

Supplementary Information

Facile Synthesis of Substituted 2-Aroylbenzo[*b*]thiophen-3-ols to Approach Novel Triazole Hybrids Using Click Chemistry

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General Information

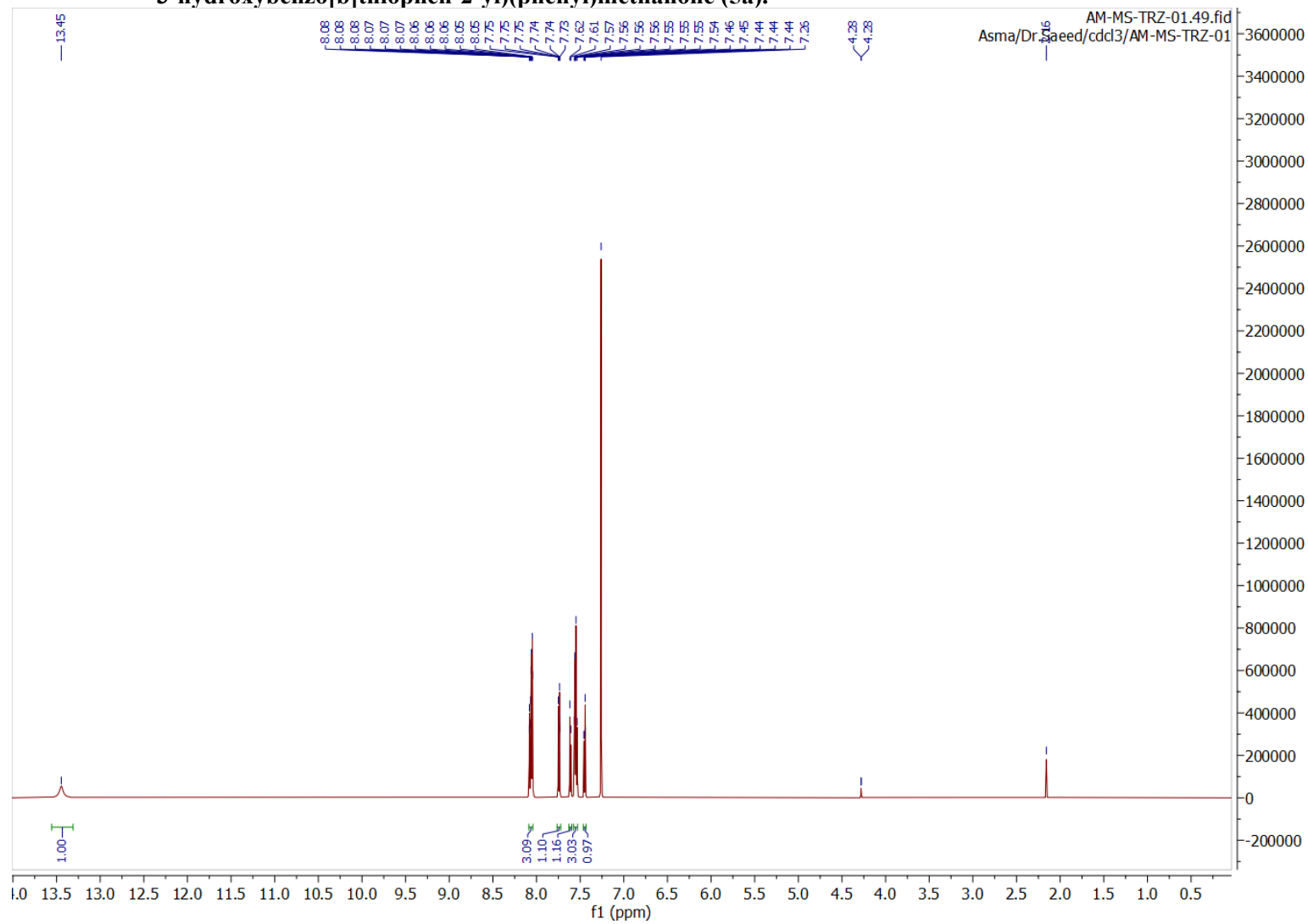
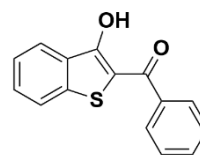
All the chemicals and reagents were purchased from different vendors (Merck, Sigma Aldrich & TCI) and were used without further purification. Solvents for syntheses and chromatographic work were distilled and properly dried before use (if required). The progress of reactions was monitored by TLC plates (Aluminium sheet pre-coated with silica gel) by visualizing under the UV lamp at 254 nm wavelength. The reaction mixtures were purified using silica gel column chromatography (pore size 60 Å, 230-400 mesh size, 40-63 µm). FTIR spectra were recorded using Bruker Alpha Platinum AT applying ATR sampling technique through neat samples. NMR spectra were recorded in deuterated solvent using Bruker 600 MHz NMR instrument (Avance Neo Bruker). GCMS data were obtained using 1300 GC-MS (Thermo Scientific). Melting points were measured by using "STUART SMP3" apparatus.

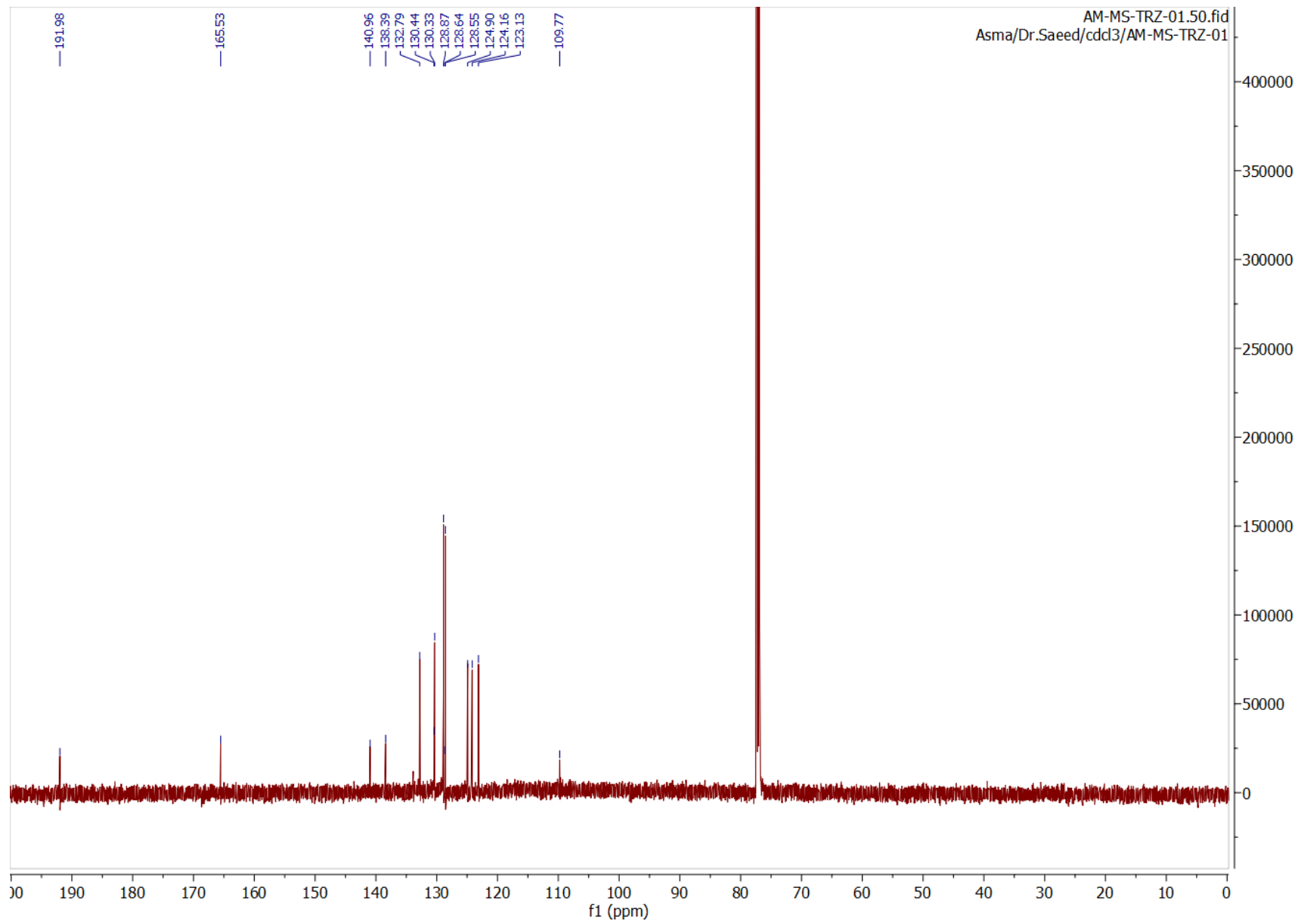
Table S1. Crystal data and structure refinement (CCDC 2297186)

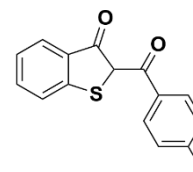
Chemical formula	C ₁₆ H ₉ F ₃ O ₂ S
M_r	322.29
Crystal system, space group	triclinic, <i>P-1</i>
Temperature (K)	100(2)
a, b, c (Å)	6.5671(10), 7.2171(11), 14.364(2)
α	85.588(4)°
β	81.019(4)°
γ	83.178(4)°
V (Å ³)	1117.9 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.27
Crystal size (mm)	0.39 × 0.27 × 0.08
Diffractionmeter	Bruker AXS <i>SMART APEX</i>
Absorption correction	Multi-scan (<i>SADABS</i> ; Sheldrick, 2004)
T_{\min}, T_{\max}	0.901, 0.979
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10330, 2652, 2171
R_{int}	0.039
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.658
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.095, 1.06
No. of reflections	2652
No. of parameters	140
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.39, -0.37

Spectroscopic Data (¹H NMR and ¹³C NMR Scans)

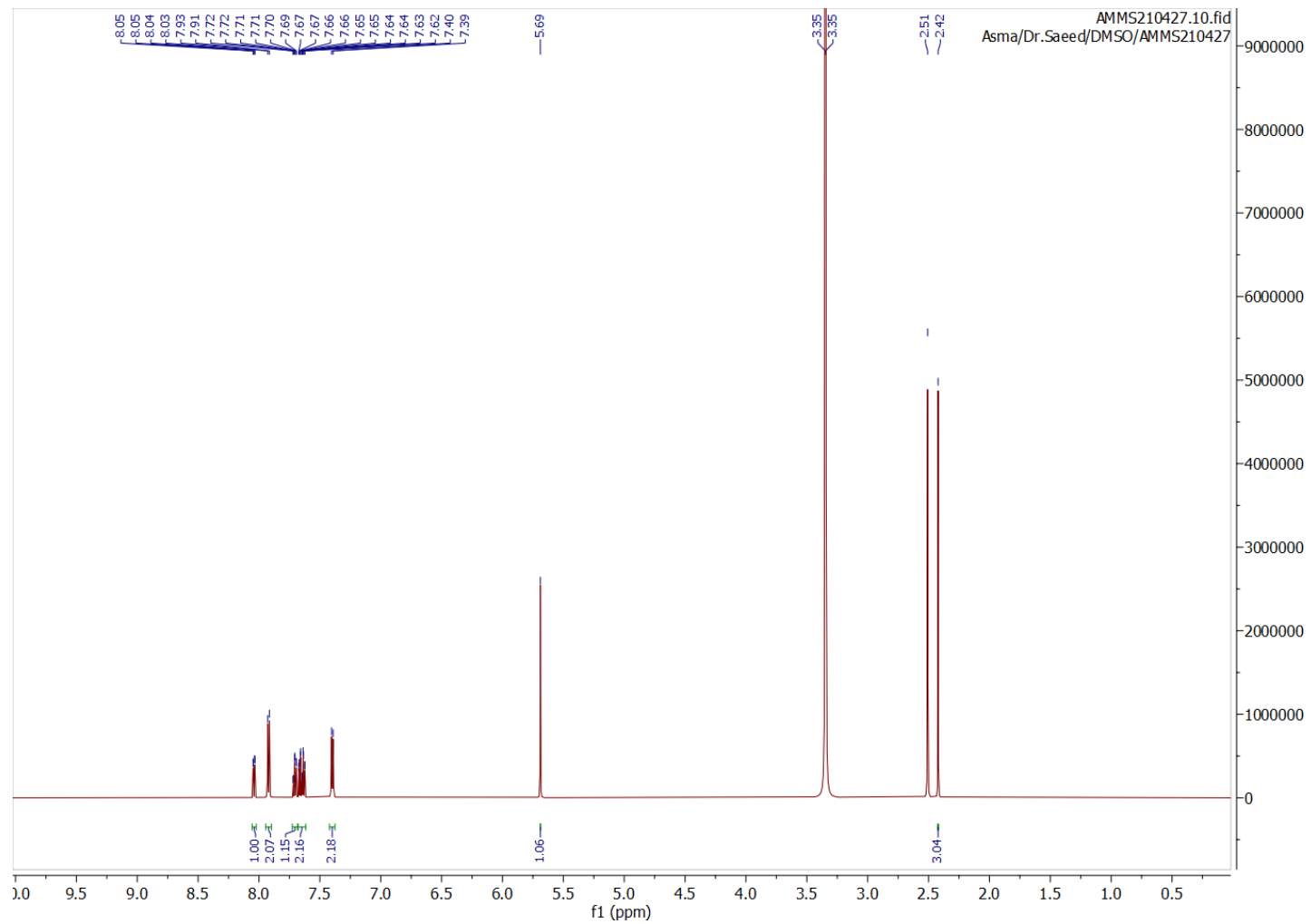
3-hydroxybenzo[b]thiophen-2-yl)(phenyl)methanone (5a).

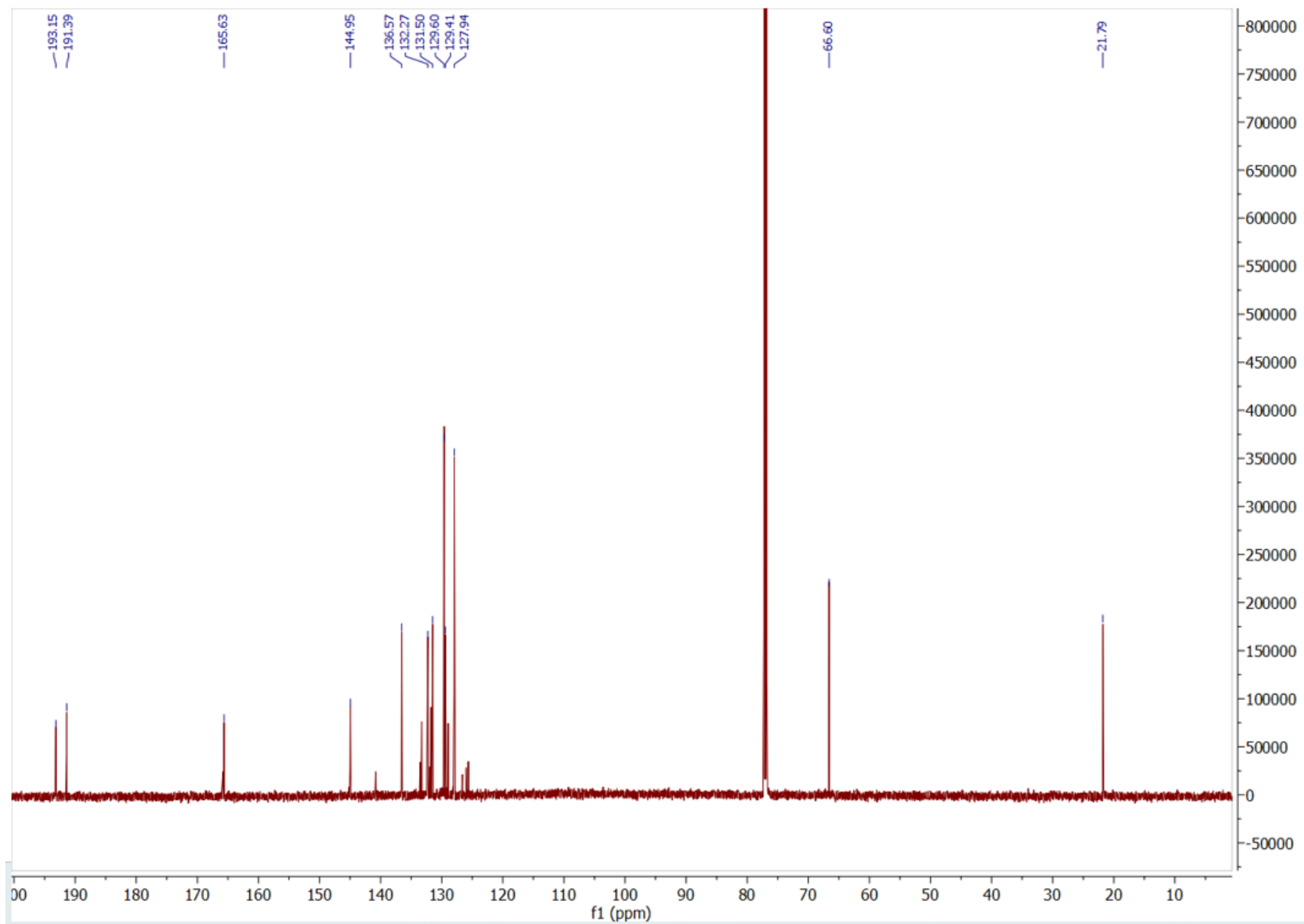




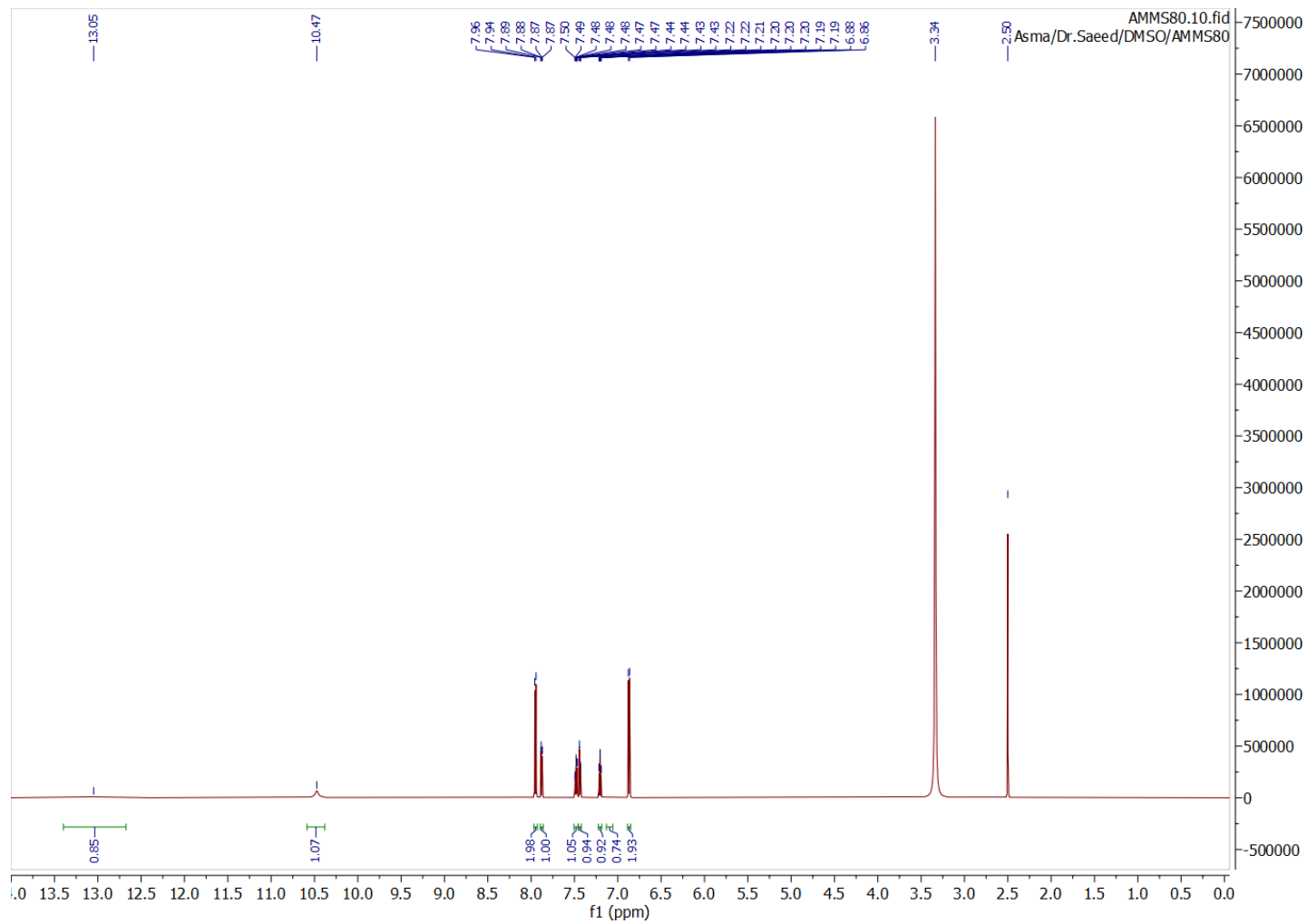
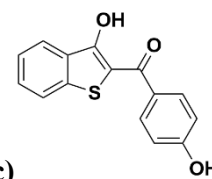


