

Supporting Information

Oxidation of Organotrifluoroborates via Oxone®

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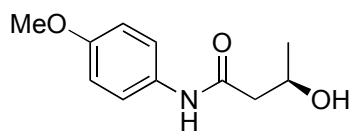
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General Considerations: All of the reagents and HPLC grade acetone were used as received. Melting points (°C) are uncorrected. ¹H, ¹³C, and ¹⁹F NMR spectra were recorded at 500.4, 125.8, and 470.8 MHz, respectively. ¹⁹F NMR chemical shifts were referenced to external CFCl₃ (0.0 ppm). Compounds **4d** and **4e** were characterized by comparison of their NMR data with commercially available samples.

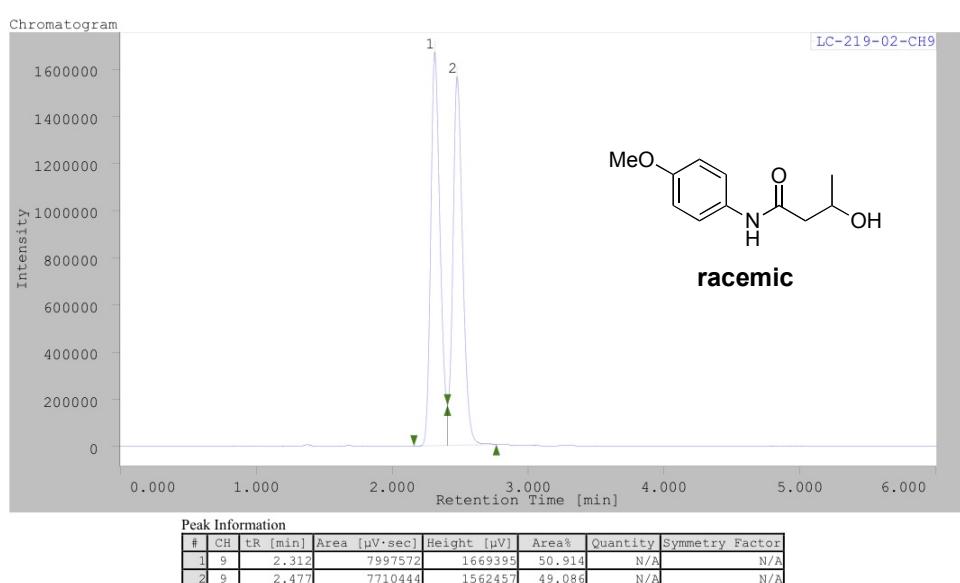


Analysis of 3-Hydroxy-N-(4-methoxyphenyl)butanamide using SFC.

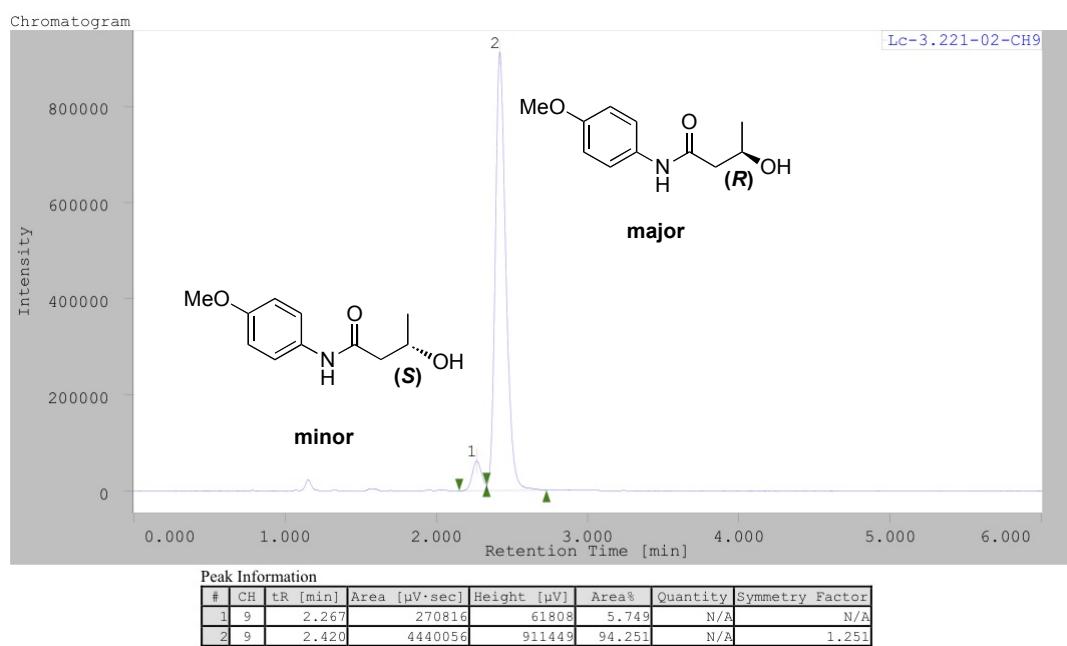
Analysis was performed using Column OD-H, 20% *i*-PrOH, 4 mL, 12MPa.

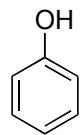
(*S*) – isomer $t_r = 2.3$ min and (*R*) – isomer $t_r = 2.4$ min.

Chromatogram of racemic 3-Hydroxy-N-(4-methoxyphenyl)butanamide product:

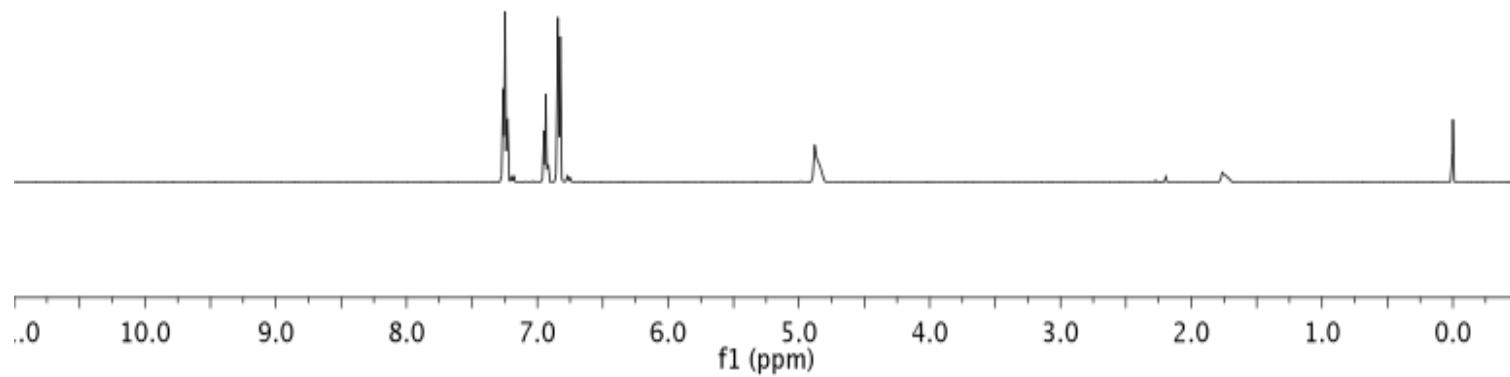


Chromatogram of enantioenriched 3-Hydroxy-N-(4-methoxyphenyl)butanamide product (5):

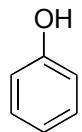




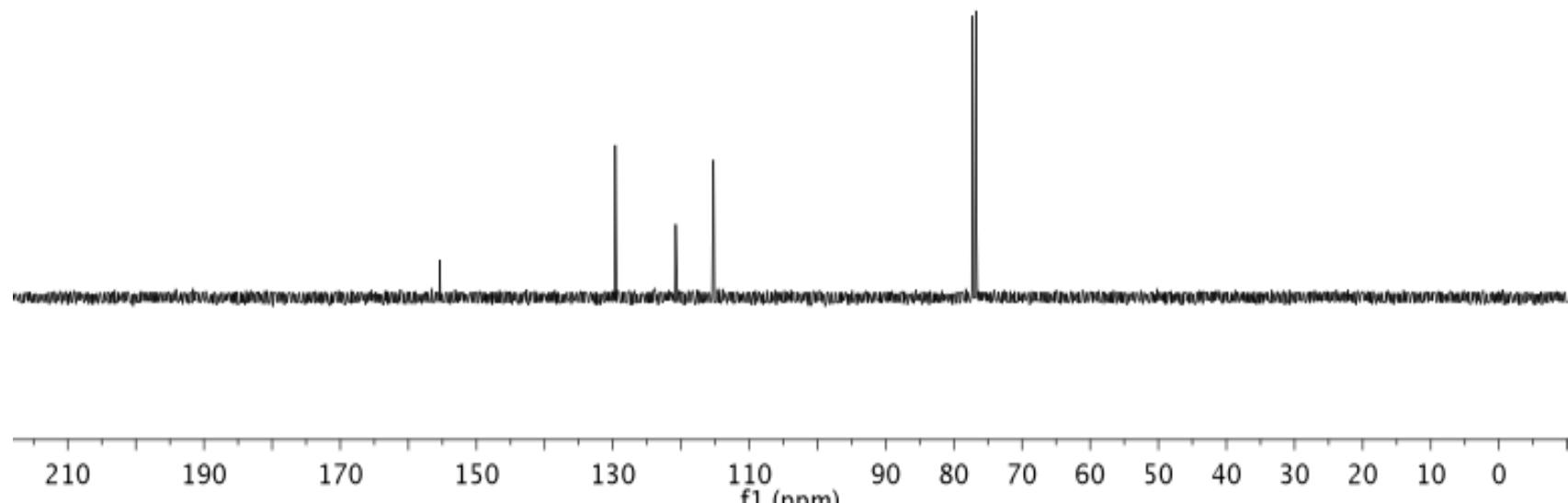
(1a)



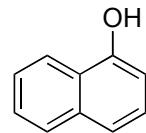
^1H NMR (500 MHz, CDCl_3) Spectrum of Phenol (1a)



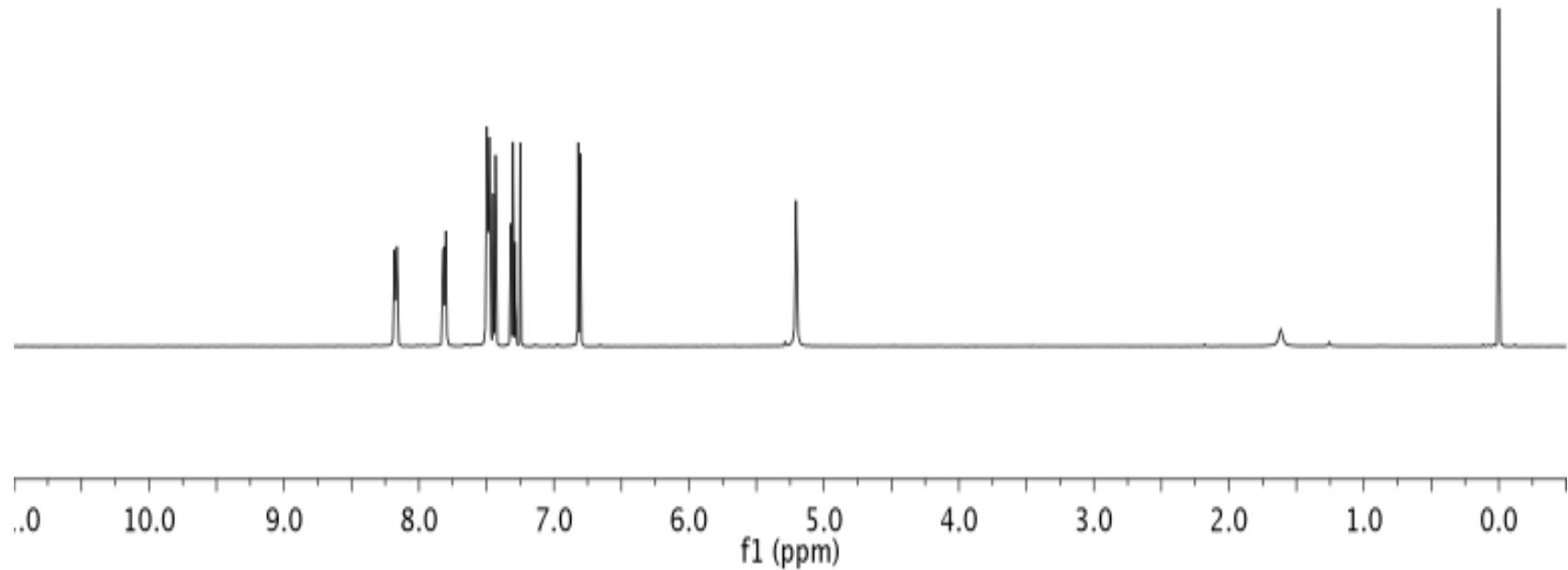
(1a)



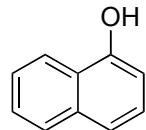
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Phenol (1a)



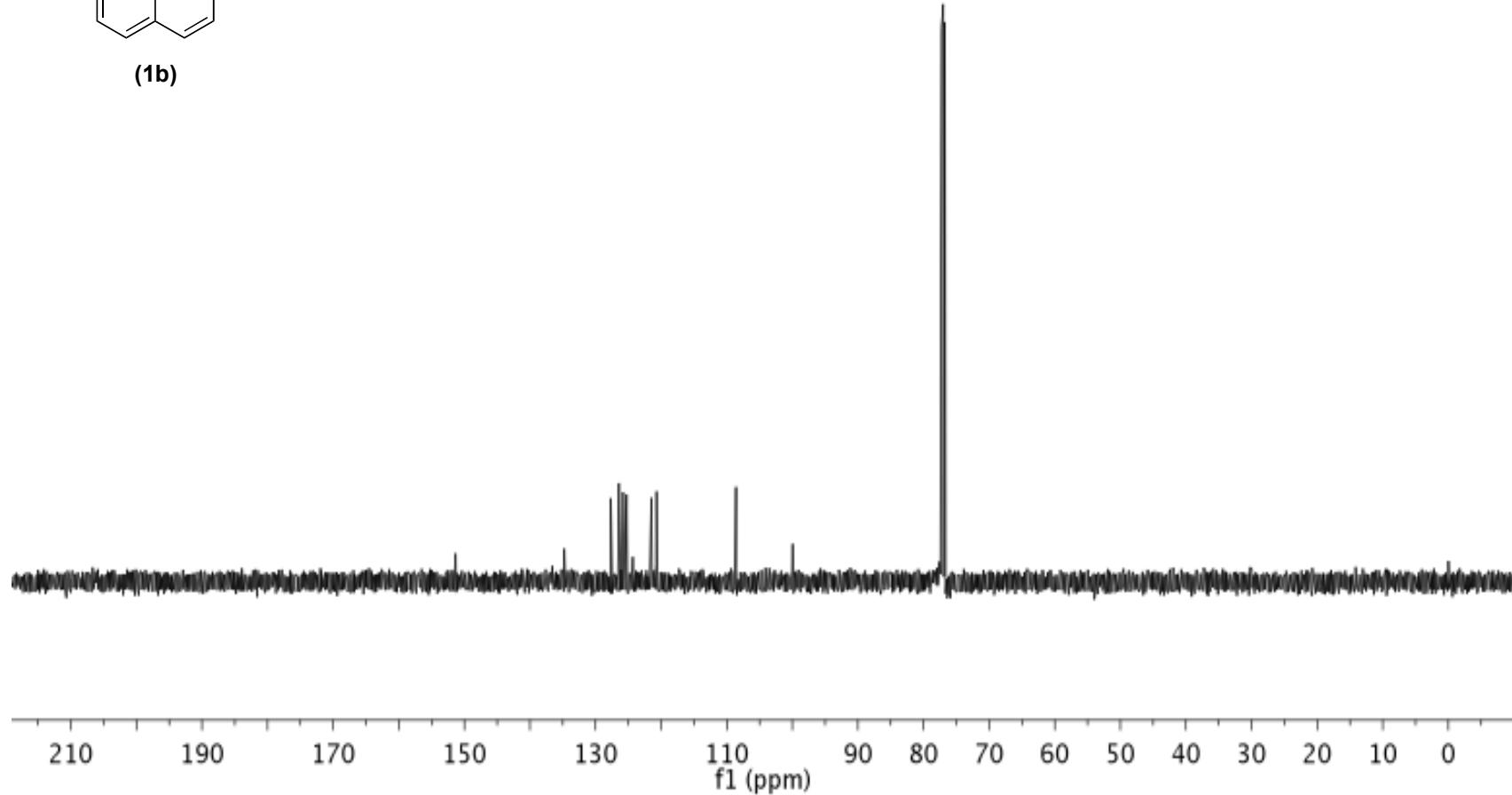
(1b)



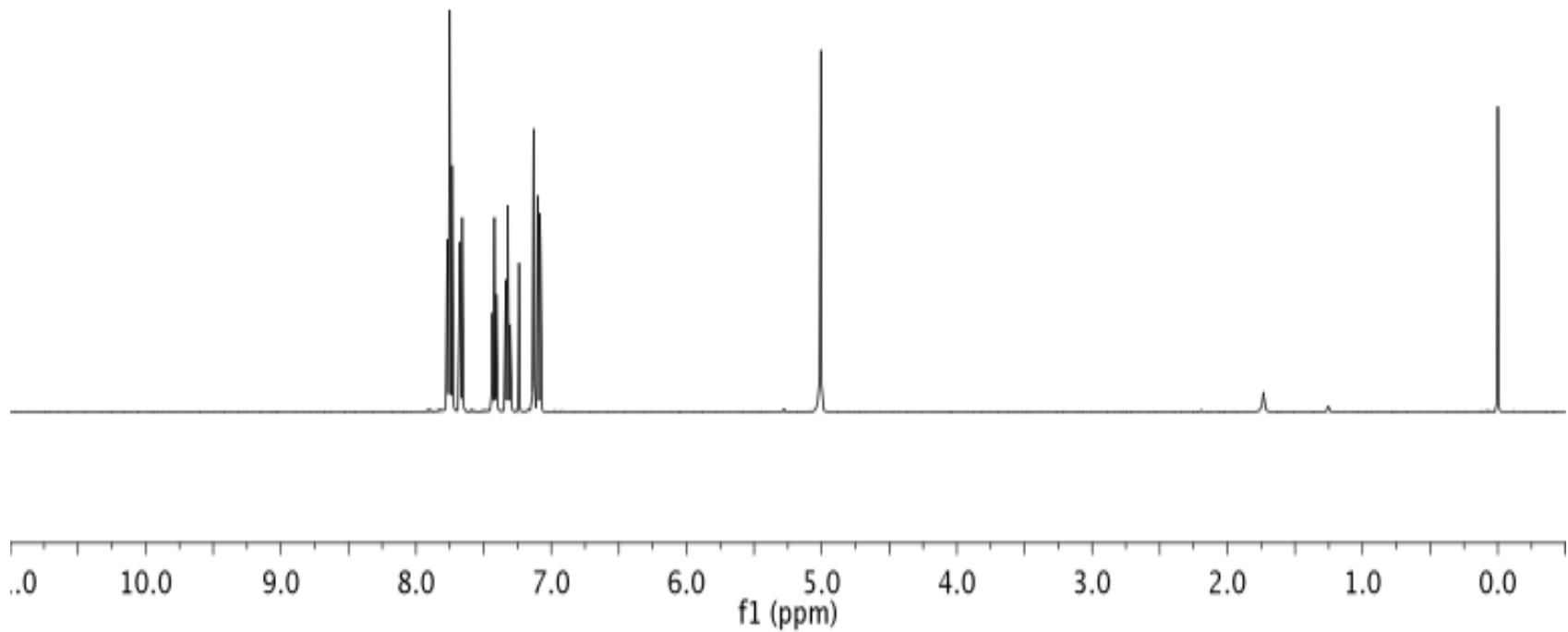
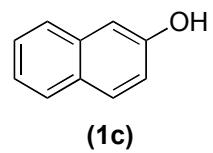
^1H NMR (500 MHz, CDCl_3) Spectrum of Naphthalen-1-ol (1b)



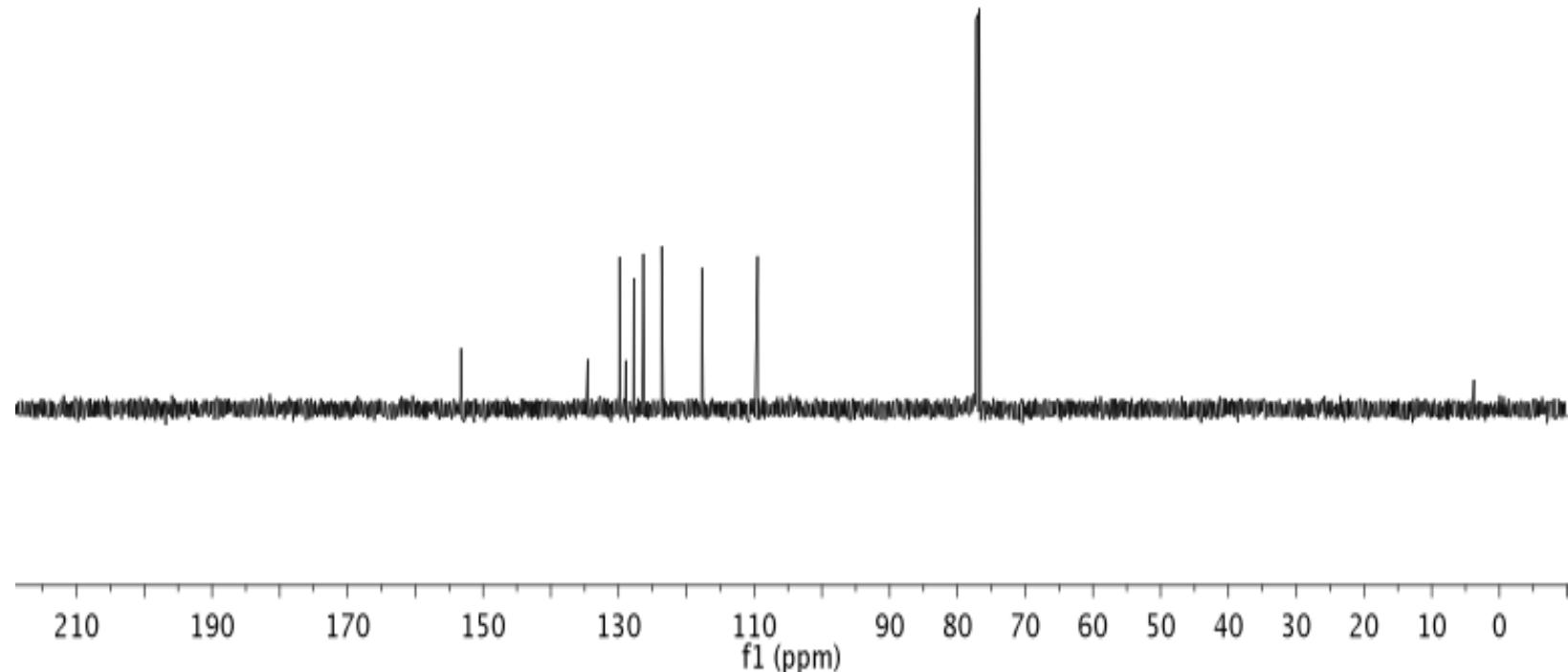
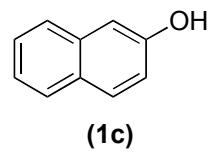
(1b)



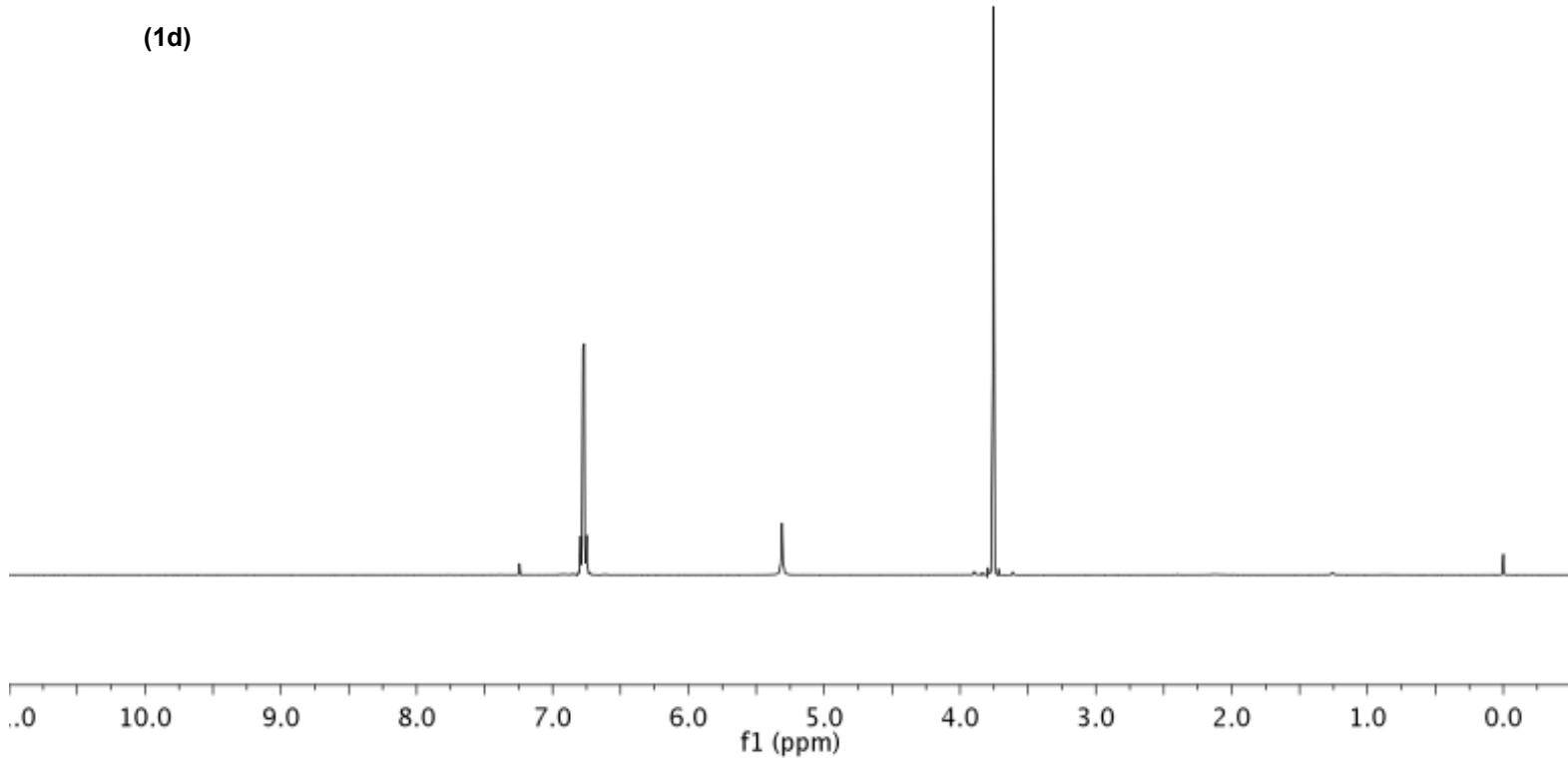
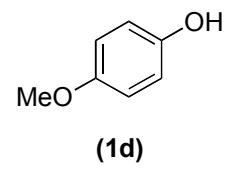
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of Naphthalen-1-ol (1b)



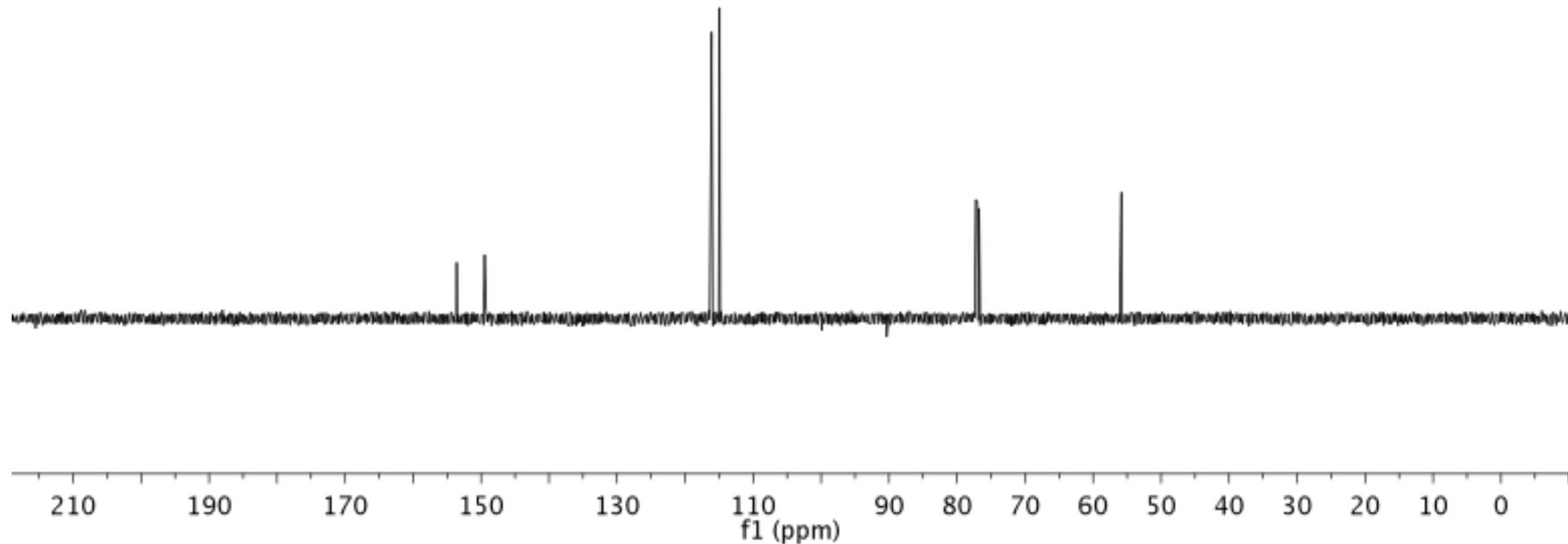
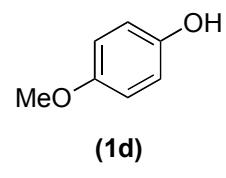
^1H NMR (500 MHz, CDCl_3) Spectrum of Naphthalen-2-ol (1c)



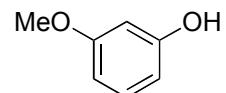
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of Naphthalen-2-ol (1c)



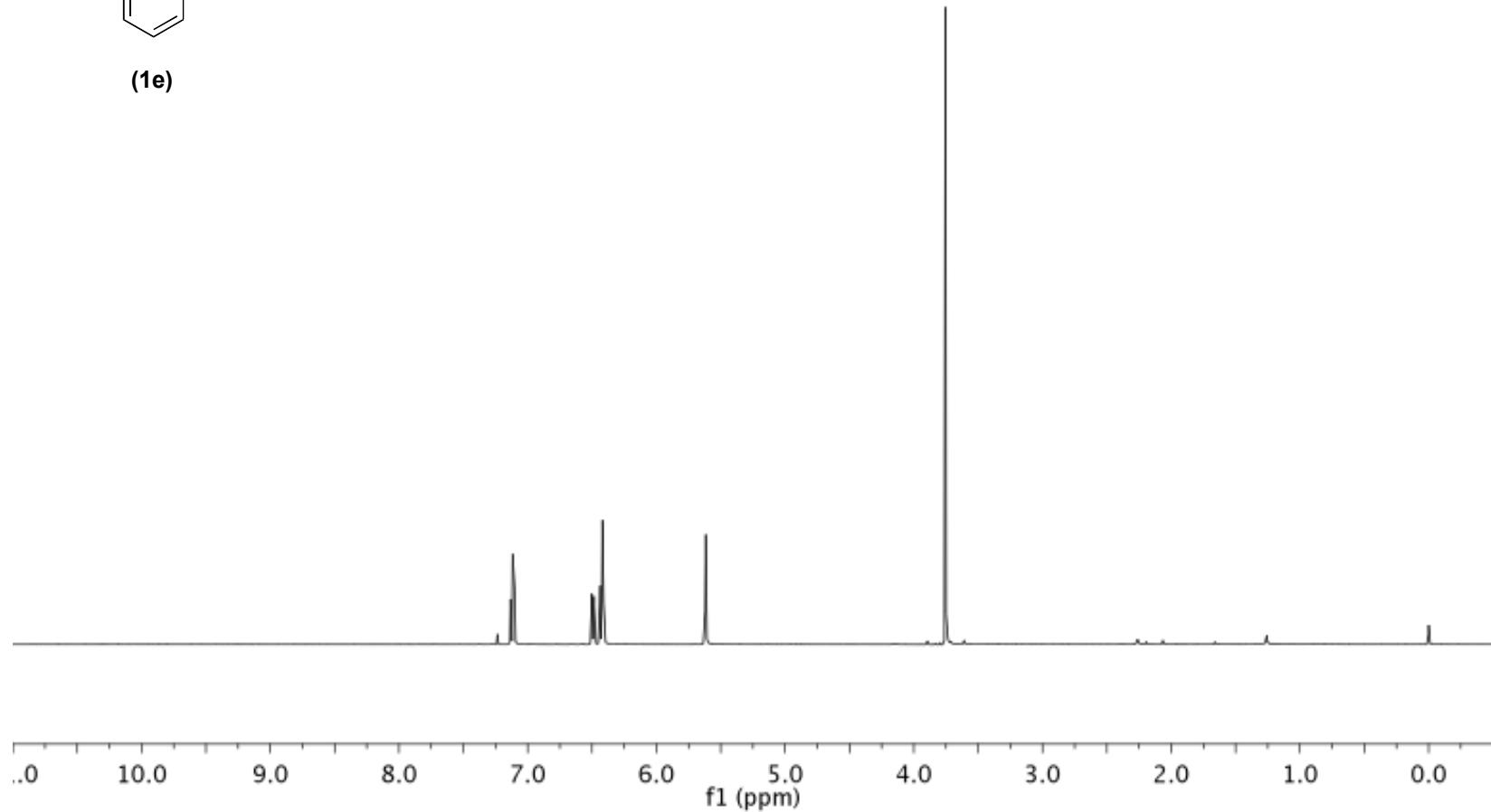
^1H NMR (500 MHz, CDCl_3) Spectrum of 4-Methoxyphenol (1d)



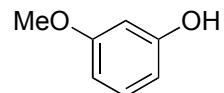
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Methoxyphenol (1d)



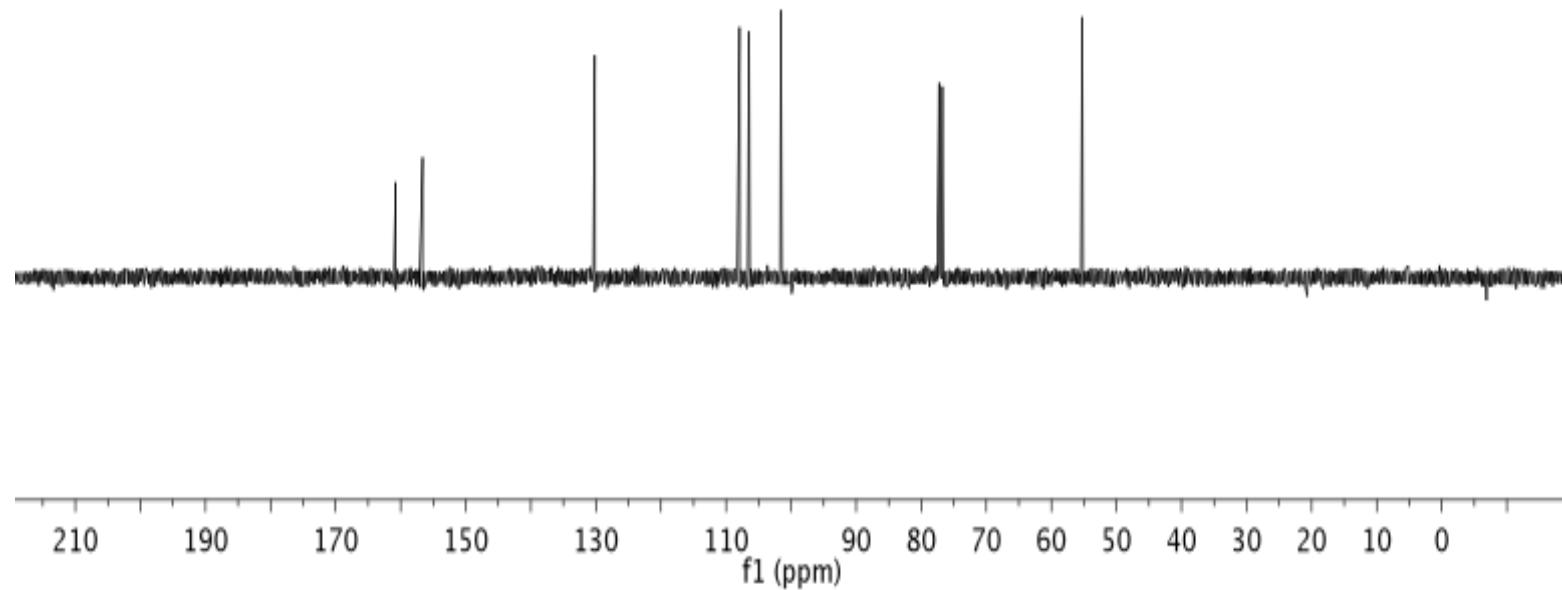
(1e)



