# Supporting Information

# $BH_3$-Promoted Stereoselective β-Lithiation of *N*-Alkyl-2-phenylaziridines

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**Content**

**General**

All air sensitive reactions were carried out under dry Ar. Tetrahydrofuran (THF) and diethylether were freshly distilled under a nitrogen or argon atmosphere over sodium/benzophenone ketyl immediately prior to use. For the $^{1}H$, $^{13}C$ and $^{11}B$ NMR spectra ($^{1}H$ NMR 300, 400, 600 MHz, $^{13}C$ NMR 75 and 100 MHz, $^{11}B$ NMR 192 MHz), $CDCl_3$, $CD_3OD$ were used as the solvents. MS-ESI analyses were performed on LC/MSD trap system. Melting points are uncorrected. Infra-red spectra of the compounds were recorded as a film or in Nujol as indicated. Analytical thin layer chromatography (TLC) was carried out on aluminium backed plates pre-coated (0.25 mm) with Silica Gel 60 $F_{254}$. Detection was accomplished by UV light (254 nm), by spraying a 5% solution of $(NH_4)_2Mo_7O_{24}{\cdot}4\ H_2O$ (phosphomolibdic acid) in EtOH or in a 5% solution (w/v) of ammonium molybdate and 0.2% (w/v) of cerium(III)sulfate in 17.6% (w/v) aqueous sulfuric acid followed by heating until dark spots appear. For flash chromatography silica Gel 60, 0.040–0.063 mm particle size was used. Optical rotation $[\alpha]_{589}^{20}$ values were measured by using a polarimeter with a cell of 1 dm path length; the concentration (c) is expressed in g/100mL. All air- and water-sensitive reactions were carried out in oven-dried glassware under argon or nitrogen atmosphere using syringe-septum cap techniques.

**Starting materials**

Aziridines **1a**[1] **1b**[1] and **1d**[2] were synthetized according to a known procedure[3]. Aziridine **1c** was synthetized by the same procedure, purified and characterized as follows.

**1-Cumyl-2-phenylaziridine, 1c.**

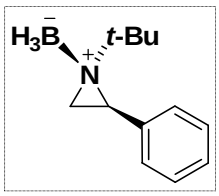
Pale yellow oil, yield 94%. Purified by flash chromatography (petroleum ether/ AcOEt 8:2; $R_f$ = 0.61). $^{1}H$-NMR (300 MHz, $CDCl_3$) δ: 1.43 (s, 3 H), 1.44 (s, 3 H,), 1.72 (dd, *J* = 3.0, 9.0 Hz, 1 H), 1.85 (dd, *J* = 0.6, 6.3 Hz, 1 H), 2.53 (dd, *J* = 3.3, 6.6 Hz, 1 H), 7.15-7.38 (m, 8 H), 7.45-7.55 (m, 2 H). $^{13}C$-NMR (75 MHz, $CDCl_3$) δ: 26.2, 26.6, 31.3, 34.3, 58.5, 126.4, 126.6, 127.8, 128.1, 141.0, 145.7. Anal. Calcd for $C_{17}H_{19}N$: C, 86.03%; N, 5.90%; H, 8.07%. Found: C, 86.11%; N, 5.85%; H, 8.12%.

**General procedure for the synthesis of the borane-complexes, 2a-2c.**

1.1 Equivalent of $BH_3{\cdot}THF$ was added dropwise at 0 °C to 6.79 mmol of aziridine neat under inert atmosphere. The mixture was stirred for 5 minutes at 0 °C. Then the solvent was evaporated *in vacuo*. The resulted white solid was purified by washing with hexane.

The products **2a-2c** were characterized as follows:

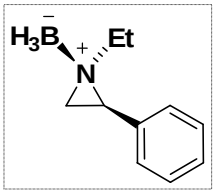
**1-Borane-1-*tert*-butyl-2-phenylaziridine, 2a.**




White solid, yield >95%, mp 95-97 °C. $^{1}H$-NMR (300 MHz, $CDCl_3$) δ: 1.40 (s, 9 H), 2.67-2.61 (m, 2 H), 3.70 (dd, *J* = 6.3, 1.5 Hz, 1 H), 7.39-7.26 (m, 5 H). $^{13}C$-NMR (75 MHz, $CDCl_3$) δ: 26.3, 36.0, 44.4, 60.7, 127.9, 128.3, 130.0, 132.0. FT-IR (nujol, $cm^{-1}$) ν: 2292, 2345, 2390 (BH). Anal. Calcd for $C_{12}H_{20}BN$: C, 76.22%; H, 10.66%; N, 7.41%. Found: C, 76.38%; H, 10.51%; N, 7.34%.

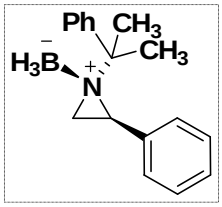
[1]Du,Y.; Wu, Y.; Liu, A. –H.; He, L. –N. *J. Org. Chem.* **2008**, *73*, 4709-4712.
[2]Barama, A.; Condom, R.; Guedj, R. J. *Fluor. Chem.* **1980**, *16*, 538-539.
[3] Okada, I.; Ichimura, K.; Sudo, R. *Bull. Chem. Soc. Jpn.* **1970**, *43*, 1185-1189.

**1-Borane-1-ethyl-2-phenylaziridine, 2b.**



White solid, yield >95%, mp 60-62 °C. $^{1}$H-NMR (300 MHz, $CDCl_3$) δ: 1.45 (t, *J* = 7.2 Hz, 3 H), 2.42 (dd, *J* = 7.8, 1.5 Hz, 1 H), 2.53 (dq, *J* = 12.3, 7.2 Hz, 1 H), 2.81 (dd, *J* = 6.6, 1.5 Hz, 1 H), 3.23 (dq, *J* =12.0, 7.2 Hz, 1 H), 3.34 (t, *J* =6.9 Hz, 1 H), 7.28-7.43 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 11.9, 41.0, 48.8, 59.3, 127.9, 128.6, 129.9, 130.88. FT-IR (nujol, $cm^{-1}$) ν: 2267, 2311, 2360 (BH). Anal. Calcd for $C_{10}H_{16}BN$: C, 74.58%; H, 10.01%; N, 8.70%. Found: C, 74.63%; H, 9.92%; N, 8.62%. $[\alpha]_{589}^{20}$ = +58 (c=0.7, $EtOH_{abs}$), er > 95:5. Enantiomeric purity determined by HPLC analysis (Cellulose LUX-2 chiral column, Hexane-*i*PrOH 90:1, 1.0 mL/min, 227 nm, for (±)-**2b** $t_1$ = 14.63 min, $t_2$ = 16.52 min; for **(1*S*, 2*S*)-2b** resulted t = 14.65 min (See Section determination of er).

**1-Borane-1-cumyl-2-phenylaziridine, 2c.**



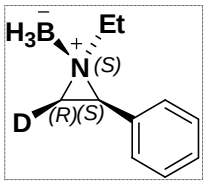
White solid, yield 92%, mp 165-167°C. $^{1}$H-NMR (300 MHz, $CDCl_3$) δ: 1.94 (s, 3 H), 1.99 (s, 3 H), 2.39 (dd, *J* = 0.6, 8.1 Hz, 1 H), 2.63 (dd, *J* = 1.8, 6.3 Hz, 1 H), 3.27 (dd, *J* = 6, 8.1 Hz, 1 H), 7.55-7.30 (m, 5 H), $^{13}$ C-NMR (75 MHz, $CDCl_3$) δ: 26.4, 26.6, 36.7, 44.9, 65.1, 128.0, 128.2, 128.3, 128.5, 128.6, 130.0, 132.0, 139.4. FT-IR (nujol, $cm^{-1}$) ν: 2300, 2340, 2373 (BH). Anal. Calcd for $C_{17}H_{22}BN$: calcd C, 81.29%; H, 8.83%; N, 5.58%. Found: C, 81.19%; H, 8.87%, N, 5.49%.

**General procedure for the lithiation-trapping sequence of aziridino-borane complexes.**

A solution of *s*-BuLi (1.2 eq., 1.4 M in cyclohexane) was added under inert atmosphere at -50°C to a stirring solution of aziridine-borane complex (3.11 mmol) in dry THF (7 mL). The reaction mixture was stirred at -50°C for 2h, then cooled at -78°C before adding the electrophile (1.4 eq., 4.35 mmol). The reaction mixture was then allowed to warm to room temperature and stirred until substrate consumption (TLC monitoring). The reaction mixture was poured into $H_2O$ and extracted with $CH_2Cl_2$ (3x15mL). The organic layers were dried under $Na_2SO_4$ and the solvent evaporated *in vacuo*. Aziridino-borane 3-functionalized was purified by crystallization from hexane.

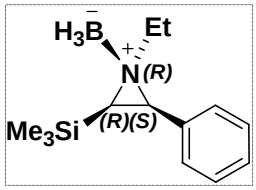
**Spectroscopic data of (*S*,*S*,*R*)-3f and (*R*,*S*,*R*)-3h functionalized *N*-borane-complexes.**

**(*S*,*S*,*R*)-1-Borane-1-ethyl-3-deutero-2-phenylaziridine, (*S*,*S*,*R*)-3f.**



White solid, yield >83%, D = 90%, mp 59-60 °C. Purified by crystallization from hexane. $^{1}$H-NMR (400 MHz, $CD_3OD$) δ: 1.32 (t, *J* = 7.1 Hz, 3 H), 2.48 (d, *J* = 7.7 Hz, 1 H), 2.50 (m overlapping d at 2.48 ppm, 1 H), 3.06 (dq, *J* =12.3, 7.1 Hz, 1 H), 3.50 (d, *J* = 7.7 Hz, 1 H), 7.29 (m, 5 H). $^{13}$C-NMR (100 MHz, $CD_3OD$) δ: 12.3, 41.6 (t, $J_{C\text{-}D}$ = 26.7 Hz), 50.0, 60.2, 128.9, 129.5, 131.4, 133.2. $^{11}$B-NMR (192 MHz, $CDCl_3$) δ: -16.58 (q, *J* = 91.9 Hz). FT-IR (film, $cm^{-1}$) ν: 3035, 2976, 2938, 2370, 2273, 1451, 1385, 1166, 971, 695. ESI-MS *m/z* (%): 185 $[M+Na]^+$ (100). Anal. Calcd for $C_{10}H_{15}DBN$: C, 74.11%; H, 10.57%; N, 8.64%. Found: C, 74.03%; H, 10.32; N, 8.62%. $[\alpha]_{589}^{20}$ = +26 (c=0.4, $EtOH_{abs}$), er=95:5. Enantiomeric purity determined by HPLC analysis (Cellulose LUX-2 chiral column, Hexane-*i*PrOH 90:1, 1.0 mL/min, 219 nm, for racemic **3f** $t_1$ = 14.69 min, $t_2$ = 16.58 min; for **(*S*,*R*,*S*)-3f** resulted t = 14.77 min (See Section determination of er).

**(*R*,*S*,*R*)-1-Borane-1-ethyl-2-phenyl-3-trimethylsilanylaziridine, (*R*,*S*,*R*)-3h.**



White solid, yield 95%, mp 65-67 °C. Purified by crystallization from hexane. $^{1}$H-NMR (600 MHz, $CDCl_3$) δ: 1.19 (s, 9 H), 1.46 (t, *J* = 7.1 Hz, 3 H), 1.63 (d, *J* = 9.6 Hz, 1 H), 2.84 (dq, *J* =14.1, 7.1 Hz, 1 H), 2.94 (dq, *J* =14.3, 7.1 Hz, 1 H), 3.54 (d, *J* = 9.6 Hz, 1 H), 7.31-7.35 (m, 3 H), 7.45-7.46 (m, 2 H). $^{13}$C-

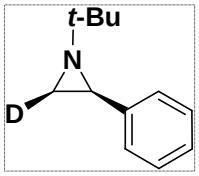
NMR (100 MHz, $CDCl_3$) δ: 0.1, 12.3, 45.8, 53.1, 64.2, 127.7, 128.0, 129.5, 132.8. $^{11}$B-NMR (192 MHz, $CDCl_3$) δ: -17.27 (q, $J$ = 91.1 Hz). FT-IR (film, $cm^{-1}$) ν: 3062, 3031, 2954, 2428, 2357, 2277, 1381, 1249, 1165, 843. ESI-MS *m/z* (%): 256 $[M+Na]^+$ (100). Anal. Calcd for $C_{13}H_{24}BNSi$: C, 66.95%; H, 10.37%; N, 6.01%. Found: C, 66.84%; H, 10.42%; N, 6.08%. $[\alpha]_{589}^{20}$ = +61 (c=0.5, $EtOH_{abs}$), er=95:5. Enantiomeric purity determined by HPLC analysis (Cellulose LUX-2 chiral column, Hexane-*i*PrOH 99.95:0.005, 0.5 mL/min, 227 nm, for racemic **3h** $t_1$ = 15.93 min, $t_2$ = 17.67 min; for **(*R*,*R*,*S*)-3h** resulted t = 16.05 min (See Section determination of er).

**General procedure for the decomplexation of the aziridine-borane 3-functionalized complexes.**

The reaction crudes of the borane-adducts 3-functionalized *N*-*tert*-Bu- and *N*-$C(CH_3)_2$Ph-substituted were treated with of $H_2O$ (1 mL) and stirred until gas evolution ceased. More $H_2O$ (15 mL) was added and the resulting mixture was extracted with $Et_2O$ (3x15mL). The organic phase was washed with brine (15 mL), dried under $K_2CO_3$ and the solvent evaporated *in vacuo*. To accomplish the decomplexation of the *N*-Ethyl borane-adducts 3-functionalized, it needed to treat the reaction crude with $NH_3$ (28% aq) at reflux for 5 h. Extraction with $Et_2O$ gave the desired aziridines.

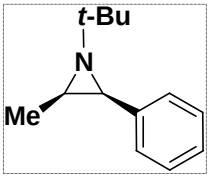
**Spectroscopic data of 4a-4m deprotected functionalized aziridines.**

**1-Butyl-3-deutero-2-phenylaziridine, 4a.**



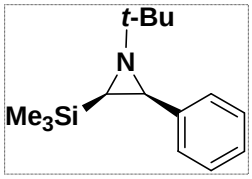

Yellow oil, yield >95%, D >98%. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 1.05 (s, 9 H), 1.86 (d, $J$ = 6.3 Hz, 1 H), 2.61 (d, $J$ = 6.3 Hz, 1 H), 7.17-7.27 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 26.5, 29.9 (t, $J_{C\text{-}D}$ = 26.5 Hz), 33.7, 53.1, 126.5, 126.5, 128.1, 141.2. Anal. Calcd for $C_{12}H_{16}DN$: C, 81.76%; H, 10.29%; N, 7.95%. Found: C, 81.82%; H, 10.20%; N, 8.01%.

**1-Butyl-3-methyl-2-phenylaziridine, 4b.**



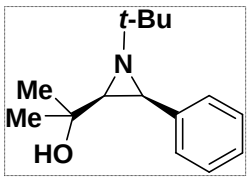

Colorless oil, yield 80%. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 0.86 (d, $J$ = 5.7 Hz, 3 H), 1.06 (s, 9 H), 1.99 (dq, $J$ = 6.6, 5.7 Hz, 1 H), 2.78 (d, $J$ = 6.6 Hz, 1 H), 7.18-7.39 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 14.0, 26.7, 33.5, 38.7, 52.9, 126.2, 127.7, 128.0, 138.7. Anal. Calcd for $C_{13}H_{19}N$: C, 82.48%; H, 10.12%; N, 7.40%. Found: C, 82.52%; H, 10.22%; N, 7.38%.

**1-Butyl-2-phenyl-3-trimethylsilanylaziridine, 4c.**



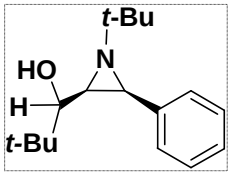

Yellow oil, yield >95%. $^1$H-NMR (300 MHz, $CDCl_3$) δ: -0.26 (s, 9 H), 0.91 (d, $J$ = 7.5 Hz, 1 H), 1.03 (s, 9 H), 2.90 (d, $J$ = 7.2 Hz, 1 H), 7.16-7.42 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: -1.8, 26.4, 29.6, 38.5, 53.1, 126.1, 127.6, 127.9, 141.0. FT-IR (nujol, $cm^{-1}$) ν: 1237 ($Si(CH_3)_3$). Anal. Calcd for $C_{15}H_{25}NSi$: C, 72.81%; H, 10.18%; N, 5.66%. Found: C, 72.85%; H, 10.27%; N, 5.69%.

**2-(1-*t*-Butyl-3-phenyl-aziridin-2-yl)-propan-2-ol, 4d.**



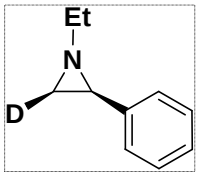

Pale yellow solid, yield 73%. Purified by flash chromatography (petroleum ether/AcOEt 7:3) $R_f$ = 0.73. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 0.99 (s, 3 H), 1.12 (s, 9 H), 1.21 (s, 3 H), 1.98 (d, $J$ = 6.6 Hz, 1 H), 2.69 (br s, 1 H), 2.93 (d, $J$ = 6.3 Hz, 1 H), 7.15-7.42 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 25.6, 27.0, 31.4, 38.3, 47.3, 52.6, 67.9, 126.4, 127.8, 127.9, 137.9. FT-IR (nujol, $cm^{-1}$) ν: 3437 (OH). Anal. Calcd for $C_{15}H_{23}NO$: C, 77.21%; H, 9.93%; N, 6.00%. Found: C, 77.28%; H, 9.96%; N, 6.13%.

**1-(1-Butyl-3-phenyl-aziridin-2-yl)-2,2-dimethyl-propan-1-ol, 4e.**



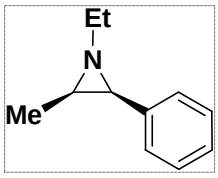

Pale yellow oil, yield 86%. Purified by flash chromatography (petroleum ether/$Et_2O$, 7:3) $R_f$ = 0,69. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 0.84 (s, 9 H), 1.09 (s, 9 H), 2.18 (t, *J* = 6.6 Hz, 1 H), 2.47 (dd, *J* = 6.3, 1.5 Hz, 1 H), 2.63 (s, 1 H), 3.04 (d, *J* = 6.3 Hz, 1 H), 7.17-7.35 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 25.4, 26.8, 34.0, 40,5, 41.3, 52.9, 72.8, 126.7, 127. 6, 127.9, 137.5. Anal. Calcd for $C_{17}H_{27}NO$: C, 78.11%; H, 10.41%; N, 5.36%. Found: C, 78.17%; H, 10.36%; N, 5.31%.

**1-Ethyl-3-deutero-2-phenylaziridine, 4f.**



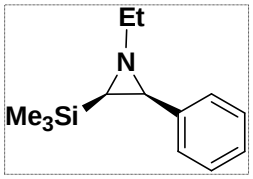

Pale yellow oil, yield >95%, %D = 90%. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 1.20 (t, *J* = 7.2 Hz, 3 H), 1.64 (d, *J* = 6.6 Hz, 1 H), 2.30 (d, *J* = 6.6 Hz, 1 H), 2.45 (q, *J* = 7.2 Hz, 2 H), 7.18-7.34 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 14.3, 37.0 (t, $J_{C-D}$ = 26.7 Hz), 40.9, 55.7, 126.1, 126.6, 128.1, 140.3. Anal. Calcd for $C_{10}H_{12}DN$: C, 81.03%; H, 9.52%; N, 9.45%. Found: C, 81.13%; H, 9.35%; N, 9.58%.

**1-Ethyl-2-methyl-3-phenylaziridine, 4g.**



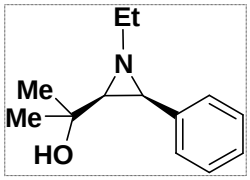

Yellow oil, yield 60%. Purified by flash chromatography (petroleum ether/$Et_2O$, 7:3) $R_f$ = 0,70. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 0.93 (d, *J* = 5.7 Hz, 3 H), 1.20 (t, *J* = 7.2 Hz, 3 H), 1.75 (quint, *J* = 6.3 Hz, 1 H), 2.28 (dq, *J* = 11.7, 6.9 Hz, 1 H), 2.46 (d, *J* = 6.9 Hz, 1 H), 2.68 (dq, *J* = 11.4, 7.2 Hz, 1 H), 7.18-7.34 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 13.1, 14.3, 41.2, 46.1, 55.3, 126.3, 127.7, 127.9, 137.8. Anal. Calcd for $C_{11}H_{15}N$: C, 81.94%; H, 9.38%; N, 8.69%. Found: C, 81.87%; H, 9.48%; N, 8.56%.

**1-Ethyl-2-phenyl-3-trimethylsilanylaziridine, 4h.**



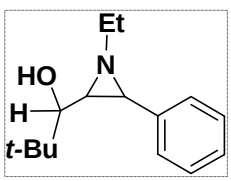

Colorless oil, yield 72%. Purified by flash chromatography (petroleum ether/$Et_2O$, 8:2) $R_f$ = 0,82. $^1$H-NMR (300 MHz, $CDCl_3$) δ: -0.23 (s, 9 H), 0.72 (d, *J* = 7.8 Hz, 1 H), 1.20 (t, *J* = 7.2 Hz, 3 H), 2.28 (dq, *J* = 11.4, 6.9 Hz, 1 H), 2.61 (dq, *J* = 11.7, 6.9 Hz, 1 H), 2.64 (d, *J* = 7.5 Hz, 1 H), 7.16-7.38 (m, 5 H), $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 1.9, 14.8, 38.1, 46.4, 58.4, 126.36, 127.7, 127.8, 140.1. FT-IR (nujol, $cm^{-1}$) ν: 1246 ($Si(CH_3)_3$). Anal. Calcd for $C_{13}H_{21}NSi$: C, 71.17%; H, 9.65%; N, 6.38%. Found: C, 71.27%; H, 9.69%; N, 6.29%.

**2-(1-Ethyl-3-phenyl-aziridin-2-yl)-propan-2-ol, 4i.**



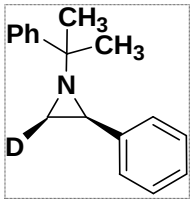

Pale yellow oil, yield 68%. Purified by flash chromatography (petroleum ether/$Et_2O$, 7:3) $R_f$ = 0,60. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 1.01 (s, 3 H), 1.24 (s, 3 H), 1.26 (t, *J* = 7.2 Hz, 3 H), 1.70 (d, *J* = 6.6 Hz, 1 H), 2.11 (s, 1 H). 2.61 (q, *J* = 7.2 Hz, 2 H), 2.64 (d, *J* = 7.2 Hz, 1 H), 7.18-7.42 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 14.6, 25.8, 30.5, 46.0, 54.2, 55.3, 68.5, 126.5, 127.55, 127.9, 137.4. FT-IR (nujol, $cm^{-1}$) ν: 3449 (OH). Anal. Calcd for $C_{13}H_{19}NO$: C, 76.06%; H, 9.33%; N, 6.82%. Found: C, 76.16%; H, 9.24%; N, 6.85%.

**1-(1-Ethyl-3-phenyl-aziridin-2-yl)-2,2-dimethyl-propan-1-ol, 4j.**



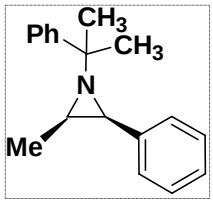

White solid, yield 48%. Purified by flash chromatography (petroleum ether/$Et_2O$, 7:3) $R_f$ = 0,49. $^1$H-NMR (300 MHz, $CDCl_3$) δ: 0.89 (s, 9 H), 1.10 (t, *J* = 7.2 Hz, 3 H), 1.78 (dd, *J* = 9.0, 6.6 Hz, 1 H), 1.83 (dq, *J* = 11.4, 7.2 Hz, 1 H), 2.42 (d, *J* = 6.6 Hz, 1 H), 2.71 (d, *J* = 7.2 Hz, 1 H), 3.0 (dq, *J* = 11.4, 6.9 Hz, 1 H), 7.12-7.36 (m, 5 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 14.3, 25.8, 34.7, 43.5, 48.4, 54.5, 77.0, 126.8, 127.5, 128.3, 137.8. Anal. Calcd for $C_{15}H_{23}NO$: C, 77.21%; H, 9.93%; N, 6.00%. Found: C, 77.31%; H, 9.87%; N, 6.09%.

**1-Cumyl-3-deutero-2-phenylaziridine, 4k.**



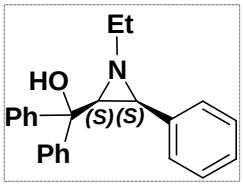

Yellow oil, yield >95%, D = 95%. $^{1}$H-NMR (300 MHz, $CDCl_3$) δ: 1.43 (s, 3 H), 1.44 (s, 3 H), 1.84 (d, *J* = 6.6 Hz, 1 H), 2.53 (d, *J* = 6.3 Hz, 1 H), 7.23-7.37 (m, 10 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 26.2, 29.5, 30.9 (t, $J_{C\text{-}D}$ = 27.5 Hz), 34.2, 58.5, 126.4, 127.8, 128.1, 128.6, 128.7, 133.0, 133.1, 141.0. Anal. Calcd for $C_{17}H_{18}DN$: C, 85.67%; H, 8.46%; N, 5.88%. Found: C, 85.75%; H, 8.41%; N, 5.79%.

**1-Cumyl-3-methyl-2-phenylaziridine, 4l.**




Yellow oil, yield 56%. Purified by flash chromatography (petroleum ether /AcOEt, 9:1) $R_f$ = 0.45. $^{1}$H-NMR (300 MHz, $CDCl_3$) δ: 0.89 (d, *J* = 5.4 Hz, 3 H), 1.44 (s, 3 H), 1.48 (s, 3 H), 1.89 (dq, *J* = 12.0, 5.7 Hz, 1 H), 2.67 (d, *J* = 6.6 Hz, 1 H), 7.17-7.39 (m, 8 H), 7.48-7.54 (m, 2 H). $^{13}$C-NMR (75 MHz, $CDCl_3$) δ: 13.4, 25.5, 27.7, 34.4, 39.0, 58.5, 126.3, 126.5, 126.6, 127.8, 128.1, 138. 5, 145.9. Anal. Calcd for $C_{18}H_{21}N$: C, 86.01%; H, 8.42%; N, 5.57%. Found: C, 86.11%; H, 8.38%; N, 5.61%.

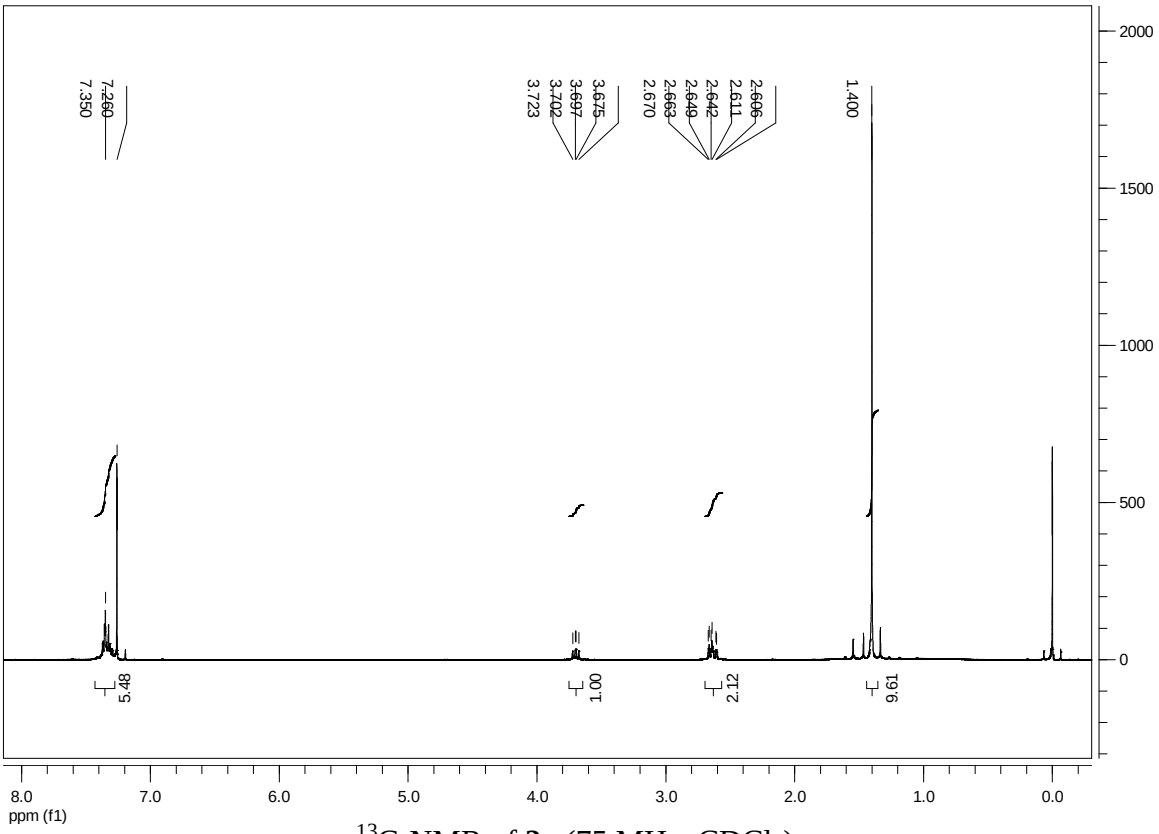
**(*S*,*S*)-1-(1-Ethyl-3-phenyl-aziridin-2-yl)-2,2-diphenyl-methanol, (*S*, *S*)-4m.**



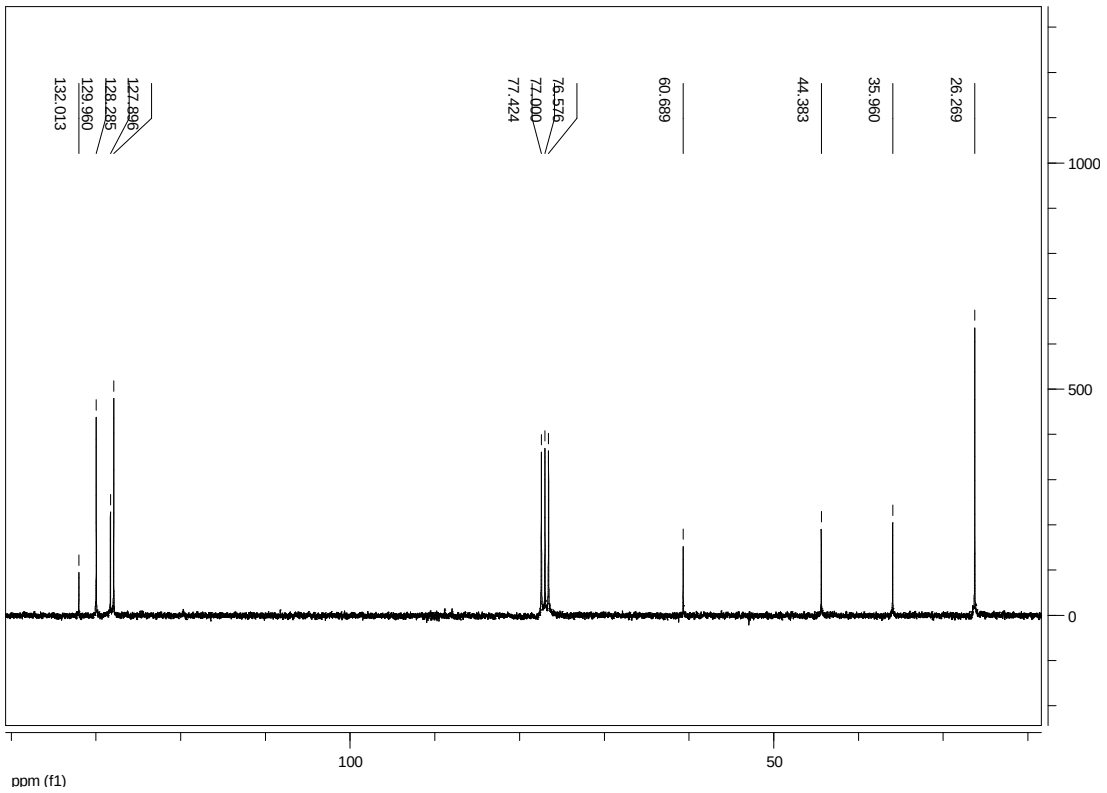

White solid, yield 70%, mp 81-83 °C. Purified by crystallization from hexane. $^{1}$H-NMR (400 MHz, $CDCl_3$) δ: 1.10 (t, *J* = 7.2 Hz, 3 H), 2.46 (dq, *J* = 11.6, 7.1 Hz, 1 H), 2.71 (d, *J* = 6.5 Hz, 1 H), 2.77 (d, *J* = 6.5 Hz, 1 H), 2.89 (dq, *J* =11.6, 7.2 Hz, 1 H), 6.97-7.00 (m, 1 H), 7.07-7.09 (m, 2 H), 7.16-7.39 (m, 12 H). $^{13}$C-NMR (100 MHz, $CDCl_3$) δ: 14.6, 45.8, 53.9, 54.7, 74.6, 126.0, 126.1, 126.4, 126.6, 126.7, 127.5, 127.6, 127.7, 128.0, 136.2, 144.5, 148.8. FT-IR (film, $cm^{-1}$) ν: 3387, 3062, 3033, 2918, 2391, 1598, 1448, 1021, 697. ESI-MS *m/z* (%): 353 $[M+Na]^+$ (100). Anal. Calcd for $C_{23}H_{23}NO$: C, 83.85%; H, 7.04%; N, 4.25%. Found: C, 84.05%; H, 7.14%; N, 4.05%. $[\alpha]_{589}^{20}$ = +25 (c=0.6, $EtOH_{abs}$), er >98:2. Enantiomeric purity determined by HPLC analysis (Cellulose LUX-2 chiral column, Hexane-*i*PrOH 90:1, 1.0 mL/min, 220 nm, for racemic **4m** $t_1$ = 3.84 min, $t_2$ = 6.82 min; for **(*S*,*S*)-4m** resulted t = 3.78 min (See Section determination of er).