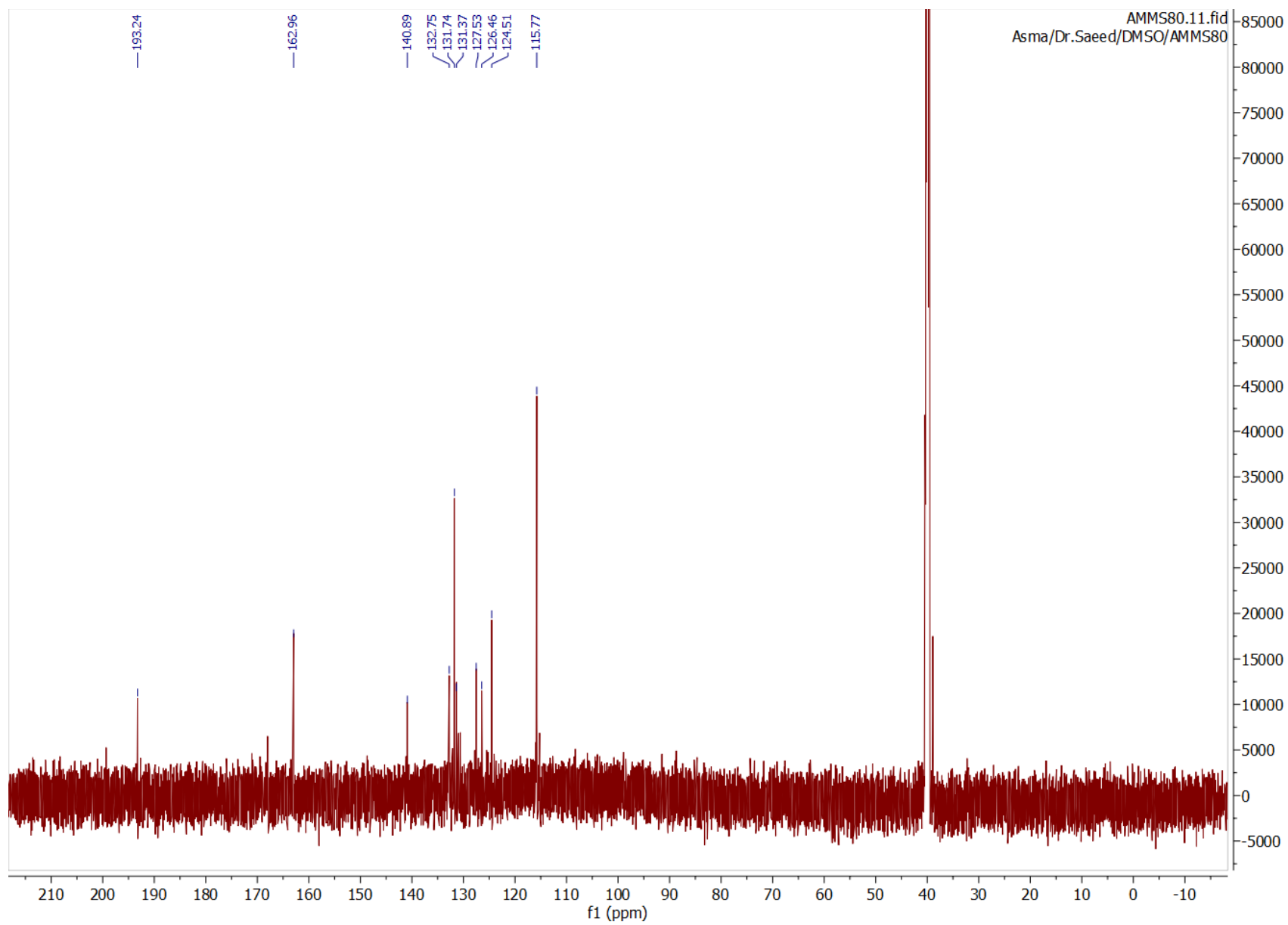
(3-hydroxybenzo[b]thiophen-2-yl)(p-tolyl)methanone (5b)

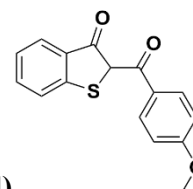




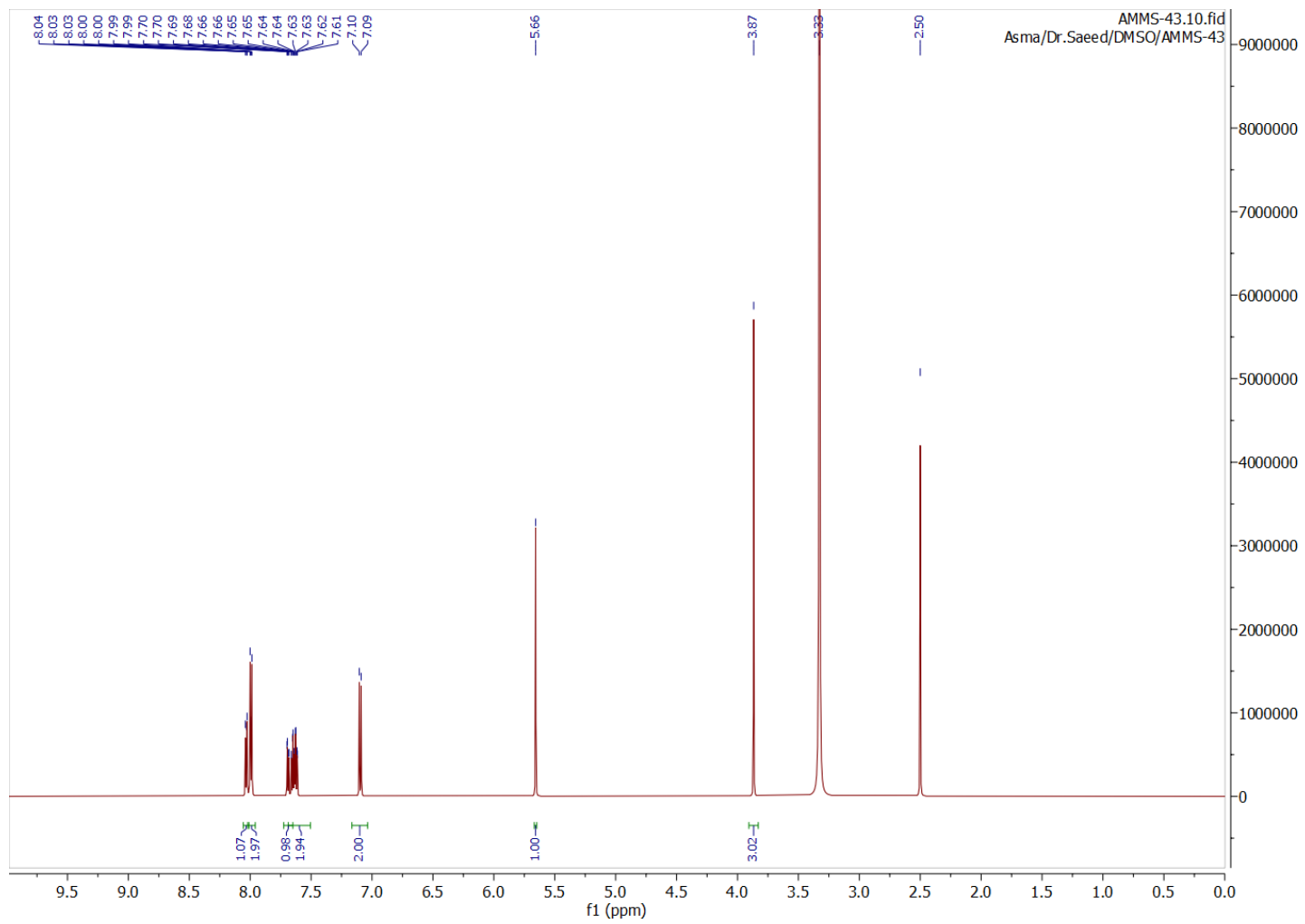
(3-hydroxybenzo[b]thiophen-2-yl)(4-hydroxyphenyl)methanone (5c)

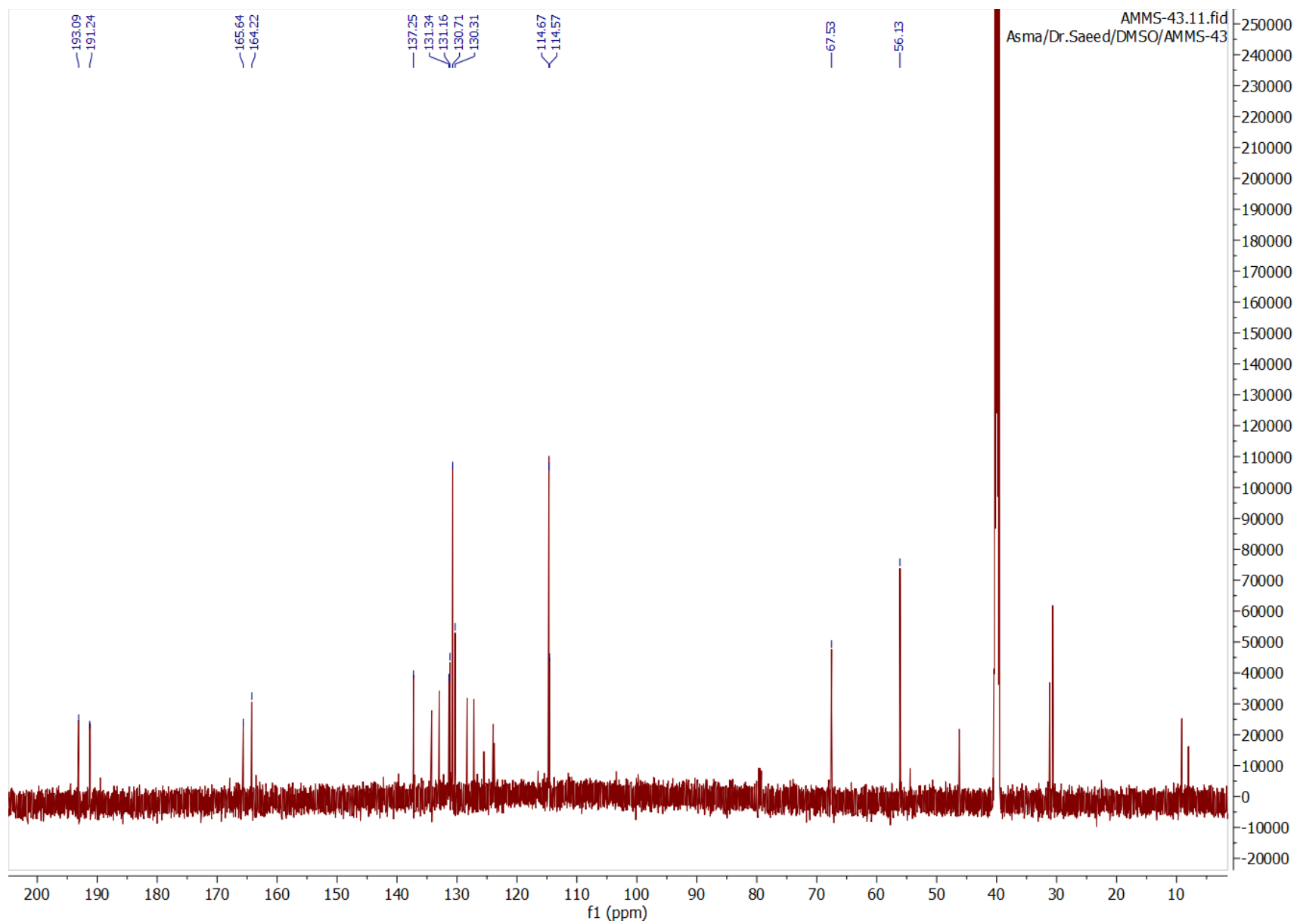


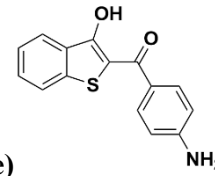




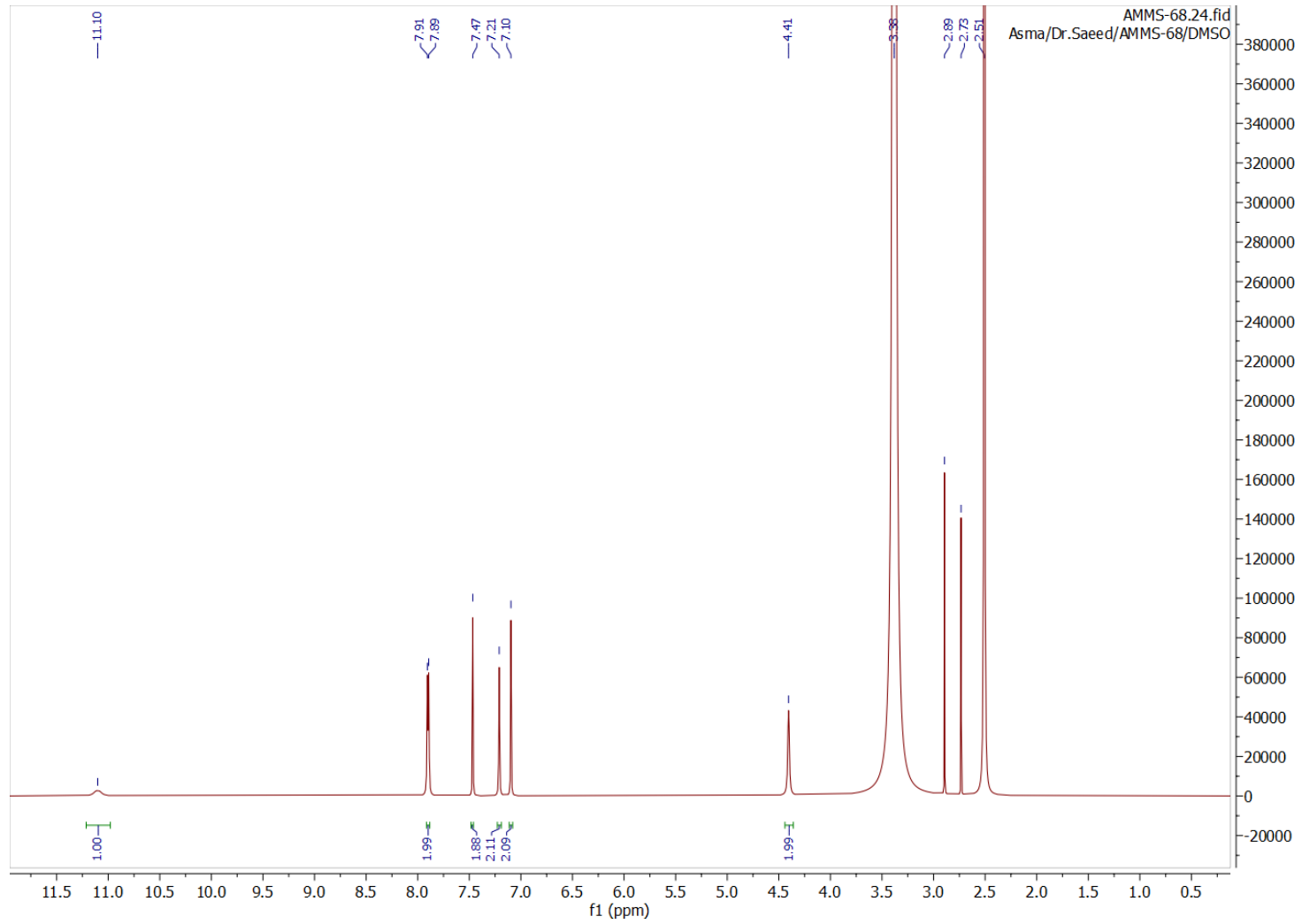
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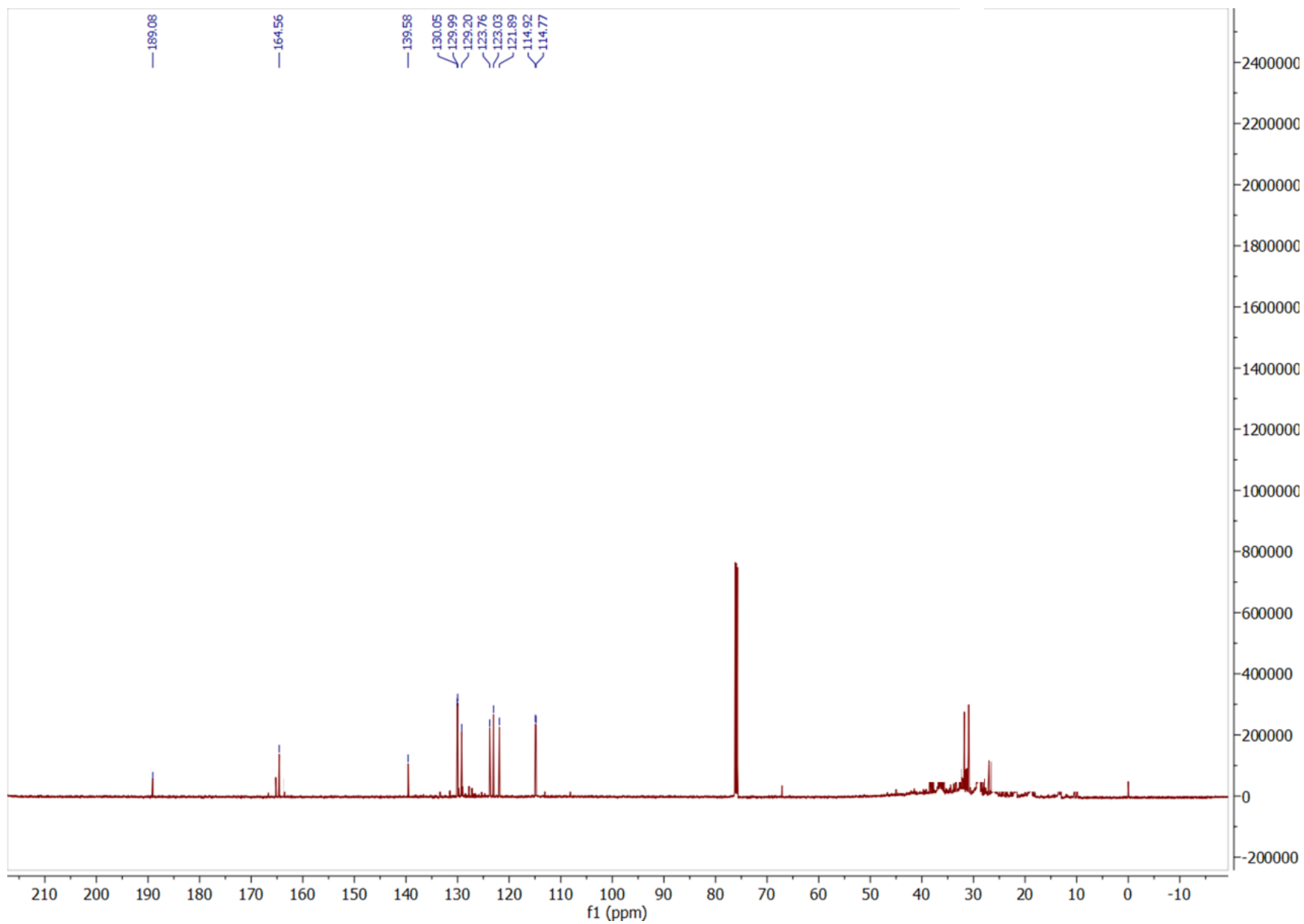


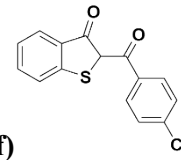




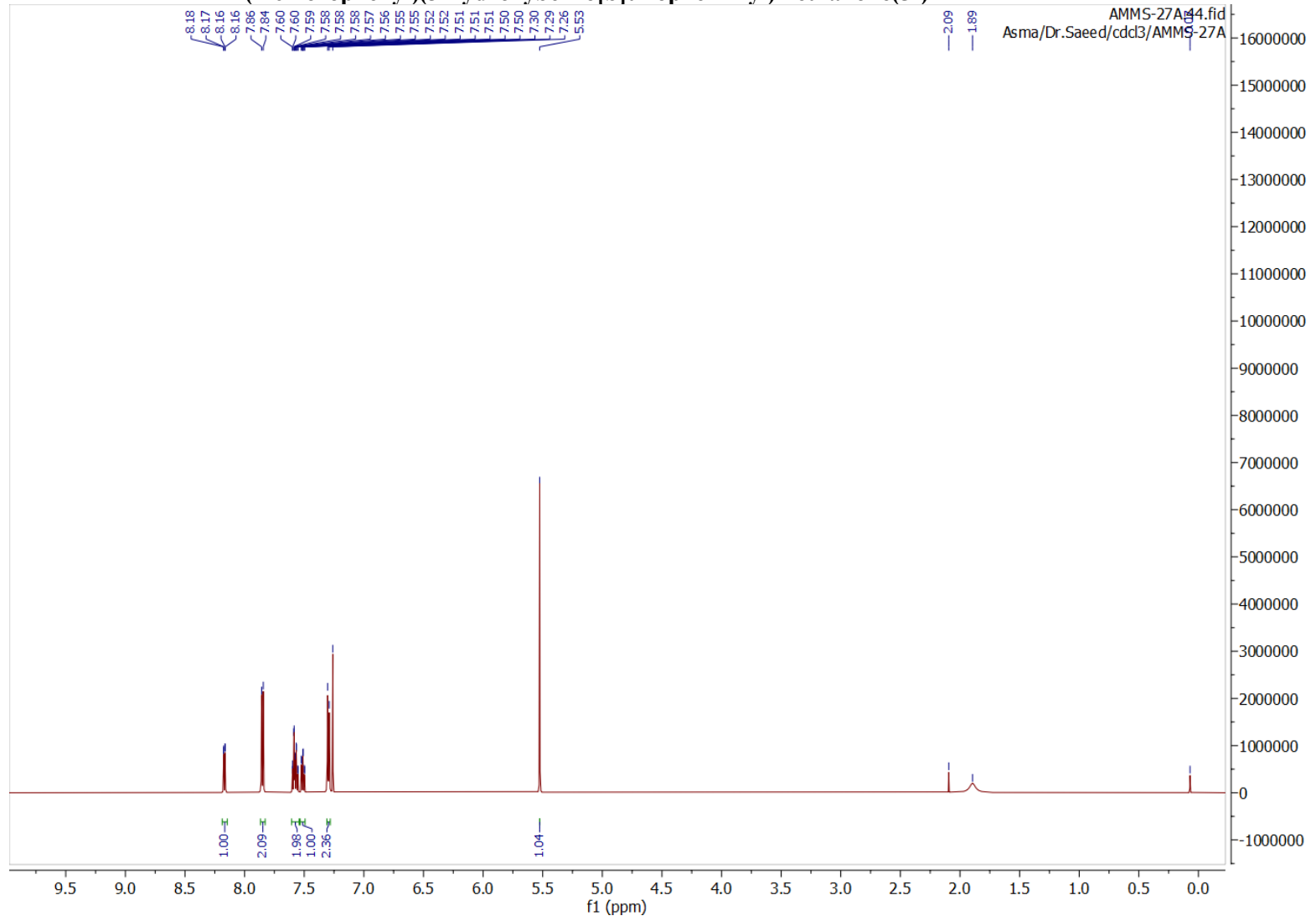
(4-aminophenyl)(3-hydroxybenzo[b]thiophen-2-yl)methanone (5e)