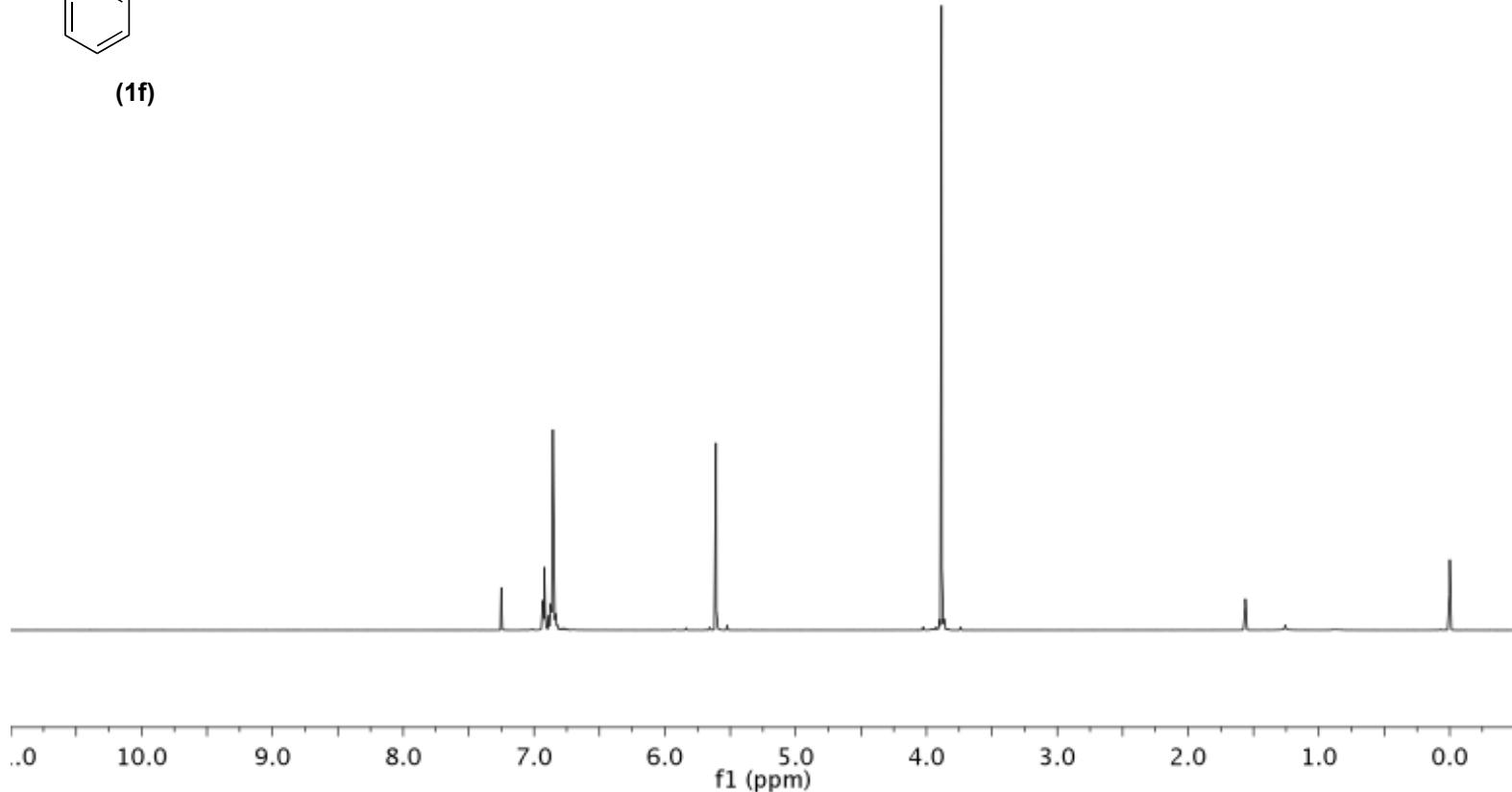
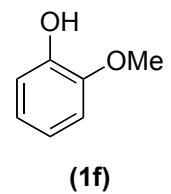
^1H NMR (500 MHz, CDCl_3) Spectrum of 3-Methoxyphenol (1e)



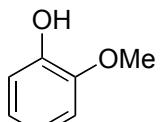
(1e)



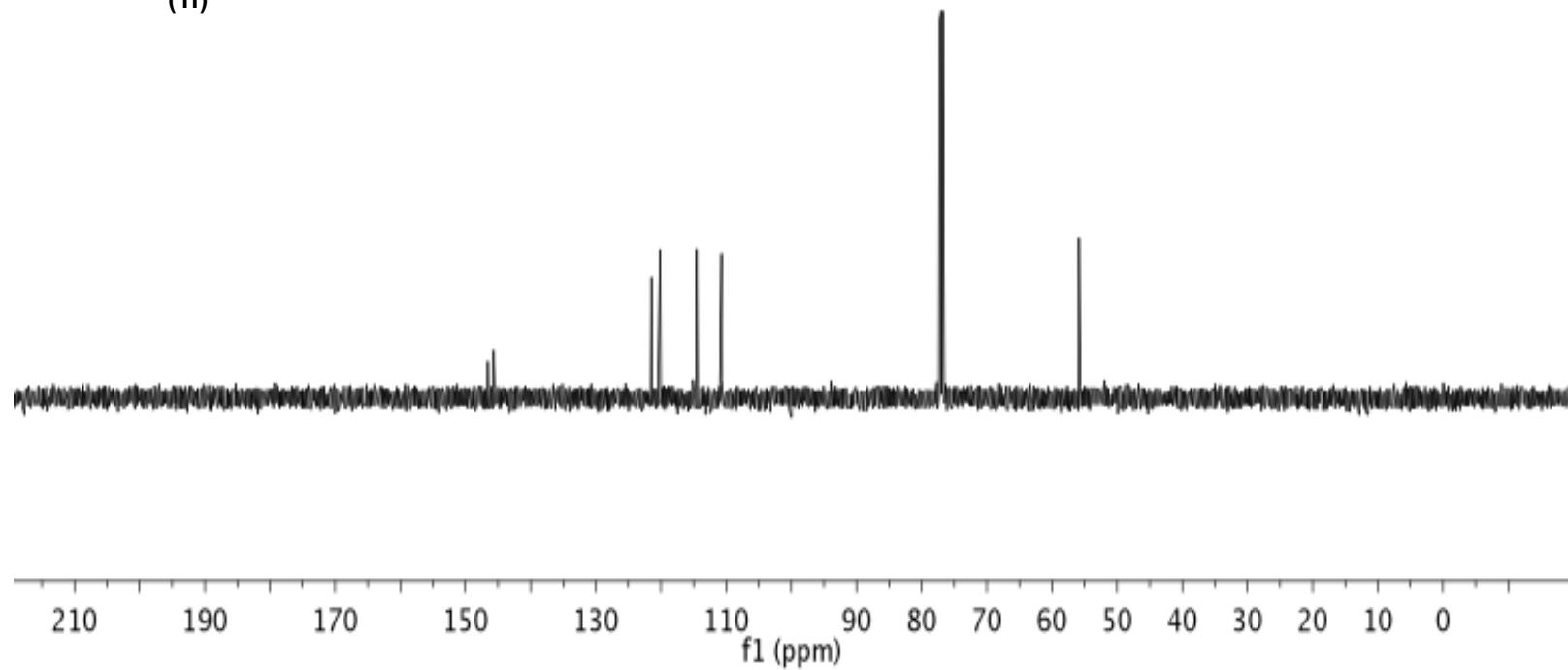
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 3-Methoxyphenol (1e)



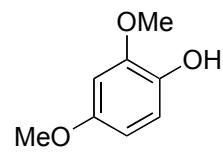
¹H NMR (500 MHz, CDCl₃) Spectrum of 2-Methoxyphenol (1f)



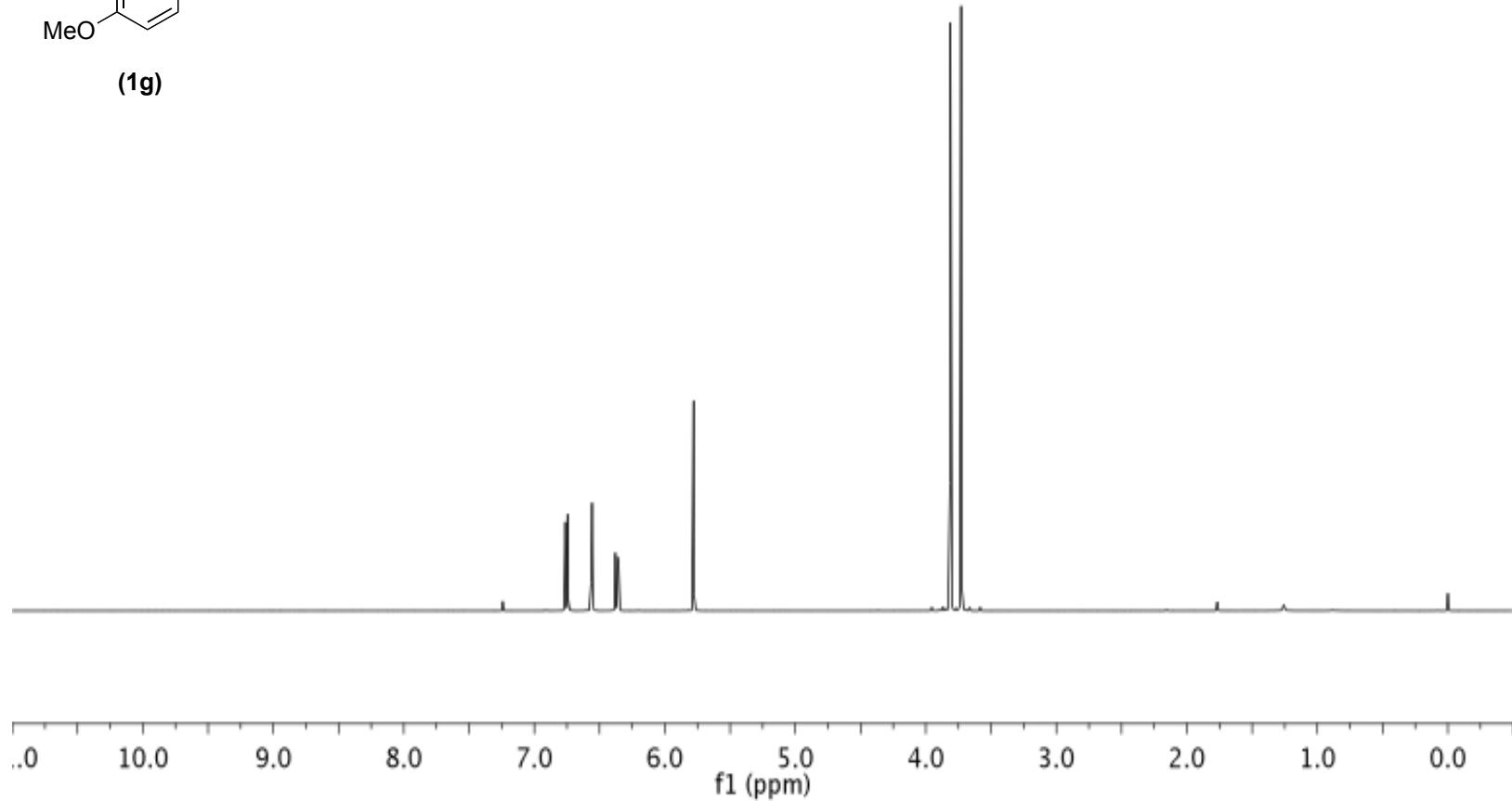
(1f)



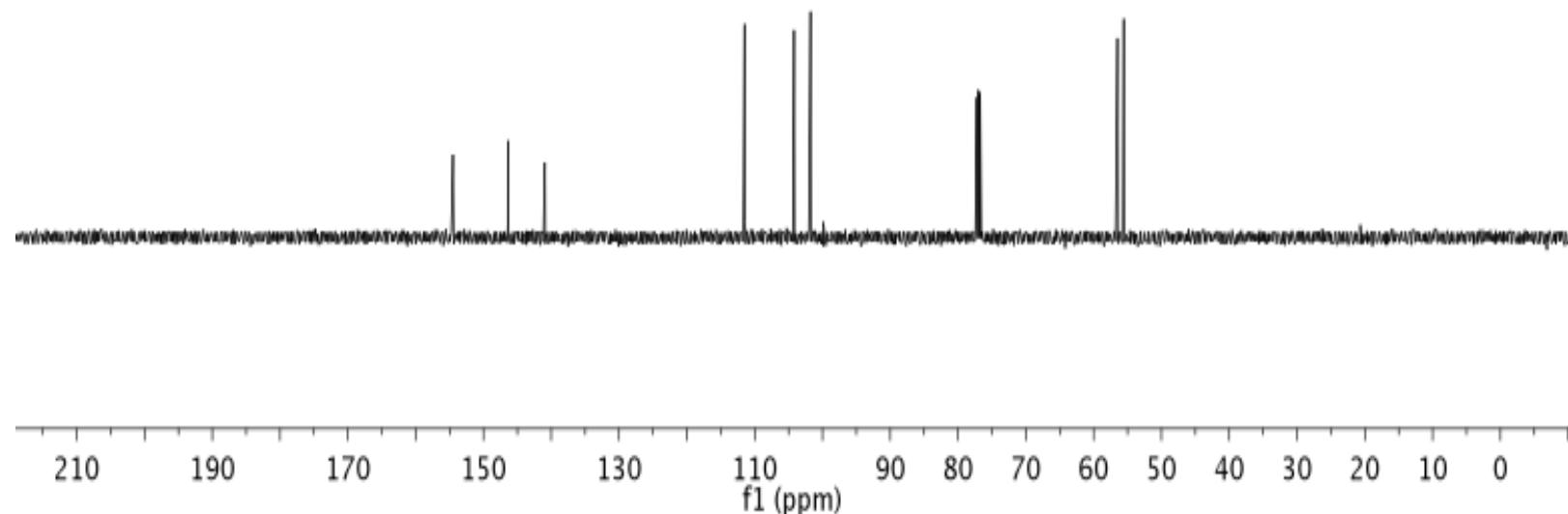
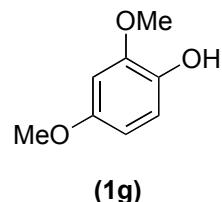
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 2-Methoxyphenol (1f)



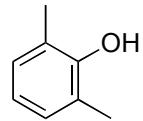
(1g)



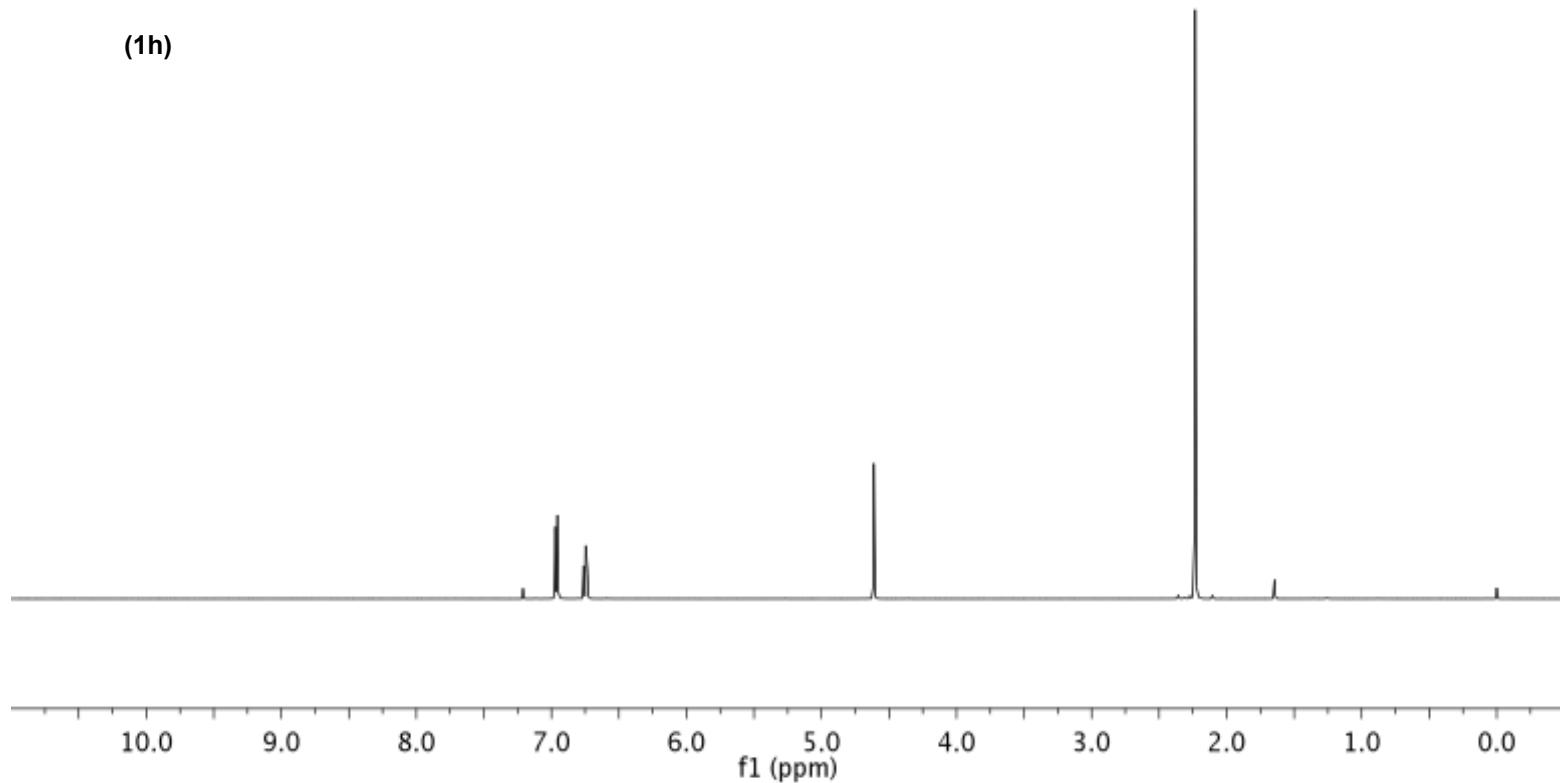
^1H NMR (500 MHz, CDCl_3) Spectrum of 2,4-Dimethoxyphenol (1g)



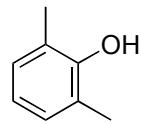
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 2,4-Dimethoxyphenol (1g)



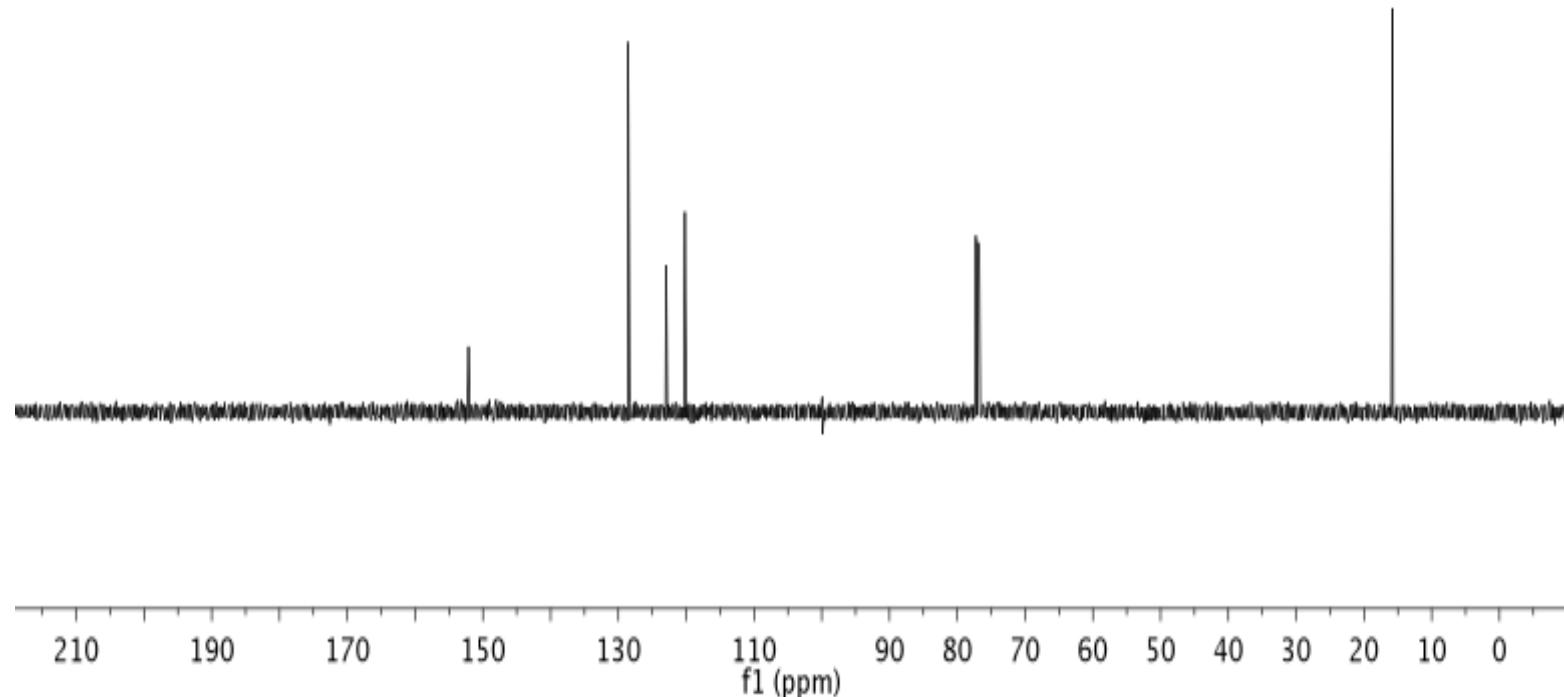
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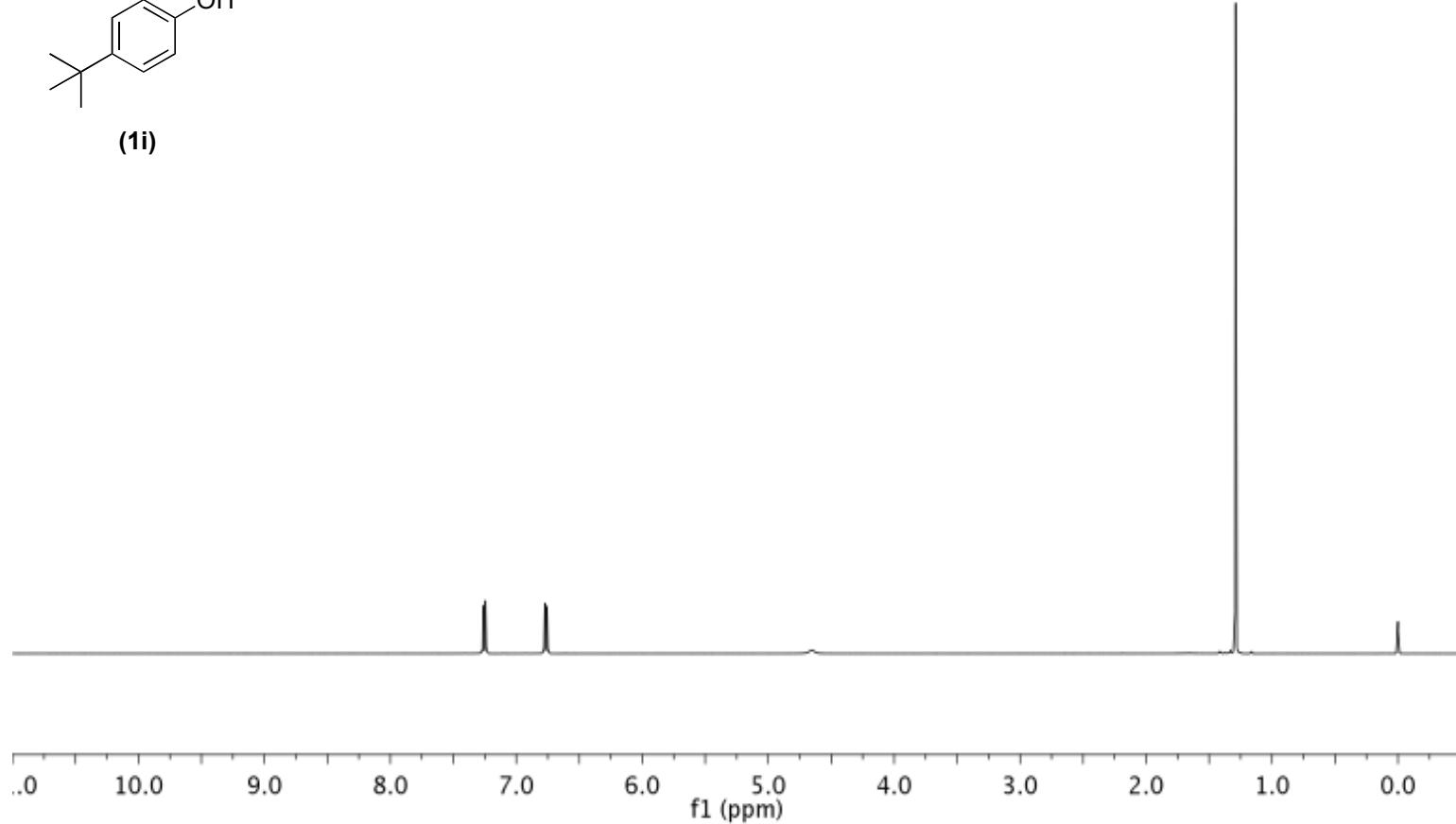
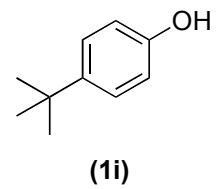
¹H NMR (500 MHz, CDCl₃) Spectrum of 2,6-Dimethylphenol (1h)



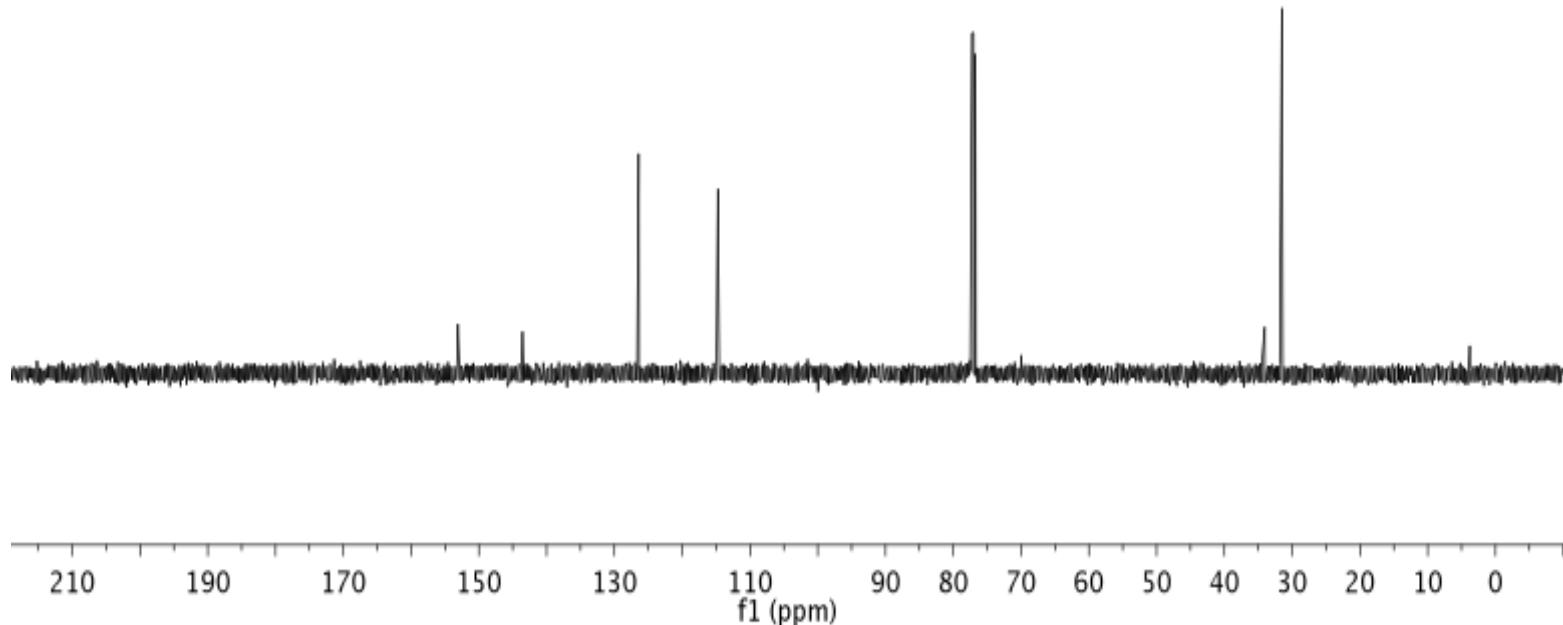
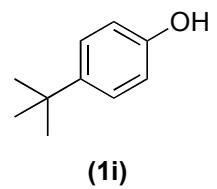
(1h)



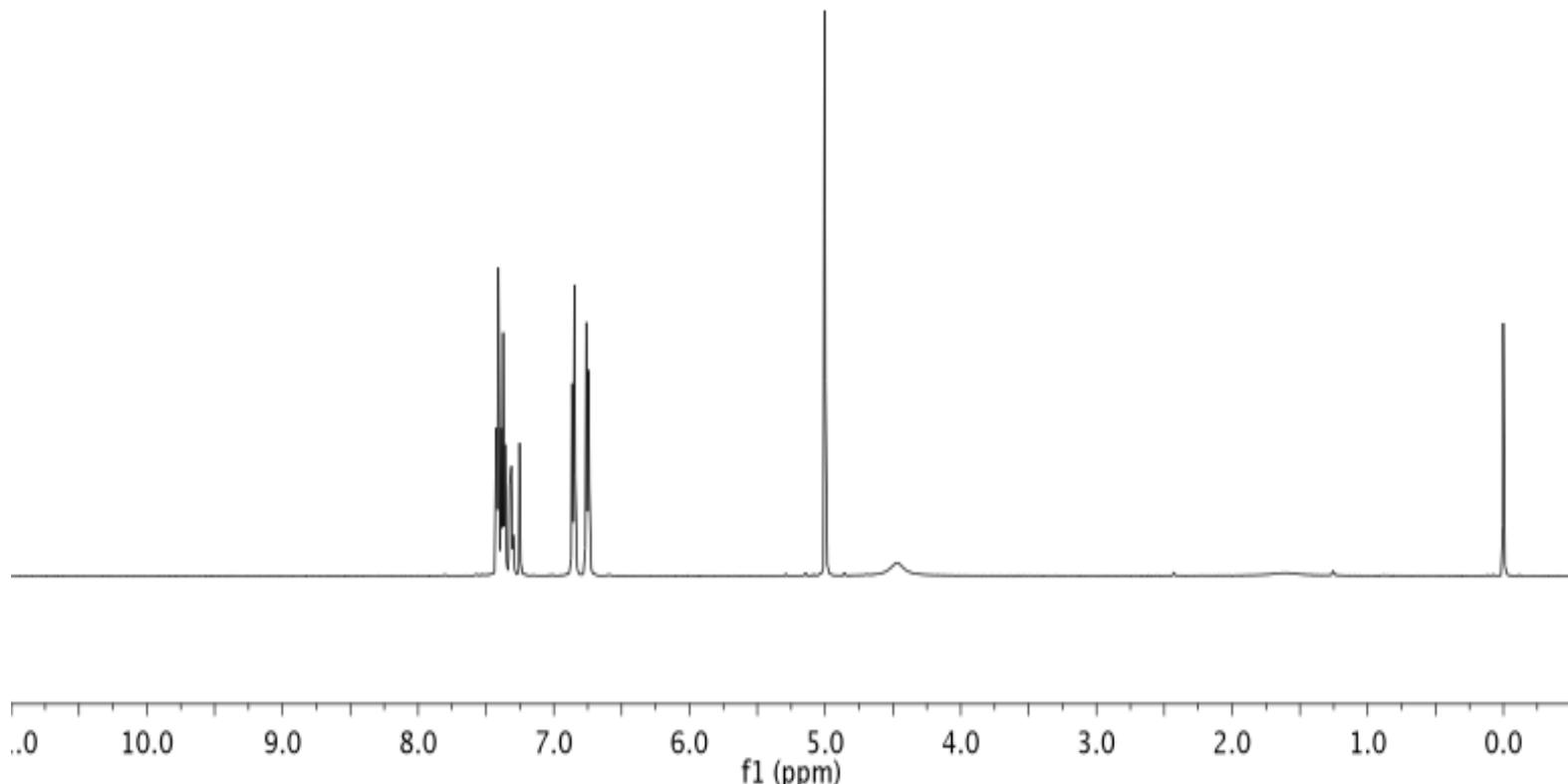
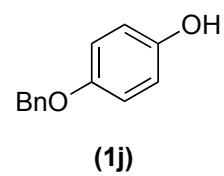
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 2,6-Dimethylphenol (1h)



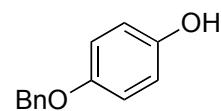
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-(*tert*-Butyl)phenol (1i)



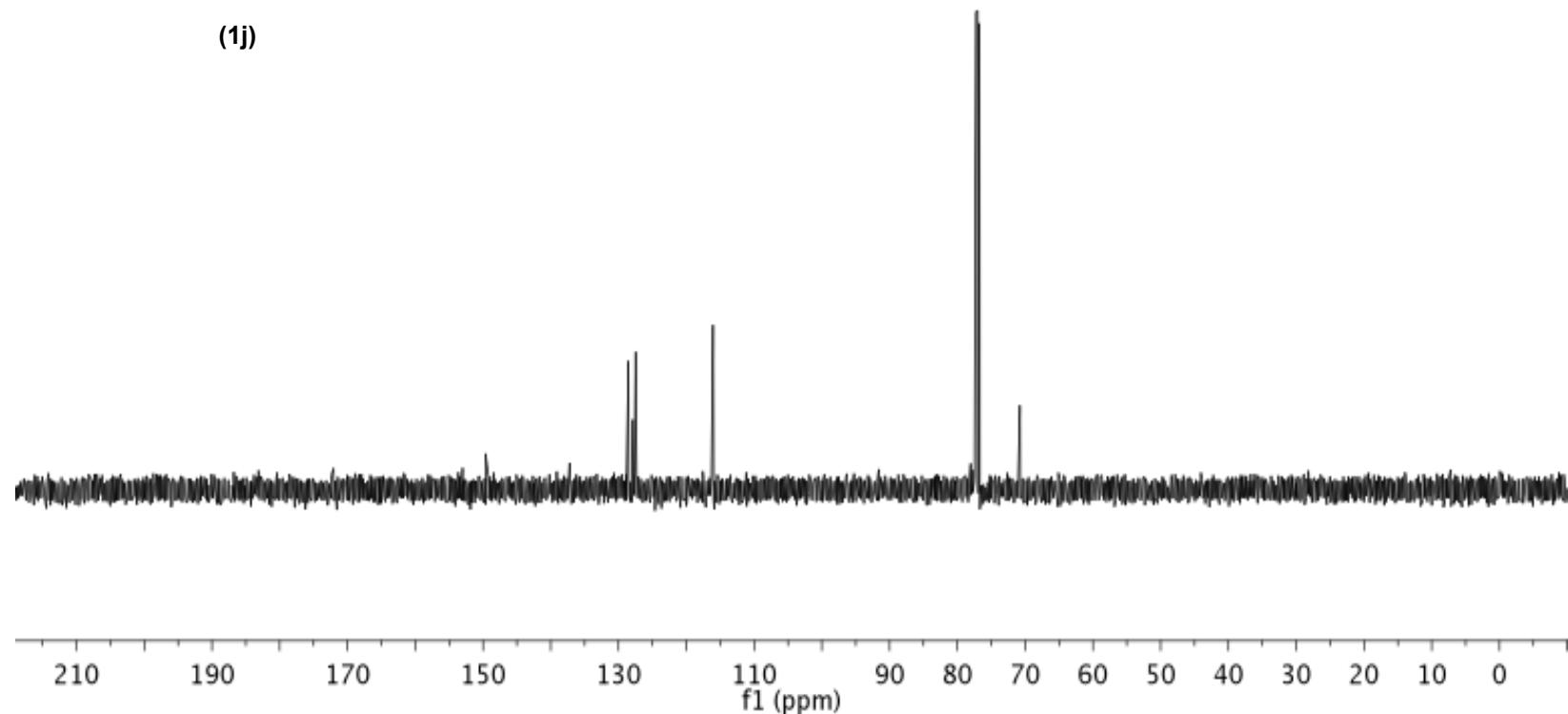
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of 4-(*tert*-Butyl)phenol (1i)



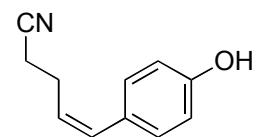
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-(Benzylxy)phenol (1j)



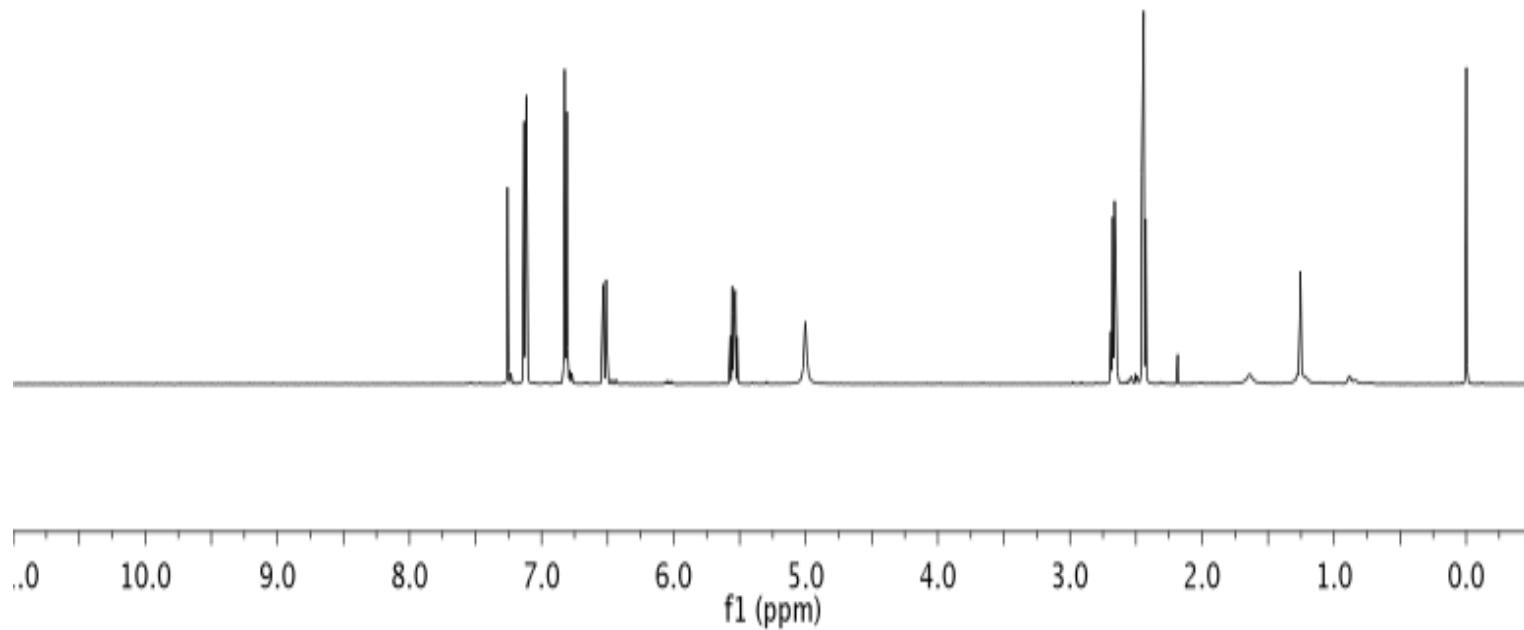
(1j)



