

Supplementary Material

Therapeutic Potential of 1,3,4-oxadiazoles as potential lead compounds for the treatment of Alzheimer's disease

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Table S1. Experimental crystal structure details of compound **4n**.

CCDC	
Chemical formula	C ₁₅ H ₁₃ N ₃ O
<i>M</i> _r	251.28
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.5156 (16), 7.2615 (15), 20.971 (4)
β (°)	93.424 (9)
<i>V</i> (Å ³)	1294.4 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.38 × 0.32 × 0.30
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2005)
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	11008, 3064, 2374
<i>R</i> _{int}	0.057
(sin θ/λ) _{max} (Å ⁻¹)	0.659
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.055, 0.160, 1.05
No. of reflections	3064
No. of parameters	173
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.24, -0.23

Table S2. Hydrogen-bond geometry (Å, °) in compound **4n**.

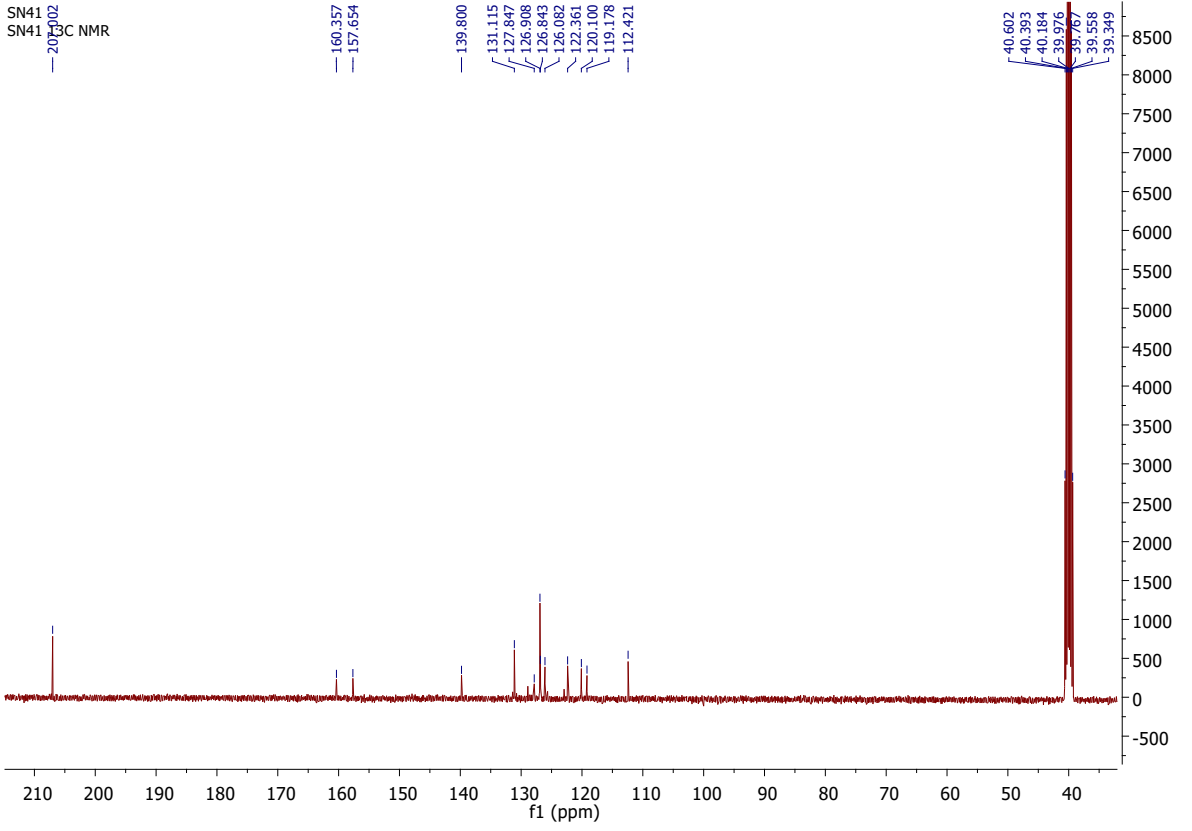
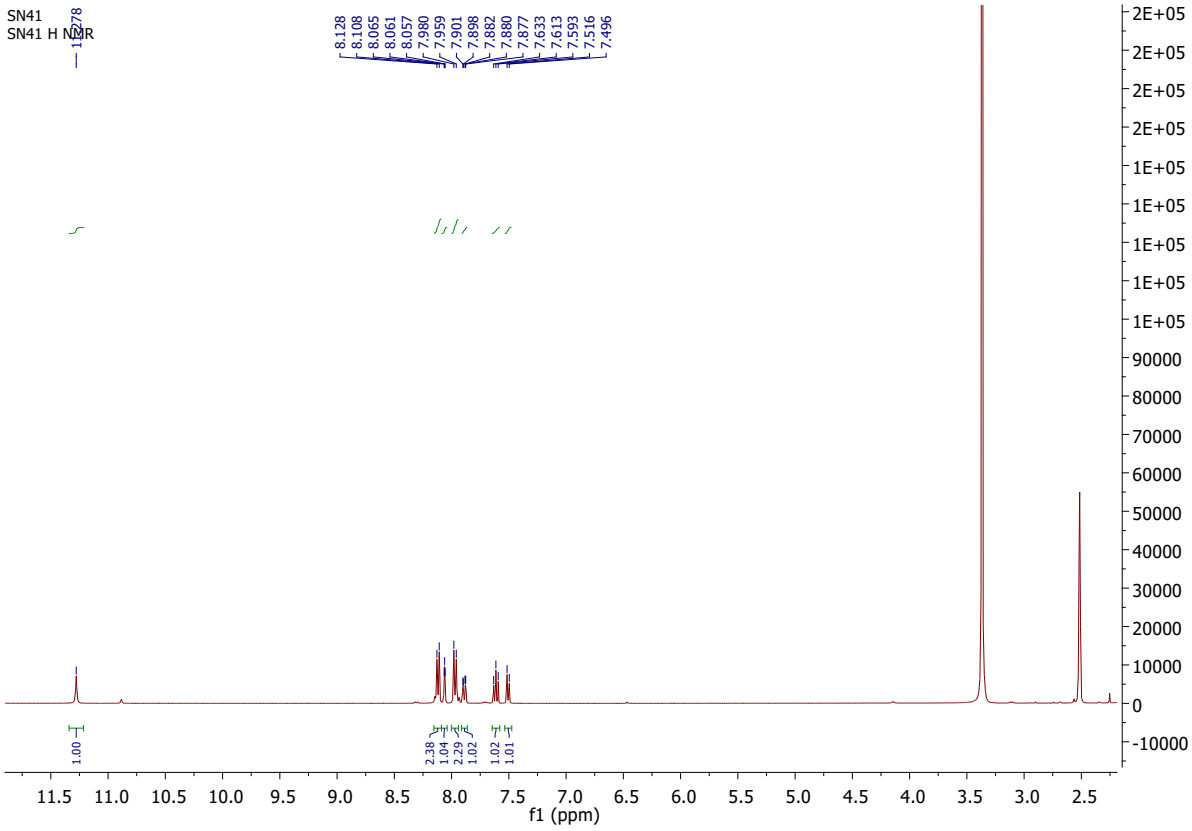
<i>D</i> —H⋯ <i>A</i>	<i>D</i> —H	H⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> —H⋯ <i>A</i>
N1—H1⋯N2 ⁱ	0.86	2.10	2.9373 (19)	163

Symmetry code: (i) -*x*+1, -*y*+1, -*z*.

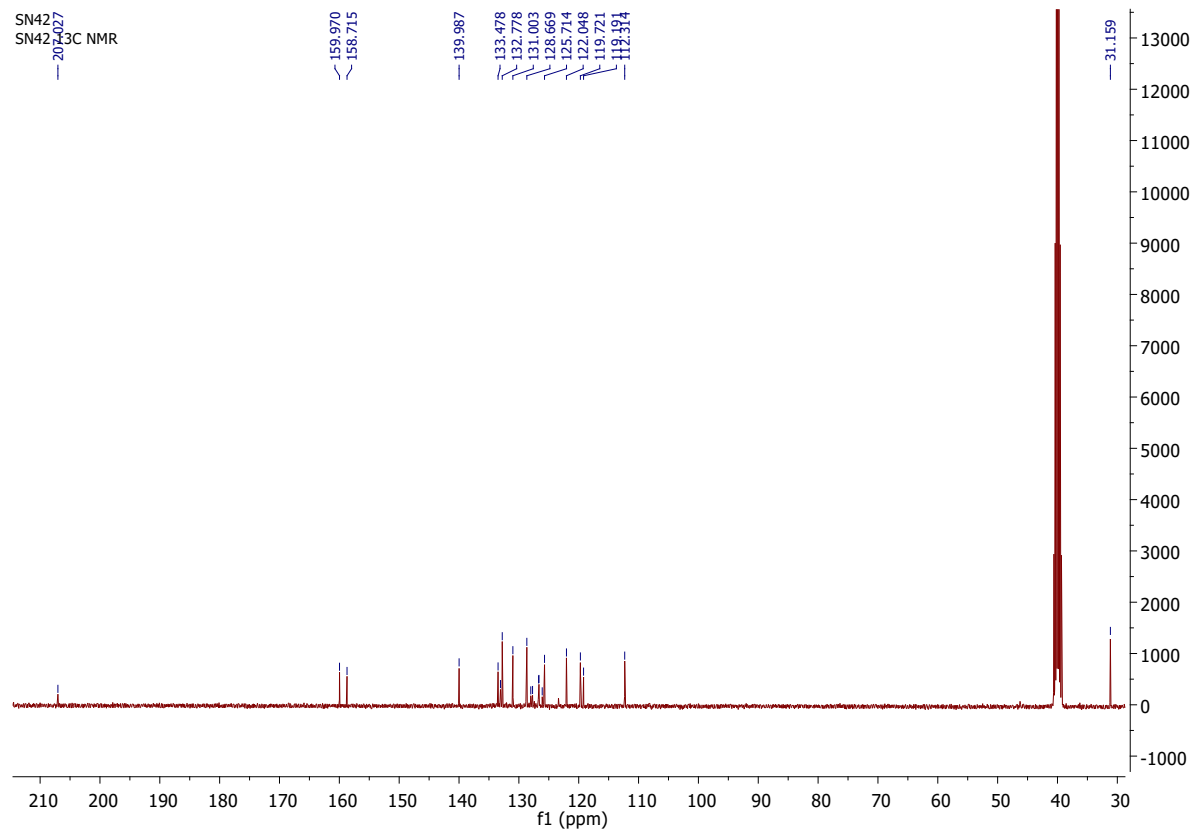
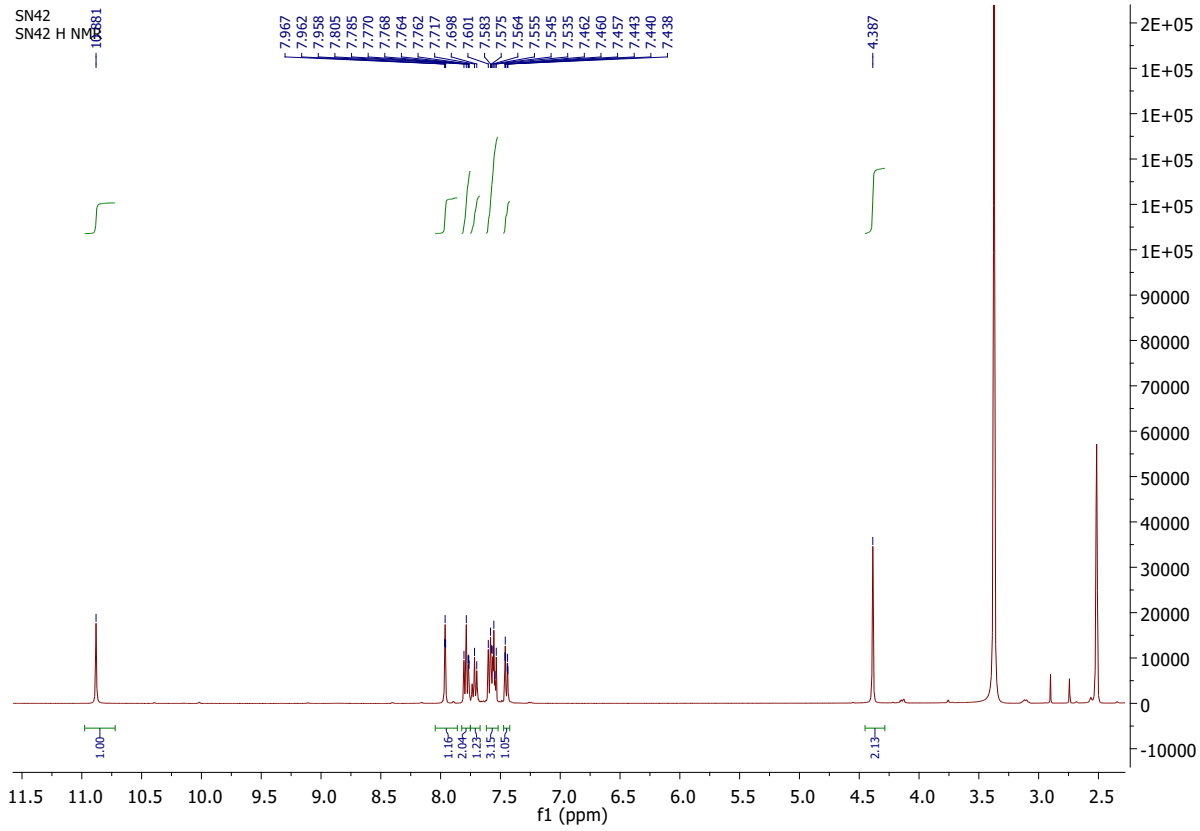
Table S3. Computational toxicological evaluation for Compounds **4a-o**.