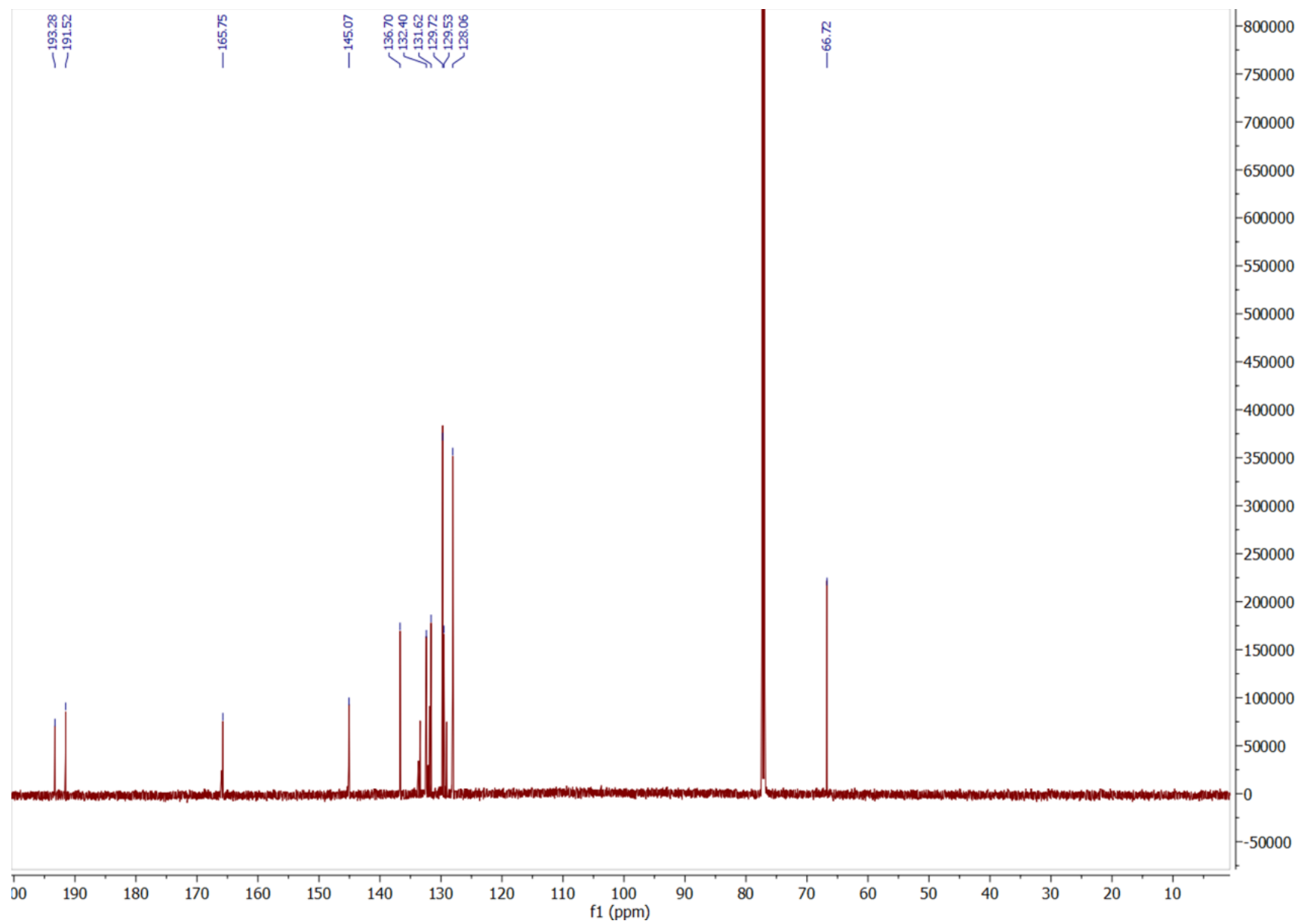


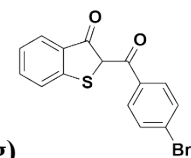




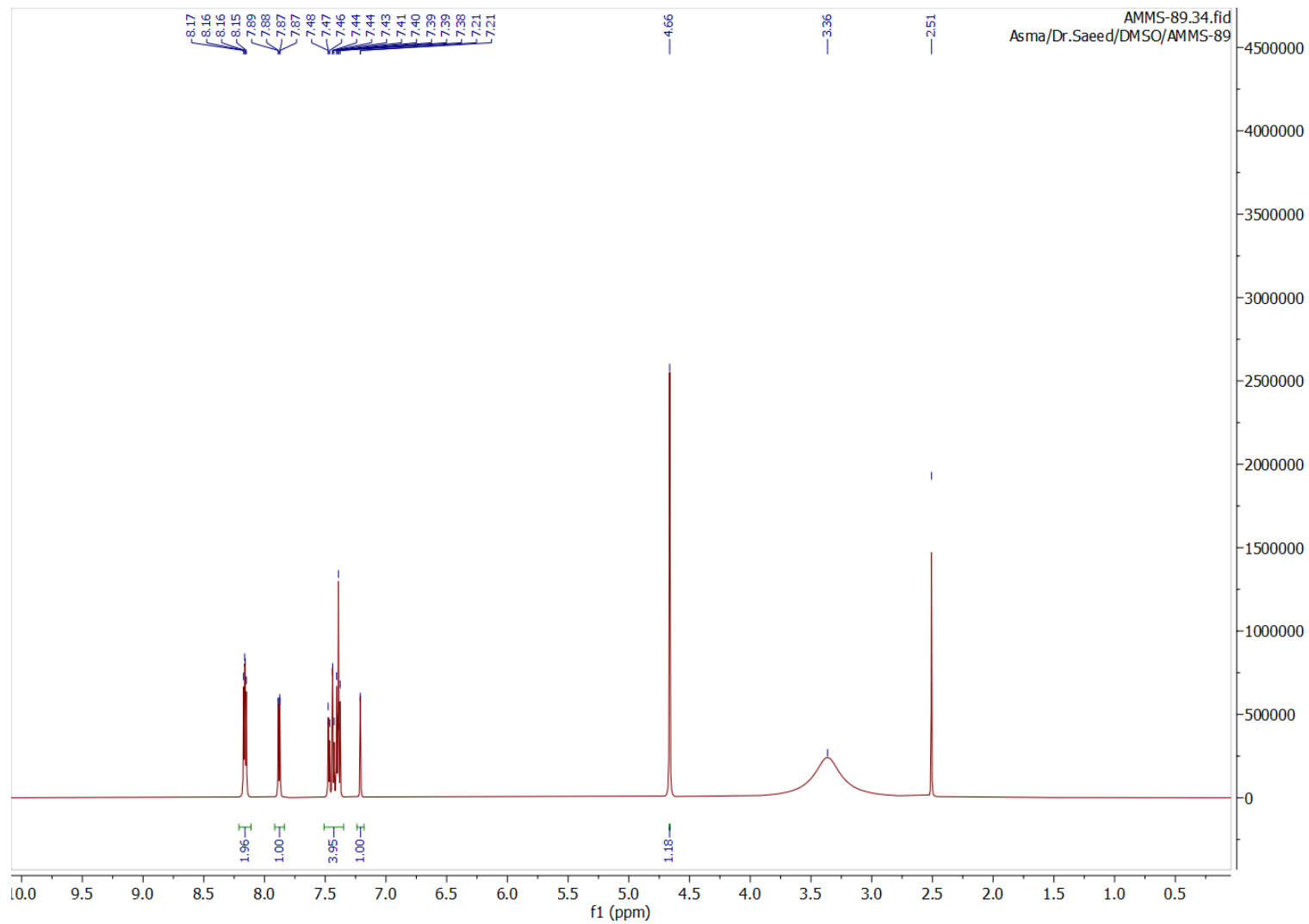
(4-chlorophenyl)(3-hydroxybenzo[b]thiophen-2-yl)methanone(5f)

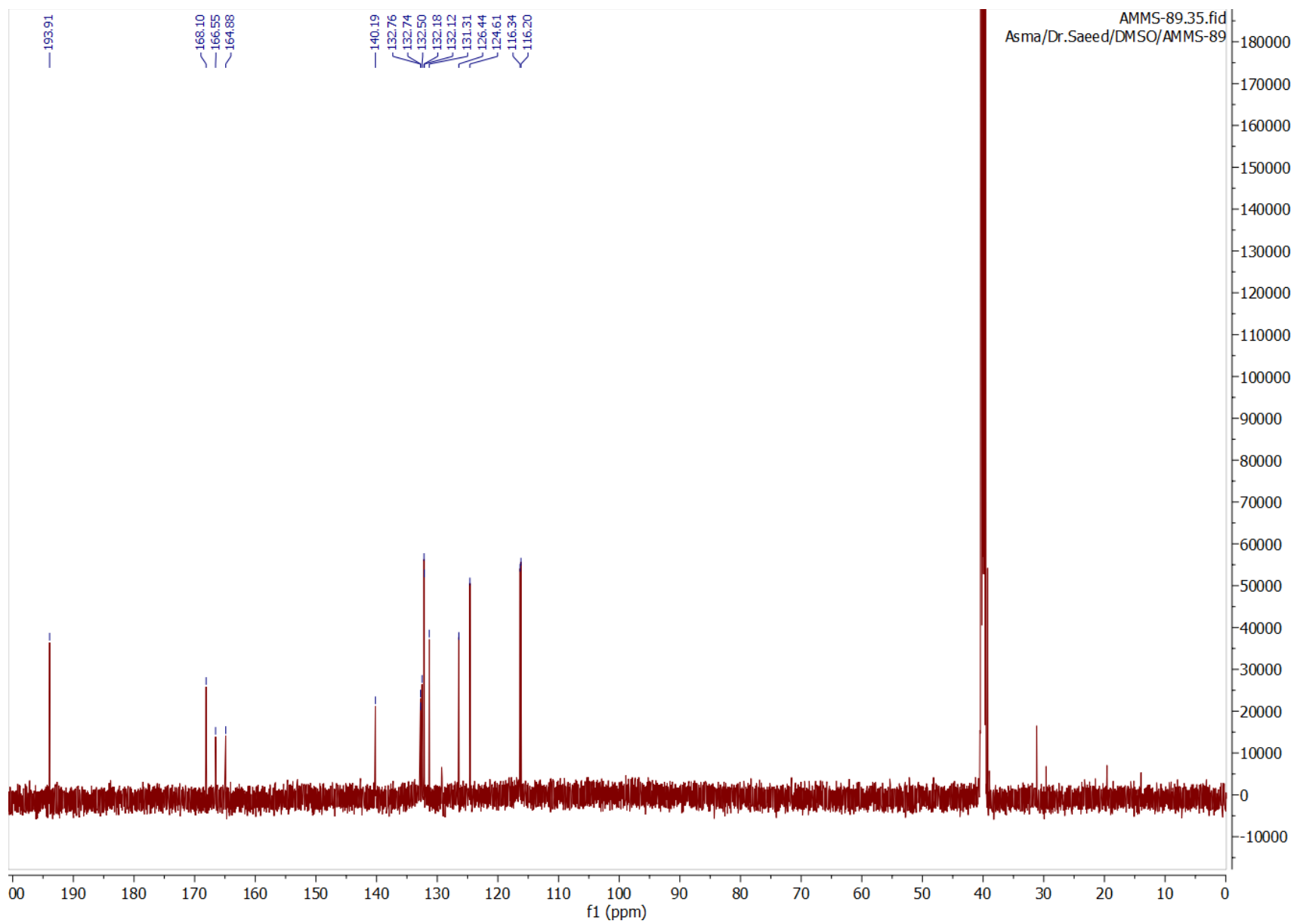


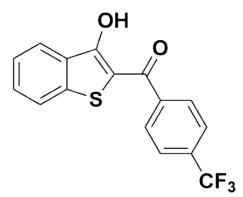




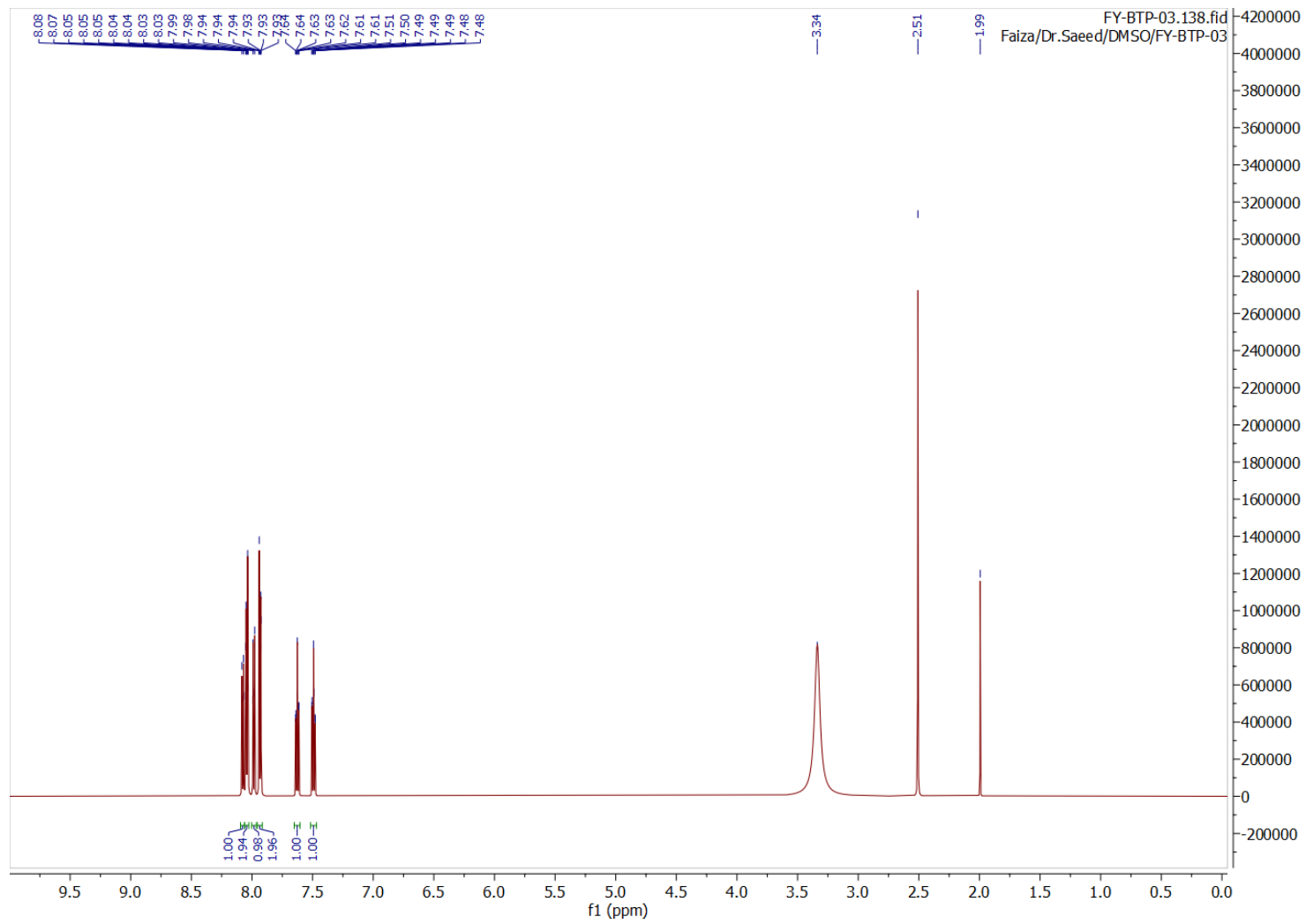
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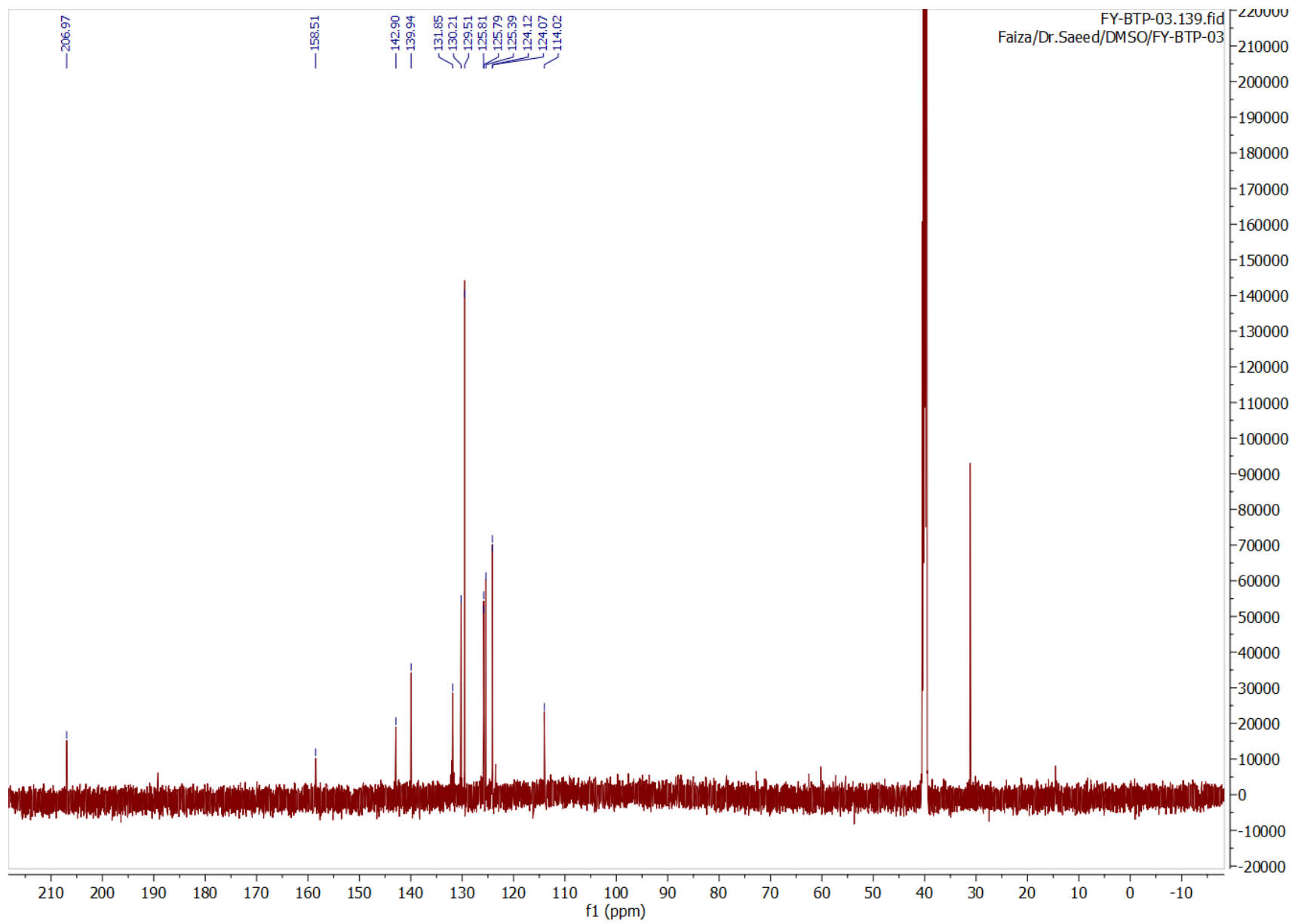


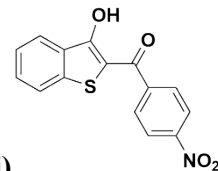




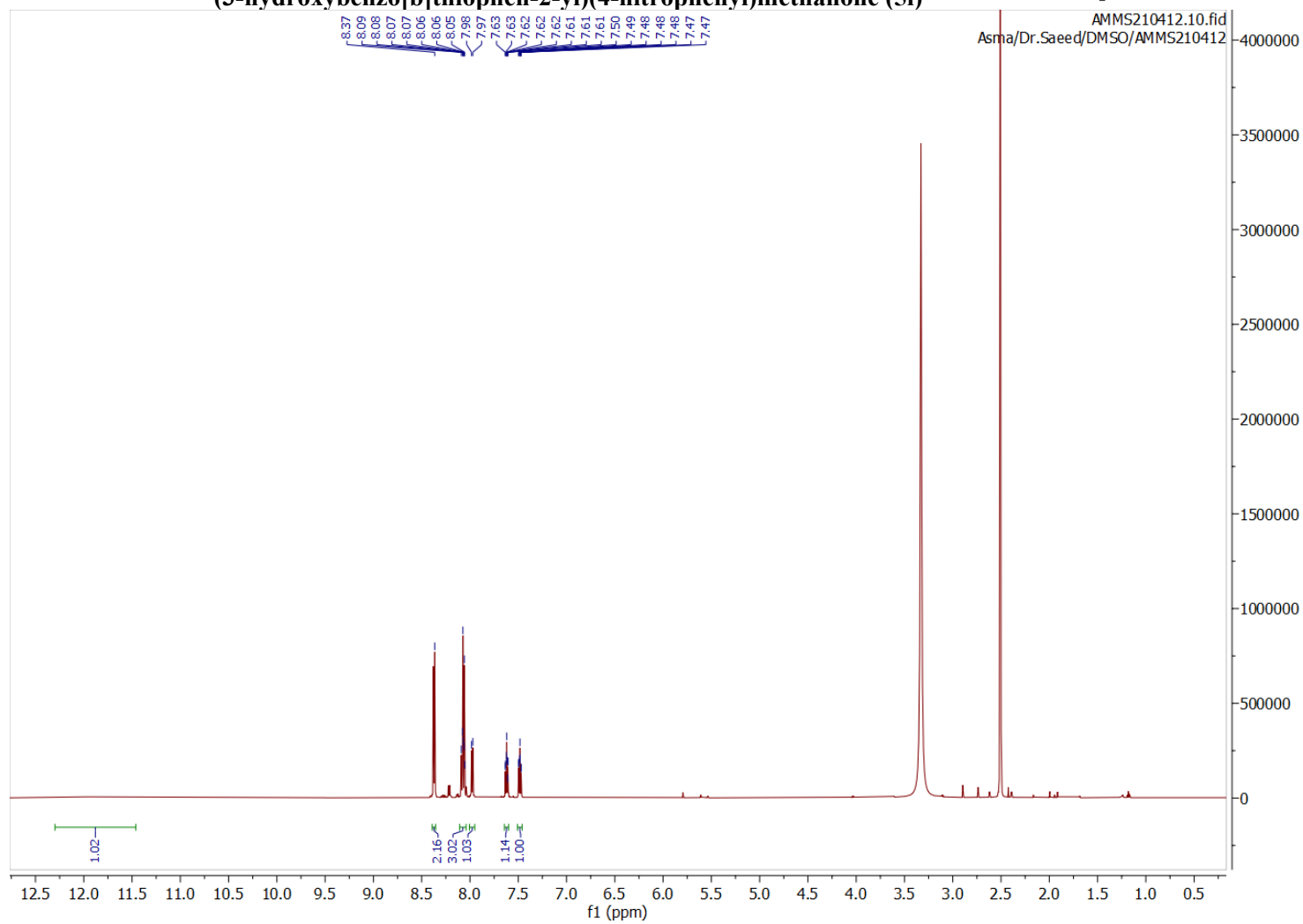
(3-hydroxybenzo[b]thiophen-2-yl)(4-(trifluoromethyl)phenyl)methanone (5h)

