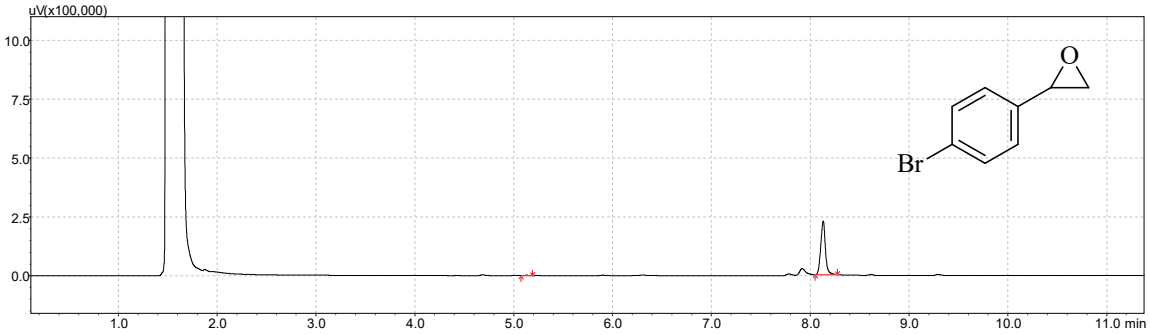
GC conditions of 4-bromostyrene (**16**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	5.121	25476778.1	4455871.2	100.00000

GC chromatogram of 4-bromostyrene oxide (17) with catalyst 1b

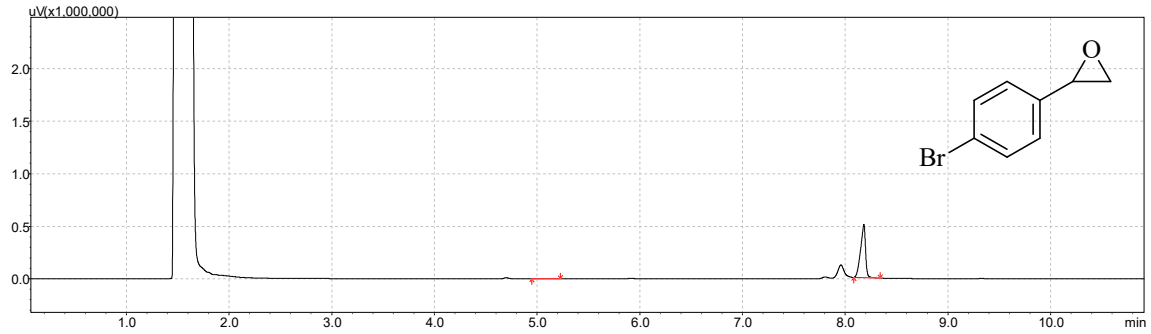
GC conditions of 4-bromostyrene oxide (**17**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	5.129	4890.2	1878.5	0.65260
2	8.131	744450.2	227569.6	99.34740

GC chromatogram of 4-bromostyrene oxide (17) with catalyst 2b

GC conditions of 4-bromostyrene oxide (**17**): column information Rtx-5, L = 30 m, 0.25 mm ID, injector temperature = 250 °C, column flow rate = 1.36 mL/min, column temperature = 100-180 °C, temperature program = 6 °C/min, detector temperature = 250 °C.



Peak	Ret.Time	Area	Height	Conc.
1	5.040	3269.6	446.8	0.19255
2	8.182	1694750.1	504684.6	99.80745