<u>Code</u>	<u>Predicted Toxicity class</u>	<u>Predicted LD50</u>	<u>Predicted end points of toxicity</u>
4a	4	550mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4b	4	800mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4c	4	800mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4d	4	580mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4e	4	550mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4f	4	550mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4g	4	550mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4h	4	550mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4i	4	1190mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4j	4	580mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4k	4	580mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4l	4	550mg/Kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4m	4	550mg/Kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4n	4	550mg/Kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity
4o	4	1190mg/kg	Inactive for the Immunotoxicity, mutagenicity and cytotoxicity, carcinogenicity

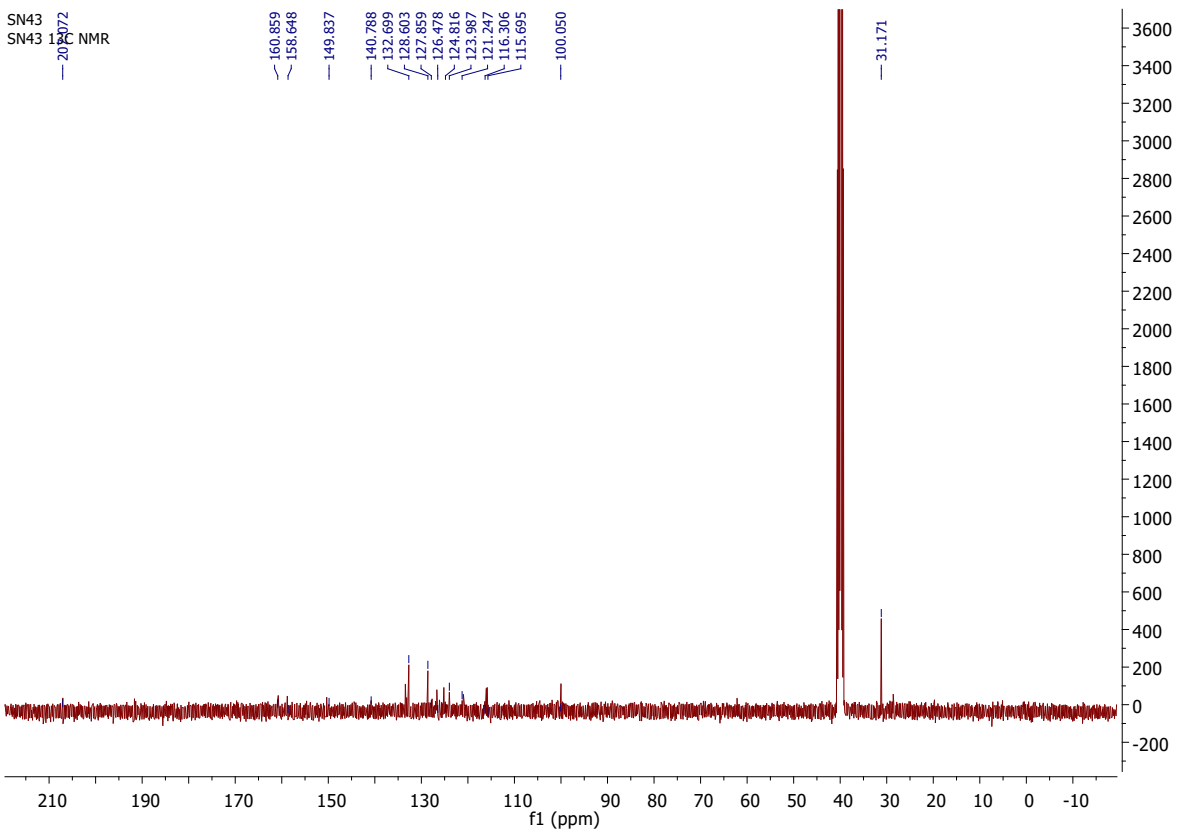
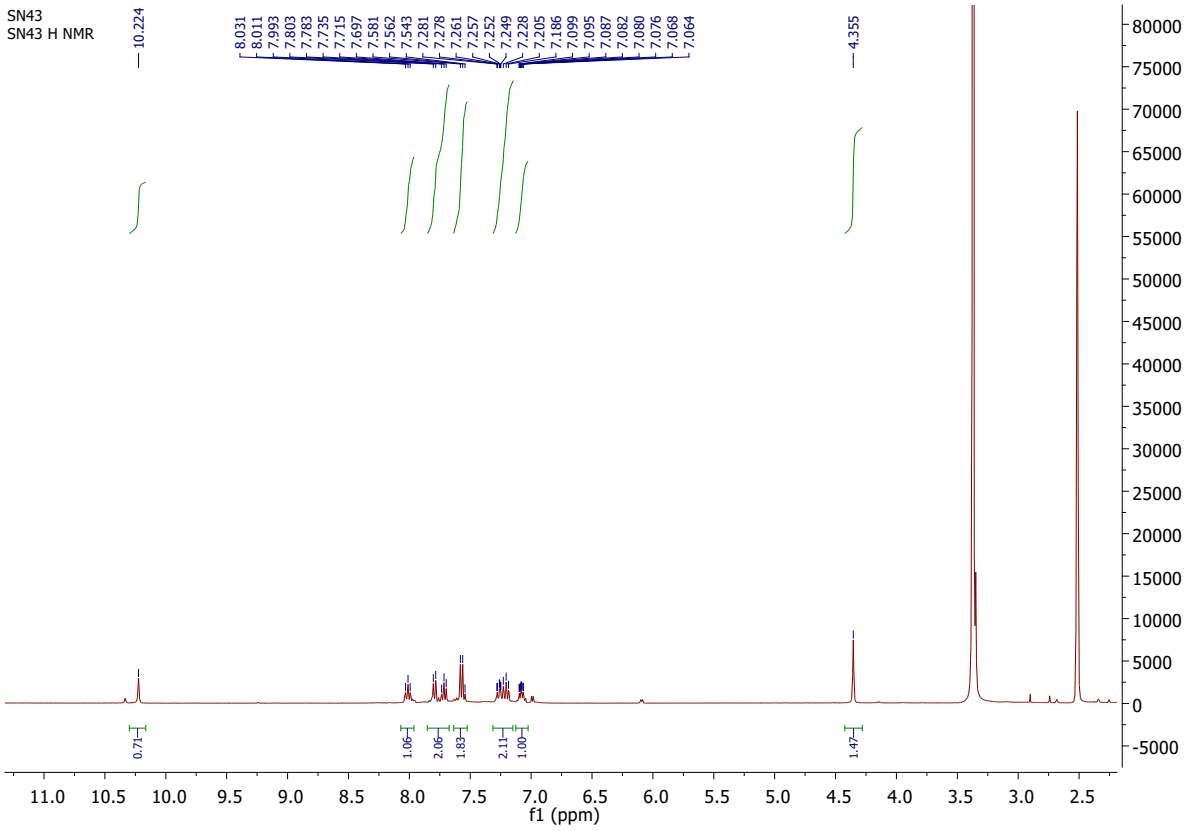
H¹ & ¹³C NMR of Compound 4a