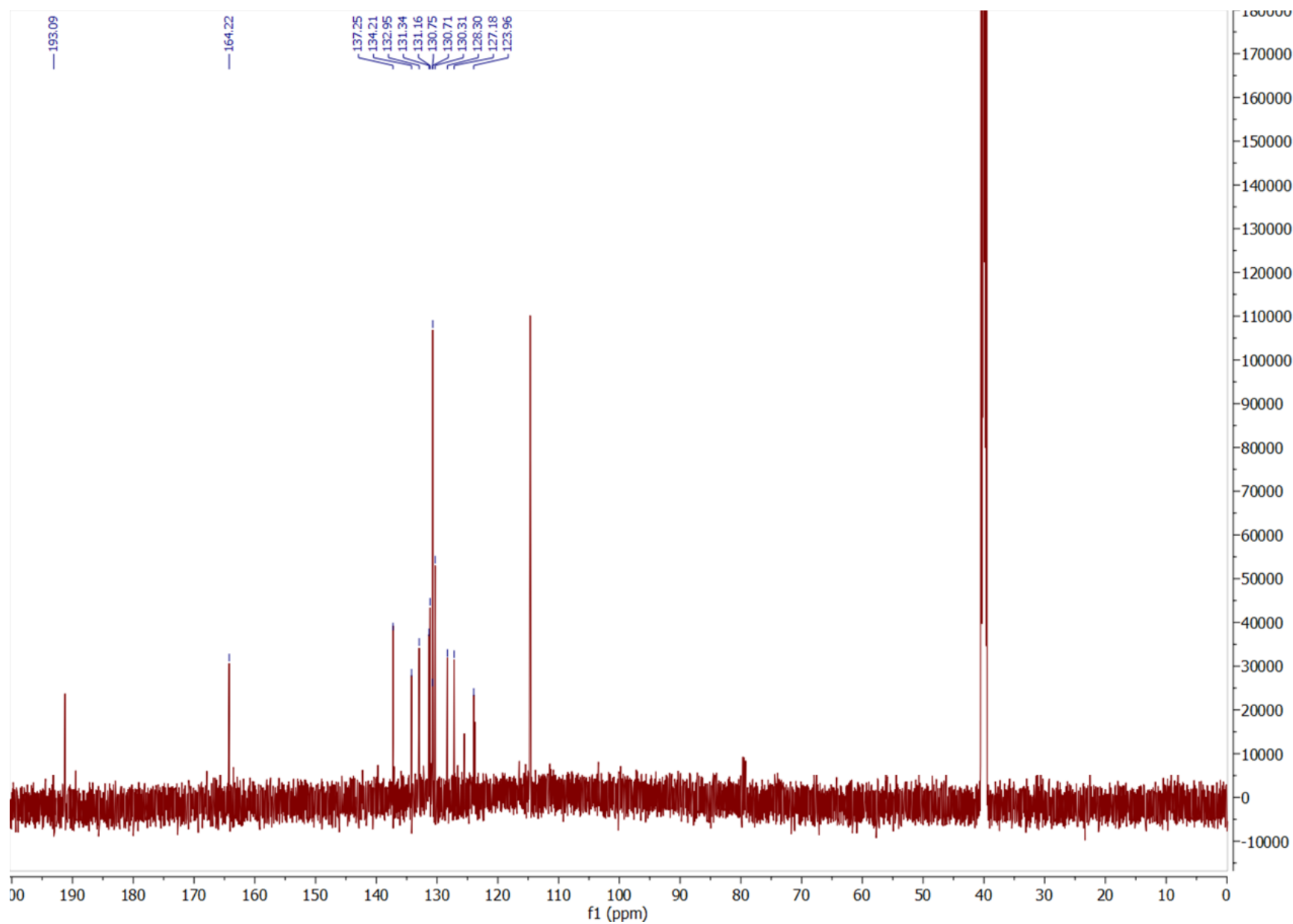


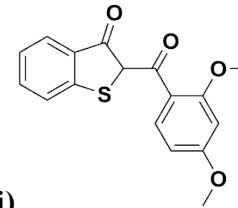




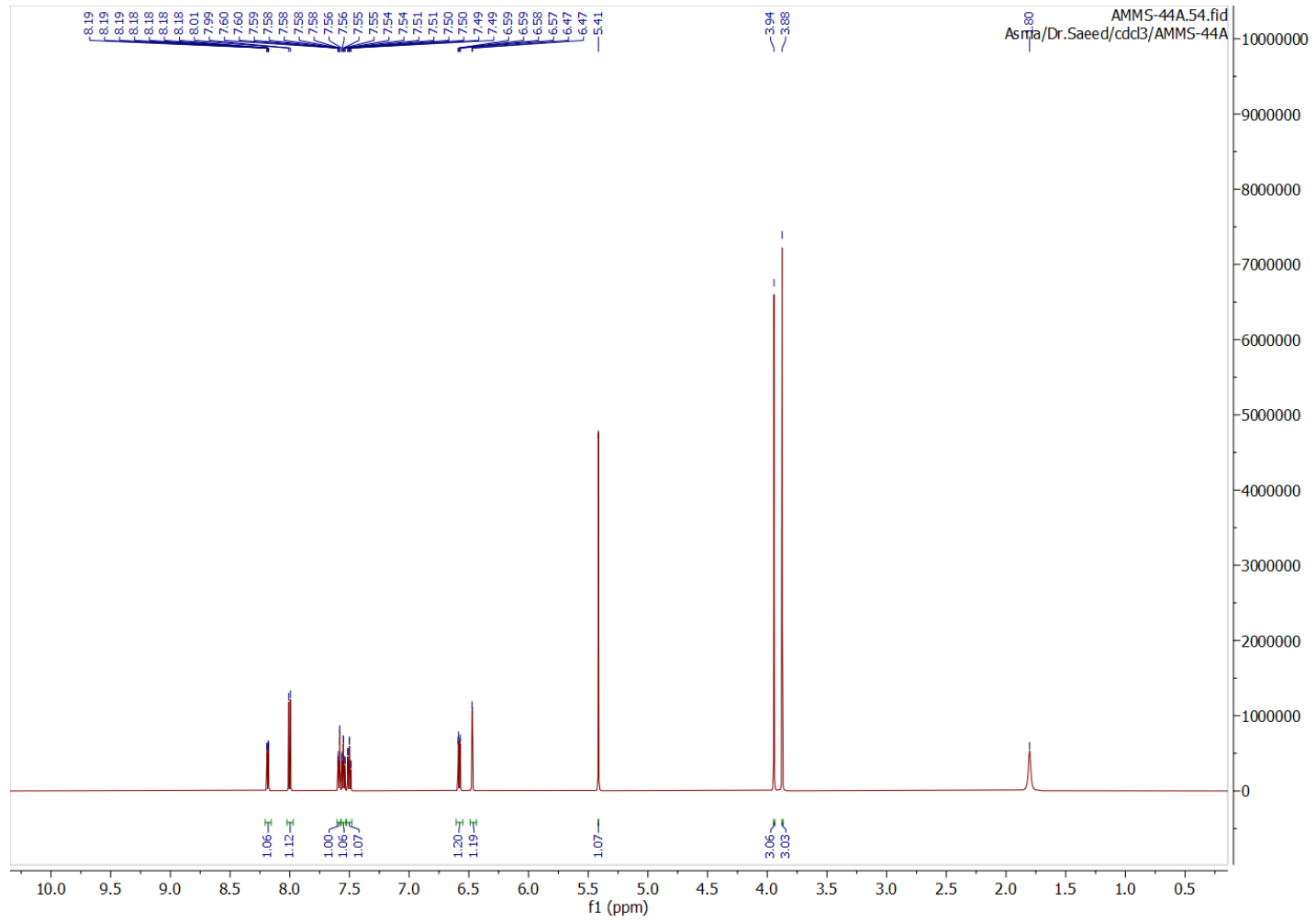
(3-hydroxybenzo[b]thiophen-2-yl)(4-nitrophenyl)methanone (5i)

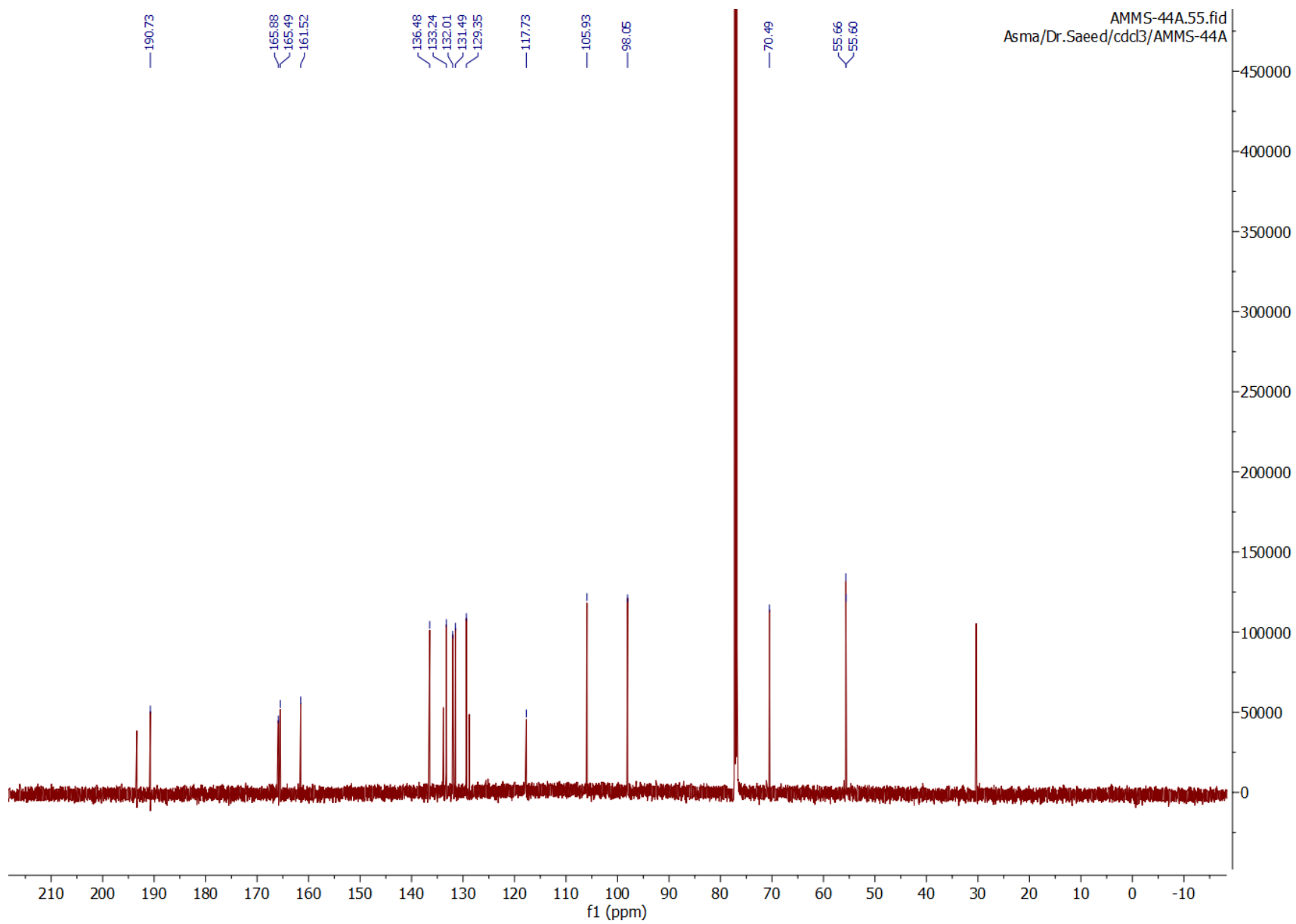


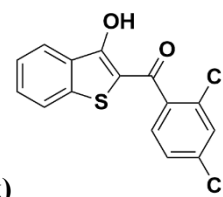




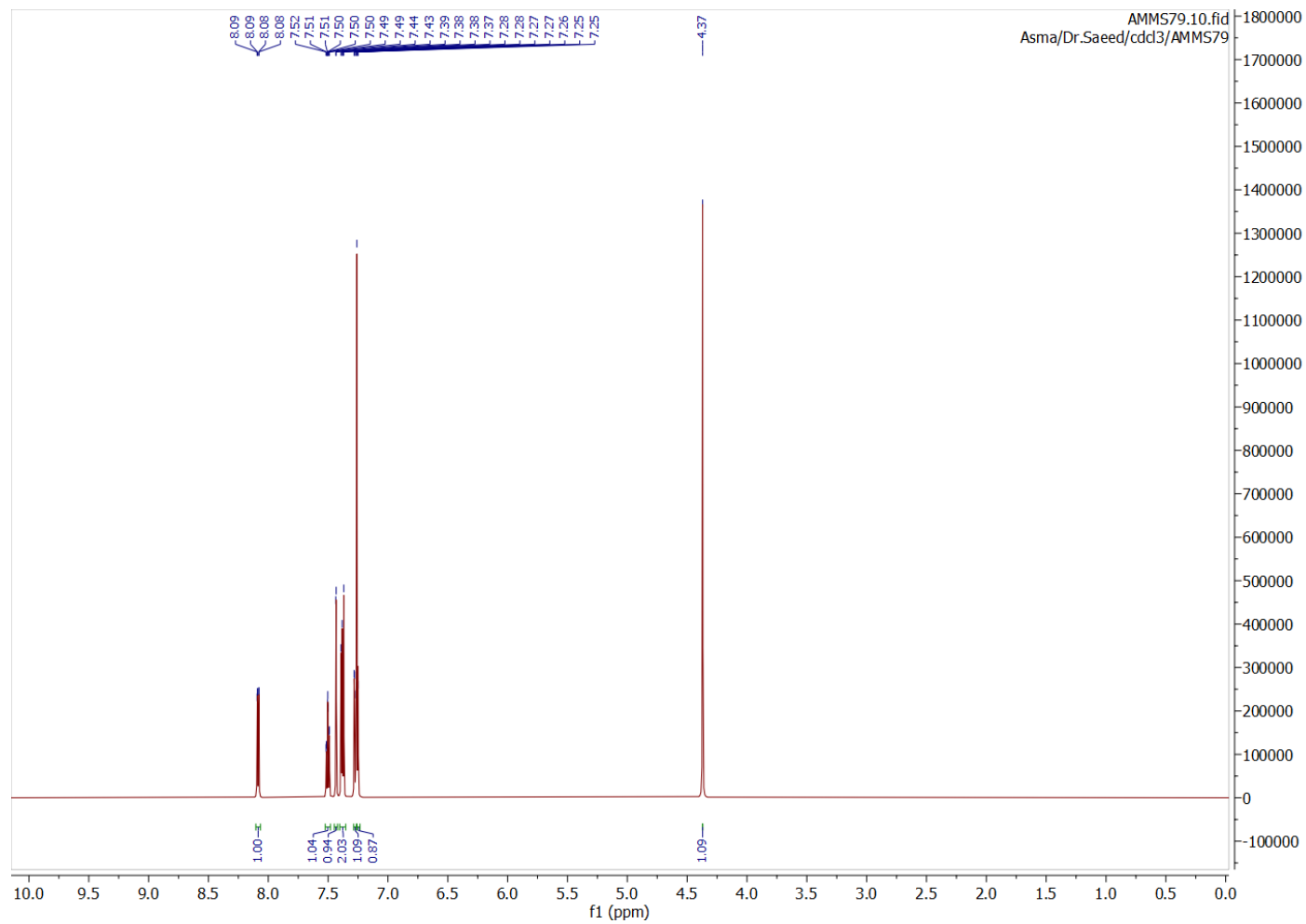
2-(2,4-dimethoxybenzoyl)benzo[b]thiophen-3(2H)-one (5j)