**Copies of $^{1}$H-NMR, $^{13}$C-NMR and $^{11}$B-NMR spectra.**

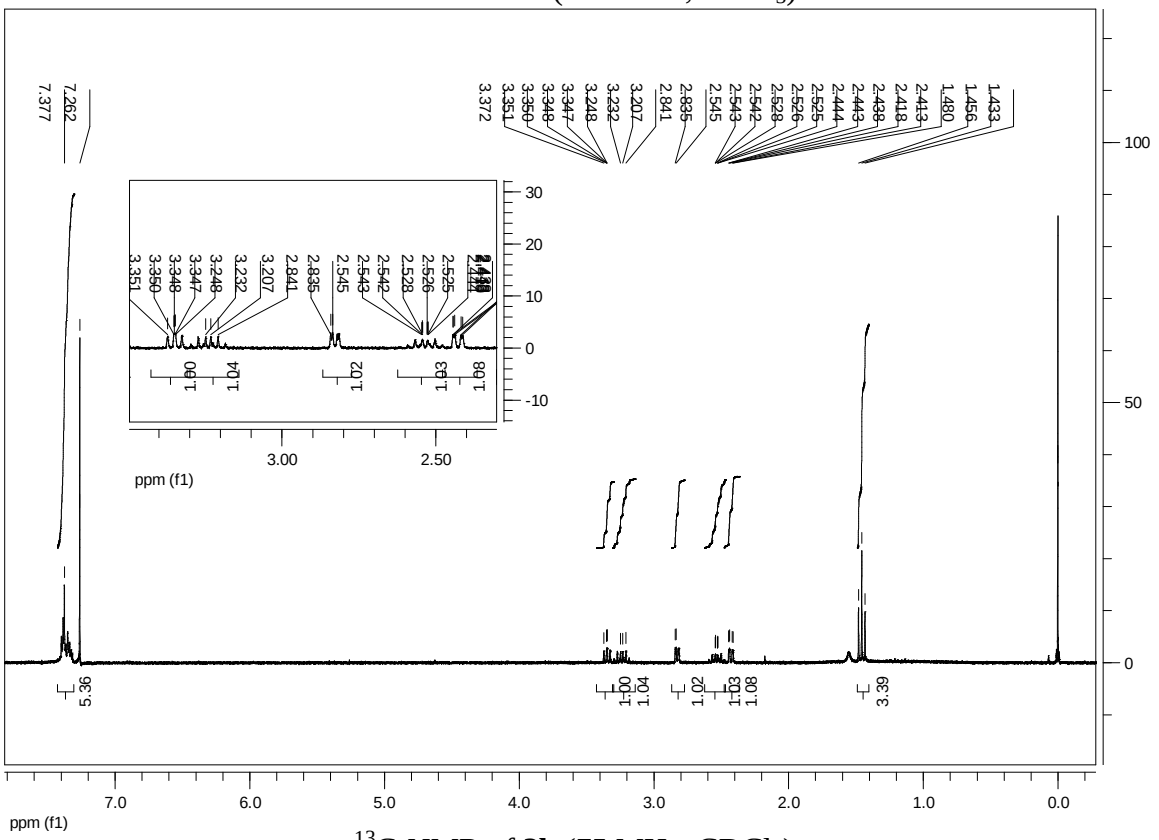
$^{1}$H-NMR of **2a** (300 MHz, $CDCl_3$)



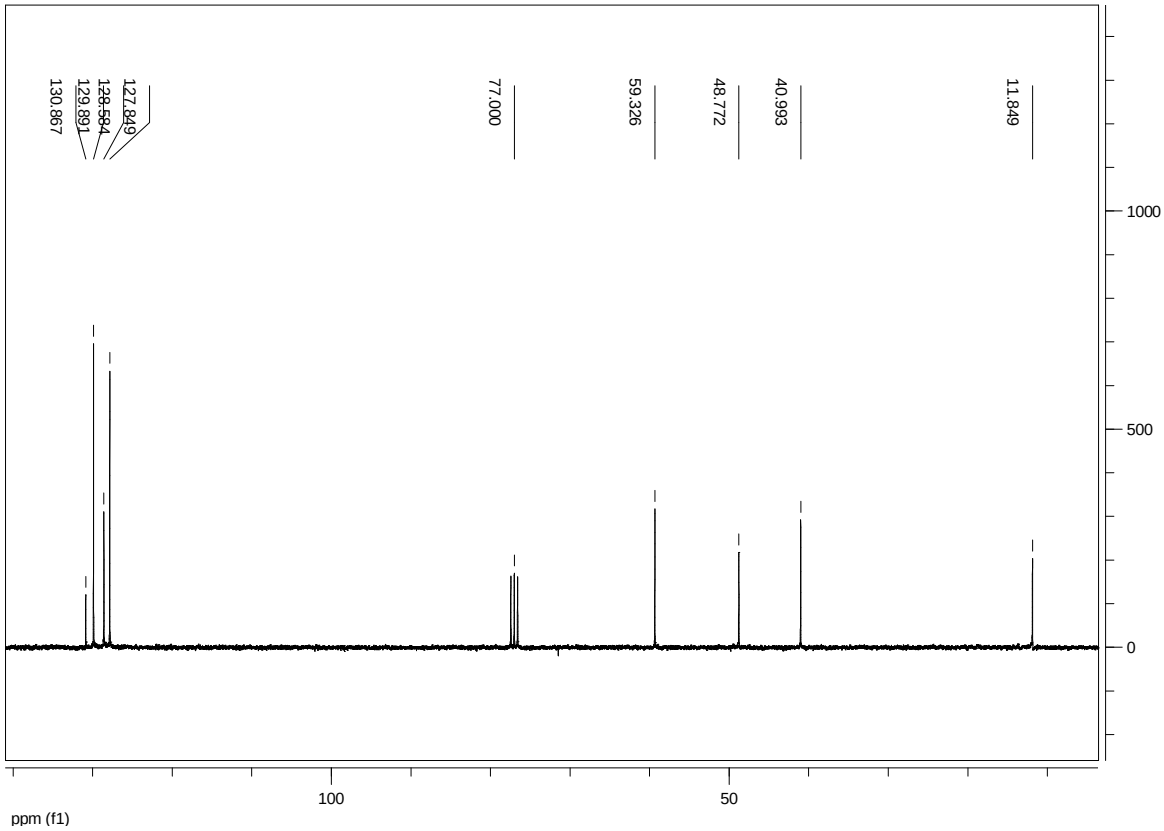

$^{13}$C-NMR of **2a** (75 MHz, $CDCl_3$)



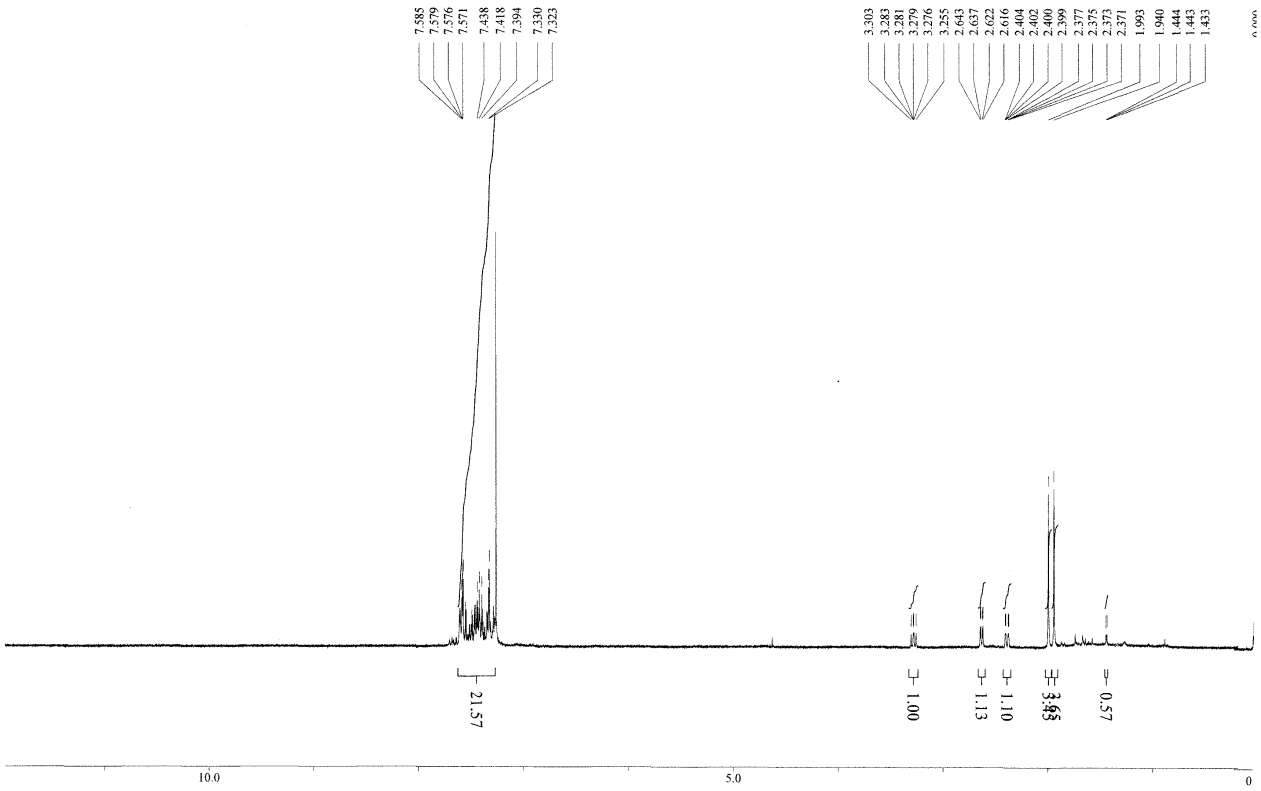
$^{1}$H-NMR of **2b** (300 MHz, $CDCl_3$)



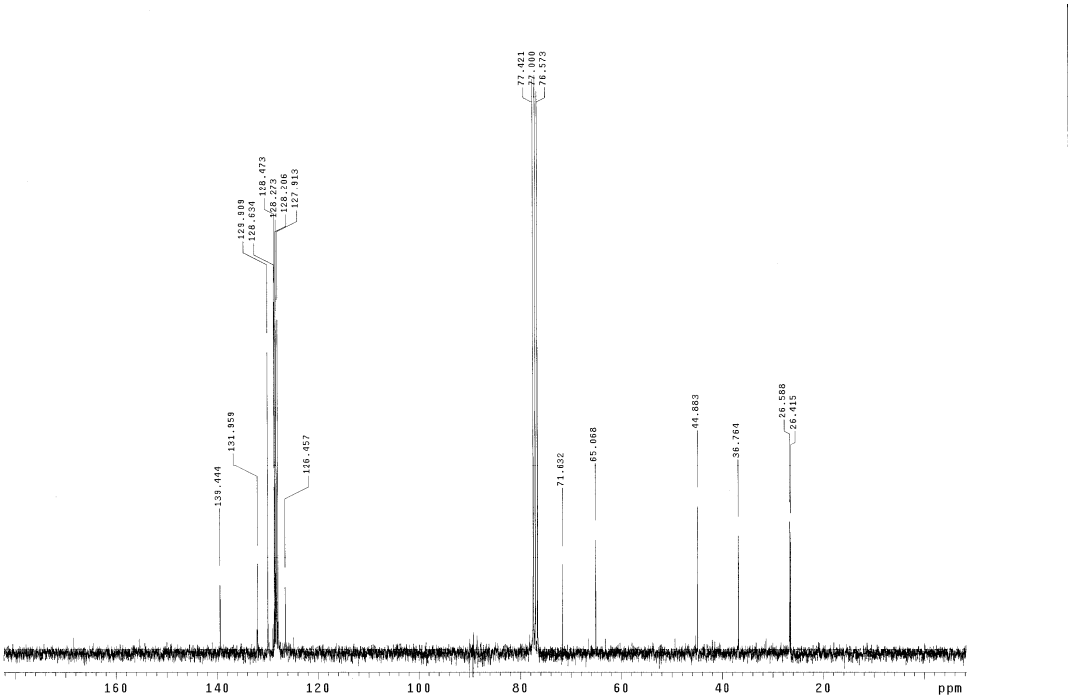

$^{13}$C-NMR of **2b** (75 MHz, $CDCl_3$)



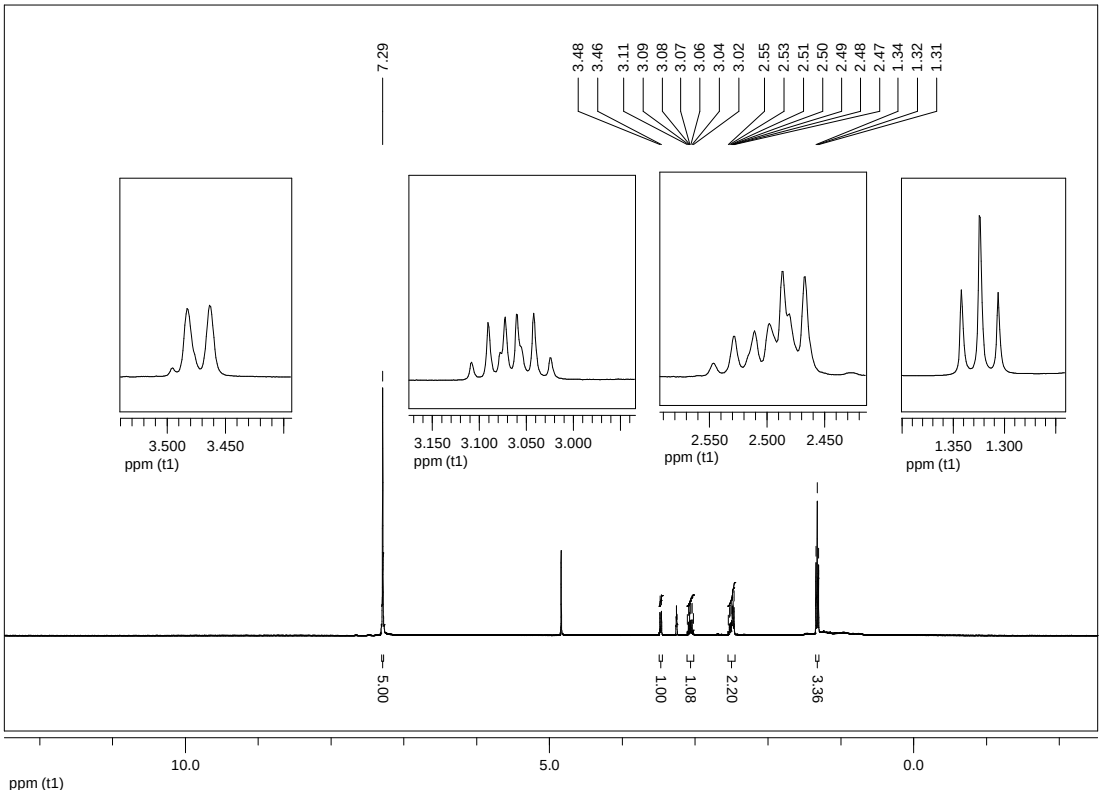
$^{1}$H-NMR of **2c** (300 MHz, $CDCl_3$)



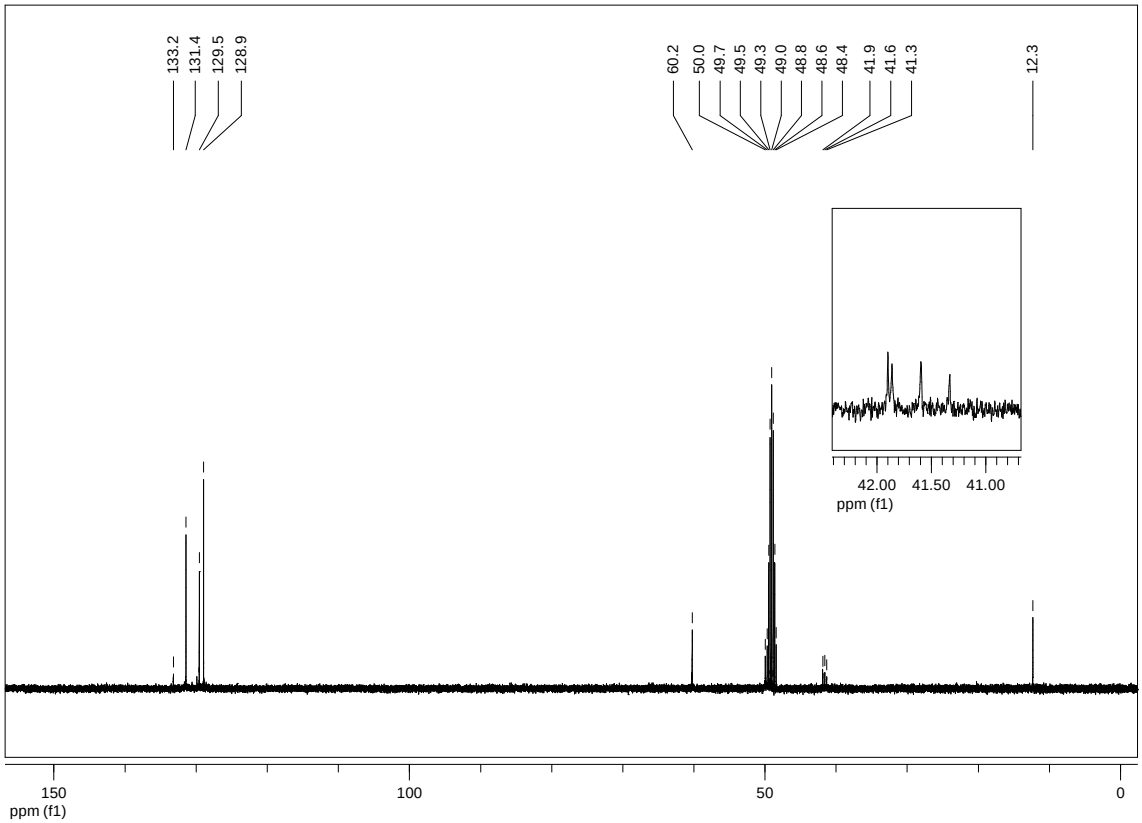

$^{13}$C-NMR of **2c** (75 MHz, $CDCl_3$)



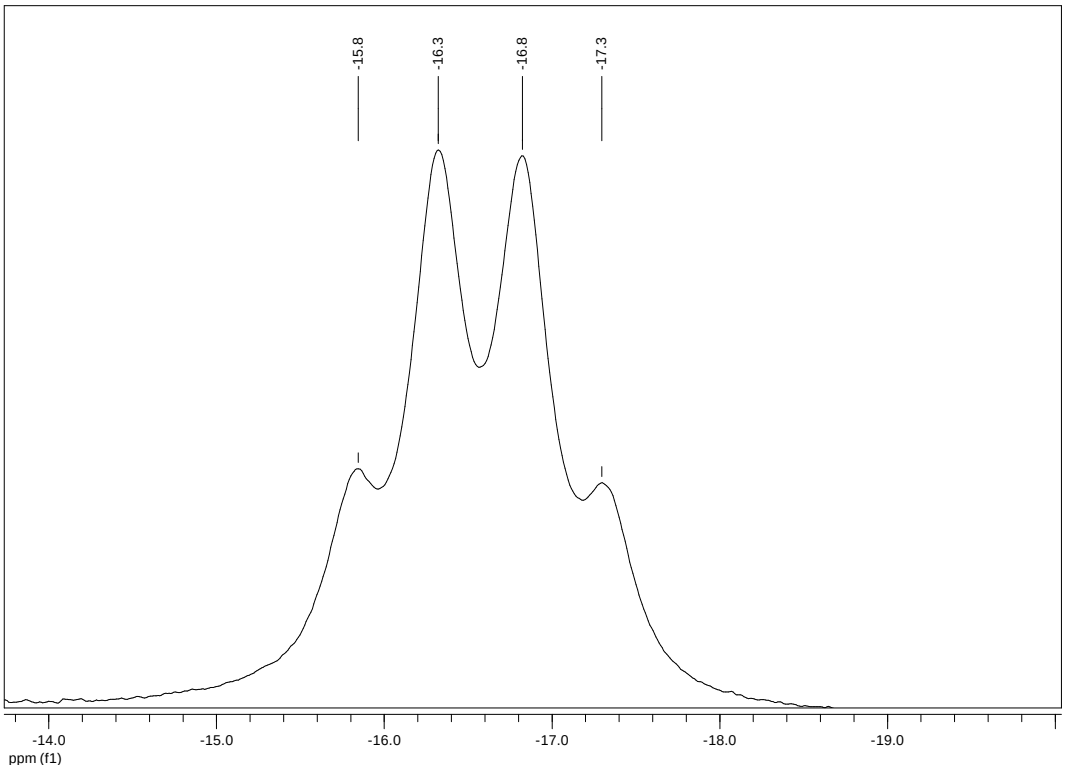
$^{1}$H-NMR of **3f** (400 MHz, $CD_3OD$)



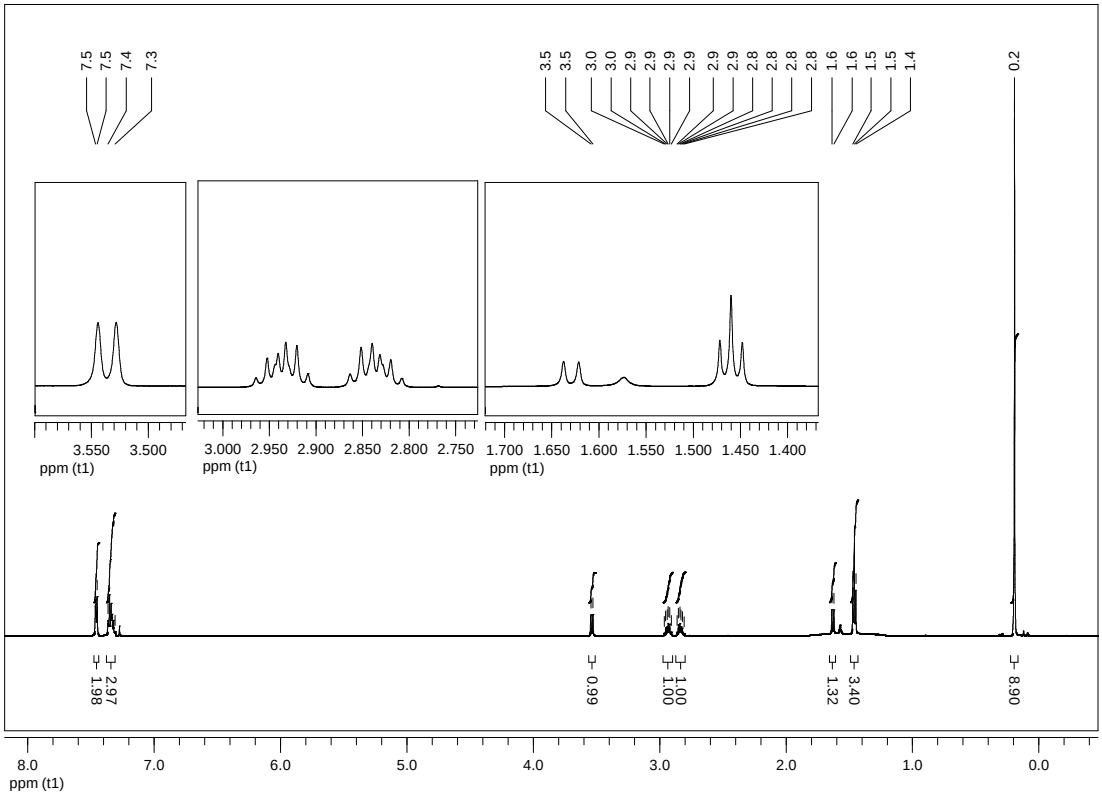

$^{13}$C-NMR of **3f** (100 MHz, $CD_3OD$)



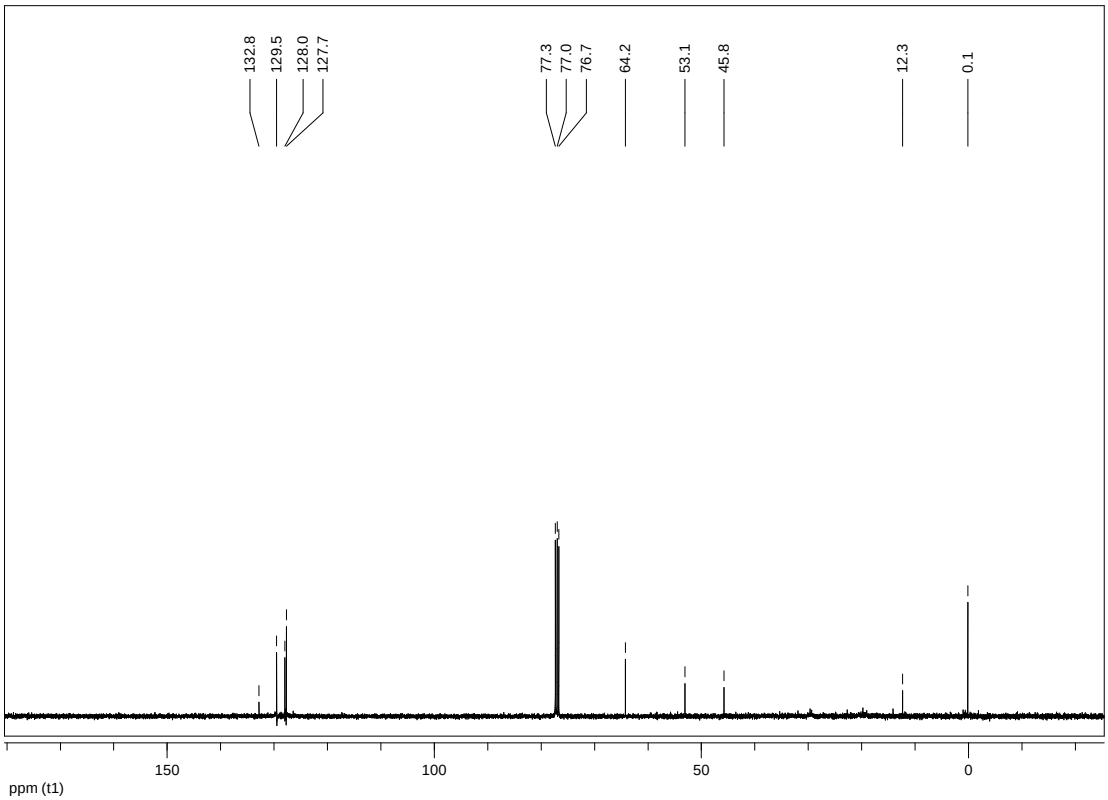
$^{11}$B-NMR of **3f** (192 MHz, $CDCl_3$)



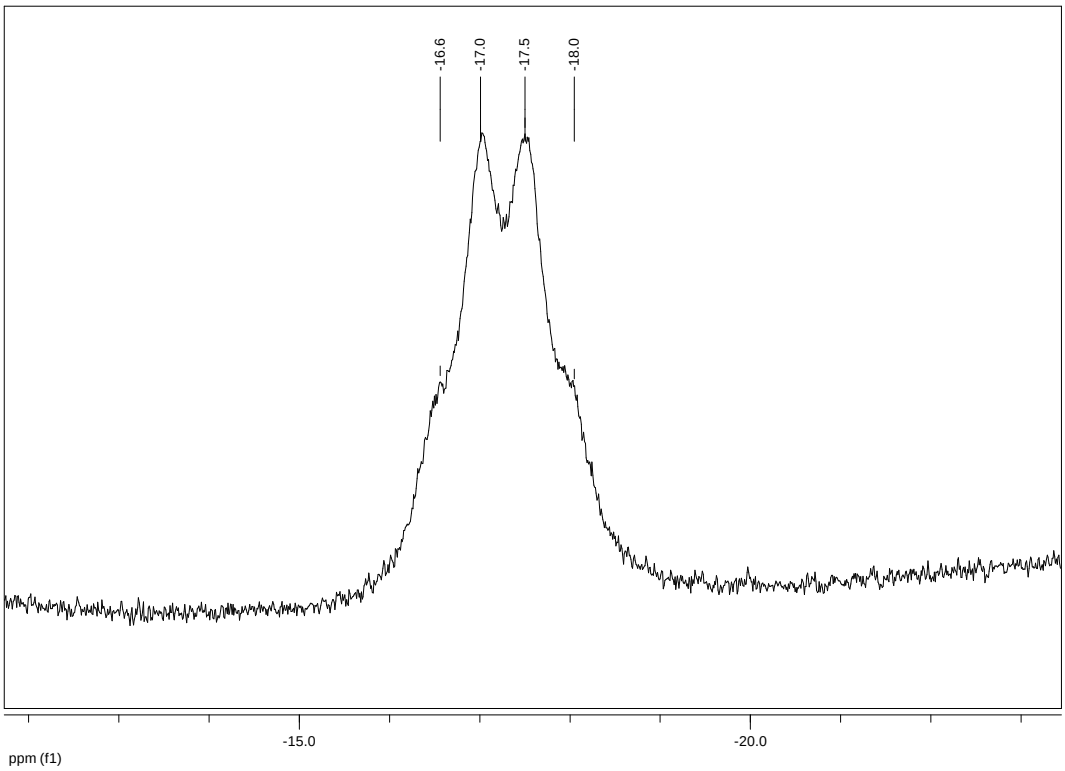

$^{1}$H-NMR of **3h** (600 MHz, $CDCl_3$)



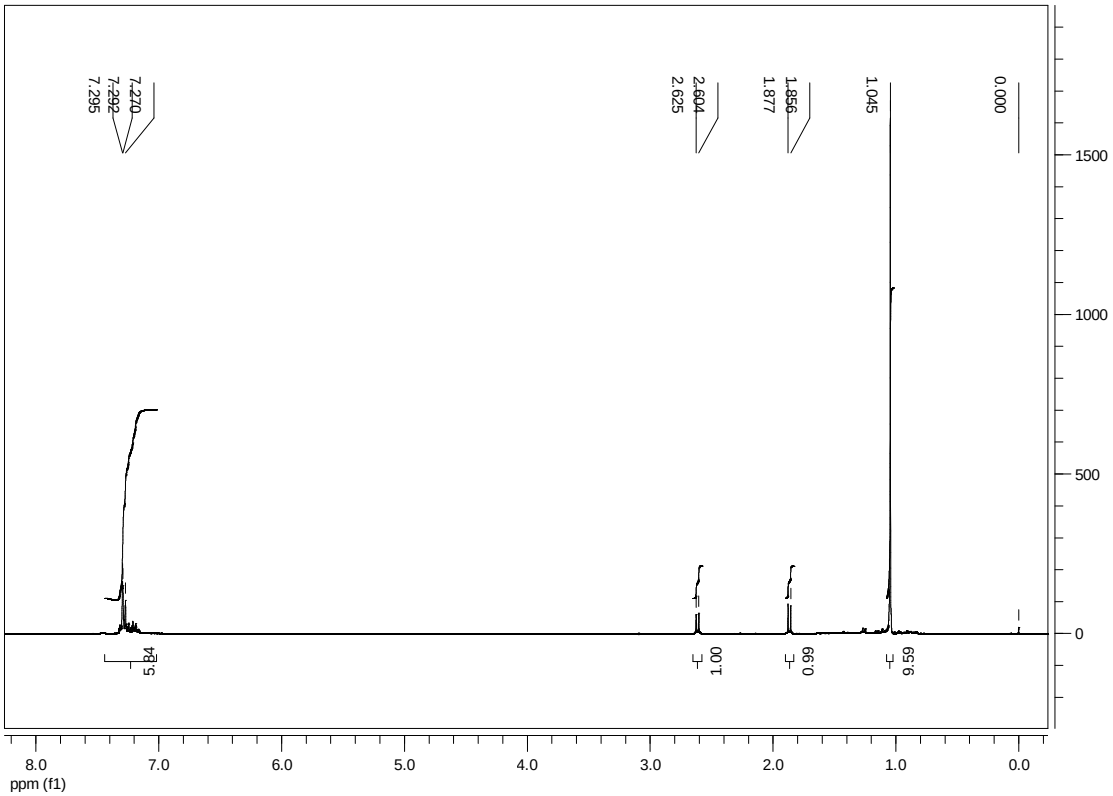
$^{13}$C-NMR of **3h** (100 MHz, $CDCl_3$)



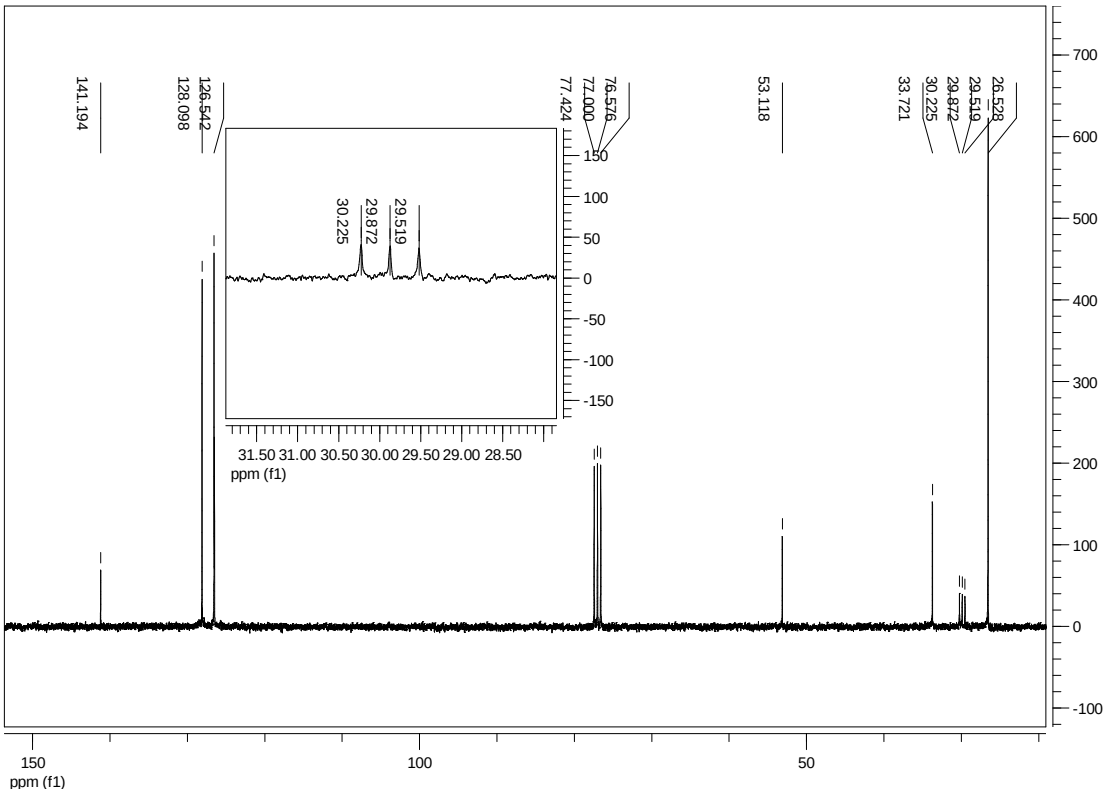

$^{11}$B-NMR of **3h** (192 MHz, $CDCl_3$)



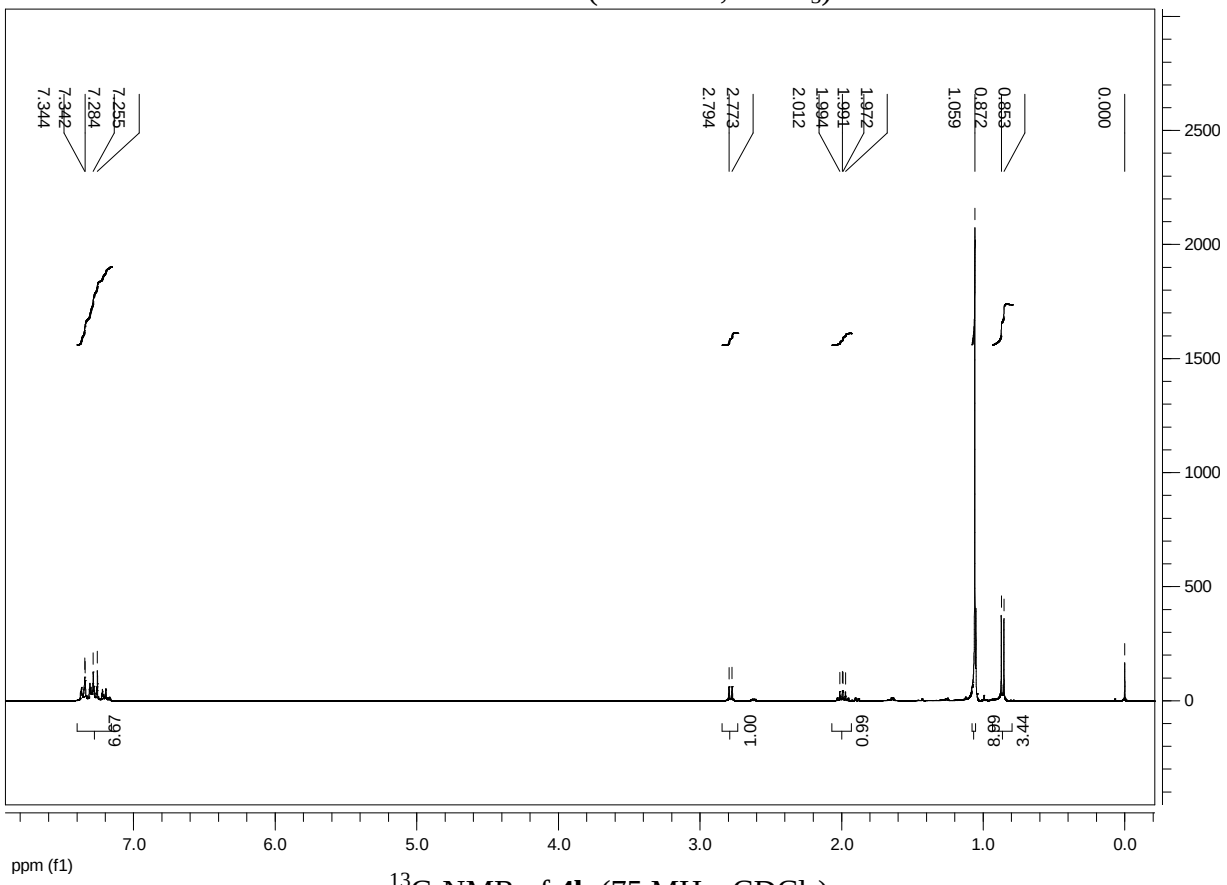
$^{1}$H-NMR of **4a** (300 MHz, $CDCl_3$)



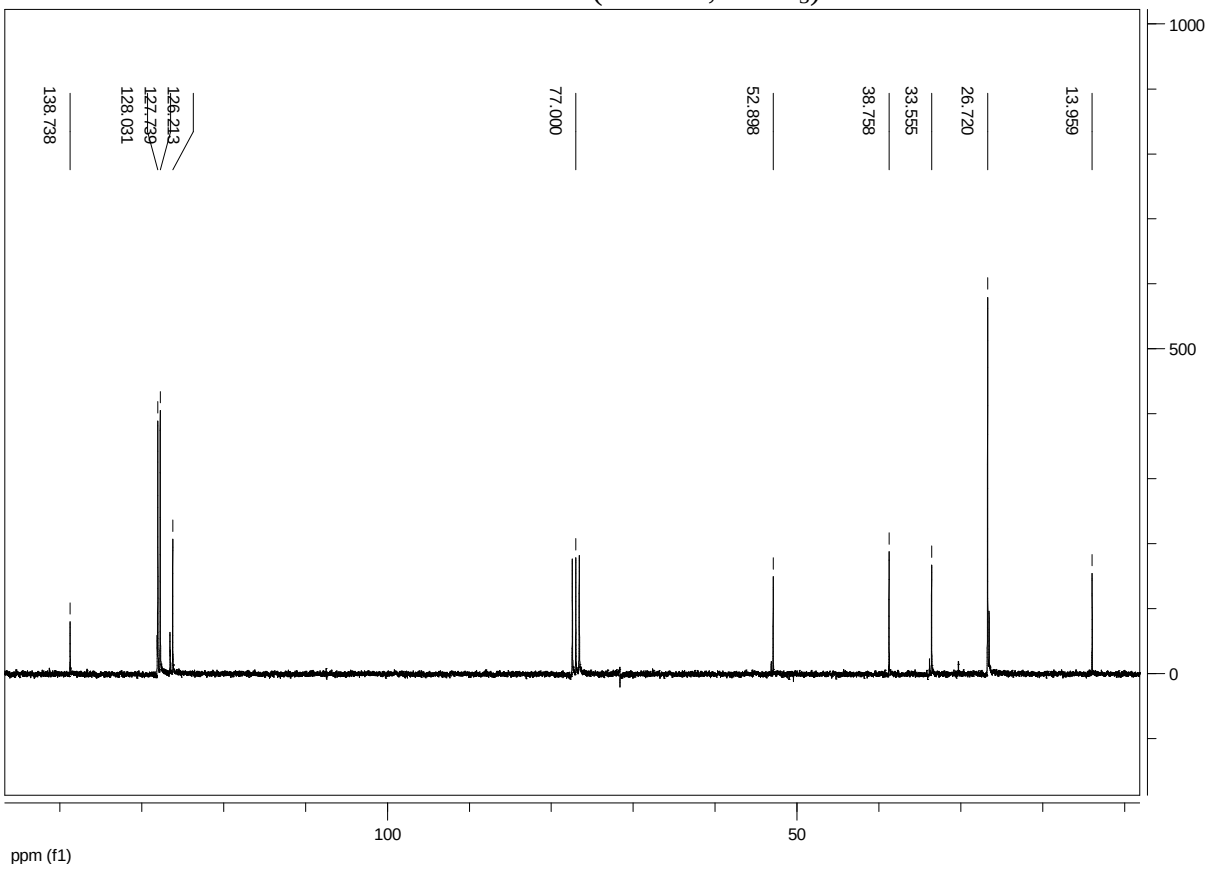

$^{13}$C-NMR of **4a** (75 MHz, $CDCl_3$)