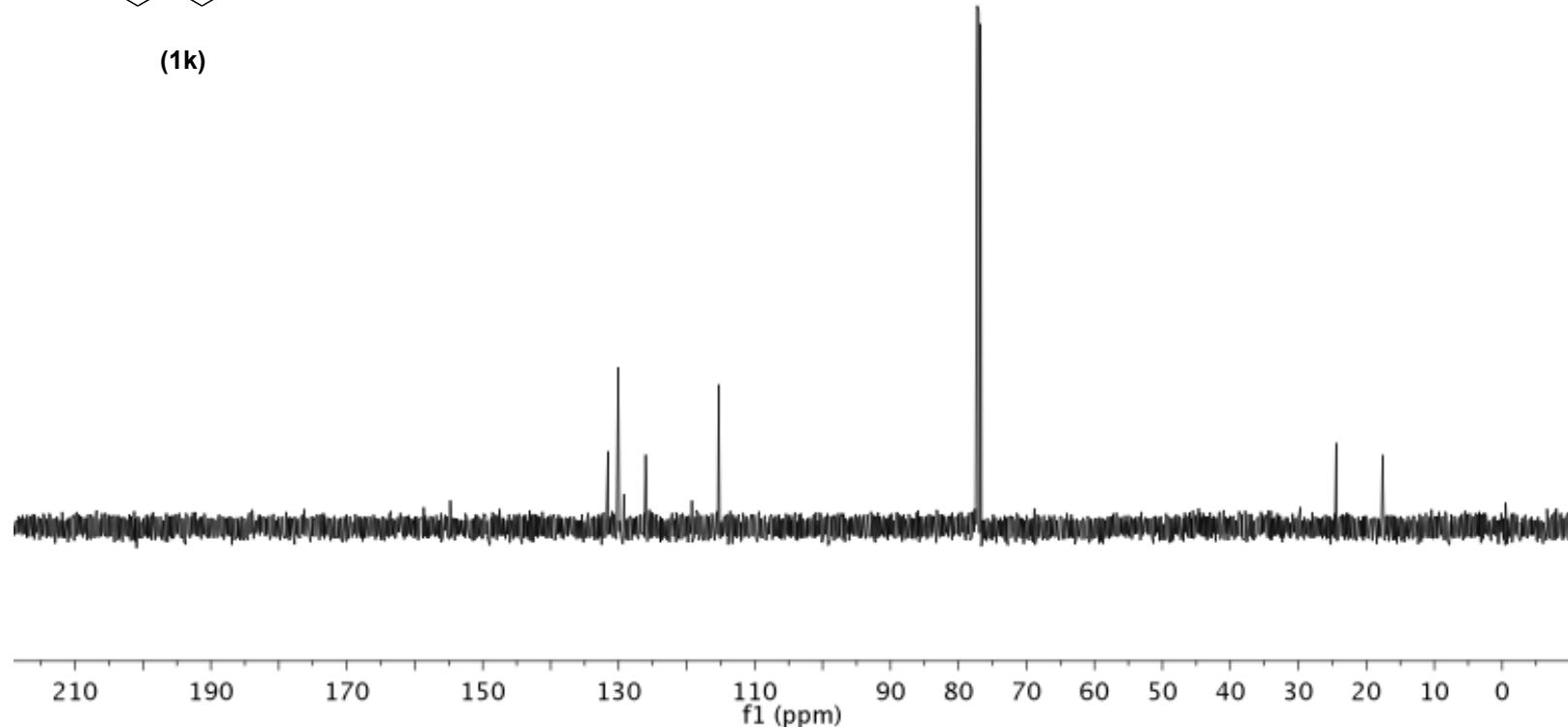
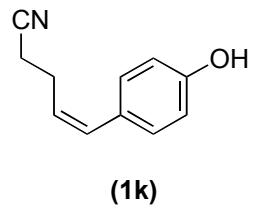
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-(Benzylxy)phenol (1j)



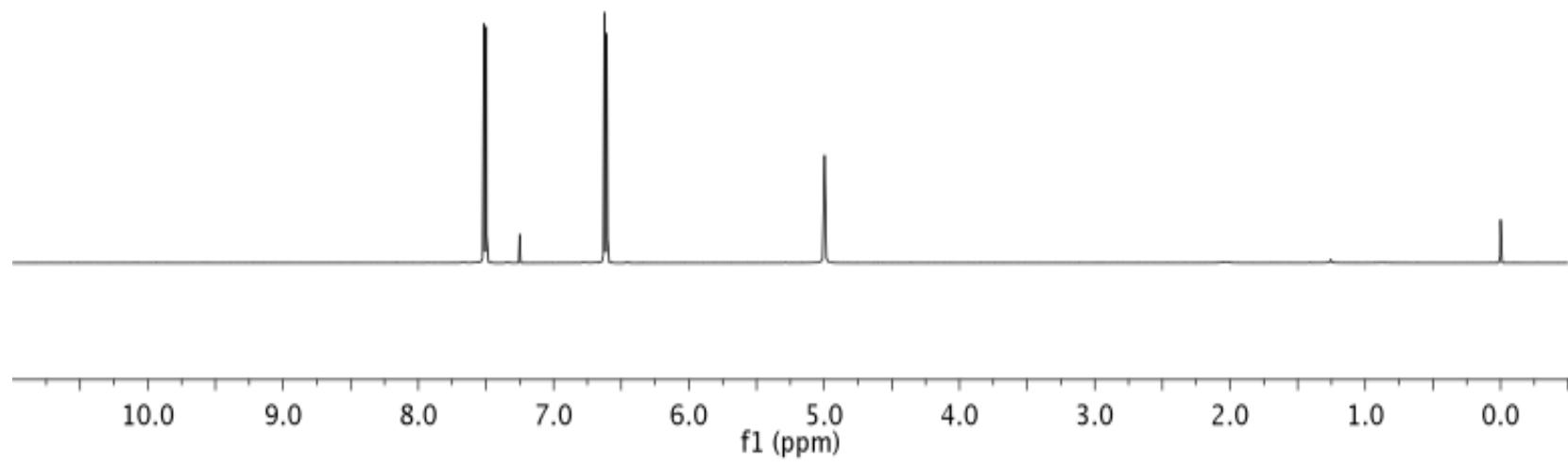
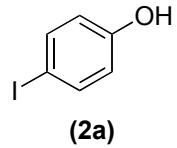
(1k)



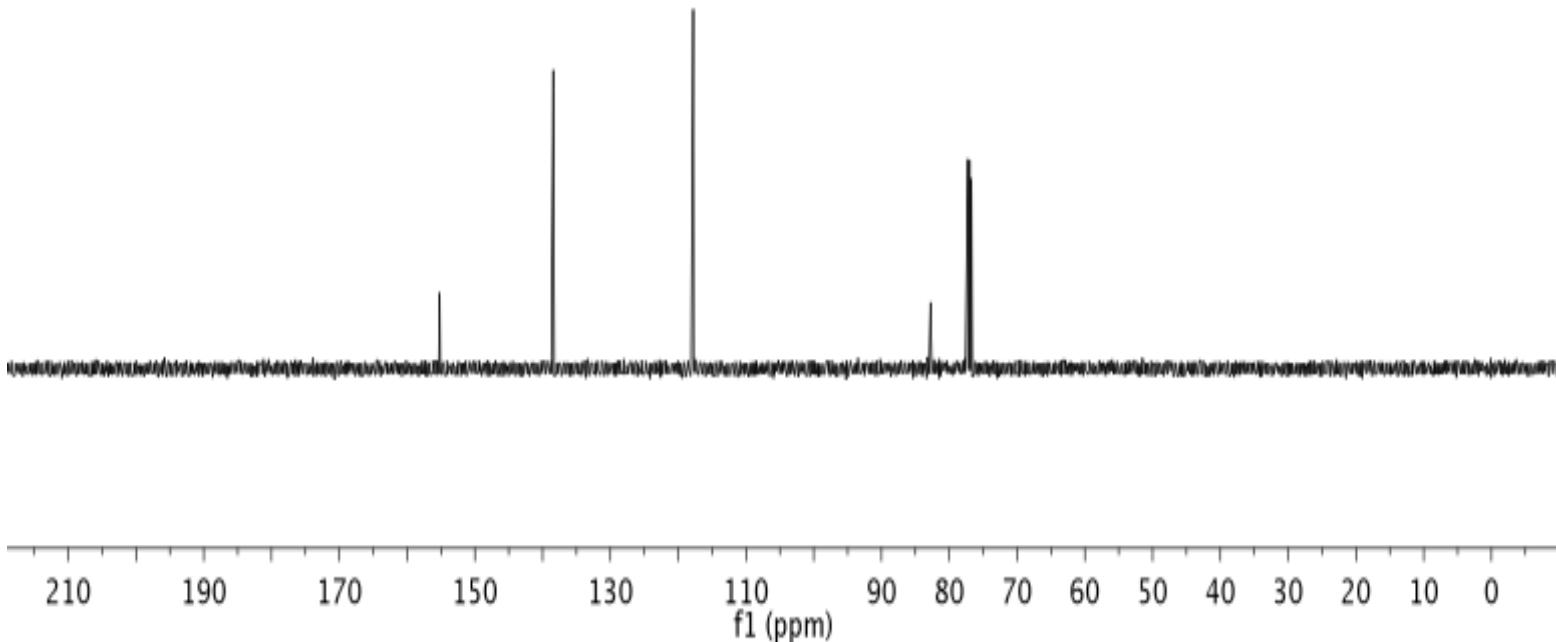
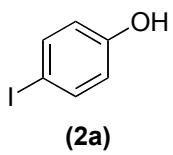
¹H NMR (500 MHz, CDCl₃) Spectrum of (Z)-5-(4-Hydroxyphenyl)pent-4-enenitrile (1k)



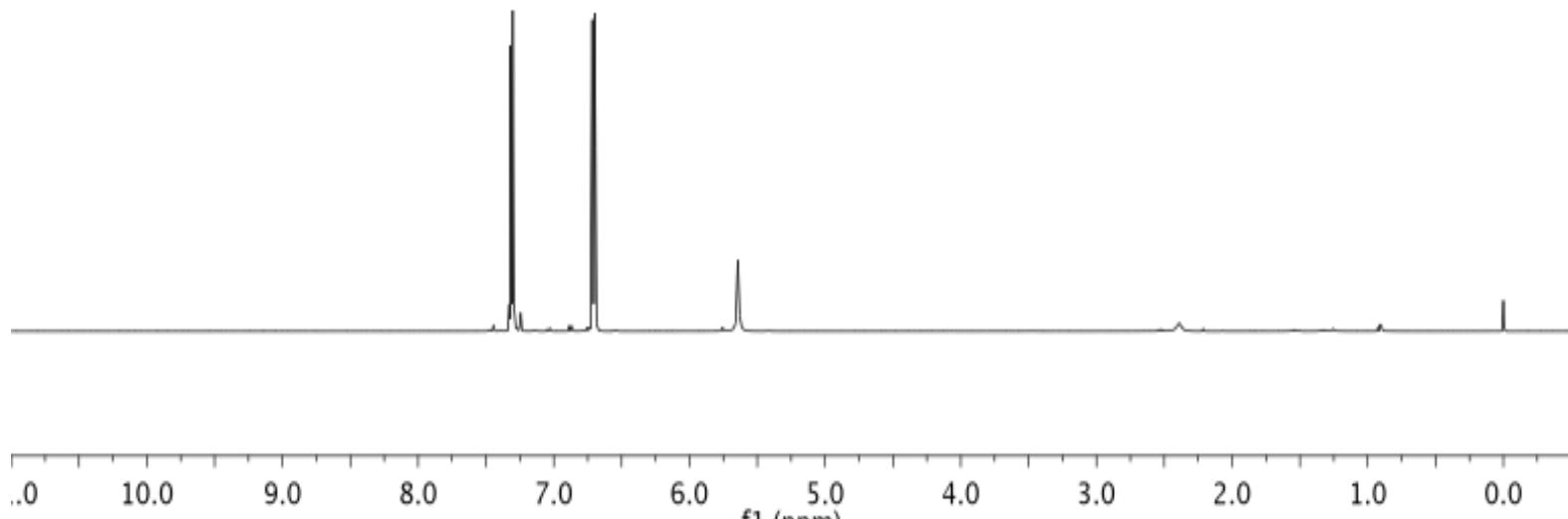
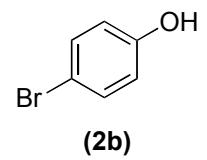
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of (Z)-5-(4-Hydroxyphenyl)pent-4-enenitrile (1k)



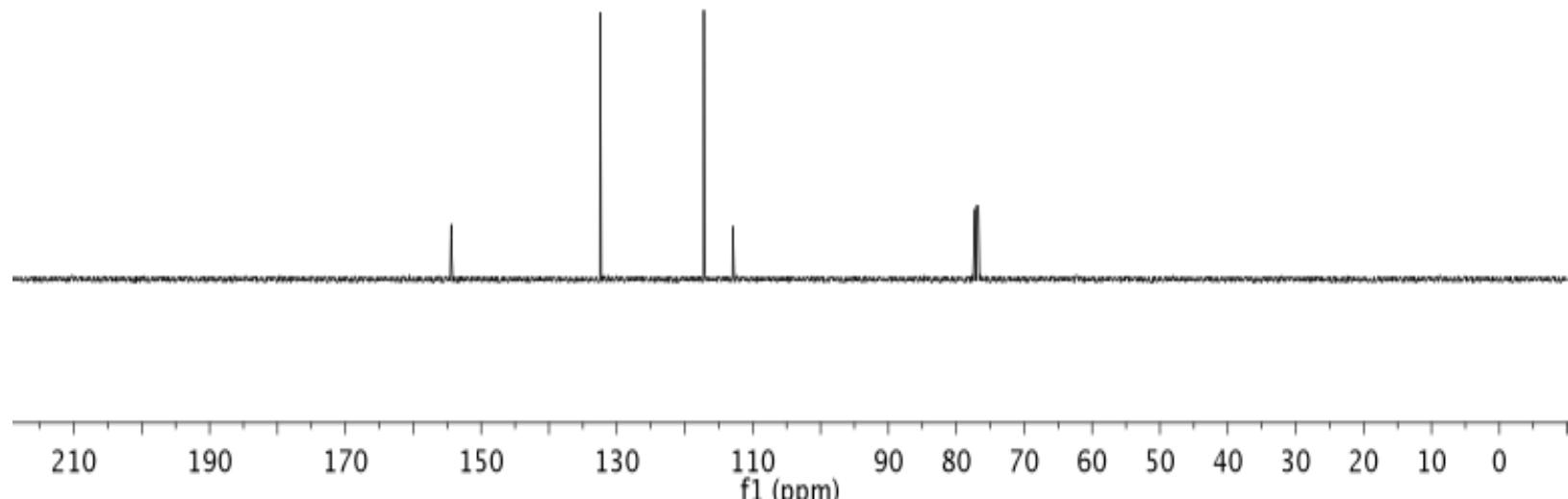
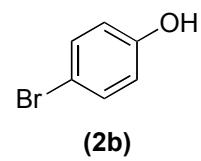
^1H NMR (500 MHz, CDCl_3) Spectrum of 4-Iodophenol (2a)



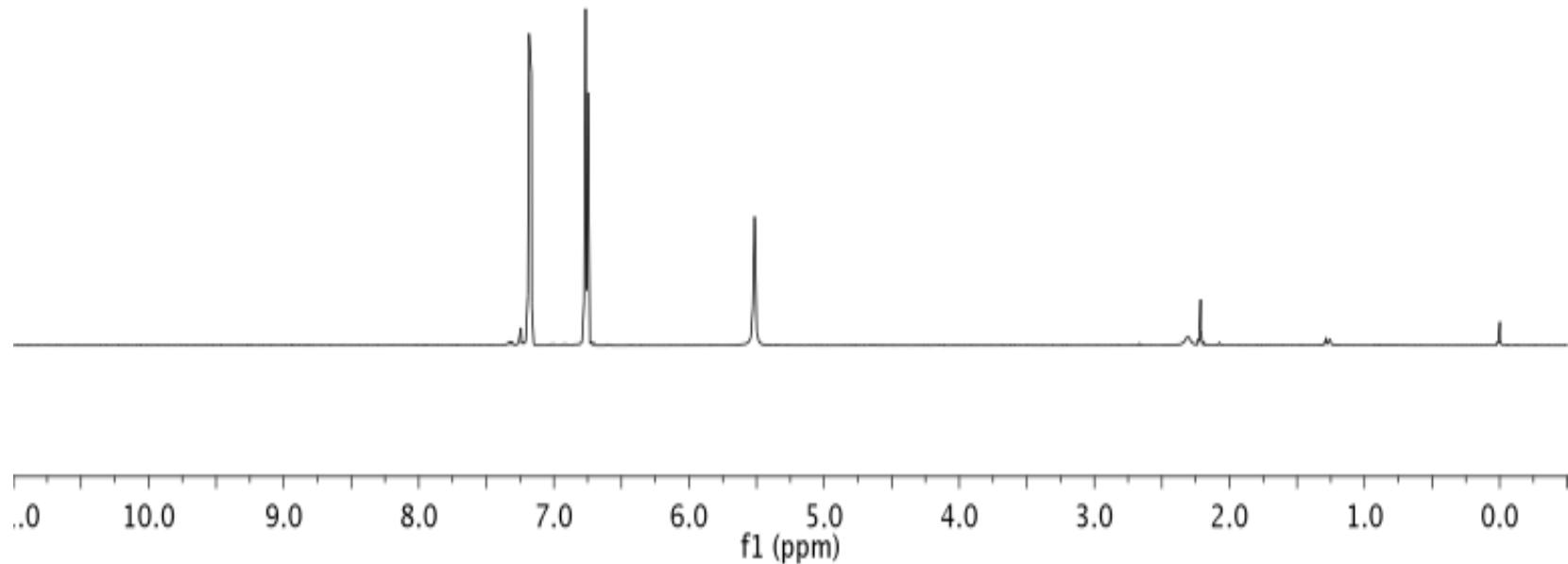
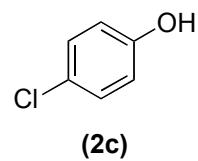
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Iodophenol (2a)



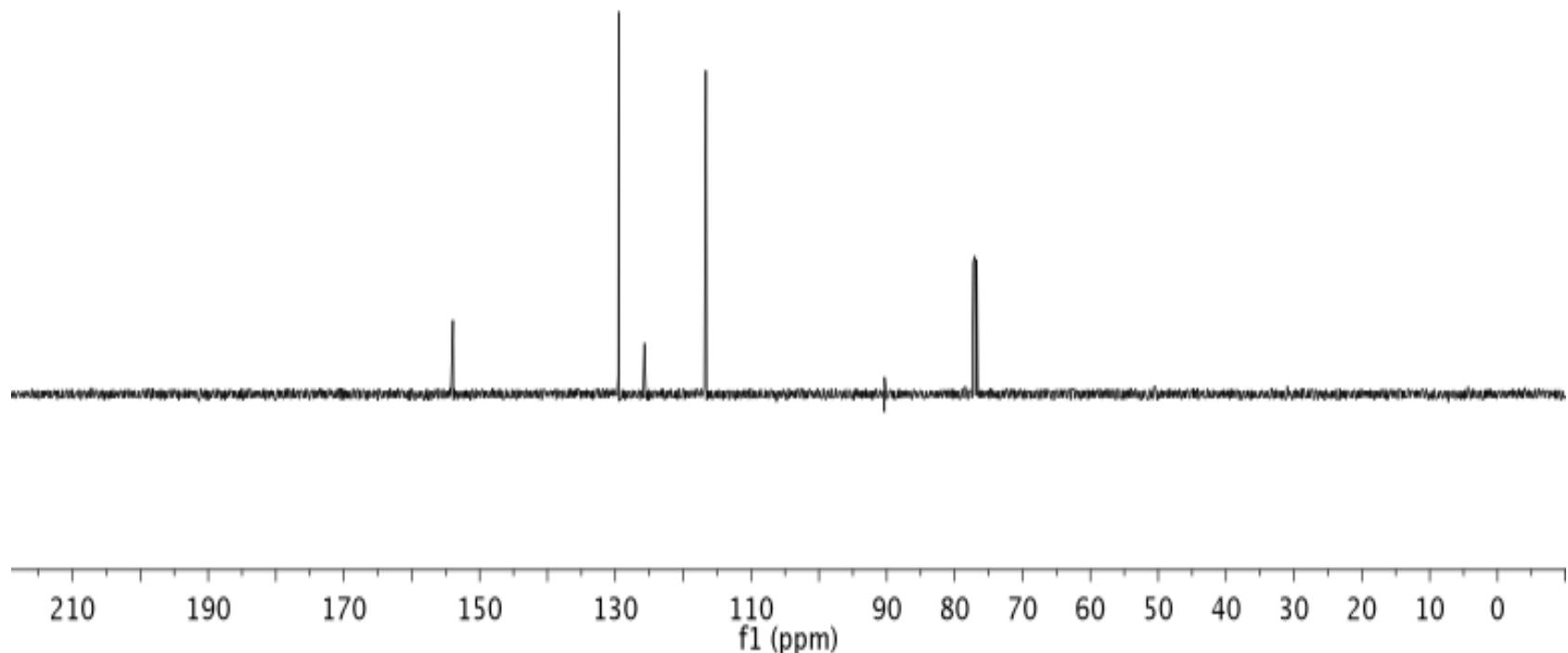
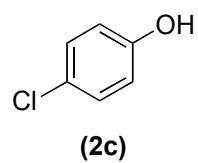
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-Bromophenol (2b)



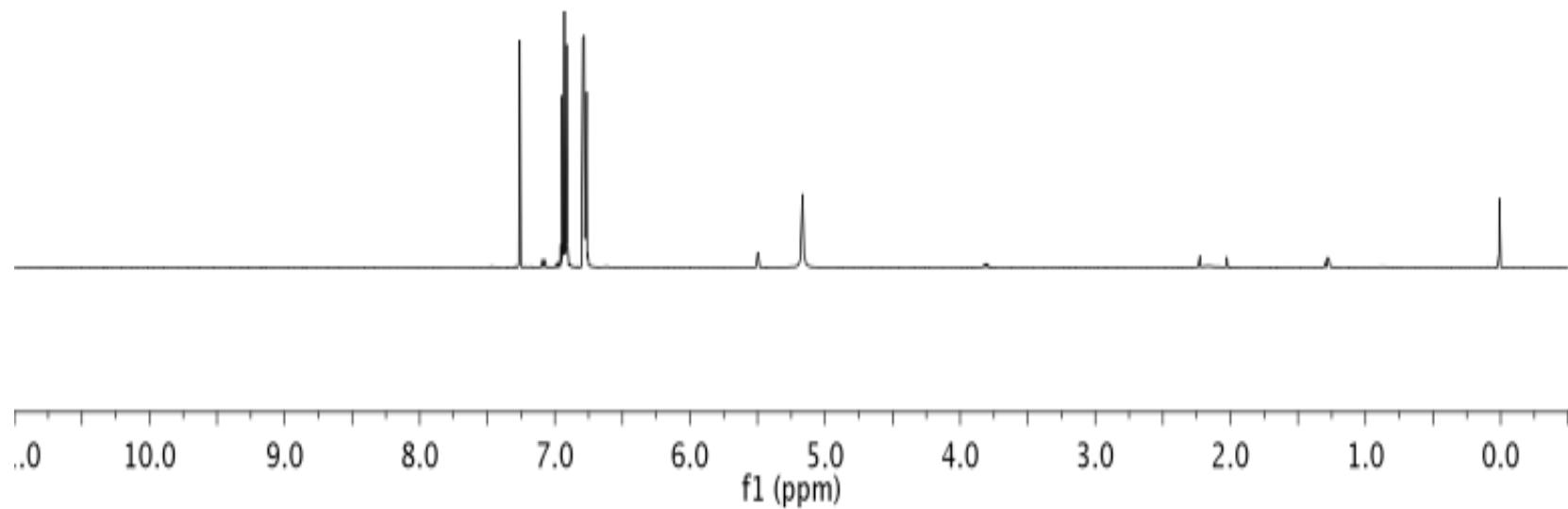
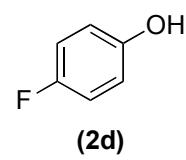
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of 4-Bromophenol (2b)



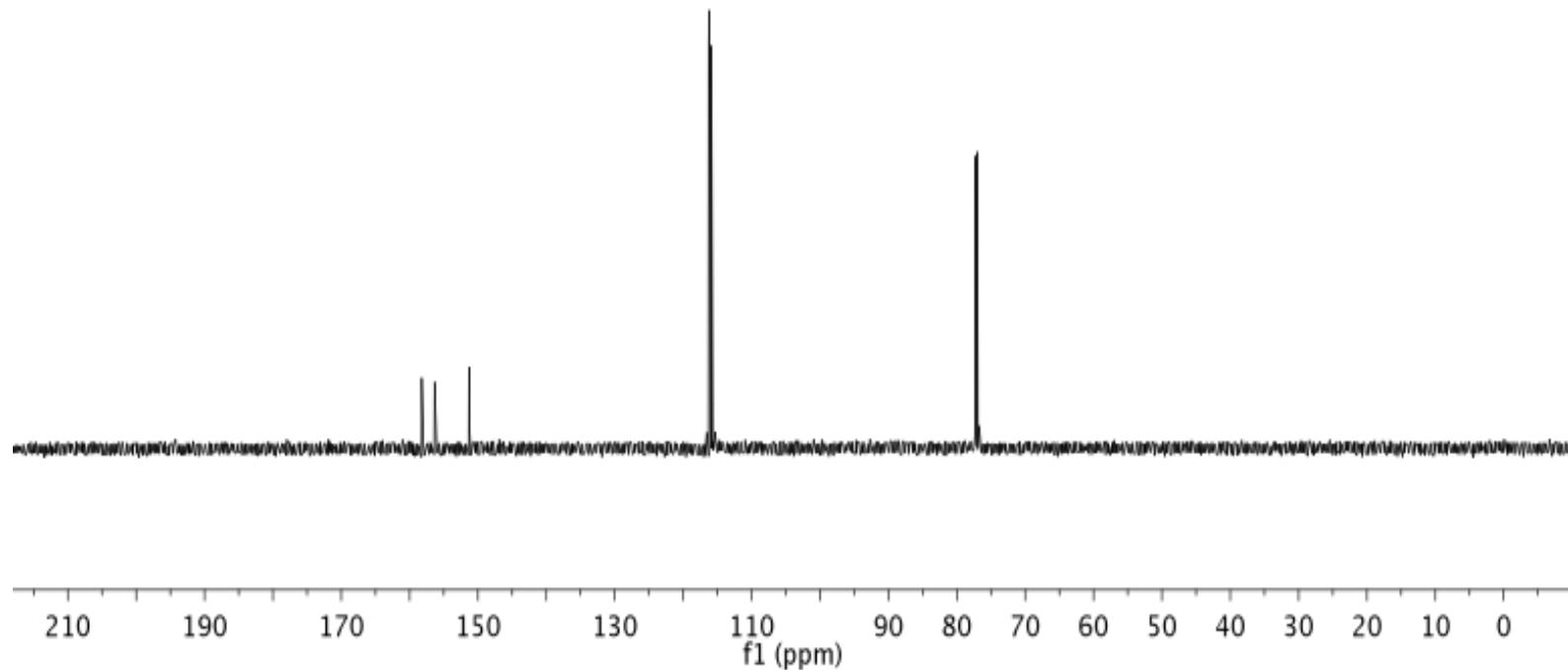
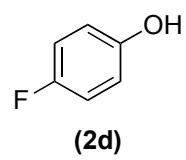
^1H NMR (500 MHz, CDCl_3) Spectrum of 4-Chlorophenol (2c)



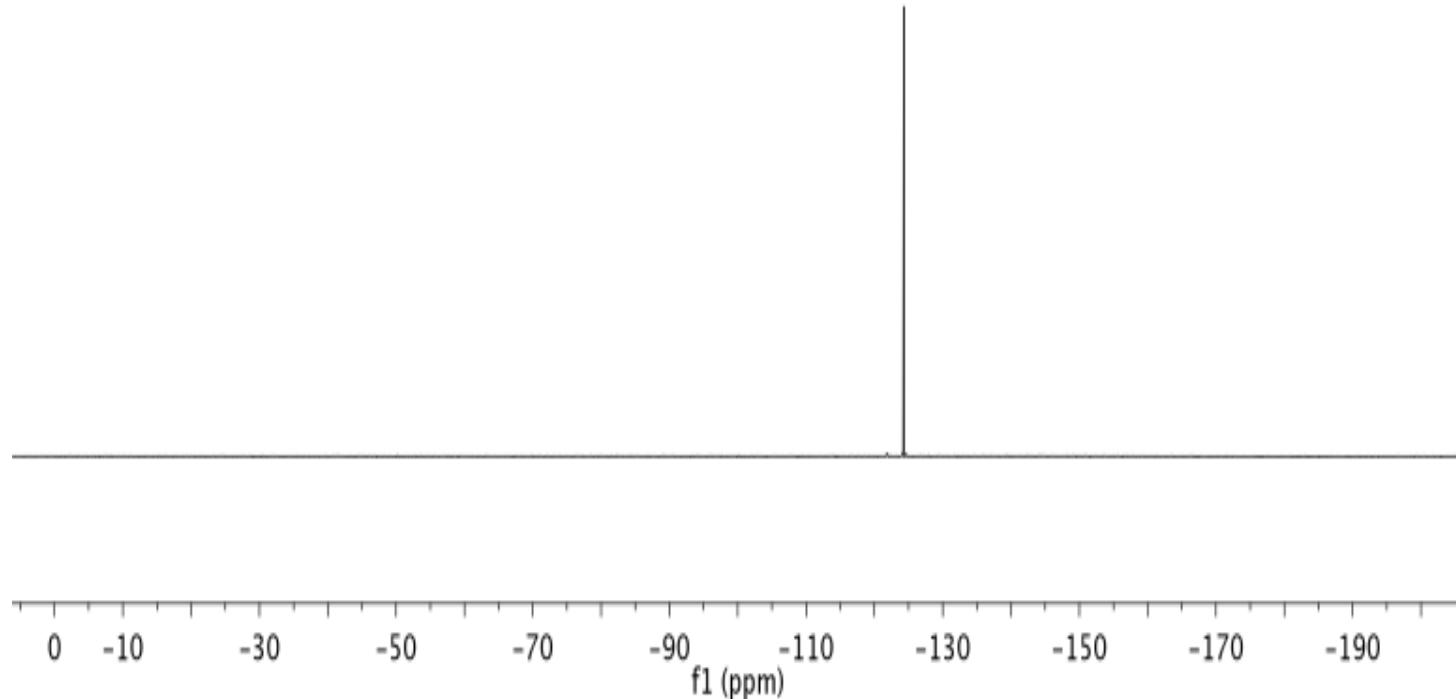
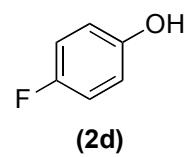
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Chlorophenol (2c)



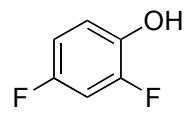
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-Fluorophenol (2d)



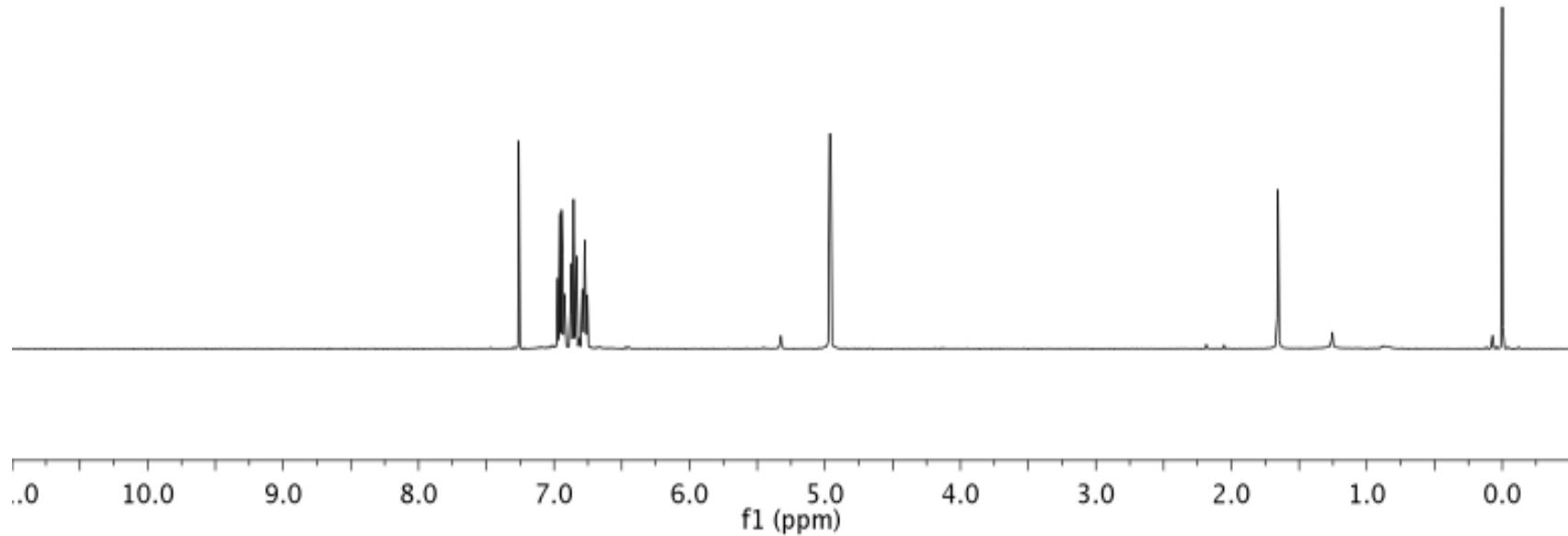
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Fluorophenol (2d)



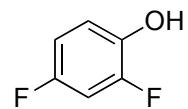
¹⁹F NMR (470.8 MHz, CDCl₃) Spectrum of 4-Fluorophenol (2d)



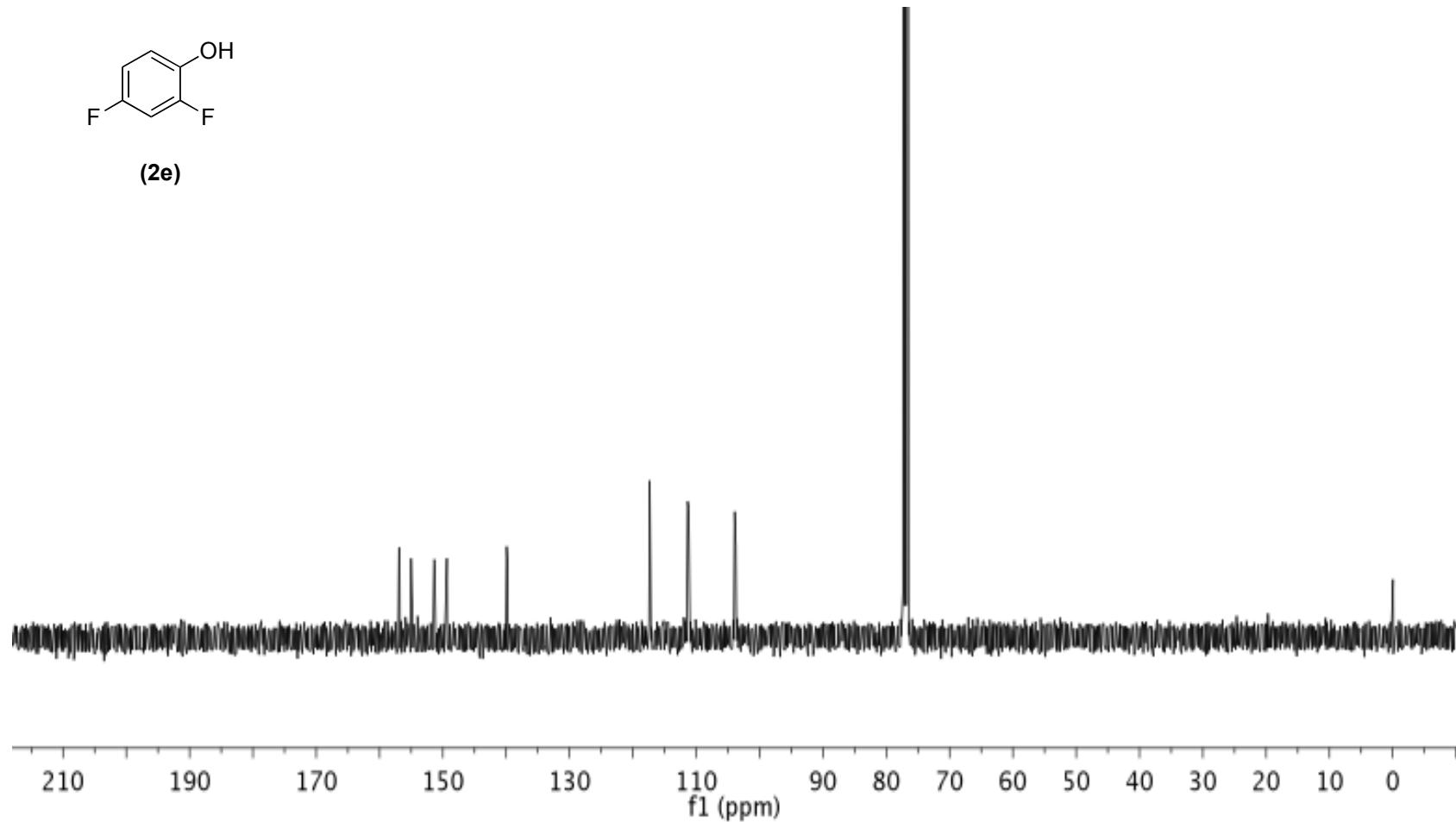
(2e)