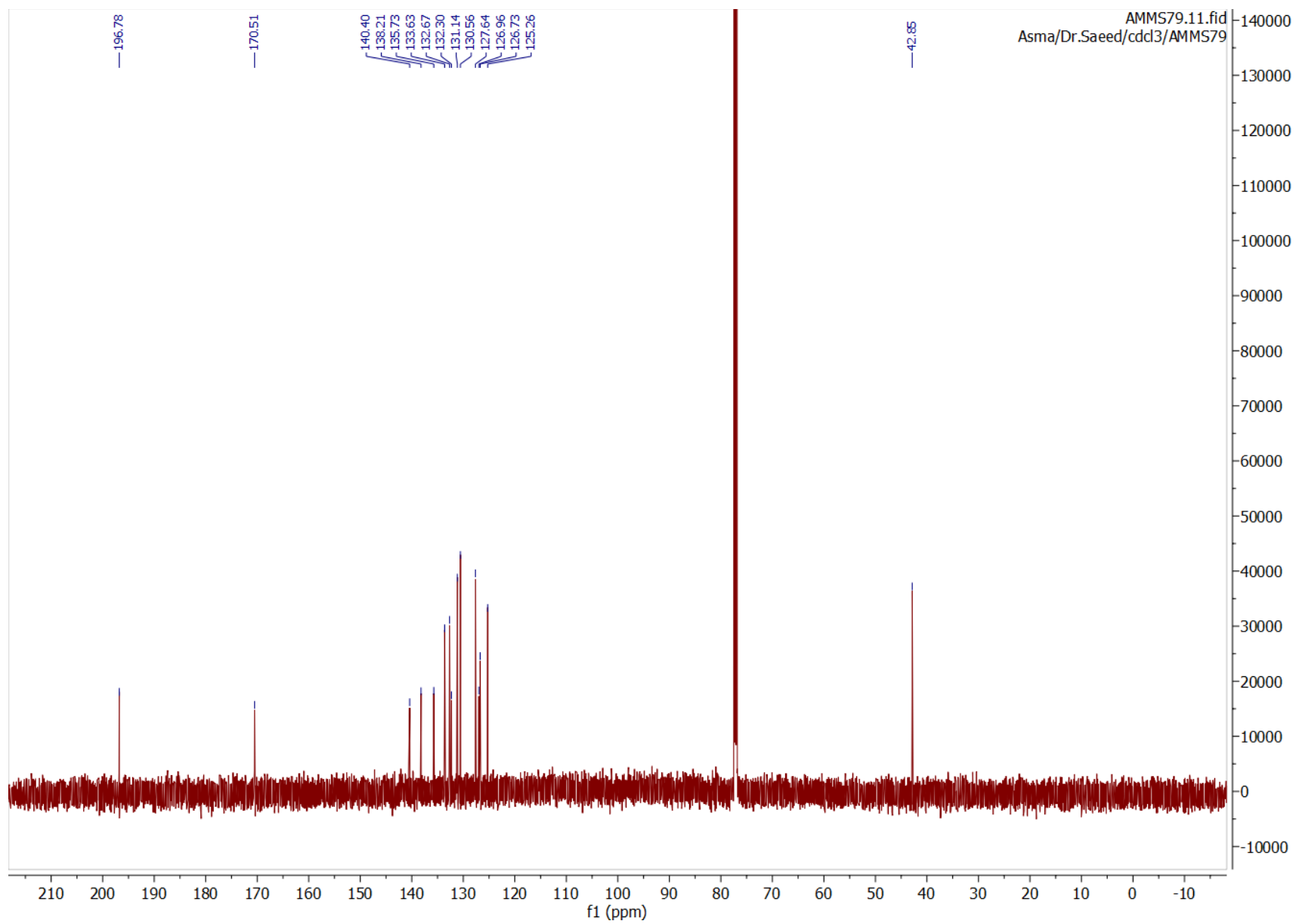


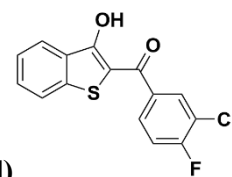




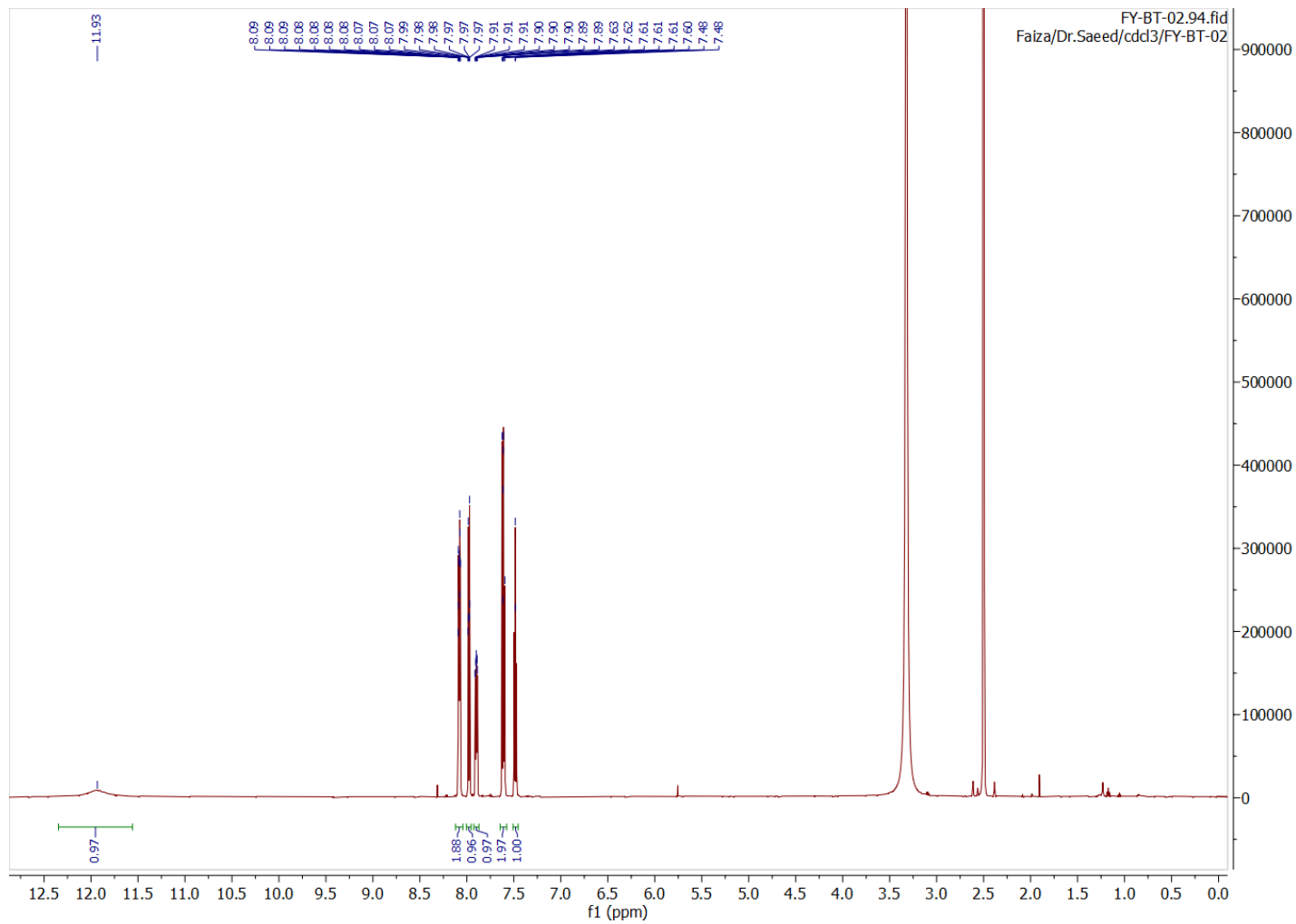
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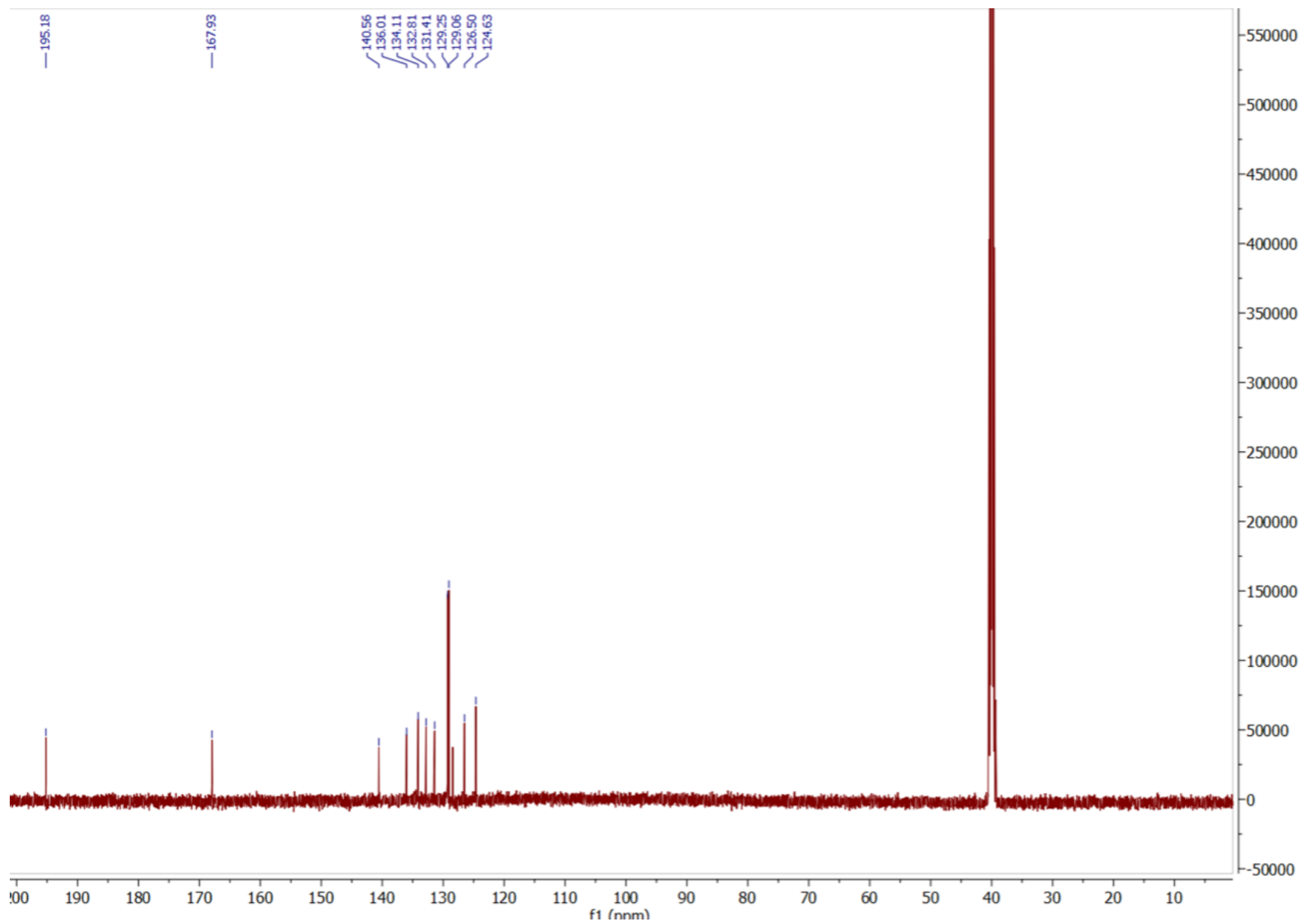


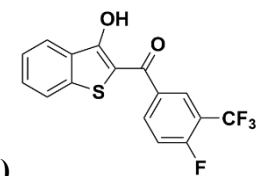




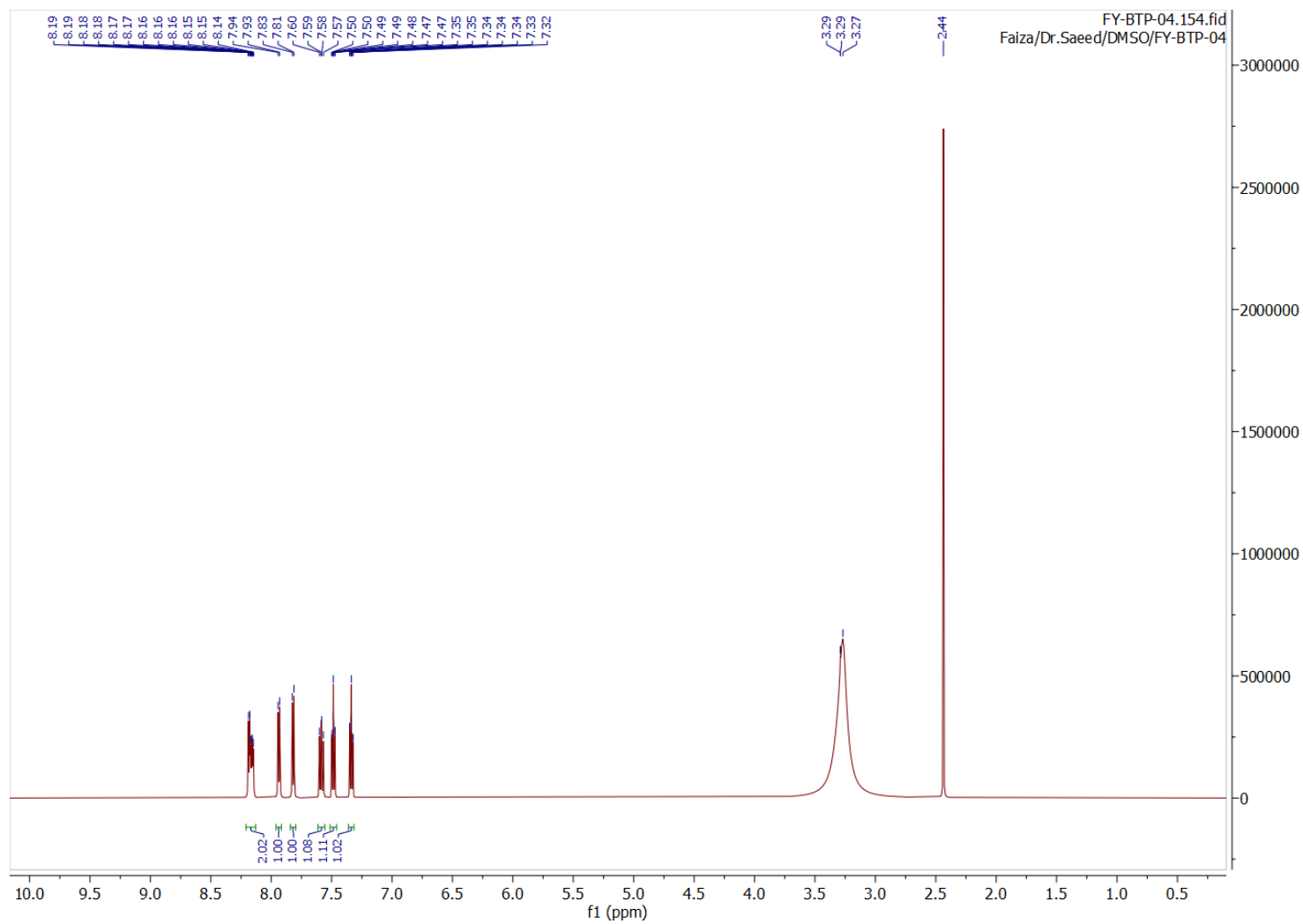
(3-chloro-4-fluorophenyl)(3-hydroxybenzo[b]thiophen-2-yl)methanone (5I)

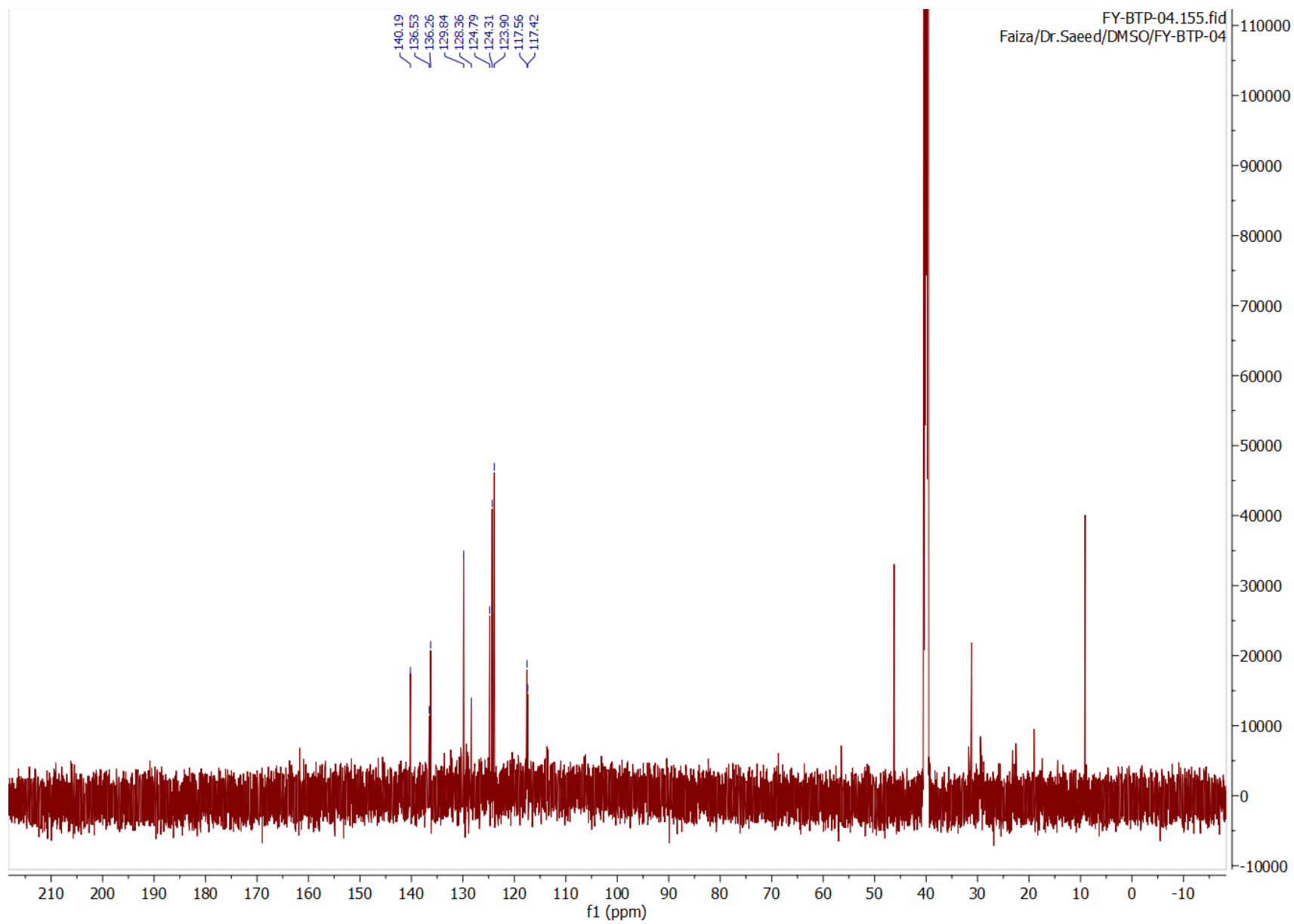


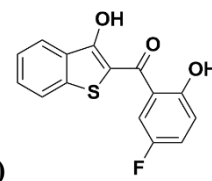




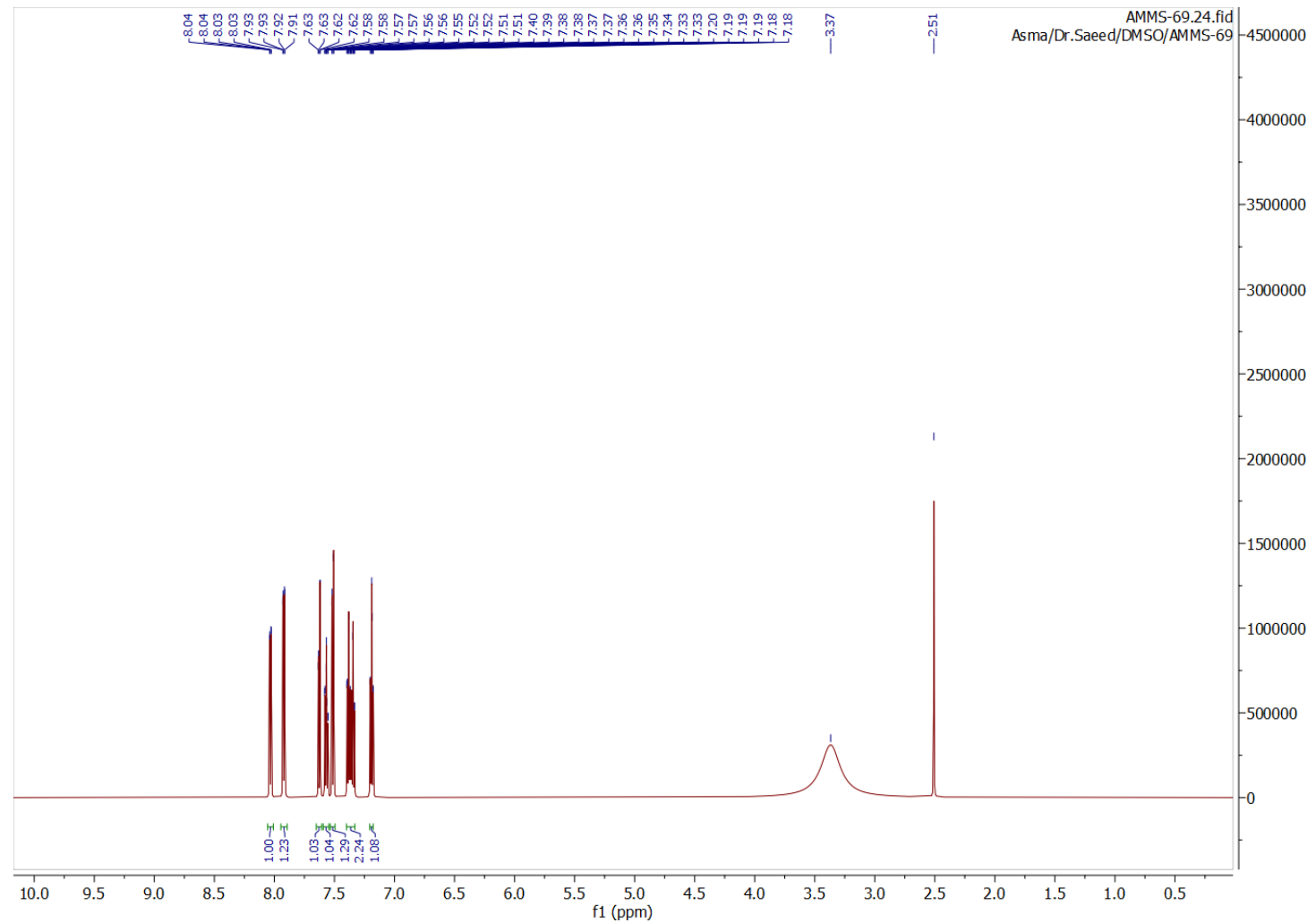
(4-fluoro-3-(trifluoromethyl)phenyl)(3-hydroxybenzo[b]thiophen-2-yl)methanone (5m)



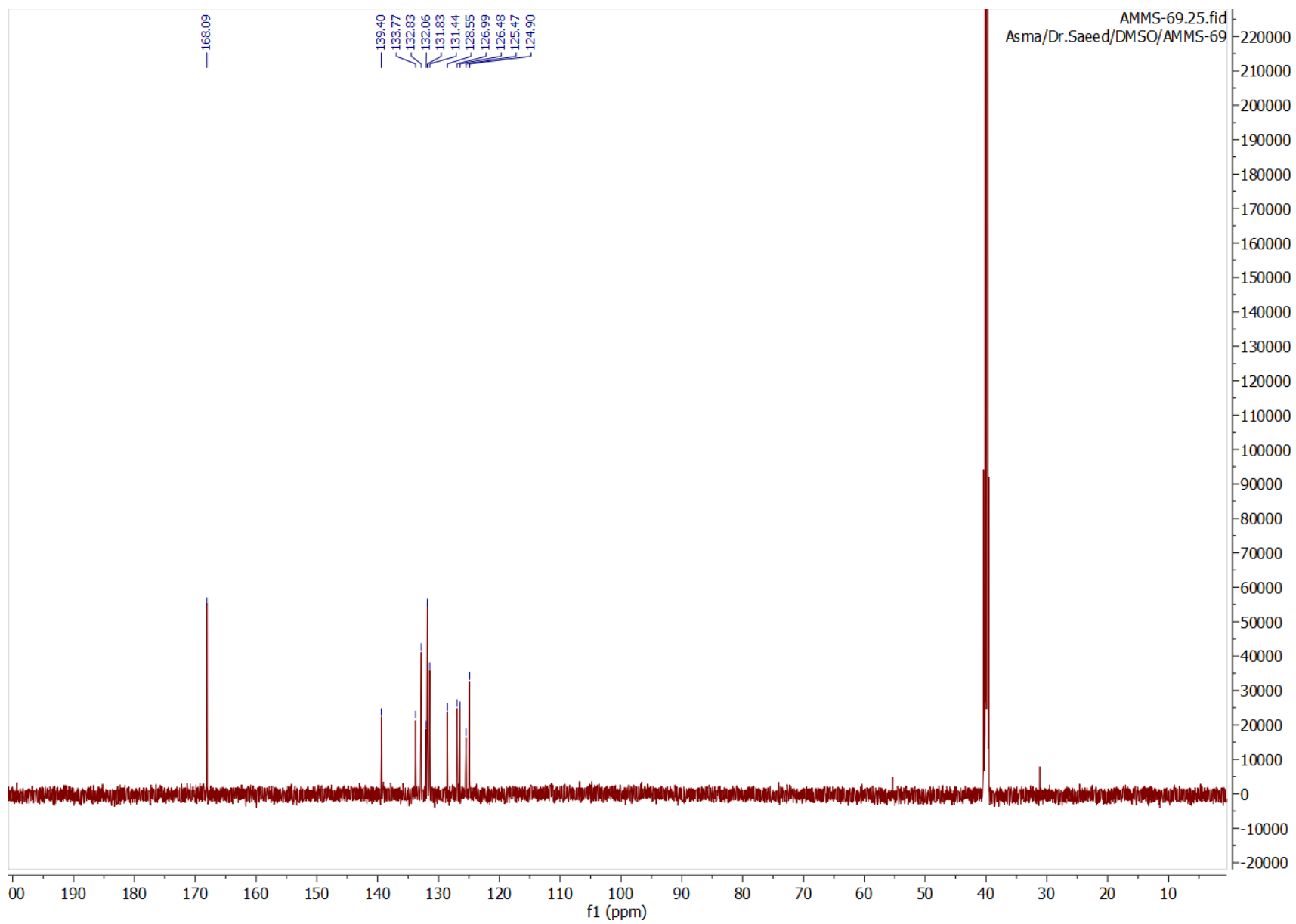


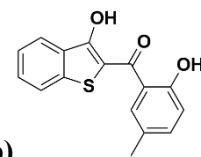


(5-fluoro-2-hydroxyphenyl)(3-hydroxybenzo[b]thiophen-2-yl)methanone (5n)