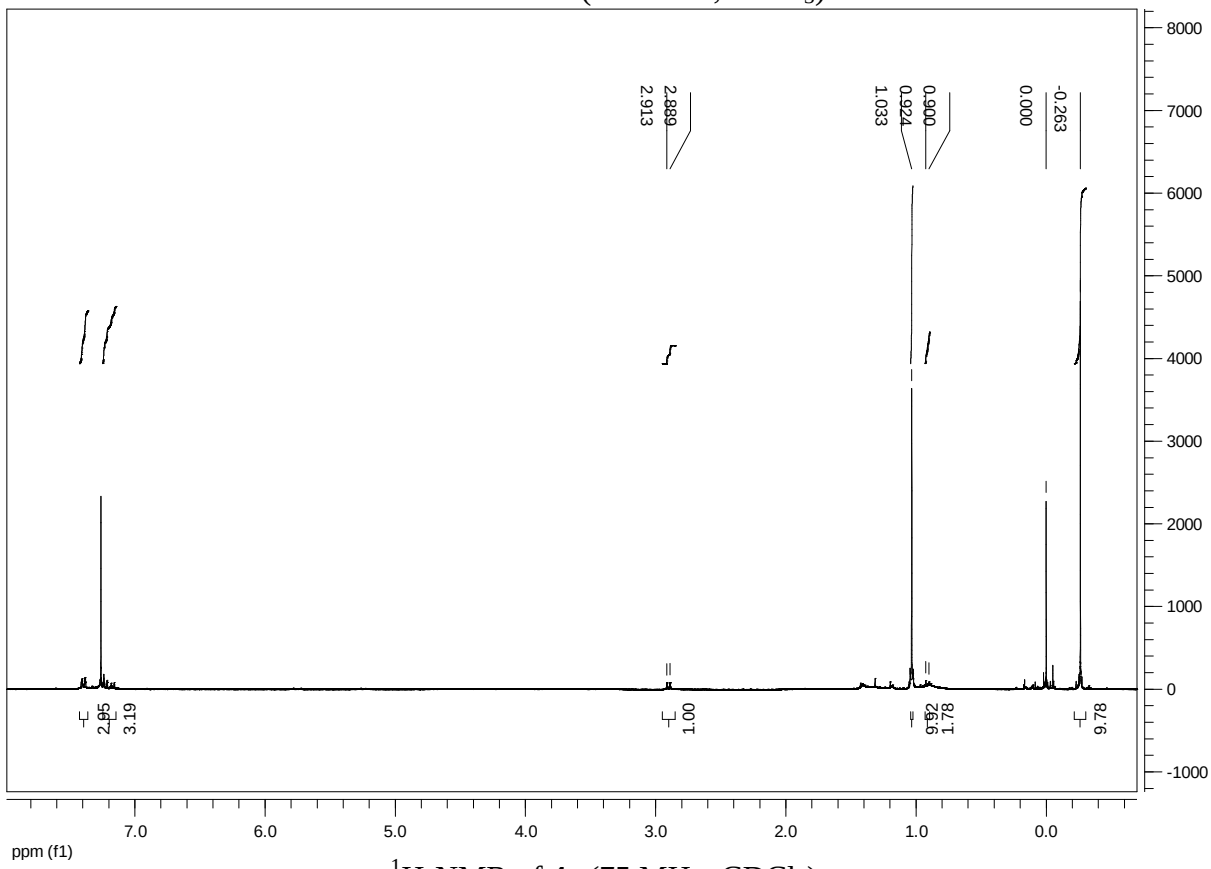
$^{1}$H-NMR of **4b** (300 MHz, $CDCl_3$)



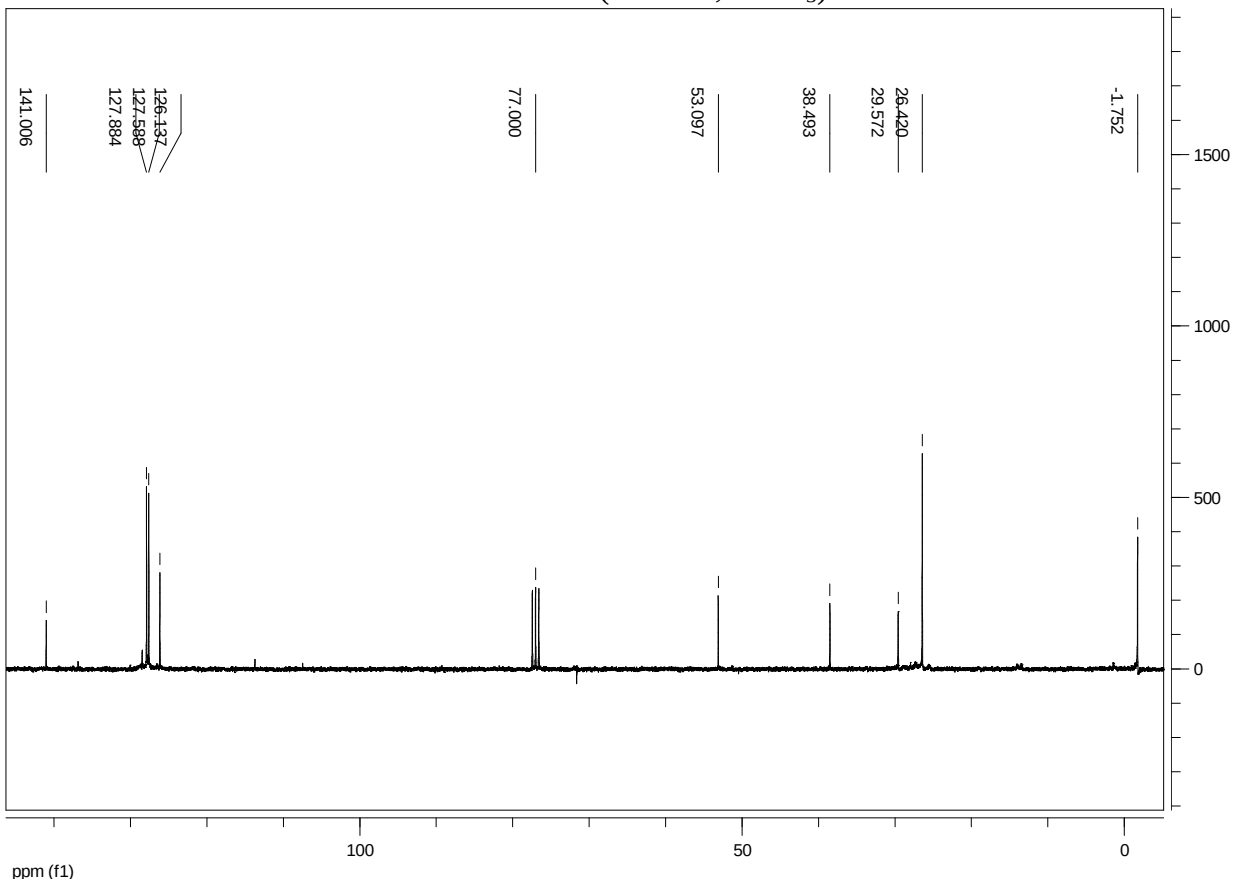

$^{13}$C-NMR of **4b** (75 MHz, $CDCl_3$)



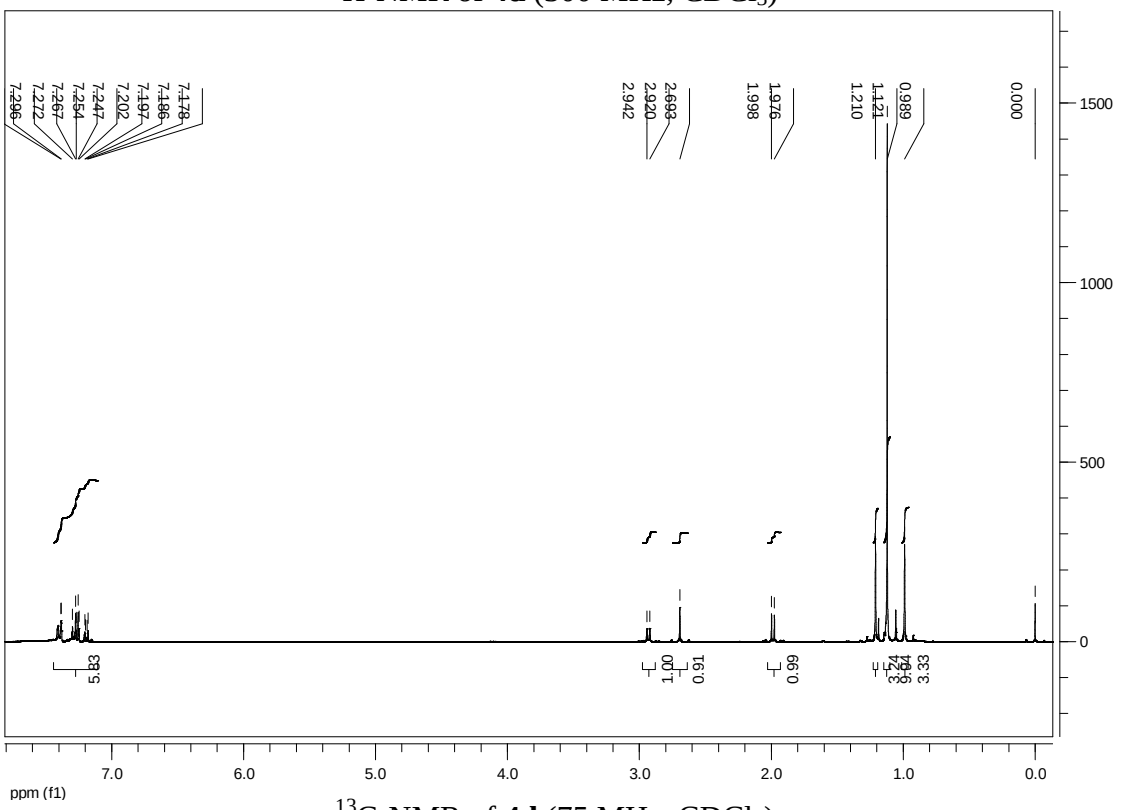
$^{1}$H-NMR of **4c** (300 MHz, $CDCl_3$)



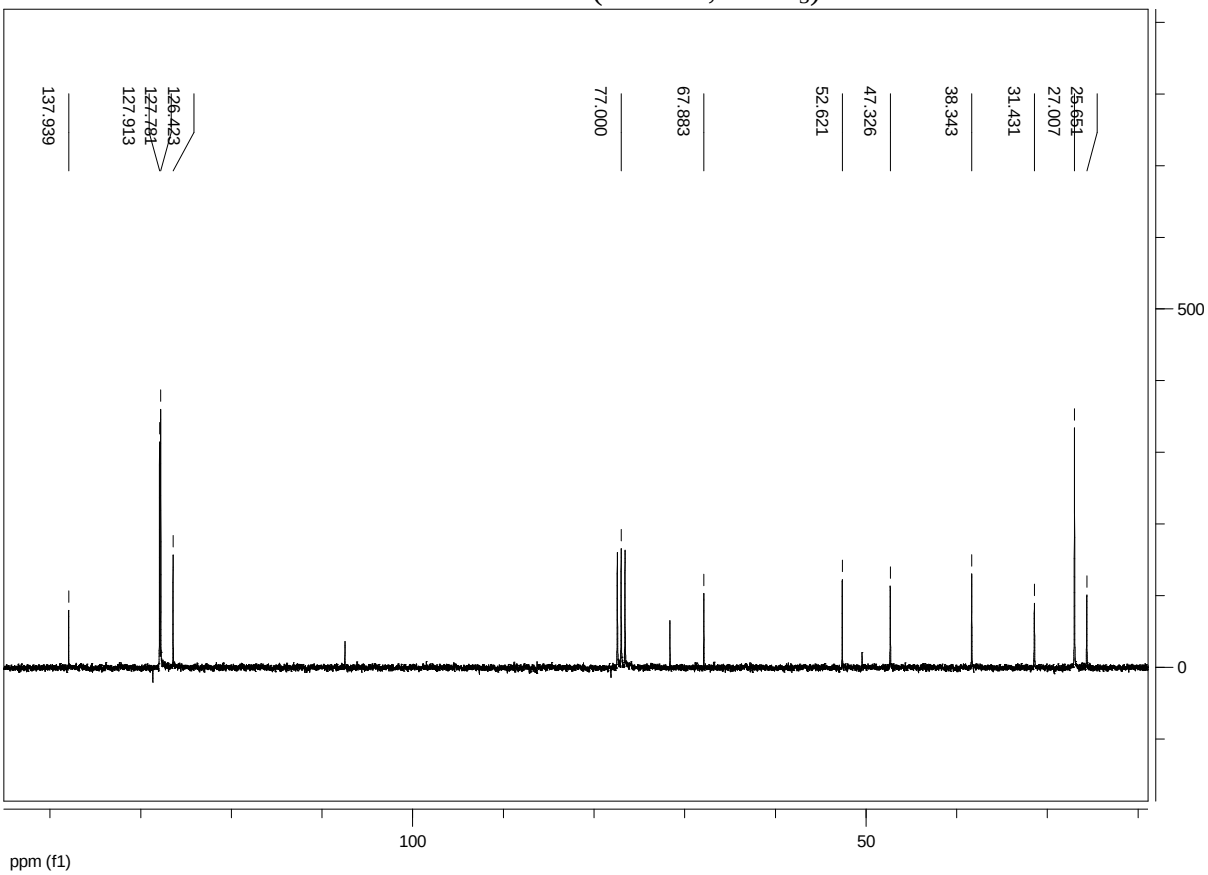

$^{1}$H-NMR of **4c** (75 MHz, $CDCl_3$)



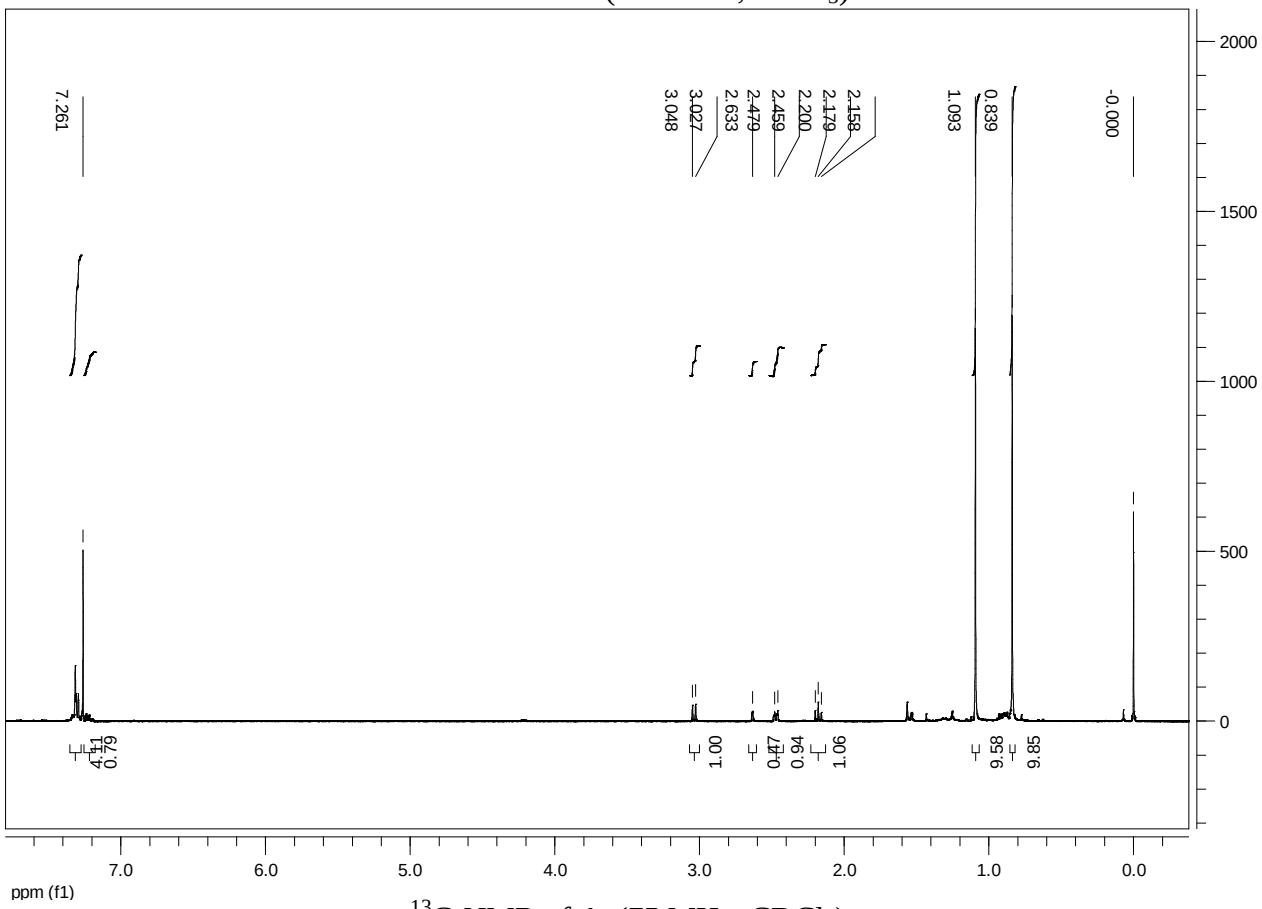
$^{1}$H-NMR of **4d** (300 MHz, $CDCl_3$)



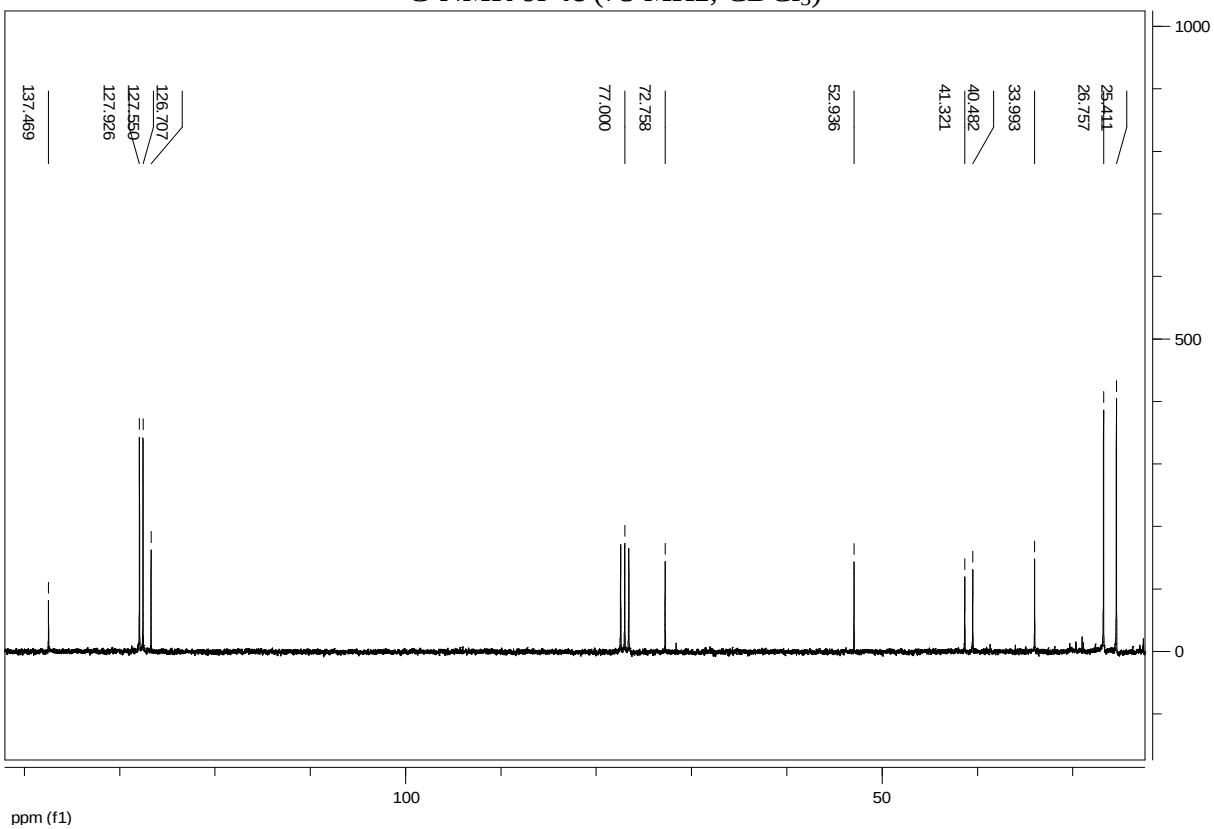

$^{13}$C-NMR of **4d** (75 MHz, $CDCl_3$)



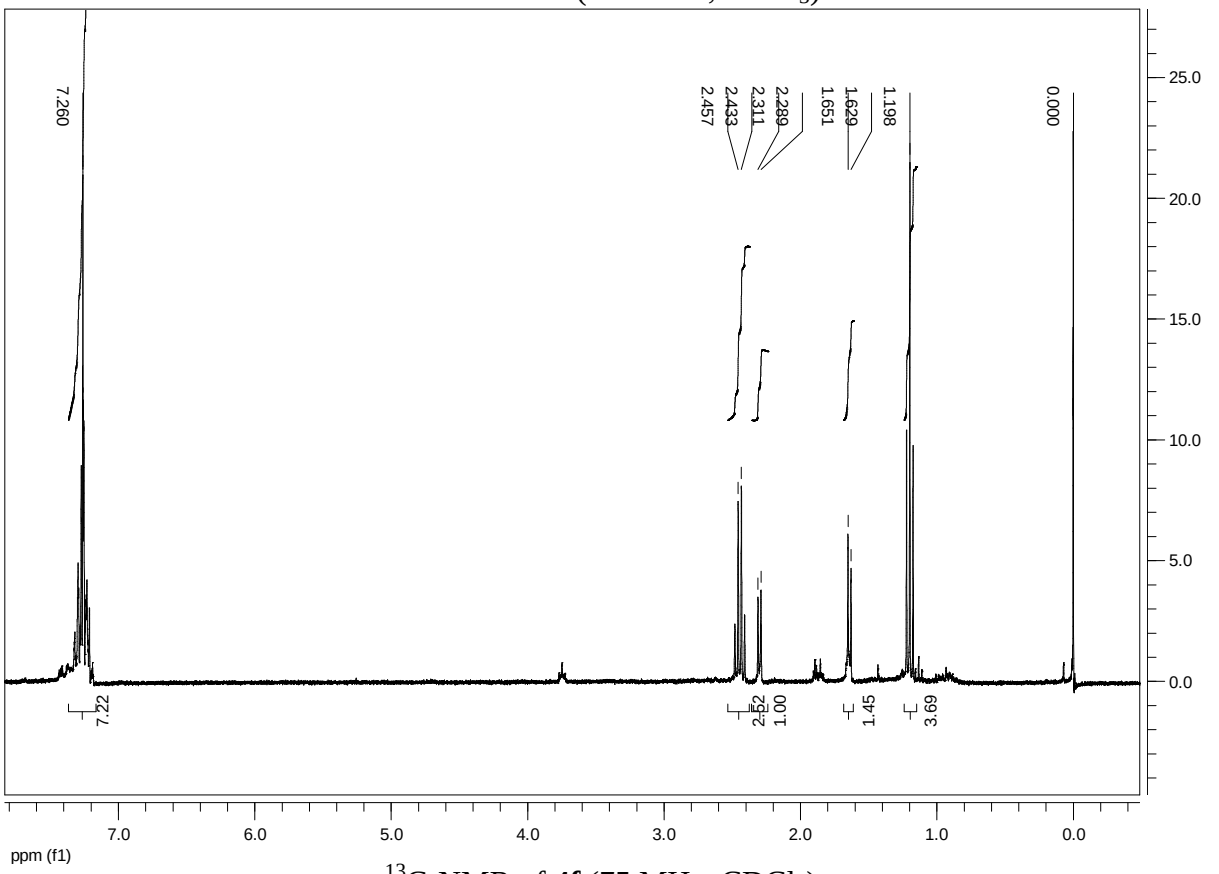
$^{1}$H-NMR of **4e** (300 MHz, $CDCl_3$)



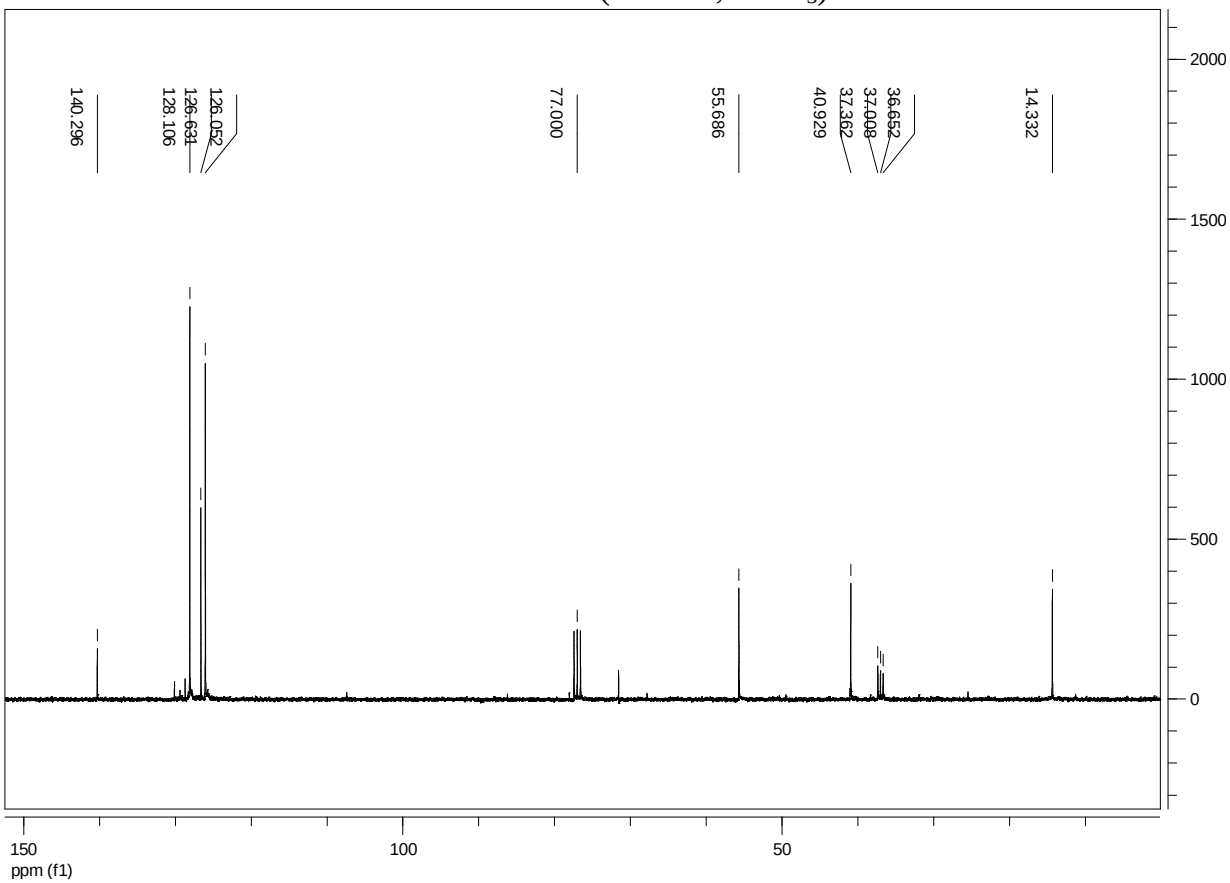

$^{13}$C-NMR of **4e** (75 MHz, $CDCl_3$)



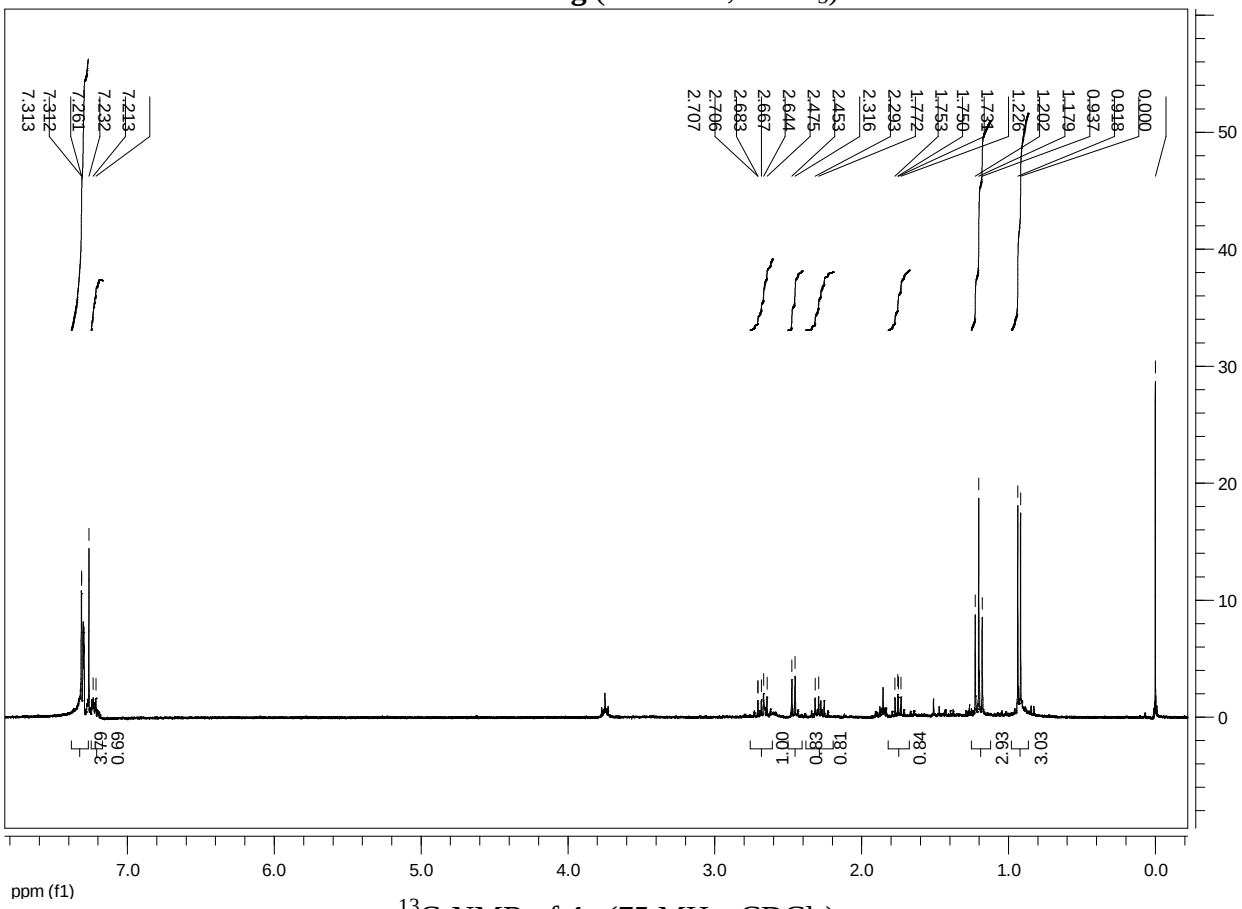
$^{1}$H-NMR of **4f** (300 MHz, $CDCl_3$)



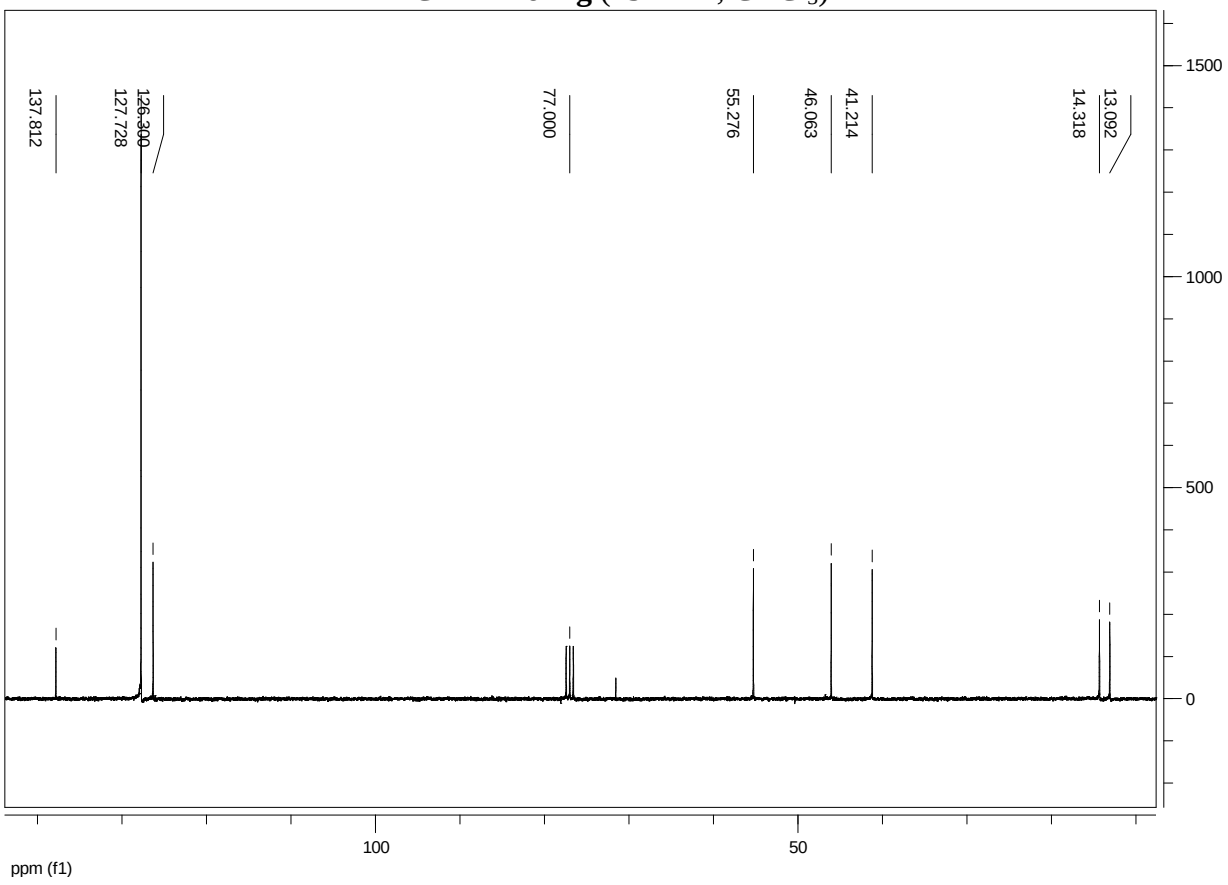

$^{13}$C-NMR of **4f** (75 MHz, $CDCl_3$)



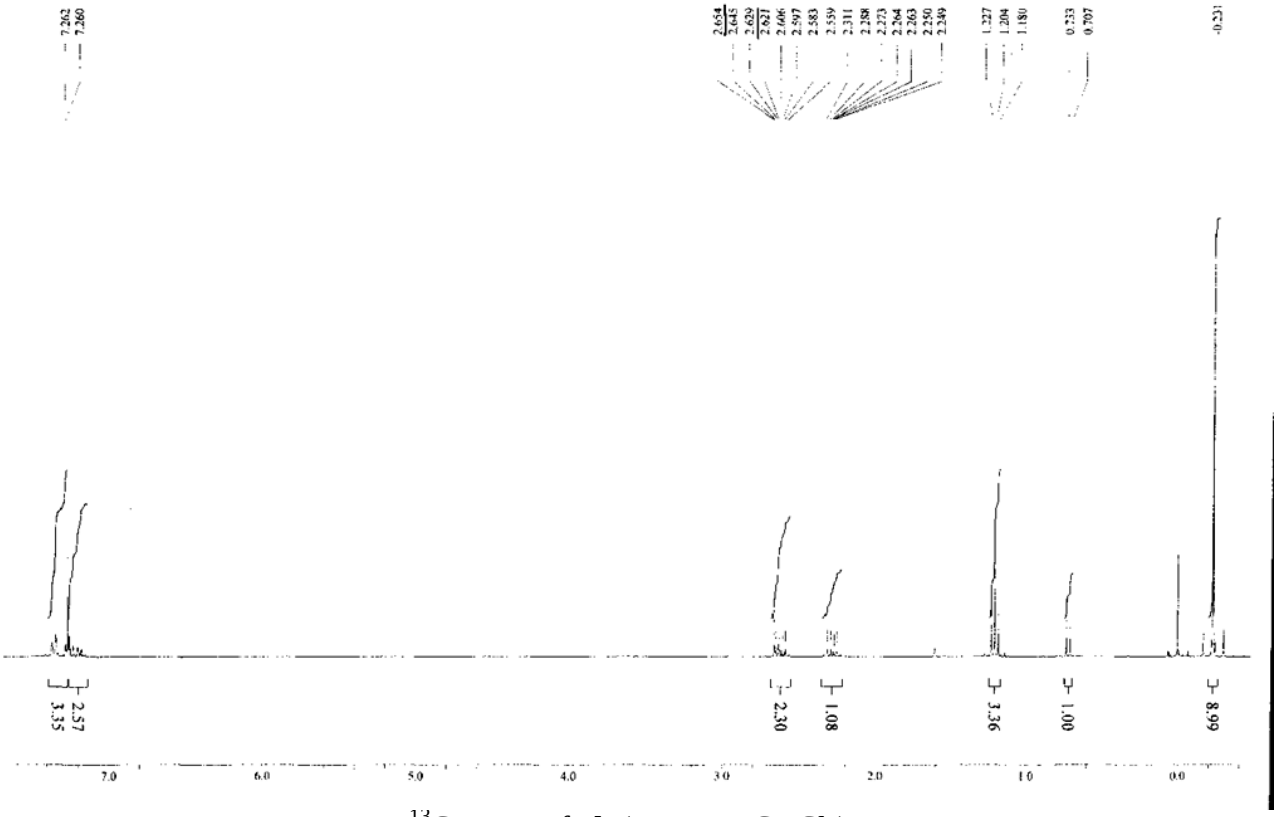
$^{1}$H-NMR of **4g** (300 MHz, $CDCl_3$)