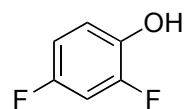
^1H NMR (500 MHz, CDCl_3) Spectrum of 2,4-Difluorophenol (2e)



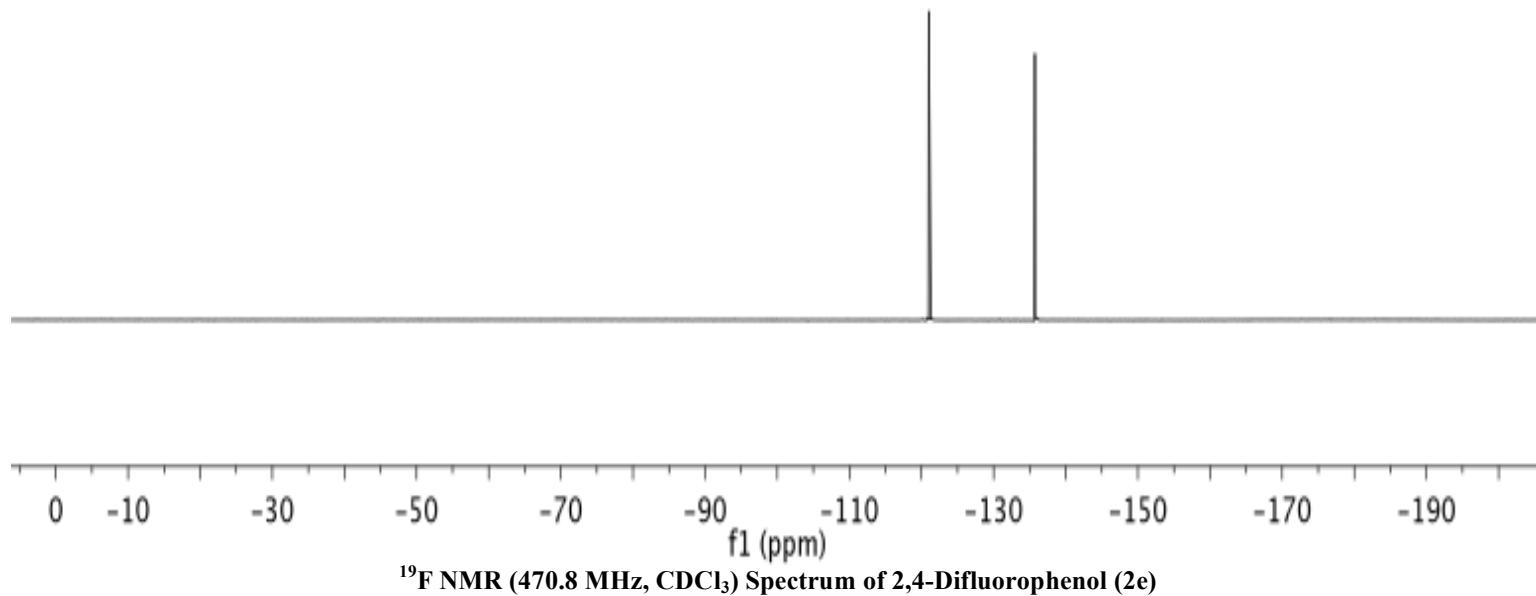
(2e)

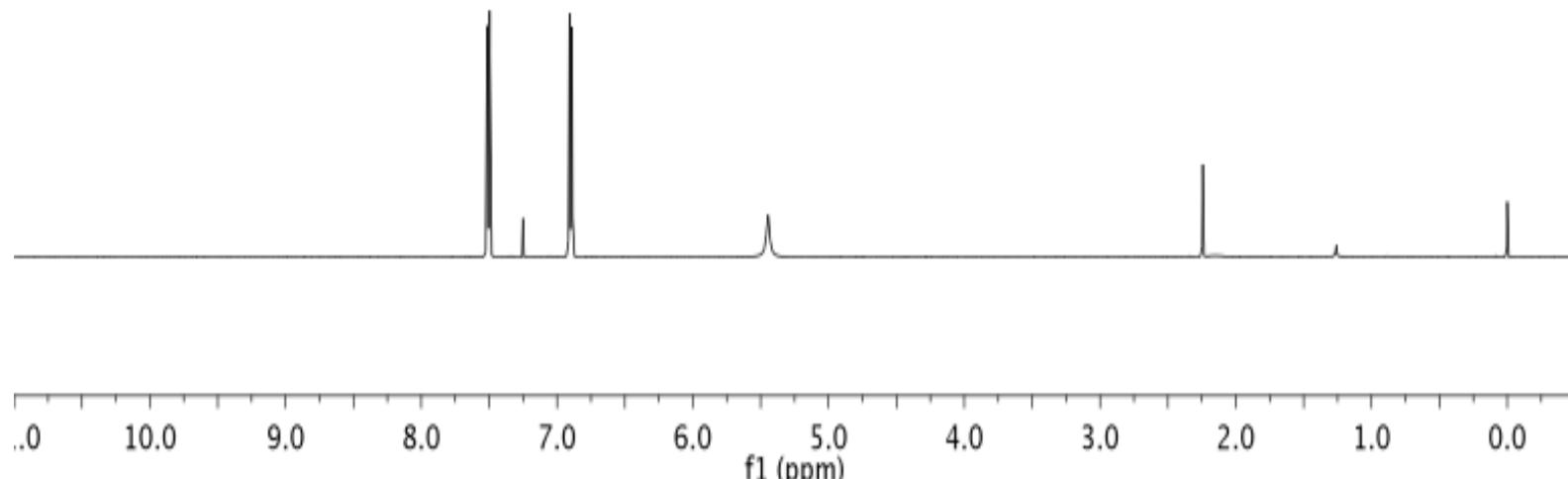
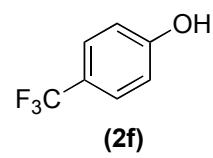


¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 2,4-Difluorophenol (2e)

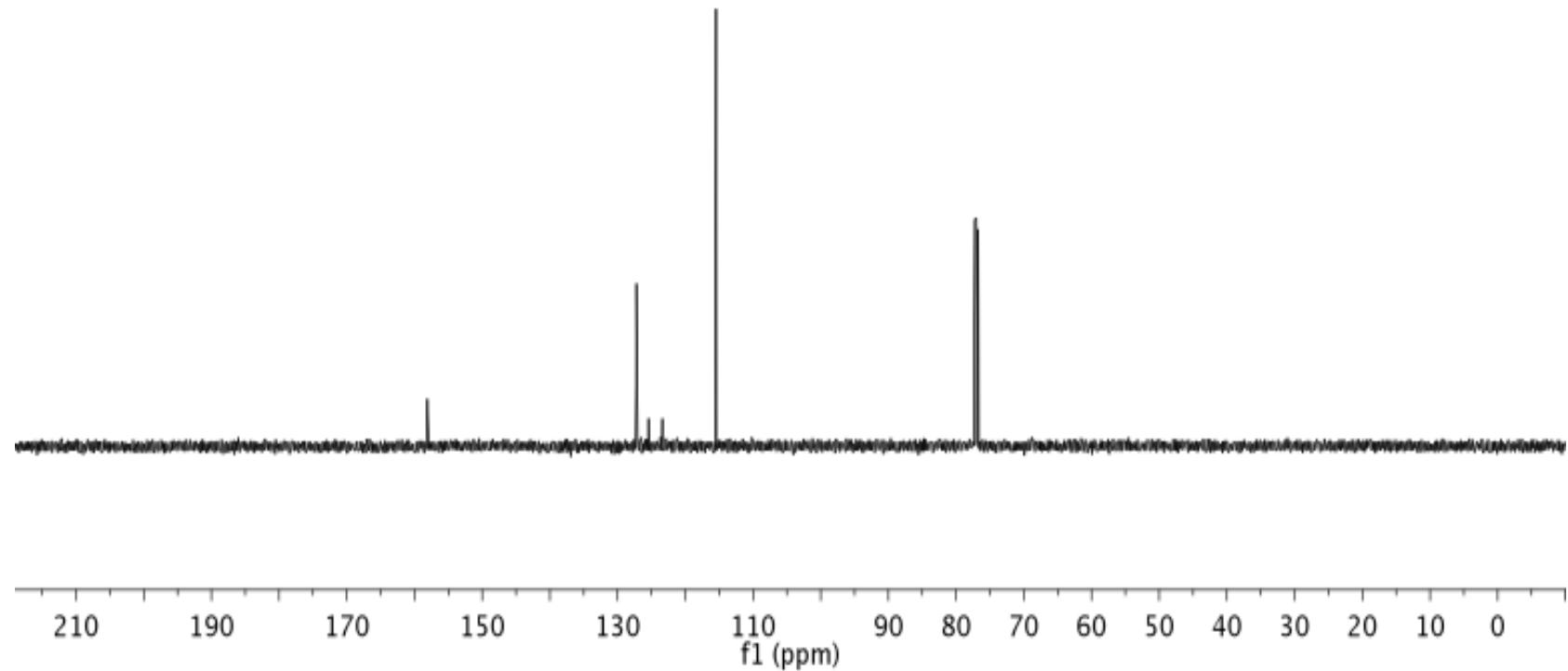
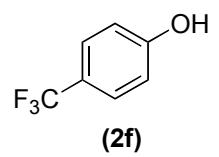


(2e)

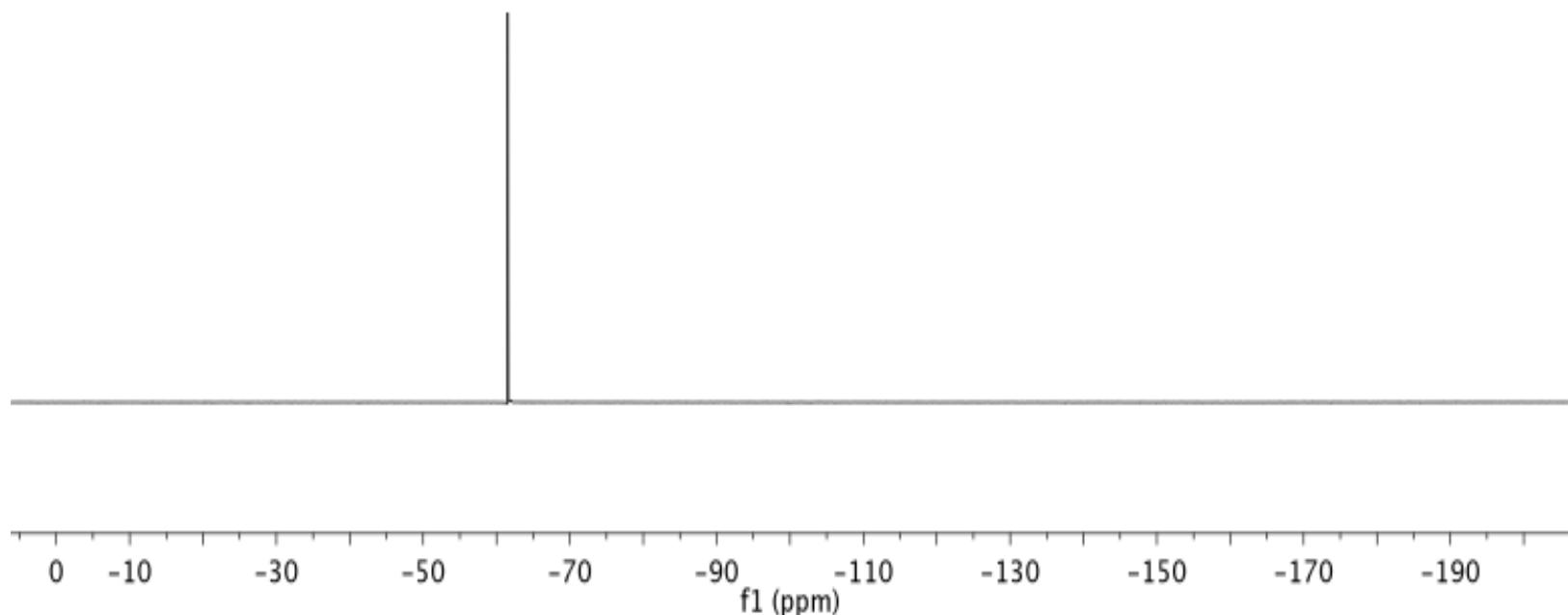
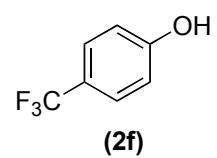




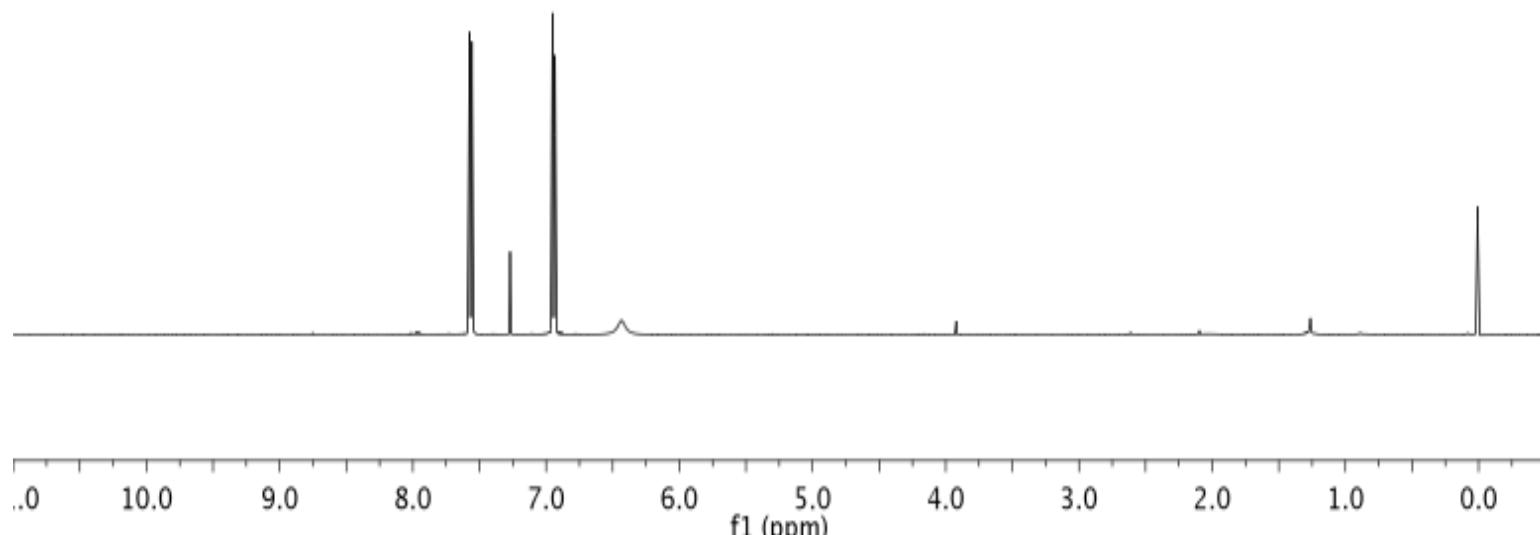
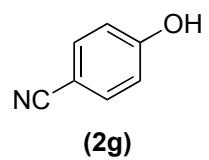
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-(Trifluoromethyl)phenol (2f)



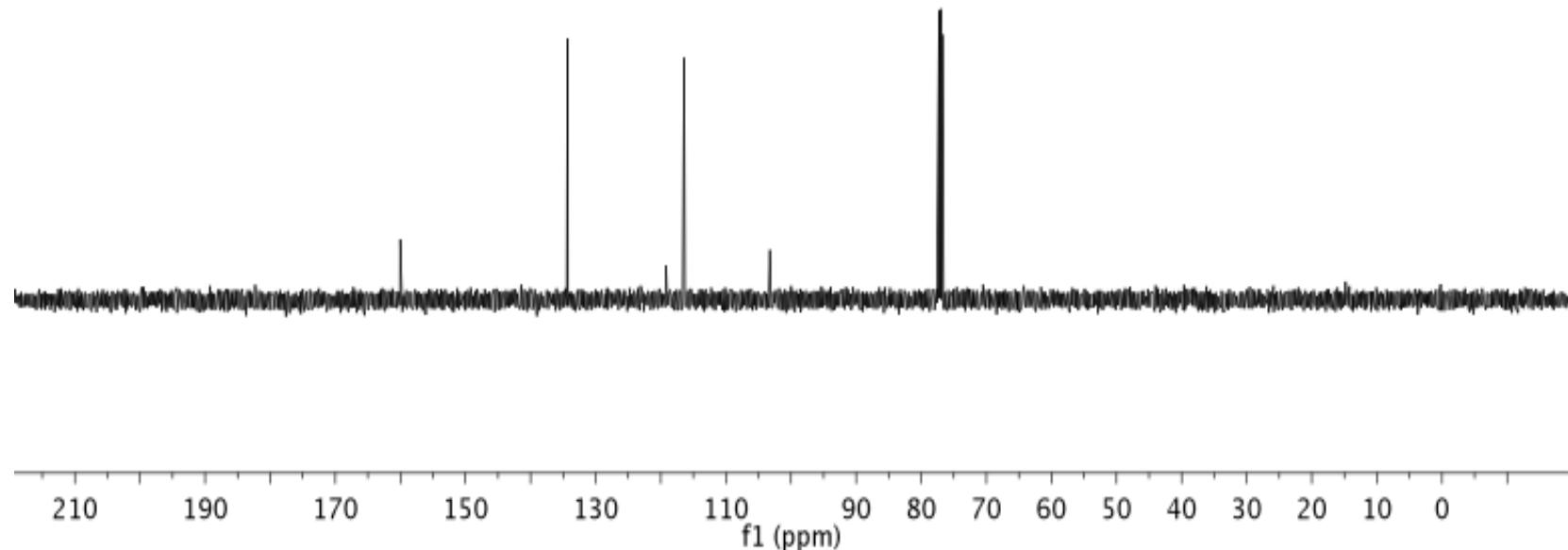
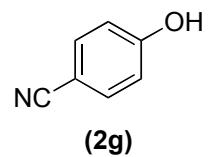
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-(Trifluoromethyl)phenol (2f)



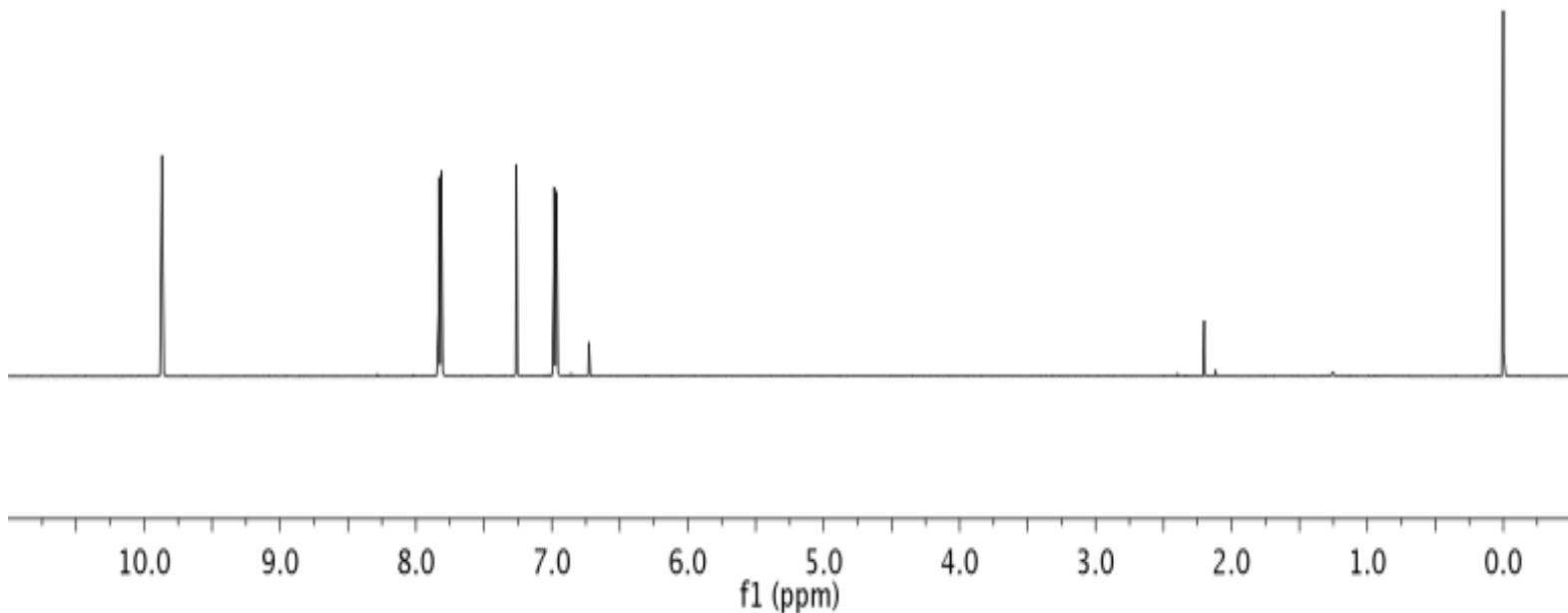
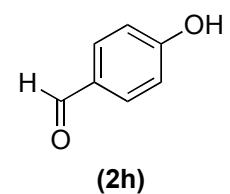
¹⁹F NMR (470.8 MHz, CDCl₃) Spectrum of 4-(Trifluoromethyl)phenol (2f)



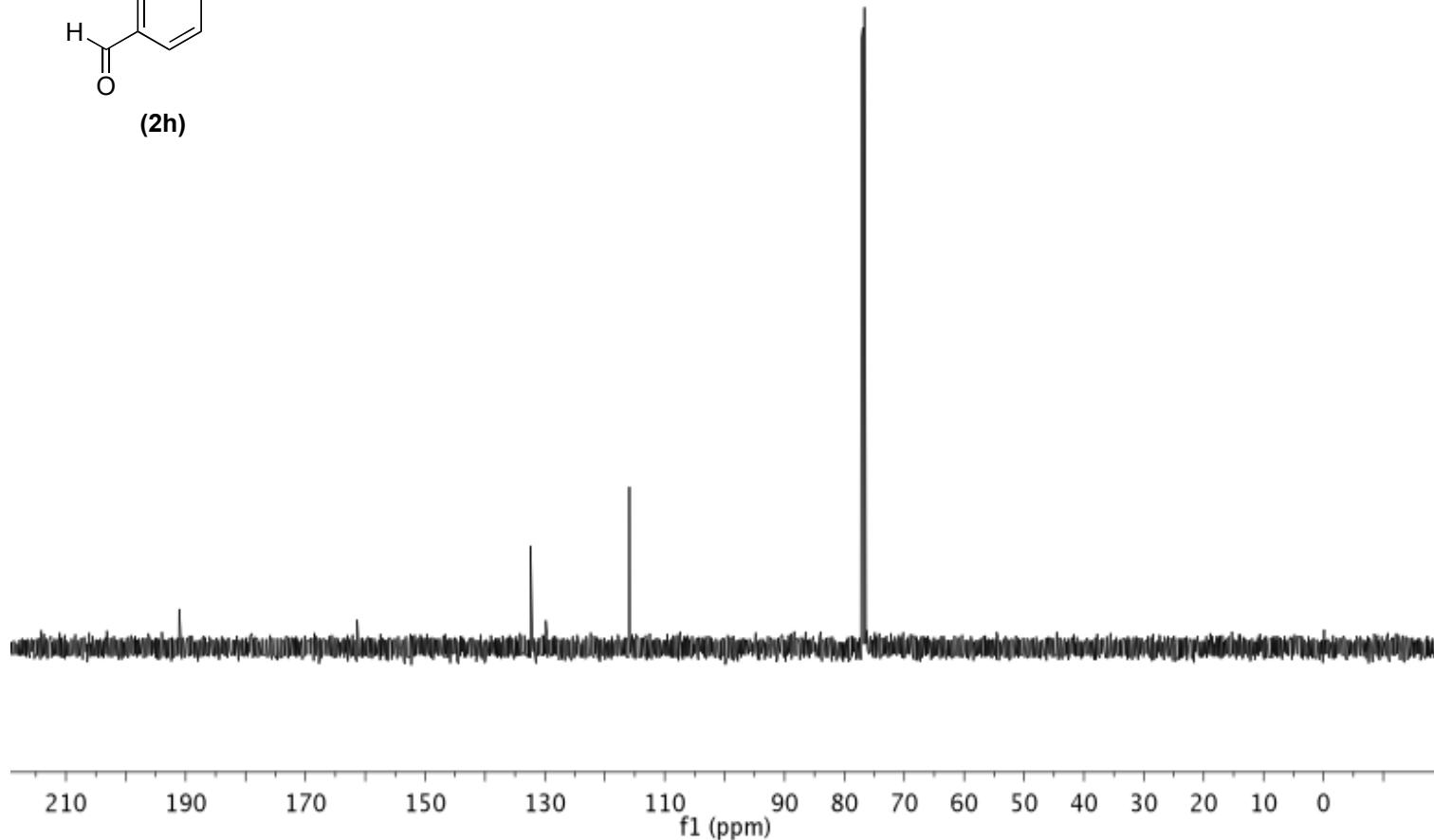
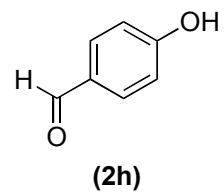
^1H NMR (500 MHz, CDCl_3) Spectrum of 4-Hydroxybenzonitrile (2g)



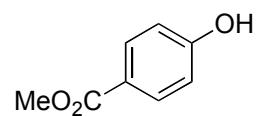
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Hydroxybenzonitrile (2g)



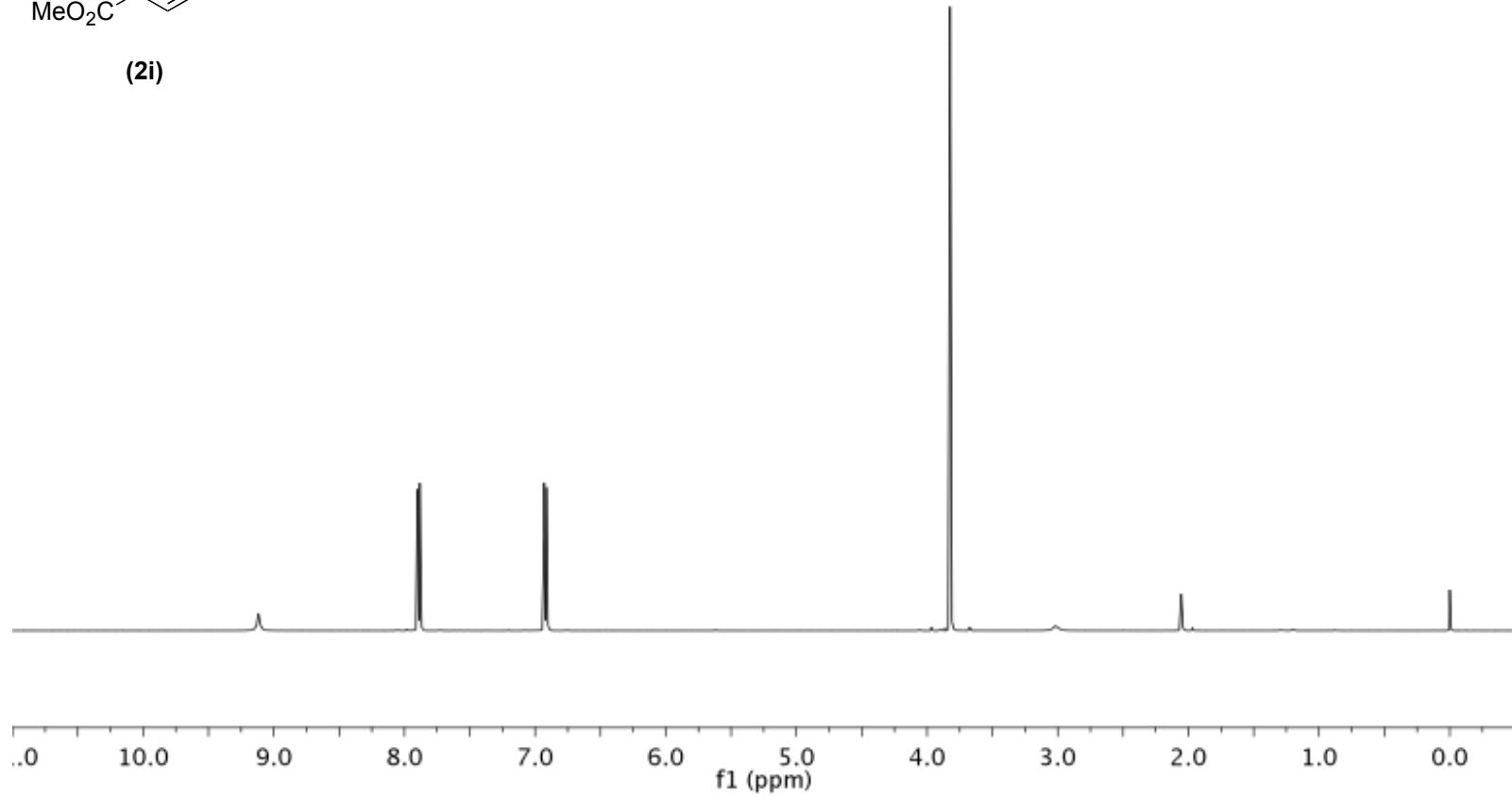
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-Hydroxybenzaldehyde (2h)



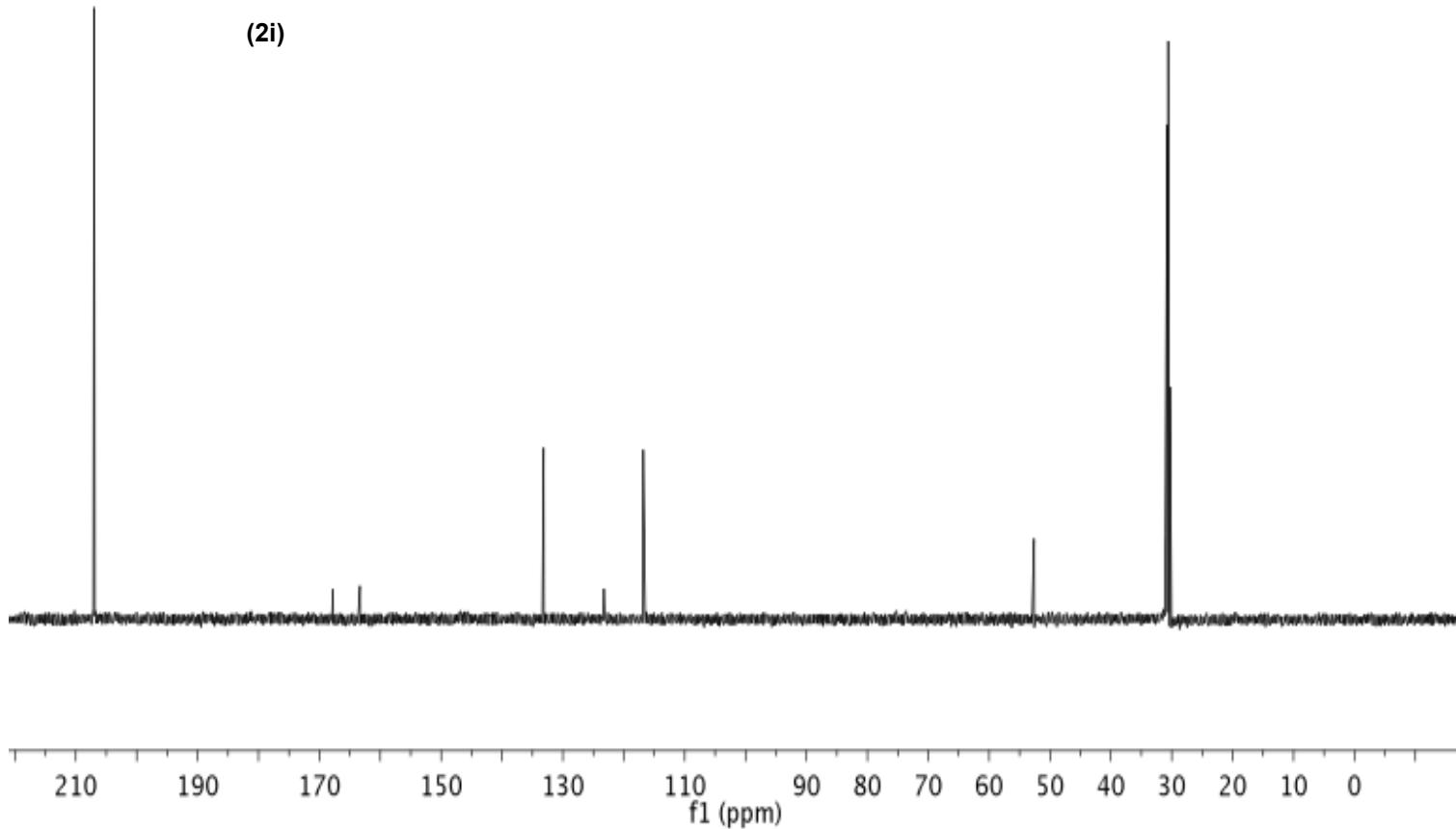
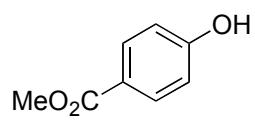
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Hydroxybenzaldehyde (2h)



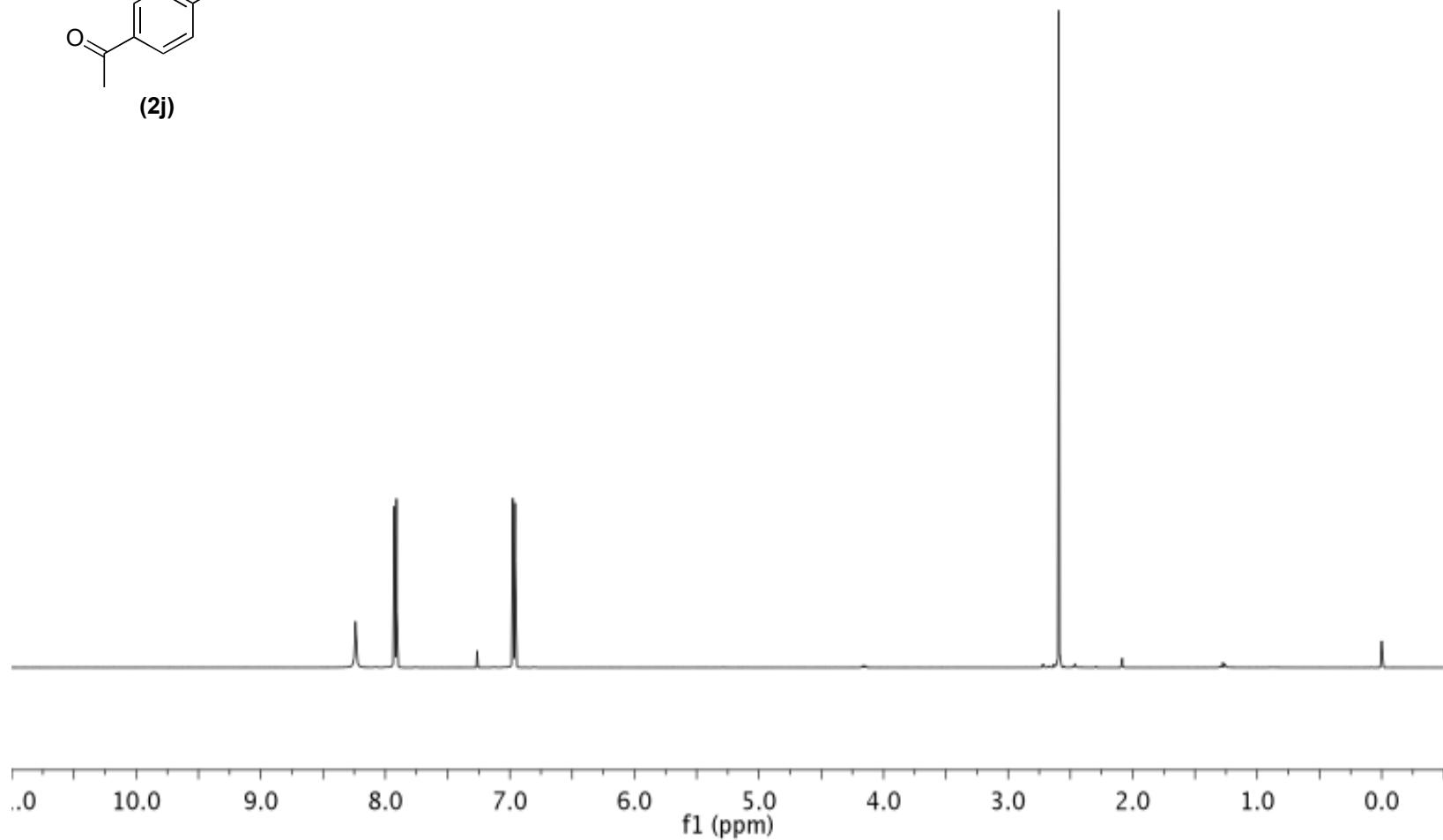
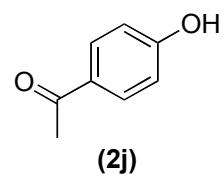
(2i)