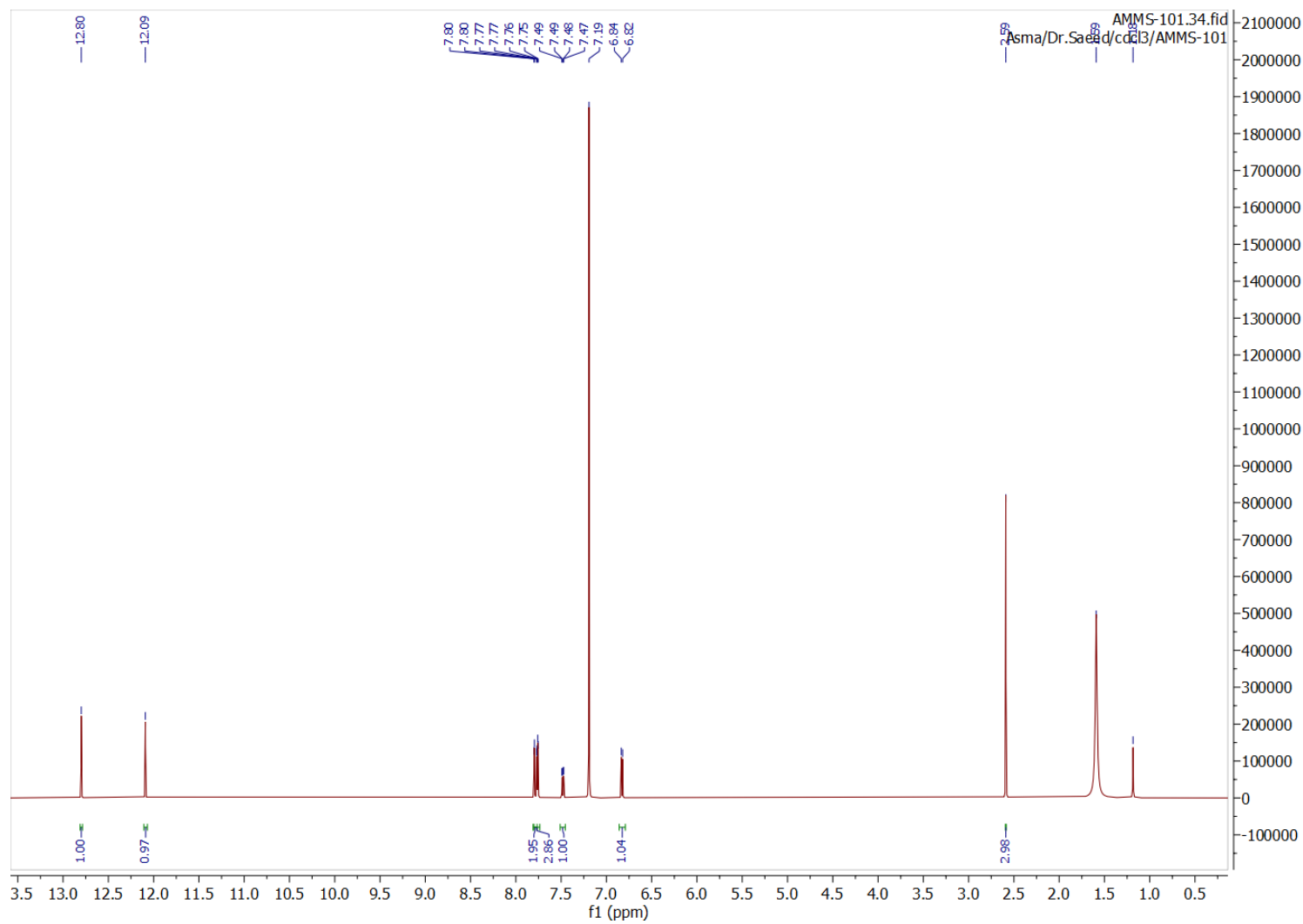


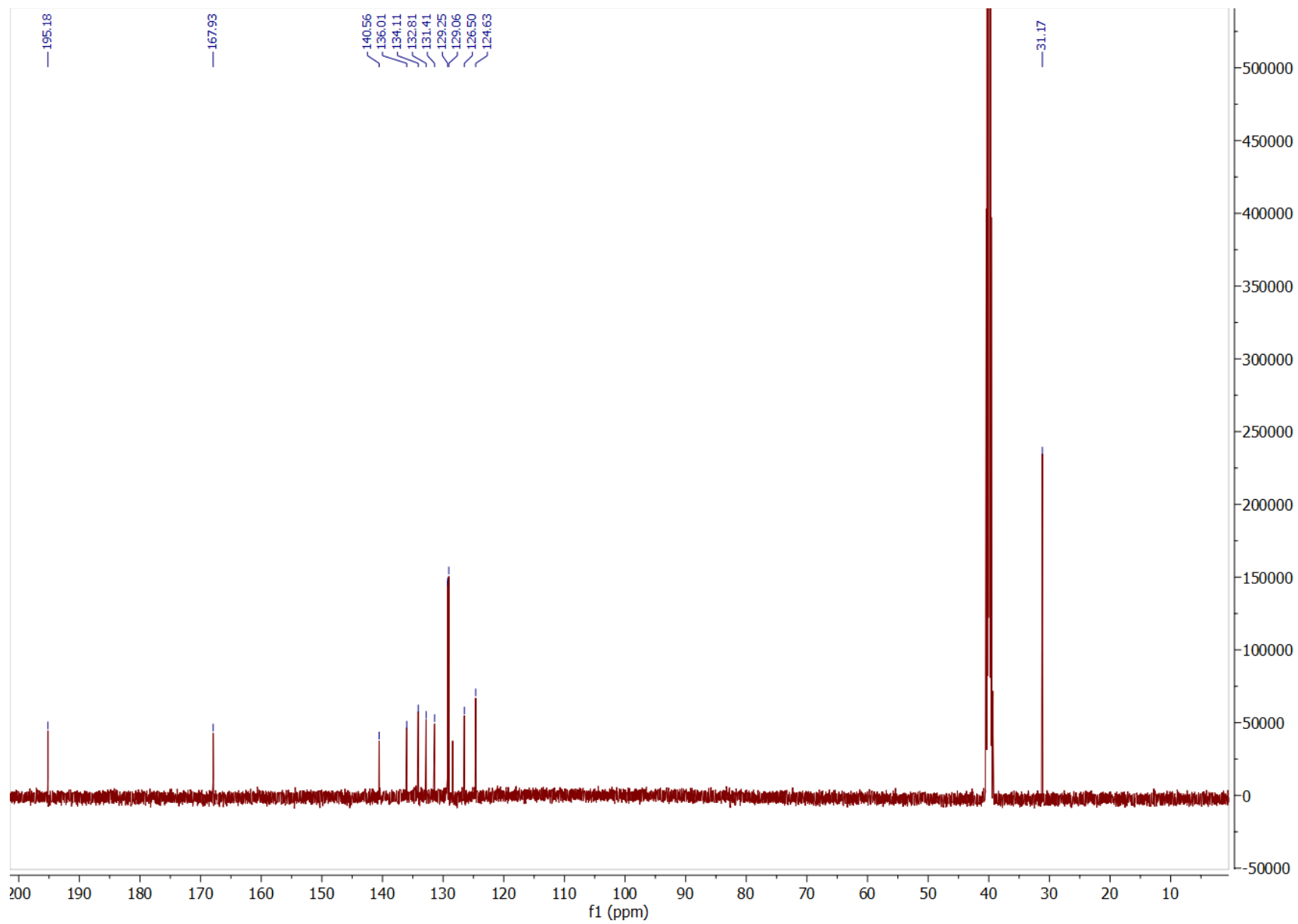
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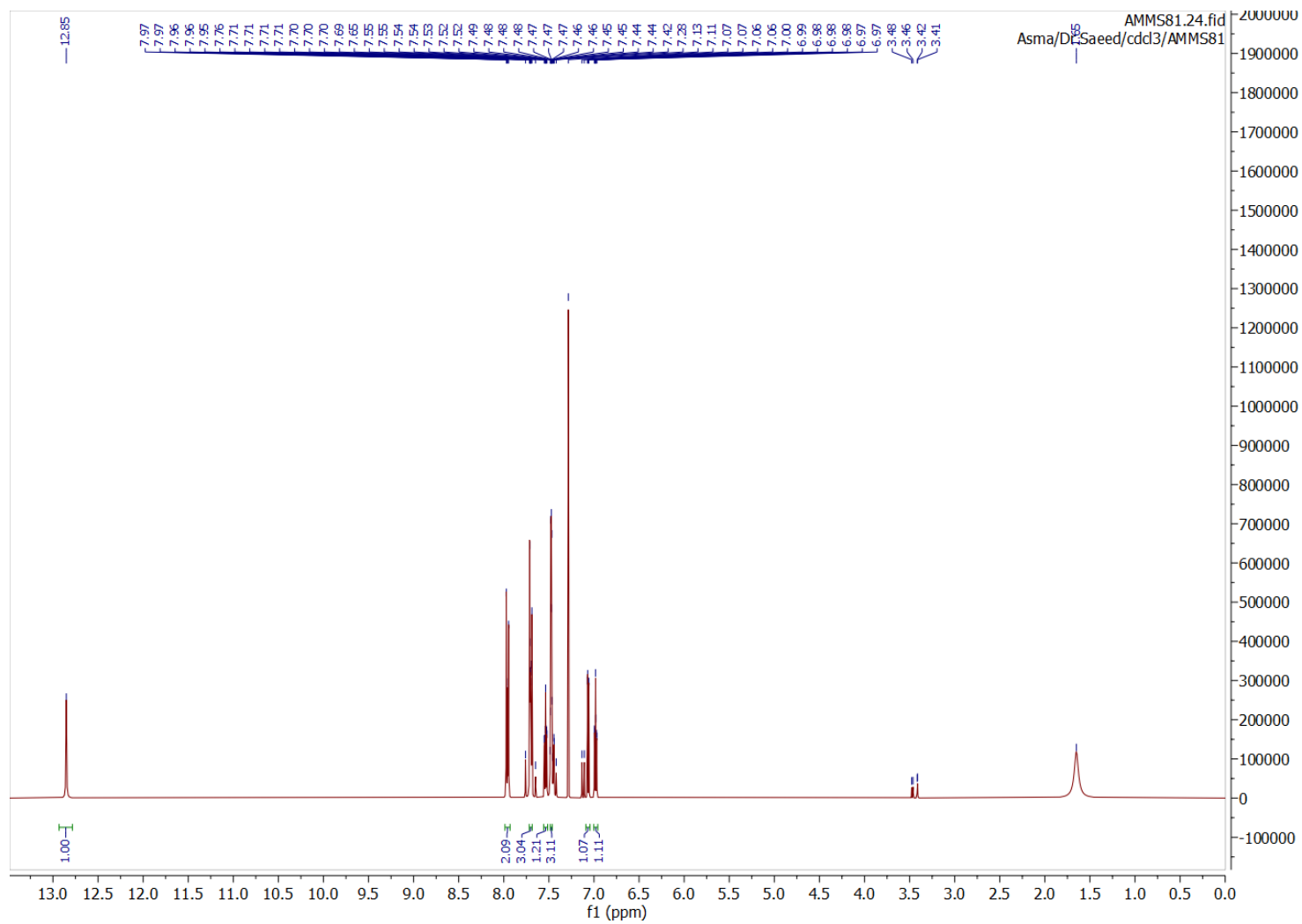
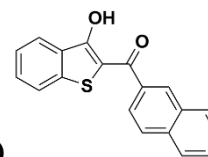


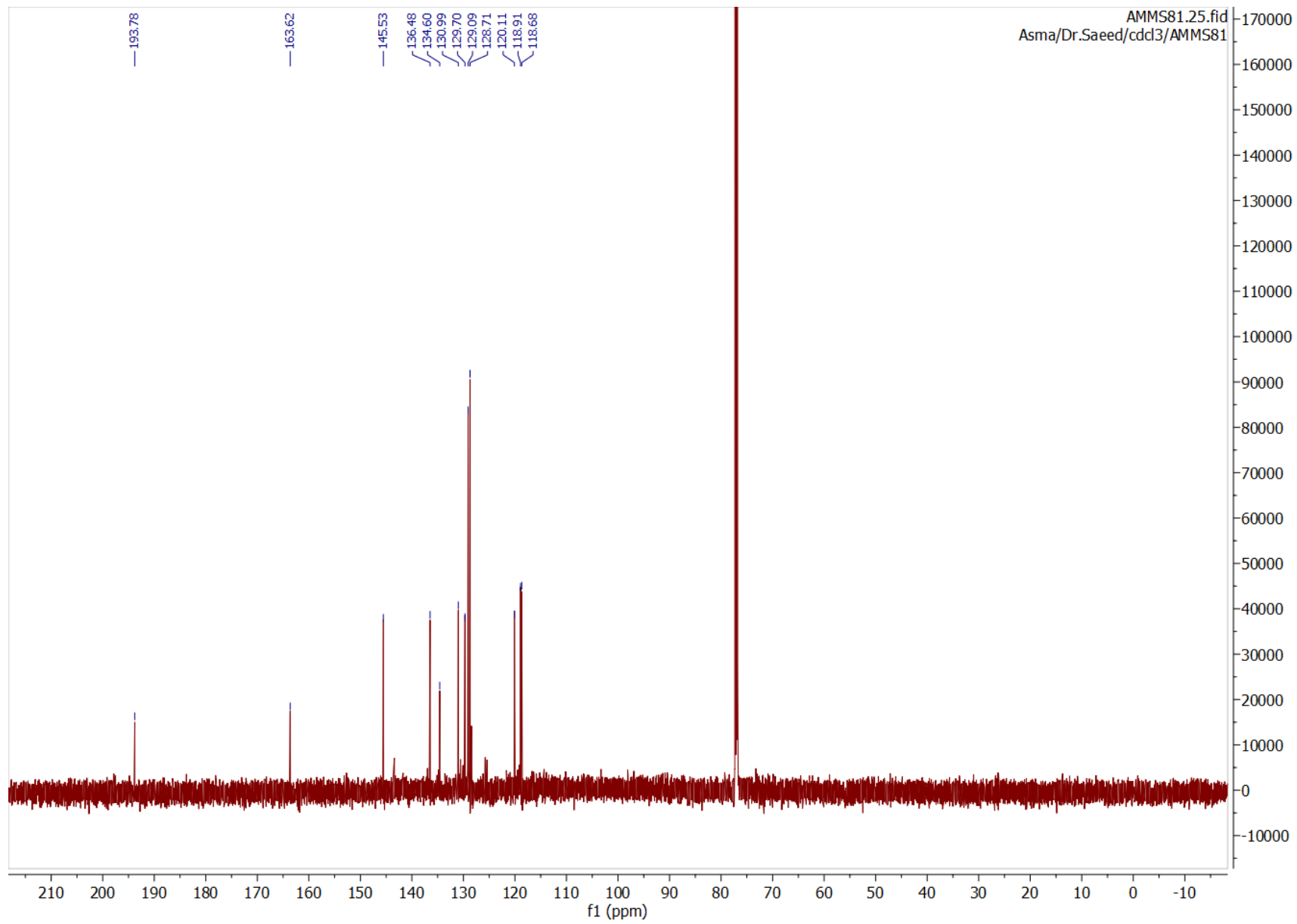
(3-hydroxybenzo[b]thiophen-2-yl)(2-hydroxyphenyl)methanone (5o)



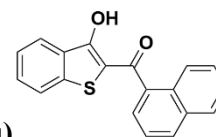


(3-hydroxybenzo[b]thiophen-2-yl)(naphthalen-2-yl)methanone (5p)

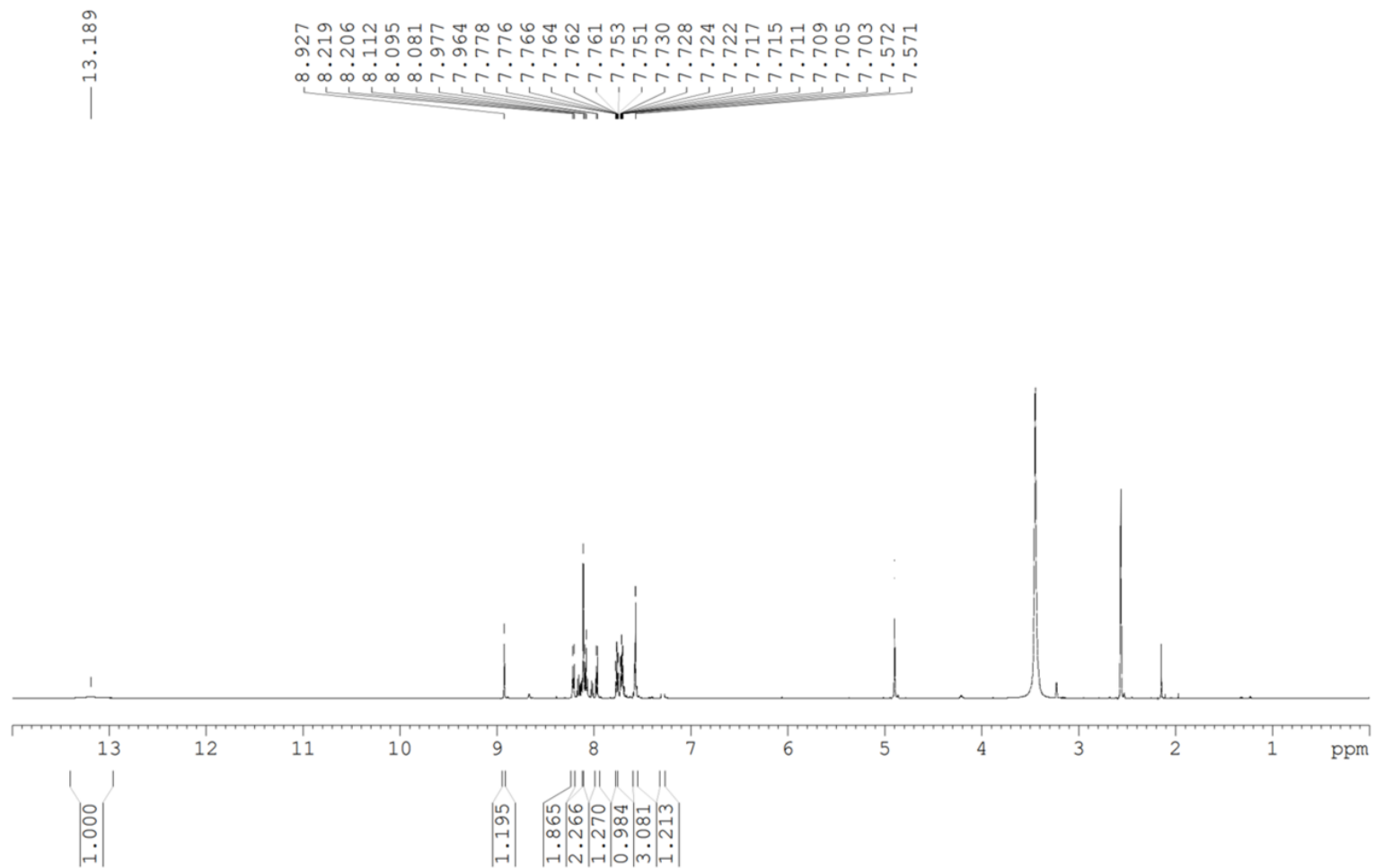




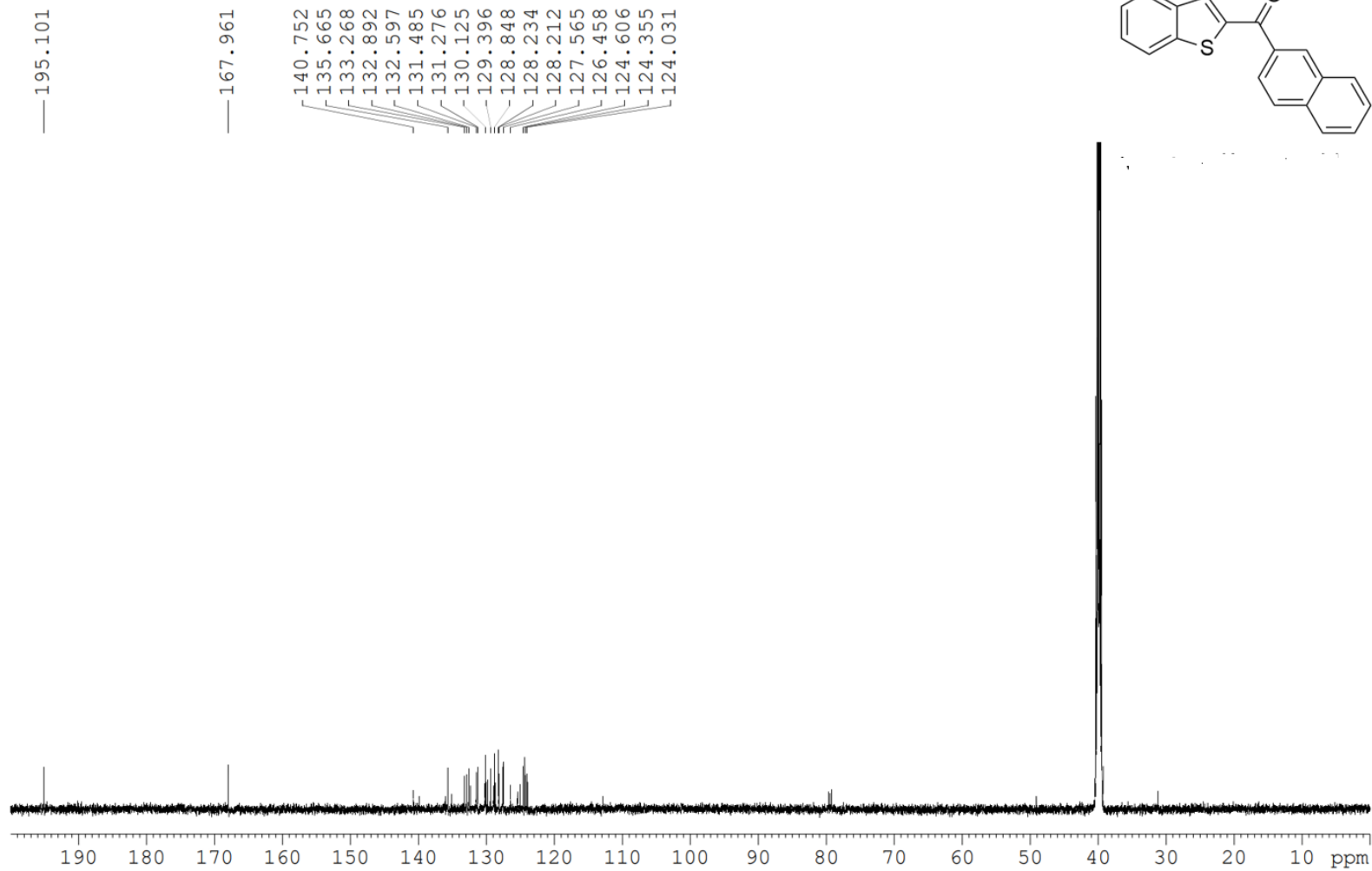
(3-hydroxybenzo[b]thiophen-2-yl)(naphthalen-1-yl)methanone (5q)