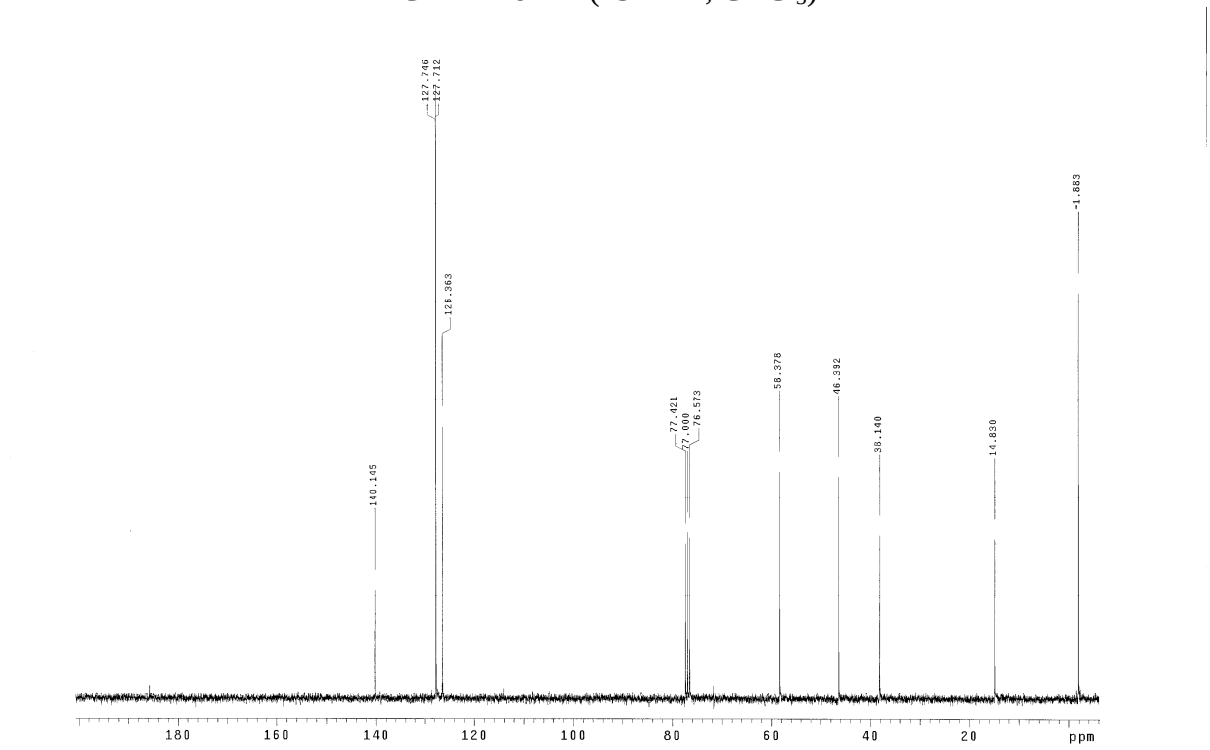

$^{13}$C-NMR of **4g** (75 MHz, $CDCl_3$)



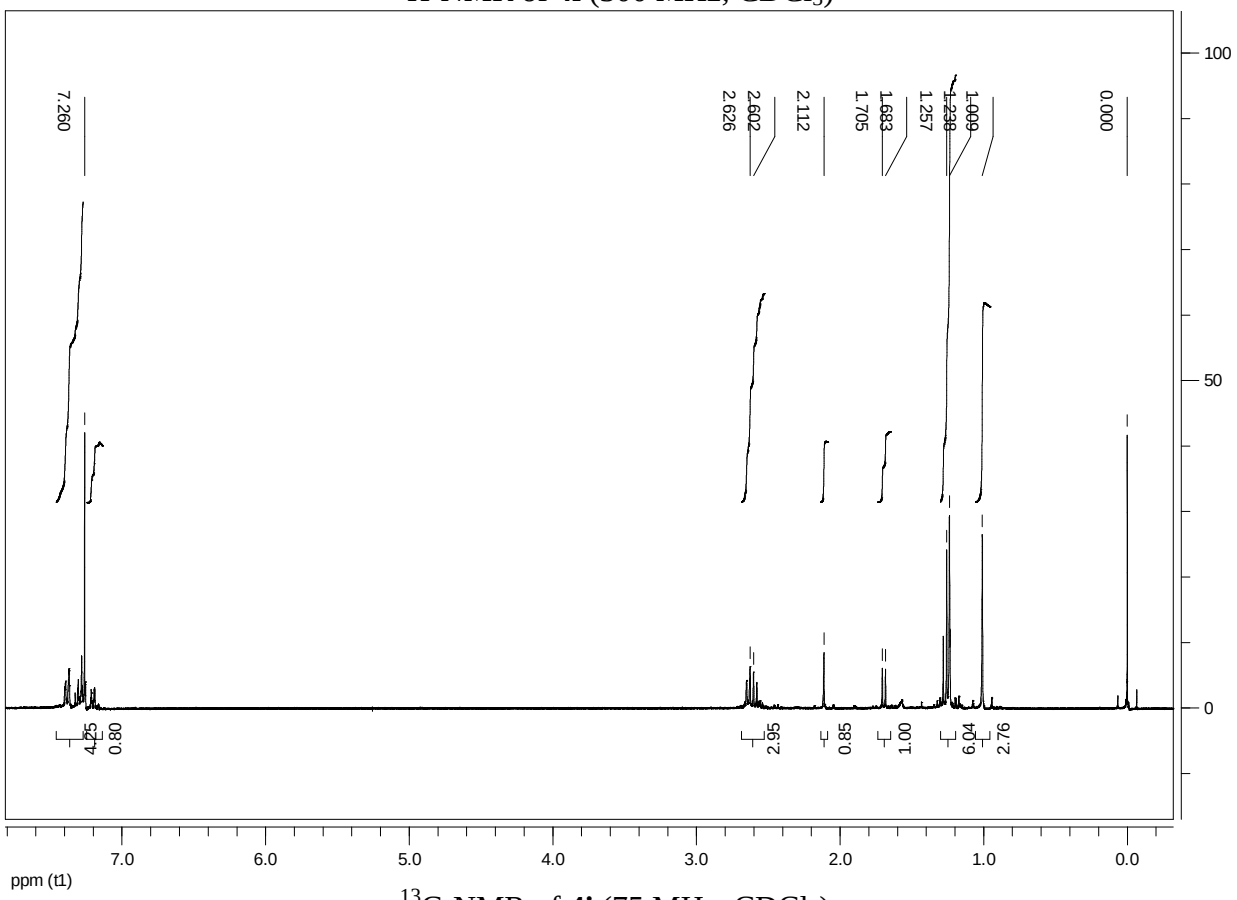
$^{1}$H-NMR of **4h** (300 MHz, $CDCl_3$)



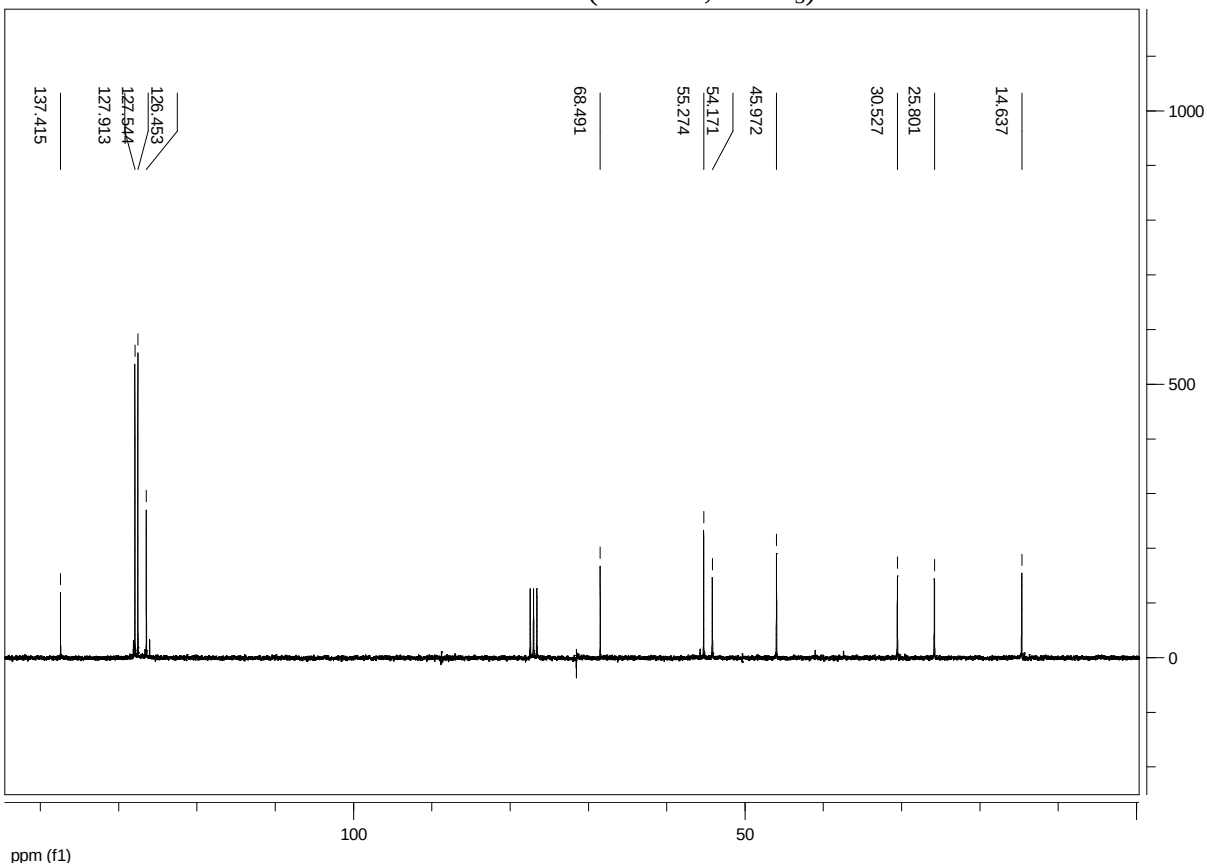

$^{13}$C-NMR of **4h** (75 MHz, $CDCl_3$)



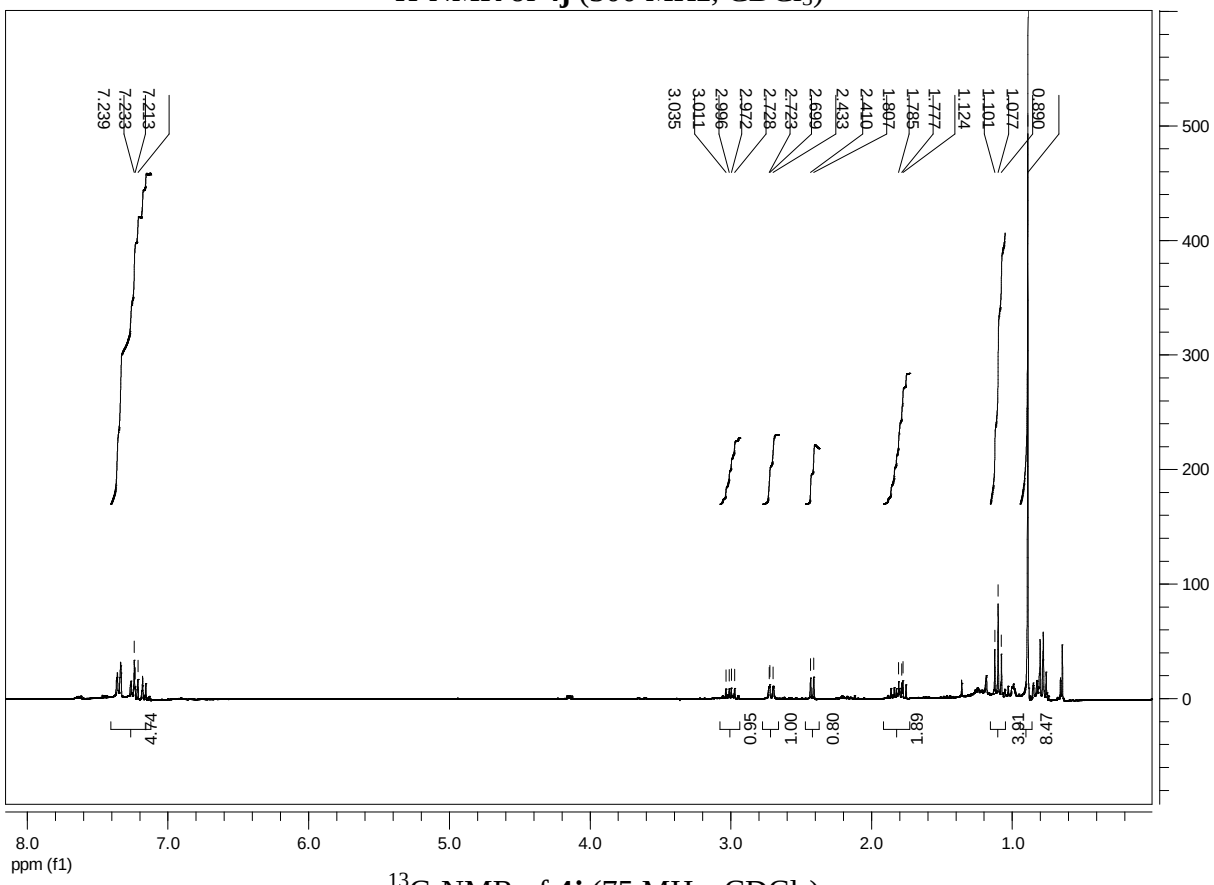
$^{1}$H-NMR of **4i** (300 MHz, $CDCl_3$)



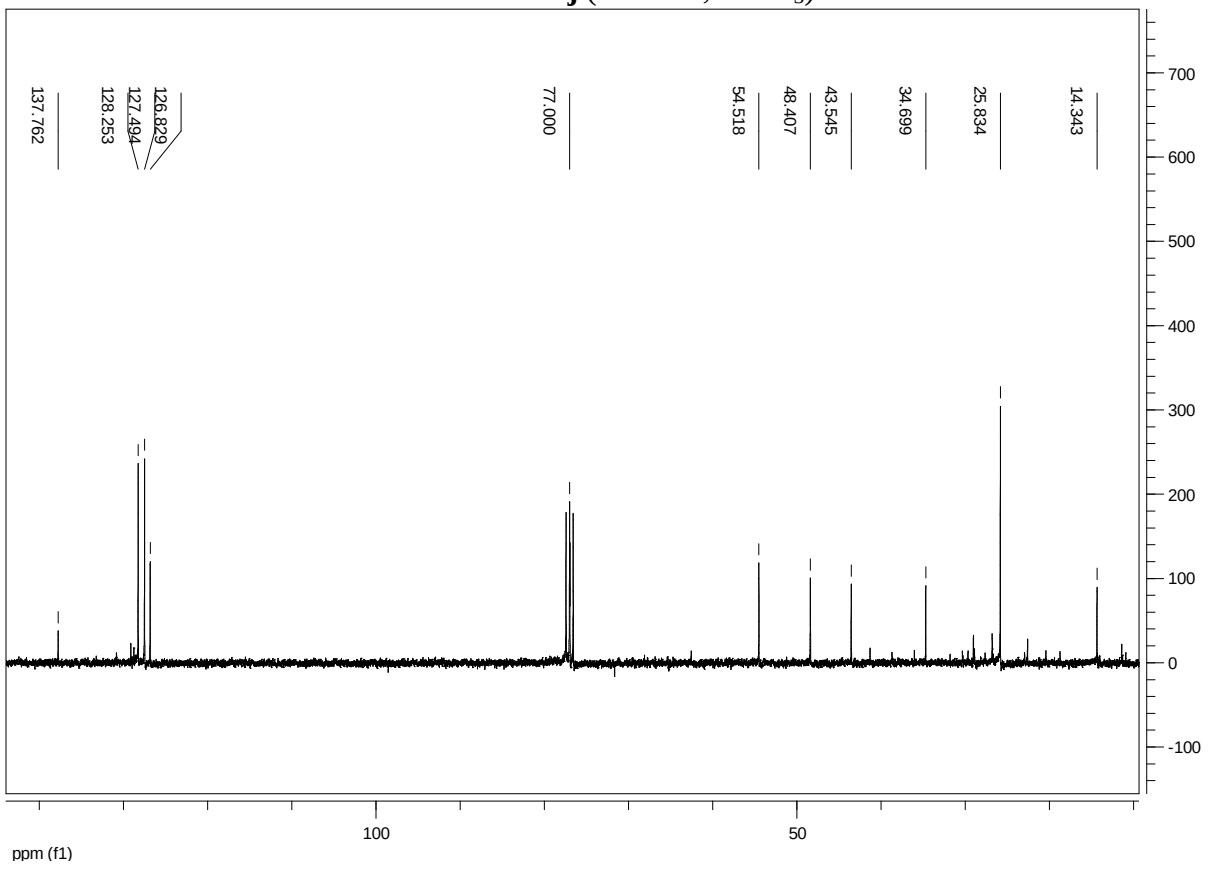

$^{13}$C-NMR of **4i** (75 MHz, $CDCl_3$)



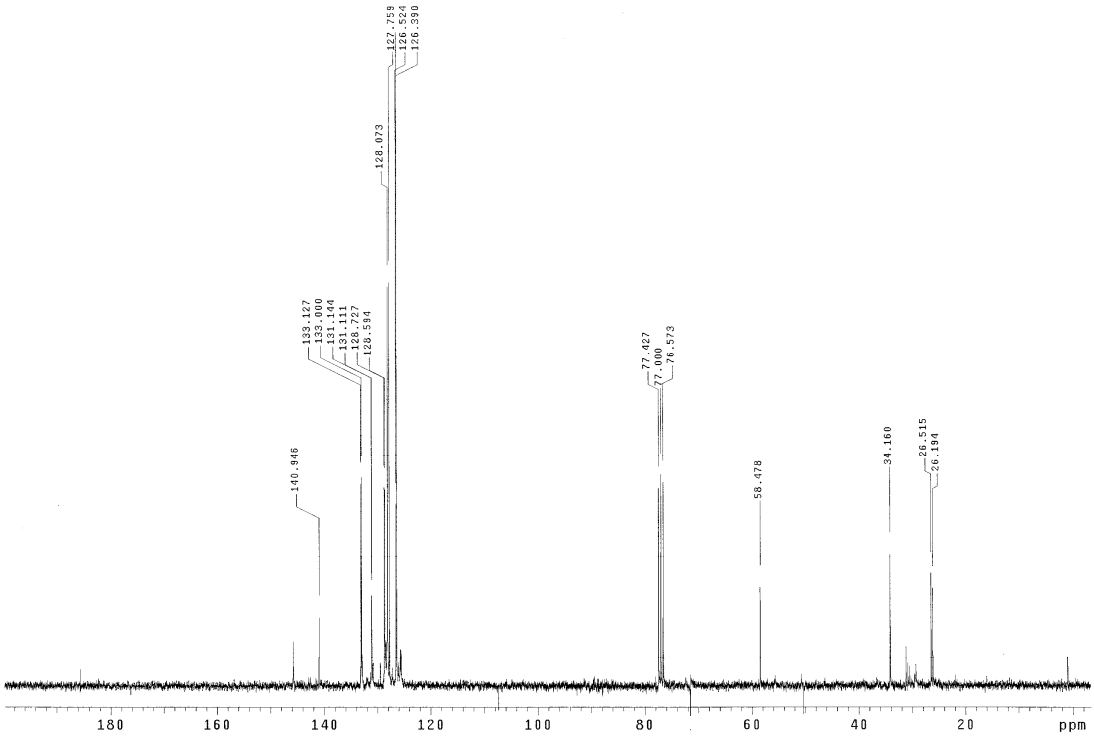
$^{1}$H-NMR of **4j** (300 MHz, $CDCl_3$)



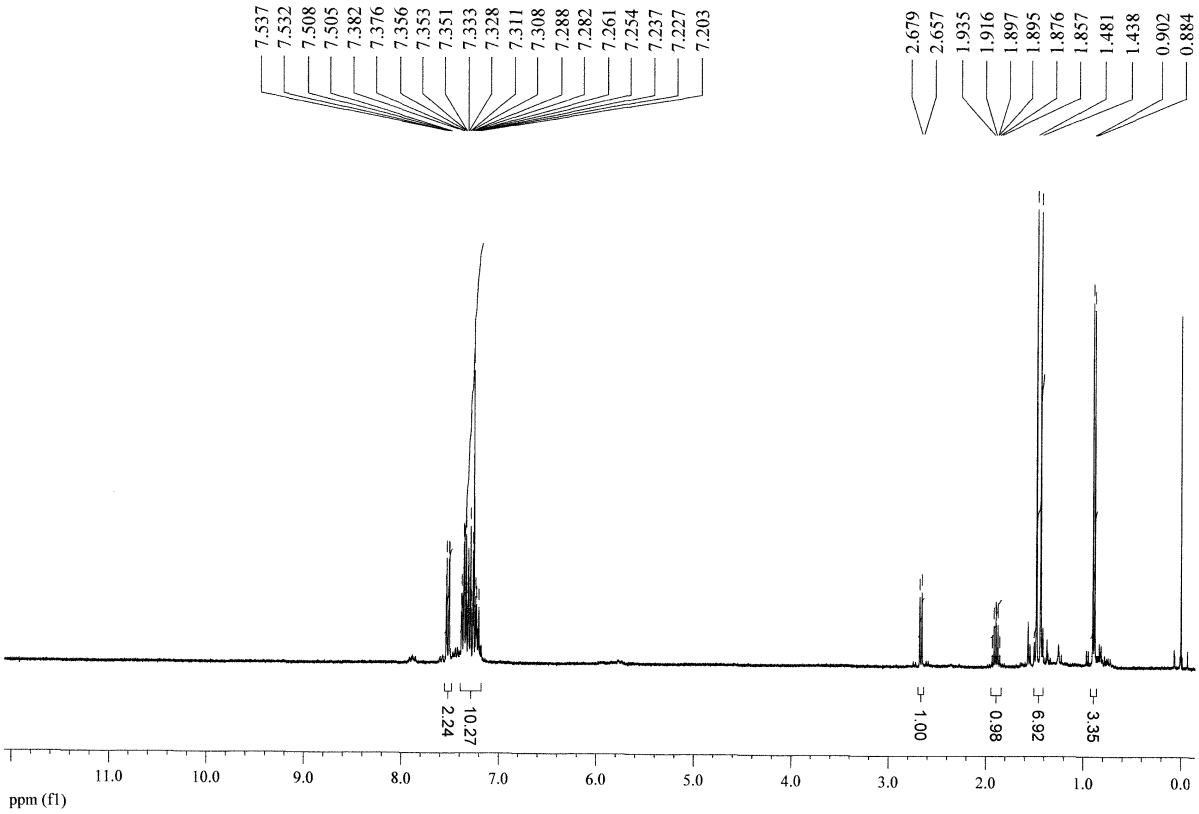

$^{13}$C-NMR of **4j** (75 MHz, $CDCl_3$)



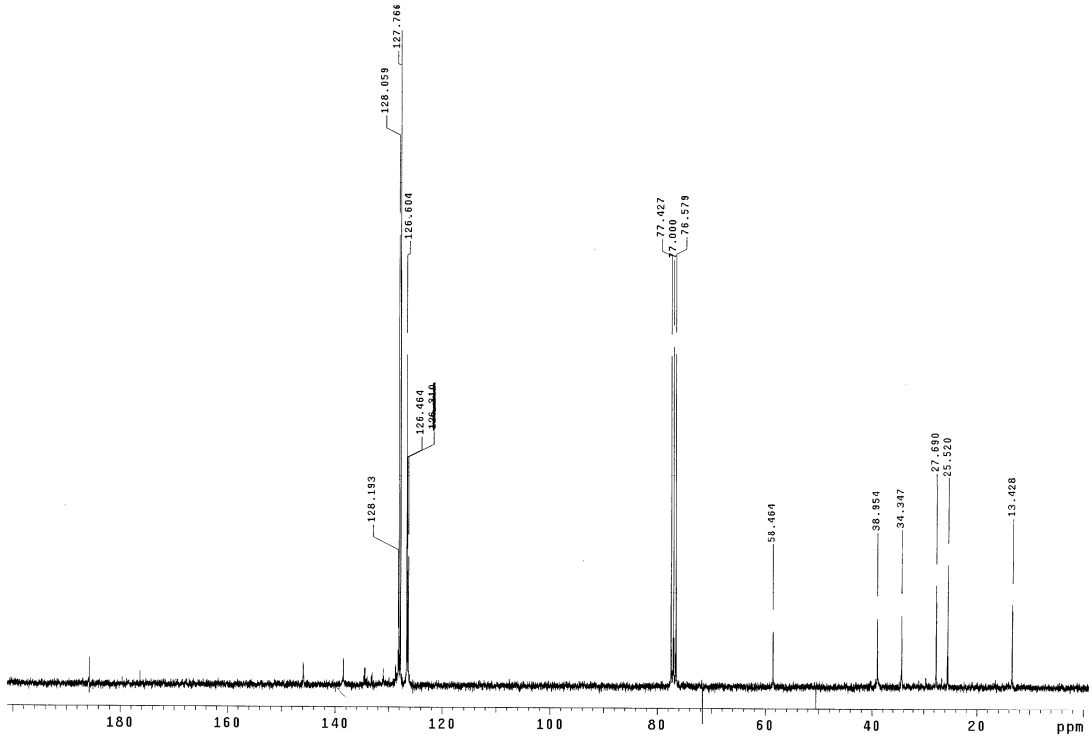
$^{13}$C-NMR of **4k** (75 MHz, $CDCl_3$)



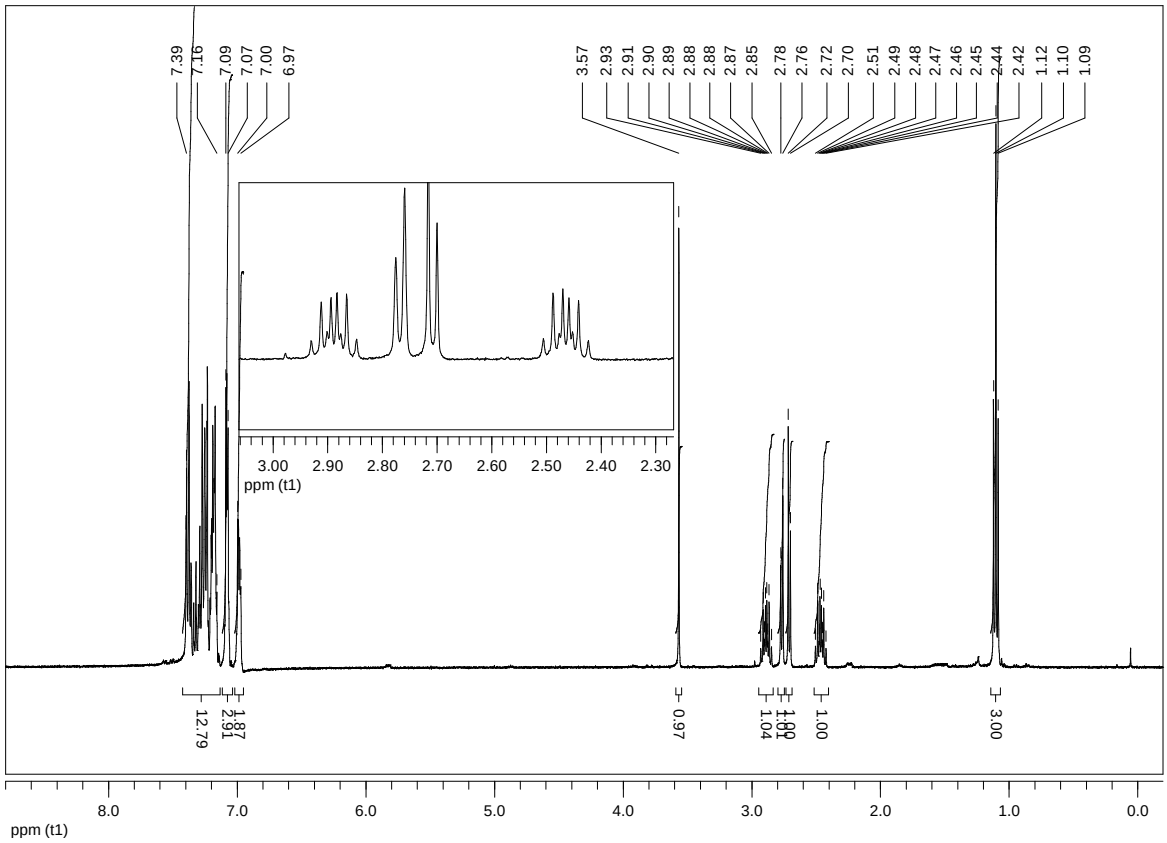
$^{1}$H-NMR of **4l** (300 MHz, $CDCl_3$)



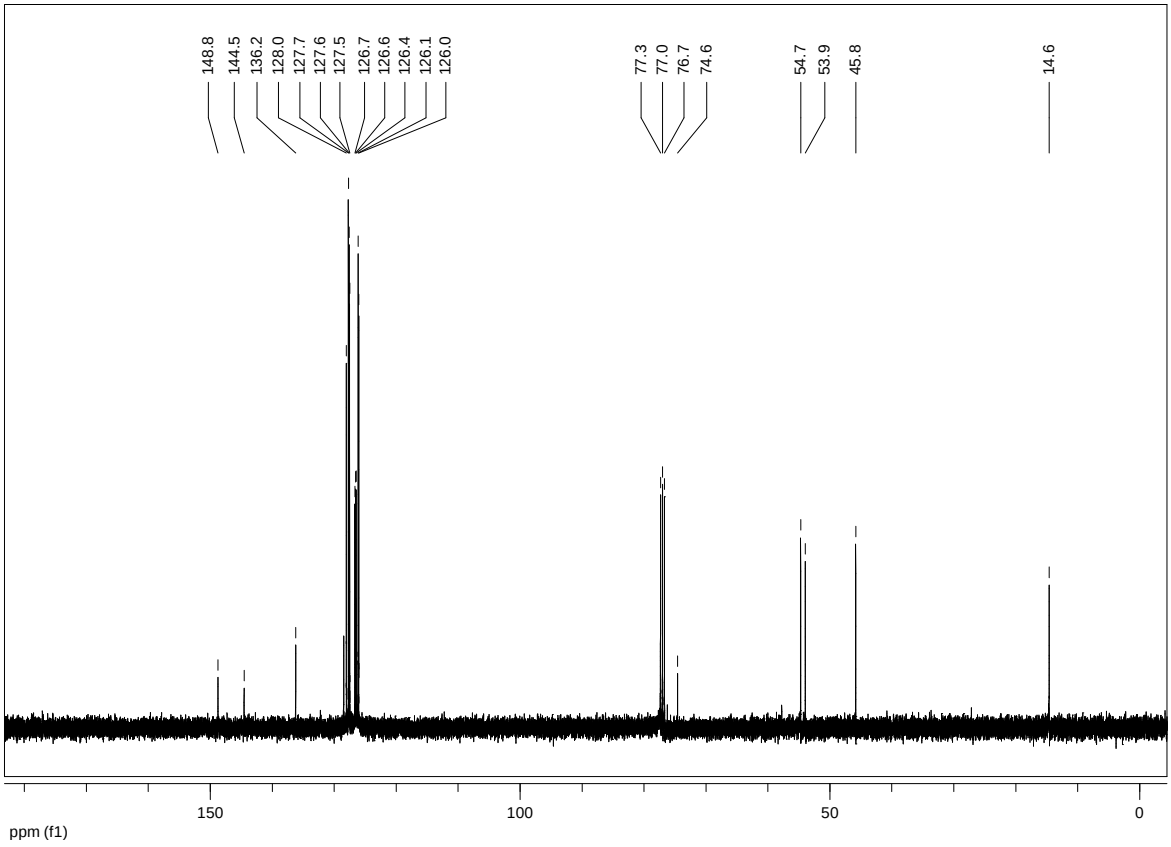

$^{13}$C-NMR of **4l** (75 MHz, $CDCl_3$)



$^{1}$H-NMR of **4m** (400 MHz, $CDCl_3$)

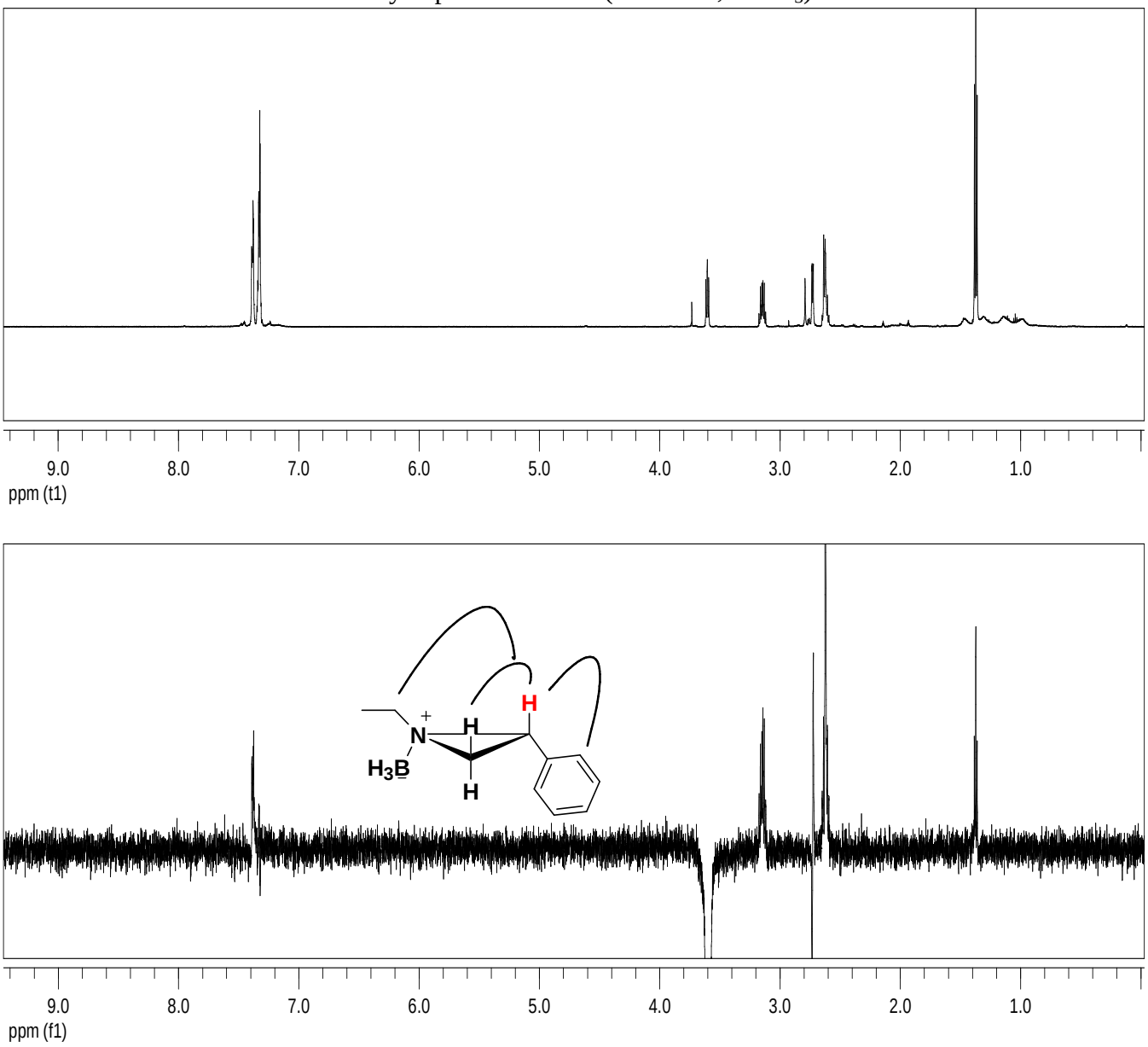



$^{13}$C-NMR of **4m** (100 MHz, $CDCl_3$)

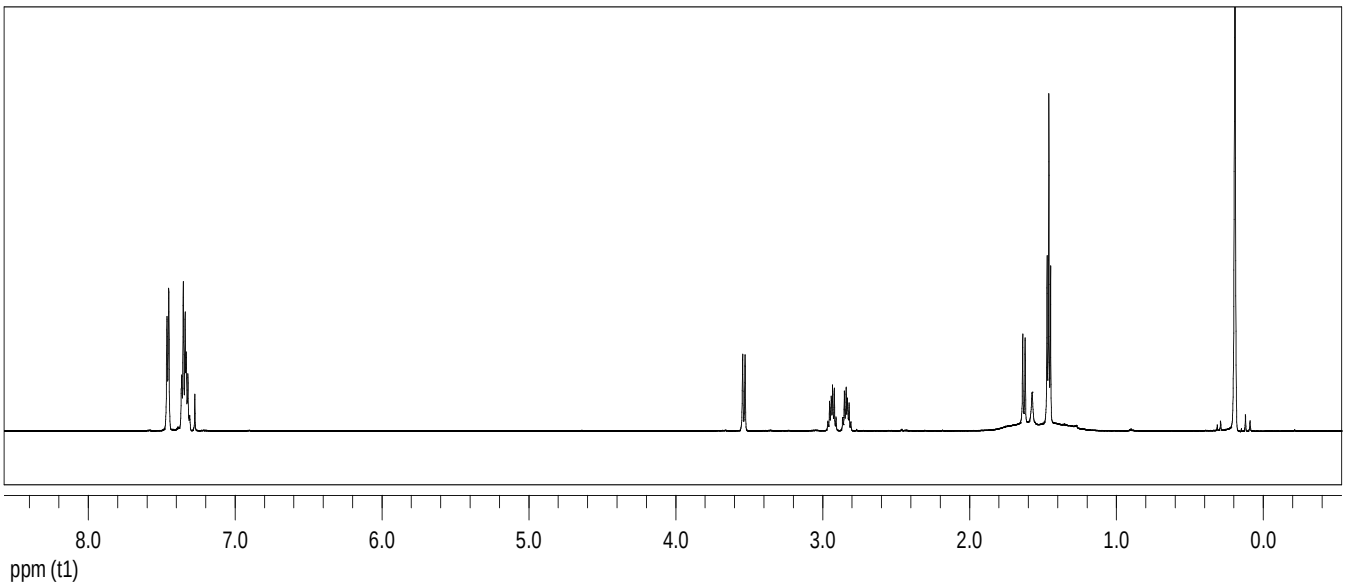


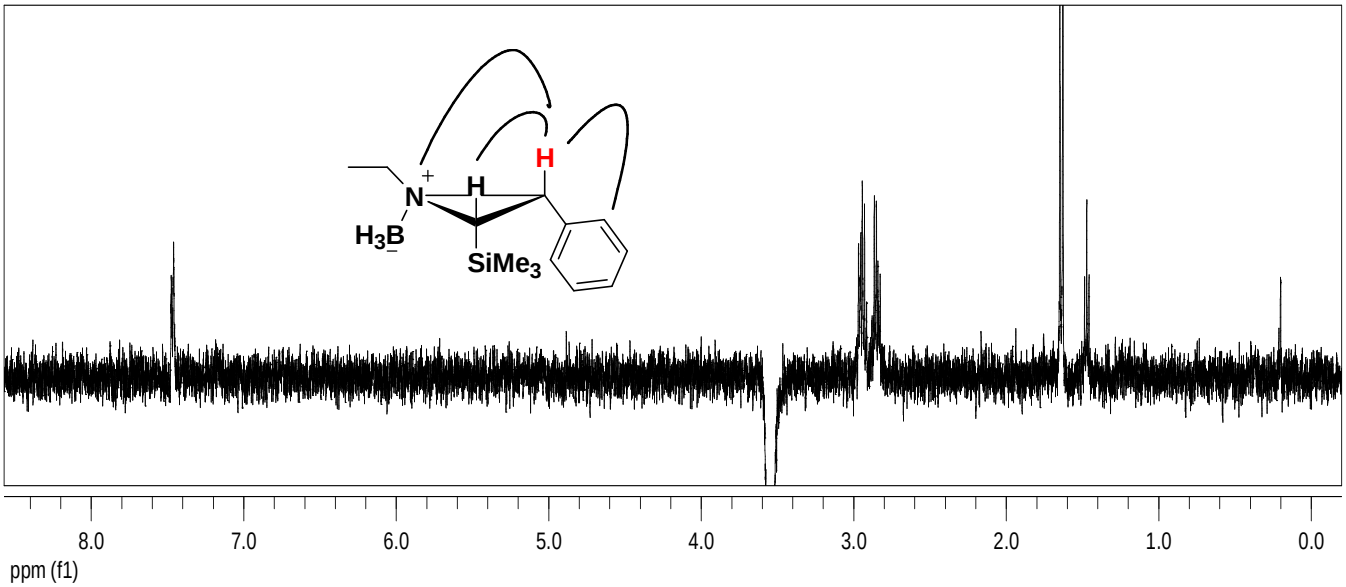
**Selected copies of 1D NOESY experiments.**