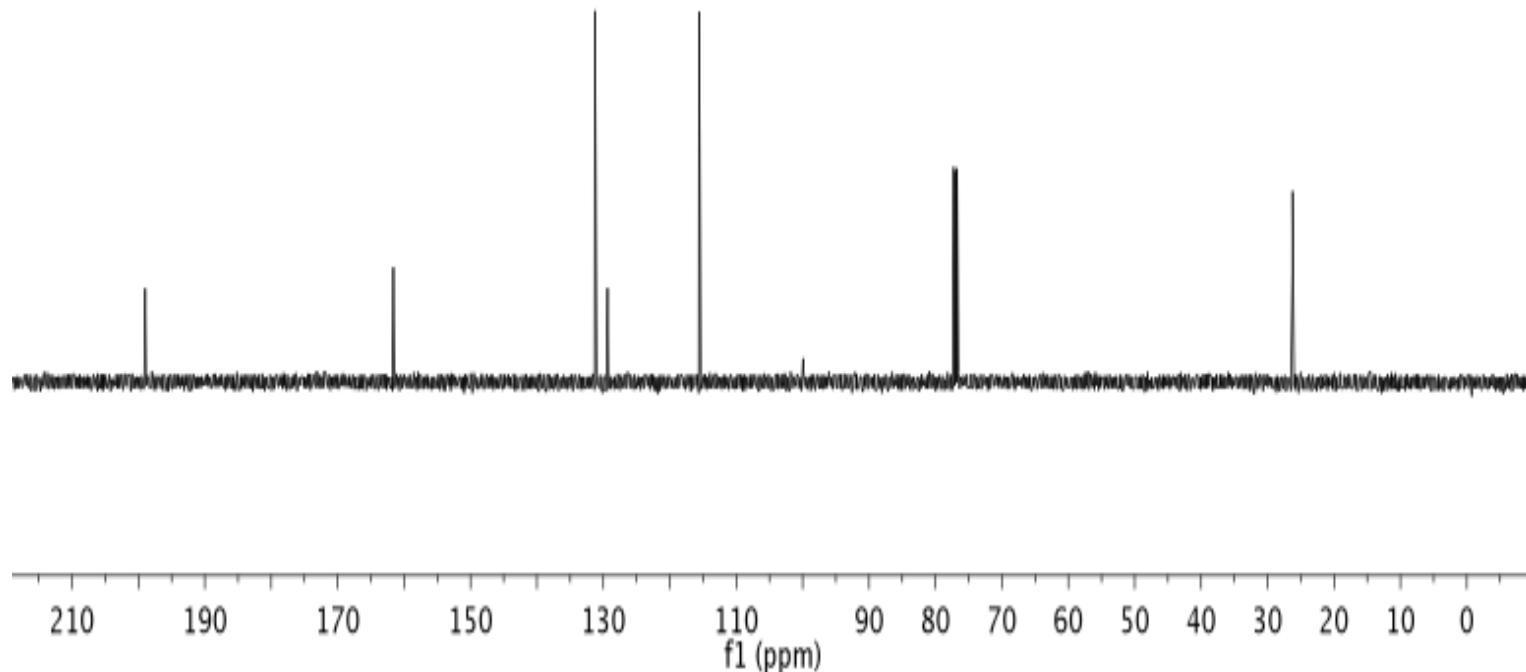
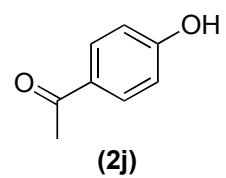
^1H NMR (500 MHz, acetone- d_6) Spectrum of Methyl 4-Hydroxybenzoate (2i)



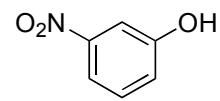
^{13}C NMR (128.5 MHz, acetone- d_6) Spectrum of Methyl 4-Hydroxybenzoate (2i)



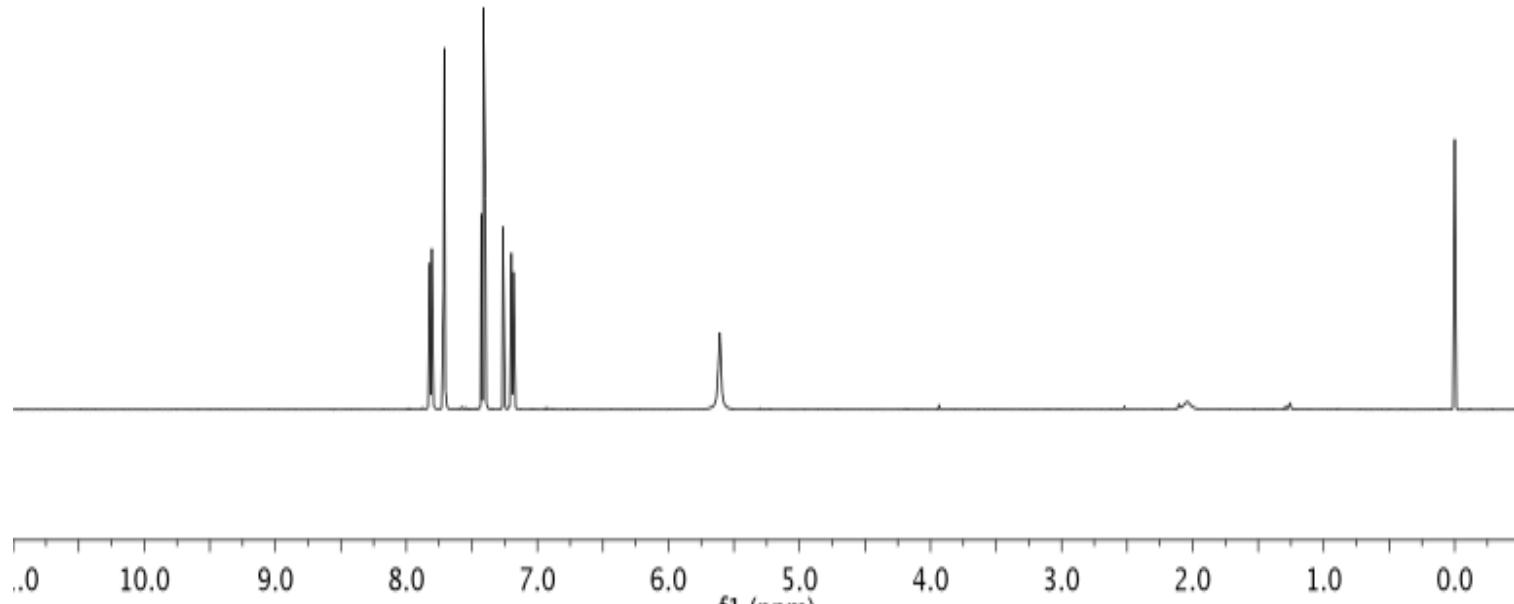
¹H NMR (500 MHz, CDCl₃) Spectrum of 1-(4-Hydroxyphenyl)ethanone (2j)



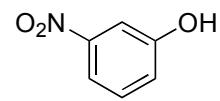
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 1-(4-Hydroxyphenyl)ethanone (2j)



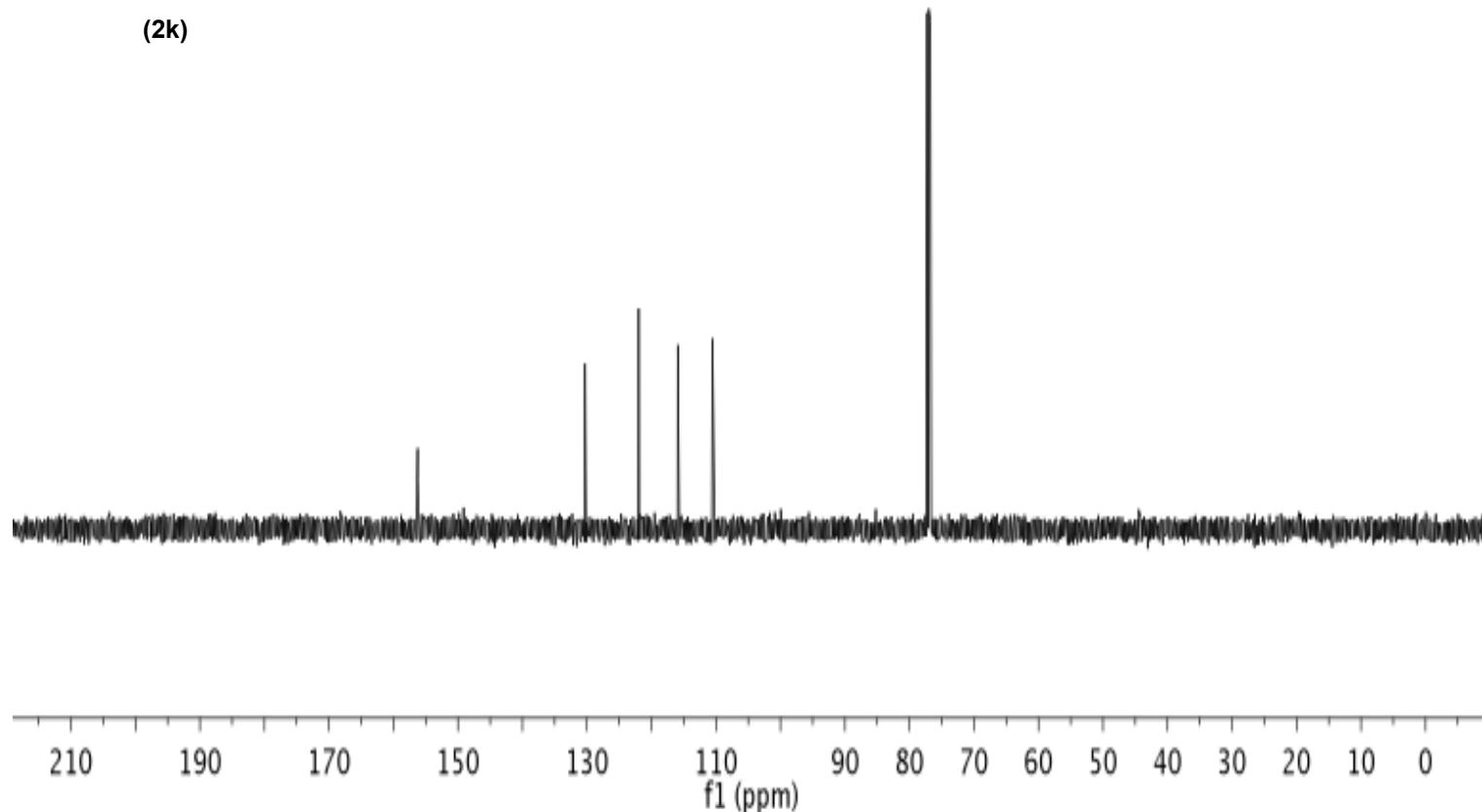
(2k)



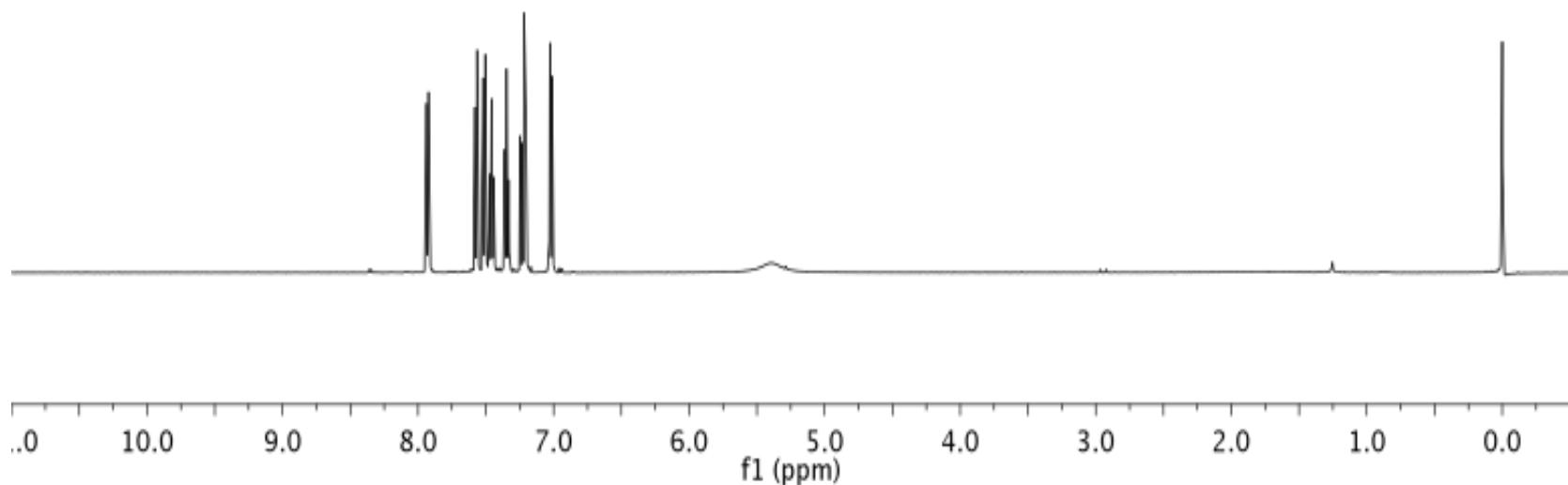
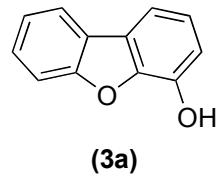
¹H NMR (500 MHz, CDCl₃) Spectrum of 3-Nitrophenol (2k)



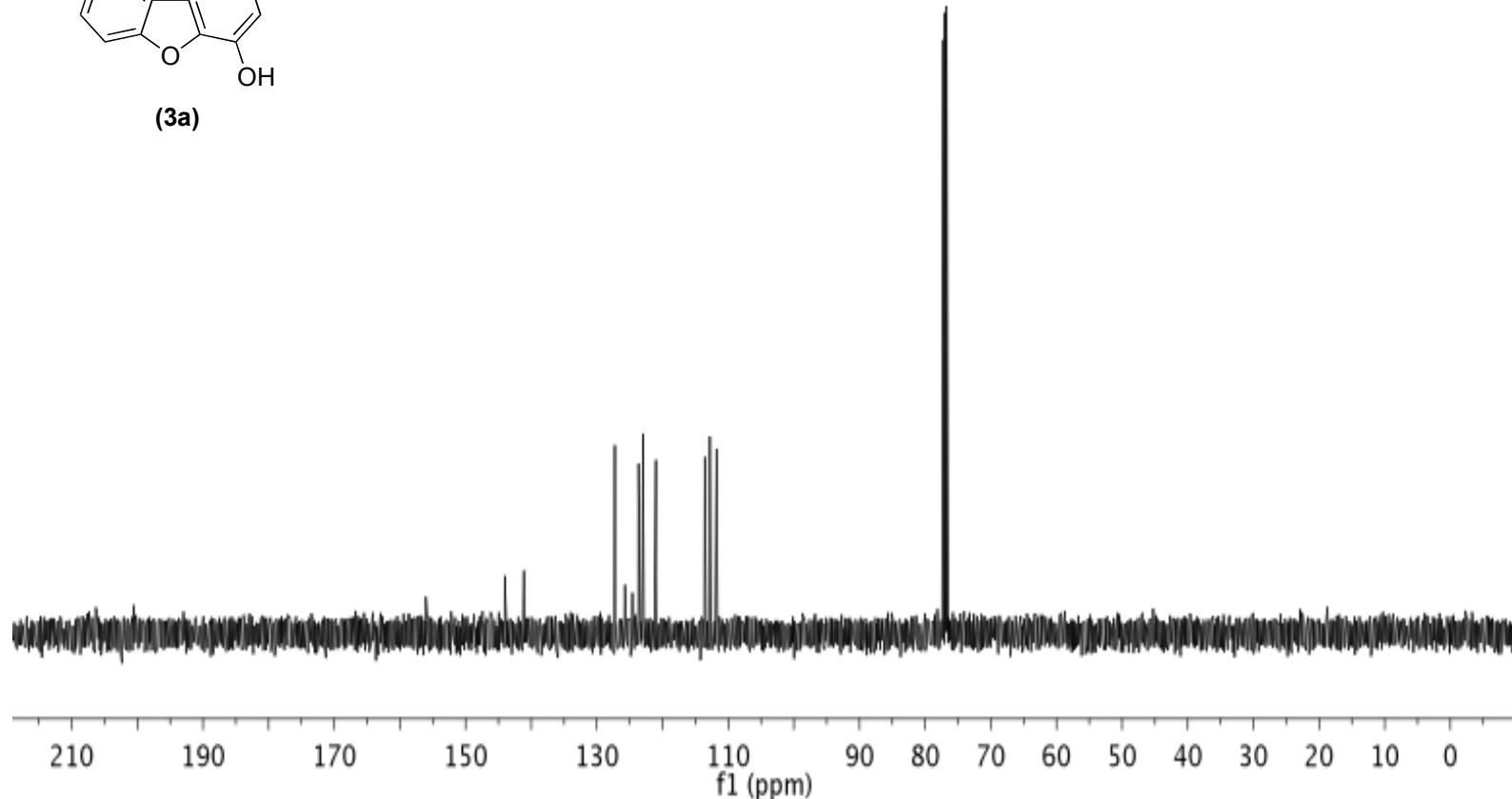
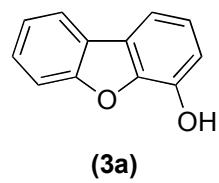
(2k)



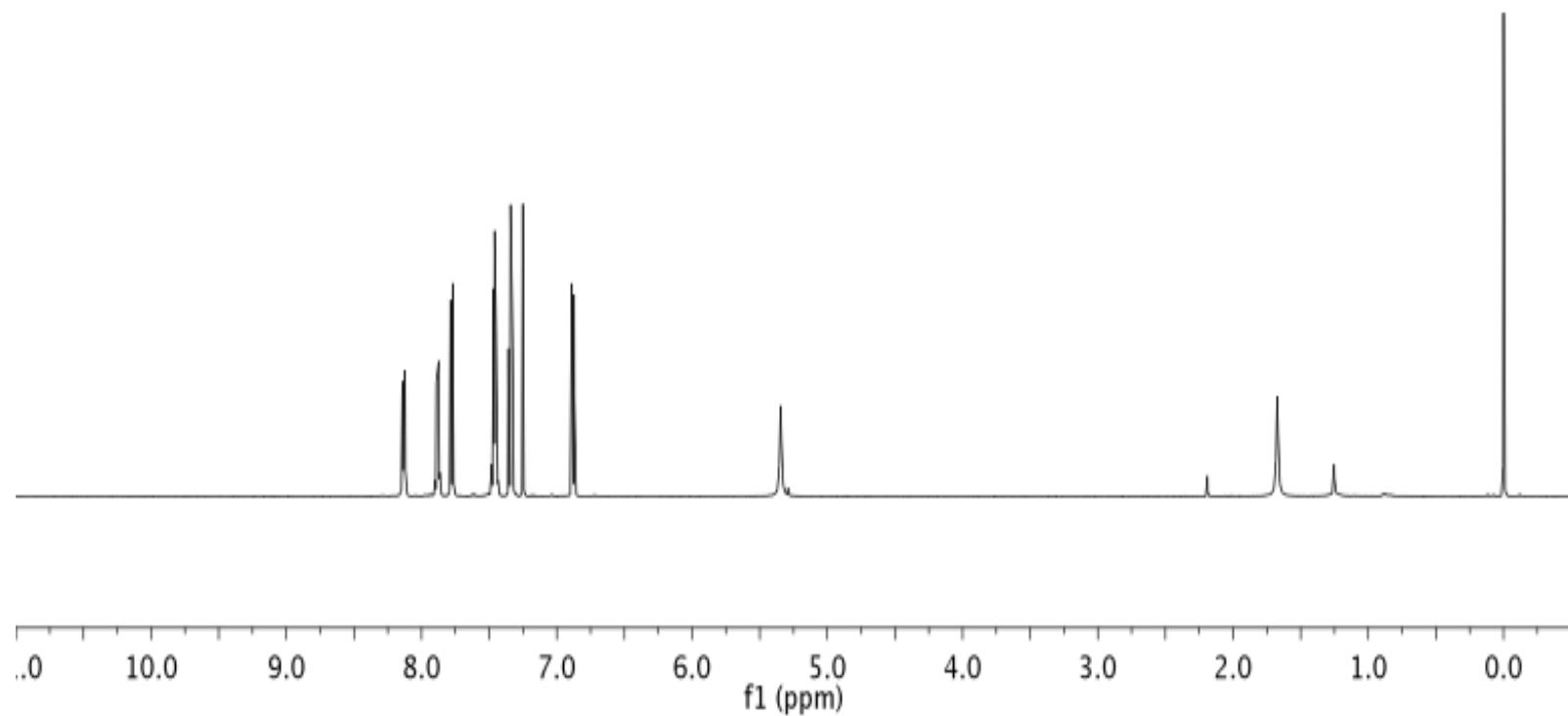
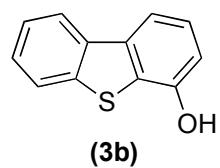
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 3-Nitrophenol (2k)



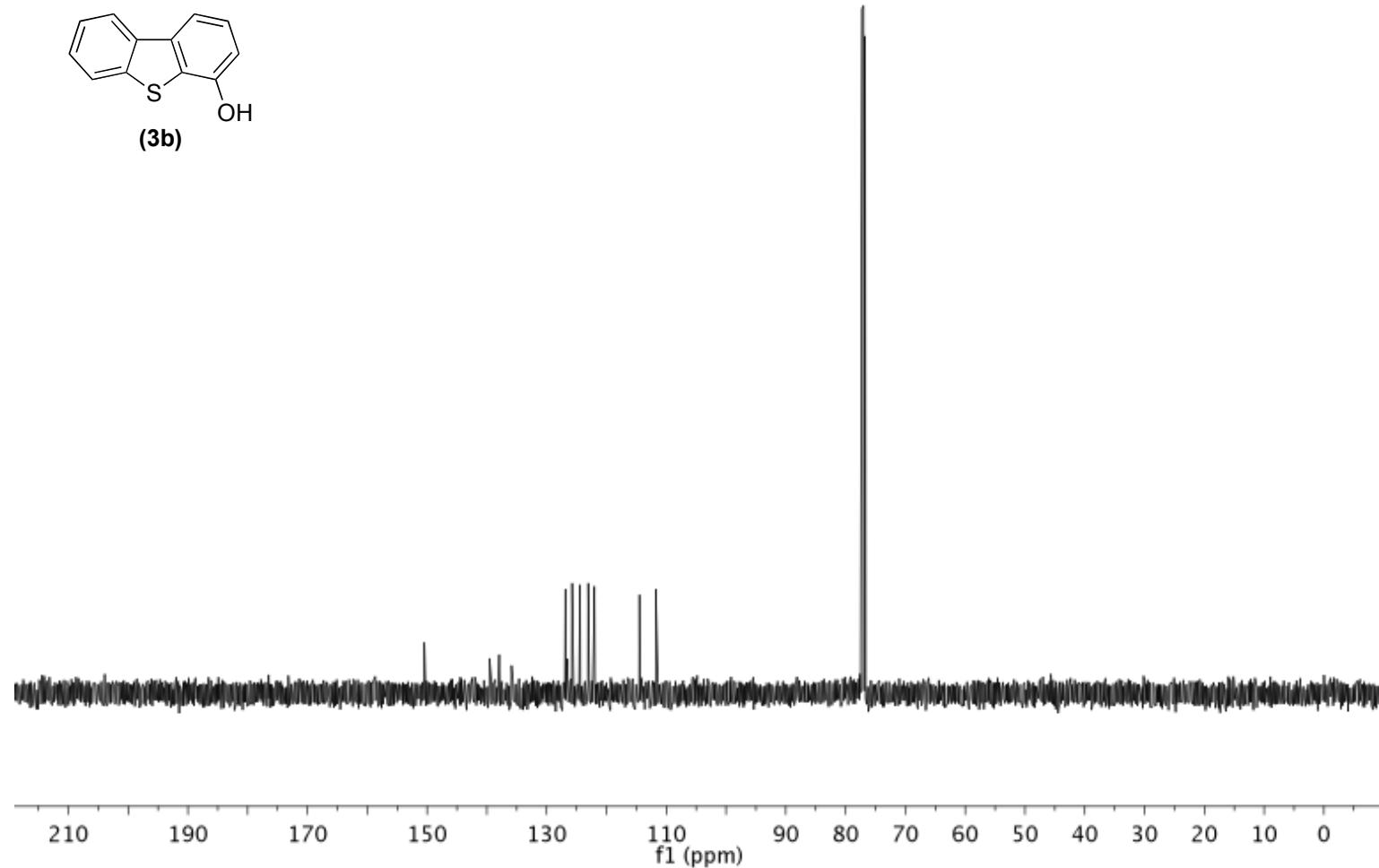
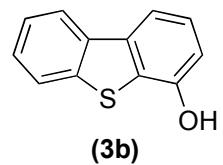
^1H NMR (500 MHz, CDCl_3) Spectrum of Dibenzo[*b,d*]furan-4-ol (3a)



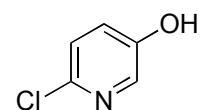
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Dibenzo[*b,d*]furan-4-ol (3a)



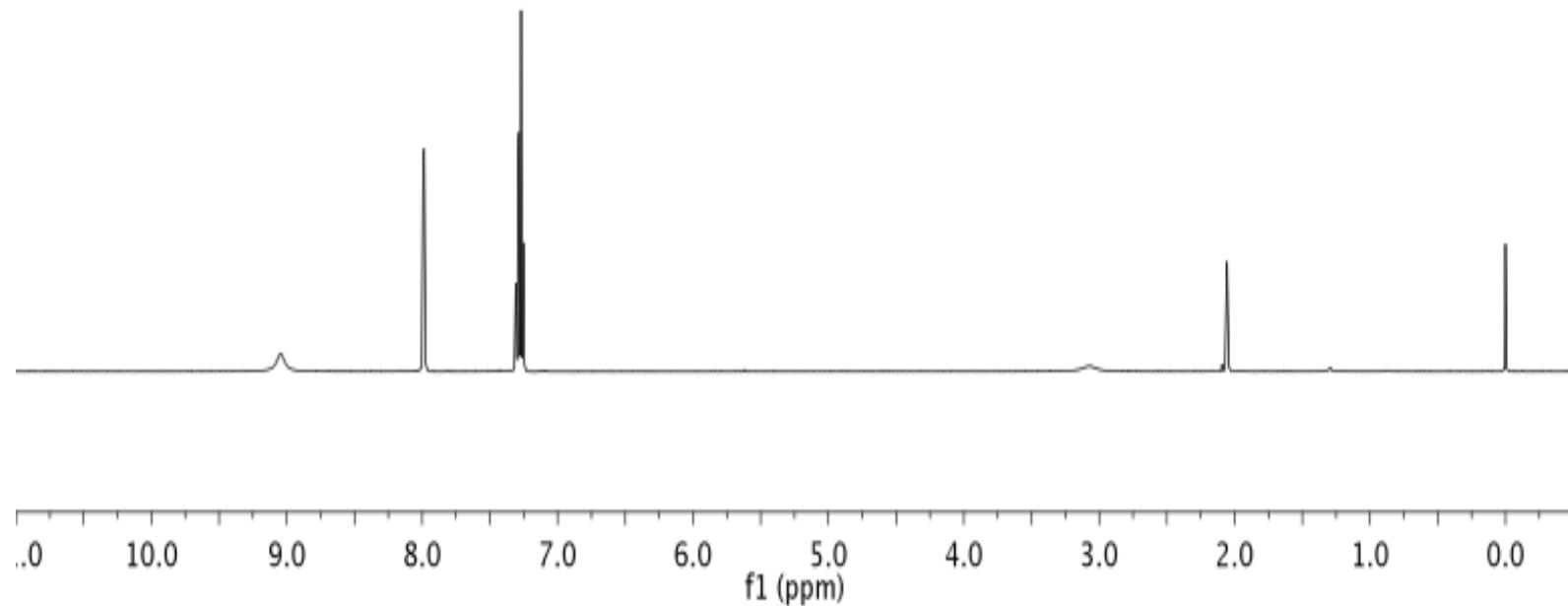
¹H NMR (500 MHz, CDCl₃) Spectrum of Dibenzo[*b,d*]thiophen-4-ol (3b)



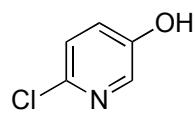
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of Dibenzo[*b,d*]thiophen-4-ol (3b)



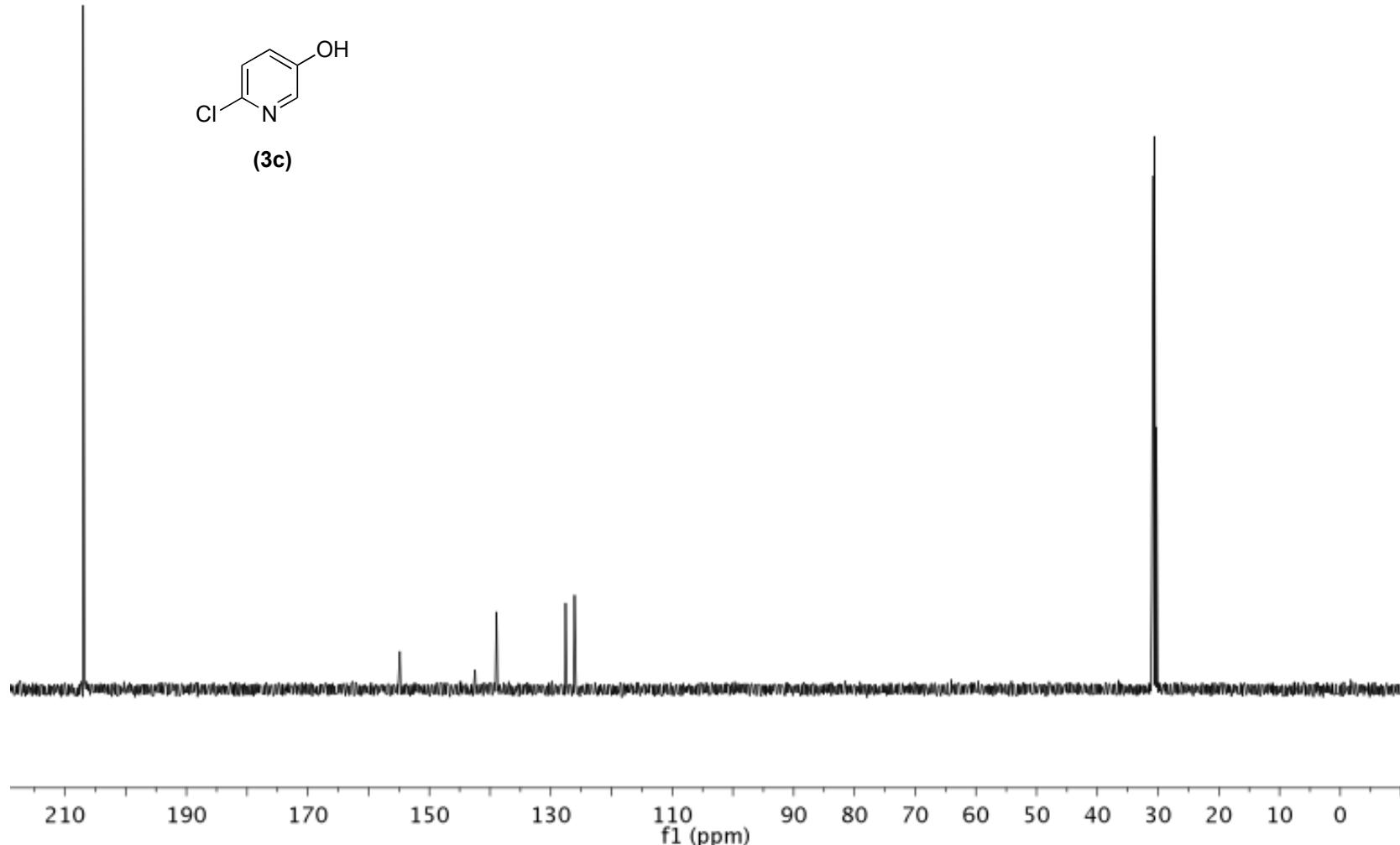
(3c)



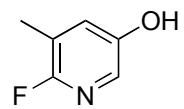
¹H NMR (500 MHz, acetone-*d*₆) Spectrum of 6-Chloropyridin-3-ol (3c)



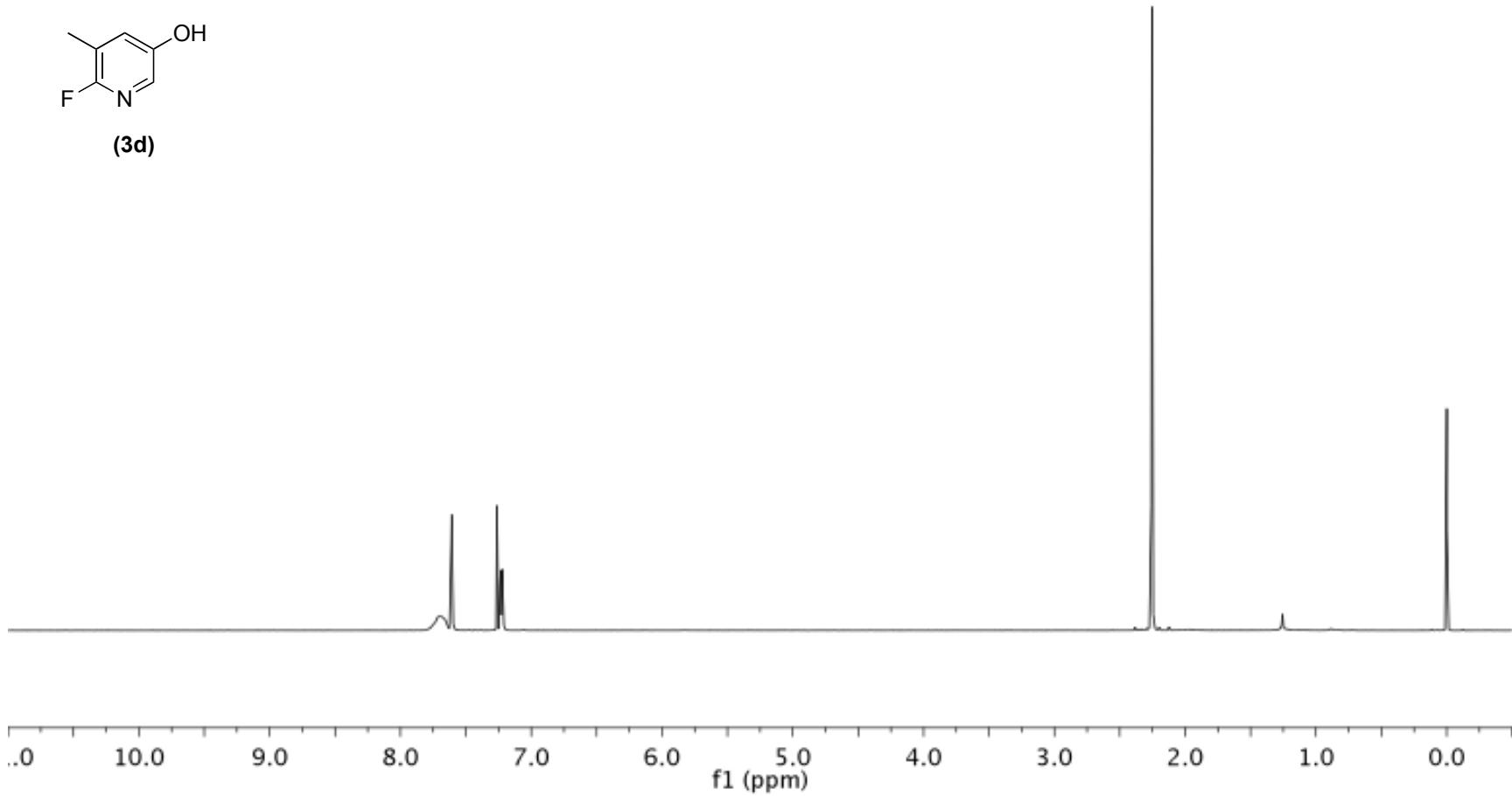
(3c)



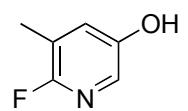
¹³C NMR (128.5 MHz, acetone-*d*₆) Spectrum of 6-Chloropyridin-3-ol (3c)



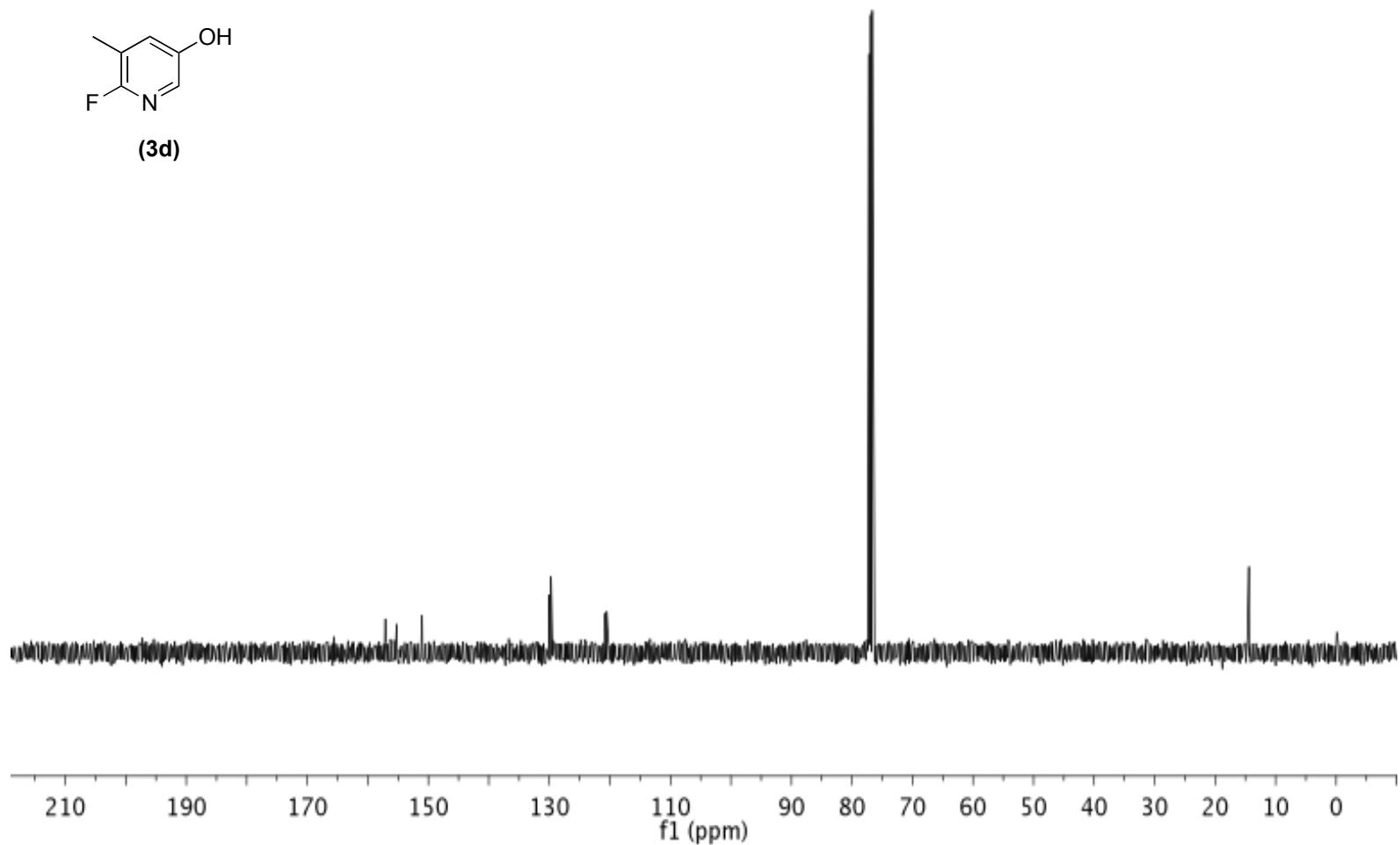
(3d)