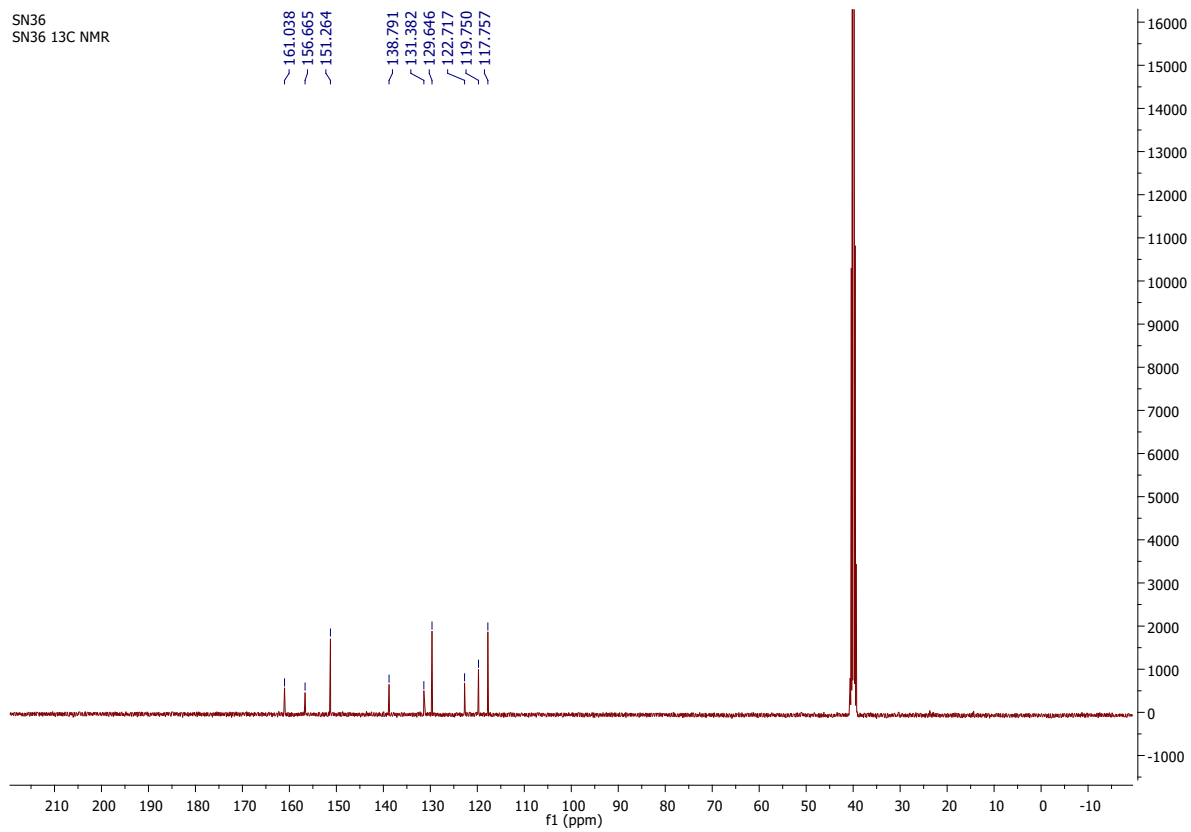
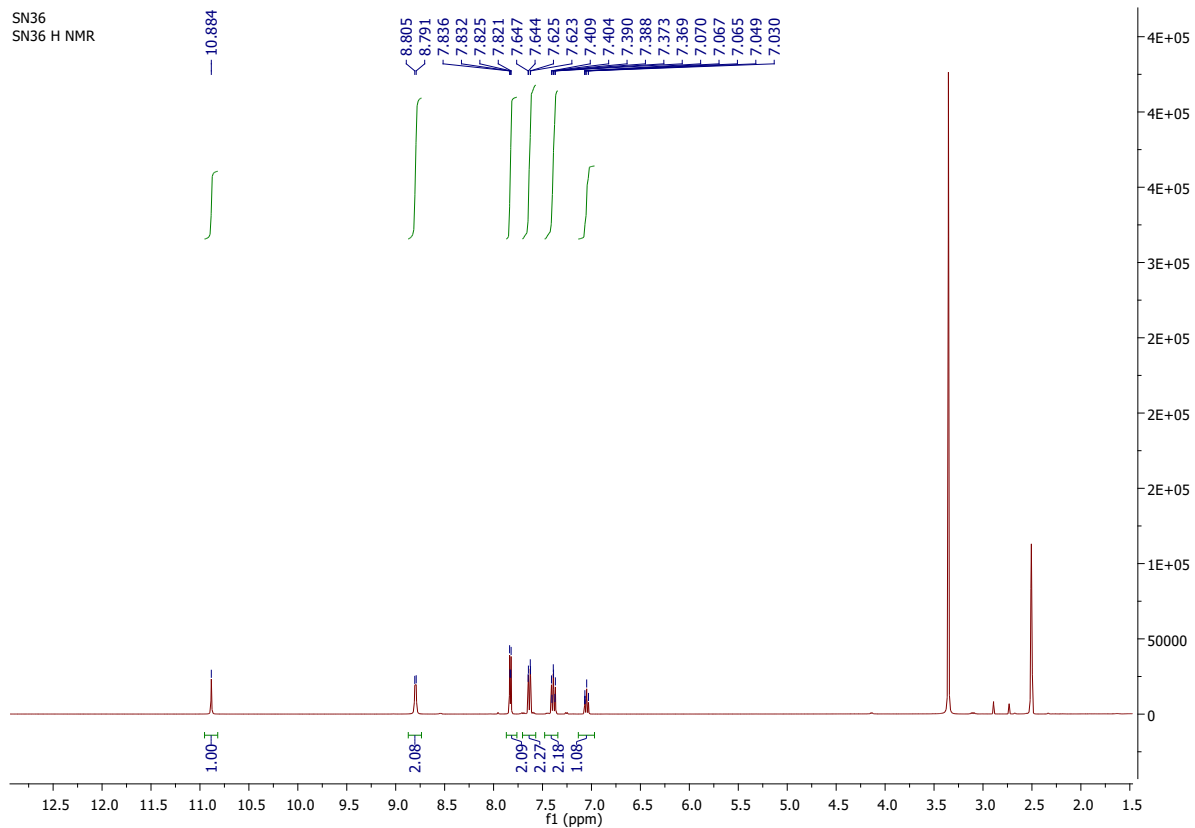
^1H & ^{13}C NMR of Compound 4b



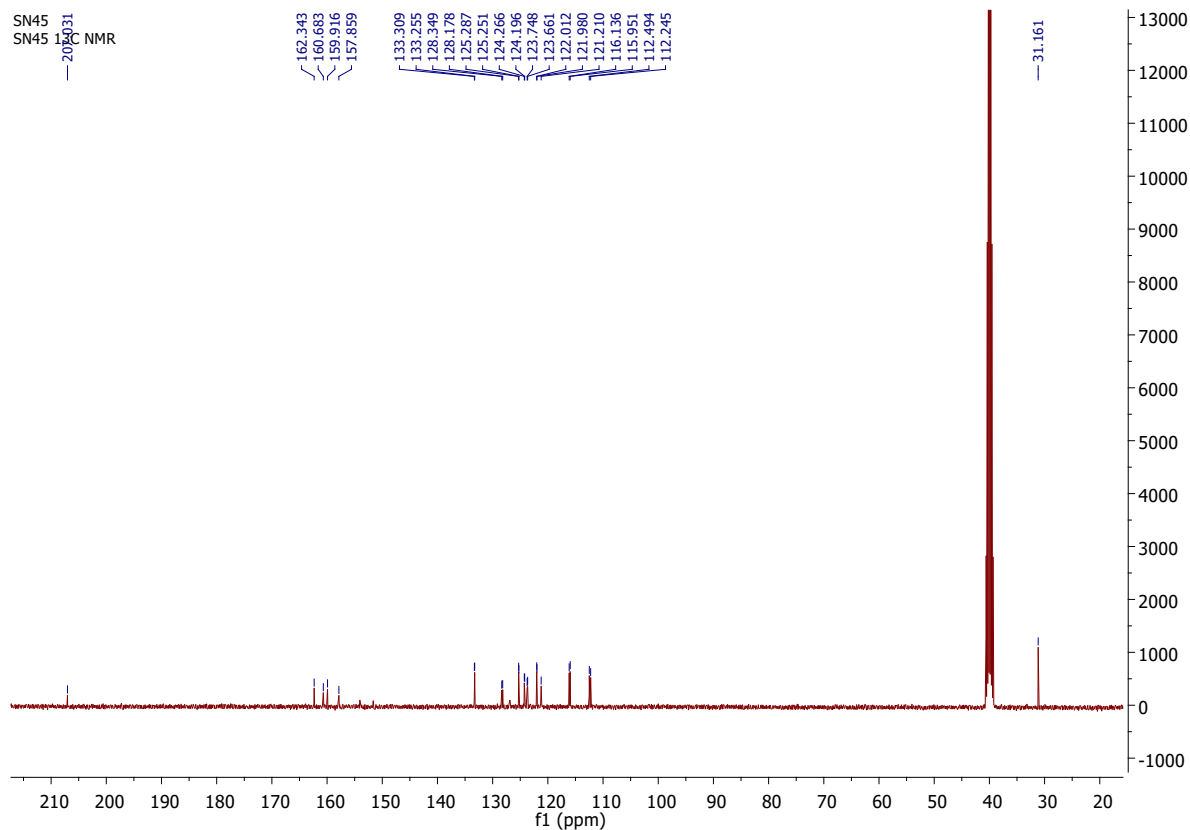
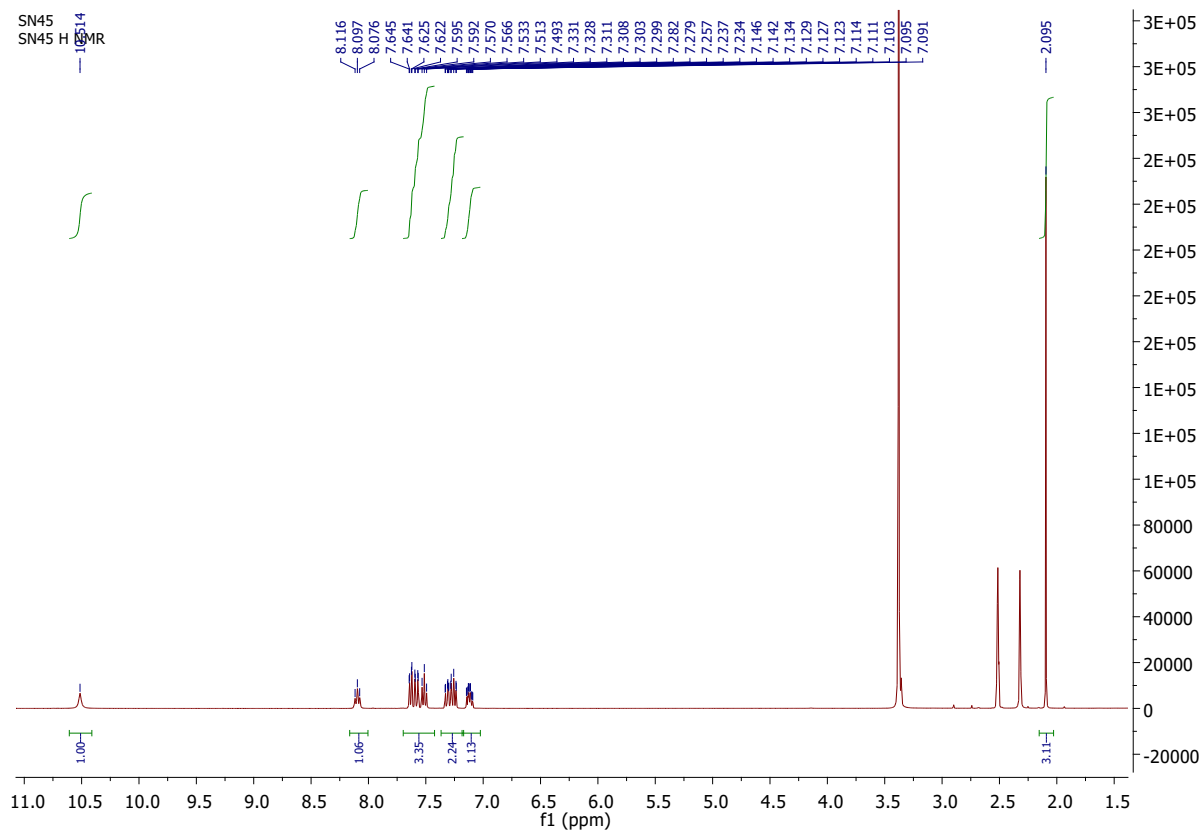
H¹ & ¹³C NMR of Compound 4c