1D Noesy experiment of **2b** (600 MHz, $CDCl_3$)

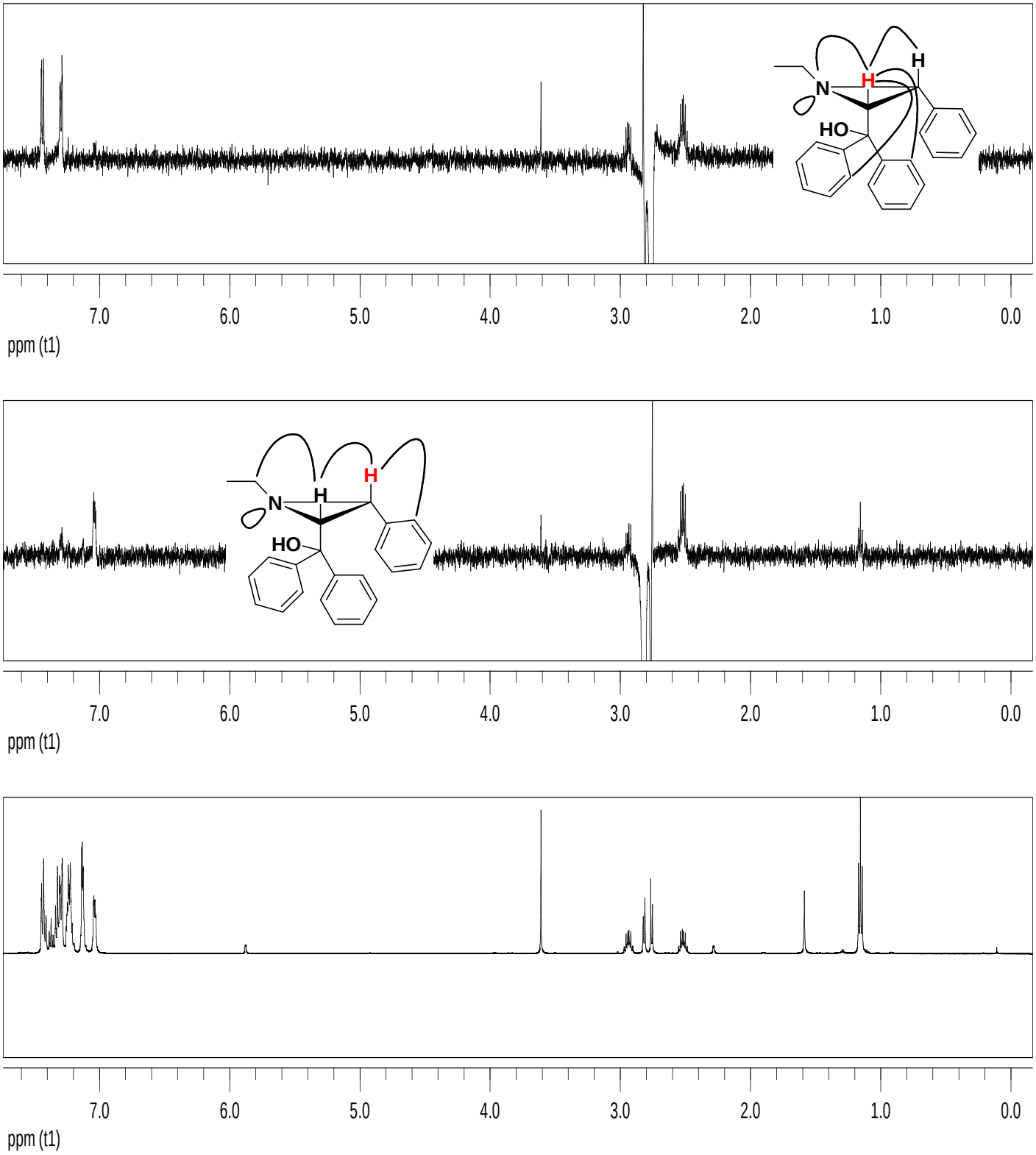


1D Noesy experiment of **3f** (500 MHz, $CDCl_3$)



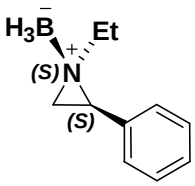



1D Noesy experiment of **4m** (500 MHz, $CDCl_3$)

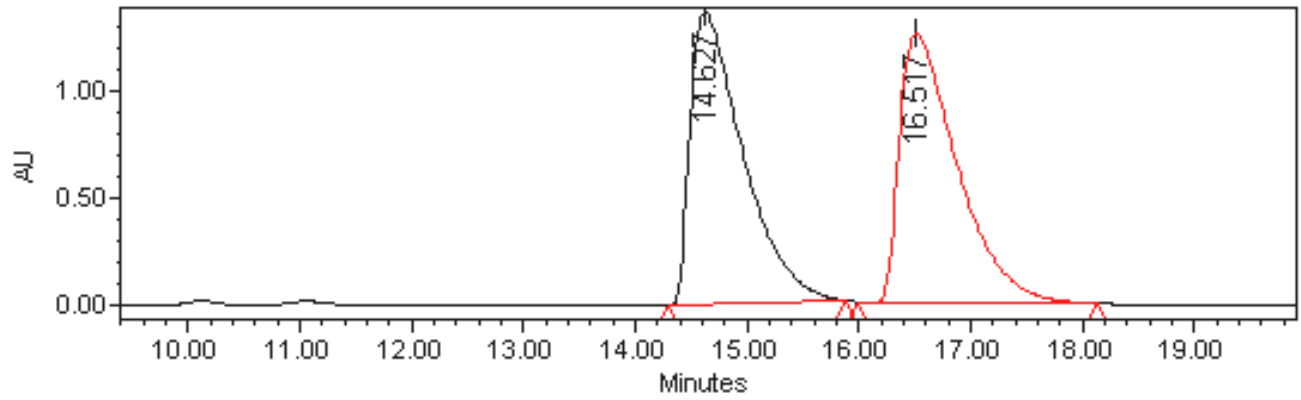


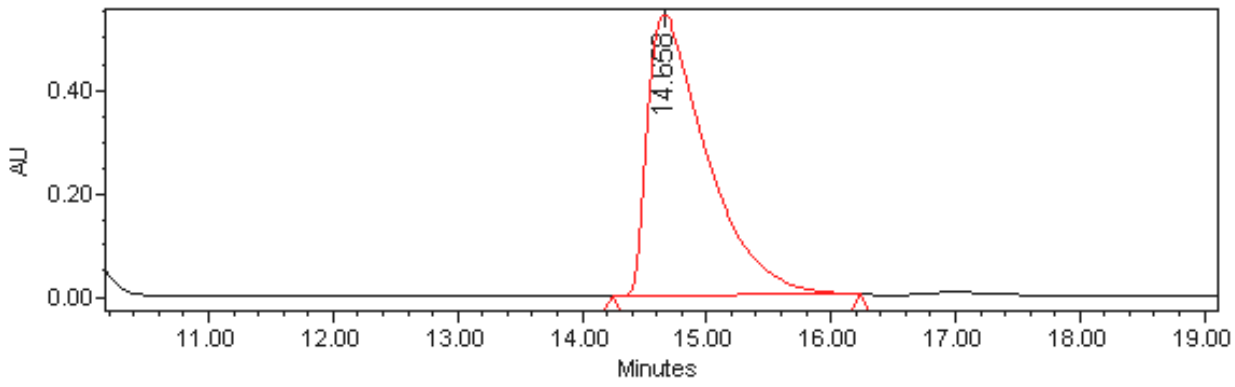
**Determination of the enantiomeric ratios by HPLC analysis.**

HPLC analysis of racemic and enantioenriched **(*S*,*S*)-2b**

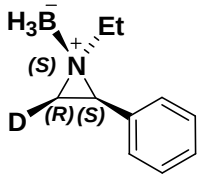



Cellulose – Lux2, Hexane-*i*PrOH 90:1, 1.0 mL/min, 227 nm er > 98:2

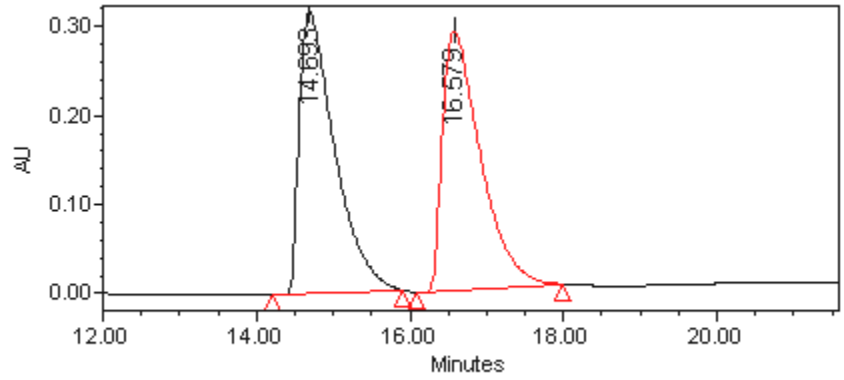


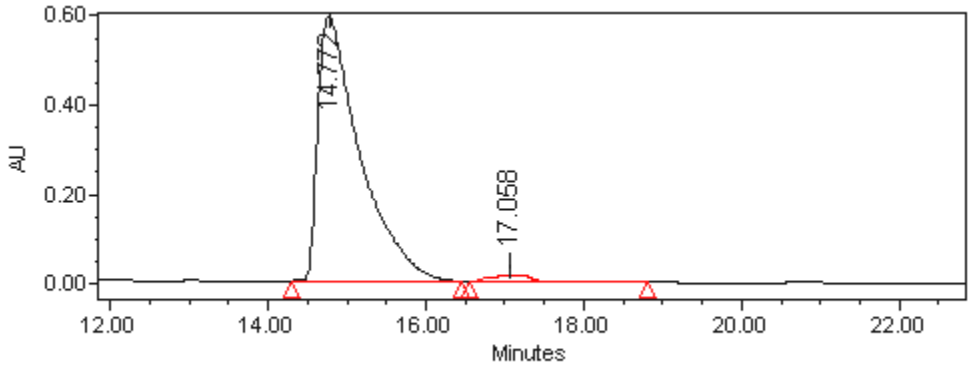



HPLC analysis of racemic and enantioenriched **(*S*,*S*,*R*)-3f**

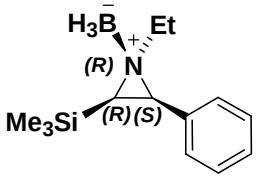



Cellulose – Lux2, Hexane-*i*PrOH 90:1, 1.0 mL/min, 227 nm; er = 91:9

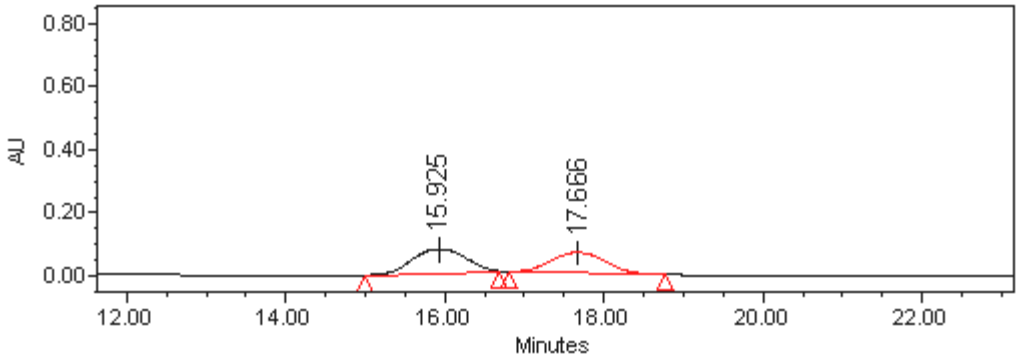


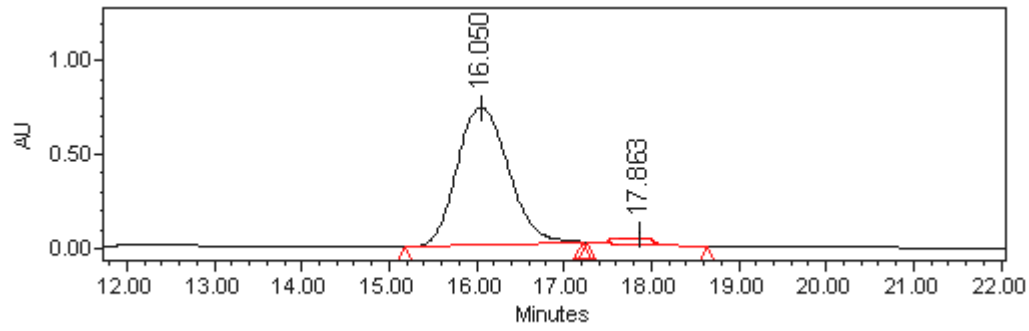



HPLC analysis of racemic and enantioenriched (*R*,*S*,*R*)-3h

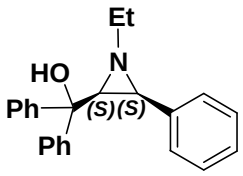



Cellulose – Lux2, Hexane-*i*PrOH 90:1, 1.0 mL/min, 227 nm; er = 96:4

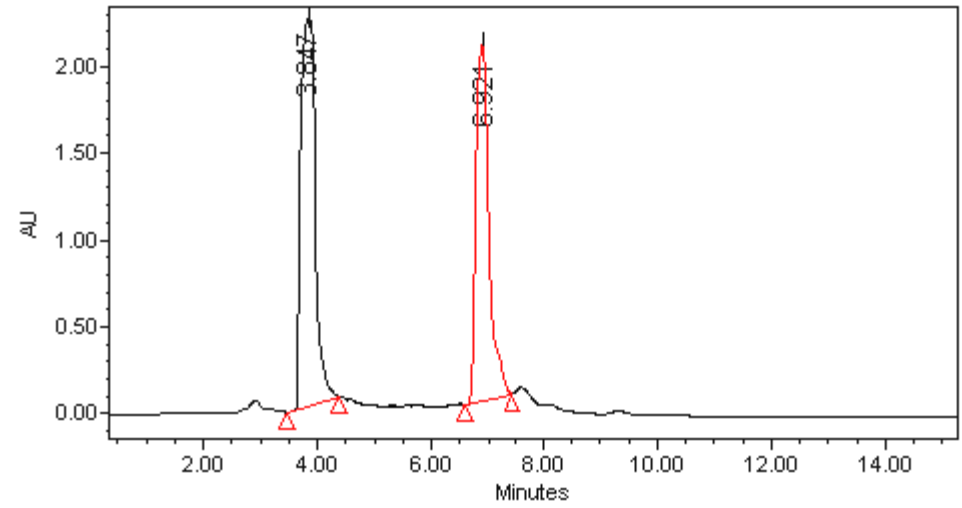


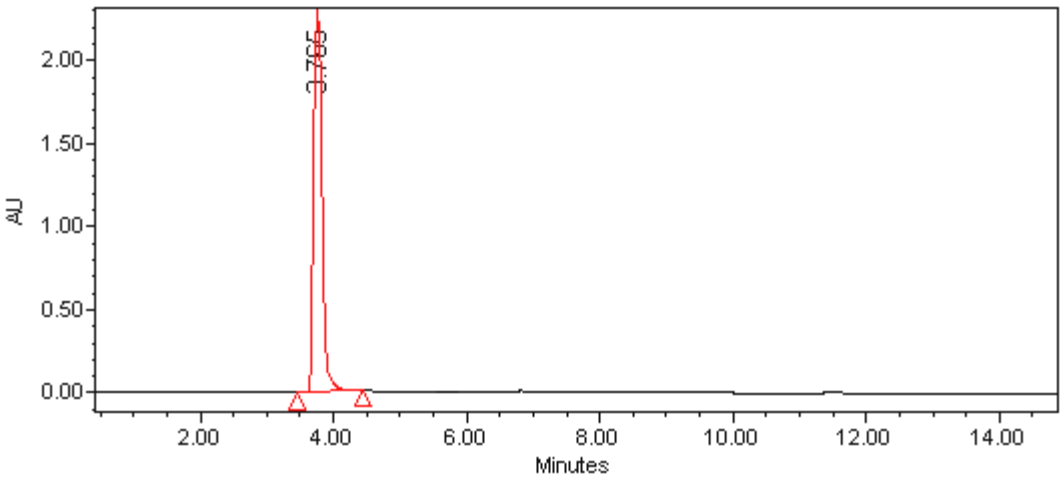



HPLC analysis of racemic and enantioenriched **(*S*,*S*)-4m**



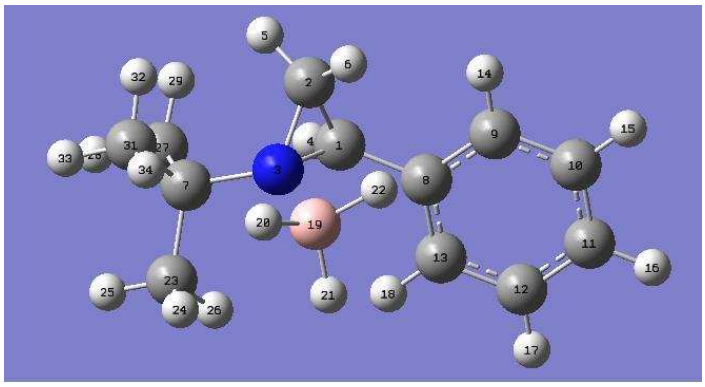

Cellulose – Lux2, Hexane-*i*PrOH 90:1, 1.0 mL/min, 219 nm er >98:2



**Cartesian coordinates of the optimized geometries at the PCM/B3LYP/6-311++G(d,p) computational level and thermochemical data.**

**2a**

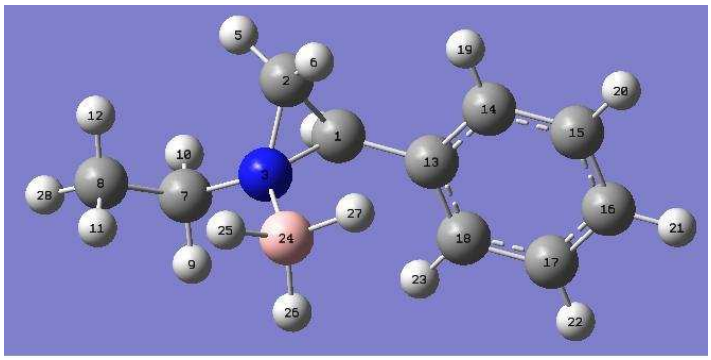


```
Charge = 0 Multiplicity = 1
 C,0,0.0235456207,-0.4164074734,-0.7161789126
 C,0,0.7690514972,-1.6459313829,-0.3582885731
 N,0,1.1315597433,-0.3740109614,0.3107649478
 H,0,0.3161345042,0.0342313513,-1.6560551227
 H,0,1.4793966553,-2.0428903804,-1.0730834808
 H,0,0.3225983653,-2.3711290218,0.3085549677
 C,0,2.482701865,0.2608396155,-0.0738010281
 C,0,-1.4008233718,-0.136846155,-0.3561527441
 C,0,-2.3171205954,-1.1735706198,-0.1607621104
 C,0,-3.659045745,-0.8945240516,0.0968373773
 C,0,-4.0989679772,0.4267219684,0.1630348258
 C,0,-3.1918021017,1.4677283664,-0.0392505326
 C,0,-1.8535256923,1.1867152616,-0.3044796269
 H,0,-1.9856066948,-2.2063149986,-0.208512562
 H,0,-4.3593876621,-1.7109710914,0.2480802529
 H,0,-5.1431217775,0.6450662676,0.367988372
 H,0,-3.5271890926,2.4998529854,0.0077774885
 H,0,-1.156466782,2.0035527853,-0.4658472034
 B,0,0.6720232131,-0.2550434067,1.8805984329
 H,0,1.6353731504,-0.5310742628,2.5579601718
 H,0,0.2844273901,0.8729682824,2.0760859147
 H,0,-0.2155731397,-1.05881926,2.0349564001
 C,0,2.5444688614,1.6642657925,0.5432048659
 H,0,2.5284923634,1.6264066197,1.6309757674
 H,0,3.4692293645,2.1509441448,0.2229695587
 H,0,1.704370137,2.2784925625,0.2094687712
 C,0,2.6822869563,0.3888099801,-1.5944801649
 H,0,3.7071712848,0.7235606666,-1.7678867525
 H,0,2.5635026362,-0.5558313007,-2.1307977119
 H,0,2.022981987,1.1364557622,-2.040658904
 C,0,3.5919680739,-0.6349516485,0.4992644549
 H,0,3.5872525863,-1.6249743626,0.0348353358
 H,0,4.5628912652,-0.176999365,0.2952417929
 H,0,3.4860648434,-0.7563315419,1.5759131586

Zero-point correction = 0.294980 (Hartree/Particle)
 Thermal correction to Energy = 0.309293
 Thermal correction to Enthalpy = 0.310237
 Thermal correction to Gibbs Free Energy = 0.254725
 Sum of electronic and zero-point Energies = -548.744550
 Sum of electronic and thermal Energies = -548.730237
 Sum of electronic and thermal Enthalpies = -548.729293
```

Sum of electronic and thermal Free Energies = -548.784805

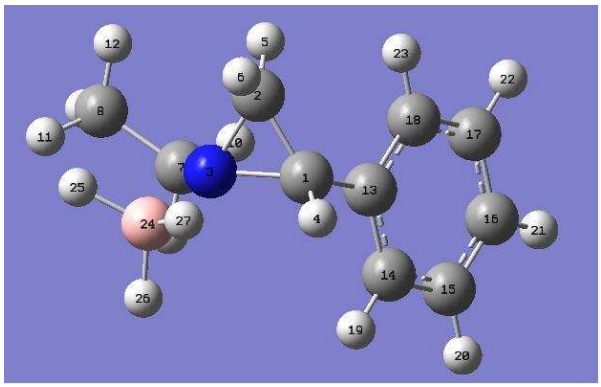
**2b**




Charge = 0 Multiplicity = 1
C,0,-0.4767841799,0.2863449463,-0.8048001714
C,0,-1.2716598712,1.468336183,-0.3869350424
N,0,-1.6092906135,0.1453919519,0.1819995099
H,0,-0.7514038084,-0.1371097311,-1.7689469024
H,0,-1.9899379705,1.8871081728,-1.0832181366
H,0,-0.8585779601,2.1593857066,0.3369344867
C,0,-2.8335838548,-0.5029481053,-0.3748393758
C,0,-4.1296025361,0.0428816985,0.2107379705
H,0,-2.7322904193,-1.5713922348,-0.1717240389
H,0,-2.8276704293,-0.3627173753,-1.4602908761
H,0,-4.2098237839,-0.16567832,1.2766497402
H,0,-4.2104059929,1.1235326981,0.0632900821
C,0,0.9435435485,0.0304495684,-0.4223371003
C,0,1.8202519648,1.0751057385,-0.1184436082
C,0,3.159990273,0.8138505875,0.1686967296
C,0,3.6351607532,-0.496654425,0.1584308692
C,0,2.7667981592,-1.5452808029,-0.1503964488
C,0,1.4319688366,-1.2817576617,-0.4475989639
H,0,1.4622349287,2.0998266866,-0.1066643576
H,0,3.8308613856,1.6354822811,0.4027989311
H,0,4.6773401512,-0.7011490369,0.3865888097
H,0,3.1309407403,-2.5685998808,-0.1635288764
H,0,0.7623063908,-2.1013871454,-0.6941850644
B,0,-1.3125441663,-0.1307434358,1.74864443
H,0,-2.2496543164,0.326670428,2.3657626822
H,0,-1.2257446932,-1.3356668914,1.8750460704
H,0,-0.2837642362,0.4343649066,2.0298418081
H,0,-4.97315342,-0.4286631131,-0.3006622281

Zero-point correction = 0.239120 (Hartree/Particle)
 Thermal correction to Energy = 0.251027
 Thermal correction to Enthalpy = 0.251971
 Thermal correction to Gibbs Free Energy = 0.201179
 Sum of electronic and zero-point Energies = -470.160378
 Sum of electronic and thermal Energies = -470.148471
 Sum of electronic and thermal Enthalpies = -470.147527
 Sum of electronic and thermal Free Energies = -470.198320

**2b’**

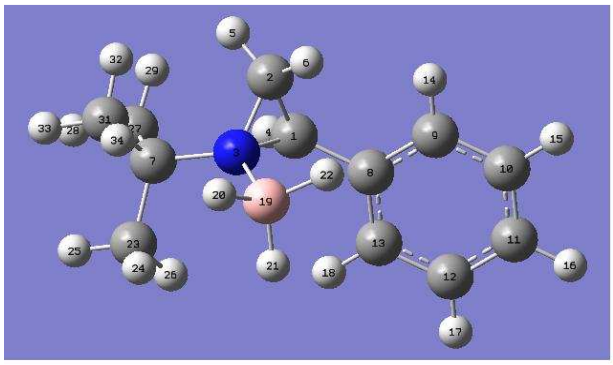



```
Charge = 0 Multiplicity = 1
C,0,-0.5114578991,-0.8240033653,0.8225417029
 C,0,-1.4851250166,0.0529303607,1.5204908953
 N,0,-1.7605767883,-0.3456112081,0.1240157916
 H,0,-0.5977223454,-1.8850550461,1.0357368645
 H,0,-1.2356131106,1.0986215045,1.6624407061
 H,0,-2.154319787,-0.3758173565,2.2557250653
 C,0,-1.6180349468,0.7143591002,-0.9129344378
 C,0,-2.8138190548,1.6582744494,-0.958941618
 H,0,-1.4914421918,0.1971251067,-1.8664554052
 H,0,-0.7033330482,1.2763764157,-0.7150654605
 H,0,-3.7306924793,1.1327234414,-1.2234253892
 H,0,-2.9666249143,2.155268685,0.0033060517
 C,0,0.8494368555,-0.3879110347,0.385603534
 C,0,1.4854632538,-1.0922347775,-0.6469236507
 C,0,2.7639553112,-0.7334250774,-1.0656320445
 C,0,3.4311330201,0.3264833353,-0.4481947851
 C,0,2.813209775,1.0213938419,0.5900259891
 C,0,1.5287795341,0.6664128225,1.0044141151
 H,0,0.9743876851,-1.9255153426,-1.1227412672
 H,0,3.2426277555,-1.2846722464,-1.87002067
 H,0,4.4305348123,0.6035337727,-0.7712698533
 H,0,3.3305785646,1.8397444156,1.0825657708
 H,0,1.0634851727,1.2100851164,1.8213419411
 B,0,-2.9064396446,-1.4675004716,-0.1386294856
 H,0,-3.9792020939,-0.9075185403,-0.1357834993
 H,0,-2.644412953,-1.9688538808,-1.2123704078
 H,0,-2.8136715849,-2.2582770852,0.7754176726
 H,0,-2.6269393877,2.4313107907,-1.7088977198


Zero-point correction = 0.239107 (Hartree/Particle)
 Thermal correction to Energy = 0.251069
 Thermal correction to Enthalpy = 0.252013
 Thermal correction to Gibbs Free Energy = 0.200895
 Sum of electronic and zero-point Energies = -470.163173
 Sum of electronic and thermal Energies = -470.151210
 Sum of electronic and thermal Enthalpies = -470.150266
 Sum of electronic and thermal Free Energies = -470.201384
```

**Cartesian coordinates of the optimized geometries at the PCM/MPW1PW91/6-311++g(d,p) computational level and thermochemical data.**

**2a**



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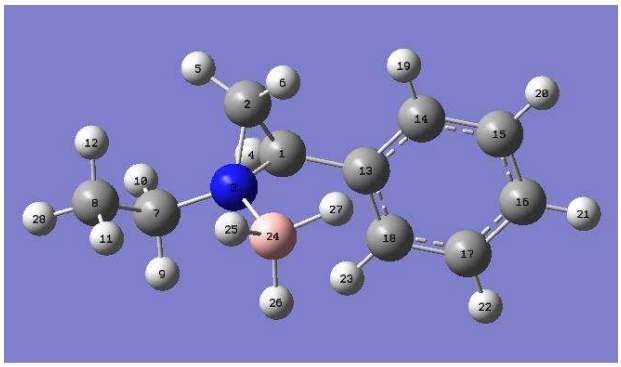
Charge = 0 Multiplicity = 1
 C,0,0.0338132903,-0.4092356973,-0.7193682938
 C,0,0.7783785021,-1.6334738135,-0.3642278947
 N,0,1.1248718451,-0.3691537358,0.3032217443
 H,0,0.3292660279,0.04570624,-1.6568226937
 H,0,1.496278856,-2.0217971796,-1.0761542366
 H,0,0.3304073333,-2.3606529335,0.2995180727
 C,0,2.4609870243,0.2649910394,-0.0670031662
 C,0,-1.38560392,-0.1386675929,-0.3598157887
 C,0,-2.2951592077,-1.1769395052,-0.17349412
 C,0,-3.6335073277,-0.9044593972,0.0870148913
 C,0,-4.0753658648,0.4113203306,0.1650657388
 C,0,-3.174190776,1.4537389182,-0.0285954258
 C,0,-1.8394503788,1.179424689,-0.2973331483
 H,0,-1.9593494414,-2.2076316434,-0.2318557992
 H,0,-4.3316444504,-1.7235692251,0.2314655115
 H,0,-5.1196577912,0.6247452148,0.3727258075
 H,0,-3.5124384261,2.4840875918,0.0277971566
 H,0,-1.1438558759,1.9983604894,-0.4530053242
 B,0,0.6567171626,-0.2526522612,1.8533719652
 H,0,1.6115156222,-0.5417707008,2.5433085415
 H,0,0.2762307655,0.8807206927,2.0501431952
 H,0,-0.2432311197,-1.0498543505,1.9956556662
 C,0,2.5238659786,1.6500993093,0.5693267445
 H,0,2.5061300906,1.5910026882,1.6560221019
 H,0,3.449265941,2.1398821185,0.2582065463
 H,0,1.6848231268,2.2701209567,0.2459188935
 C,0,2.6590343028,0.416136227,-1.5768587583
 H,0,3.6854765955,0.7472629275,-1.7442817867
 H,0,2.5355783283,-0.5180308028,-2.1297867991
 H,0,2.0047944264,1.1758420737,-2.0091705986
 C,0,3.5632925436,-0.6341760785,0.4911444043
 H,0,3.5682712257,-1.6120260157,0.0029992667
 H,0,4.5332196466,-0.1668176897,0.3094033358
 H,0,3.44466539,-0.7807935687,1.5633700093

Zero-point correction = 0.297146 (Hartree/Particle)
 Thermal correction to Energy = 0.311316
 Thermal correction to Enthalpy = 0.312261
 Thermal correction to Gibbs Free Energy = 0.257109
 Sum of electronic and zero-point Energies = -548.602907
```

Sum of electronic and thermal Energies = -548.588737
Sum of electronic and thermal Enthalpies = -548.587793
Sum of electronic and thermal Free Energies = -548.642945

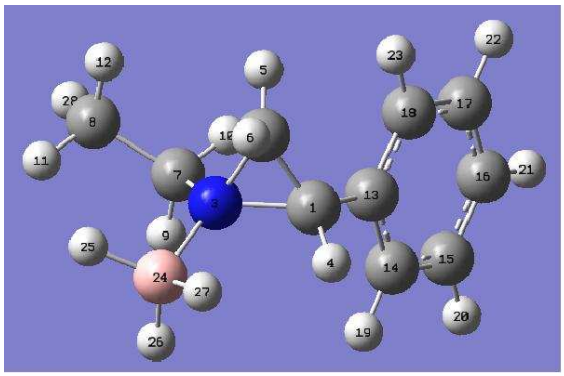
**2b**




Charge = 0 Multiplicity = 1
C,0,-0.4792181,0.2852008788,-0.8080062261
C,0,-1.2682595516,1.4606731935,-0.3817142011
N,0,-1.5987218844,0.140982292,0.170790559
H,0,-0.7538997719,-0.1283701538,-1.7765057389
H,0,-1.9889816631,1.8831440082,-1.07263375
H,0,-0.8505231146,2.1432086923,0.3474060468
C,0,-2.8167020942,-0.4961046975,-0.3806112161
C,0,-4.0983075169,0.0447601161,0.2193695056
H,0,-2.7161161103,-1.5664773605,-0.1898591723
H,0,-2.8173783209,-0.3442690919,-1.46455048
H,0,-4.1661400834,-0.1743196711,1.2834015372
H,0,-4.1751996322,1.1262750466,0.083984315
C,0,0.9345212898,0.0305099737,-0.4245154992
C,0,1.8076588295,1.0749146675,-0.1310806326
C,0,3.1413047845,0.8162272107,0.1654338924
C,0,3.6132221085,-0.4909269958,0.1715733569
C,0,2.7479578294,-1.538918735,-0.1286568403
C,0,1.4185440908,-1.2785176105,-0.4328520208
H,0,1.4488339993,2.0991747548,-0.131905201
H,0,3.8119561318,1.6391462729,0.393795111
H,0,4.6538739443,-0.693981003,0.4060548503
H,0,3.110907294,-2.5623307792,-0.1277592329
H,0,0.7474390095,-2.0991781517,-0.6703627575
B,0,-1.2945398899,-0.1438582278,1.7221558243
H,0,-2.2244964131,0.3191711273,2.350534431
H,0,-1.215613084,-1.3523328203,1.8397618759
H,0,-0.2559741801,0.4138082119,1.9947138656
H,0,-4.9492653839,-0.4171619958,-0.2860294469

Zero-point correction = 0.240892 (Hartree/Particle)
Thermal correction to Energy = 0.252771
Thermal correction to Enthalpy = 0.253715
Thermal correction to Gibbs Free Energy = 0.202873
Sum of electronic and zero-point Energies = -470.035830
Sum of electronic and thermal Energies = -470.023951
Sum of electronic and thermal Enthalpies = -470.023007
Sum of electronic and thermal Free Energies = -470.073849

**inv-2b**



```
Charge = 0 Multiplicity = 1
 C,0,-0.5134331775,-0.8324021275,0.820390885
 C,0,-1.4817997274,0.0422400693,1.5154449408
 N,0,-1.7479640735,-0.3497754031,0.1255755122
 H,0,-0.6032289535,-1.8957495655,1.0214478688
 H,0,-1.2304984201,1.0872571292,1.6581007018
 H,0,-2.1586141392,-0.3863258139,2.243152143
 C,0,-1.5945390091,0.7056995809,-0.8982301877
 C,0,-2.7727835429,1.6584951999,-0.9321735899
 H,0,-1.4795246509,0.18991997,-1.8536160081
 H,0,-0.6698879823,1.2521843173,-0.7015903223
 H,0,-3.6973679236,1.1435018904,-1.188445411
 H,0,-2.9104325541,2.1557219937,0.0311667029
 C,0,0.8402539045,-0.3929162412,0.3849541468
 C,0,1.4805033866,-1.1002636871,-0.6361925877
 C,0,2.751193878,-0.7337095278,-1.0585897272
 C,0,3.4048789553,0.3375798687,-0.4561923651
 C,0,2.7821198943,1.0359354023,0.571147306
 C,0,1.5058052692,0.6728338323,0.9893611193
 H,0,0.977931114,-1.9440103912,-1.1015775821
 H,0,3.2351996647,-1.2889809382,-1.8564661321
 H,0,4.4008164825,0.6213719749,-0.7829098852
 H,0,3.291032274,1.8649118734,1.0538089991
 H,0,1.0368440807,1.2200282088,1.8009944539
 B,0,-2.8815265605,-1.4527352802,-0.1443756644
 H,0,-3.9530777439,-0.8852357967,-0.1903883466
 H,0,-2.5952686147,-1.9864499467,-1.199468019
 H,0,-2.8286203514,-2.2263670665,0.7917526513
 H,0,-2.5851199517,2.4293721652,-1.6826317198