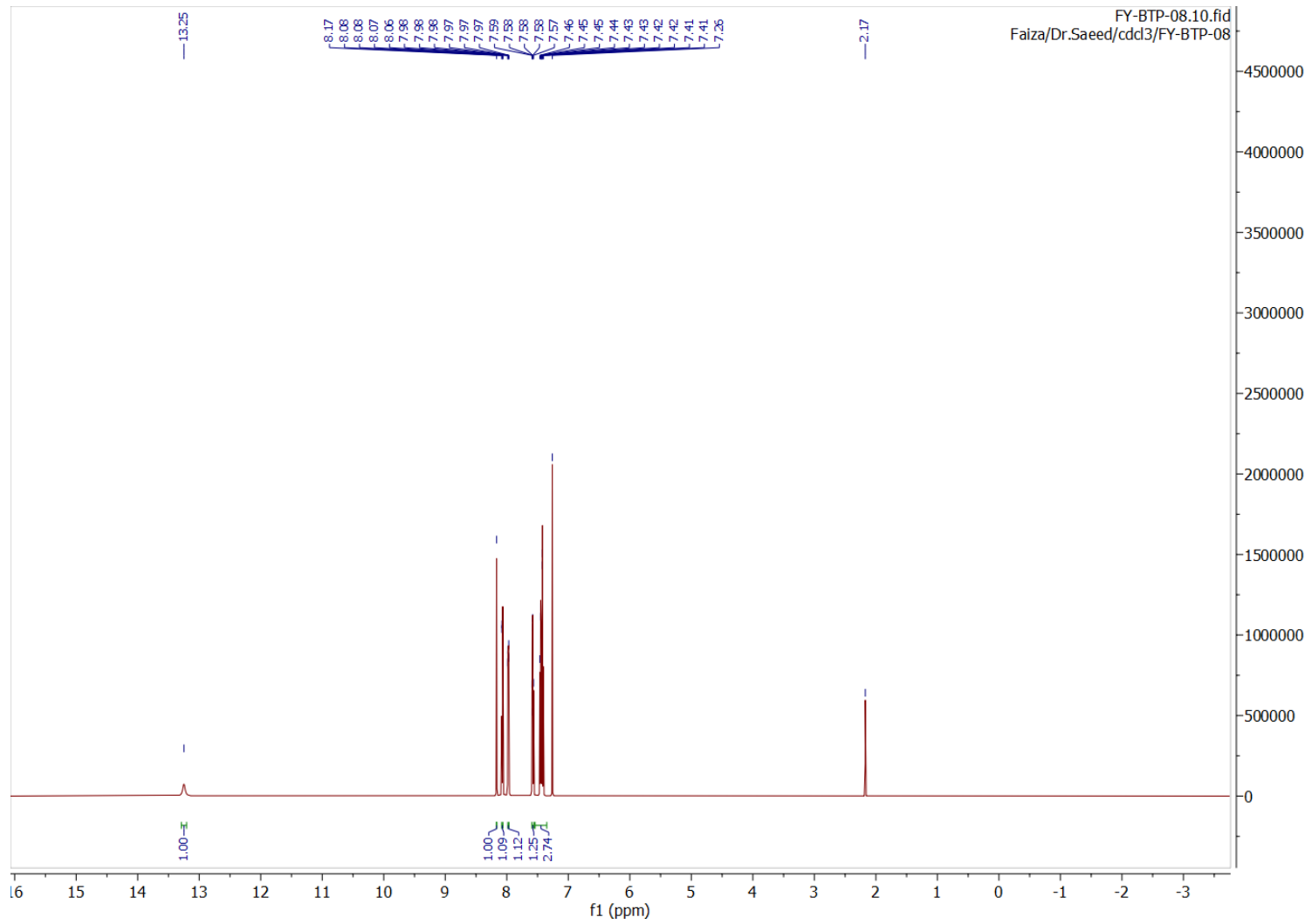
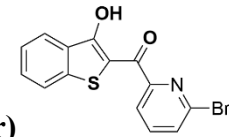
Asma/Dr. Saeed/DMSO/AMMS84

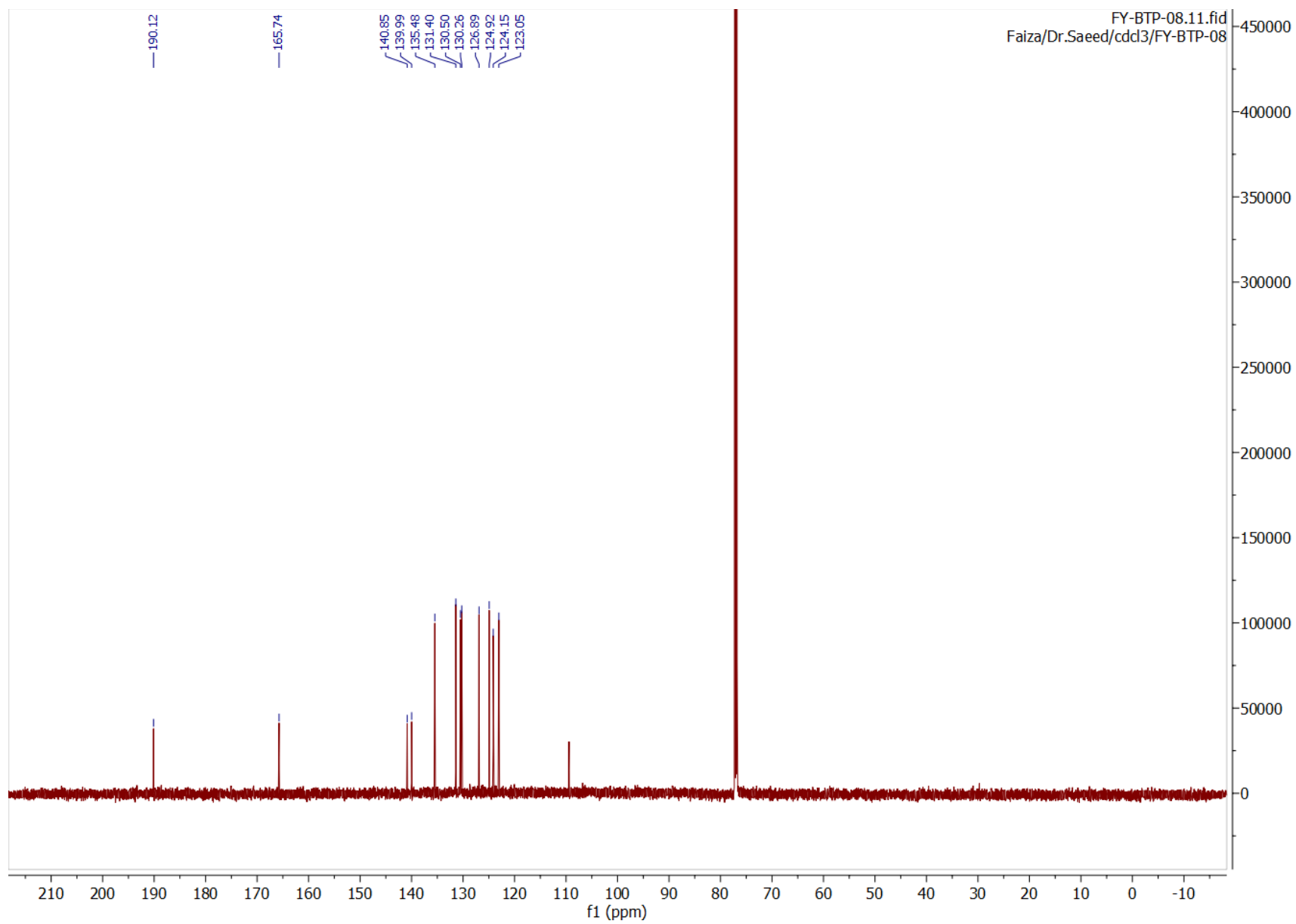


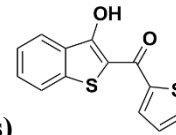
Asma/Dr. Saeed/DMSO/AMMS84



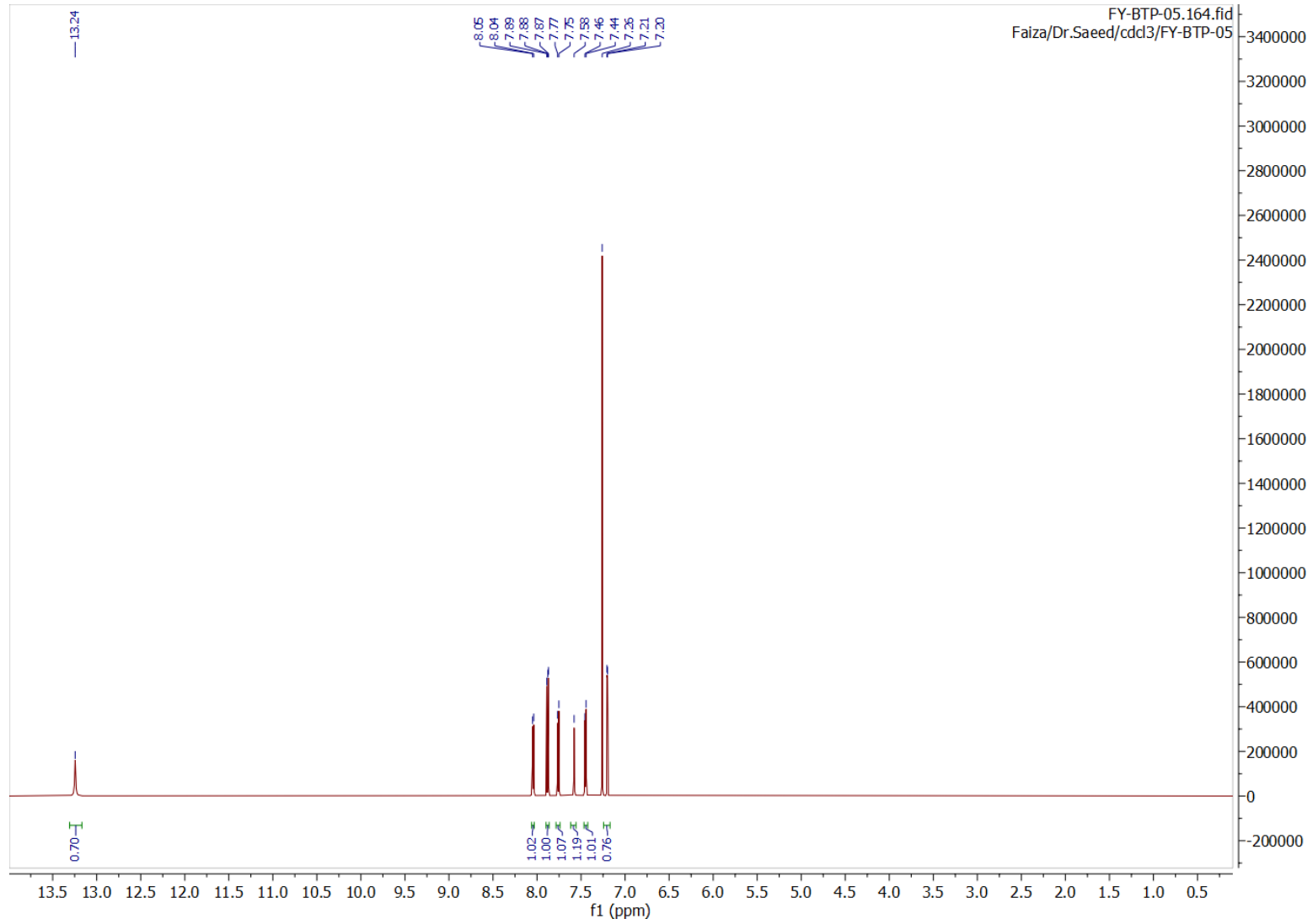
(6-bromopyridin-2-yl)(3-hydroxybenzo[b]thiophen-2-yl)methanone (5r)

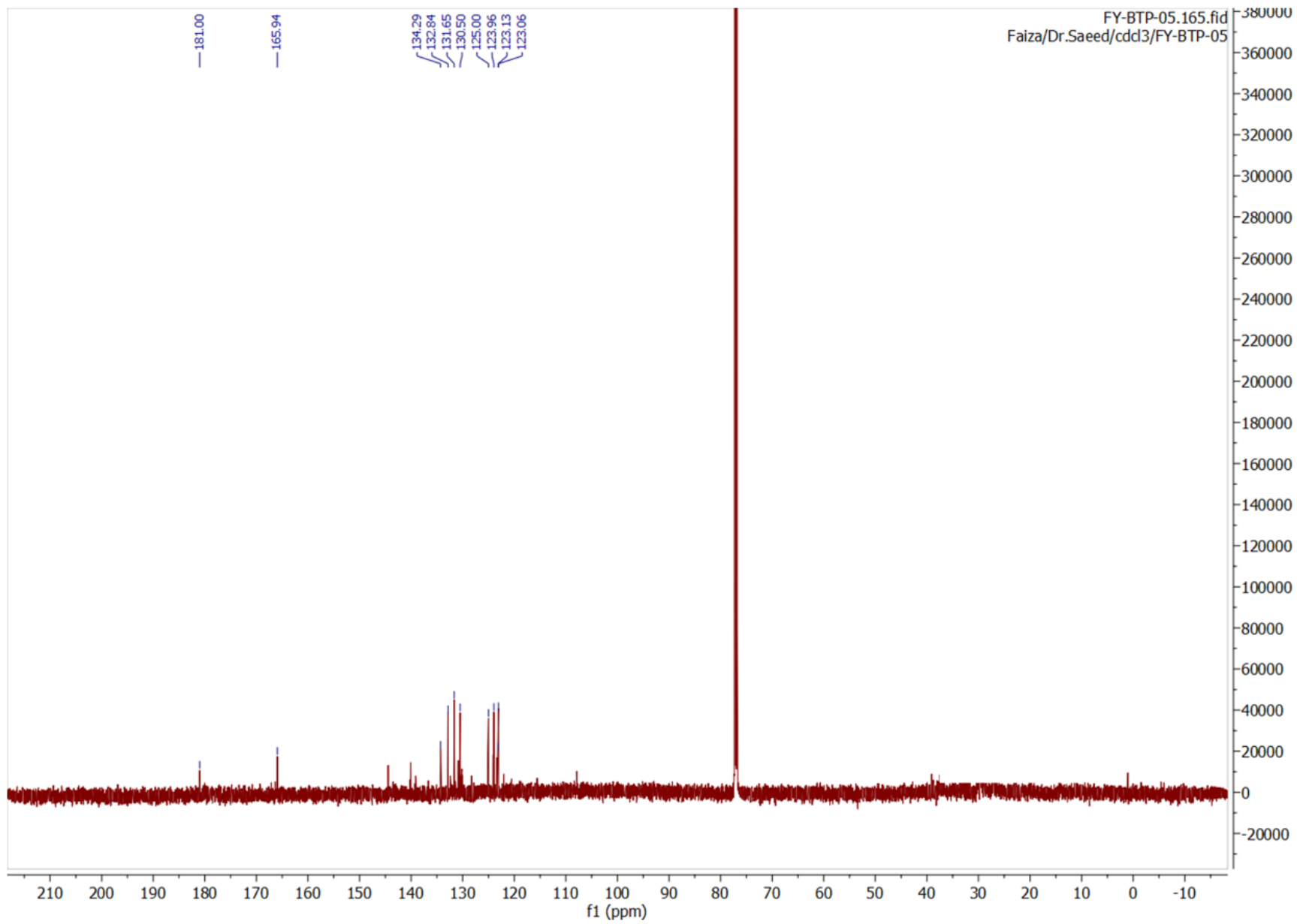


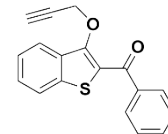




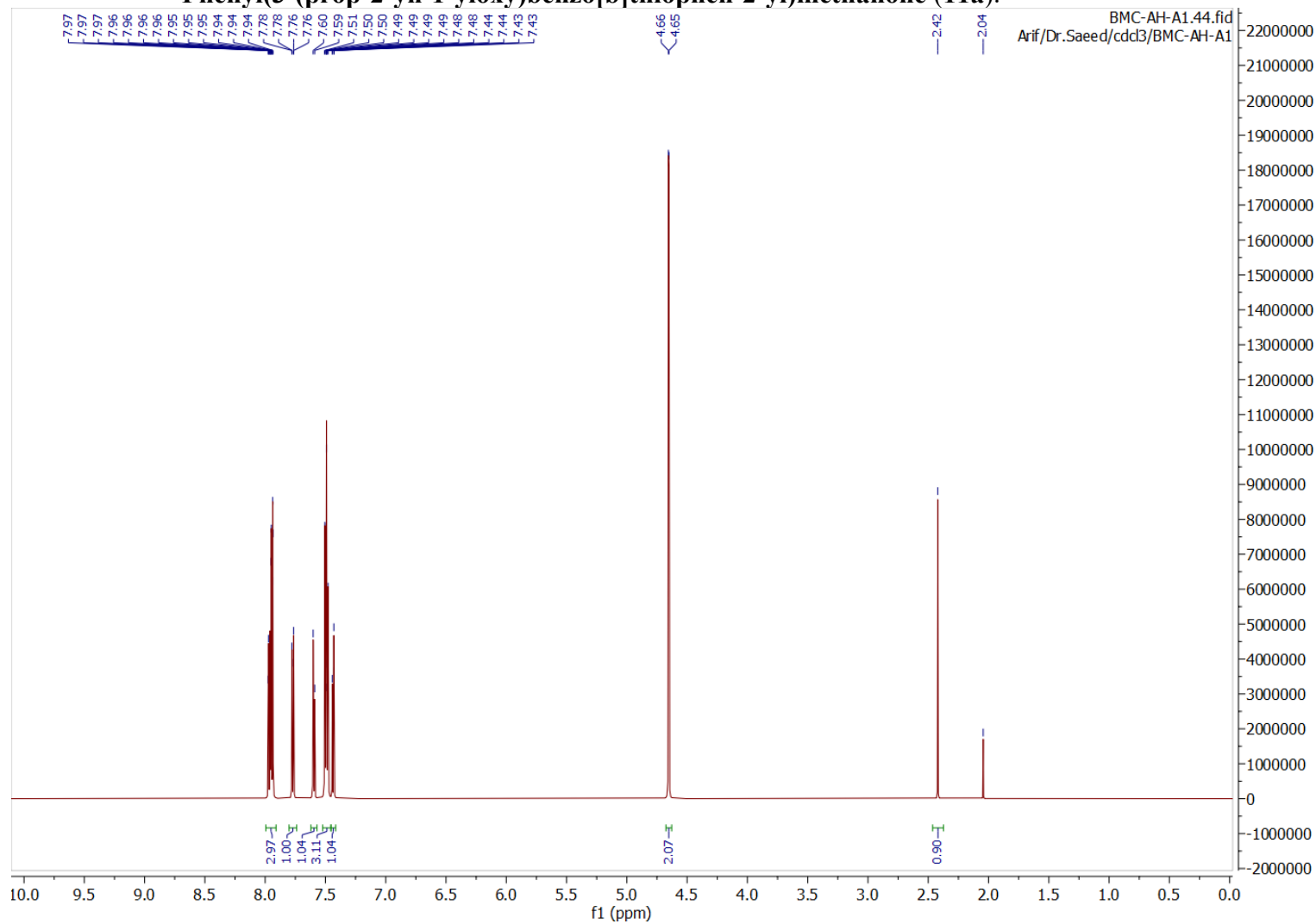
(3-hydroxybenzo[b]thiophen-2-yl)(thiophen-2-yl)methanone (5s)