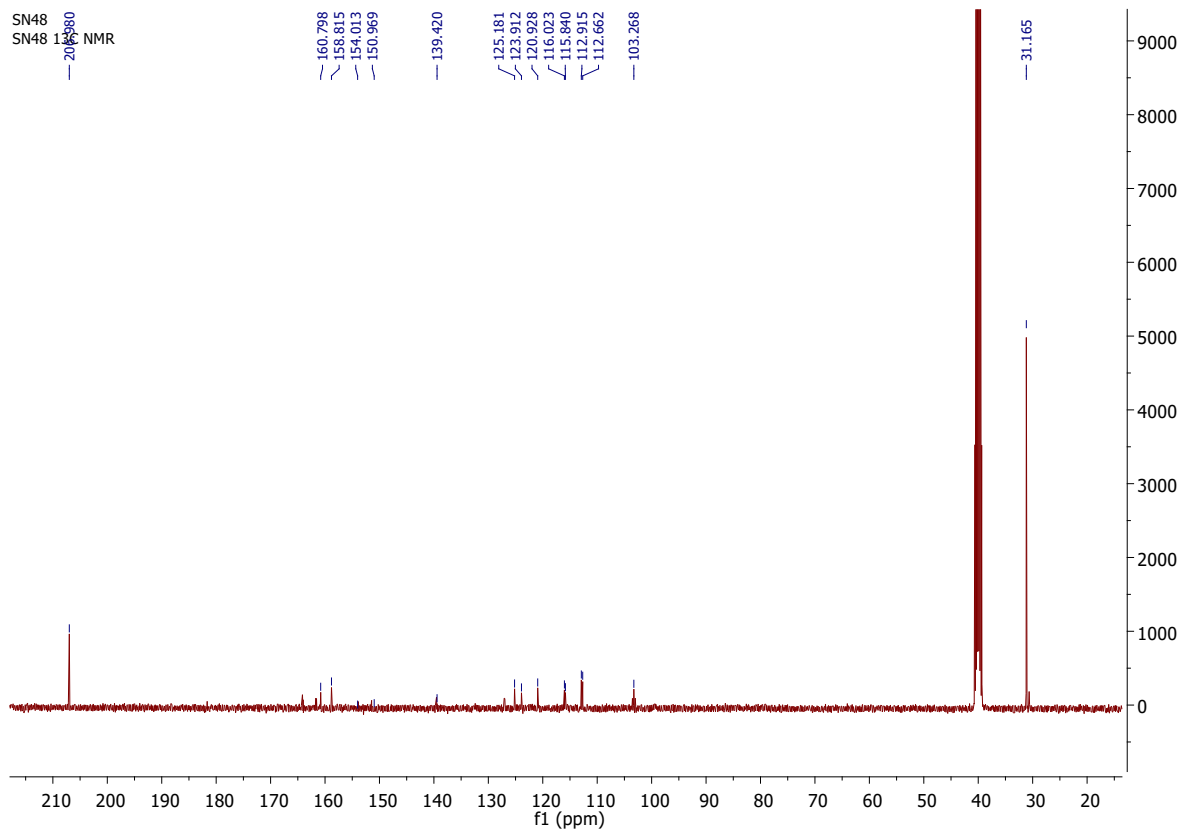
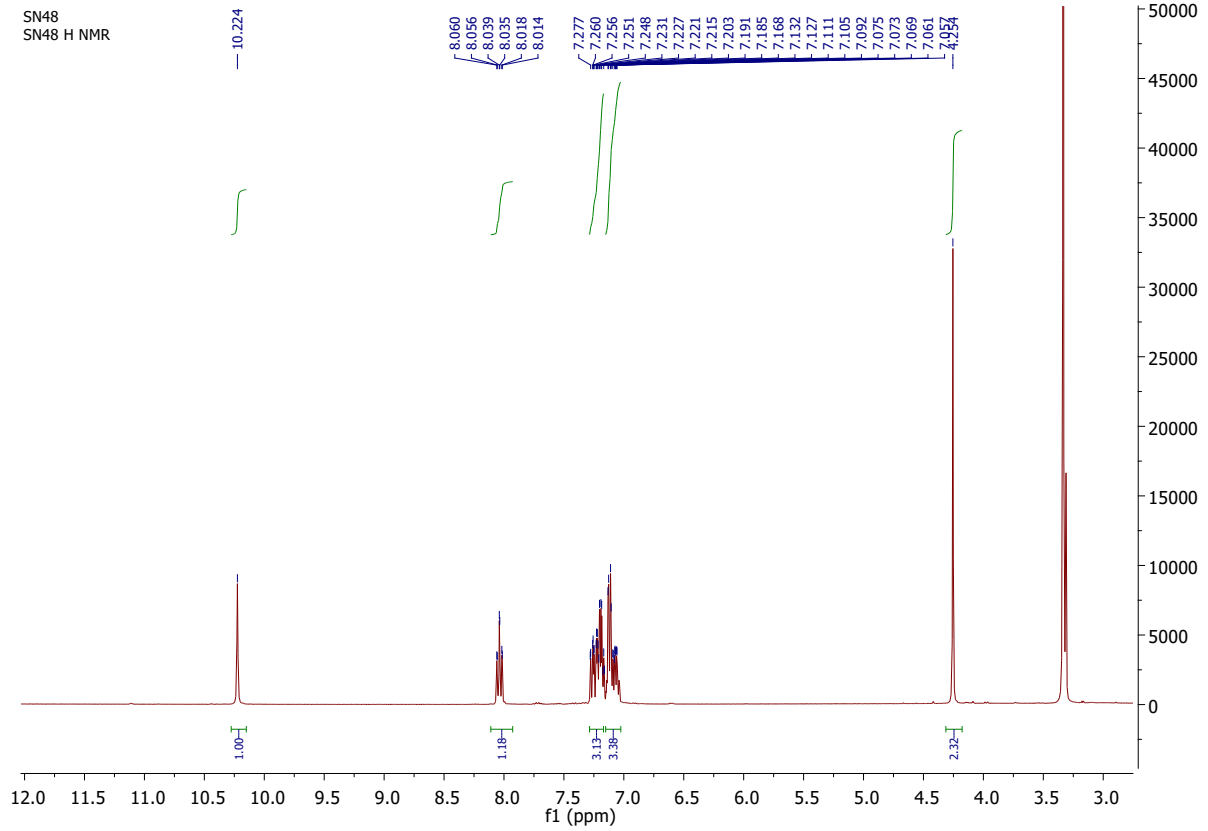
H¹ & ¹³C NMR of Compound 4d



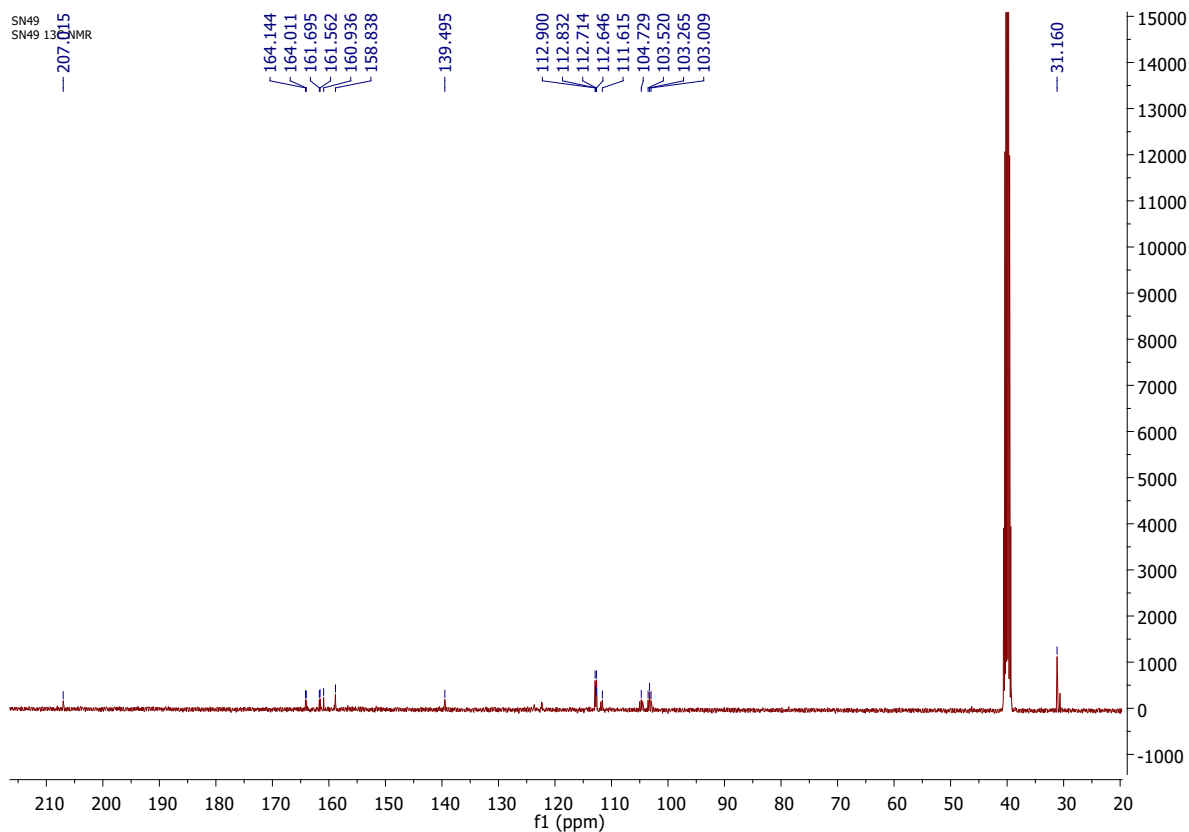
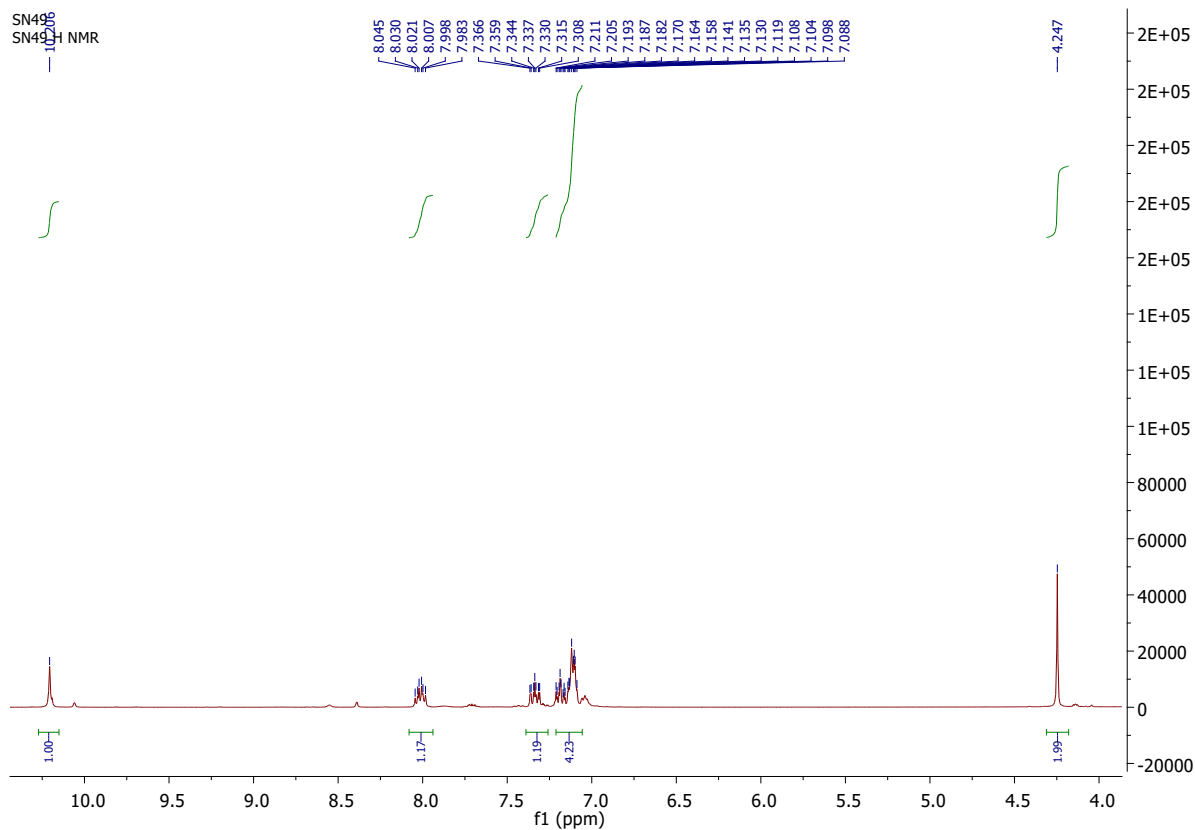
H¹ & ¹³CNMR of Compound 4e