Zero-point correction = 0.240908 (Hartree/Particle)
 Thermal correction to Energy = 0.252830
 Thermal correction to Enthalpy = 0.253774
 Thermal correction to Gibbs Free Energy = 0.202530
 Sum of electronic and zero-point Energies = -470.038875
 Sum of electronic and thermal Energies = -470.026953
 Sum of electronic and thermal Enthalpies = -470.026009
 Sum of electronic and thermal Free Energies = -470.077253
```

**SCF GIAO magnetic shielding tensor (ppm) and total nuclear spin-spin coupling *J* (Hz) calculated at the PCM/B3LYP/6-311++g(d,p) level of theory.**

**2a**

```
GIAO nuclear magnetic shielding tensors:
1C    Isotropic = 133.6787    Anisotropy = 56.1942
      XX = 157.7211     YX = 14.0285      ZX = -13.3533
      XY = 18.7145      YY = 110.9402     ZY = 20.9766
      XZ = -31.5191     YZ = 19.5361      ZZ = 132.3749
      Eigenvalues: 88.9181    140.9766    171.1415
2C    Isotropic = 145.5539    Anisotropy = 39.9084
      XX = 145.0664     YX = 30.5814      ZX = -6.5330
      XY = 26.5393      YY = 124.2297     ZY = 6.0301
      XZ = -15.5281     YZ = 12.5780      ZZ = 167.3655
      Eigenvalues: 101.2931   163.2090    172.1594
3N    Isotropic = 189.0207    Anisotropy = 122.3181
      XX = 236.3771     YX = 11.1844      ZX = -43.8925
      XY = -0.3172      YY = 162.7908     ZY = -29.2358
      XZ = -64.1713     YZ = -39.5554     ZZ = 167.8943
      Eigenvalues: 119.3817   177.1143    270.5661
4H    Isotropic = 28.1119     Anisotropy = 8.5980
      XX = 31.1563      YX = 2.1558       ZX = -3.0300
      XY = -0.3990      YY = 23.4360      ZY = -2.5259
      XZ = -1.7567      YZ = -4.8381      ZZ = 29.7433
      Eigenvalues: 21.7370    28.7548     33.8438
5H    Isotropic = 29.5322     Anisotropy = 8.9273
      XX = 28.9680      YX = -1.3474      ZX = -3.4146
      XY = 1.0393       YY = 30.4607      ZY = 2.3478
      XZ = -5.4670      YZ = 5.5686       ZZ = 29.1680
      Eigenvalues: 23.4738    29.6391     35.4837
6H    Isotropic = 29.3090     Anisotropy = 11.1265
      XX = 28.1563      YX = 4.5974       ZX = -3.9431
      XY = 2.9443       YY = 33.2486      ZY = -1.2378
      XZ = -1.2310      YZ = -4.7662      ZZ = 26.5222
      Eigenvalues: 24.6178    26.5826     36.7267
7C    Isotropic = 114.8421    Anisotropy = 57.0152
      XX = 140.7430     YX = 22.5400      ZX = -10.3261
      XY = 20.9666      YY = 103.9139     ZY = -2.5016
      XZ = -8.5900      YZ = -5.9233      ZZ = 99.8693
      Eigenvalues: 93.8216    97.8524     152.8522
8C    Isotropic = 43.0759     Anisotropy = 186.9290
      XX = -46.9846     YX = 16.1282      ZX = 44.7606
      XY = 16.3155      YY = 17.3635      ZY = -1.1769
      XZ = 42.3820      YZ = -6.7783      ZZ = 158.8489
      Eigenvalues: -59.4538   20.9863     167.6953
9C    Isotropic = 47.6191     Anisotropy = 179.7589
      XX = 34.2088      YX = 29.5001      ZX = 26.8953
      XY = 28.0184      YY = -52.7493     ZY = -3.9460
      XZ = 29.8053      YZ = -3.3217      ZZ = 161.3977
      Eigenvalues: -62.0253   37.4242     167.4584
10C   Isotropic = 49.4745     Anisotropy = 185.4845
      XX = 0.8637       YX = -47.9432     ZX = 34.4266
      XY = -48.4642     YY = -18.5592     ZY = 10.5975
      XZ = 35.0513      YZ = 10.9882      ZZ = 166.1191
      Eigenvalues: -62.1280   37.4207     173.1309
11C   Isotropic = 48.8691     Anisotropy = 188.0326
      XX = -49.7473     YX = 17.2805      ZX = 44.6607
      XY = 18.1999      YY = 31.0900      ZY = -2.8303
```

```
      XZ = 44.9274      YZ = -4.9111      ZZ = 165.2647
      Eigenvalues: -62.2378   34.6209     174.2242
12C   Isotropic = 49.1998     Anisotropy = 185.6750
      XX = 33.1273      YX = 29.7658      ZX = 28.1289
      XY = 30.1901      YY = -52.7664     ZY = -3.4223
      XZ = 28.2941      YZ = -1.7928      ZZ = 167.2384
      Eigenvalues: -62.7309   37.3470     172.9831
13C   Isotropic = 44.6854     Anisotropy = 179.9718
      XX = -0.2889      YX = -47.0040     ZX = 36.6970
      XY = -48.9371     YY = -22.3096     ZY = 11.9529
      XZ = 35.4801      YZ = 18.0187      ZZ = 156.6546
      Eigenvalues: -65.8580   35.2475     164.6666
14H   Isotropic = 24.4194     Anisotropy = 10.6848
      XX = 30.2905      YX = 3.4245       ZX = -0.6790
      XY = 2.9367       YY = 22.8279      ZY = -0.2359
      XZ = -1.0449      YZ = -0.6261      ZZ = 20.1397
      Eigenvalues: 20.0522    21.6633     31.5426
15H   Isotropic = 24.2224     Anisotropy = 5.3369
      XX = 26.8138      YX = -1.5784      ZX = -0.9296
      XY= -1.4127       YY = 25.0087      ZY = 0.2894
      XZ = -0.7814      YZ = 0.4259       ZZ = 20.8447
      Eigenvalues: 20.7190    24.1678     27.7803
16H   Isotropic = 24.1880     Anisotropy = 4.4499
      XX = 24.4836      YX = 0.4797       ZX = -0.4816
      XY = 0.6062       YY = 27.0213      ZY = -0.2093
      XZ = -0.5097      YZ = -0.3314      ZZ = 21.0591
      Eigenvalues: 20.9826    24.4267     27.1546
17H   Isotropic = 24.0720     Anisotropy = 5.6648
      XX = 27.5958      YX = 0.4693       ZX = -1.0941
      XY = 0.4994       YY = 23.8529      ZY = -0.2154
      XZ = -1.2010      YZ = -0.1779      ZZ = 20.7674
      Eigenvalues: 20.5756    23.7920     27.8485
18H   Isotropic = 24.0517     Anisotropy = 10.0354
      XX = 27.0245      YX = -4.8902      ZX = -0.1915
      XY = -4.1920      YY = 25.1939      ZY = -0.0841
      XZ = -0.0227      YZ = 0.0144       ZZ = 19.9368
      Eigenvalues: 19.9306    21.4825     30.7420
19B   Isotropic = 122.0889    Anisotropy = 34.7714
      XX = 110.6641     YX = 5.2316       ZX = -11.1756
      XY = 4.4851       YY = 114.0398     ZY = 1.1384
      XZ = -11.0299     YZ = 6.1861       ZZ = 141.5629
      Eigenvalues: 103.8243   117.1726    145.2699
20H   Isotropic = 29.8022     Anisotropy = 7.2968
      XX = 28.4822      YX = 0.3774       ZX = -2.3080
      XY = 0.2061       YY = 26.4615      ZY = -0.9961
      XZ = 0.8674       YZ = -0.9185      ZZ = 34.4628
      Eigenvalues: 26.3283    28.4115     34.6667
21H   Isotropic = 30.4495     Anisotropy = 6.4070
      XX = 30.0600      YX = -0.4370      ZX = -2.4866
      XY = -0.1268      YY = 27.9885      ZY = 1.3519
      XZ = 0.3368       YZ = 4.1311       ZZ = 33.3001
      Eigenvalues: 26.8191    29.8086     34.7208
      22H   Isotropic = 31.4236     Anisotropy = 7.5666
      XX = 30.9674      YX = 1.1336       ZX = -2.2998
      XY = 1.2739       YY = 27.6019      ZY = -0.8118
      XZ = 0.4679       YZ = -3.3838      ZZ = 35.7015
      Eigenvalues: 26.8615    30.9413     36.4680
23C   Isotropic = 154.2669    Anisotropy = 35.1726
      XX = 143.3846     YX = 2.2845       ZX = 0.8567
      XY = -1.0637      YY = 171.8621     ZY = 15.8584
      XZ = -2.2724      YZ = 10.7094      ZZ = 147.5539
```

```
      Eigenvalues: 141.3162   143.7691    177.7153
24H   Isotropic = 29.7450     Anisotropy = 6.9693
      XX = 27.1113      YX = 1.8901       ZX = 0.2117
      XY = 1.7344       YY = 29.3638      ZY = 3.6146
      XZ = 0.1183       YZ = 1.7614       ZZ = 32.7601
      Eigenvalues: 25.8623    28.9816     34.3912
25H   Isotropic = 30.9497     Anisotropy = 9.5996
      XX = 32.1861      YX = 4.5647       ZX = -0.5602
      XY = 4.6744       YY = 33.2162      ZY = 0.4997
      XZ = -0.5488      YZ = 0.5542       ZZ = 27.4466
      Eigenvalues: 26.9273    28.5723     37.3494
26H   Isotropic = 30.5076     Anisotropy = 8.0079
      XX = 30.6334      YX = -1.6800      ZX = 0.4866
      XY = -3.0211      YY = 34.7861      ZY = -0.2032
      XZ = 0.6418       YZ = 0.6386       ZZ = 26.1032
      Eigenvalues: 26.0011    29.6755     35.8462
27C   Isotropic = 158.5911    Anisotropy = 38.8535
      XX = 148.1190     YX = -0.7557      ZX = -4.0690
      XY = -5.7374      YY = 143.5645     ZY = -3.4102
      XZ = 0.6459       YZ = -4.1419      ZZ = 184.0899
      Eigenvalues: 141.4739   149.8060    184.4935
28H   Isotropic = 30.8639     Anisotropy = 9.7186
      XX = 33.9639      YX = 2.4744       ZX = -3.4938
      XY = 2.0632       YY = 27.6692      ZY = -1.6909
      XZ = -4.0354      YZ = -1.7040      ZZ = 30.9587
      Eigenvalues: 26.8308    28.4180     37.3430
29H   Isotropic = 30.9802     Anisotropy = 7.6225
      XX = 29.0051      YX = 0.6610       ZX = -2.6976
      XY = 1.0593       YY = 30.0952      ZY = 2.1709
      XZ=    -2.5876   YZ=     3.8479   ZZ=    33.8403
      Eigenvalues: 26.4787    30.4001     36.0619
30H   Isotropic = 30.8405     Anisotropy = 7.7567
      XX = 29.8850      YX = -0.4630      ZX = 0.0232
      XY = -1.2923      YY = 30.3706      ZY = -3.6687
      XZ = 1.3877       YZ = -5.1205      ZZ = 32.2660
      Eigenvalues: 26.8032    29.7067     36.0117
31C   Isotropic = 157.2448    Anisotropy = 43.0148
      XX = 166.5373     YX = -17.4091     ZX = 11.3130
      XY = -13.9252     YY = 159.6831     ZY = -13.3100
      XZ = 11.3533      YZ = -11.1996     ZZ = 145.5142
      Eigenvalues: 138.1871   147.6260    185.9214
32H   Isotropic = 30.8376     Anisotropy = 8.2086
      XX = 31.4747      YX = -4.1476      ZX =    0.4350
      XY = -2.3556      YY = 34.0161      ZY = 1.8201
      XZ = 0.6235       YZ = 0.8827       ZZ = 27.0222
      Eigenvalues: 26.4425    29.7603     36.3100
33H   Isotropic = 31.0819     Anisotropy = 10.0065
      XX = 37.7013      YX = 0.7077       ZX = 0.5040
      XY = 0.3057       YY = 28.3937      ZY = -0.6775
      XZ = 0.5750       YZ = -0.5988      ZZ =    27.1508
      Eigenvalues: 26.8370    28.6559     37.7529
34H   Isotropic = 29.4769     Anisotropy = 7.4331
      XX = 29.7309      YX = -1.9734      ZX = 2.1938
      XY = -1.5253      YY = 25.8295      ZY = -3.0753
      XZ = 0.6623       YZ = -1.8525      ZZ = 32.8702

Total nuclear spin-spin coupling J (Hz):
                1             2             3             4             5
      1  0.000000D+00
      2  0.236855D+02  0.000000D+00
      3 -0.552163D+01 -0.413734D+01  0.000000D+00
```

```
 4  0.158737D+03 -0.184598D+01 -0.223498D+00  0.000000D+00
 5 -0.867247D+00  0.158616D+03 -0.404981D+00  0.765256D+01  0.000000D+00
 6 -0.285704D+01  0.168018D+03  0.990360D+00  0.484706D+01 -0.193417D+01
 7 -0.102930D+01 -0.949085D+00 -0.182866D+00  0.344589D+01  0.378708D+01
 8  0.595537D+02 -0.102820D+01 -0.540217D-01  0.133424D+00  0.236191D+01
 9  0.368813D+01  0.303497D+01  0.741033D+00  0.268006D+01 -0.119208D+00
10  0.427076D+01  0.345091D+00 -0.694250D-01 -0.484900D+00 -0.338178D-01
11 -0.832944D+00  0.106801D-01  0.189474D+00  0.717540D+00 -0.618619D-01
12  0.415055D+01  0.533841D+00 -0.220633D+00 -0.914447D+00  0.856948D-01
13  0.338400D+01  0.270368D+01  0.184664D+00  0.235016D+01  0.745202D-01
14  0.460560D+01  0.373332D+00 -0.736201D-01 -0.898876D+00 -0.499529D-01
15  0.691813D+00 -0.497527D-01  0.102878D+00  0.269892D+00 -0.111465D+00
16  0.524200D+00 -0.293369D-01 -0.163518D+00 -0.758693D+00 -0.134974D+00
17  0.607472D+00  0.107447D+00  0.578457D-01  0.154782D+00 -0.101739D+00
18  0.466374D+01 -0.886229D-01 -0.180027D+00 -0.488732D+00 -0.986004D-01
19 -0.405512D+00  0.115154D+00  0.417792D+01  0.414290D+00  0.125802D+01
20  0.664623D+01 -0.130785D+00  0.996351D+00  0.455253D+00 -0.255666D+00
21  0.180007D+01  0.672898D+01  0.325476D+00 -0.296698D+00  0.108005D+01
22  0.118029D+01  0.642171D+01  0.585876D+00 -0.589261D+00  0.629793D+00
23 -0.114504D+00  0.908499D+00  0.144028D+01 -0.892095D-01 -0.360299D+00
24 -0.516585D-01 -0.232276D+00  0.298956D+00 -0.153491D+00 -0.156488D+00
25 -0.195122D+00  0.697556D+00  0.445167D+01  0.202741D-01 -0.586855D-01
26 -0.231907D-02 -0.137792D+00  0.986548D+00  0.150333D+00 -0.137027D+00
27  0.343430D+01  0.694371D+00 -0.364473D+00 -0.240697D+00  0.112075D+00
28  0.206935D+01 -0.101383D+00  0.255969D+01 -0.610966D+00 -0.113328D+00
29  0.611431D+00  0.641323D+00  0.577485D+00  0.273105D+00  0.743295D-01
30  0.136639D+01 -0.347459D-02  0.212832D+00 -0.182193D+00  0.712563D-01
31  0.118266D+01  0.112529D+01  0.915872D+00 -0.362048D+00  0.568356D-01
32  0.190404D+00  0.390229D+00  0.690622D+00 -0.484420D-01  0.286827D+00
33  0.127664D+01  0.267858D+00  0.406352D+01 -0.123554D+00 -0.118698D+00
34 -0.365454D+00 -0.961562D-01  0.612255D+00 -0.166802D+00 -0.732965D-01
           6             7             8             9            10
 6  0.000000D+00
 7  0.182331D+01  0.000000D+00
 8  0.310551D+01  0.294104D+00  0.000000D+00
 9 -0.652399D-01  0.536974D+00  0.648447D+02  0.000000D+00
10  0.646613D-02  0.145486D+00 -0.120745D+01  0.609984D+02  0.000000D+00
11 -0.257421D-02 -0.398978D-01  0.942182D+01 -0.203741D+01  0.601433D+02
12 -0.111630D+00  0.945567D-02 -0.144321D+01  0.869423D+01 -0.157830D+01
13 -0.438746D+00 -0.479718D-01  0.626347D+02 -0.317802D+00  0.884718D+01
14  0.242879D+00  0.147097D+00 -0.719084D-01  0.150103D+03  0.933563D+00
15  0.787423D-01 -0.986038D-02  0.704213D+01  0.185558D+01  0.151160D+03
16 -0.106021D+00  0.730528D-03 -0.130179D+01  0.697294D+01  0.166765D+01
17 -0.160073D+00 -0.276483D-01  0.707386D+01 -0.119036D+01  0.704437D+01
18 -0.177060D+00  0.290318D-01  0.480341D+00  0.575849D+01 -0.931761D+00
19  0.247236D+01  0.194007D+00  0.121875D+01  0.223407D+00 -0.288748D-01
20 -0.530131D-01  0.194894D+01  0.380448D+00  0.348746D+00 -0.334151D-01
21 -0.137961D+00  0.104442D+00  0.952158D-01 -0.283996D-01  0.315957D-01
22  0.150702D+00  0.490322D+01  0.456160D+00  0.116733D+01 -0.153637D-01
23  0.319992D-01  0.380856D+02 -0.114049D-01 -0.260259D-01 -0.121124D-01
24 -0.140279D+00 -0.440984D+01 -0.160385D-01 -0.181468D-01 -0.266656D-01
25  0.133408D+00 -0.512285D+00 -0.342006D-01 -0.591851D-02 -0.205642D-01
26 -0.559107D-01 -0.454342D+01 -0.369453D-02 -0.763409D-02 -0.320026D-01
27 -0.194238D+00  0.369218D+02 -0.380748D-02  0.119288D+00  0.121424D-01
28 -0.276264D+00 -0.178663D+00 -0.540337D-01  0.633264D-02 -0.473245D-01
29 -0.160696D+00 -0.379797D+01  0.311858D-01 -0.111715D-01 -0.259401D-01
30  0.428049D-01 -0.375226D+01  0.736371D-02  0.153518D-01 -0.484487D-01
31 -0.155815D+00  0.379407D+02  0.386668D+00  0.417312D-01 -0.331931D-01
32  0.366905D-01 -0.422712D+01  0.835562D-01 -0.318416D-01 -0.129685D-01
33 -0.145271D+00 -0.145636D+00  0.387709D+00  0.498792D-01 -0.167840D-01
34  0.362436D-02 -0.446819D+01 -0.276262D-01 -0.154500D-01 -0.200497D-01
```

| | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|
| 11 | 0.000000D+00 | | | | |
| 12 | 0.599291D+02 | 0.000000D+00 | | | |
| 13 | -0.196115D+01 | 0.613856D+02 | 0.000000D+00 | | |
| 14 | 0.668386D+01 | -0.891964D+00 | 0.564979D+01 | 0.000000D+00 | |
| 15 | 0.145185D+01 | 0.701882D+01 | -0.119006D+01 | 0.718578D+01 | 0.000000D+00 |
| 16 | 0.151100D+03 | 0.174251D+01 | 0.704245D+01 | 0.620077D+00 | 0.688162D+01 |
| 17 | 0.148288D+01 | 0.151129D+03 | 0.167023D+01 | 0.376517D+00 | 0.749769D+00 |
| 18 | 0.667022D+01 | 0.840106D+00 | 0.149025D+03 | 0.135270D+01 | 0.413608D+00 |
| 19 | -0.248461D-02 | -0.134507D-02 | 0.832720D-01 | 0.836537D-02 | -0.300074D-01 |
| 20 | -0.205863D-01 | -0.667843D-02 | 0.206340D-01 | -0.541758D-01 | -0.837964D-01 |
| 21 | -0.588231D-01 | 0.115202D+00 | 0.645591D+00 | -0.868296D-01 | -0.140706D+00 |
| 22 | 0.831299D-01 | -0.104594D+00 | 0.234836D+00 | 0.319903D+00 | -0.107580D-01 |
| 23 | -0.844509D-02 | 0.106609D-01 | 0.201583D-01 | -0.276551D-01 | -0.242557D-01 |
| 24 | -0.243259D-01 | -0.198846D-02 | -0.296384D-02 | -0.813799D-01 | -0.824589D-01 |
| 25 | -0.355655D-01 | -0.857739D-02 | 0.737825D-02 | -0.101946D+00 | -0.103013D+00 |
| 26 | -0.261975D-01 | 0.226674D-01 | 0.129211D+00 | -0.750335D-01 | -0.845711D-01 |
| 27 | -0.505268D-02 | -0.116049D-01 | 0.206052D-01 | -0.300569D-01 | -0.102242D-01 |
| 28 | -0.169427D-01 | -0.412054D-01 | -0.123203D-01 | -0.117091D+00 | -0.877983D-01 |
| 29 | -0.330459D-01 | -0.274406D-01 | -0.287307D-01 | -0.349914D-02 | -0.657791D-01 |
| 30 | -0.191346D-01 | -0.123806D-01 | 0.101439D-01 | -0.710754D-01 | -0.741037D-01 |
| 31 | 0.393056D-01 | -0.514964D-01 | 0.520027D-01 | -0.530170D-01 | 0.636362D-02 |
| 32 | -0.380626D-01 | -0.148548D-01 | -0.148215D-01 | 0.151622D-01 | -0.587345D-01 |
| 33 | -0.125578D-01 | -0.387670D-01 | -0.209097D-01 | -0.882573D-01 | -0.704067D-01 |
| 34 | -0.231589D-01 | -0.204416D-01 | -0.127359D-01 | -0.358756D-01 | -0.637821D-01 |

| | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|
| 16 | 0.000000D+00 | | | | |
| 17 | 0.683370D+01 | 0.000000D+00 | | | |
| 18 | 0.601165D+00 | 0.719235D+01 | 0.000000D+00 | | |
| 19 | -0.368417D-01 | -0.203867D-01 | 0.437037D-01 | 0.000000D+00 | |
| 20 | -0.101790D+00 | -0.100057D+00 | -0.536386D-01 | 0.923249D+02 | 0.000000D+00 |
| 21 | -0.644460D-01 | -0.513898D-01 | 0.477011D+00 | 0.976191D+02 | -0.637510D+01 |
| 22 | -0.166948D+00 | -0.762477D-01 | -0.194233D+00 | 0.960707D+02 | -0.693672D+01 |
| 23 | -0.188498D-01 | -0.527576D-02 | 0.974186D-01 | 0.212661D+01 | 0.100157D+01 |
| 24 | -0.721747D-01 | -0.297299D-01 | 0.491281D-01 | 0.103477D+00 | 0.124715D+00 |
| 25 | -0.892315D-01 | -0.565113D-01 | 0.134090D-01 | 0.450039D+00 | -0.118121D+00 |
| 26 | -0.603788D-01 | 0.489411D-01 | 0.349894D+00 | 0.972828D-01 | -0.815392D-01 |
| 27 | -0.247661D-01 | -0.129559D-01 | 0.145708D-01 | 0.295456D+00 | -0.172746D+00 |
| 28 | -0.109703D+00 | -0.681842D-01 | -0.484765D-01 | 0.232572D+00 | 0.224216D-01 |
| 29 | -0.907989D-01 | -0.776445D-01 | -0.263336D-01 | -0.132190D+00 | -0.830982D-01 |
| 30 | -0.855440D-01 | -0.180349D-02 | 0.209323D+00 | -0.702253D-01 | -0.142468D+00 |
| 31 | -0.583552D-01 | 0.285962D-02 | -0.497126D-01 | 0.104971D+01 | 0.244721D+01 |
| 32 | -0.783706D-01 | -0.875369D-01 | -0.683898D-01 | -0.115306D+00 | -0.142196D+00 |
| 33 | -0.103031D+00 | -0.679189D-01 | -0.705341D-01 | -0.165026D-01 | 0.352955D-01 |
| 34 | -0.743310D-01 | -0.694104D-01 | -0.554089D-01 | 0.268131D-01 | -0.262077D+00 |

| | 21 | 22 | 23 | 24 | 25 |
|---|---|---|---|---|---|
| 21 | 0.000000D+00 | | | | |
| 22 | -0.712973D+01 | 0.000000D+00 | | | |
| 23 | 0.246622D+01 | 0.176264D+01 | 0.000000D+00 | | |
| 24 | 0.659506D+00 | -0.403169D-01 | 0.126860D+03 | 0.000000D+00 | |
| 25 | 0.105035D+01 | 0.529502D-01 | 0.117939D+03 | -0.116576D+02 | 0.000000D+00 |
| 26 | 0.479325D+00 | -0.175282D+00 | 0.120636D+03 | -0.116066D+02 | -0.121029D+02 |
| 27 | -0.103595D+00 | 0.366651D+00 | 0.175423D+01 | 0.905722D+01 | 0.226342D+01 |
| 28 | -0.131624D+00 | 0.659085D+00 | 0.114465D+01 | -0.771920D-01 | 0.668429D+00 |
| 29 | -0.132979D+00 | 0.706380D-01 | 0.782004D+01 | 0.394253D+01 | 0.626975D+00 |
| 30 | -0.515602D-01 | -0.137413D+00 | 0.320138D+01 | 0.974380D-01 | -0.144989D+00 |
| 31 | 0.659039D-01 | 0.171923D-01 | 0.143866D+01 | 0.281521D+01 | 0.112385D+01 |
| 32 | -0.196889D+00 | -0.923721D-02 | 0.792568D+01 | -0.107819D+00 | -0.137184D+00 |
| 33 | -0.714560D-01 | -0.204590D+00 | 0.179177D+01 | -0.239159D+00 | 0.438695D+00 |
| 34 | -0.106349D-02 | -0.139027D+00 | 0.205162D+01 | 0.139747D+00 | -0.292951D+00 |

| | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|

```
    26  0.000000D+00
    27  0.218537D+01  0.000000D+00
    28 -0.280907D+00  0.120820D+03  0.000000D+00
    29 -0.370314D+00  0.119166D+03 -0.135698D+02  0.000000D+00
    30  0.180682D+00  0.121332D+03 -0.132696D+02 -0.954362D+01  0.000000D+00
    31  0.785724D+01  0.164042D+01  0.246878D+01  0.145747D+01  0.787017D+01
    32  0.347578D+01  0.262443D+01 -0.243113D+00  0.145767D+00 -0.125832D+00
    33  0.180673D+00  0.163979D+01  0.662035D+00 -0.244378D+00  0.301871D-01
    34 -0.341771D+00  0.877303D+01  0.553041D+00 -0.422850D+00  0.364485D+01
              31            32            33            34
    31  0.000000D+00
    32  0.118889D+03  0.000000D+00
    33  0.119180D+03 -0.124203D+02  0.000000D+00
    34  0.125825D+03 -0.111269D+02 -0.121633D+02  0.000000D+00
```

**2b**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   124.9816   Anisotropy =    62.7428
   XX=   143.6445   YX=    21.5388   ZX=    16.7330
   XY=    42.0192   YY=    98.5691   ZY=   -17.6536
   XZ=    28.5013   YZ=   -10.0087   ZZ=   132.7313
   Eigenvalues:    73.1883   134.9464   166.8101
  2  C    Isotropic =   144.5079   Anisotropy =    39.8564
   XX=   139.1095   YX=    40.1440   ZX=    15.4330
   XY=    27.0651   YY=   129.7896   ZY=    -9.8723
   XZ=    12.5525   YZ=   -16.7397   ZZ=   164.6247
   Eigenvalues:    95.1970   167.2479   171.0789
  3  N    Isotropic =   199.6154   Anisotropy =   110.6326
   XX=   236.1227   YX=     1.8639   ZX=    44.6221
   XY=    -3.3484   YY=   164.6359   ZY=    27.5247
   XZ=    55.1663   YZ=    35.0778   ZZ=   198.0876
   Eigenvalues:   136.8683   188.6075   273.3705
  4  H    Isotropic =    28.4419   Anisotropy =     7.9674
   XX=    29.1532   YX=     1.3882   ZX=     2.0807
   XY=    -2.4441   YY=    24.3851   ZY=     2.6636
   XZ=     1.1764   YZ=     4.9030   ZZ=    31.7873
   Eigenvalues:    22.5982    28.9739    33.7535
  5  H    Isotropic =    29.5986   Anisotropy =    10.2398
   XX=    29.5550   YX=    -3.3427   ZX=     3.2426
   XY=    -0.4316   YY=    30.1285   ZY=    -2.5123
   XZ=     5.4617   YZ=    -5.3583   ZZ=    29.1121
   Eigenvalues:    24.3693    28.0012    36.4251
  6  H    Isotropic =    29.3812   Anisotropy =    10.2947
   XX=    28.0079   YX=     3.8871   ZX=     4.1288
   XY=     1.7268   YY=    33.1109   ZY=     1.8846
   XZ=     0.6067   YZ=     5.1242   ZZ=    27.0249
   Eigenvalues:    24.8943    27.0050    36.2443
  7  C    Isotropic =   119.2927   Anisotropy =    74.4848
   XX=   136.8772   YX=    33.8286   ZX=    21.4824
   XY=    29.1482   YY=   106.5681   ZY=    18.2550
   XZ=    16.1229   YZ=    18.8117   ZZ=   114.4327
   Eigenvalues:    85.1591   103.7697   168.9492
  8  C    Isotropic =   170.5785   Anisotropy =    20.0632
   XX=   182.2209   YX=    -1.4891   ZX=    -3.1871
   XY=    -3.2166   YY=   166.3240   ZY=     7.7218
   XZ=    -5.0625   YZ=     6.2189   ZZ=   163.1906
   Eigenvalues:   157.4820   170.2995   183.9540
  9  H    Isotropic =    28.2755   Anisotropy =     7.2677
   XX=    29.2246   YX=     2.6259   ZX=    -0.0016
   XY=     0.5253   YY=    32.0920   ZY=     0.9639
```

```
  XZ=     0.5872   YZ=     2.6745   ZZ=    23.5100
  Eigenvalues:    23.1402    28.5657    33.1207
10  H    Isotropic =    29.7855   Anisotropy =     8.2650
  XX=    31.8818   YX=     2.3052   ZX=     2.6979
  XY=     1.7607   YY=    25.5520   ZY=     3.3732
  XZ=     1.4795   YZ=     2.5945   ZZ=    31.9227
  Eigenvalues:    24.1895    29.8716    35.2955
11  H    Isotropic =    29.9435   Anisotropy =     7.5208
  XX=    31.1161   YX=     0.5284   ZX=    -2.8965
  XY=     0.7560   YY=    25.4044   ZY=    -1.1389
  XZ=    -1.6178   YZ=    -1.5893   ZZ=    33.3100
  Eigenvalues:    25.1629    29.7102    34.9574
12  H    Isotropic =    30.7744   Anisotropy =     7.6220
  XX=    32.5436   YX=    -3.3870   ZX=    -0.4924
  XY=    -2.0284   YY=    33.5770   ZY=    -1.2318
  XZ=    -0.0167   YZ=    -0.7679   ZZ=    26.2025
  Eigenvalues:    26.0033    30.4641    35.8557
13  C    Isotropic =    43.6469   Anisotropy =   186.9740
  XX=   -44.2609   YX=    13.7066   ZX=   -55.0754
  XY=    15.2363   YY=    22.5491   ZY=   -14.0349
  XZ=   -54.8458   YZ=    -7.2844   ZZ=   152.6524
  Eigenvalues:   -60.1286    22.7730   168.2962
14  C    Isotropic =    47.7040   Anisotropy =   178.6421
  XX=    31.9856   YX=    39.8668   ZX=   -31.1132
  XY=    36.9762   YY=   -45.2914   ZY=   -14.8874
  XZ=   -32.5981   YZ=   -14.8704   ZZ=   156.4178
  Eigenvalues:   -61.1553    37.4685   166.7987
15  C    Isotropic =    49.1954   Anisotropy =   186.6487
  XX=    13.0277   YX=   -40.6206   ZX=   -45.8020
  XY=   -41.2788   YY=   -23.3815   ZY=   -32.6865
  XZ=   -46.3584   YZ=   -33.7134   ZZ=   157.9401
  Eigenvalues:   -62.9246    36.8829   173.6279
16  C    Isotropic =    48.3311   Anisotropy =   189.0260
  XX=   -47.1647   YX=    14.1390   ZX=   -56.0969
  XY=    15.8762   YY=    33.9634   ZY=   -11.9944
  XZ=   -57.0023   YZ=   -11.2850   ZZ=   158.1946
  Eigenvalues:   -63.1155    33.7603   174.3485
17  C    Isotropic =    49.0802   Anisotropy =   187.2502
  XX=    29.7117   YX=    40.5659   ZX=   -33.2715
  XY=    40.2414   YY=   -45.6255   ZY=   -15.6063
  XZ=   -33.0436   YZ=   -16.9119   ZZ=   163.1545
  Eigenvalues:   -63.2094    36.5364   173.9137
18  C    Isotropic =    44.4241   Anisotropy =   179.9951
  XX=    11.4088   YX=   -38.0373   ZX=   -47.5999
  XY=   -42.0102   YY=   -25.8277   ZY=   -34.2898
  XZ=   -41.4534   YZ=   -41.0876   ZZ=   147.6914
  Eigenvalues:   -66.0745    34.9260   164.4209
19  H    Isotropic =    24.4542   Anisotropy =    10.1477
  XX=    29.3806   YX=     3.5476   ZX=     1.5542
  XY=     3.1477   YY=    23.4428   ZY=     0.7095
  XZ=     1.7457   YZ=     1.1484   ZZ=    20.5391
  Eigenvalues:    20.1900    21.9532    31.2193
20  H    Isotropic =    24.1654   Anisotropy =     5.3986
  XX=    26.7845   YX=    -1.6057   ZX=     1.1591
  XY=    -1.4703   YY=    24.7437   ZY=     0.0158
  XZ=     1.1019   YZ=    -0.1194   ZZ=    20.9681
  Eigenvalues:    20.7412    23.9906    27.7645
21  H    Isotropic =    24.1460   Anisotropy =     4.5884
  XX=    24.1683   YX=     0.1038   ZX=     0.6235
  XY=     0.2644   YY=    27.0747   ZY=     0.8252
  XZ=     0.6146   YZ=     0.7733   ZZ=    21.1949
```

```
  Eigenvalues:    20.9789    24.2541    27.2049
22  H    Isotropic =    24.1566   Anisotropy =     5.2359
  XX=    27.1106   YX=     0.7394   ZX=     1.4922
  XY=     0.6434   YY=    24.0377   ZY=     0.6594
  XZ=     1.4561   YZ=     0.5173   ZZ=    21.3216
  Eigenvalues:    20.9120    23.9106    27.6472
23  H    Isotropic =    23.9743   Anisotropy =     9.2561
  XX=    26.8695   YX=    -4.5705   ZX=     0.1970
  XY=    -3.9069   YY=    24.6386   ZY=     0.3262
  XZ=    -0.2996   YZ=     0.4531   ZZ=    20.4148
  Eigenvalues:    20.3329    21.4451    30.1451
24  B    Isotropic =   124.1164   Anisotropy =    37.8057
  XX=   108.3187   YX=     1.5042   ZX=     7.9552
  XY=     2.3523   YY=   119.4328   ZY=    -8.8661
  XZ=     8.5647   YZ=   -11.0032   ZZ=   144.5978
  Eigenvalues:   105.2125   117.8166   149.3202
25  H    Isotropic =    29.9319   Anisotropy =     6.6364
  XX=    28.8619   YX=     0.0333   ZX=     0.9082
  XY=     0.2531   YY=    26.6267   ZY=     0.1144
  XZ=    -1.9368   YZ=     0.0815   ZZ=    34.3071
  Eigenvalues:    26.6153    28.8242    34.3562
26  H    Isotropic =    30.5795   Anisotropy =     7.2580
  XX=    29.0428   YX=    -0.9109   ZX=     1.0049
  XY=    -0.4231   YY=    30.1029   ZY=    -2.4107
  XZ=    -1.2836   YZ=    -5.3139   ZZ=    32.5926
  Eigenvalues:    27.0911    29.2291    35.4182
27  H    Isotropic =    31.3258   Anisotropy =     7.0519
  XX=    30.7987   YX=     0.2892   ZX=     1.1371
  XY=     1.1853   YY=    27.1783   ZY=    -0.4540
  XZ=    -1.6277   YZ=     1.2511   ZZ=    36.0005
  Eigenvalues:    27.0126    30.9378    36.0271
28  H    Isotropic =    30.9724   Anisotropy =    11.1560
  XX=    36.3616   YX=     3.1343   ZX=     2.7069
  XY=     3.1523   YY=    28.5304   ZY=     1.6731
  XZ=     2.7214   YZ=     1.7114   ZZ=    28.0252
  Eigenvalues:    26.5667    27.9407    38.4097


Total nuclear spin-spin coupling J (Hz):
              1             2             3             4             5
     1  0.000000D+00
     2  0.238325D+02  0.000000D+00
     3 -0.492658D+01 -0.390960D+01  0.000000D+00
     4  0.159829D+03 -0.174700D+01 -0.202917D+00  0.000000D+00
     5 -0.116500D+01  0.161261D+03 -0.417452D+00  0.726187D+01  0.000000D+00
     6 -0.261717D+01  0.166703D+03  0.924914D+00  0.508931D+01 -0.207750D+01
     7 -0.402918D+00 -0.942032D+00  0.181522D+01  0.495158D+01  0.420625D+01
     8  0.221483D+01  0.102429D+01  0.118138D+00 -0.114639D+00 -0.264413D-01
     9 -0.151116D+00  0.614225D+01  0.116872D+01 -0.185501D+00 -0.606021D+00
    10  0.386725D+01  0.160709D+01 -0.634876D+00  0.789434D-02  0.131529D+00
    11 -0.106365D-01 -0.109261D+00  0.266626D+00 -0.175075D+00 -0.775361D-01
    12 -0.114677D+00  0.437773D-01  0.117393D+01 -0.706521D-01  0.243037D+00
    13  0.598151D+02 -0.921422D+00 -0.112819D+00  0.445688D+00  0.229460D+01
    14  0.345092D+01  0.314430D+01  0.693292D+00  0.278934D+01 -0.423656D-01
    15  0.423094D+01  0.340177D+00 -0.107735D+00 -0.420323D+00 -0.295662D-01
    16 -0.848117D+00  0.116927D-01  0.213947D+00  0.681177D+00 -0.652124D-01
    17  0.423418D+01  0.556888D+00 -0.245146D+00 -0.867261D+00  0.875092D-01
    18  0.361638D+01  0.283784D+01  0.218043D+00  0.242734D+01  0.117864D+00
    19  0.454628D+01  0.407438D+00 -0.106527D+00 -0.905659D+00 -0.697234D-01
    20  0.678253D+00 -0.495450D-01  0.104229D+00  0.260080D+00 -0.123553D+00
    21  0.535624D+00 -0.308174D-01 -0.184048D+00 -0.742179D+00 -0.136643D+00
```

```
22  0.596727D+00  0.116121D+00  0.665957D-01  0.136473D+00 -0.102332D+00
23  0.481382D+01 -0.708598D-01 -0.203125D+00 -0.470787D+00 -0.103338D+00
24 -0.503246D+00  0.104585D-01  0.458437D+01  0.349689D+00  0.908397D+00
25  0.724007D+01  0.770309D+00  0.894822D+00  0.119316D+00 -0.263956D+00
26  0.503887D+00  0.698345D+01  0.834494D+00 -0.276508D+00  0.928698D+00
27  0.229931D+01  0.320866D+01  0.756732D-01 -0.462723D+00  0.279778D-01
28  0.204207D+00 -0.773288D-01  0.470369D+01 -0.914083D-01 -0.237406D-01
          6             7             8             9            10
 6  0.000000D+00
 7  0.217260D+01  0.000000D+00
 8  0.577506D-01  0.365515D+02  0.000000D+00
 9  0.673281D+00  0.134891D+03 -0.229023D+01  0.000000D+00
10 -0.521197D+00  0.129065D+03 -0.258267D+01 -0.113496D+02  0.000000D+00
11 -0.894877D-01 -0.508281D+01  0.126551D+03  0.470542D+01  0.126425D+02
12  0.810056D-01 -0.508585D+01  0.119523D+03  0.125393D+02  0.323152D+01
13  0.307301D+01  0.516333D+00  0.539505D+00 -0.581138D-01 -0.871076D-01
14 -0.512745D-01  0.690136D+00  0.858160D-01 -0.234146D-01  0.821941D-01
15  0.519176D-02  0.170411D+00 -0.837780D-03 -0.560581D-01 -0.945380D-02
16 -0.333025D-02 -0.423385D-01  0.172037D-01 -0.329964D-01 -0.482530D-01
17 -0.115871D+00  0.861101D-02 -0.282341D-01 -0.449673D-02 -0.164429D-01
18 -0.445609D+00 -0.891749D-01  0.115453D-01 -0.125966D-01 -0.340001D-02
19  0.242948D+00  0.156639D+00 -0.433374D-01 -0.129597D+00 -0.726497D-01
20  0.698037D-01 -0.683363D-02  0.123641D-01 -0.102165D+00 -0.976312D-01
21 -0.107998D+00  0.513573D-02 -0.420394D-01 -0.970929D-01 -0.967349D-01
22 -0.160011D+00 -0.319568D-01 -0.832037D-02 -0.168227D-01 -0.682404D-01
23 -0.184300D+00  0.430976D-01 -0.925209D-02  0.207981D+00  0.658616D-01
24  0.223448D+01  0.692276D+00  0.112610D+01  0.980381D+00  0.235377D+01
25 -0.117453D+00  0.103274D+01  0.256232D+01 -0.125353D+00 -0.476683D+00
26 -0.470844D-01  0.279649D+01 -0.155268D+00  0.178553D+00  0.109612D+00
27  0.287269D+00  0.656354D+01  0.758557D+00 -0.692540D-02  0.142798D+01
28 -0.732224D-01  0.417825D+00  0.118085D+03  0.203160D+01  0.345631D+01
          11            12            13            14            15
11  0.000000D+00
12 -0.110701D+02  0.000000D+00
13 -0.387940D-01  0.640715D-01  0.000000D+00
14 -0.212665D-01 -0.335920D-01  0.650961D+02  0.000000D+00
15 -0.290380D-01 -0.138856D-01 -0.120634D+01  0.609519D+02  0.000000D+00
16 -0.186800D-01 -0.358311D-01  0.944769D+01 -0.203919D+01  0.602747D+02
17 -0.206853D-01 -0.201445D-01 -0.146592D+01  0.864597D+01 -0.160878D+01
18 -0.101487D-01 -0.353794D-01  0.624028D+02 -0.377966D+00  0.881217D+01
19 -0.620672D-01  0.473053D-02  0.102696D-01  0.149927D+03  0.866428D+00
20 -0.703429D-01 -0.623519D-01  0.704911D+01  0.184460D+01  0.151436D+03
21 -0.767712D-01 -0.788249D-01 -0.129702D+01  0.699054D+01  0.166525D+01
22 -0.580274D-01 -0.807967D-01  0.711180D+01 -0.119685D+01  0.702179D+01
23 -0.336025D-01 -0.690131D-01  0.492911D+00  0.574214D+01 -0.937940D+00
24  0.966136D-01 -0.636695D-01  0.116973D+01  0.191941D+00 -0.349537D-01
25  0.304533D+00  0.315097D-02  0.750429D-01  0.247781D+00 -0.252590D-01
26  0.117166D+00 -0.164550D+00  0.693604D-02 -0.342195D-01  0.180826D-01
27 -0.217762D+00 -0.126367D+00  0.441420D+00  0.114199D+01 -0.921378D-02
28 -0.123531D+02 -0.128739D+02  0.155379D+00  0.274071D-01 -0.354290D-01
          16            17            18            19            20
16  0.000000D+00
17  0.598935D+02  0.000000D+00
18 -0.197194D+01  0.613642D+02  0.000000D+00
19  0.665472D+01 -0.897317D+00  0.564188D+01  0.000000D+00
20  0.143322D+01  0.702184D+01 -0.118984D+01  0.716673D+01  0.000000D+00
21  0.151264D+03  0.172713D+01  0.702184D+01  0.609964D+00  0.691093D+01
22  0.151095D+01  0.151427D+03  0.167124D+01  0.377414D+00  0.740663D+00
23  0.671732D+01  0.895054D+00  0.149763D+03  0.133431D+01  0.410082D+00
24  0.521195D-02 -0.415403D-02  0.646502D-01 -0.238775D-01 -0.264363D-01
25 -0.258393D-01 -0.157511D-01  0.504119D-01 -0.508674D-01 -0.806760D-01
```

```
    26 -0.515844D-01  0.811713D-01  0.480534D+00 -0.895559D-01 -0.143805D+00
    27  0.776171D-01 -0.656500D-01  0.272023D+00  0.266904D+00 -0.104746D-01
    28 -0.399346D-02 -0.451128D-01  0.462814D-02 -0.921407D-01 -0.724599D-01
              21            22            23            24            25
    21  0.000000D+00
    22  0.682516D+01  0.000000D+00
    23  0.611481D+00  0.720081D+01  0.000000D+00
    24 -0.429006D-01 -0.183057D-01  0.852148D-02  0.000000D+00
    25 -0.100856D+00 -0.110815D+00 -0.391843D-01  0.924240D+02  0.000000D+00
    26 -0.760413D-01 -0.475073D-01  0.391245D+00  0.932653D+02 -0.652138D+01
    27 -0.133134D+00 -0.626866D-01 -0.103438D+00  0.959345D+02 -0.717912D+01
    28 -0.103755D+00 -0.539126D-01 -0.528251D-01  0.157743D+00  0.446383D+00
              26            27            28
    26  0.000000D+00
    27 -0.724186D+01  0.000000D+00
    28 -0.122554D+00 -0.280055D+00  0.000000D+00
```