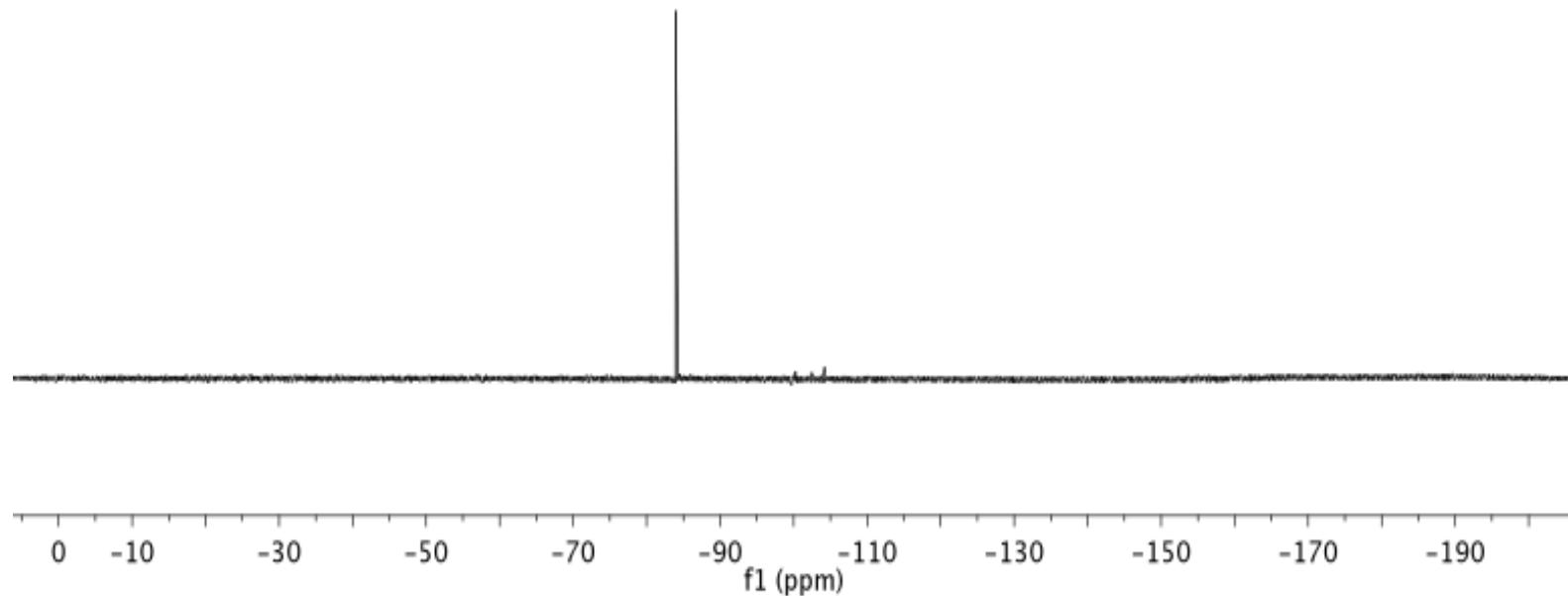
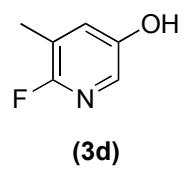
¹H NMR (500 MHz, CDCl₃) Spectrum of 6-Fluoro-5-methylpyridin-3-ol (3d)



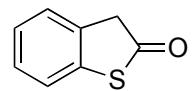
(3d)



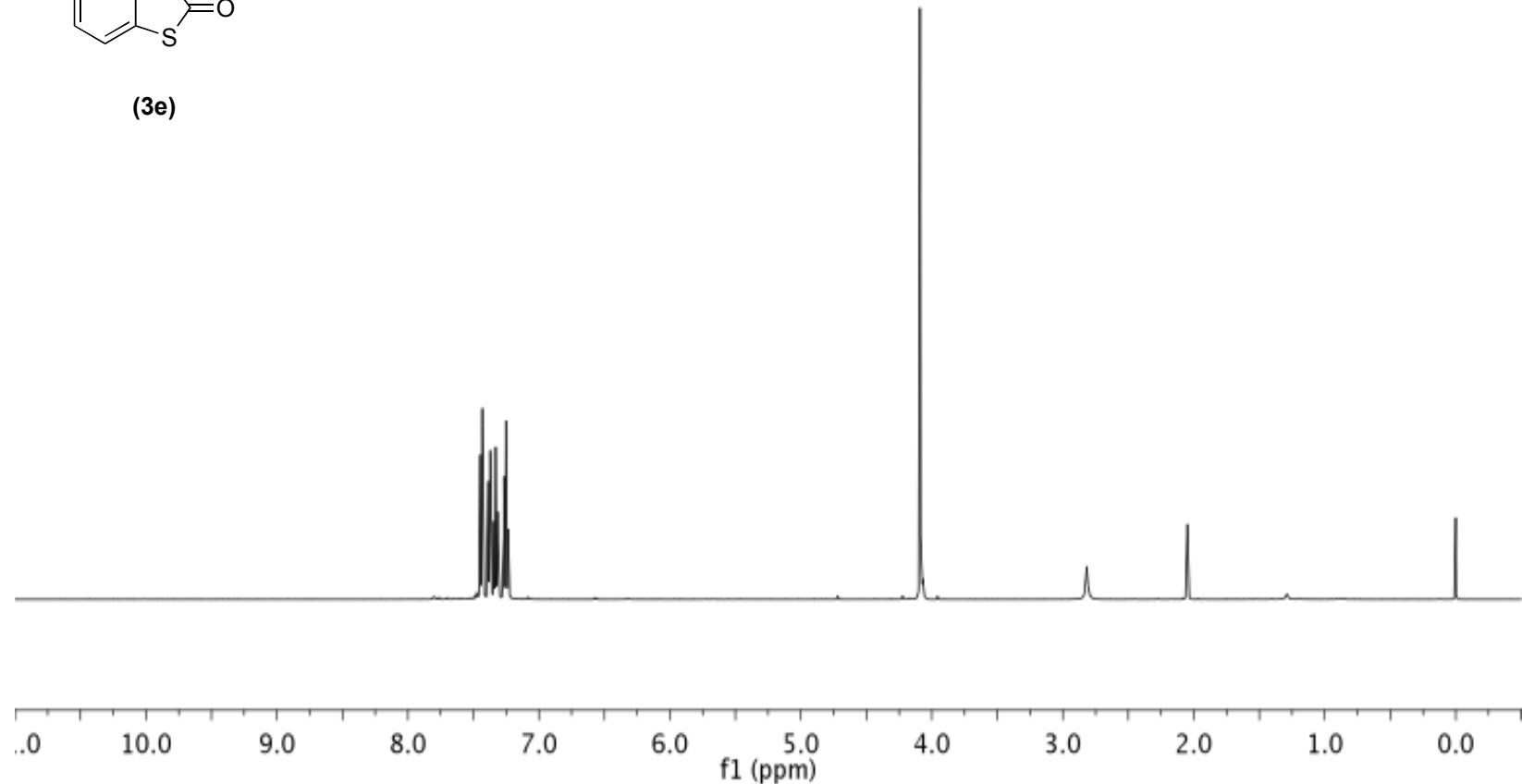
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 6-Fluoro-5-methylpyridin-3-ol (3d)



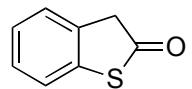
¹⁹F NMR (470.8 MHz, CDCl₃) Spectrum of 6-Fluoro-5-methylpyridin-3-ol (3d)



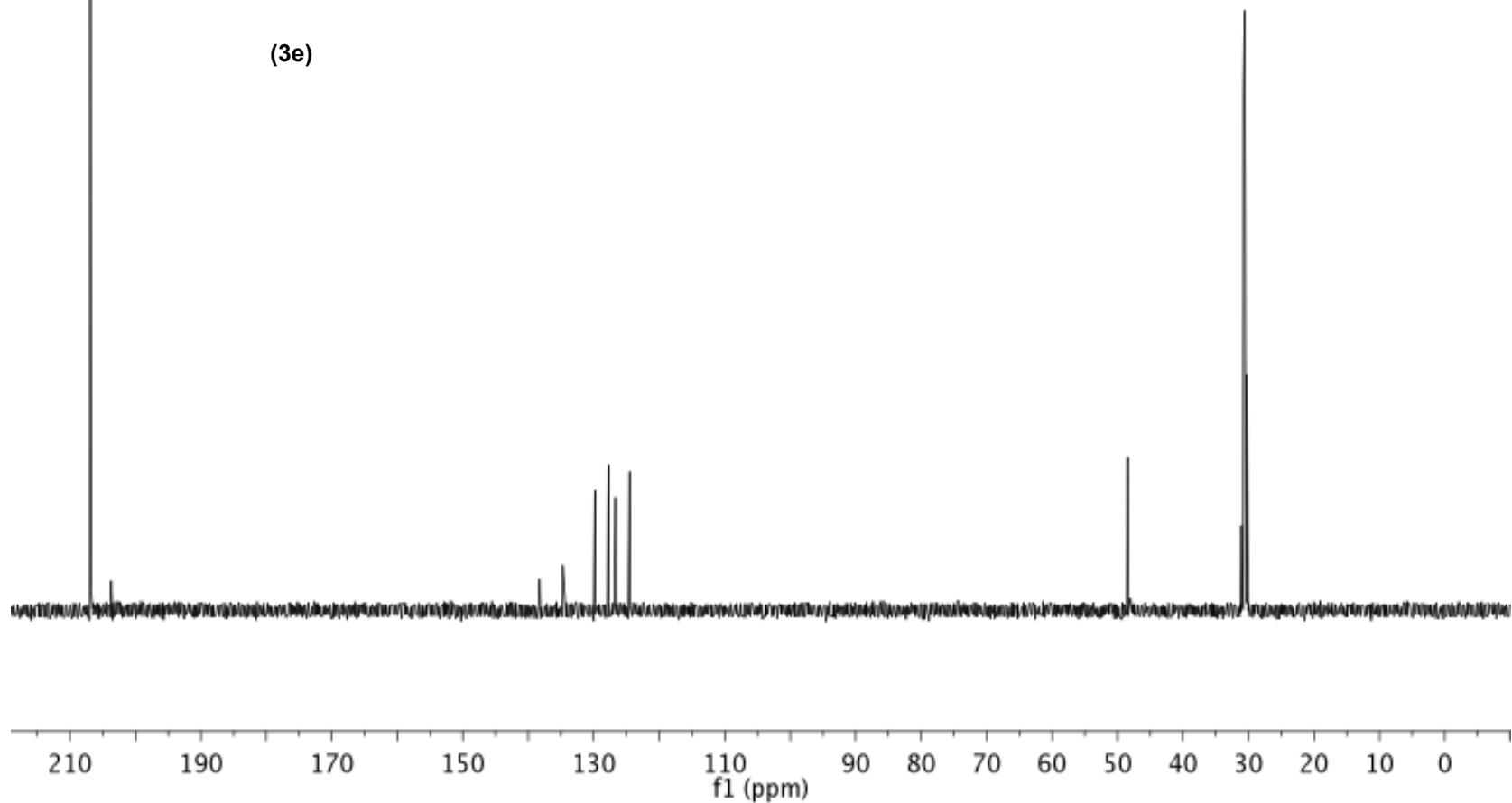
(3e)



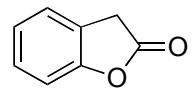
^1H NMR (500 MHz, acetone- d_6) Spectrum of Benzo[*b*]thiophen-2(*3H*)-one (3e)



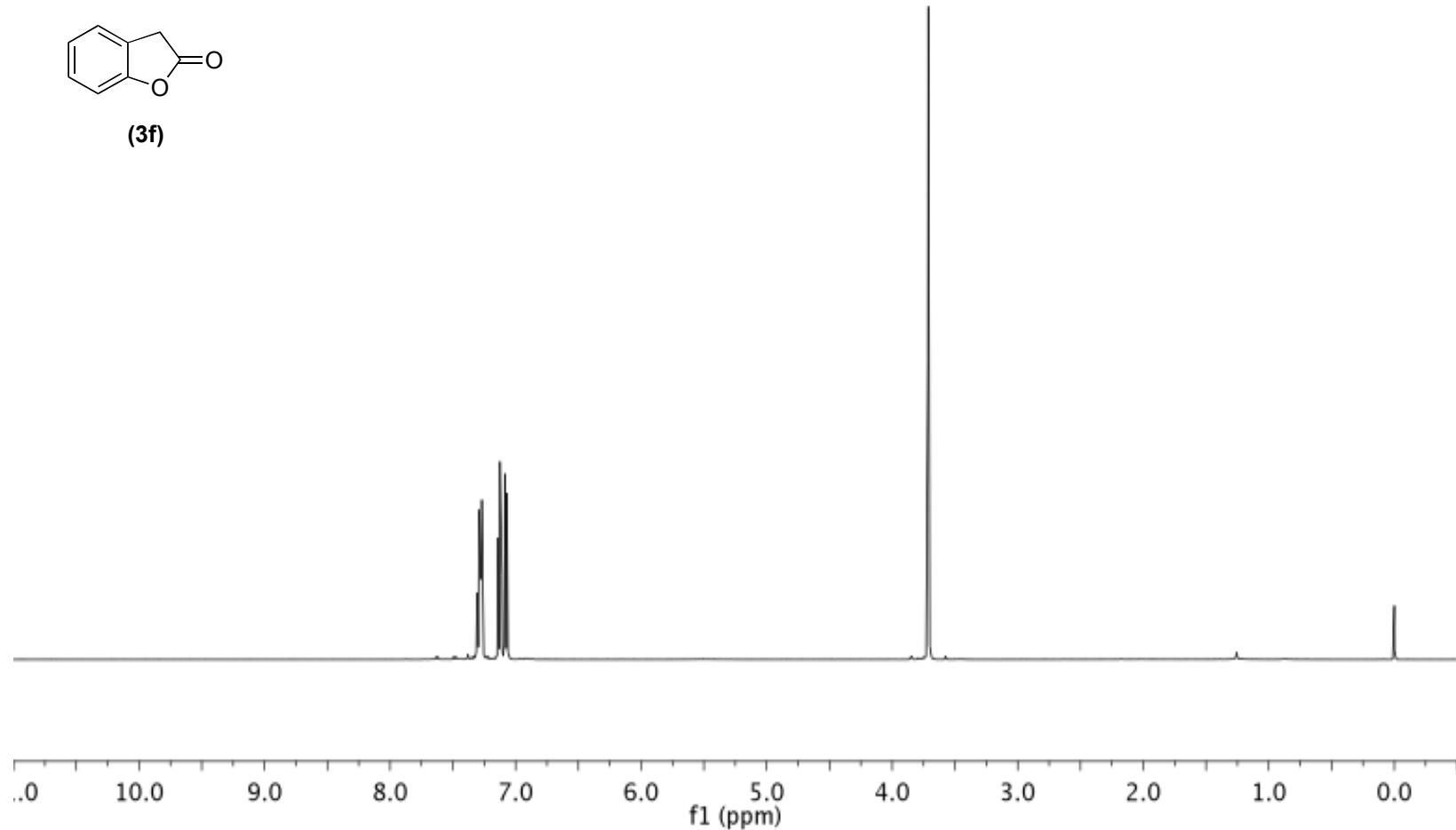
(3e)



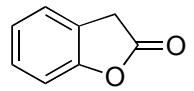
¹³C NMR (128.5 MHz, acetone-*d*₆) Spectrum of Benzo[*b*]thiophen-2(*3H*)-one (3e)



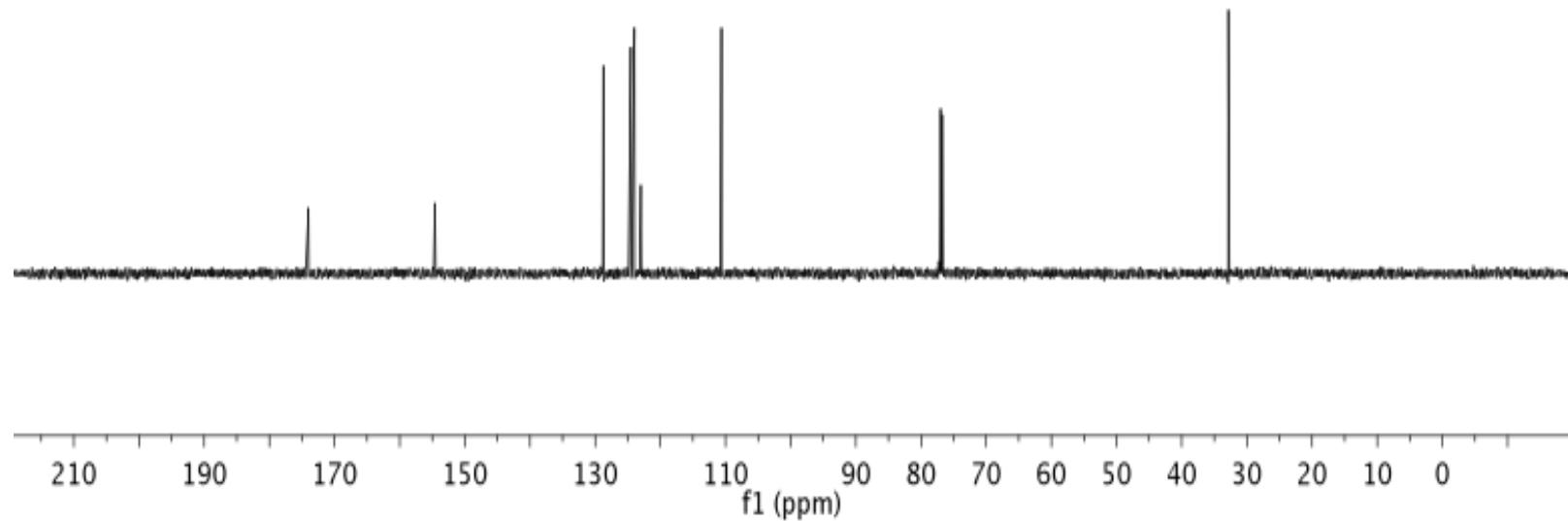
(3f)



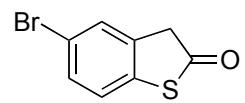
^1H NMR (500 MHz, CDCl_3) Spectrum of Benzofuran-2(*3H*)-one (3f)



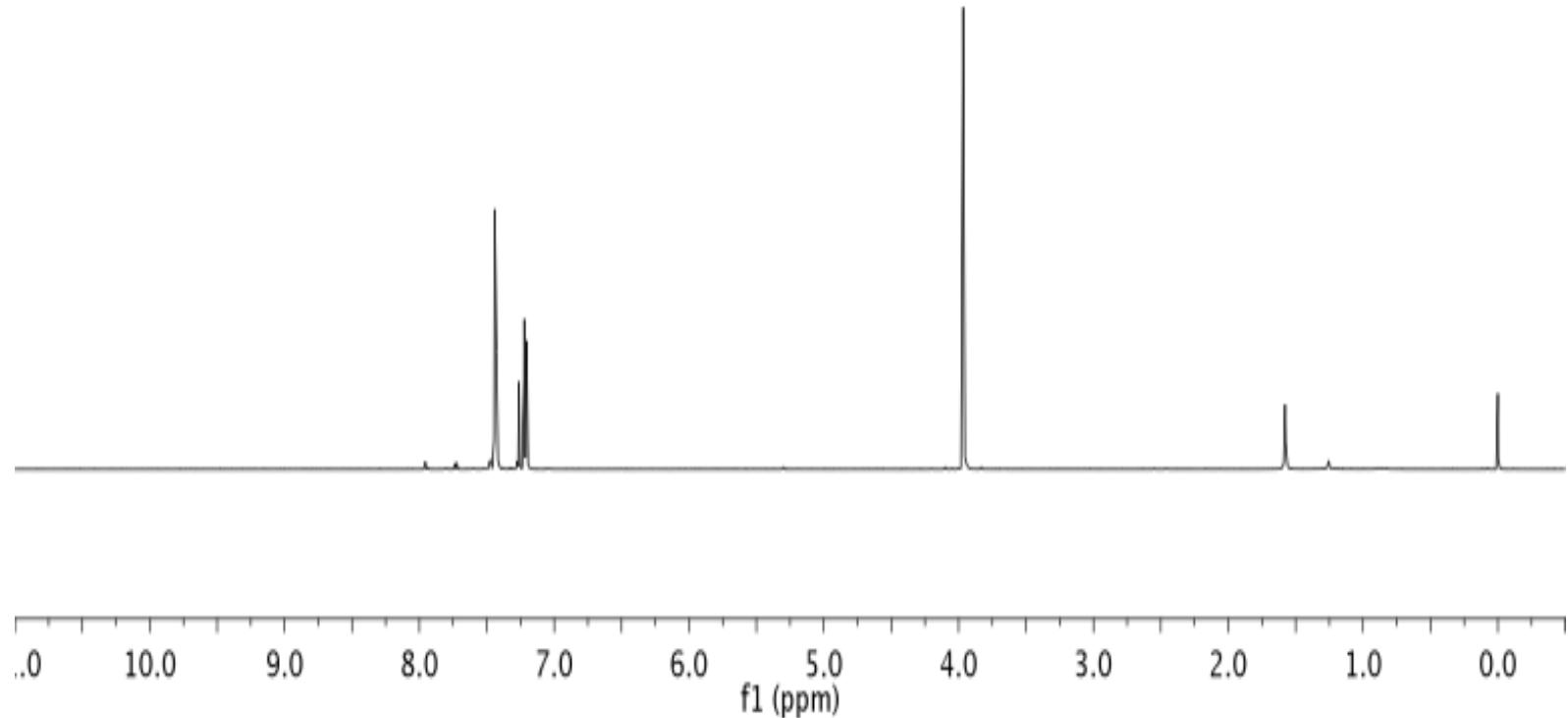
(3f)



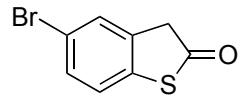
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Benzofuran-2(3H)-one (3f)



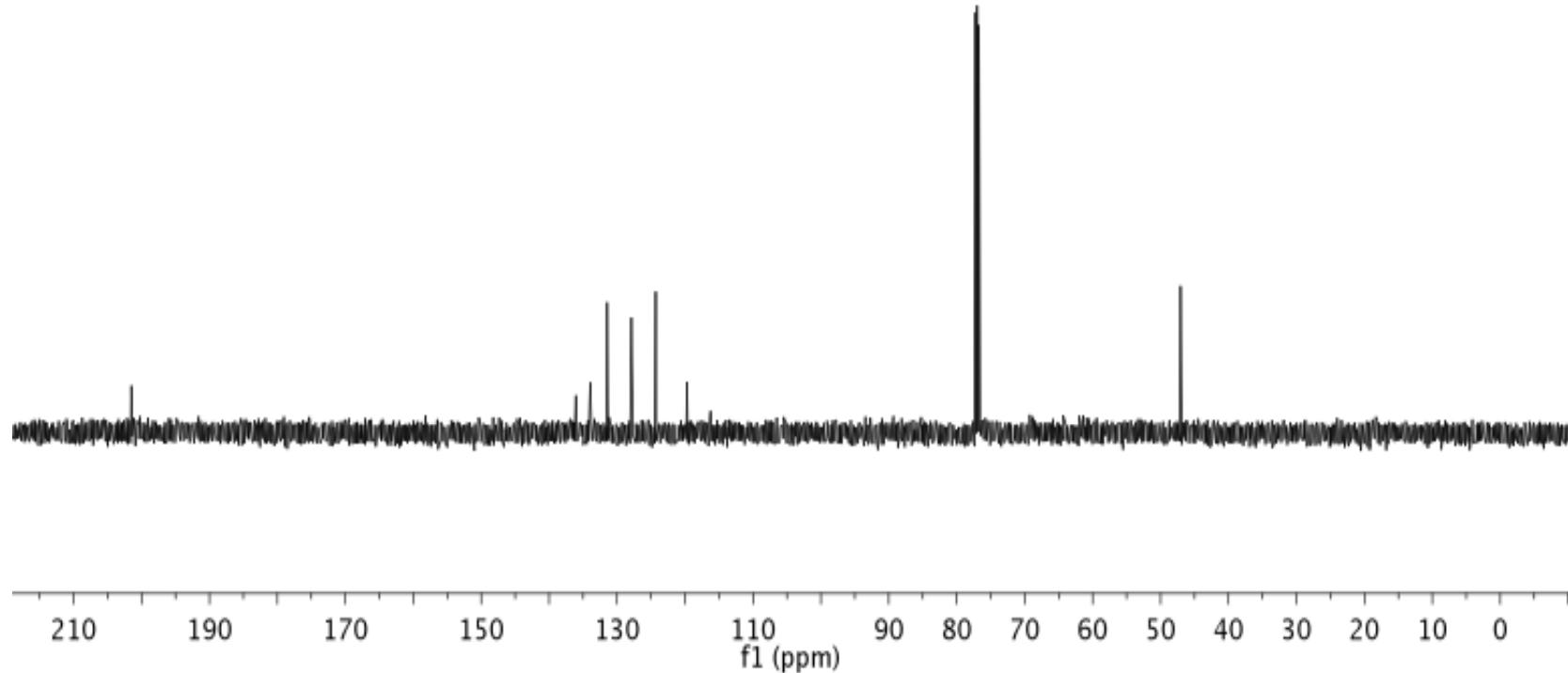
(3g)



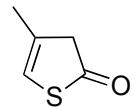
¹H NMR (500 MHz, CDCl₃) Spectrum of 5-Bromobenzo[*b*]thiophen-2(*3H*)-one (3g)



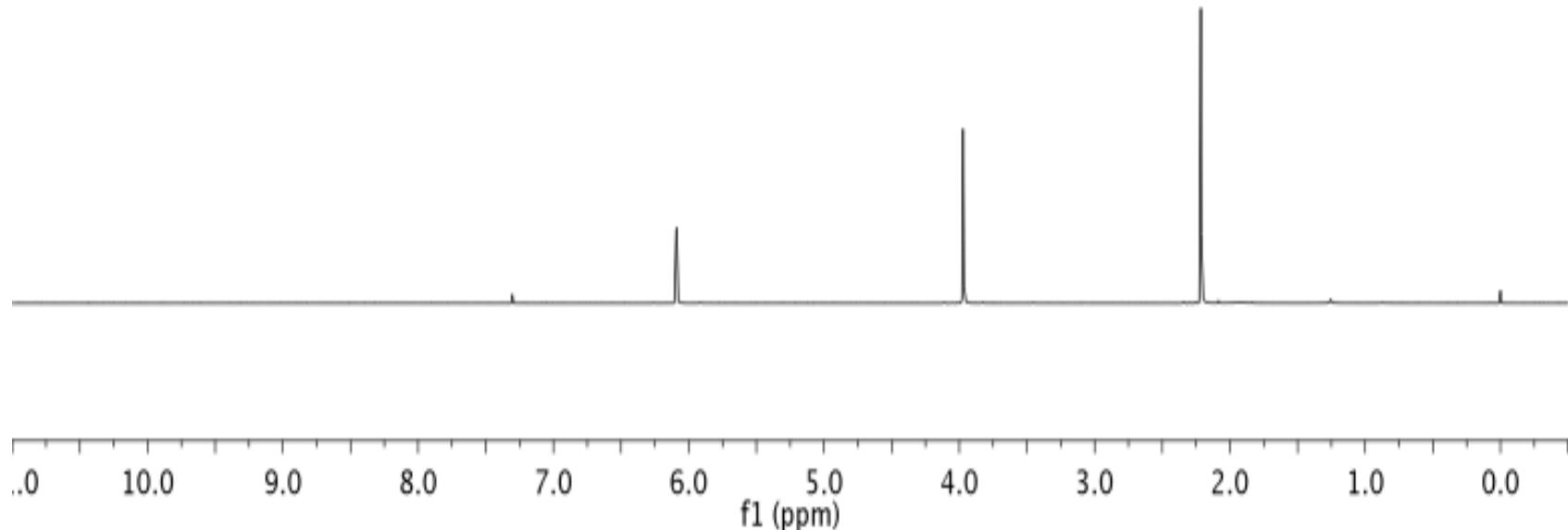
(3g)



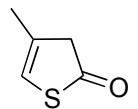
^{13}C NMR (128.5 MHz, CDCl₃) Spectrum of 5-Bromobenzo[*b*]thiophen-2(*3H*)-one (3g)



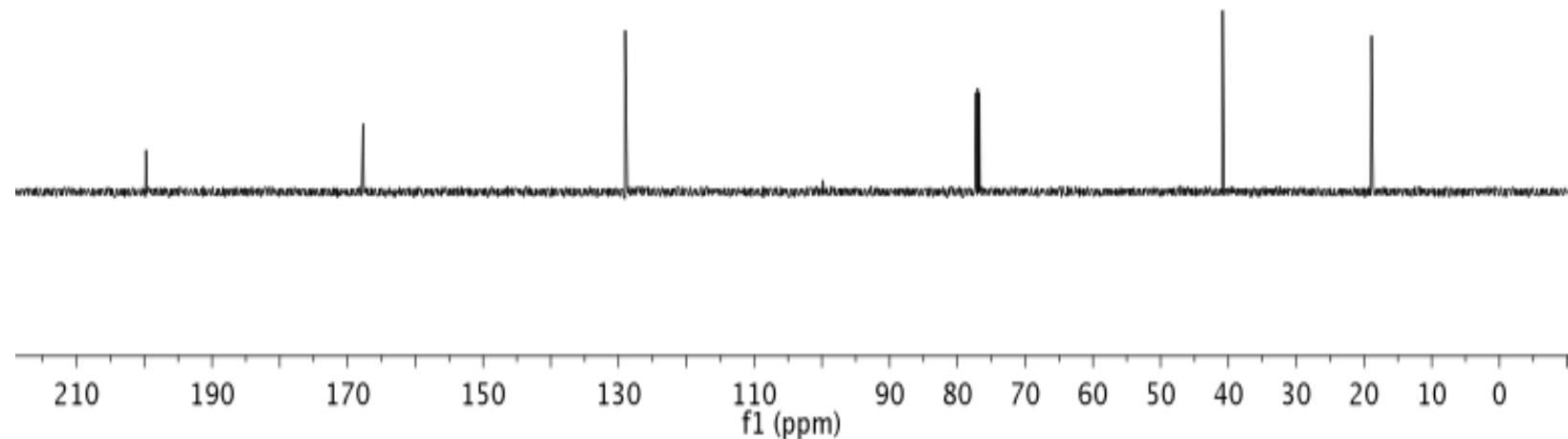
(3h)



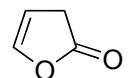
^1H NMR (500 MHz, CDCl_3) Spectrum of 4-Methylthiophen-2(3*H*)-one (3h)



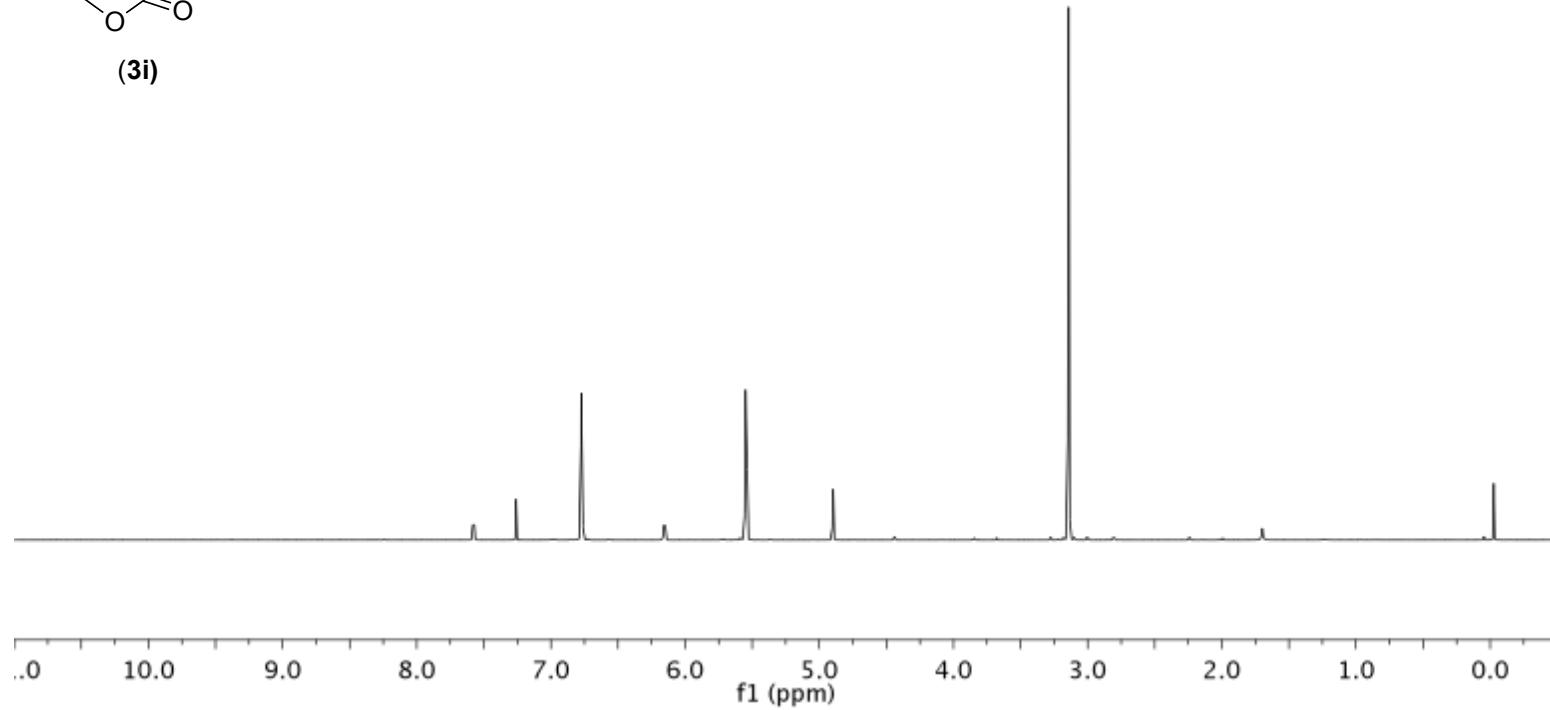
(3h)



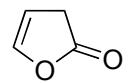
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 4-Methylthiophen-2(3*H*)-one (3h)



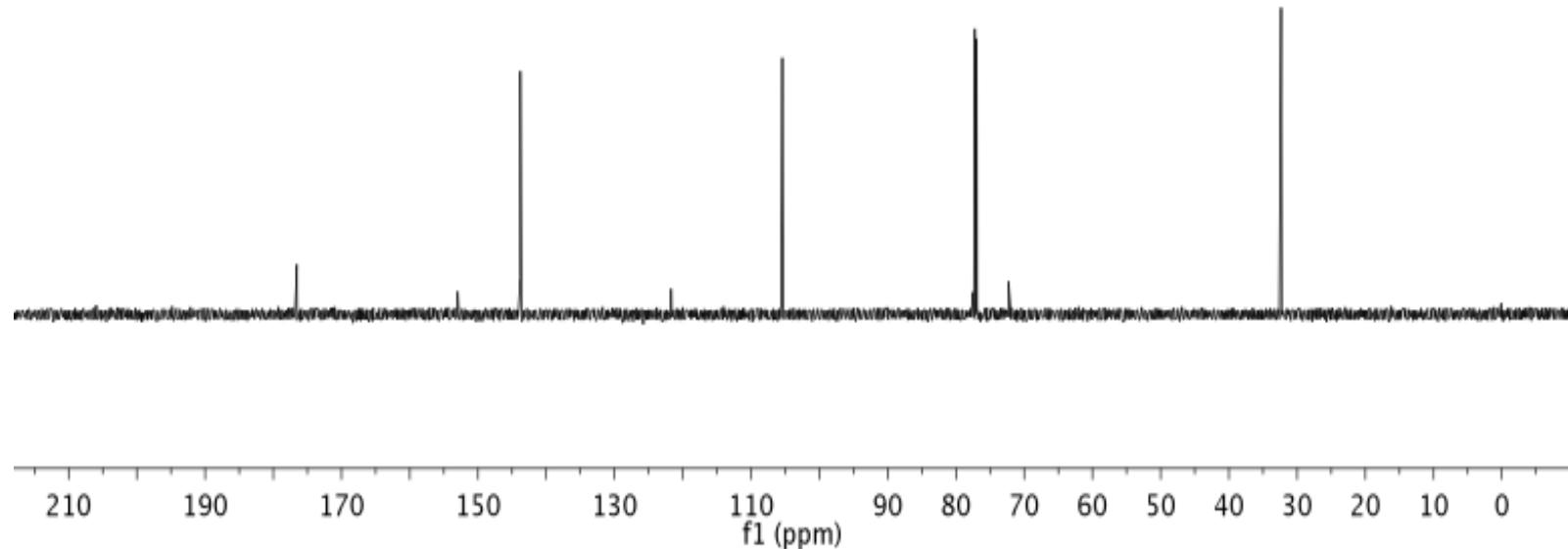
(3i)



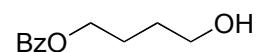
^1H NMR (500 MHz, CDCl_3) Spectrum of Furan-2(*3H*)-one (3i)