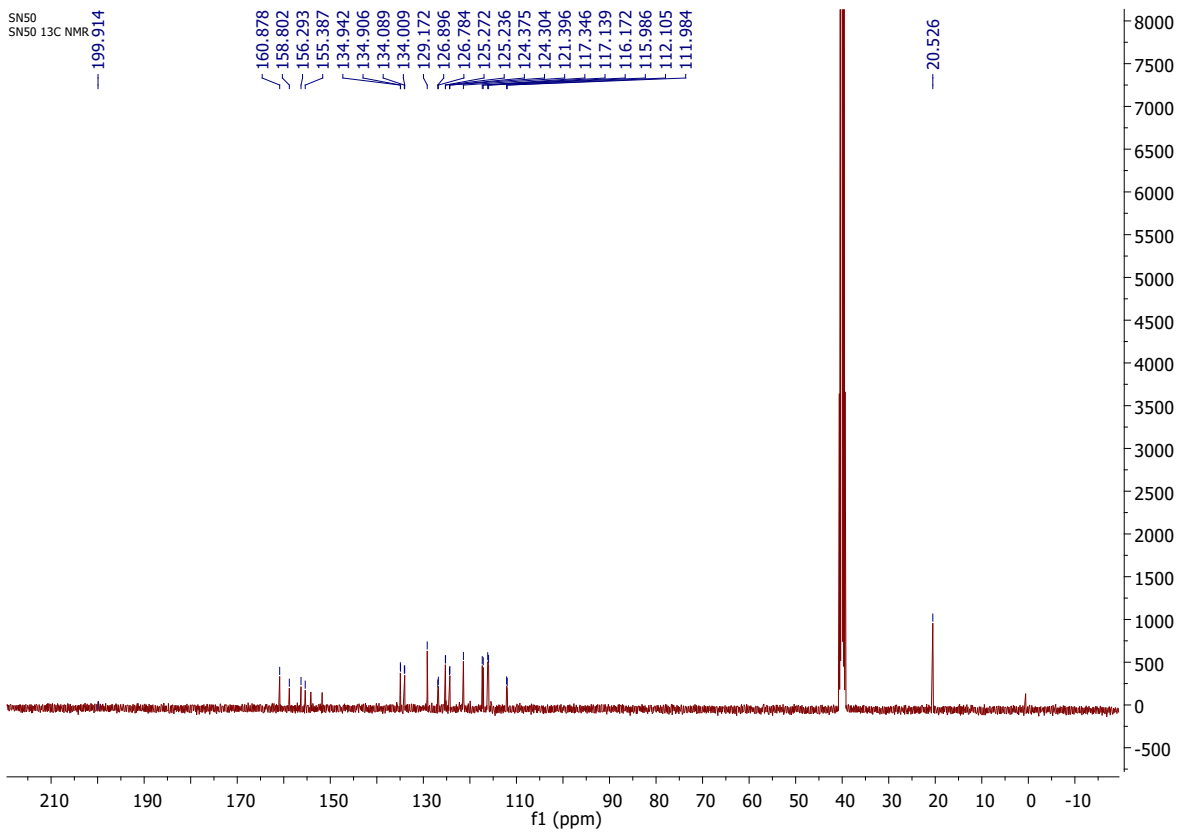
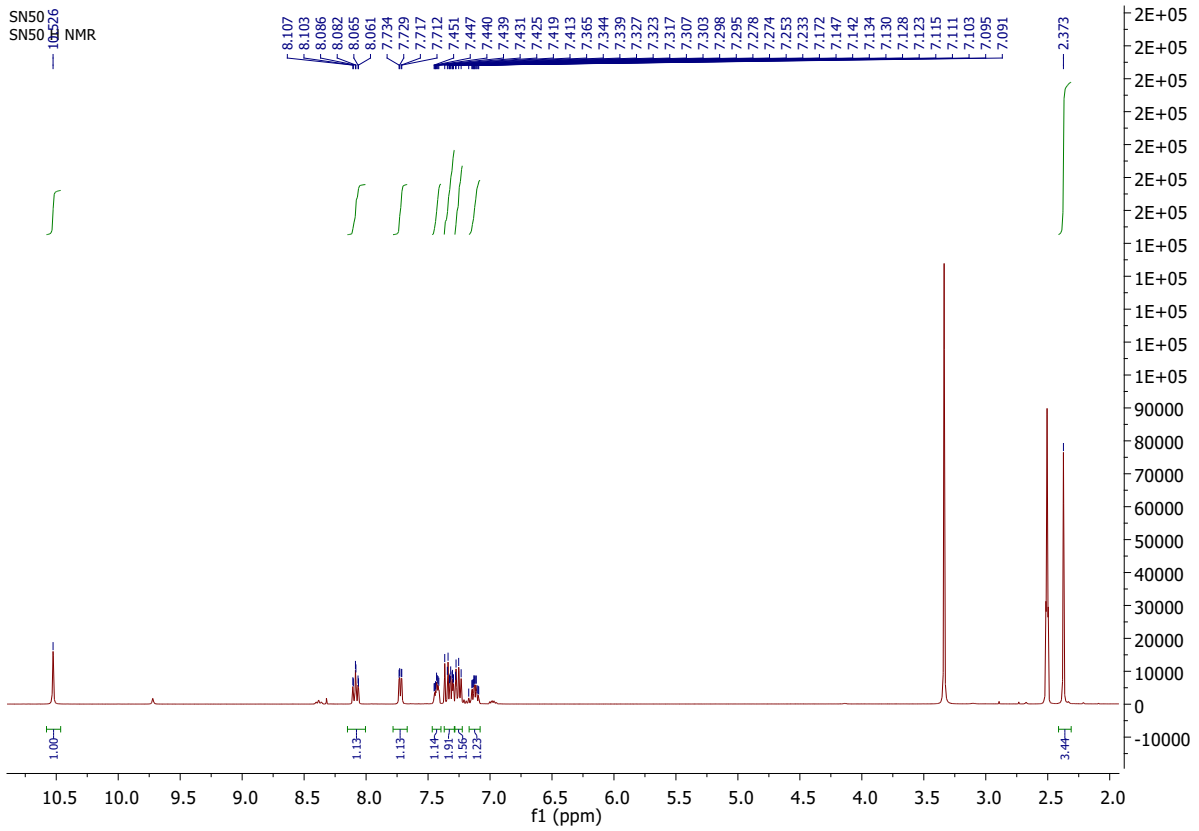
H¹ & ¹³CNMR of Compound 4f



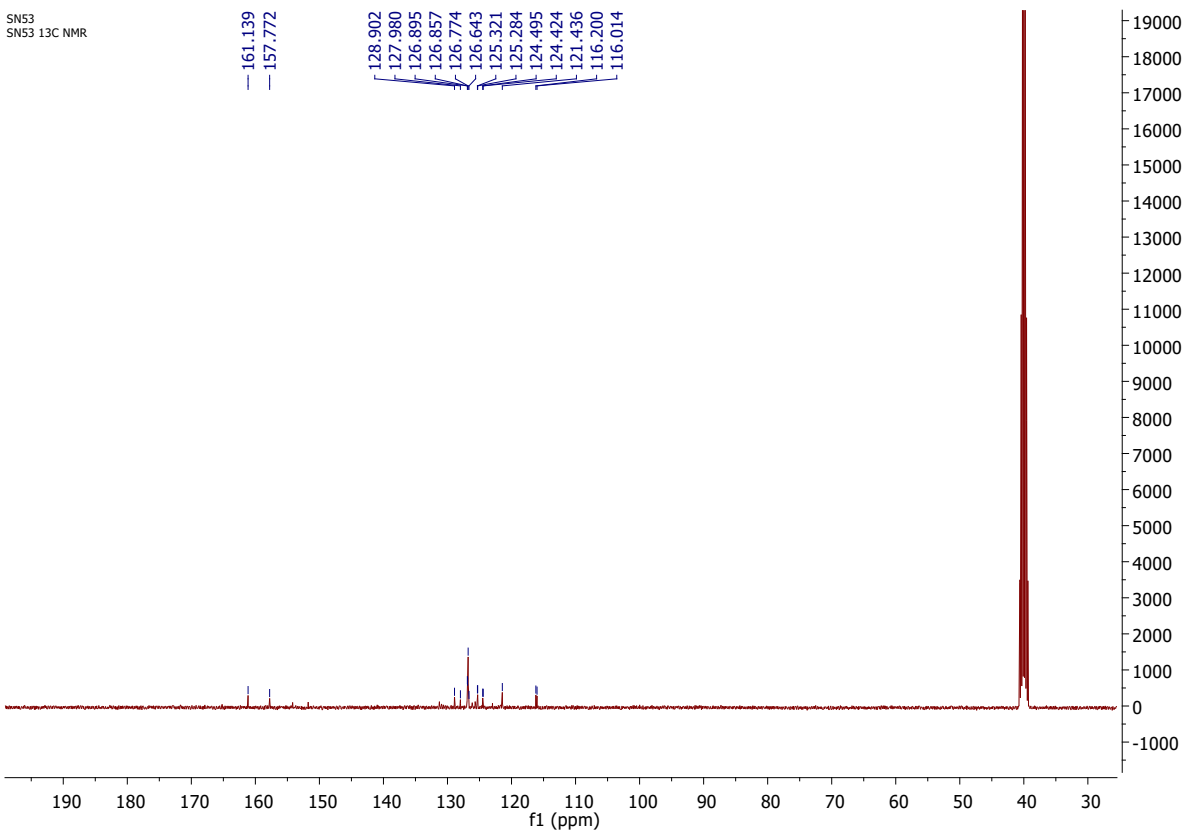
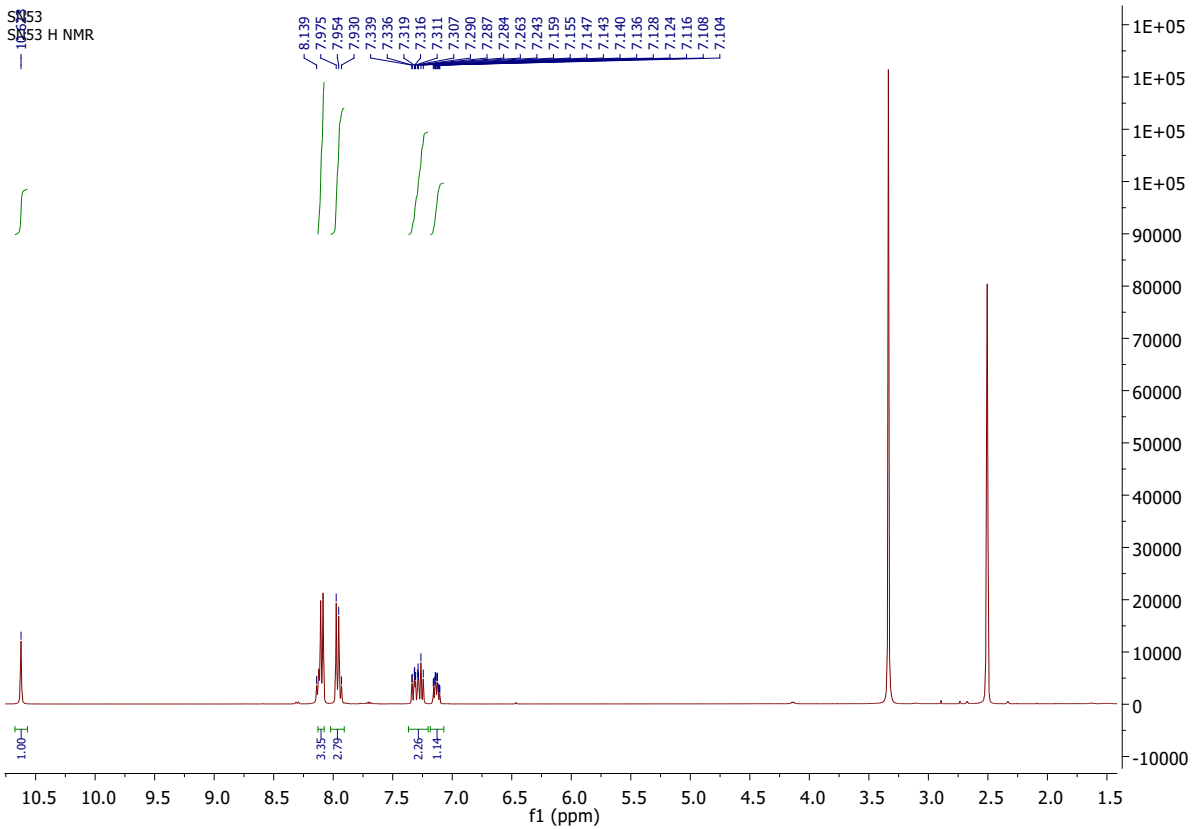
H^1 & ^{13}C NMR of Compound 4g