**inv-2b**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   125.8373   Anisotropy =    59.2073
   XX=   131.8725   YX=    29.7221   ZX=     9.8928
   XY=    46.2022   YY=   121.9435   ZY=   -17.8380
   XZ=    19.3028   YZ=   -21.4189   ZZ=   123.6960
   Eigenvalues:    76.1169   136.0863   165.3089
  2  C    Isotropic =   145.0830   Anisotropy =    41.0153
   XX=   139.9291   YX=    33.7191   ZX=    23.1198
   XY=    29.9200   YY=   141.2111   ZY=   -24.5203
   XZ=    16.3406   YZ=   -12.8871   ZZ=   154.1089
   Eigenvalues:    96.0227   166.7998   172.4266
  3  N    Isotropic =   201.2760   Anisotropy =    94.8719
   XX=   197.1148   YX=    36.0248   ZX=   -50.0919
   XY=     6.0932   YY=   240.4098   ZY=   -34.4243
   XZ=   -20.7141   YZ=   -18.1891   ZZ=   166.3033
   Eigenvalues:   141.8204   197.4835   264.5239
  4  H    Isotropic =    27.8931   Anisotropy =     9.2595
   XX=    27.7979   YX=     2.1073   ZX=    -0.1906
   XY=    -0.3239   YY=    33.2755   ZY=    -1.2559
   XZ=    -2.0086   YZ=    -3.9007   ZZ=    22.6058
   Eigenvalues:    21.8843    27.7288    34.0660
  5  H    Isotropic =    29.5523   Anisotropy =     9.4476
   XX=    27.8342   YX=     4.4728   ZX=     0.8204
   XY=     0.6526   YY=    32.4386   ZY=     5.6670
   XZ=     1.0228   YZ=     2.4810   ZZ=    28.3840
   Eigenvalues:    25.6377    27.1685    35.8506
  6  H    Isotropic =    29.5126   Anisotropy =    11.3539
   XX=    28.0930   YX=     1.5299   ZX=    -4.9819
   XY=     4.9605   YY=    27.0133   ZY=    -2.9336
   XZ=    -4.2979   YZ=    -0.4002   ZZ=    33.4314
   Eigenvalues:    23.8103    27.6457    37.0819
  7  C    Isotropic =   130.0154   Anisotropy =    53.1108
   XX=   114.1593   YX=     2.5326   ZX=    -5.0209
   XY=     8.6681   YY=   136.2073   ZY=   -27.8637
   XZ=   -11.5249   YZ=   -23.1738   ZZ=   139.6797
   Eigenvalues:   110.7835   113.8402   165.4227
  8  C    Isotropic =   170.7277   Anisotropy =    21.0518
   XX=   173.5693   YX=   -12.5743   ZX=    -1.3248
   XY=   -11.0208   YY=   172.0901   ZY=    -4.1137
   XZ=    -2.4964   YZ=    -4.0371   ZZ=   166.5237
   Eigenvalues:   158.6589   168.7620   184.7622
```

```
 9  H    Isotropic =    29.2375   Anisotropy =     6.7393
  XX=    27.3362   YX=    -1.4983   ZX=    -2.0581
  XY=    -3.3849   YY=    26.7526   ZY=    -1.9777
  XZ=     0.4184   YZ=     1.1535   ZZ=    33.6236
  Eigenvalues:    24.5055    29.4765    33.7303
10  H    Isotropic =    30.3829   Anisotropy =     7.6161
  XX=    34.7051   YX=     0.8366   ZX=     0.5042
  XY=    -1.3092   YY=    30.6745   ZY=    -3.8091
  XZ=     3.1538   YZ=    -5.0045   ZZ=    25.7691
  Eigenvalues:    22.9952    32.6932    35.4603
11  H    Isotropic =    30.0222   Anisotropy =     8.2842
  XX=    34.3333   YX=     1.5933   ZX=     3.0192
  XY=    -0.3981   YY=    29.3853   ZY=    -0.5977
  XZ=     3.5845   YZ=    -0.4960   ZZ=    26.3481
  Eigenvalues:    25.0410    29.4807    35.5450
12  H    Isotropic =    30.9957   Anisotropy =     7.9740
  XX=    29.0879   YX=    -3.1258   ZX=    -1.3225
  XY=    -4.2868   YY=    32.2864   ZY=     3.4053
  XZ=     0.4491   YZ=     2.4468   ZZ=    31.6130
  Eigenvalues:    26.3036    30.3718    36.3118
13  C    Isotropic =    44.9011   Anisotropy =   186.6174
  XX=   -23.3161   YX=   -57.6243   ZX=    56.0129
  XY=   -59.0471   YY=    82.1862   ZY=   -50.9485
  XZ=    62.1312   YZ=   -57.9768   ZZ=    75.8331
  Eigenvalues:   -59.1417    24.5323   169.3127
14  C    Isotropic =    44.6492   Anisotropy =   183.9064
  XX=    32.1473   YX=   -67.7168   ZX=    17.5020
  XY=   -68.1259   YY=    27.2221   ZY=   -94.7582
  XZ=    10.3419   YZ=   -87.8255   ZZ=    74.5780
  Eigenvalues:   -67.1044    33.7984   167.2534
15  C    Isotropic =    47.6321   Anisotropy =   188.1756
  XX=    37.0378   YX=   -13.6505   ZX=    69.4859
  XY=   -13.0933   YY=    65.9336   ZY=   -96.8837
  XZ=    67.8509   YZ=   -93.8176   ZZ=    39.9249
  Eigenvalues:   -64.4473    34.2611   173.0825
16  C    Isotropic =    47.7829   Anisotropy =   192.1027
  XX=   -27.4879   YX=   -60.6899   ZX=    61.1235
  XY=   -60.1654   YY=    86.0109   ZY=   -53.2710
  XZ=    63.1599   YZ=   -53.7124   ZZ=    84.8258
  Eigenvalues:   -64.4480    31.9454   175.8514
17  C    Isotropic =    48.3439   Anisotropy =   187.3676
  XX=    33.0483   YX=   -71.6292   ZX=    13.3183
  XY=   -70.2320   YY=    39.2588   ZY=   -91.5863
  XZ=    12.3569   YZ=   -92.8896   ZZ=    72.7246
  Eigenvalues:   -63.6805    35.4566   173.2557
18  C    Isotropic =    48.0567   Anisotropy =   179.7331
  XX=    41.8371   YX=   -11.3227   ZX=    66.3960
  XY=   -13.8271   YY=    67.2103   ZY=   -91.4276
  XZ=    65.0878   YZ=   -93.3320   ZZ=    35.1228
  Eigenvalues:   -62.1790    38.4703   167.8788
19  H    Isotropic =    23.8803   Anisotropy =     9.1811
  XX=    26.9056   YX=    -1.9856   ZX=    -4.1501
  XY=    -1.4885   YY=    21.7503   ZY=     1.6864
  XZ=    -3.6449   YZ=     1.7731   ZZ=    22.9850
  Eigenvalues:    20.2301    21.4098    30.0010
20  H    Isotropic =    24.0209   Anisotropy =     5.3084
  XX=    26.3687   YX=     2.1633   ZX=    -0.7927
  XY=     2.2746   YY=    23.4007   ZY=     1.2805
  XZ=    -0.9559   YZ=     1.2933   ZZ=    22.2932
  Eigenvalues:    20.7048    23.7981    27.5598
21  H    Isotropic =    24.1773   Anisotropy =     4.4422
```

```
   XX=    23.8936   YX=     0.6529   ZX=    -0.7491
   XY=     0.6684   YY=    24.4838   ZY=     2.8706
   XZ=    -0.5562   YZ=     2.7584   ZZ=    24.1545
   Eigenvalues:    21.1821    24.2109    27.1388
 22  H    Isotropic =    24.1011   Anisotropy =     5.3298
   XX=    26.5129   YX=     0.6461   ZX=    -2.2727
   XY=     0.6371   YY=    22.3727   ZY=     1.3651
   XZ=    -2.1209   YZ=     1.5147   ZZ=    23.4178
   Eigenvalues:    20.7505    23.8986    27.6543
 23  H    Isotropic =    24.3913   Anisotropy =    10.1276
   XX=    28.3924   YX=     4.0759   ZX=     1.5886
   XY=     4.1898   YY=    23.2934   ZY=     1.8707
   XZ=     1.1237   YZ=     1.7319   ZZ=    21.4882
   Eigenvalues:    20.1231    21.9078    31.1430
 24  B    Isotropic =   118.1296   Anisotropy =    50.7456
   XX=   121.4626   YX=    26.4275   ZX=     9.0139
   XY=    26.3305   YY=   124.7620   ZY=     6.8329
   XZ=     9.4819   YZ=     3.9713   ZZ=   108.1642
   Eigenvalues:    95.7930   106.6358   151.9600
 25  H    Isotropic =    29.5713   Anisotropy =     8.1066
   XX=    32.8219   YX=     2.4412   ZX=     1.0635
   XY=     4.2918   YY=    29.4083   ZY=     0.1863
   XZ=     1.0769   YZ=    -0.4151   ZZ=    26.4835
   Eigenvalues:    26.0629    27.6752    34.9756
 26  H    Isotropic =    29.8187   Anisotropy =     8.5108
   XX=    29.6693   YX=     3.3848   ZX=     2.8384
   XY=     2.3769   YY=    31.3468   ZY=     3.7546
   XZ=     1.2392   YZ=     2.5336   ZZ=    28.4400
   Eigenvalues:    26.4109    27.5527    35.4926
 27  H    Isotropic =    30.6051   Anisotropy =     9.4202
   XX=    31.2658   YX=     5.2219   ZX=    -0.5493
   XY=     4.1935   YY=    32.9272   ZY=    -0.3317
   XZ=    -0.0038   YZ=     0.0678   ZZ=    27.6224
   Eigenvalues:    27.2693    27.6608    36.8853
 28  H    Isotropic =    31.1125   Anisotropy =    11.0441
   XX=    28.3769   YX=    -1.3395   ZX=     0.3487
   XY=    -1.9691   YY=    34.0068   ZY=    -5.5138
   XZ=     0.9416   YZ=    -5.4816   ZZ=    30.9539
   Eigenvalues:    26.6170    28.2453    38.4752


Total nuclear spin-spin coupling J (Hz):
              1             2             3             4             5
     1  0.000000D+00
     2  0.237941D+02  0.000000D+00
     3 -0.498760D+01 -0.371133D+01  0.000000D+00
     4  0.167973D+03 -0.188321D+01  0.973391D+00  0.000000D+00
     5 -0.240647D+01  0.157856D+03 -0.396218D+00  0.493771D+01  0.000000D+00
     6 -0.145397D+01  0.169889D+03  0.618422D+00  0.645816D+01 -0.199214D+01
     7 -0.709927D+00 -0.561108D+00  0.203314D+01  0.123023D+01  0.435651D+01
     8  0.178837D+01  0.850109D+00  0.268560D+00  0.598843D+00  0.183363D-01
     9 -0.666727D-01  0.593151D+01  0.120238D+01 -0.305326D+00 -0.568826D+00
    10  0.258072D+01  0.157515D+01 -0.713225D+00 -0.557135D+00  0.186167D+00
    11 -0.236077D+00 -0.967931D-01  0.341805D+00 -0.179864D+00 -0.924449D-01
    12 -0.777142D-01  0.494026D-01  0.107521D+01  0.382903D-01  0.279093D+00
    13  0.563149D+02 -0.720284D+00 -0.675350D+00  0.846416D+00  0.344113D+01
    14  0.389795D+01  0.286392D+01  0.238058D+00  0.262478D+01 -0.459256D+00
    15  0.410571D+01  0.574624D+00 -0.215310D+00 -0.813930D+00 -0.106800D+00
    16 -0.814712D+00  0.139147D-01  0.194036D+00  0.650303D+00  0.717863D-03
    17  0.388521D+01  0.318842D+00 -0.171941D+00 -0.287215D+00  0.357920D-02
    18  0.314381D+01  0.315251D+01  0.385679D+00  0.314365D+01  0.390022D-02
```

```
19  0.476321D+01 -0.459436D-01 -0.175175D+00 -0.431462D+00 -0.182911D+00
20  0.562748D+00  0.116927D+00  0.599653D-01  0.127498D+00 -0.154387D+00
21  0.514722D+00 -0.320368D-01 -0.170544D+00 -0.727469D+00 -0.108105D+00
22  0.642571D+00 -0.491799D-01  0.817230D-01  0.277391D+00  0.663202D-01
23  0.426041D+01  0.441899D+00 -0.178373D+00 -0.904287D+00  0.222507D+00
24  0.862599D-01 -0.242961D+00  0.439849D+01  0.218393D+01  0.916999D+00
25  0.834173D+01  0.115090D+01  0.755690D+00 -0.143454D+00 -0.266268D+00
26  0.475448D+00  0.728254D+01  0.870676D+00 -0.132007D+00  0.121688D+01
27  0.530205D+01  0.284062D+01  0.239374D+00 -0.198476D+00 -0.128225D+00
28  0.349464D+00 -0.899534D-01  0.480923D+01  0.215230D+00 -0.584965D-01
          6             7             8             9            10
 6  0.000000D+00
 7  0.217845D+01  0.000000D+00
 8  0.104464D+00  0.365508D+02  0.000000D+00
 9  0.601727D+00  0.134794D+03 -0.227656D+01  0.000000D+00
10 -0.473454D+00  0.129279D+03 -0.266549D+01 -0.115846D+02  0.000000D+00
11 -0.972608D-01 -0.514596D+01  0.125825D+03  0.442469D+01  0.128119D+02
12  0.684941D-01 -0.506003D+01  0.119340D+03  0.125153D+02  0.353541D+01
13  0.242293D+01  0.195162D+01 -0.429279D-01 -0.446460D-01  0.189211D-01
14  0.196974D+00 -0.145361D-01 -0.386602D-02  0.163347D+00  0.206278D+00
15  0.112669D+00 -0.905786D-02 -0.518052D-02  0.447244D-01 -0.497309D-02
16 -0.598009D-01  0.259844D-01 -0.650101D-02 -0.222311D-01  0.383835D-01
17 -0.229647D-01 -0.603949D-01 -0.292135D-02 -0.121857D-01  0.736082D-01
18  0.164335D+00  0.800595D-01  0.319955D-01  0.283503D-01  0.647352D+00
19 -0.108519D+00 -0.476738D-01  0.355118D-02  0.246698D+00  0.103458D-01
20 -0.100538D+00  0.133217D-01 -0.223779D-01 -0.189180D-01 -0.726791D-01
21 -0.140427D+00 -0.481019D-01 -0.197723D-01 -0.859280D-01 -0.591609D-01
22 -0.133333D+00 -0.350828D-02 -0.189132D-01 -0.127603D+00 -0.162668D-02
23 -0.903408D-01 -0.655209D-01 -0.133548D-01 -0.114811D+00  0.273189D+00
24  0.208158D+01  0.863998D+00  0.104050D+01  0.111672D+01  0.262003D+01
25 -0.919225D-01  0.694782D+00  0.226107D+01 -0.126019D+00 -0.529238D+00
26 -0.987033D-01  0.271163D+01 -0.145823D+00  0.193958D+00  0.131533D+00
27  0.191186D+00  0.543675D+01  0.668747D+00  0.309374D-01  0.128239D+01
28 -0.144902D+00  0.655170D+00  0.118666D+03  0.224857D+01  0.331574D+01
          11            12            13            14            15
11  0.000000D+00
12 -0.110546D+02  0.000000D+00
13  0.134238D-01  0.886216D-03  0.000000D+00
14  0.254213D-01 -0.545029D-02  0.607893D+02  0.000000D+00
15 -0.439234D-01 -0.222064D-01 -0.140521D+01  0.607482D+02  0.000000D+00
16 -0.289382D-02 -0.270037D-01  0.937685D+01 -0.193561D+01  0.594205D+02
17 -0.503043D-01  0.199858D-02 -0.120129D+01  0.880543D+01 -0.155220D+01
18  0.690647D-01 -0.552279D-02  0.633963D+02 -0.275160D+00  0.858540D+01
19 -0.731543D-01 -0.854643D-01  0.698062D+00  0.151152D+03  0.952683D+00
20 -0.750756D-01 -0.104053D+00  0.711150D+01  0.171754D+01  0.152196D+03
21 -0.116319D+00 -0.839877D-01 -0.127022D+01  0.698459D+01  0.172286D+01
22 -0.921886D-01 -0.411687D-01  0.697703D+01 -0.117734D+01  0.702660D+01
23 -0.103107D+00  0.720971D-01  0.314291D+00  0.562123D+01 -0.887408D+00
24  0.805947D-01 -0.877950D-01  0.190664D+00 -0.686203D-01  0.530315D-02
25  0.320342D+00 -0.265233D-01  0.959655D+00 -0.148867D-01 -0.685199D-01
26  0.101364D+00 -0.173982D+00 -0.729040D-01  0.986305D-01  0.997187D-02
27 -0.231240D+00 -0.141275D+00  0.173008D+00  0.118878D-01 -0.239252D-01
28 -0.123065D+02 -0.127584D+02 -0.709752D-01  0.534889D-01 -0.306603D-01
          16            17            18            19            20
16  0.000000D+00
17  0.599374D+02  0.000000D+00
18 -0.197276D+01  0.603343D+02  0.000000D+00
19  0.676046D+01 -0.918640D+00  0.575135D+01  0.000000D+00
20  0.153885D+01  0.703300D+01 -0.119048D+01  0.723748D+01  0.000000D+00
21  0.151910D+03  0.169244D+01  0.701571D+01  0.634752D+00  0.683228D+01
22  0.140374D+01  0.152000D+03  0.189554D+01  0.419361D+00  0.751231D+00
```