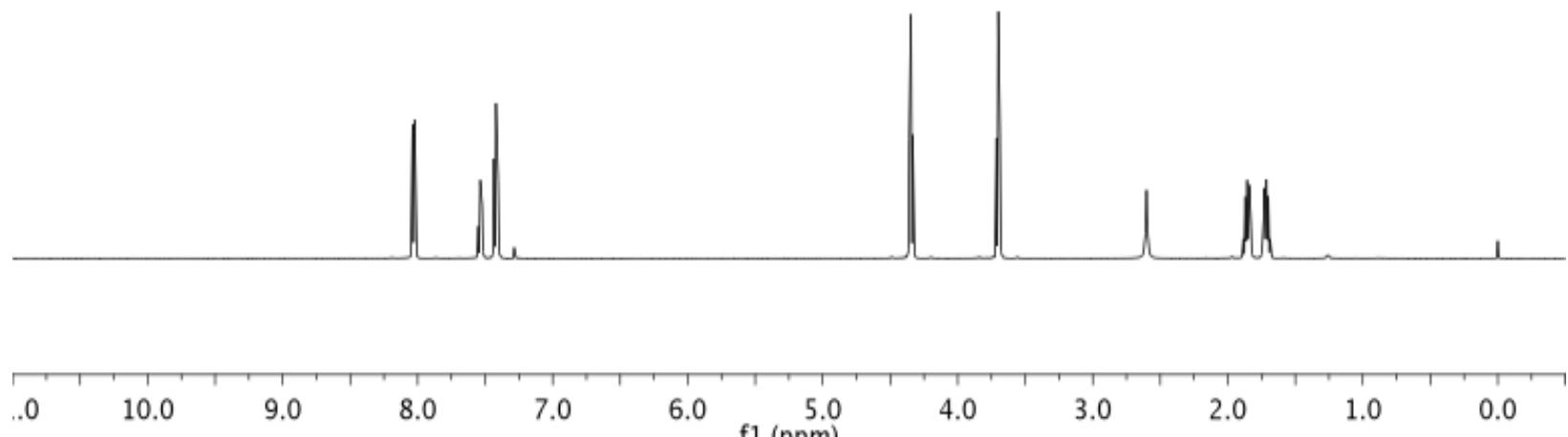
(3i)



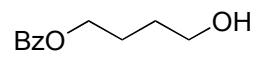
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Furan-2(3*H*)-one (3i)



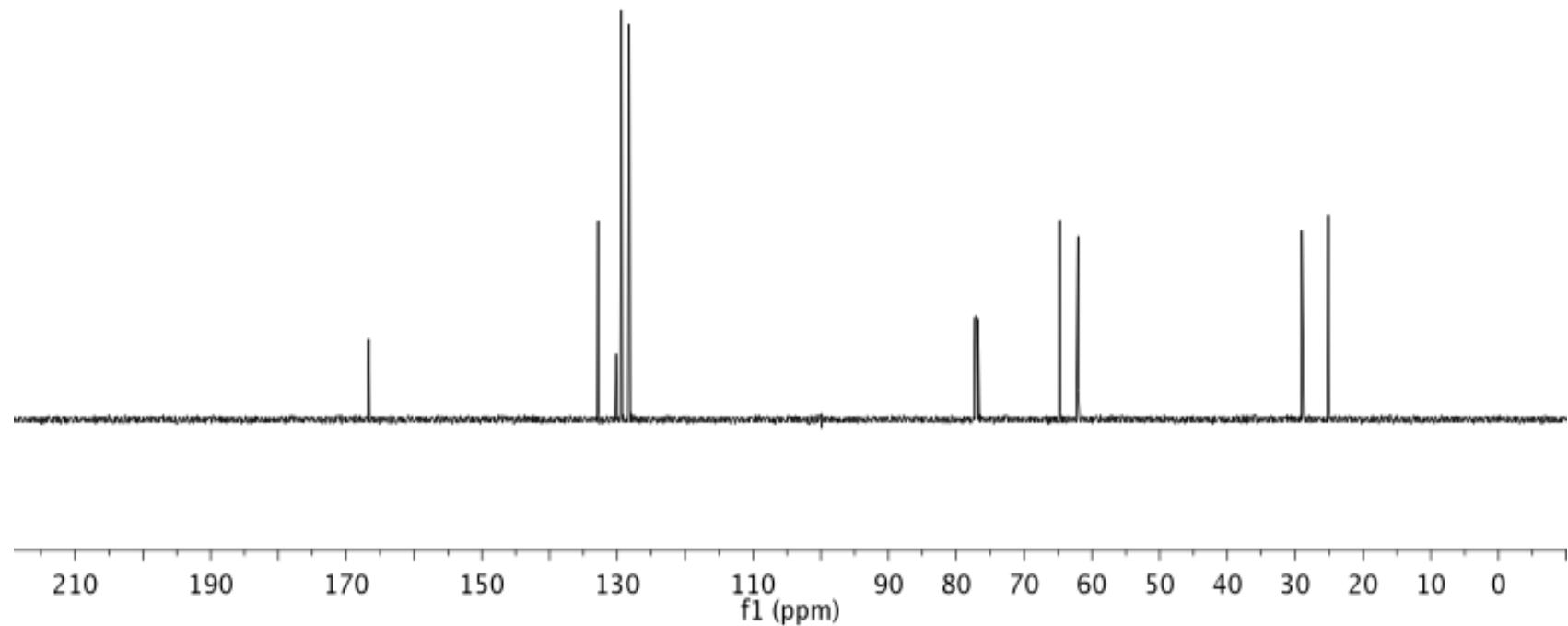
(4a)



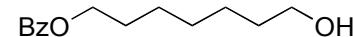
¹H NMR (500 MHz, CDCl₃) Spectrum of 4-hydroxybutyl benzoate (4a)



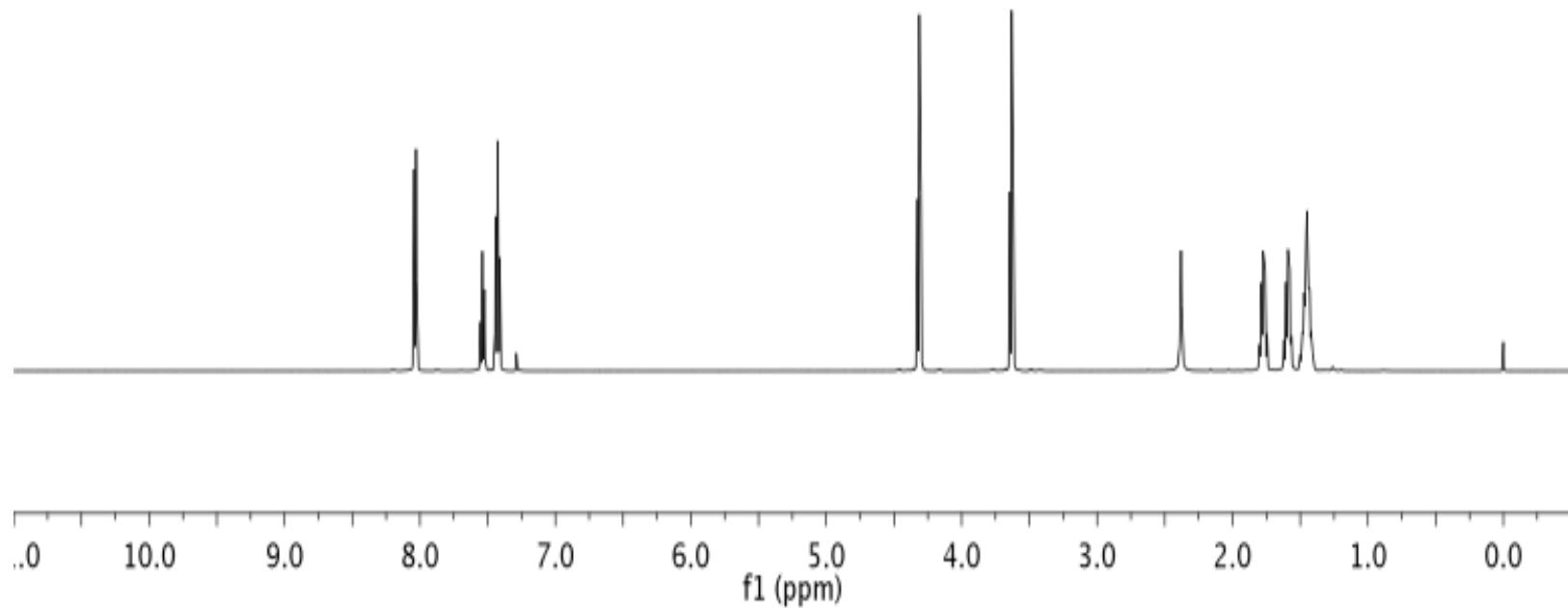
(4a)



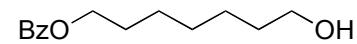
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of 4-Hydroxybutyl benzoate (4a)



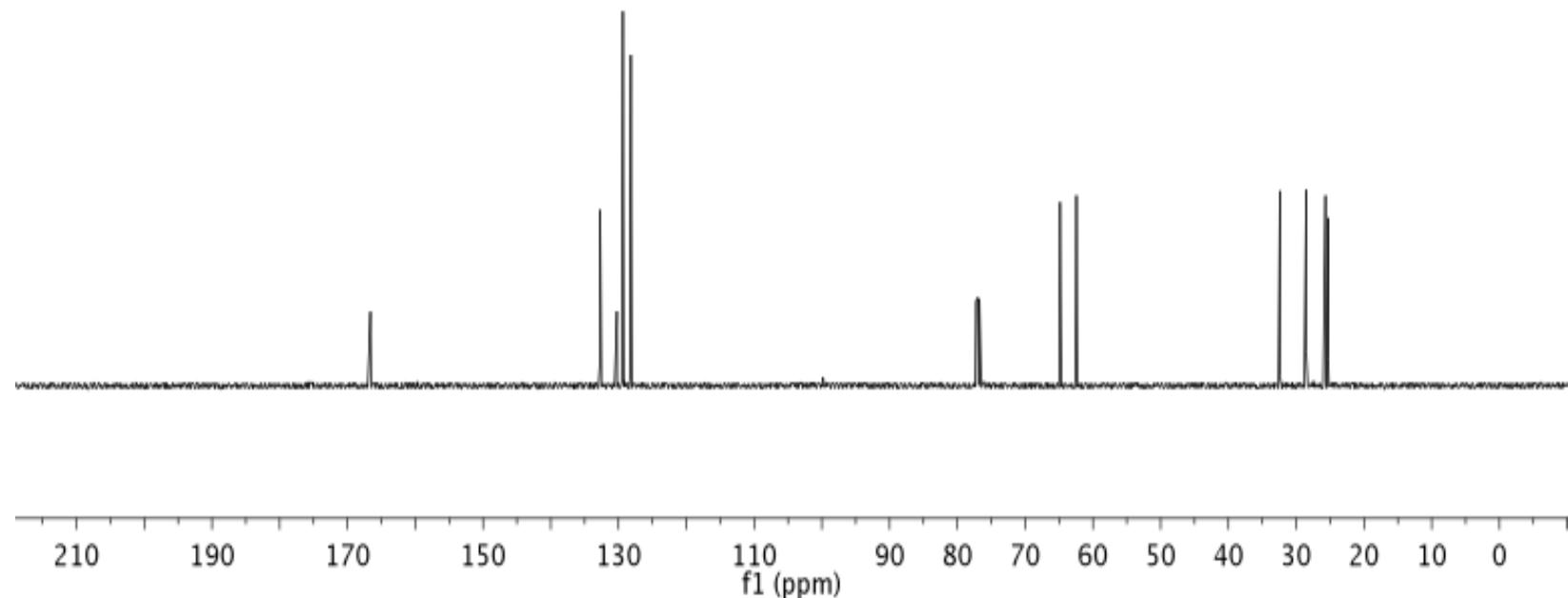
(4b)



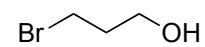
¹H NMR (500 MHz, CDCl₃) Spectrum of 7-Hydroxyheptylbenzoate (4b)



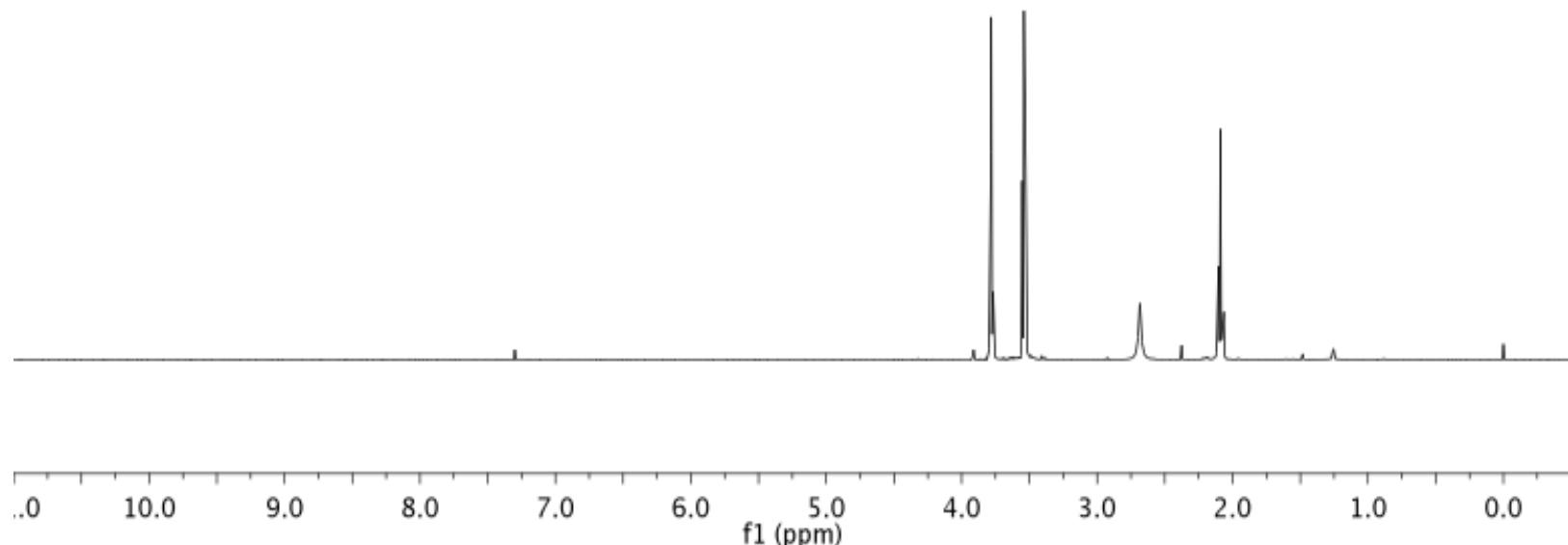
(4b)



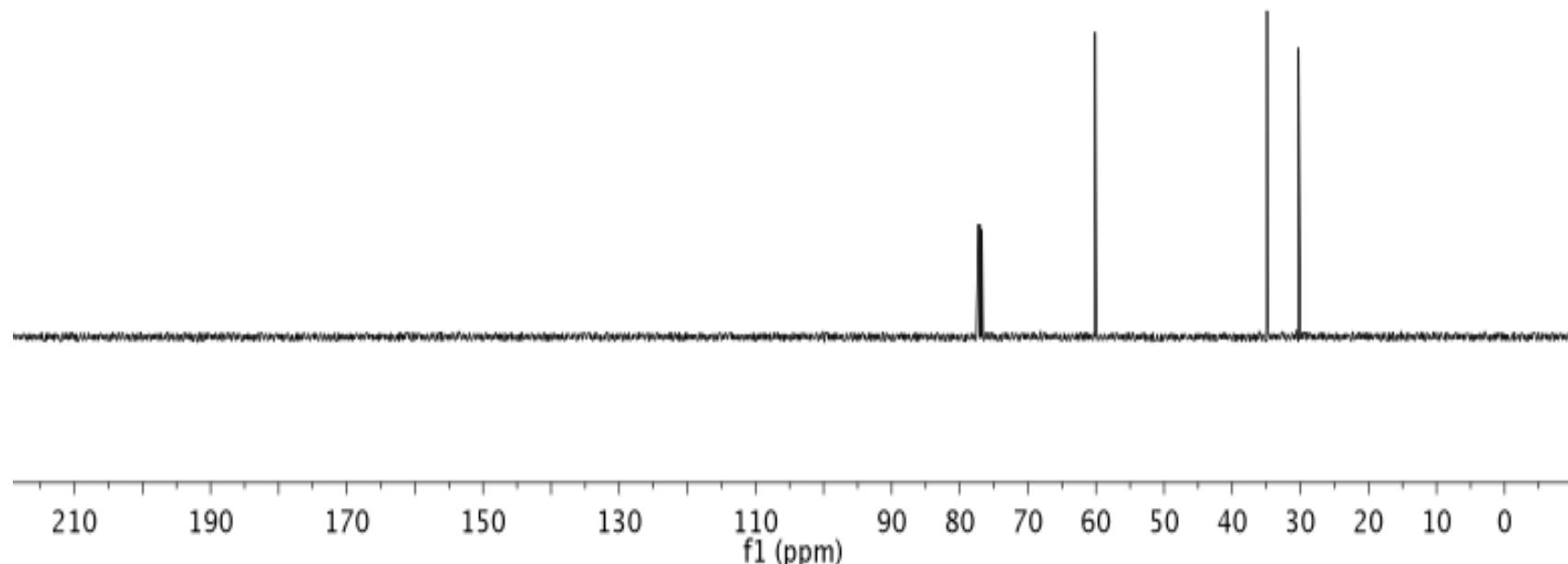
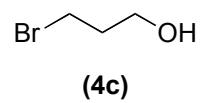
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 7-Hydroxyheptylbenzoate (4b)



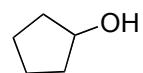
(4c)



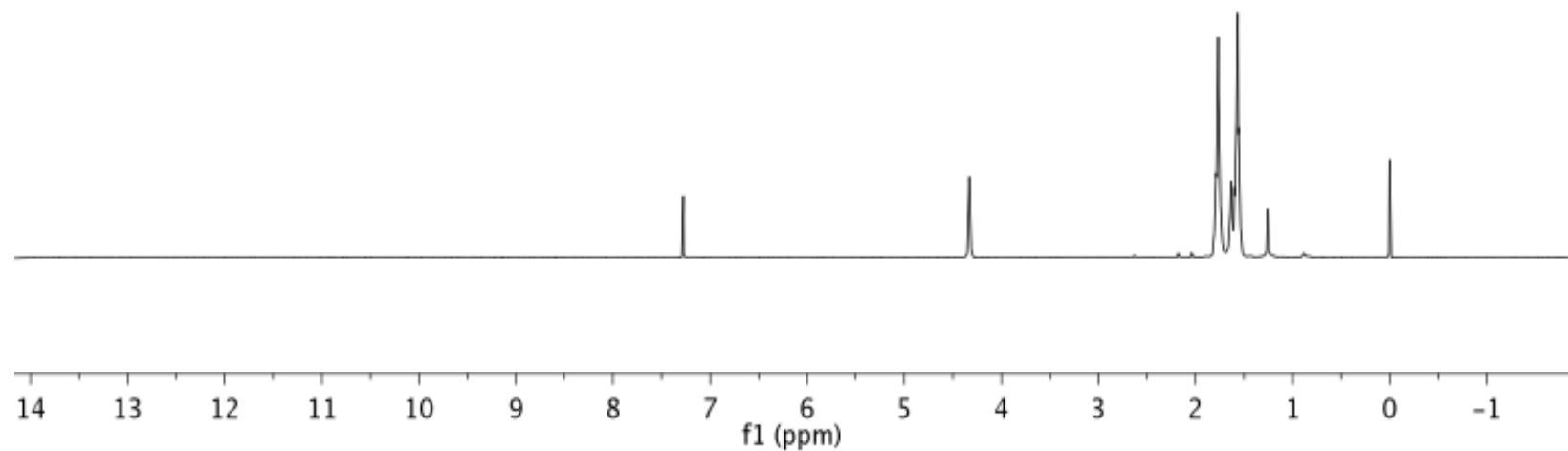
¹H NMR (500 MHz, CDCl₃) Spectrum of 3-Bromopropan-1-ol (4c)



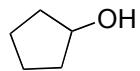
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 3-Bromopropan-1-ol (4c)



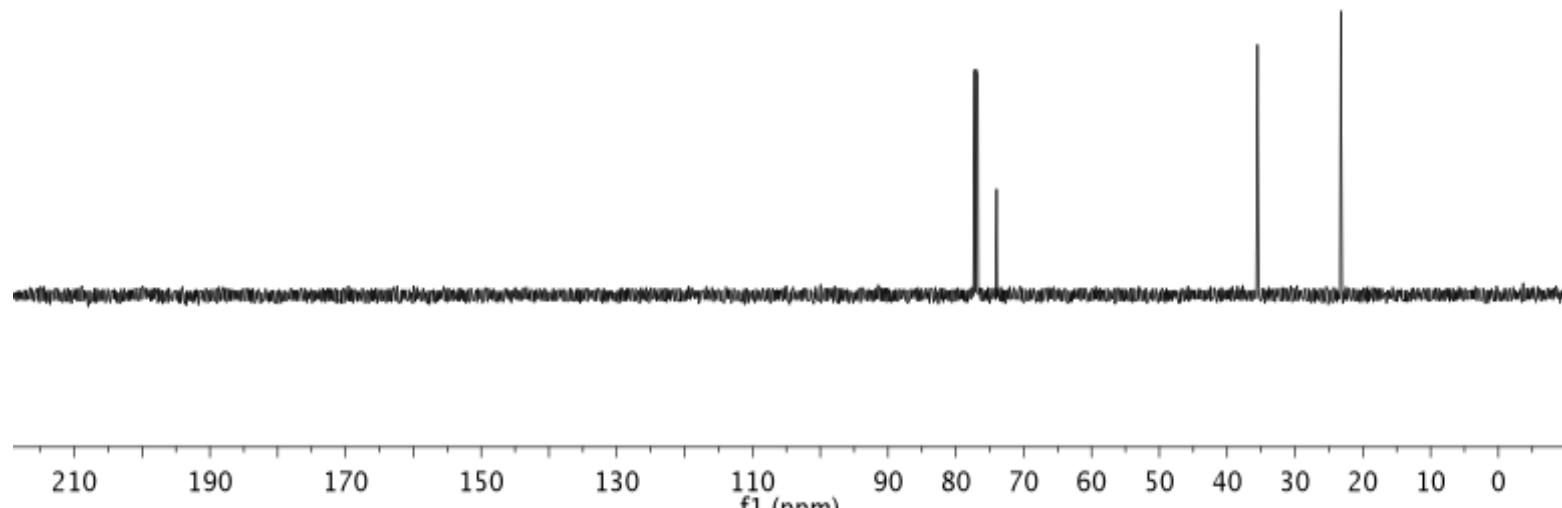
(4d)



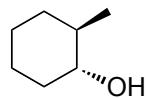
¹H NMR (500 MHz, CDCl₃) Spectrum of Cyclopentanol (4d)



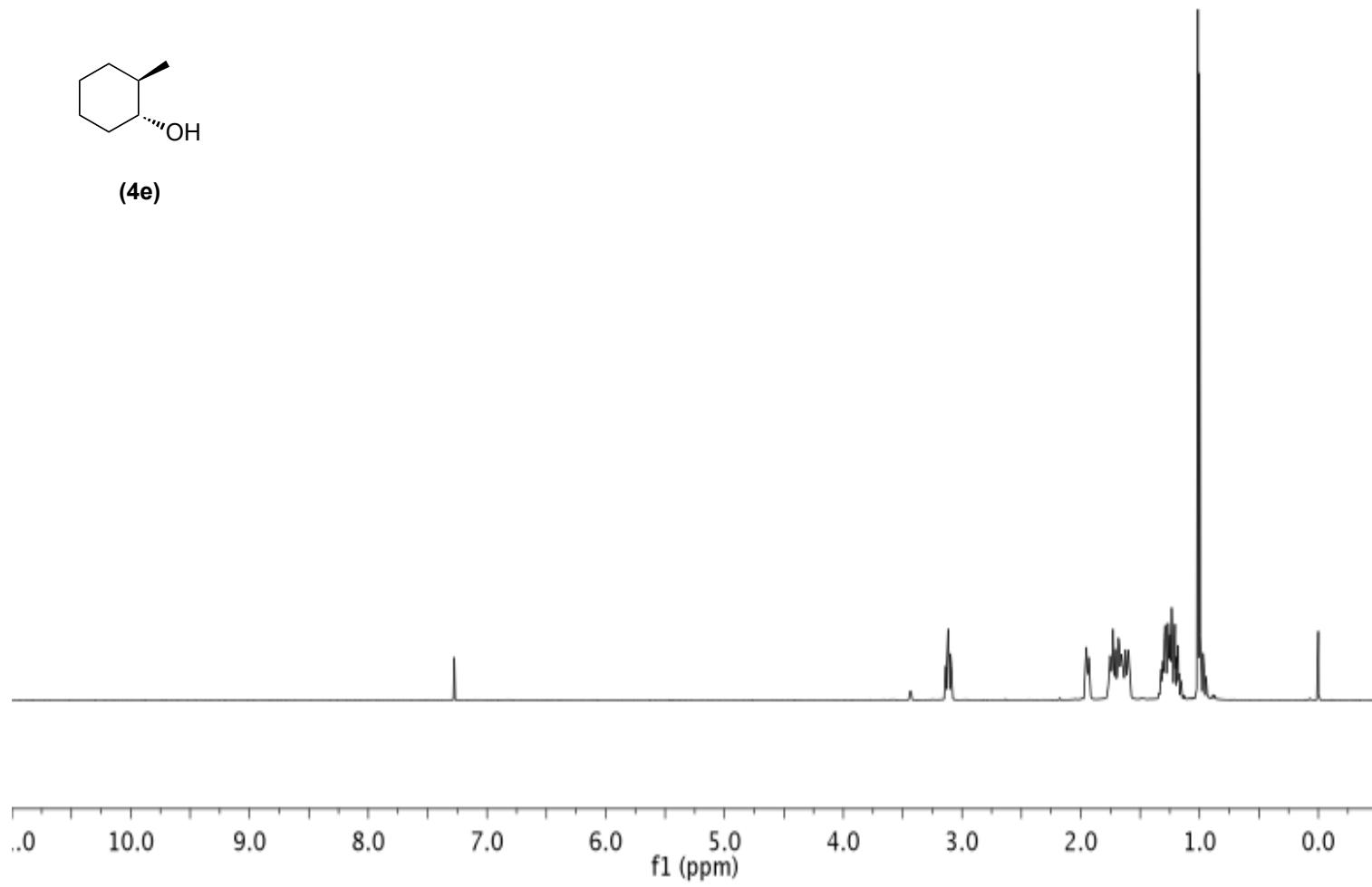
(4d)



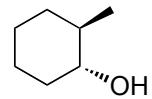
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Cyclopentanol (4d)



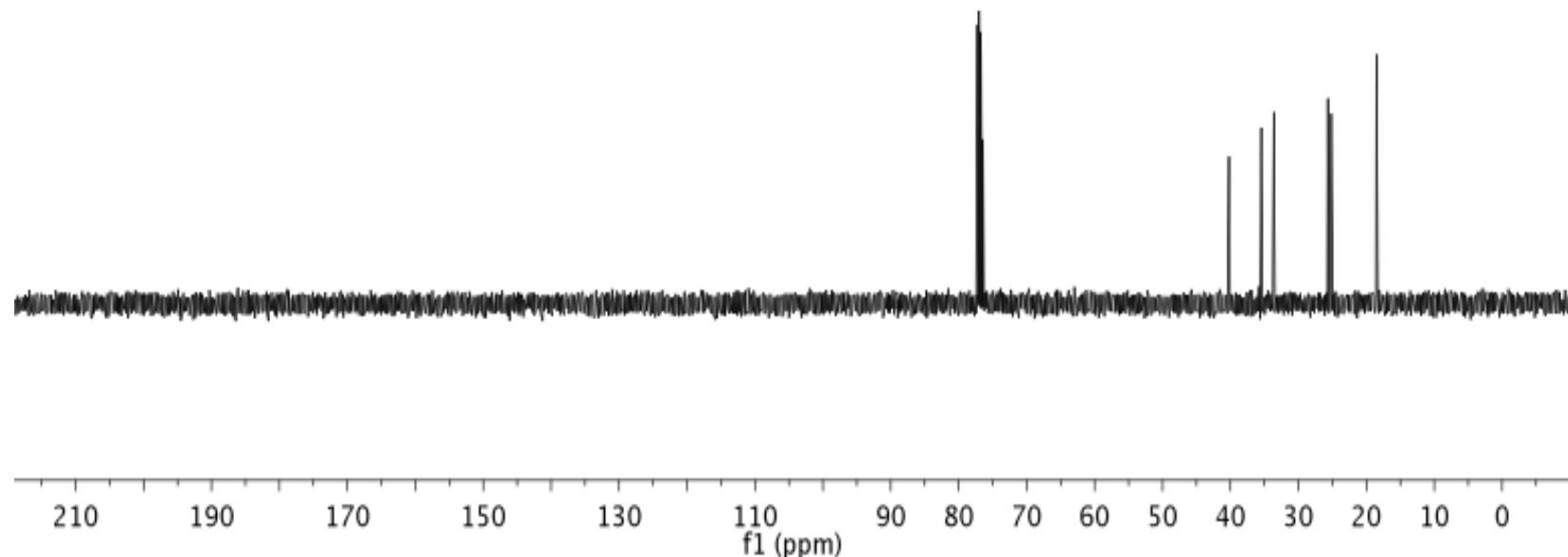
(4e)



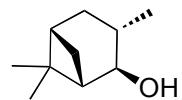
^1H NMR (500 MHz, CDCl_3) Spectrum of *trans*-2-Methylcyclohexanol (4e)



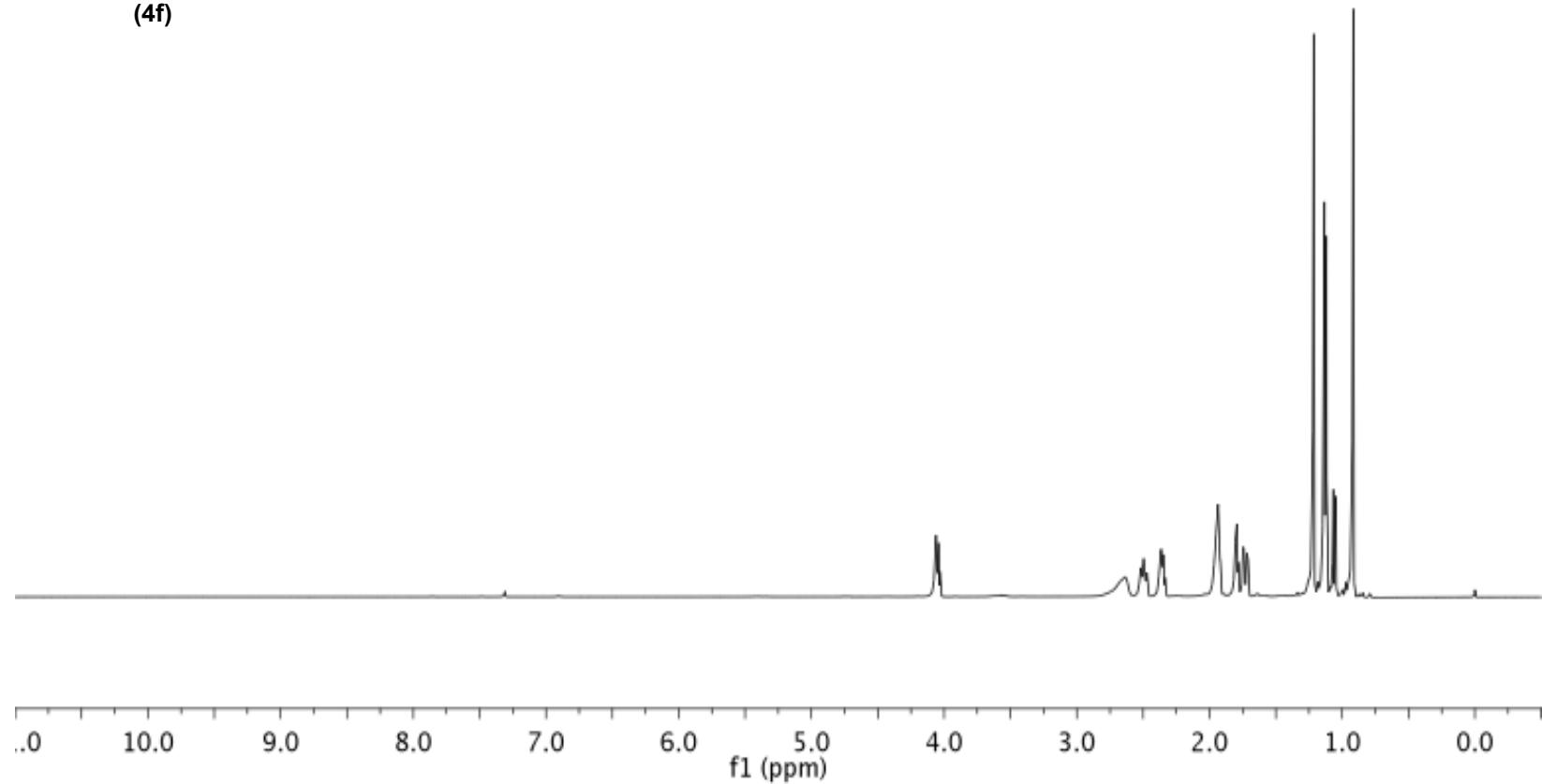
(4e)



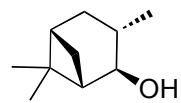
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of *trans*-2-Methylcyclohexanol (4e)



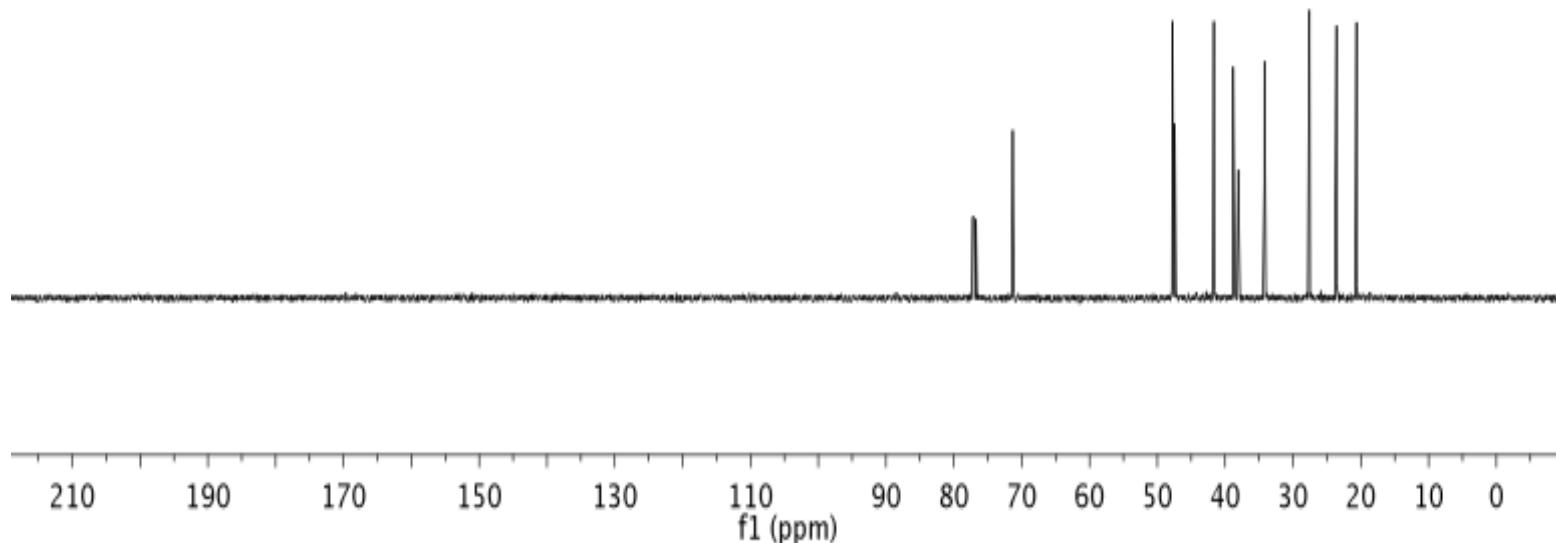
(4f)



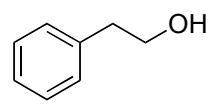
¹H NMR (500 MHz, CDCl₃) Spectrum of 3,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol (4f)



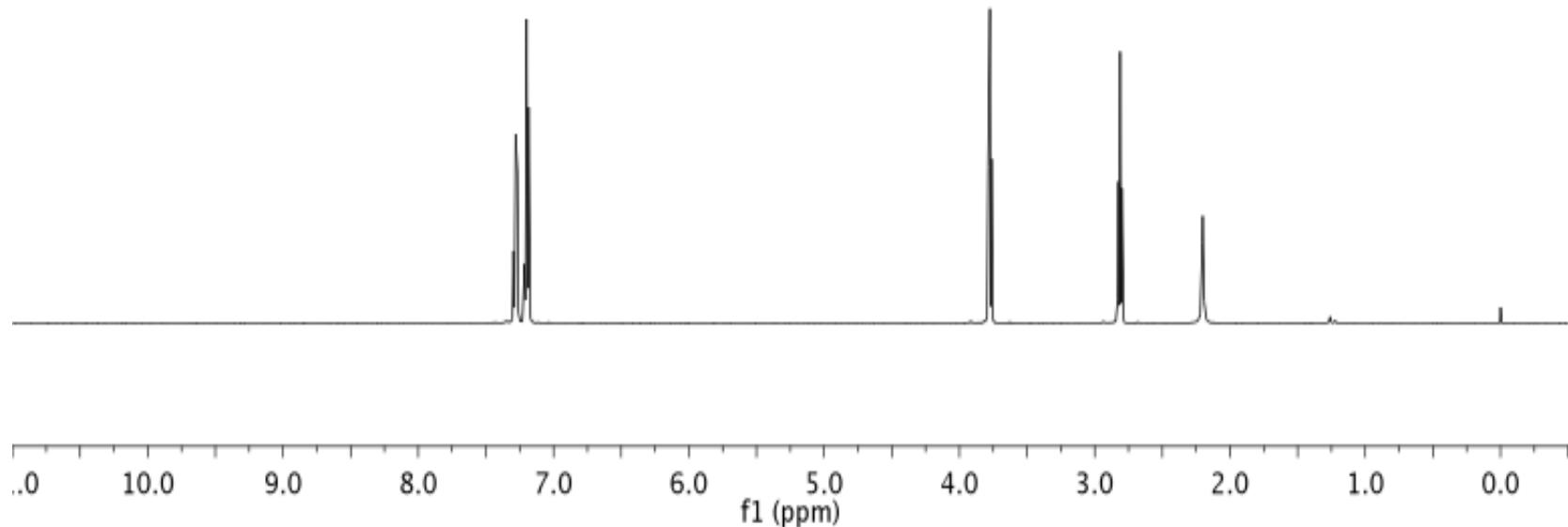
(4f)