H^1 & ^{13}C NMR of Compound 4h

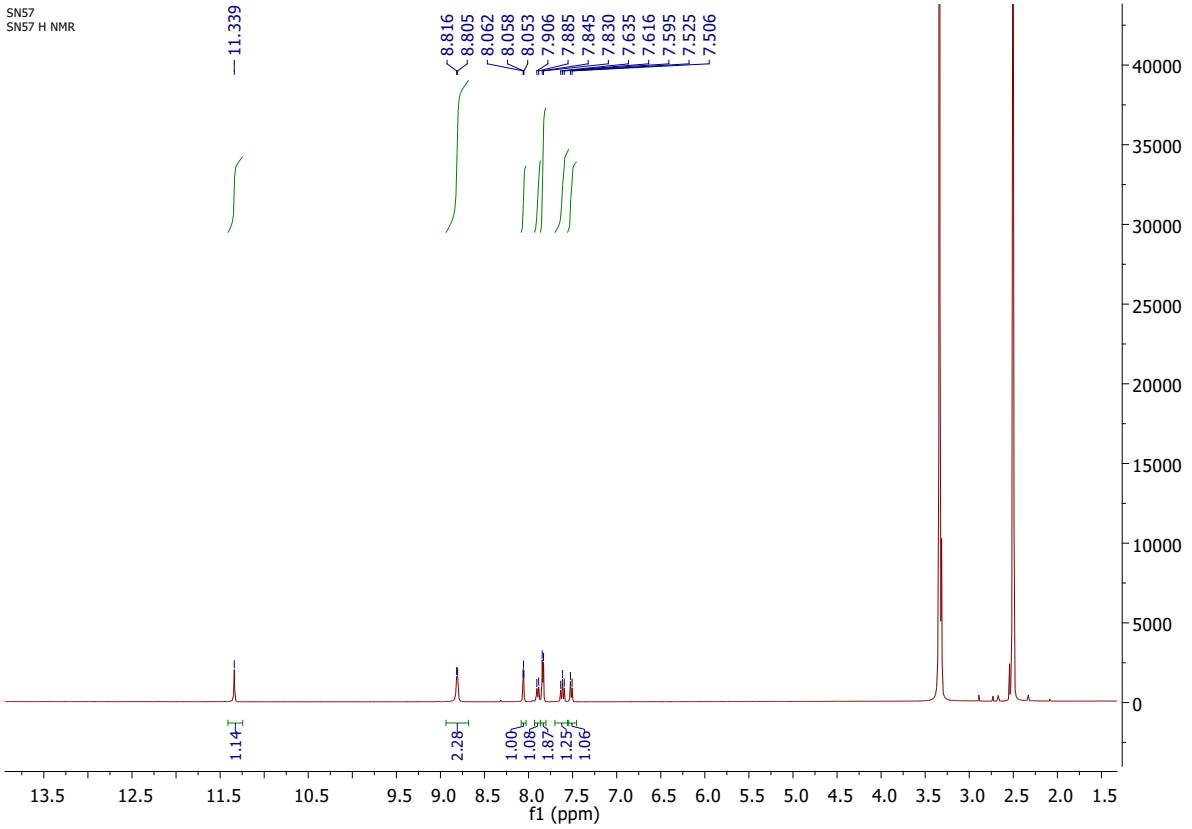


^1H & ^{13}C NMR of Compound 4i

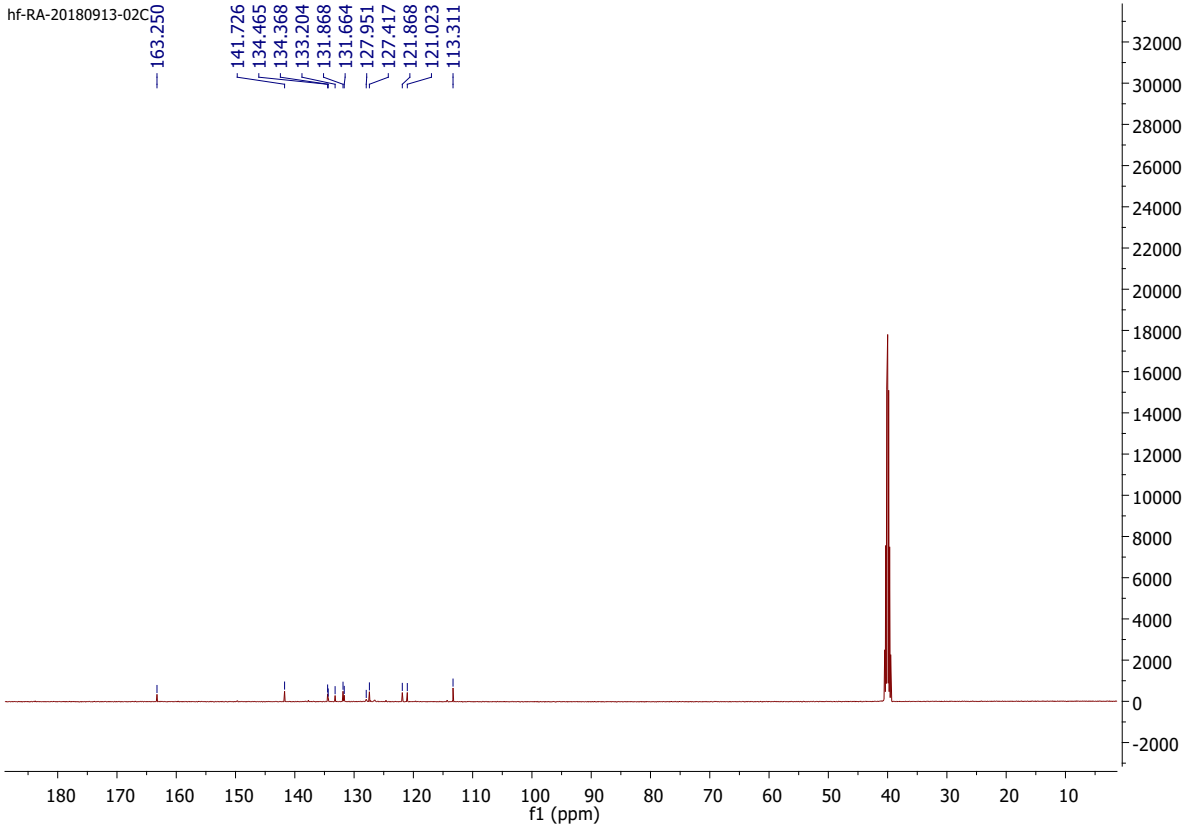


H^1 & ^{13}C NMR of Compound 4j

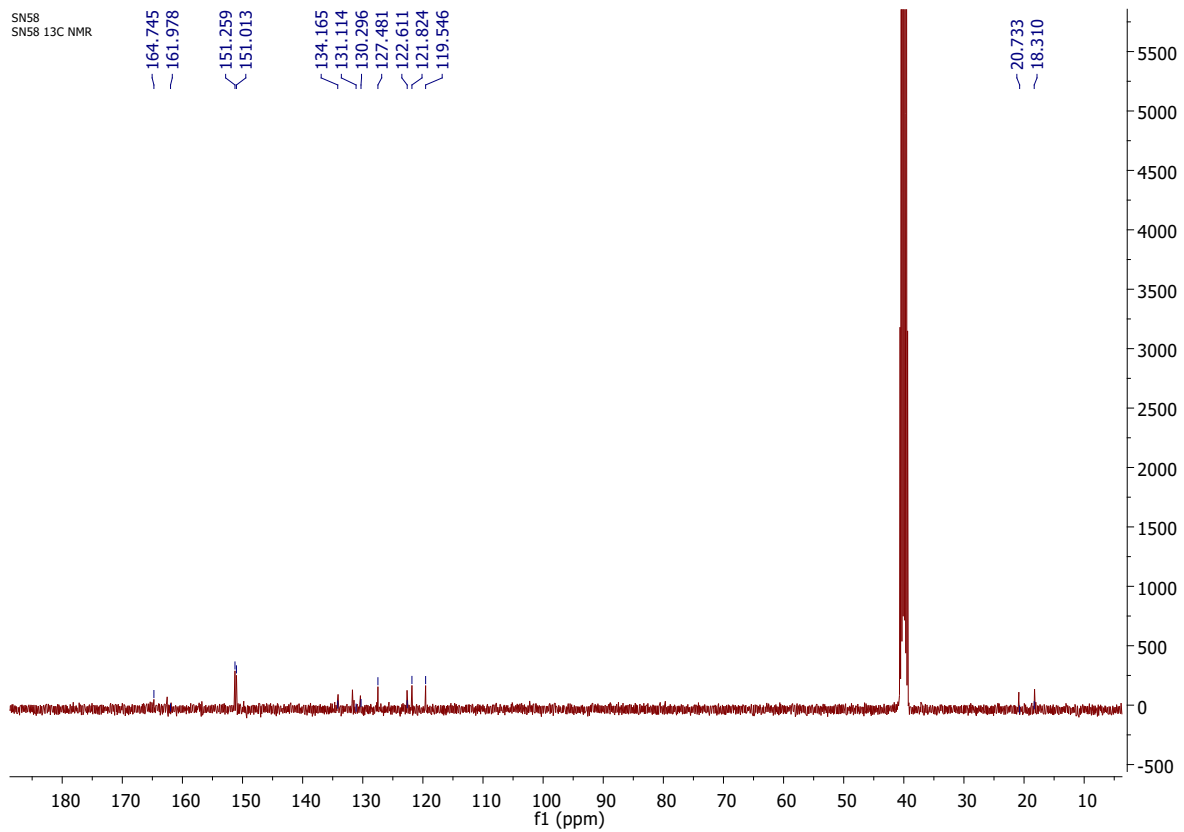
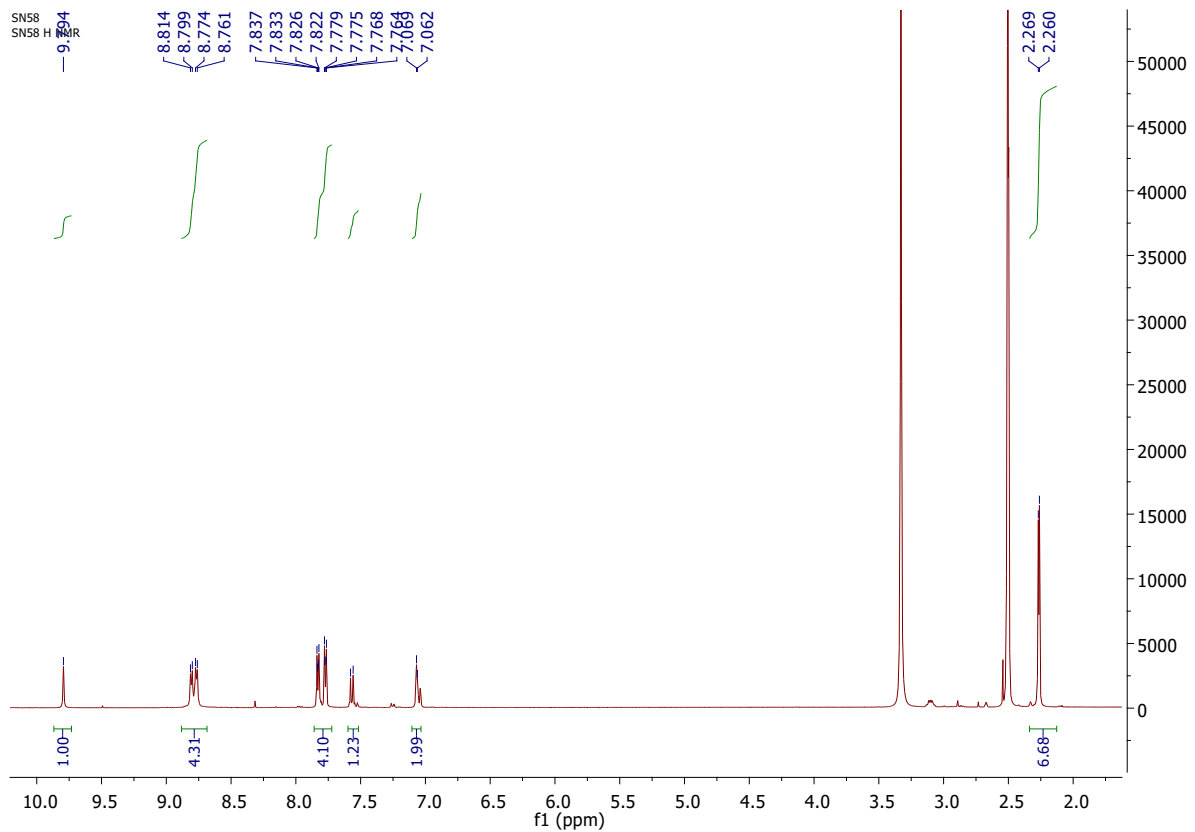