```
23  0.659812D+01  0.893369D+00  0.149829D+03  0.135441D+01  0.381415D+00
24 -0.349368D-01  0.789146D-01  0.359115D+00  0.321457D-01 -0.334054D-01
25  0.992234D-02  0.938173D-02  0.259159D+00 -0.552906D-01 -0.762849D-01
26 -0.299838D-01 -0.496570D-01 -0.123460D-01  0.221842D+00 -0.178371D-01
27 -0.427885D-01  0.340018D-01  0.178822D+00  0.484933D-01 -0.694278D-01
28  0.208966D-01 -0.293415D-01  0.353168D-01 -0.783434D-01 -0.506835D-01
          21            22            23            24            25
21  0.000000D+00
22  0.693841D+01  0.000000D+00
23  0.615069D+00  0.716389D+01  0.000000D+00
24 -0.139929D-01 -0.328149D-01  0.633286D-01  0.000000D+00
25 -0.136751D+00 -0.342661D-01 -0.926626D-01  0.943409D+02  0.000000D+00
26 -0.933937D-01 -0.955239D-01 -0.123642D+00  0.935821D+02 -0.624579D+01
27 -0.973468D-01 -0.850162D-01 -0.531311D-01  0.940839D+02 -0.672064D+01
28 -0.826198D-01 -0.379979D-01 -0.564749D-01  0.821903D-01  0.348253D+00
          26            27            28
26  0.000000D+00
27 -0.663763D+01  0.000000D+00
28 -0.125086D+00 -0.276890D+00  0.000000D+00
```

**SCF GIAO magnetic shielding tensor (ppm) and total nuclear spin-spin coupling *J* (Hz) calculated at the PCM/MPW1PW91/6-311++g(d,p) level of theory**

**2a**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   140.2554   Anisotropy =    55.2537
   XX=   164.0351   YX=    13.2821   ZX=   -13.4368
   XY=    18.3341   YY=   118.3778   ZY=    20.2868
   XZ=   -30.7615   YZ=    18.7064   ZZ=   138.3534
   Eigenvalues:    96.8457   146.8293   177.0912
  2  C    Isotropic =   151.5397   Anisotropy =    40.2320
   XX=   151.3436   YX=    29.5522   ZX=    -7.7271
   XY=    25.8221   YY=   130.8054   ZY=     6.4597
   XZ=   -16.6570   YZ=    13.0654   ZZ=   172.4701
   Eigenvalues:   108.0456   168.2124   178.3611
  3  N    Isotropic =   199.8518   Anisotropy =   113.8956
   XX=   244.8587   YX=     9.2176   ZX=   -40.6075
   XY=    -1.9208   YY=   175.8353   ZY=   -27.9848
   XZ=   -60.0015   YZ=   -37.6447   ZZ=   178.8613
   Eigenvalues:   133.2841   190.4890   275.7822
  4  H    Isotropic =    28.0111   Anisotropy =     9.0047
   XX=    31.0499   YX=     2.2931   ZX=    -3.1086
   XY=    -0.3111   YY=    23.1322   ZY=    -2.7094
   XZ=    -1.8741   YZ=    -4.9697   ZZ=    29.8511
   Eigenvalues:    21.3881    28.6309    34.0142
  5  H    Isotropic =    29.4774   Anisotropy =     9.4452
   XX=    28.9698   YX=    -1.5650   ZX=    -3.5889
   XY=     0.8883   YY=    30.4785   ZY=     2.4978
   XZ=    -5.7057   YZ=     5.7782   ZZ=    28.9841
   Eigenvalues:    23.1906    29.4675    35.7742
  6  H    Isotropic =    29.2052   Anisotropy =    11.7016
   XX=    27.9470   YX=     4.7214   ZX=    -4.1738
   XY=     3.1046   YY=    33.2858   ZY=    -1.4206
   XZ=    -1.3635   YZ=    -5.0986   ZZ=    26.3829
   Eigenvalues:    24.2754    26.3340    37.0063
  7  C    Isotropic =   124.5237   Anisotropy =    54.9989
   XX=   149.5590   YX=    21.8087   ZX=   -10.0013
   XY=    20.1587   YY=   113.7076   ZY=    -2.1511
   XZ=    -8.2730   YZ=    -5.8981   ZZ=   110.3046
   Eigenvalues:   104.0289   108.3526   161.1897
  8  C    Isotropic =    49.6970   Anisotropy =   186.0686
   XX=   -39.2709   YX=    16.1192   ZX=    44.8168
   XY=    15.9558   YY=    23.5563   ZY=    -0.4154
   XZ=    42.4472   YZ=    -6.0524   ZZ=   164.8055
   Eigenvalues:   -51.7618    27.1100   173.7427
  9  C    Isotropic =    52.8162   Anisotropy =   180.1440
   XX=    38.2884   YX=    28.8451   ZX=    27.4480
   XY=    27.6233   YY=   -46.5883   ZY=    -2.8784
   XZ=    29.8986   YZ=    -2.2003   ZZ=   166.7487
   Eigenvalues:   -55.6565    41.1929   172.9122
 10  C    Isotropic =    54.8621   Anisotropy =   185.8021
   XX=     6.1711   YX=   -45.8589   ZX=    35.0670
   XY=   -46.4879   YY=   -13.1025   ZY=    11.2790
   XZ=    35.3757   YZ=    11.6661   ZZ=   171.5177
   Eigenvalues:   -54.9879    40.8440   178.7301
 11  C    Isotropic =    54.2196   Anisotropy =   188.5048
   XX=   -42.8219   YX=    16.7834   ZX=    44.6759
   XY=    17.8634   YY=    34.6497   ZY=    -1.9541
```

```
  XZ=    45.1411   YZ=    -3.7329   ZZ=   170.8310
  Eigenvalues:   -55.2994    38.0687   179.8895
12  C    Isotropic =    54.6198   Anisotropy =   186.0378
  XX=    37.2071   YX=    28.7718   ZX=    28.6387
  XY=    29.1639   YY=   -46.0724   ZY=    -2.1033
  XZ=    28.7492   YZ=    -0.3464   ZZ=   172.7249
  Eigenvalues:   -55.5878    40.8023   178.6450
13  C    Isotropic =    50.1884   Anisotropy =   180.6434
  XX=     4.9653   YX=   -45.4623   ZX=    37.5223
  XY=   -46.9889   YY=   -16.6561   ZY=    12.8518
  XZ=    36.1745   YZ=    18.4298   ZZ=   162.2560
  Eigenvalues:   -58.9967    38.9445   170.6173
14  H    Isotropic =    24.2361   Anisotropy =    10.7656
  XX=    30.1134   YX=     3.4405   ZX=    -0.6746
  XY=     2.9961   YY=    22.8314   ZY=    -0.2345
  XZ=    -1.0813   YZ=    -0.6270   ZZ=    19.7636
  Eigenvalues:    19.6779    21.6173    31.4132
15  H    Isotropic =    24.0568   Anisotropy =     5.2526
  XX=    26.7253   YX=    -1.4251   ZX=    -0.9599
  XY=    -1.2392   YY=    24.9195   ZY=     0.2354
  XZ=    -0.8433   YZ=     0.3953   ZZ=    20.5257
  Eigenvalues:    20.3936    24.2183    27.5586
16  H    Isotropic =    24.0132   Anisotropy =     4.3273
  XX=    24.5261   YX=     0.4215   ZX=    -0.5668
  XY=     0.5392   YY=    26.7746   ZY=    -0.2127
  XZ=    -0.5774   YZ=    -0.3496   ZZ=    20.7390
  Eigenvalues:    20.6473    24.4943    26.8981
17  H    Isotropic =    23.9161   Anisotropy =     5.6002
  XX=    27.4089   YX=     0.3684   ZX=    -1.1521
  XY=     0.3649   YY=    23.8844   ZY=    -0.2181
  XZ=    -1.2347   YZ=    -0.1920   ZZ=    20.4550
  Eigenvalues:    20.2503    23.8484    27.6495
18  H    Isotropic =    23.8677   Anisotropy =    10.1247
  XX=    26.8924   YX=    -4.8394   ZX=    -0.1901
  XY=    -4.1805   YY=    25.1574   ZY=    -0.1254
  XZ=    -0.0237   YZ=    -0.0840   ZZ=    19.5534
  Eigenvalues:    19.5417    21.4440    30.6175
19  B    Isotropic =   125.9171   Anisotropy =    32.4034
  XX=   115.4225   YX=     5.0972   ZX=   -10.7910
  XY=     4.3929   YY=   118.5996   ZY=     1.3980
  XZ=   -10.6552   YZ=     6.6156   ZZ=   143.7292
  Eigenvalues:   108.4799   121.7519   147.5194
20  H    Isotropic =    29.6562   Anisotropy =     7.3860
  XX=    28.3810   YX=     0.3287   ZX=    -2.2160
  XY=     0.1502   YY=    26.1873   ZY=    -1.0127
  XZ=     0.9740   YZ=    -0.9264   ZZ=    34.4003
  Eigenvalues:    26.0623    28.3261    34.5802
21  H    Isotropic =    30.3150   Anisotropy =     6.4981
  XX=    29.9701   YX=    -0.5294   ZX=    -2.5878
  XY=    -0.1845   YY=    28.0148   ZY=     1.5583
  XZ=     0.3306   YZ=     4.3830   ZZ=    32.9600
  Eigenvalues:    26.6148    29.6831    34.6470
22  H    Isotropic =    31.3171   Anisotropy =     7.5651
  XX=    31.0513   YX=     1.2353   ZX=    -2.3624
  XY=     1.4298   YY=    27.3073   ZY=    -0.7700
  XZ=     0.5789   YZ=    -3.4256   ZZ=    35.5925
  Eigenvalues:    26.5351    31.0555    36.3605
23  C    Isotropic =   158.9504   Anisotropy =    32.6688
  XX=   148.8546   YX=     2.2839   ZX=     0.8467
  XY=    -1.0433   YY=   175.2244   ZY=    15.0072
  XZ=    -2.4044   YZ=     9.7995   ZZ=   152.7721
```

```
  Eigenvalues:   146.8137   149.3079   180.7296
 24  H    Isotropic =    29.6159   Anisotropy =     7.2692
  XX=    26.8680   YX=     2.0264   ZX=     0.2025
  XY=     1.8626   YY=    29.1100   ZY=     3.6488
  XZ=     0.1143   YZ=     1.8247   ZZ=    32.8698
  Eigenvalues:    25.4960    28.8897    34.4621
 25  H    Isotropic =    30.8862   Anisotropy =    10.0550
  XX=    32.2874   YX=     4.8118   ZX=    -0.6248
  XY=     4.8862   YY=    33.1547   ZY=     0.5068
  XZ=    -0.6291   YZ=     0.5213   ZZ=    27.2167
  Eigenvalues:    26.6648    28.4044    37.5896
 26  H    Isotropic =    30.4179   Anisotropy =     8.3994
  XX=    30.5766   YX=    -1.8642   ZX=     0.5037
  XY=    -3.1609   YY=    34.8565   ZY=    -0.2356
  XZ=     0.7231   YZ=     0.6284   ZZ=    25.8207
  Eigenvalues:    25.7098    29.5264    36.0175
 27  C    Isotropic =   163.6711   Anisotropy =    36.6970
  XX=   153.7590   YX=    -0.9139   ZX=    -3.6859
  XY=    -6.2394   YY=   149.5189   ZY=    -3.3345
  XZ=     0.7844   YZ=    -4.1702   ZZ=   187.7354
  Eigenvalues:   147.0914   155.7862   188.1358
 28  H    Isotropic =    30.7757   Anisotropy =    10.2328
  XX=    34.1373   YX=     2.6156   ZX=    -3.6937
  XY=     2.1445   YY=    27.3743   ZY=    -1.7717
  XZ=    -4.1673   YZ=    -1.7425   ZZ=    30.8155
  Eigenvalues:    26.5083    28.2213    37.5975
 29  H    Isotropic =    30.9026   Anisotropy =     7.9842
  XX=    28.7791   YX=     0.7243   ZX=    -2.7697
  XY=     1.0862   YY=    30.0465   ZY=     2.3790
  XZ=    -2.6438   YZ=     4.0234   ZZ=    33.8822
  Eigenvalues:    26.1906    30.2917    36.2254
 30  H    Isotropic =    30.7657   Anisotropy =     8.2187
  XX=    29.6857   YX=    -0.5946   ZX=     0.0898
  XY=    -1.4524   YY=    30.4415   ZY=    -3.9354
  XZ=     1.4416   YZ=    -5.3110   ZZ=    32.1699
  Eigenvalues:    26.5723    29.4800    36.2449
 31  C    Isotropic =   162.2333   Anisotropy =    41.2718
  XX=   171.1071   YX=   -16.4685   ZX=    10.8319
  XY=   -13.2395   YY=   165.0294   ZY=   -12.5922
  XZ=    11.3428   YZ=   -10.7166   ZZ=   150.5634
  Eigenvalues:   143.6819   153.2702   189.7478
 32  H    Isotropic =    30.7767   Anisotropy =     8.6075
  XX=    31.3840   YX=    -4.2856   ZX=     0.4469
  XY=    -2.4973   YY=    34.1245   ZY=     2.0109
  XZ=     0.6019   YZ=     1.0777   ZZ=    26.8214
  Eigenvalues:    26.1537    29.6613    36.5150
 33  H    Isotropic =    31.0213   Anisotropy =    10.4948
  XX=    37.9469   YX=     0.8225   ZX=     0.5821
  XY=     0.4539   YY=    28.2448   ZY=    -0.7092
  XZ=     0.6412   YZ=    -0.5795   ZZ=    26.8722
  Eigenvalues:    26.5600    28.4860    38.0178
 34  H    Isotropic =    29.3559   Anisotropy =     7.8109
  XX=    29.5574   YX=    -2.0687   ZX=     2.1595
  XY=    -1.6108   YY=    25.5451   ZY=    -3.2422
  XZ=     0.6924   YZ=    -2.0159   ZZ=    32.9651
  Eigenvalues:    24.3465    29.1580    34.5631

Total nuclear spin-spin coupling J (Hz):
               1             2             3             4             5
      1  0.000000D+00
      2  0.215940D+02  0.000000D+00
```

```
 3 -0.506315D+01 -0.389280D+01  0.000000D+00
 4  0.150848D+03 -0.241903D+01 -0.434151D+00  0.000000D+00
 5 -0.145739D+01  0.151134D+03 -0.587716D+00  0.760670D+01  0.000000D+00
 6 -0.340873D+01  0.160434D+03  0.729584D+00  0.470101D+01 -0.305715D+01
 7 -0.107977D+01 -0.103240D+01  0.384680D+00  0.353190D+01  0.375891D+01
 8  0.572038D+02 -0.131164D+01 -0.153147D+00 -0.653914D+00  0.229809D+01
 9  0.299563D+01  0.293365D+01  0.739572D+00  0.275490D+01 -0.155273D+00
10  0.433550D+01  0.321627D+00 -0.106619D+00 -0.656902D+00 -0.333050D-01
11 -0.963468D+00  0.817283D-02  0.201206D+00  0.788209D+00 -0.647308D-01
12  0.422645D+01  0.506605D+00 -0.255960D+00 -0.107550D+01  0.797205D-01
13  0.273796D+01  0.263245D+01  0.196352D+00  0.240644D+01  0.269959D-01
14  0.466274D+01  0.246559D+00 -0.118741D+00 -0.107398D+01 -0.572341D-01
15  0.543839D+00 -0.475615D-01  0.132012D+00  0.395710D+00 -0.114471D+00
16  0.650652D+00 -0.365652D-01 -0.197612D+00 -0.912314D+00 -0.133466D+00
17  0.476172D+00  0.109793D+00  0.861264D-01  0.279270D+00 -0.106600D+00
18  0.467033D+01 -0.122646D+00 -0.215618D+00 -0.668244D+00 -0.993277D-01
19 -0.487976D+00  0.743106D-02  0.418994D+01  0.383830D+00  0.123990D+01
20  0.638170D+01 -0.127673D+00  0.424632D+00  0.424142D+00 -0.295228D+00
21  0.169386D+01  0.648583D+01 -0.193075D+00 -0.342333D+00  0.108081D+01
22  0.129513D+01  0.603645D+01  0.987415D-01 -0.636232D+00  0.541042D+00
23 -0.122318D+00  0.822732D+00  0.124980D+01 -0.985247D-01 -0.387834D+00
24 -0.561854D-01 -0.247767D+00  0.336962D+00 -0.158395D+00 -0.155725D+00
25 -0.203037D+00  0.604723D+00  0.438232D+01  0.193839D-01 -0.586565D-01
26 -0.676126D-02 -0.168084D+00  0.984075D+00  0.139702D+00 -0.138686D+00
27  0.356059D+01  0.610540D+00 -0.469032D+00 -0.444373D+00  0.874154D-02
28  0.213125D+01 -0.167851D+00  0.255271D+01 -0.752948D+00 -0.130450D+00
29  0.643919D+00  0.487382D+00  0.610685D+00  0.210279D+00  0.400727D-01
30  0.124519D+01 -0.302765D-01  0.222179D+00 -0.246428D+00  0.701099D-01
31  0.116235D+01  0.115840D+01  0.759176D+00 -0.385653D+00  0.274696D-01
32  0.162704D+00  0.316420D+00  0.668414D+00 -0.428880D-01  0.238143D+00
33  0.124088D+01  0.276413D+00  0.399633D+01 -0.126079D+00 -0.148646D+00
34 -0.376017D+00 -0.110174D+00  0.690896D+00 -0.170696D+00 -0.705385D-01
           6             7             8             9            10
 6  0.000000D+00
 7  0.176365D+01  0.000000D+00
 8  0.311402D+01  0.285298D+00  0.000000D+00
 9 -0.130738D+00  0.537227D+00  0.624748D+02  0.000000D+00
10  0.519381D-02  0.154188D+00 -0.207923D+01  0.584015D+02  0.000000D+00
11 -0.116116D-01 -0.459320D-01  0.987198D+01 -0.286049D+01  0.576596D+02
12 -0.113475D+00  0.165342D-01 -0.231403D+01  0.904253D+01 -0.243099D+01
13 -0.497466D+00 -0.555945D-01  0.601798D+02 -0.115379D+01  0.920596D+01
14  0.216702D+00  0.149804D+00 -0.111450D+01  0.143117D+03 -0.110407D+00
15  0.734617D-01 -0.157925D-01  0.723496D+01  0.721086D+00  0.144067D+03
16 -0.106851D+00  0.731636D-02 -0.153652D+01  0.710358D+01  0.578270D+00
17 -0.168800D+00 -0.326138D-01  0.725516D+01 -0.139134D+01  0.716469D+01
18 -0.177808D+00  0.373328D-01 -0.591213D+00  0.590643D+01 -0.112280D+01
19  0.239926D+01  0.887990D-01  0.125216D+01  0.232217D+00 -0.366421D-01
20 -0.791761D-01  0.194438D+01  0.376691D+00  0.321529D+00 -0.366392D-01
21 -0.174686D+00  0.171260D+00  0.572131D-01 -0.430183D-01  0.331232D-01
22  0.371688D-01  0.481511D+01  0.351152D+00  0.112946D+01 -0.489130D-01
23 -0.305072D-01  0.361510D+02 -0.115470D-01 -0.313152D-01 -0.125541D-01
24 -0.143091D+00 -0.515763D+01 -0.161429D-01 -0.193538D-01 -0.266197D-01
25  0.102878D+00 -0.150070D+01 -0.330675D-01 -0.106974D-01 -0.203952D-01
26 -0.655274D-01 -0.527641D+01 -0.218626D-02 -0.828342D-02 -0.320507D-01
27 -0.257569D+00  0.352238D+02 -0.183885D-01  0.122461D+00  0.114550D-01
28 -0.301398D+00 -0.115725D+01 -0.656279D-01  0.727764D-02 -0.511271D-01
29 -0.216953D+00 -0.444531D+01  0.323776D-01 -0.125676D-01 -0.271197D-01
30  0.490644D-01 -0.444824D+01 -0.956155D-02  0.135001D-01 -0.524693D-01
31 -0.165964D+00  0.359952D+02  0.389974D+00  0.388794D-01 -0.422890D-01
32  0.230554D-01 -0.490880D+01  0.815171D-01 -0.358349D-01 -0.120688D-01
33 -0.159694D+00 -0.114707D+01  0.394869D+00  0.434643D-01 -0.203180D-01
```

```
34  0.112209D-01 -0.519113D+01 -0.289642D-01 -0.153950D-01 -0.209087D-01
          11            12            13            14            15
11  0.000000D+00
12  0.574051D+02  0.000000D+00
13 -0.279808D+01  0.587303D+02  0.000000D+00
14  0.680774D+01 -0.108558D+01  0.580188D+01  0.000000D+00
15  0.361970D+00  0.713481D+01 -0.138707D+01  0.730281D+01  0.000000D+00
16  0.143987D+03  0.642988D+00  0.716683D+01  0.415627D+00  0.701644D+01
17  0.394820D+00  0.144134D+03  0.562369D+00  0.630665D+00  0.543733D+00
18  0.680022D+01 -0.206386D+00  0.142154D+03  0.112692D+01  0.669556D+00
19  0.234666D-02 -0.935029D-02  0.765499D-01  0.116402D-02 -0.262278D-01
20 -0.191419D-01 -0.114936D-01  0.259622D-02 -0.595038D-01 -0.824821D-01
21 -0.696365D-01  0.111435D+00  0.557497D+00 -0.864709D-01 -0.151899D+00
22  0.100556D+00 -0.140437D+00  0.260680D+00  0.274920D+00 -0.529723D-04
23 -0.941009D-02  0.932532D-02  0.137520D-01 -0.304581D-01 -0.250414D-01
24 -0.246725D-01 -0.210392D-02 -0.330837D-02 -0.824970D-01 -0.837036D-01
25 -0.367020D-01 -0.898764D-02 -0.386736D-03 -0.104665D+00 -0.104578D+00
26 -0.276808D-01  0.205385D-01  0.107807D+00 -0.771133D-01 -0.858878D-01
27 -0.487588D-02 -0.130893D-01  0.241995D-01 -0.326669D-01 -0.997978D-02
28 -0.157020D-01 -0.454596D-01 -0.102878D-01 -0.123129D+00 -0.855602D-01
29 -0.335082D-01 -0.289025D-01 -0.303207D-01 -0.577246D-02 -0.657038D-01
30 -0.191923D-01 -0.157158D-01  0.820532D-02 -0.768319D-01 -0.736512D-01
31  0.421065D-01 -0.596795D-01  0.473654D-01 -0.619902D-01  0.133111D-01
32 -0.396273D-01 -0.141275D-01 -0.196893D-01  0.161266D-01 -0.604351D-01
33 -0.124060D-01 -0.412866D-01 -0.241386D-01 -0.925282D-01 -0.687040D-01
34 -0.228468D-01 -0.216167D-01 -0.130673D-01 -0.358294D-01 -0.641742D-01
          16            17            18            19            20
16  0.000000D+00
17  0.696247D+01  0.000000D+00
18  0.397556D+00  0.731706D+01  0.000000D+00
19 -0.391050D-01 -0.160974D-01  0.307781D-01  0.000000D+00
20 -0.997995D-01 -0.990345D-01 -0.608809D-01  0.852515D+02  0.000000D+00
21 -0.579738D-01 -0.646100D-01  0.440886D+00  0.905588D+02 -0.781429D+01
22 -0.191334D+00 -0.568823D-01 -0.227452D+00  0.890861D+02 -0.857559D+01
23 -0.198736D-01 -0.686777D-02  0.825582D-01  0.223795D+01  0.960606D+00
24 -0.729144D-01 -0.309557D-01  0.476611D-01  0.159329D-02  0.110617D-01
25 -0.899154D-01 -0.577295D-01  0.975188D-02  0.475894D+00 -0.142510D+00
26 -0.624016D-01  0.483981D-01  0.348759D+00  0.980167D-01 -0.106897D+00
27 -0.256288D-01 -0.125237D-01  0.121957D-01  0.260255D+00 -0.211187D+00
28 -0.114479D+00 -0.659106D-01 -0.531112D-01  0.196954D+00  0.122783D-01
29 -0.928572D-01 -0.774411D-01 -0.275153D-01 -0.146109D+00 -0.845631D-01
30 -0.904122D-01  0.130350D-02  0.209586D+00 -0.769147D-01 -0.151099D+00
31 -0.671482D-01  0.880264D-02 -0.607491D-01  0.991956D+00  0.202087D+01
32 -0.784621D-01 -0.899691D-01 -0.698141D-01 -0.130416D+00 -0.152588D+00
33 -0.107133D+00 -0.659406D-01 -0.744141D-01 -0.538412D-01 -0.734320D-01
34 -0.754092D-01 -0.704859D-01 -0.582698D-01 -0.920003D-01 -0.404250D+00
          21            22            23            24            25
21  0.000000D+00
22 -0.861492D+01  0.000000D+00
23  0.234165D+01  0.181112D+01  0.000000D+00
24  0.519755D+00 -0.140380D+00  0.119893D+03  0.000000D+00
25  0.972177D+00  0.540865D-01  0.111474D+03 -0.126851D+02  0.000000D+00
26  0.437976D+00 -0.190286D+00  0.114026D+03 -0.125870D+02 -0.130888D+02
27 -0.129721D+00  0.311516D+00  0.132666D+01  0.881845D+01  0.217887D+01
28 -0.127973D+00  0.655230D+00  0.109566D+01 -0.125809D+00  0.576444D+00
29 -0.137352D+00  0.681200D-01  0.757851D+01  0.387332D+01  0.561899D+00
30 -0.500602D-01 -0.143477D+00  0.316626D+01  0.311776D-01 -0.175355D+00
31  0.165248D-01 -0.305063D-01  0.100755D+01  0.278898D+01  0.113826D+01
32 -0.198968D+00 -0.256257D-01  0.771053D+01 -0.164065D+00 -0.189499D+00
33 -0.921624D-01 -0.216012D+00  0.184896D+01 -0.267586D+00  0.364201D+00
34 -0.137028D-01 -0.153464D+00  0.196516D+01  0.836957D-01 -0.323240D+00
```

```
            26            27            28            29            30
    26  0.000000D+00
    27  0.217244D+01  0.000000D+00
    28 -0.320910D+00  0.114175D+03  0.000000D+00
    29 -0.423370D+00  0.112239D+03 -0.146514D+02  0.000000D+00
    30  0.108790D+00  0.114726D+03 -0.142889D+02 -0.104984D+02  0.000000D+00
    31  0.768268D+01  0.119189D+01  0.241736D+01  0.141693D+01  0.763605D+01
    32  0.337760D+01  0.266648D+01 -0.270846D+00  0.758916D-01 -0.172788D+00
    33  0.146630D+00  0.151266D+01  0.551264D+00 -0.272791D+00 -0.584528D-01
    34 -0.414836D+00  0.850768D+01  0.504785D+00 -0.487118D+00  0.352555D+01
            31            32            33            34
    31  0.000000D+00
    32  0.112146D+03  0.000000D+00
    33  0.112789D+03 -0.134100D+02  0.000000D+00
    34  0.118596D+03 -0.121077D+02 -0.132578D+02  0.000000D+00
```

**2b**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   131.9214   Anisotropy =    61.6789
   XX=   150.5679   YX=    20.4296   ZX=    17.1037
   XY=    40.5016   YY=   106.6378   ZY=   -17.9986
   XZ=    28.5790   YZ=   -10.2984   ZZ=   138.5585
   Eigenvalues:    81.4040   141.3195   173.0407
  2  C    Isotropic =   150.1408   Anisotropy =    40.4554
   XX=   145.0753   YX=    38.8150   ZX=    17.0846
   XY=    26.2409   YY=   136.2129   ZY=   -10.4250
   XZ=    13.9882   YZ=   -17.3940   ZZ=   169.1342
   Eigenvalues:   101.4765   171.8348   177.1111
  3  N    Isotropic =   209.3971   Anisotropy =   103.7333
   XX=   244.6749   YX=    -0.6868   ZX=    41.6055
   XY=    -5.5884   YY=   175.4771   ZY=    24.9396
   XZ=    52.0703   YZ=    32.3884   ZZ=   208.0393
   Eigenvalues:   149.5832   200.0554   278.5526
  4  H    Isotropic =    28.3505   Anisotropy =     8.5575
   XX=    28.8937   YX=     1.4425   ZX=     2.1804
   XY=    -2.3622   YY=    23.9559   ZY=     2.6517
   XZ=     1.2132   YZ=     4.8712   ZZ=    32.2020
   Eigenvalues:    22.3279    28.6681    34.0555
  5  H    Isotropic =    29.5396   Anisotropy =    10.7737
   XX=    29.5902   YX=    -3.5988   ZX=     3.3529
   XY=    -0.6717   YY=    30.2016   ZY=    -2.6744
   XZ=     5.6520   YZ=    -5.5319   ZZ=    28.8270
   Eigenvalues:    24.0908    27.8060    36.7221
  6  H    Isotropic =    29.3081   Anisotropy =    10.7789
   XX=    27.8291   YX=     3.9242   ZX=     4.4114
   XY=     1.8101   YY=    33.0018   ZY=     2.1552
   XZ=     0.7070   YZ=     5.5293   ZZ=    27.0933
   Eigenvalues:    24.6319    26.7983    36.4940
  7  C    Isotropic =   126.1624   Anisotropy =    72.2937
   XX=   143.1034   YX=    32.4517   ZX=    21.8666
   XY=    28.1323   YY=   112.9358   ZY=    17.0349
   XZ=    16.5691   YZ=    17.4223   ZZ=   122.4482
   Eigenvalues:    93.1483   110.9808   174.3583
  8  C    Isotropic =   175.4527   Anisotropy =    18.5851
   XX=   186.2177   YX=    -1.0634   ZX=    -2.9061
   XY=    -2.8864   YY=   171.3092   ZY=     7.5098
   XZ=    -4.9904   YZ=     5.9694   ZZ=   168.8311
   Eigenvalues:   163.0750   175.4403   187.8428
  9  H    Isotropic =    28.2069   Anisotropy =     7.6753
```

```
  XX=    29.0117   YX=     2.6707   ZX=     0.0638
  XY=     0.5157   YY=    32.2858   ZY=     1.1950
  XZ=     0.5884   YZ=     2.7984   ZZ=    23.3233
  Eigenvalues:    22.8985    28.3985    33.3237
10  H    Isotropic =    29.7371   Anisotropy =     8.5603
  XX=    31.7391   YX=     2.3128   ZX=     2.8886
  XY=     1.8202   YY=    25.1320   ZY=     3.1353
  XZ=     1.5983   YZ=     2.3585   ZZ=    32.3402
  Eigenvalues:    23.9823    29.7850    35.4440
11  H    Isotropic =    29.8499   Anisotropy =     7.8692
  XX=    30.9528   YX=     0.5963   ZX=    -2.8654
  XY=     0.8265   YY=    25.1625   ZY=    -1.4801
  XZ=    -1.6283   YZ=    -1.9191   ZZ=    33.4343
  Eigenvalues:    24.8144    29.6392    35.0960
12  H    Isotropic =    30.7223   Anisotropy =     7.9573
  XX=    32.4430   YX=    -3.4586   ZX=    -0.6599
  XY=    -2.1406   YY=    33.8149   ZY=    -1.0404
  XZ=    -0.1416   YZ=    -0.5995   ZZ=    25.9091
  Eigenvalues:    25.7438    30.3960    36.0272
13  C    Isotropic =    50.2377   Anisotropy =   186.0853
  XX=   -36.6191   YX=    14.1019   ZX=   -54.9011
  XY=    15.3480   YY=    28.7399   ZY=   -14.7468
  XZ=   -54.1967   YZ=    -7.9947   ZZ=   158.5923
  Eigenvalues:   -52.4431    28.8616   174.2946
14  C    Isotropic =    52.9950   Anisotropy =   178.6736
  XX=    36.7006   YX=    39.1943   ZX=   -31.6017
  XY=    36.5760   YY=   -38.8707   ZY=   -16.1612
  XZ=   -33.0572   YZ=   -16.6836   ZZ=   161.1552
  Eigenvalues:   -54.6303    41.5047   172.1107
15  C    Isotropic =    54.6146   Anisotropy =   186.8785
  XX=    18.1160   YX=   -38.3852   ZX=   -46.7490
  XY=   -39.2332   YY=   -17.0145   ZY=   -33.7040
  XZ=   -47.0688   YZ=   -34.6289   ZZ=   162.7422
  Eigenvalues:   -55.7406    40.3841   179.2002
16  C    Isotropic =    53.7708   Anisotropy =   189.4845
  XX=   -39.8151   YX=    14.3370   ZX=   -56.2911
  XY=    16.0638   YY=    37.7213   ZY=   -13.1620
  XZ=   -57.5480   YZ=   -12.2123   ZZ=   163.4063
  Eigenvalues:   -56.0988    37.3174   180.0939
17  C    Isotropic =    54.4837   Anisotropy =   187.5507
  XX=    34.3225   YX=    39.1625   ZX=   -33.9998
  XY=    39.1040   YY=   -38.9863   ZY=   -17.0533
  XZ=   -33.8745   YZ=   -18.3804   ZZ=   168.1150
  Eigenvalues:   -55.9867    39.9203   179.5175
18  C    Isotropic =    49.9622   Anisotropy =   180.8765
  XX=    16.2269   YX=   -36.6253   ZX=   -48.3676
  XY=   -39.9447   YY=   -19.4642   ZY=   -34.8786
  XZ=   -42.6994   YZ=   -41.3719   ZZ=   153.1240
  Eigenvalues:   -59.1906    38.5307   170.5465
19  H    Isotropic =    24.2902   Anisotropy =    10.1973
  XX=    29.2228   YX=     3.5089   ZX=     1.5805
  XY=     3.1478   YY=    23.4566   ZY=     0.7719
  XZ=     1.7947   YZ=     1.1732   ZZ=    20.1911
  Eigenvalues:    19.8305    21.9516    31.0883
20  H    Isotropic =    24.0050   Anisotropy =     5.3146
  XX=    26.6552   YX=    -1.4865   ZX=     1.2320
  XY=    -1.3226   YY=    24.6892   ZY=     0.1130
  XZ=     1.1678   YZ=    -0.0367   ZZ=    20.6705
  Eigenvalues:    20.4158    24.0511    27.5481
21  H    Isotropic =    23.9787   Anisotropy =     4.4665
  XX=    24.1956   YX=     0.0633   ZX=     0.7292
```

```
   XY=     0.2220   YY=    26.8194   ZY=     0.8571
   XZ=     0.7067   YZ=     0.8099   ZZ=    20.9212
   Eigenvalues:    20.6697    24.3101    26.9564
 22  H    Isotropic =    23.9923   Anisotropy =     5.1789
   XX=    26.9424   YX=     0.6071   ZX=     1.5195
   XY=     0.5058   YY=    24.0322   ZY=     0.6910
   XZ=     1.5050   YZ=     0.5589   ZZ=    21.0022
   Eigenvalues:    20.5721    23.9600    27.4449
 23  H    Isotropic =    23.7965   Anisotropy =     9.2769
   XX=    26.6960   YX=    -4.4984   ZX=     0.2065
   XY=    -3.8636   YY=    24.6298   ZY=     0.4574
   XZ=    -0.2747   YZ=     0.5464   ZZ=    20.0636
   Eigenvalues:    19.9526    21.4557    29.9810
 24  B    Isotropic =   127.6689   Anisotropy =    36.3883
   XX=   112.5169   YX=     1.2696   ZX=     8.1899
   XY=     2.0917   YY=   123.9102   ZY=    -9.2371
   XZ=     8.6177   YZ=   -11.4173   ZZ=   146.5797
   Eigenvalues:   109.2629   121.8161   151.9278
 25  H    Isotropic =    29.7881   Anisotropy =     6.7124
   XX=    28.7977   YX=    -0.0326   ZX=     0.8862
   XY=     0.2207   YY=    26.3619   ZY=     0.0045
   XZ=    -2.0137   YZ=    -0.0526   ZZ=    34.2048
   Eigenvalues:    26.3583    28.7431    34.2630
 26  H    Isotropic =    30.4613   Anisotropy =     7.4653
   XX=    28.8669   YX=    -0.9830   ZX=     1.0420
   XY=    -0.4561   YY=    30.3415   ZY=    -2.5738
   XZ=    -1.3014   YZ=    -5.5440   ZZ=    32.1754
   Eigenvalues:    26.8870    29.0587    35.4382
 27  H    Isotropic =    31.2339   Anisotropy =     7.0634
   XX=    30.8802   YX=     0.3481   ZX=     1.1975
   XY=     1.2656   YY=    26.8956   ZY=    -0.6167
   XZ=    -1.7110   YZ=     1.0721   ZZ=    35.9259
   Eigenvalues:    26.7303    31.0285    35.9428
 28  H    Isotropic =    30.9013   Anisotropy =    11.6707
   XX=    36.5643   YX=     3.2155   ZX=     2.8482
   XY=     3.2588   YY=    28.2504   ZY=     1.7352
   XZ=     2.9010   YZ=     1.7682   ZZ=    27.8893
   Eigenvalues:    26.3086    27.7136    38.6818


Total nuclear spin-spin coupling J (Hz):
               1             2             3             4             5
     1  0.000000D+00
     2  0.217405D+02  0.000000D+00
     3 -0.452039D+01 -0.371700D+01  0.000000D+00
     4  0.152018D+03 -0.235941D+01 -0.410870D+00  0.000000D+00
     5 -0.179343D+01  0.153879D+03 -0.600501D+00  0.722922D+01  0.000000D+00
     6 -0.319422D+01  0.159001D+03  0.663671D+00  0.492655D+01 -0.319747D+01
     7 -0.443499D+00 -0.106658D+01  0.207041D+01  0.481292D+01  0.409801D+01
     8  0.217835D+01  0.974455D+00  0.732724D-05 -0.135584D+00 -0.518125D-01
     9 -0.165318D+00  0.594613D+01  0.724978D+00 -0.211174D+00 -0.668974D+00
    10  0.372722D+01  0.157582D+01 -0.925259D+00 -0.476036D-01  0.712628D-01
    11 -0.558094D-01 -0.124755D+00  0.313723D+00 -0.191430D+00 -0.842141D-01
    12 -0.140879D+00 -0.124615D-01  0.118102D+01 -0.734922D-01  0.211599D+00
    13  0.574688D+02 -0.121725D+01 -0.211033D+00 -0.359370D+00  0.223225D+01
    14  0.281364D+01  0.307111D+01  0.711923D+00  0.279115D+01 -0.820008D-01
    15  0.431783D+01  0.320799D+00 -0.142247D+00 -0.616388D+00 -0.272814D-01
    16 -0.981027D+00  0.954822D-02  0.224690D+00  0.765186D+00 -0.718595D-01
    17  0.429159D+01  0.522825D+00 -0.281908D+00 -0.105007D+01  0.873601D-01
    18  0.287493D+01  0.274362D+01  0.233401D+00  0.239353D+01  0.813941D-01
    19  0.462610D+01  0.283213D+00 -0.152887D+00 -0.108390D+01 -0.748959D-01
```

```
20  0.527731D+00 -0.472752D-01  0.136974D+00  0.385735D+00 -0.128485D+00
21  0.664479D+00 -0.380853D-01 -0.220076D+00 -0.904203D+00 -0.133071D+00
22  0.464346D+00  0.118177D+00  0.967811D-01  0.261149D+00 -0.109531D+00
23  0.477736D+01 -0.111270D+00 -0.240577D+00 -0.670192D+00 -0.100491D+00
24 -0.577590D+00 -0.936187D-01  0.432709D+01  0.317087D+00  0.879517D+00
25  0.682332D+01  0.752315D+00  0.288773D+00  0.816049D-01 -0.290768D+00
26  0.440194D+00  0.662521D+01  0.273460D+00 -0.310988D+00  0.876363D+00
27  0.237148D+01  0.302798D+01 -0.408407D+00 -0.509971D+00 -0.417252D-01
28  0.165134D+00 -0.993873D-01  0.465091D+01 -0.100079D+00 -0.356719D-01
          6             7             8             9            10
 6  0.000000D+00
 7  0.208015D+01  0.000000D+00
 8  0.457854D-01  0.345363D+02  0.000000D+00
 9  0.593177D+00  0.127750D+03 -0.306175D+01  0.000000D+00
10 -0.568230D+00  0.121781D+03 -0.332027D+01 -0.123259D+02  0.000000D+00
11 -0.954164D-01 -0.585266D+01  0.119507D+03  0.470998D+01  0.124673D+02
12  0.782430D-01 -0.585948D+01  0.112722D+03  0.123580D+02  0.327159D+01
13  0.311094D+01  0.498888D+00  0.527393D+00 -0.631056D-01 -0.107807D+00
14 -0.121298D+00  0.682026D+00  0.840973D-01 -0.298044D-01  0.762182D-01
15  0.379778D-02  0.177444D+00 -0.485487D-02 -0.610493D-01 -0.967156D-02
16 -0.130537D-01 -0.475474D-01  0.182108D-01 -0.320401D-01 -0.496558D-01
17 -0.115938D+00  0.146886D-01 -0.329163D-01 -0.920332D-02 -0.164622D-01
18 -0.503869D+00 -0.946058D-01  0.116337D-01 -0.208204D-01 -0.242997D-02
19  0.215026D+00  0.157612D+00 -0.489043D-01 -0.138951D+00 -0.739248D-01
20  0.641224D-01 -0.123261D-01  0.161429D-01 -0.102130D+00 -0.996105D-01
21 -0.108934D+00  0.103640D-01 -0.466957D-01 -0.101874D+00 -0.967460D-01
22 -0.168822D+00 -0.369847D-01 -0.533111D-02 -0.156345D-01 -0.703823D-01
23 -0.183067D+00  0.457162D-01 -0.154533D-01  0.206530D+00  0.607922D-01
24  0.217250D+01  0.532700D+00  0.109744D+01  0.946588D+00  0.229612D+01
25 -0.148913D+00  0.100157D+01  0.220654D+01 -0.161624D+00 -0.538267D+00
26 -0.866175D-01  0.265862D+01 -0.188642D+00  0.703924D-01  0.519188D-01
27  0.188585D+00  0.623239D+01  0.700544D+00 -0.538329D-01  0.135890D+01
28 -0.829994D-01 -0.760042D+00  0.111708D+03  0.206978D+01  0.343524D+01
          11            12            13            14            15
11  0.000000D+00
12 -0.121326D+02  0.000000D+00
13 -0.456068D-01  0.642421D-01  0.000000D+00
14 -0.227223D-01 -0.367111D-01  0.627162D+02  0.000000D+00
15 -0.314931D-01 -0.132265D-01 -0.207650D+01  0.583620D+02  0.000000D+00
16 -0.175367D-01 -0.368830D-01  0.989711D+01 -0.286302D+01  0.577579D+02
17 -0.223684D-01 -0.199285D-01 -0.234198D+01  0.901324D+01 -0.246054D+01
18 -0.899031D-02 -0.403712D-01  0.599688D+02 -0.120981D+01  0.916026D+01
19 -0.650539D-01  0.580541D-02 -0.102502D+01  0.142837D+03 -0.181012D+00
20 -0.706729D-01 -0.634366D-01  0.723722D+01  0.702014D+00  0.144364D+03
21 -0.786297D-01 -0.791042D-01 -0.152981D+01  0.712152D+01  0.562323D+00
22 -0.570034D-01 -0.827716D-01  0.730078D+01 -0.139498D+01  0.714322D+01
23 -0.346841D-01 -0.718740D-01 -0.594176D+00  0.590942D+01 -0.113552D+01
24  0.434191D-02 -0.856652D-01  0.118156D+01  0.193191D+00 -0.454018D-01
25  0.150175D+00 -0.262088D-01  0.680055D-01  0.221758D+00 -0.236774D-01
26  0.105075D+00 -0.193502D+00 -0.122553D-01 -0.435278D-01  0.176673D-01
27 -0.275074D+00 -0.140207D+00  0.315570D+00  0.107149D+01 -0.406167D-01
28 -0.134639D+02 -0.139017D+02  0.148128D+00  0.282939D-01 -0.398525D-01
          16            17            18            19            20
16  0.000000D+00
17  0.574668D+02  0.000000D+00
18 -0.280759D+01  0.587877D+02  0.000000D+00
19  0.677563D+01 -0.108549D+01  0.578113D+01  0.000000D+00
20  0.332126D+00  0.714134D+01 -0.138645D+01  0.728442D+01  0.000000D+00
21  0.144137D+03  0.618984D+00  0.714829D+01  0.407034D+00  0.705941D+01
22  0.421415D+00  0.144315D+03  0.554689D+00  0.627912D+00  0.533690D+00
23  0.684697D+01 -0.166144D+00  0.142912D+03  0.110630D+01  0.669895D+00
```

```
24  0.120774D-01 -0.145667D-01  0.702731D-01 -0.382826D-01 -0.201155D-01
25 -0.294747D-01 -0.147453D-01  0.297044D-01 -0.513007D-01 -0.829880D-01
26 -0.584471D-01  0.788237D-01  0.420510D+00 -0.919878D-01 -0.151655D+00
27  0.966456D-01 -0.928803D-01  0.300319D+00  0.217941D+00  0.596246D-03
28 -0.265003D-02 -0.502120D-01  0.490546D-02 -0.982338D-01 -0.692065D-01
          21            22            23            24            25
21  0.000000D+00
22  0.696212D+01  0.000000D+00
23  0.403923D+00  0.733647D+01  0.000000D+00
24 -0.486892D-01 -0.111903D-01 -0.587550D-02  0.000000D+00
25 -0.952900D-01 -0.113251D+00 -0.447094D-01  0.857089D+02  0.000000D+00
26 -0.736014D-01 -0.561646D-01  0.359426D+00  0.864341D+02 -0.796169D+01
27 -0.149159D+00 -0.456024D-01 -0.115101D+00  0.890997D+02 -0.874330D+01
28 -0.109586D+00 -0.509949D-01 -0.591483D-01  0.134807D+00  0.309748D+00
          26            27            28
26  0.000000D+00
27 -0.876411D+01  0.000000D+00
28 -0.136646D+00 -0.311683D+00  0.000000D+00
```

**Linear fitting correlation coefficient index $R^2$ of the $^1$H- and $^{13}$C-NMR chemical shift experimental and calculated (PCM/B3LYP/6-311++g(d,p) and PCM/MPW1PW91/6-311++g(d,p) level of theory) for the complexes 2a, 2b and inv-2b**

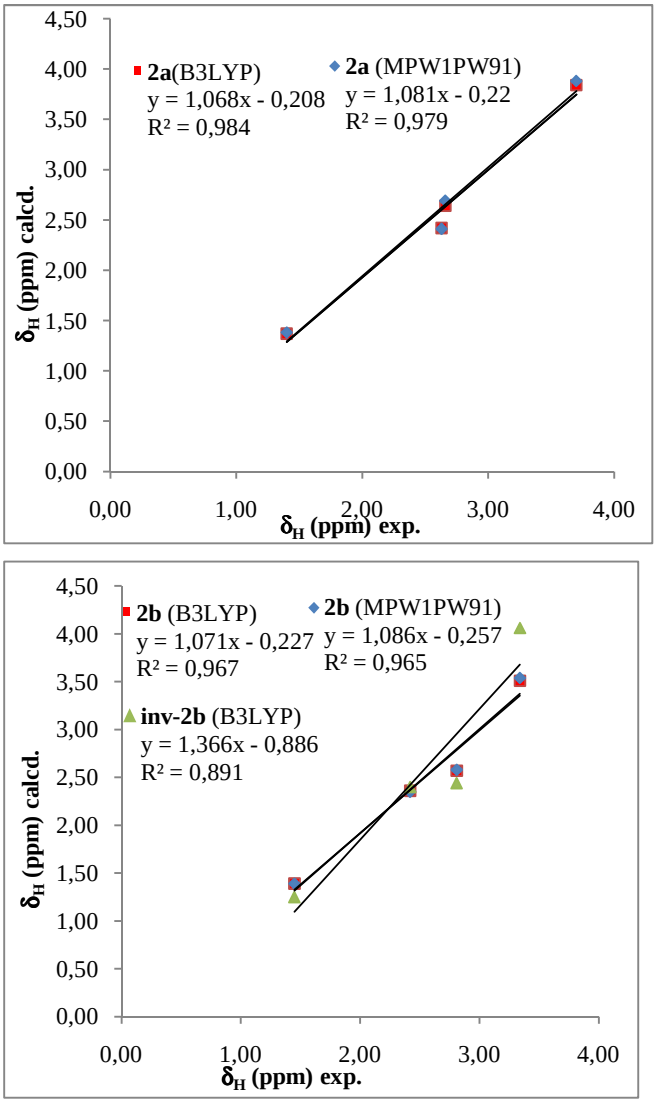



Figure 1. Comparison of $\delta_H$ exp. vs. $\delta_H$ calcd for the complexes **2a**, **2b** and **inv-2b.**

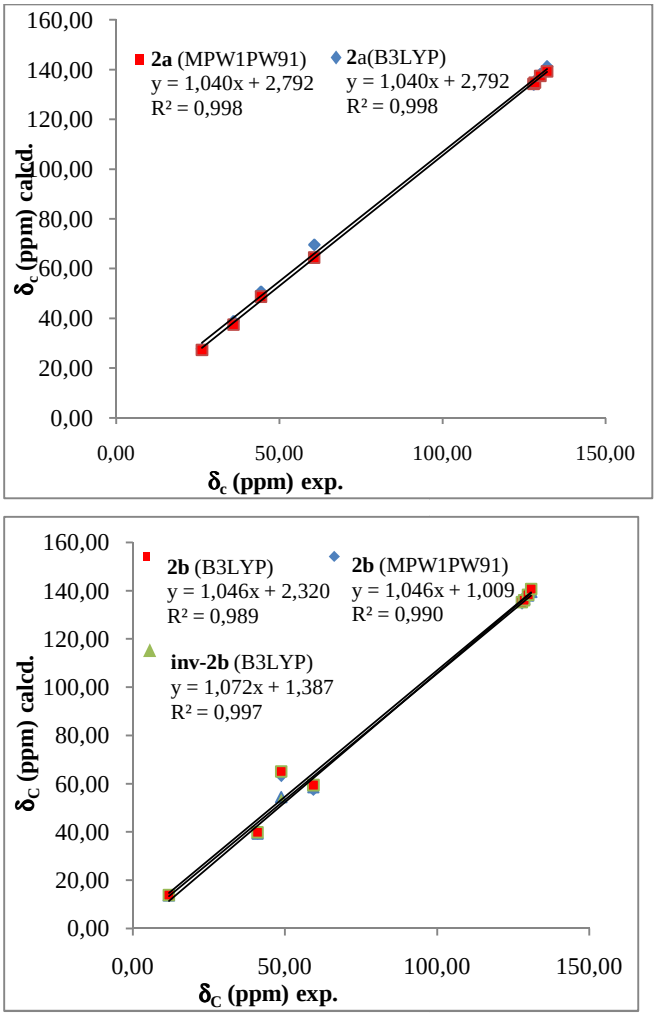



Figure 2. Comparison of $\delta_C$ exp. vs. $\delta_C$ calcd for the complexes **2a**, **2b** and **inv-2b**

The plots related to the $^1$H-NMR chemical shift calculated and experimental (Figure 1) showed an evident poor correlation ($R^2$=0.89) only for the "wrong" *N*-invertomer **inv-2b** showing that the proposed method may be used to establish the correct stereochemistry.