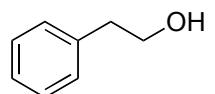
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of 3,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol (4f)



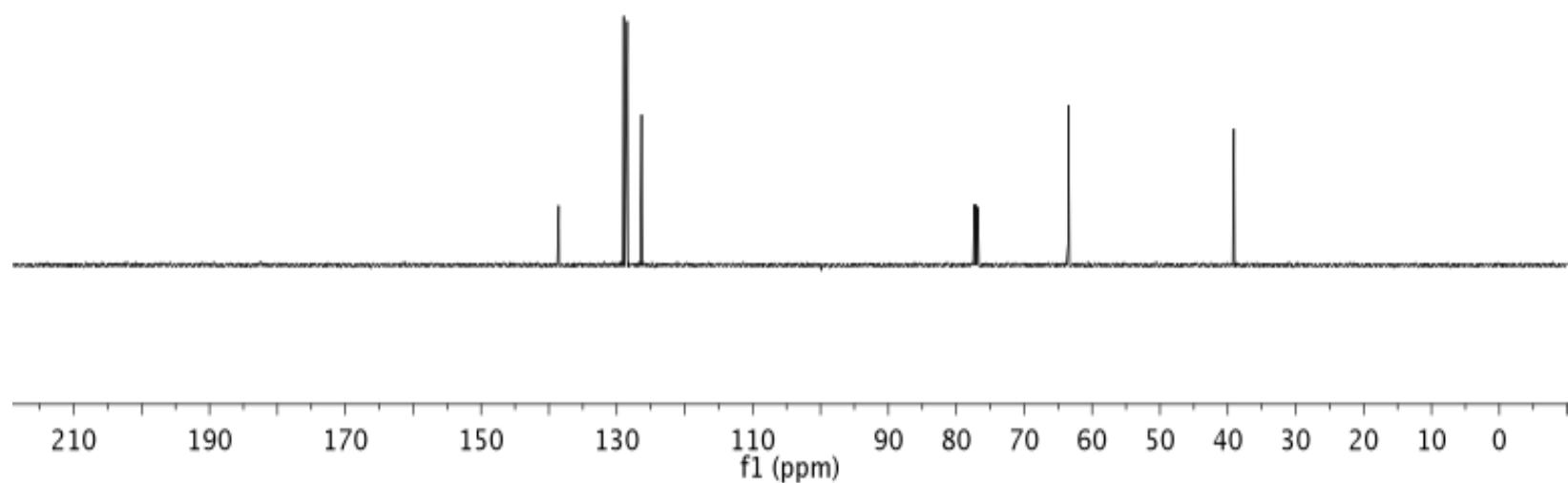
(4g)



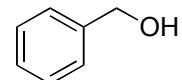
¹H NMR (500 MHz, CDCl₃) Spectrum of 2-Phenylethanol (4g)



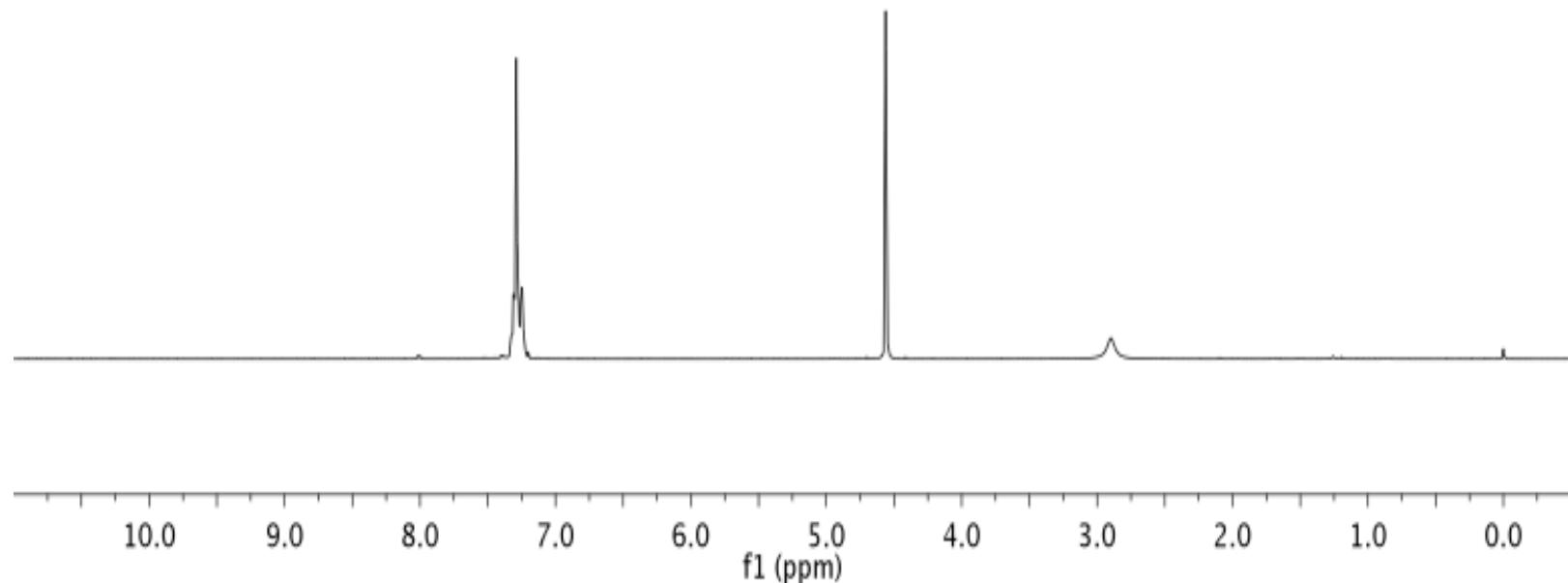
(4g)



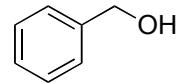
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 2-Phenylethanol (4g)



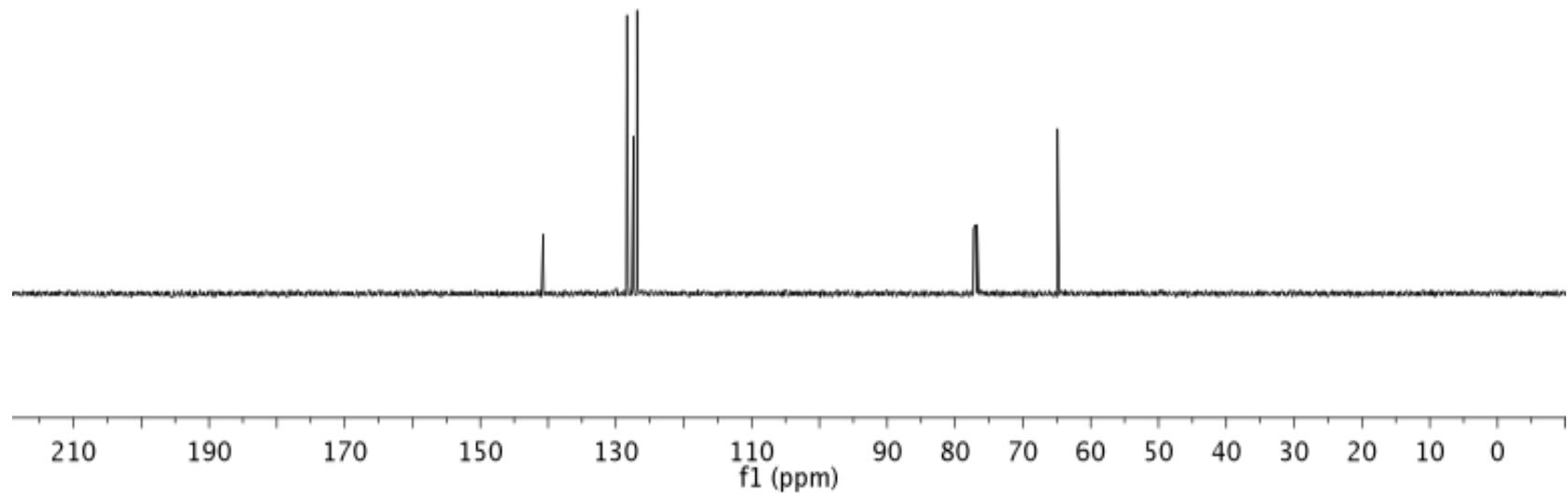
(4h)



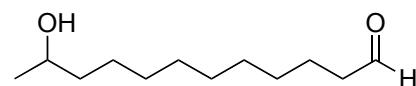
¹H NMR (500 MHz, CDCl₃) Spectrum of Phenylmethanol (4h)



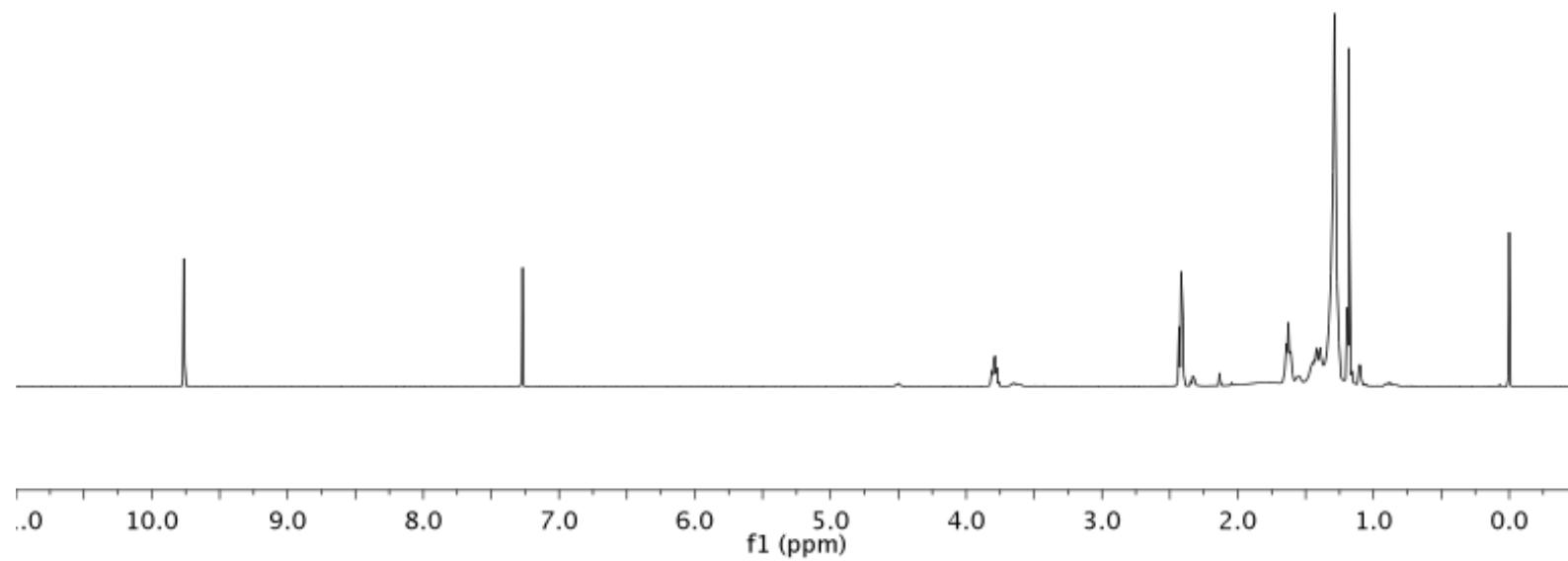
(4h)

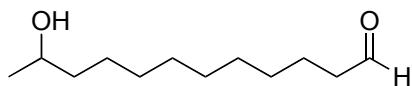


¹³C NMR (128.5 MHz, CDCl₃) Spectrum of Phenylmethanol (4h)

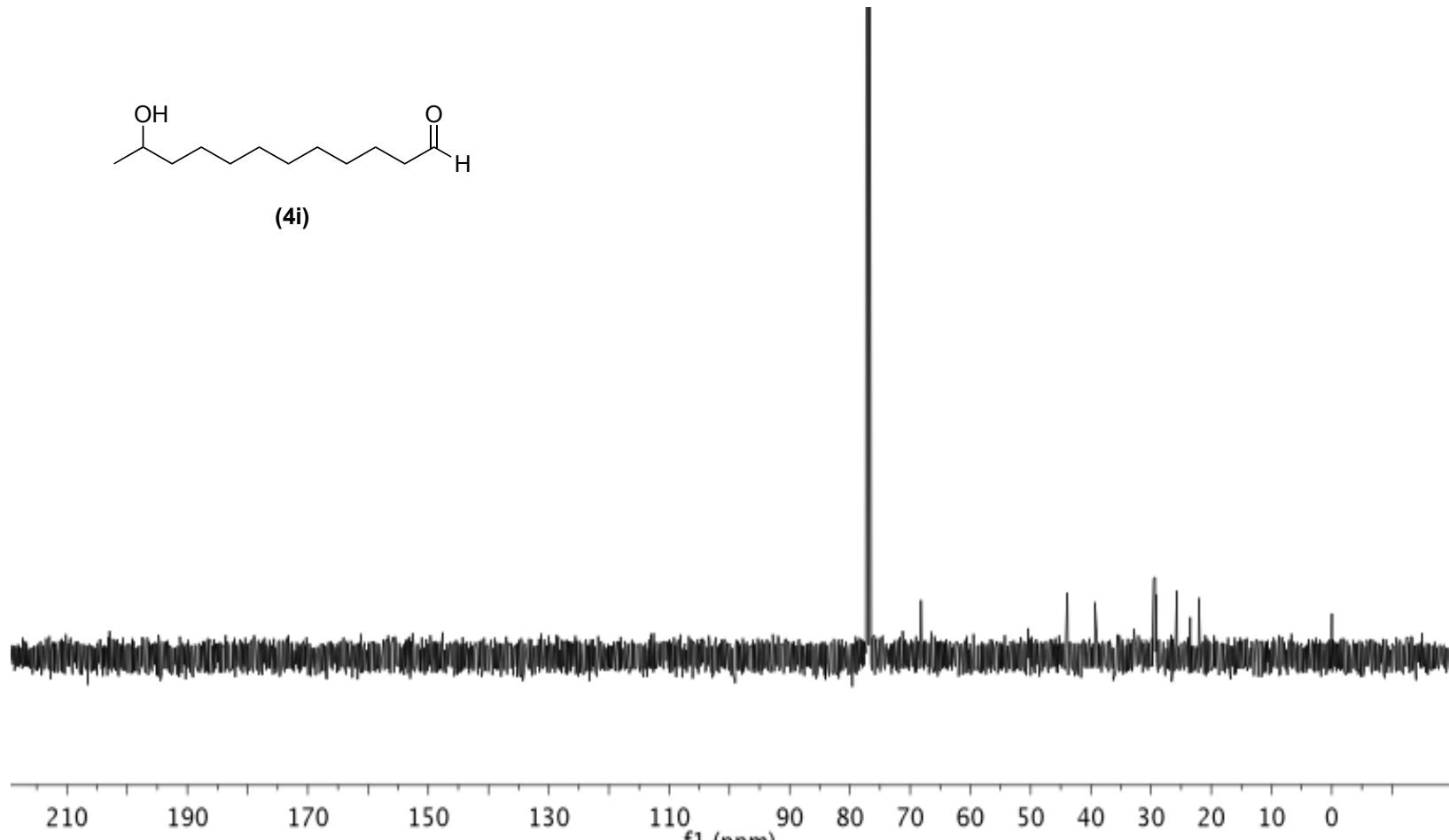


(4i)

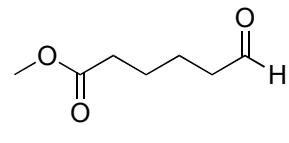




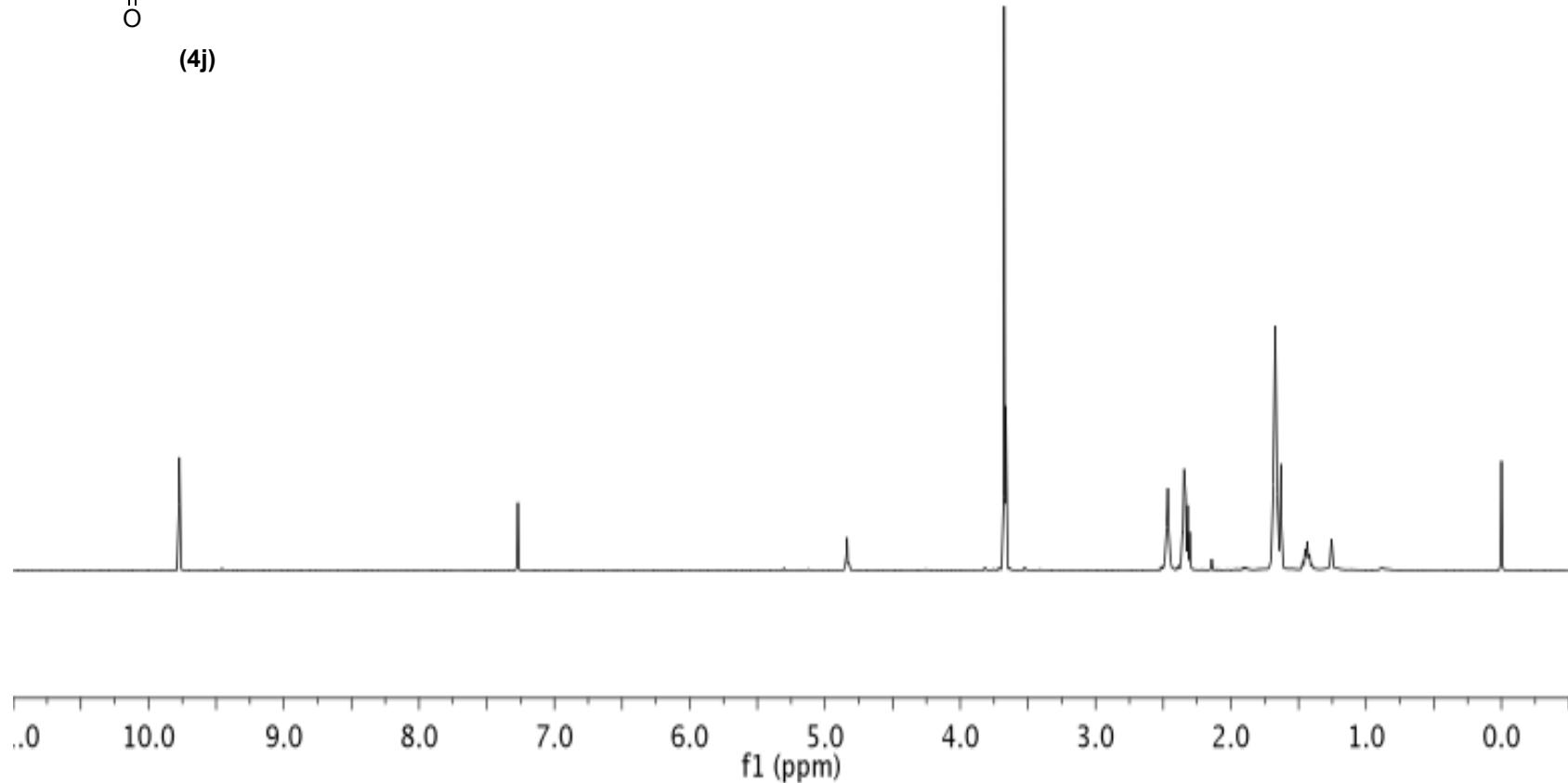
(4i)



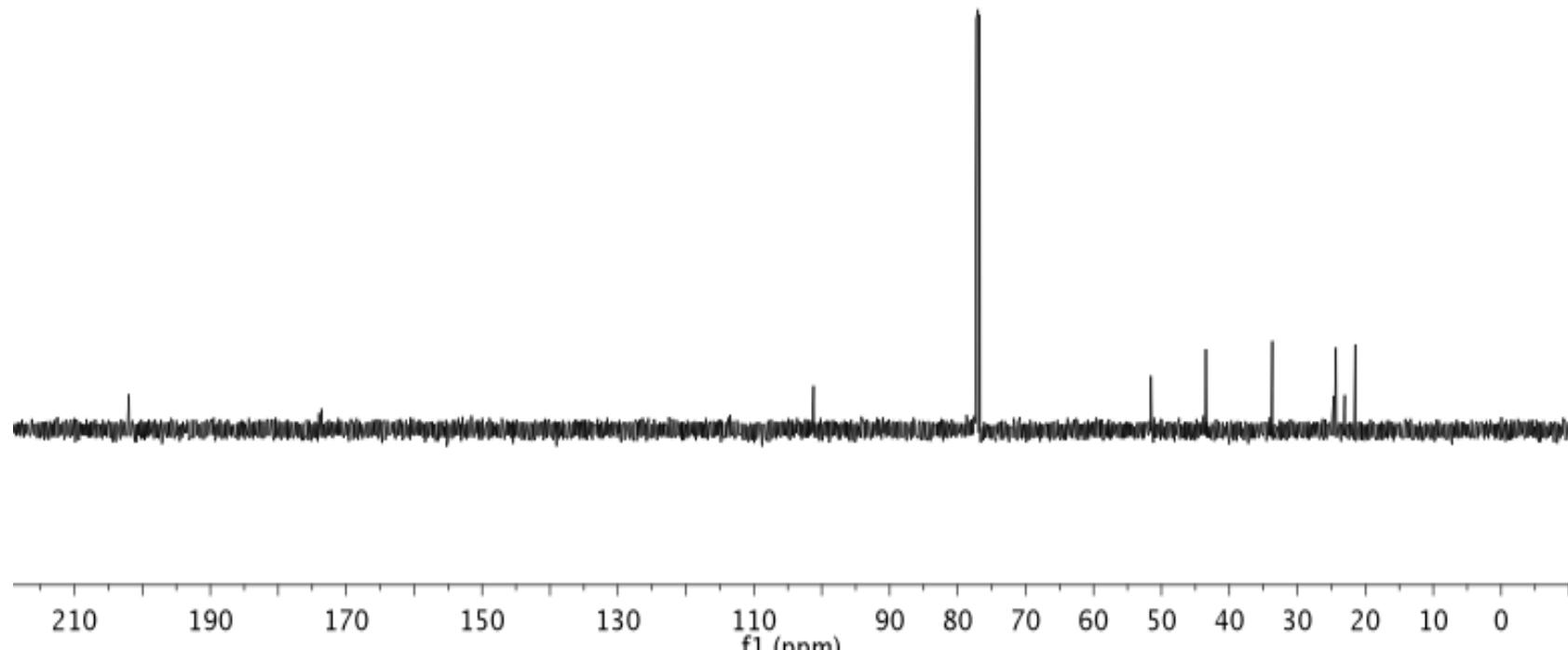
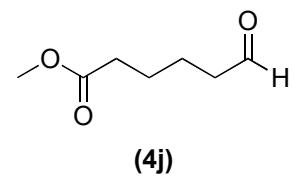
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of 11-Hydroxydodecanal (4i)



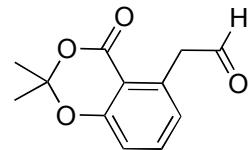
(4j)



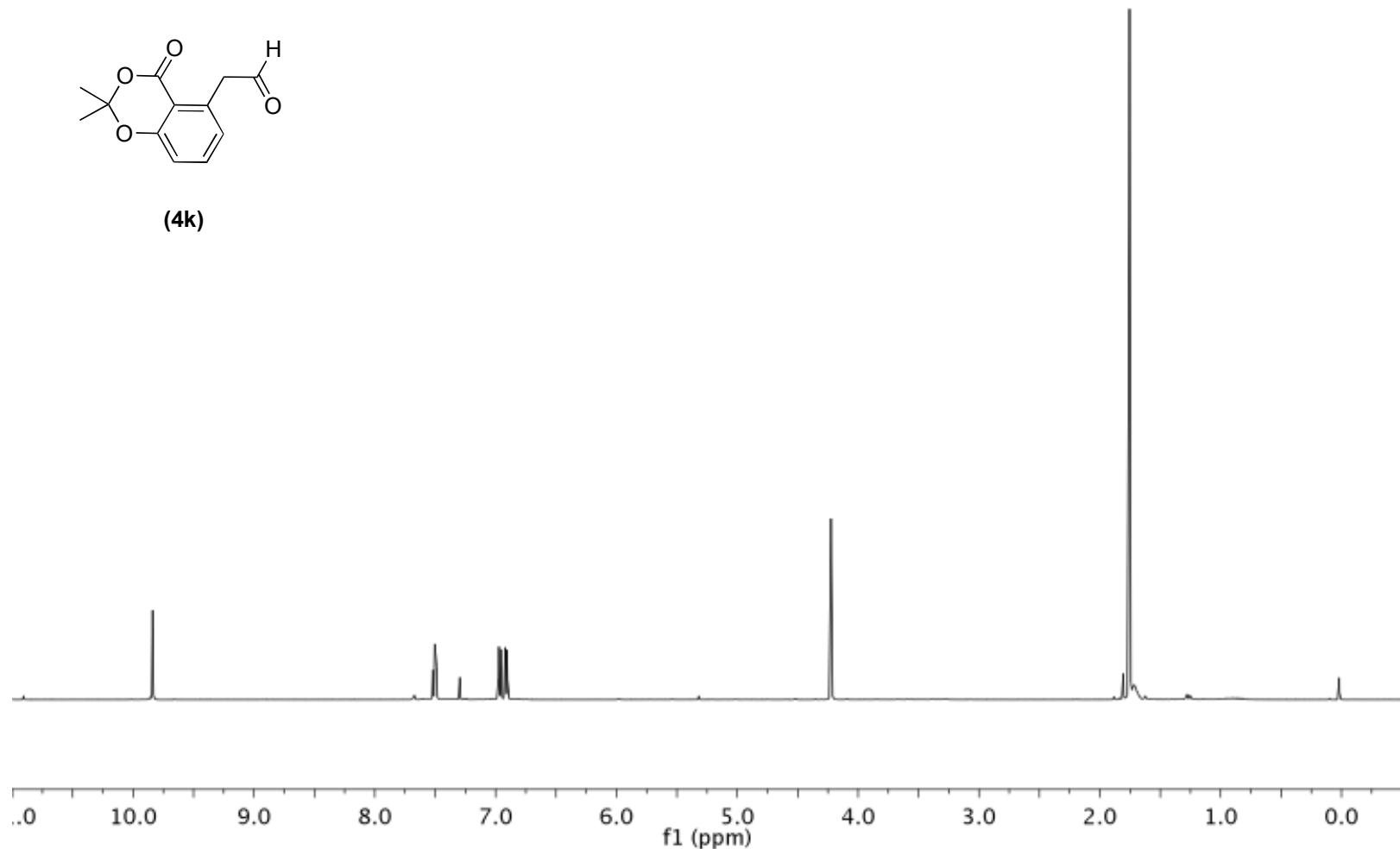
^1H NMR (500 MHz, CDCl_3) Spectrum of Methyl 6-Oxohexanoate (4j)



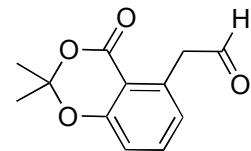
¹³C NMR (128.5 MHz, CDCl₃) Spectrum of methyl 6-oxohexanoate (4j)



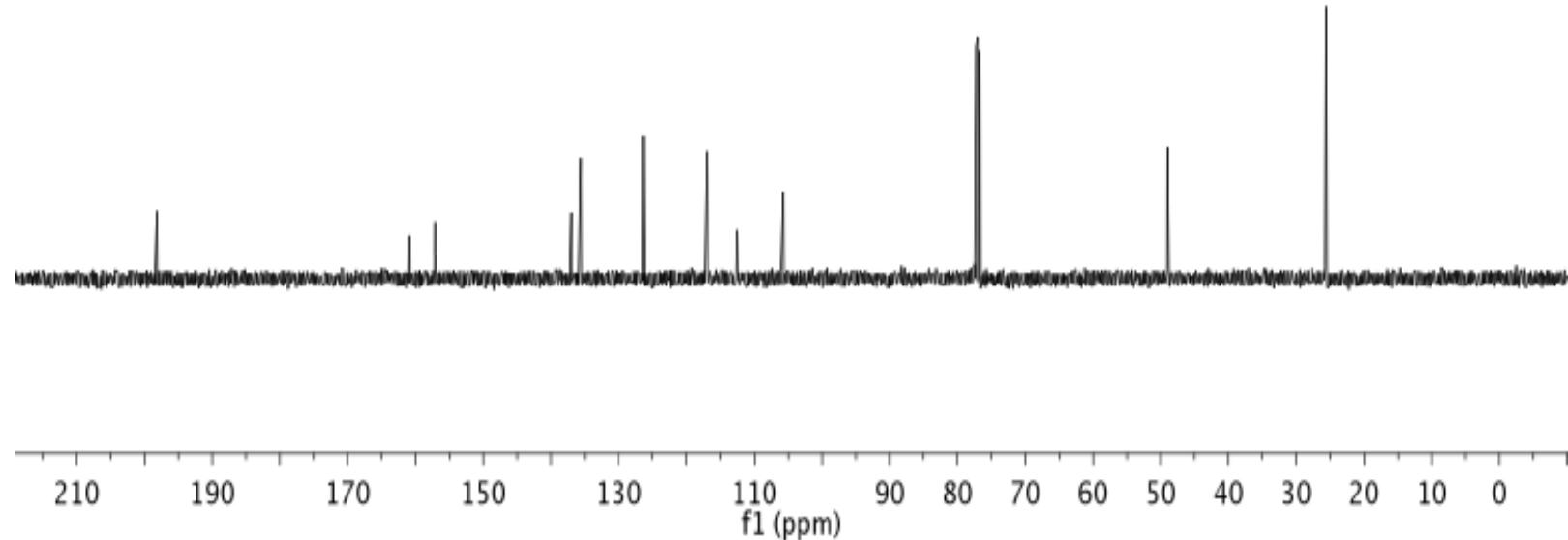
(4k)



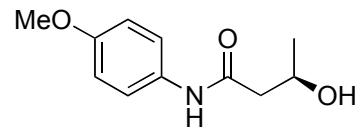
^1H NMR (500 MHz, CDCl_3) Spectrum of 2-(2,2-Dimethyl-4-oxo-4*H*-benzo[*d*][1,3]dioxin-5-yl)acetaldehyde (4k)



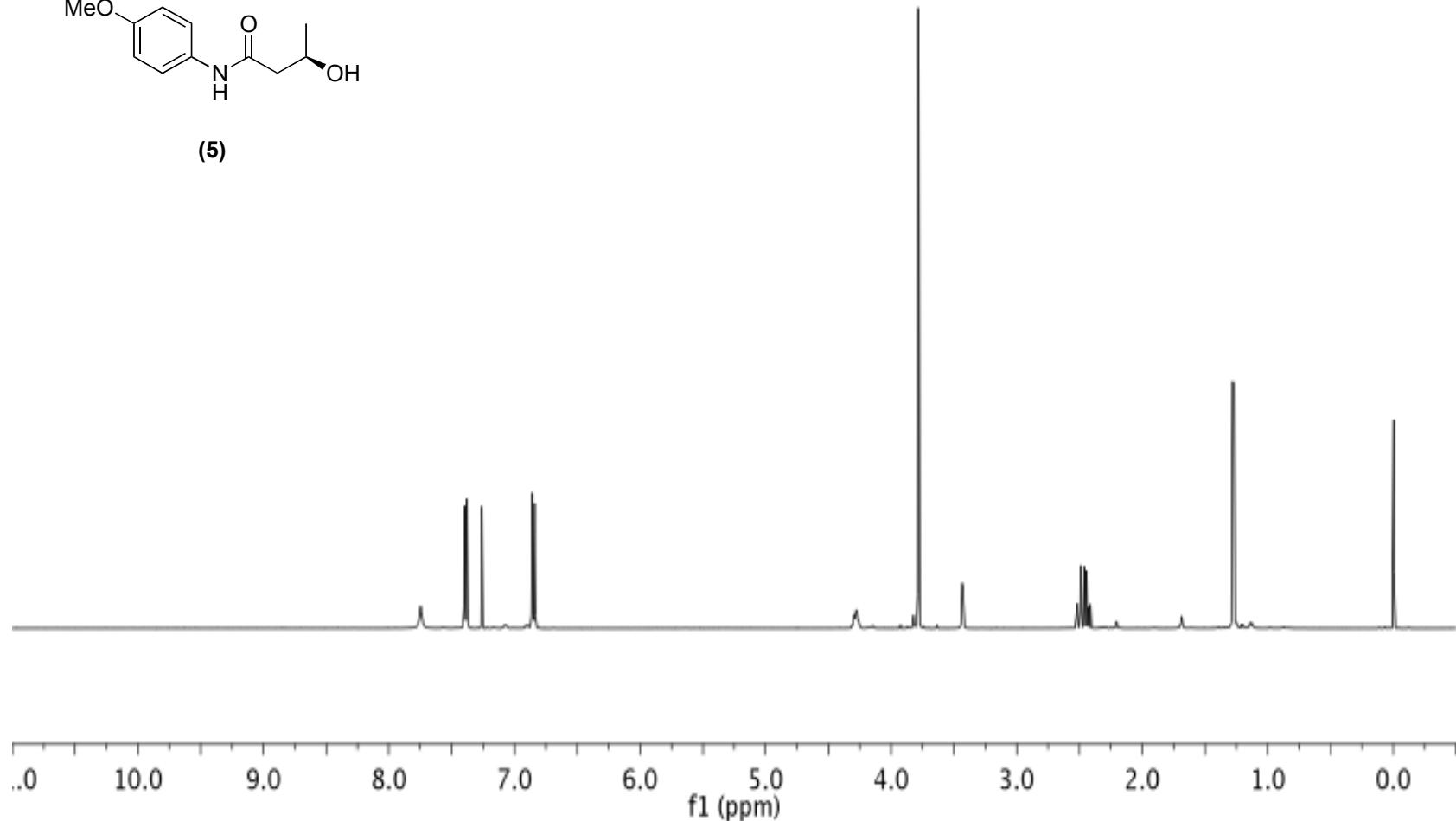
(4k)



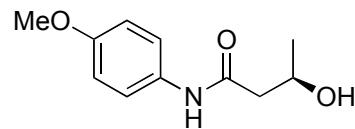
^{13}C NMR (128.5 MHz, CDCl_3) Spectrum of 2-(2,2-Dimethyl-4-oxo-4*H*-benzo[*d*][1,3]dioxin-5-yl)acetaldehyde (4k)



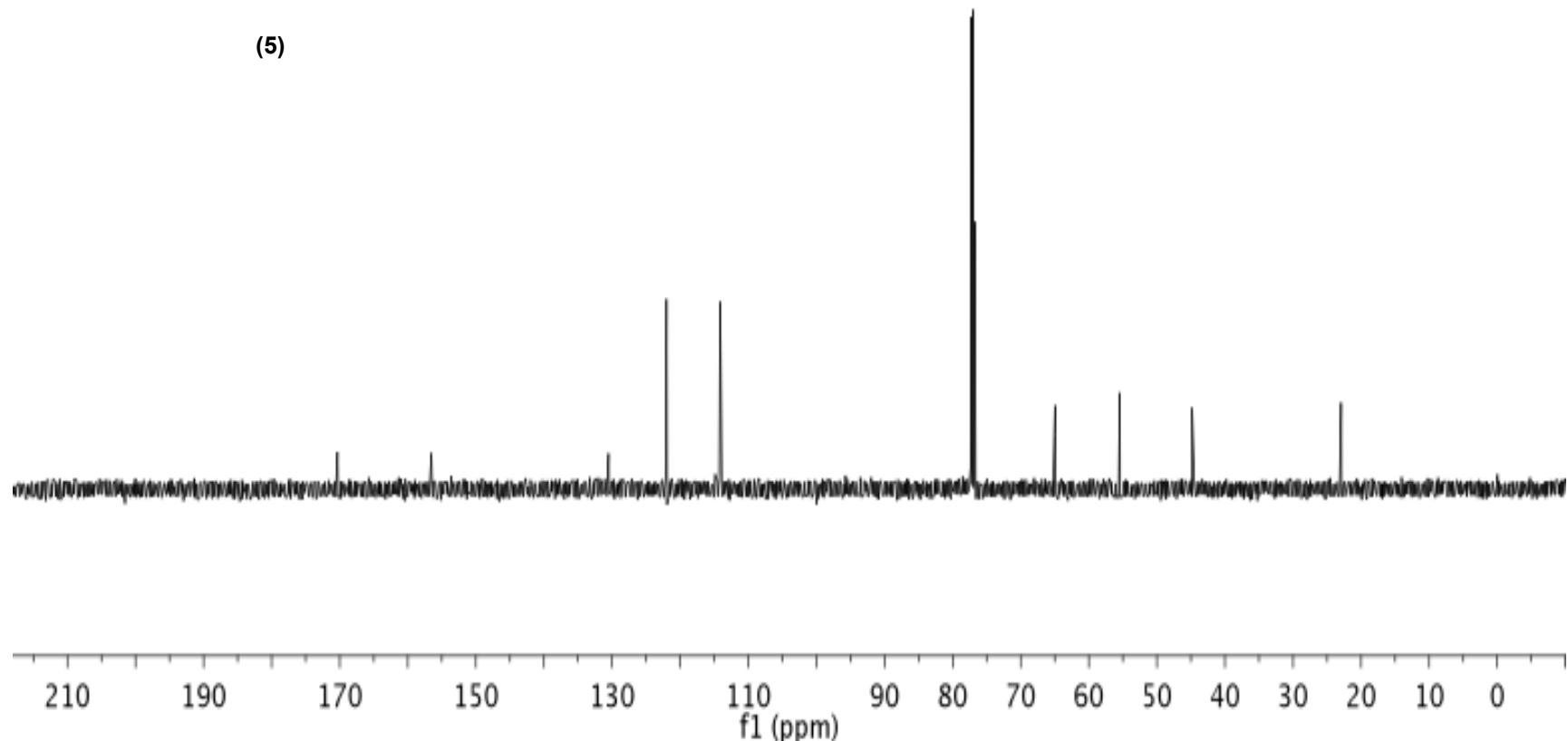
(5)



^1H NMR (500 MHz, CDCl_3) Spectrum of (*R*)-3-Hydroxy-*N*-(4-methoxyphenyl)butanamide (5)



(5)



¹³C NMR (128.5 MHz, CDCl₃) Spectrum of (*R*)-3-Hydroxy-*N*-(4-methoxyphenyl)butanamide (5)