SN57
SN57 H NMR



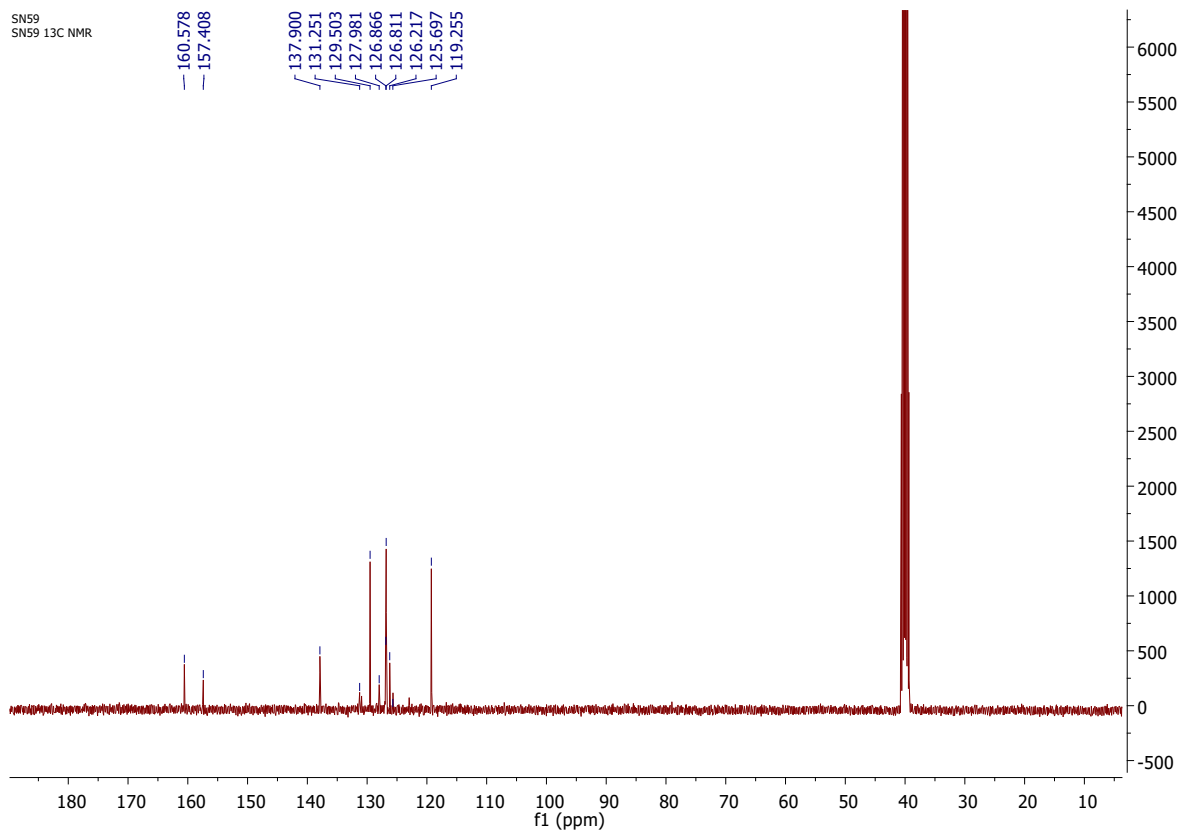
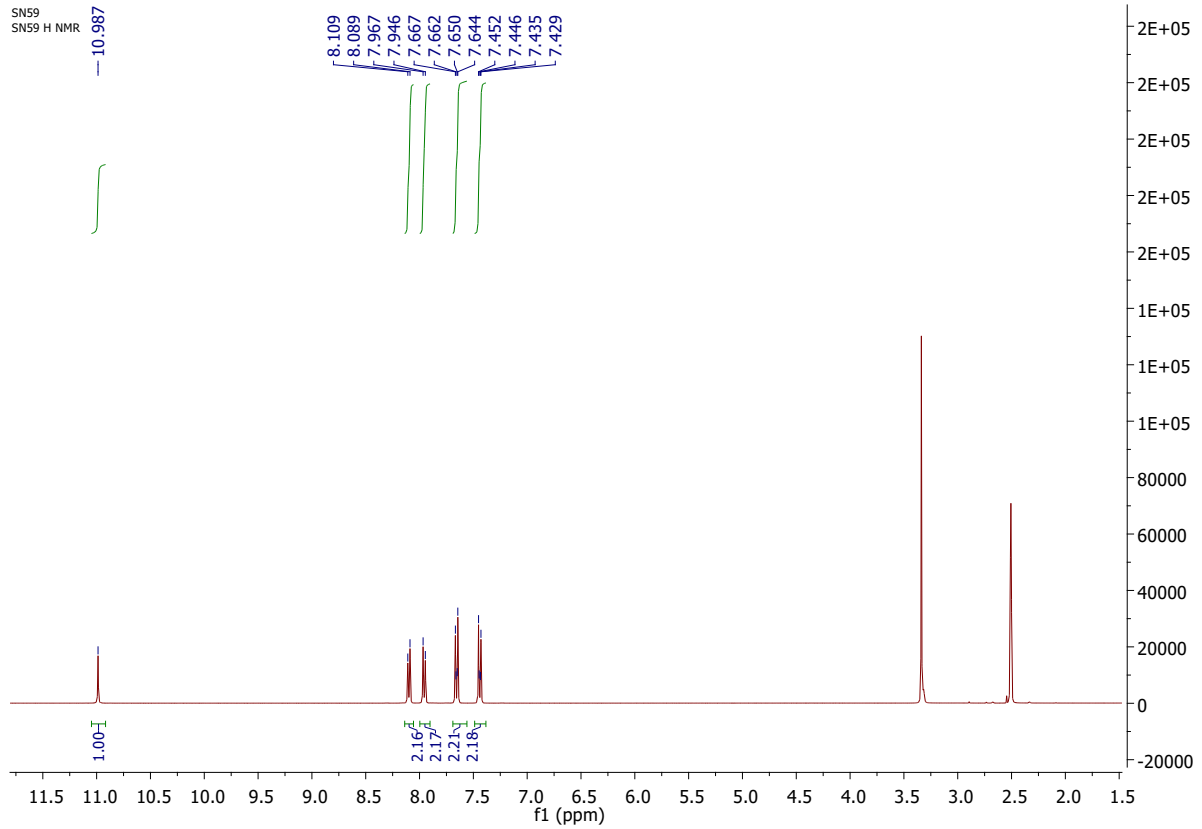
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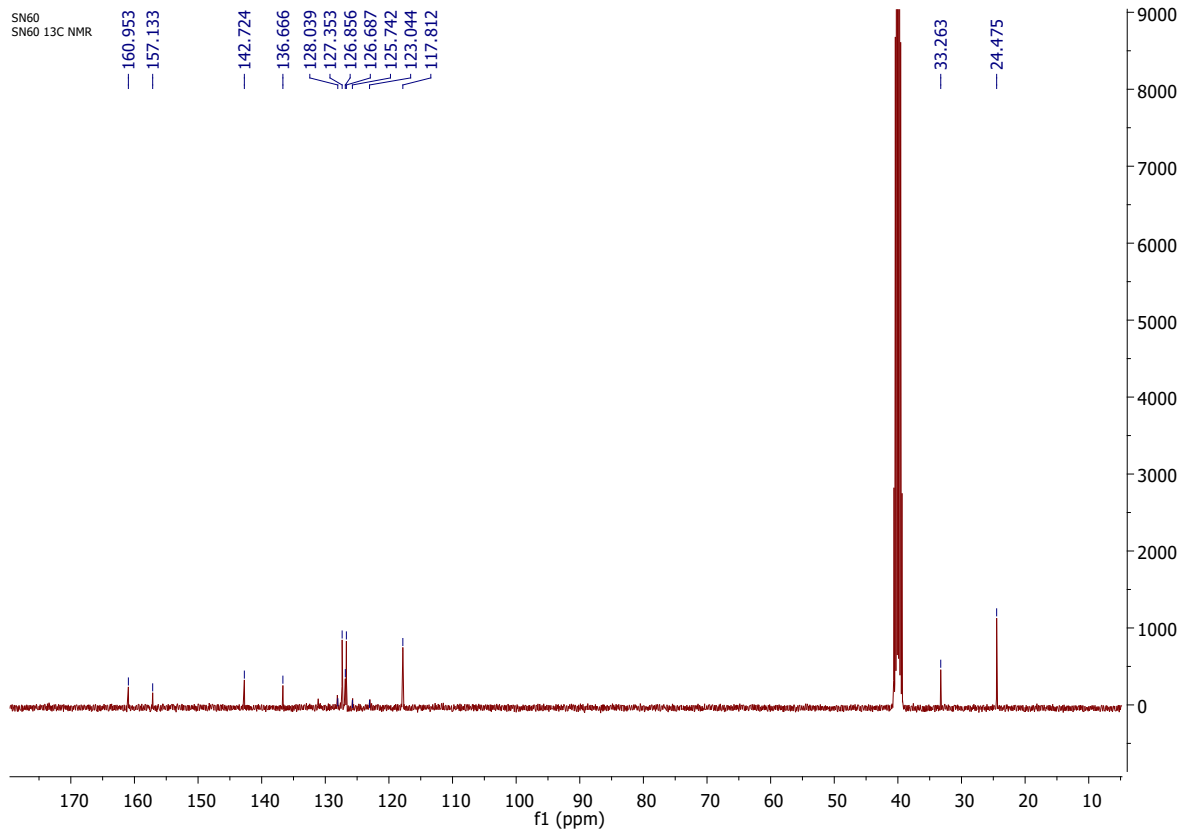
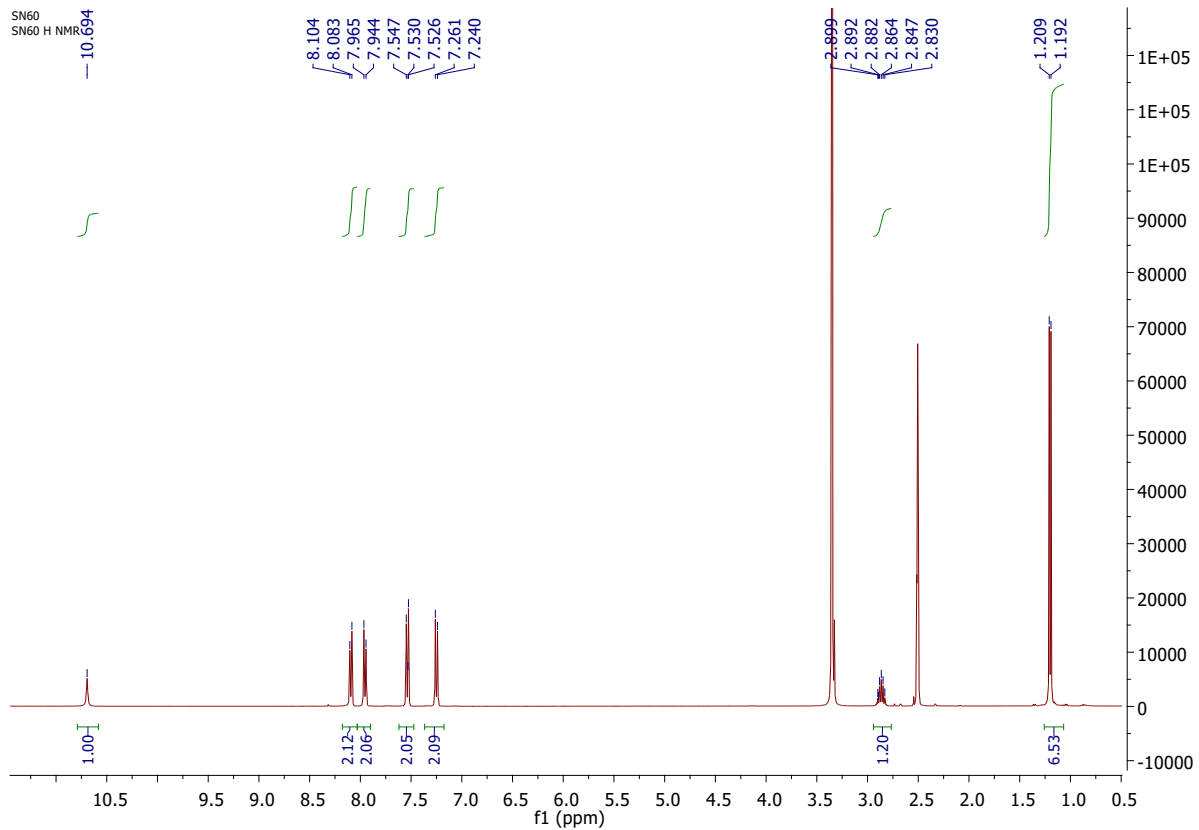
^1H & ^{13}C NMR of Compound 4k



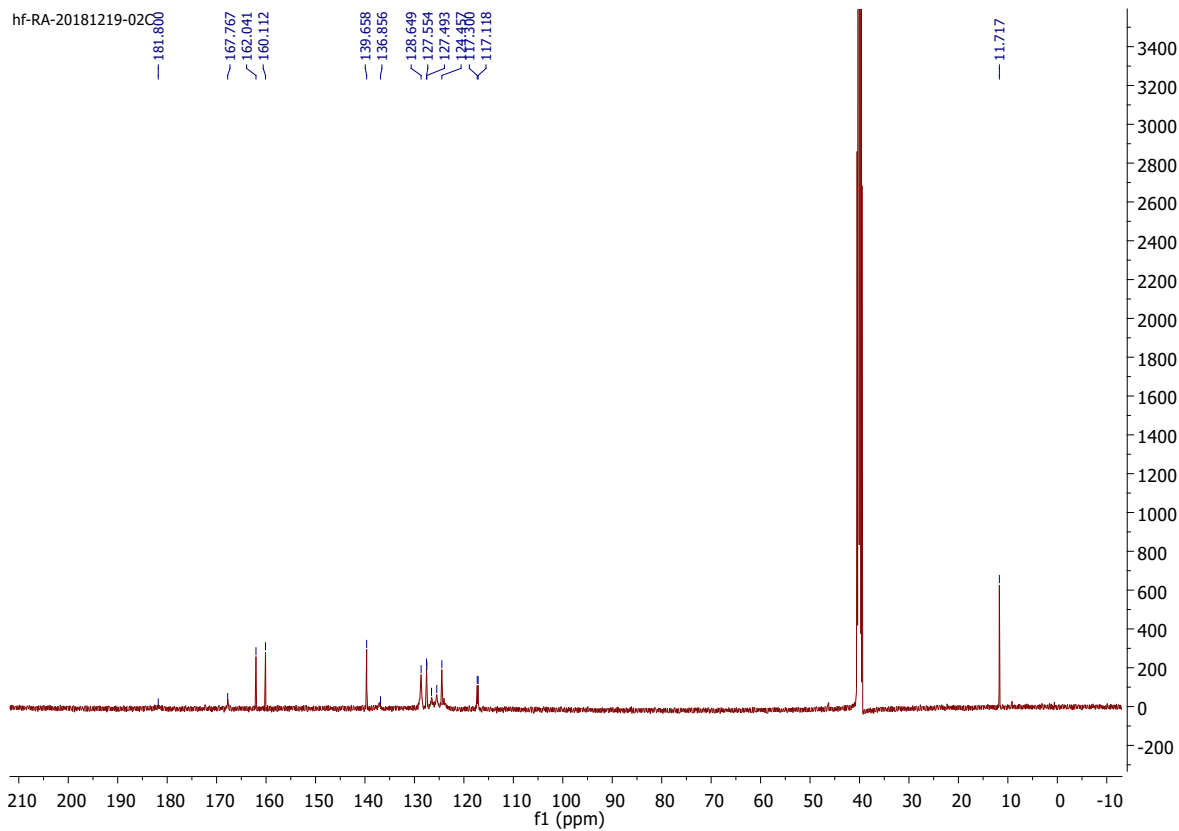
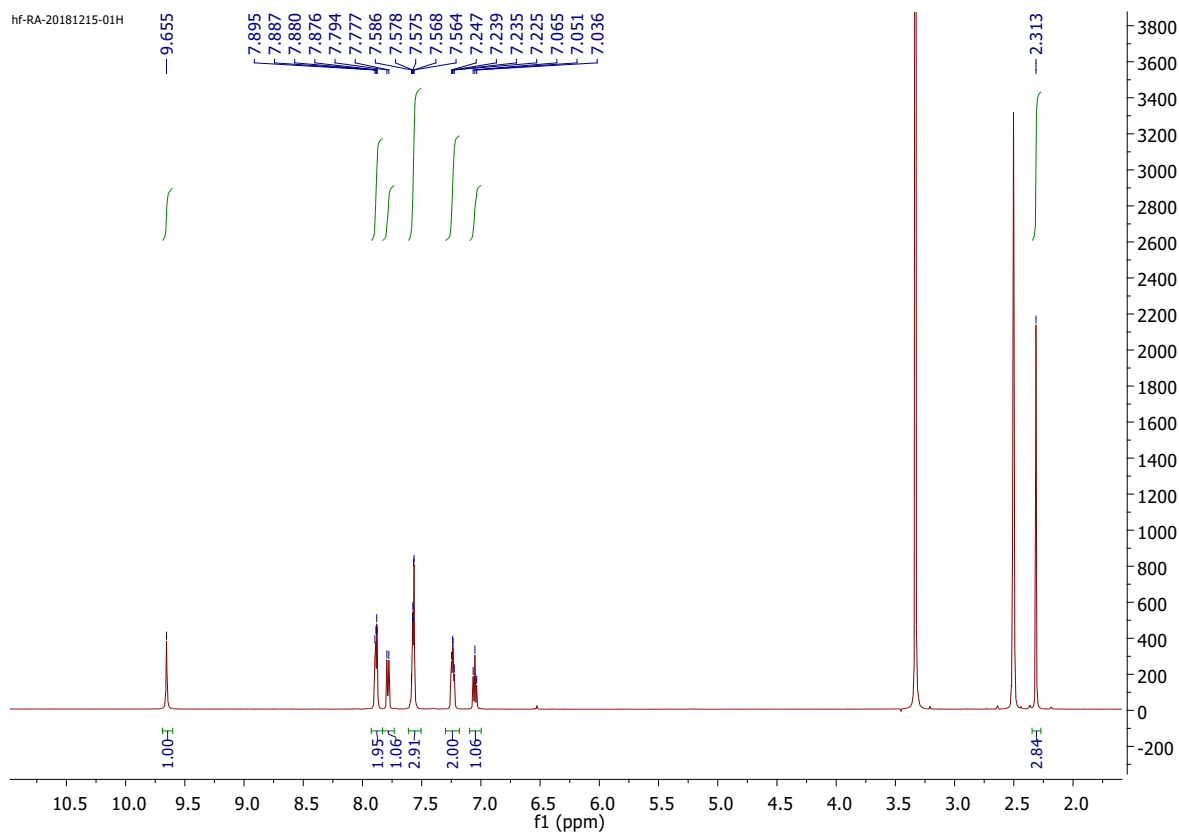
^1H & ^{13}C NMR of Compound 4l



H¹ & ¹³CNMR of Compound 4m



H¹ & ¹³CNMR of Compound 4n



^1H & ^{13}C NMR of Compound 4o