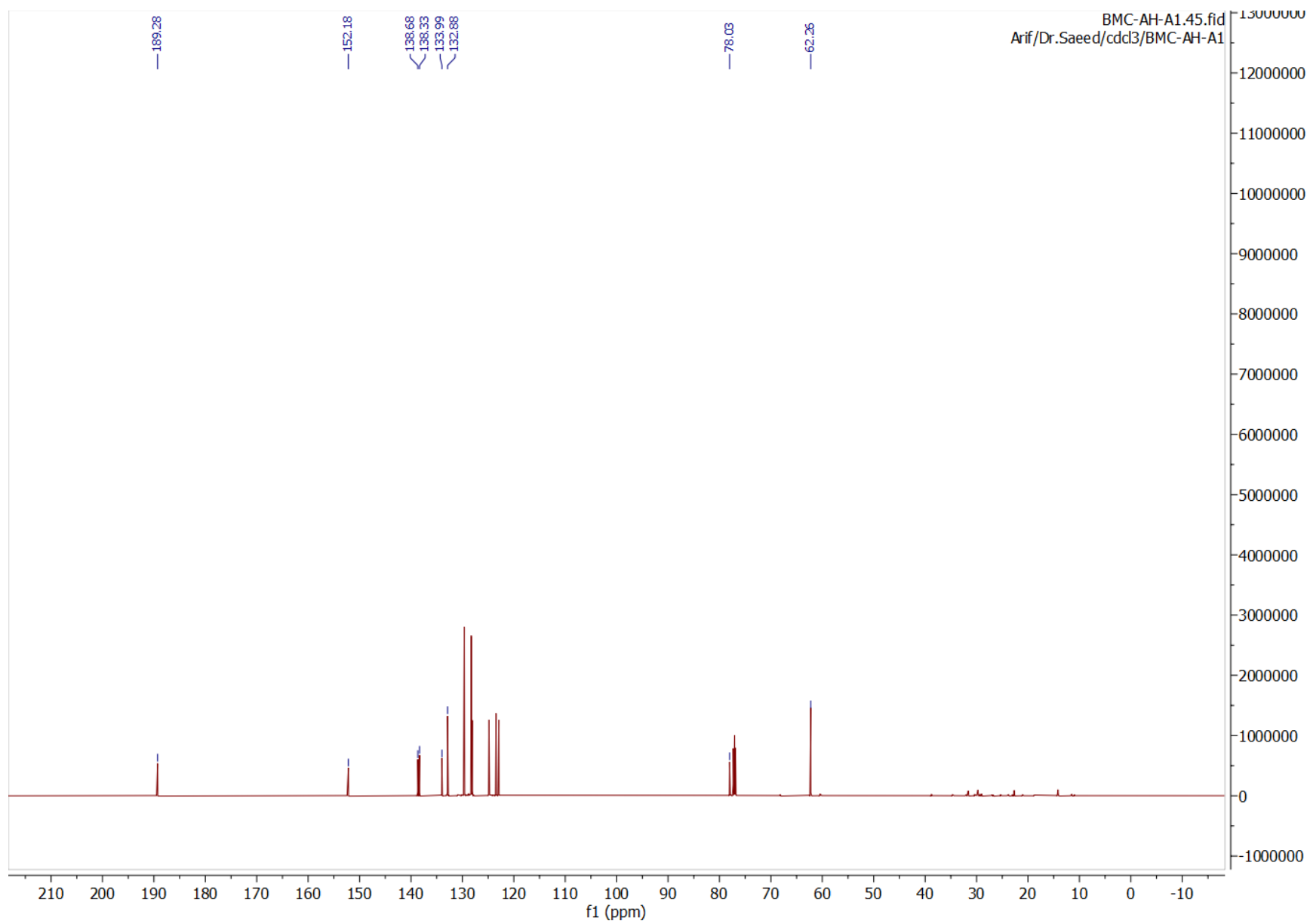


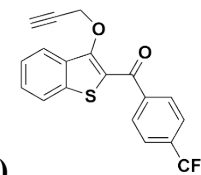




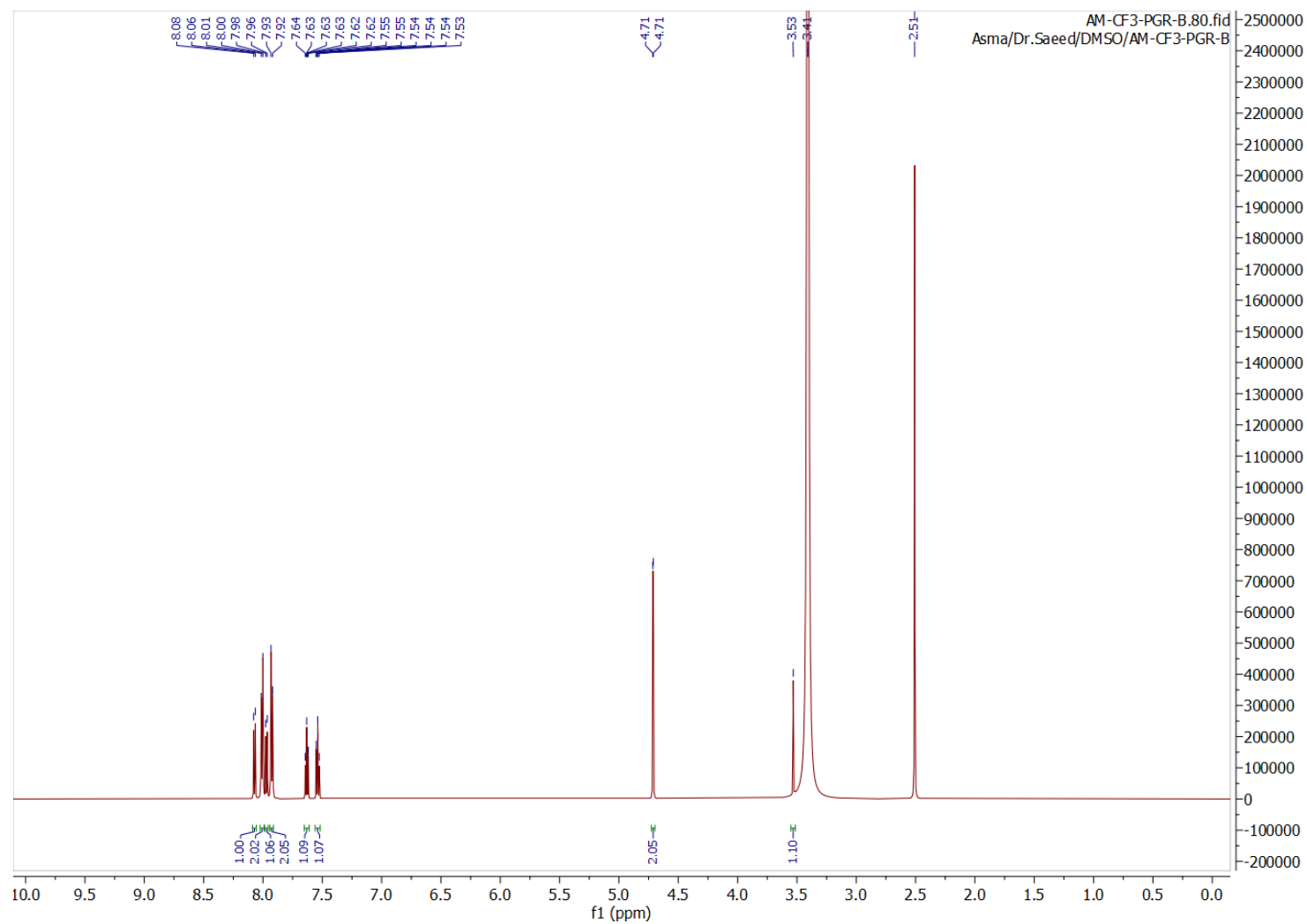
Phenyl(3-(prop-2-yn-1-yloxy)benzo[b]thiophen-2-yl)methanone (11a).

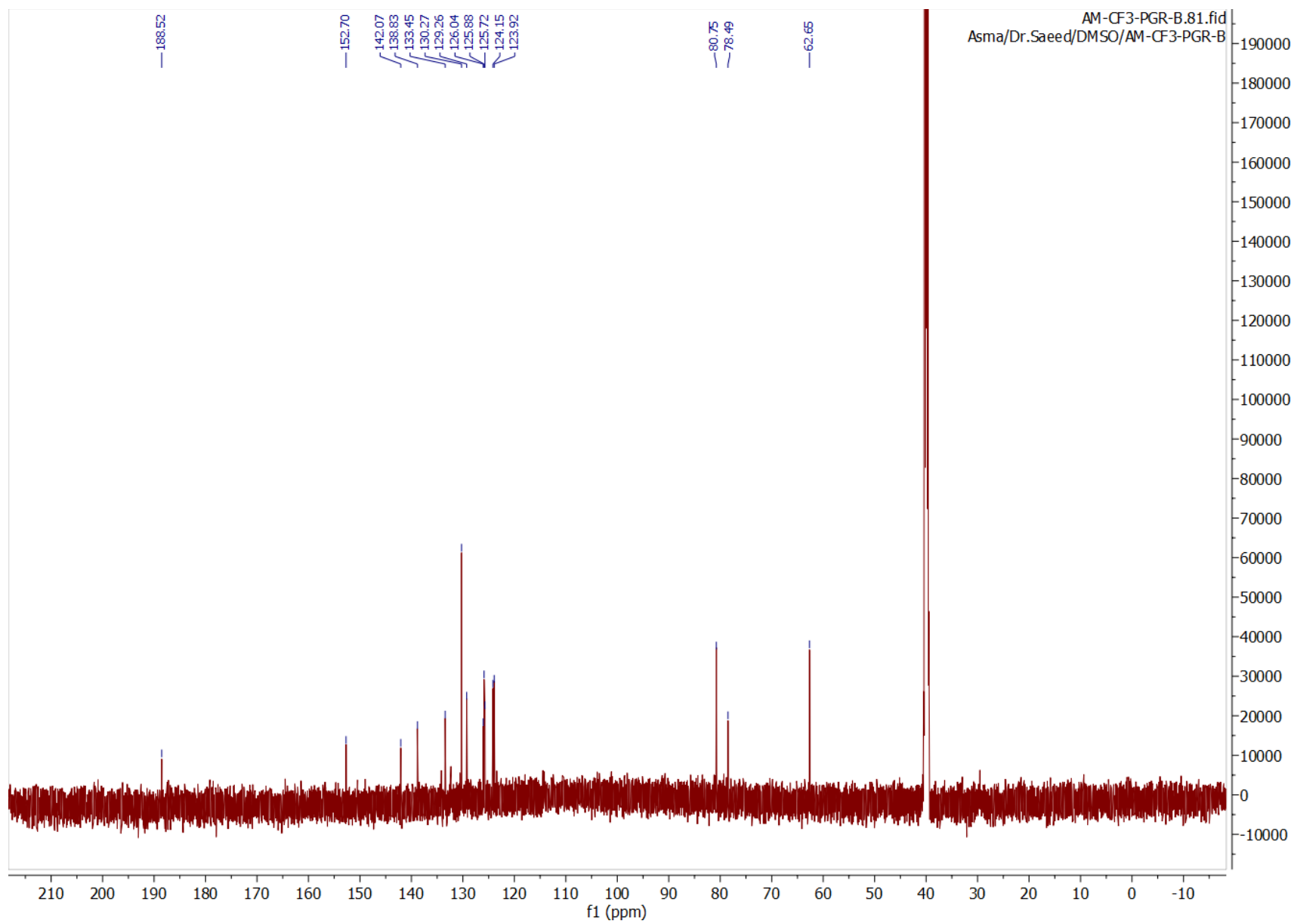


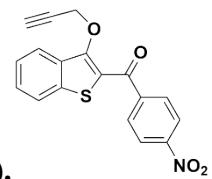




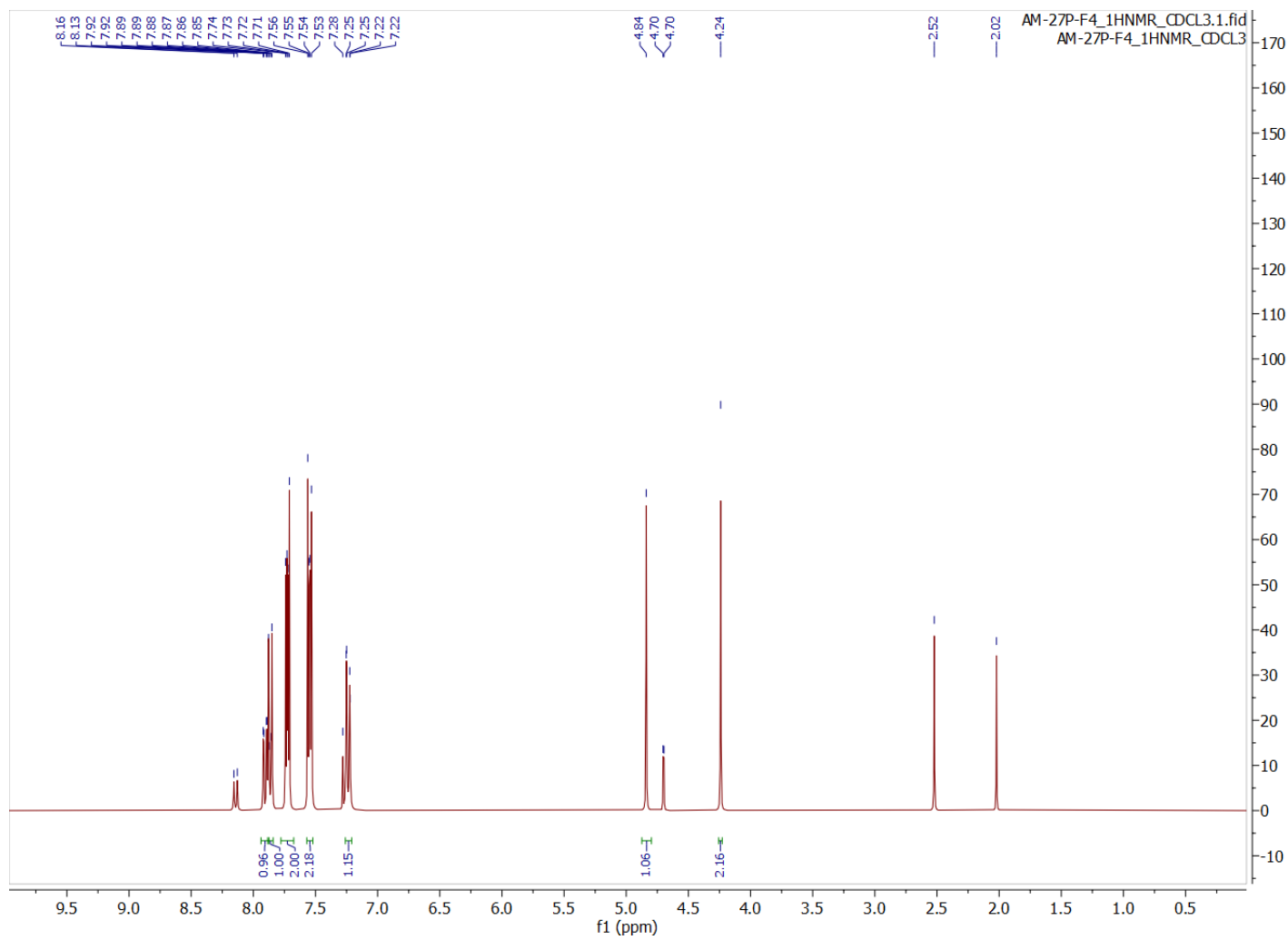
(3-(prop-2-yn-1-yloxy)benzo[b]thiophen-2-yl)(4-(trifluoromethyl)phenyl)methanone (11b).

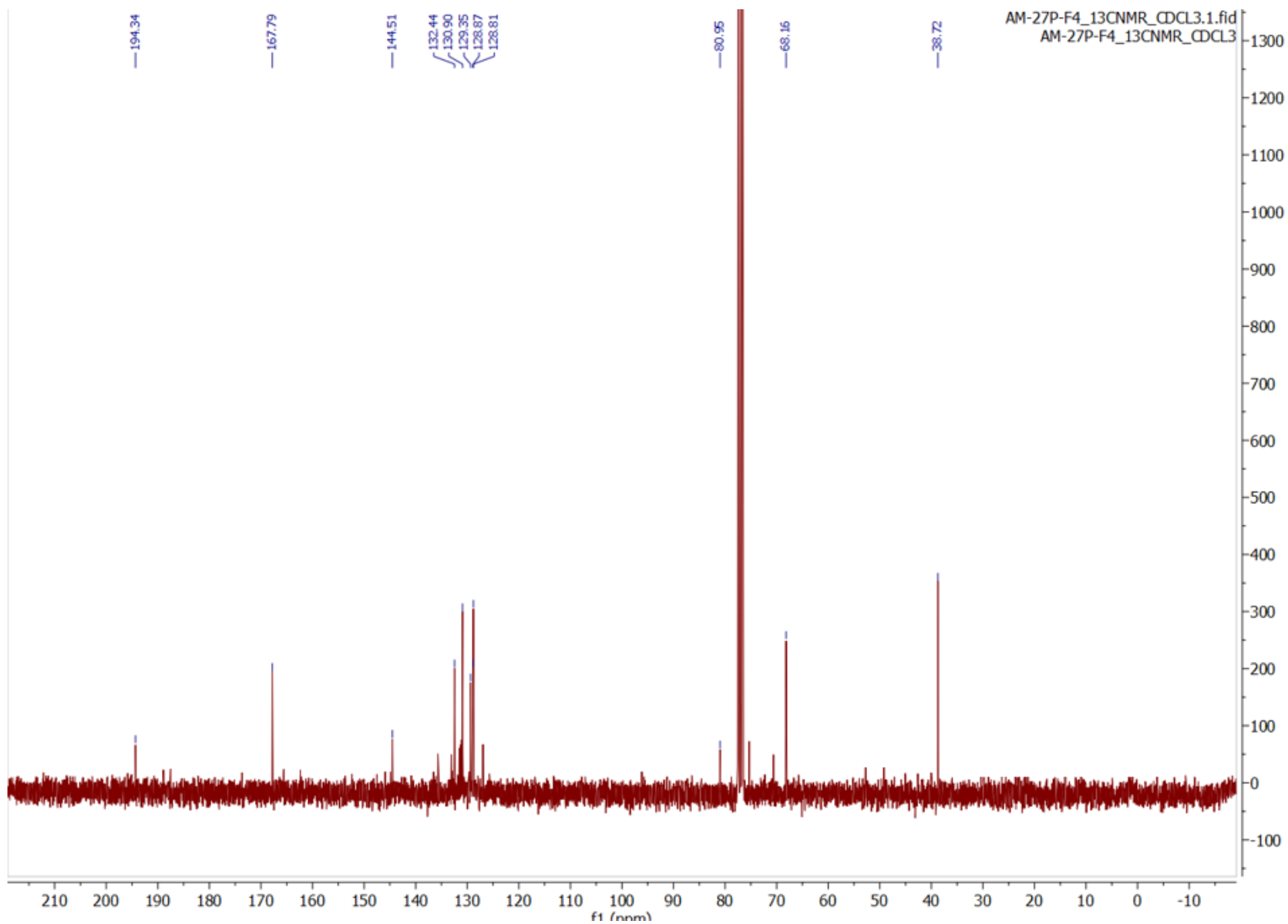


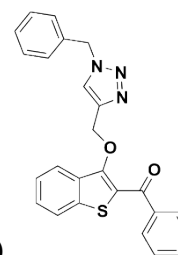




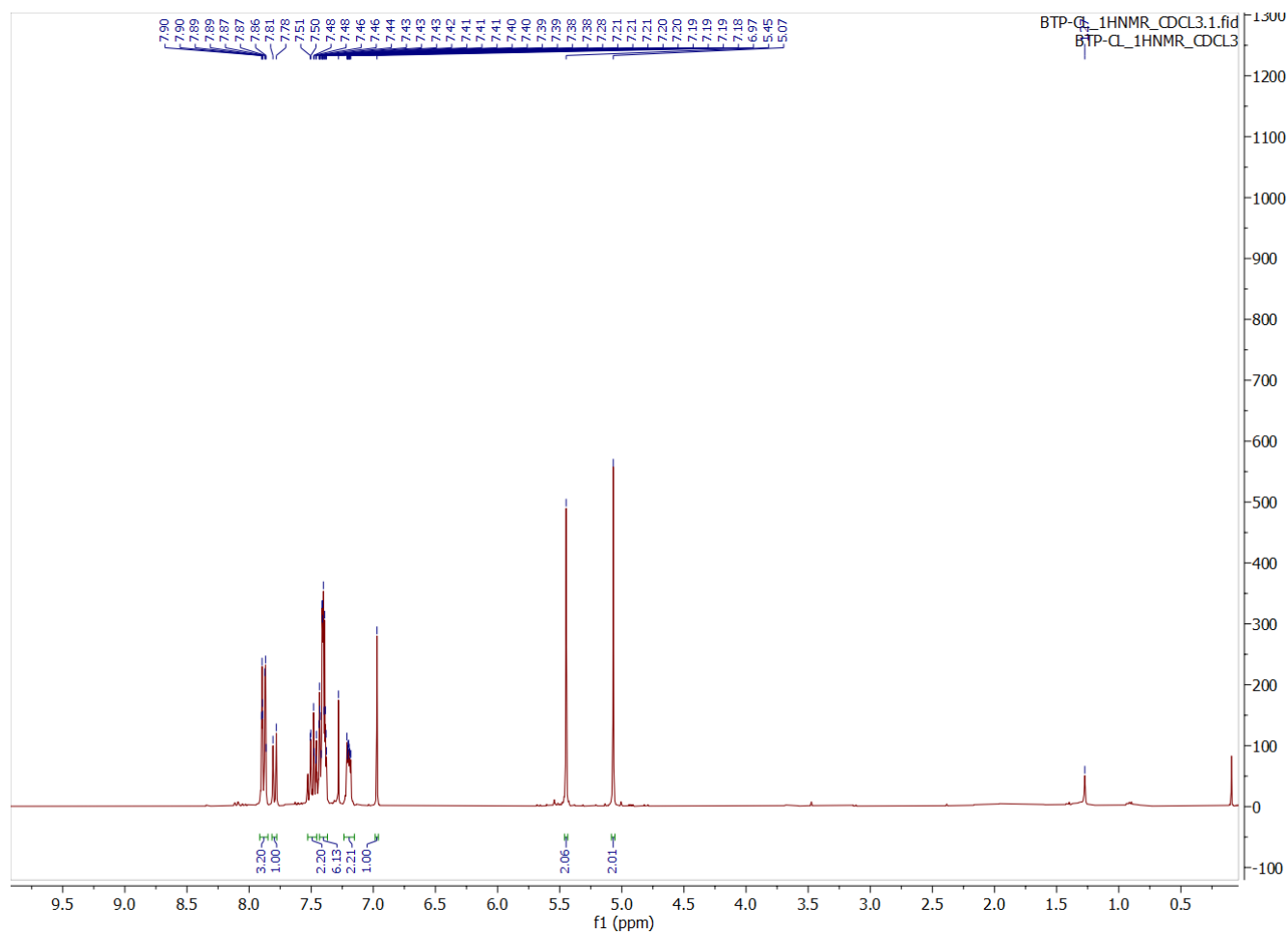
(4-nitrophenyl)(3-(prop-2-yn-1-yloxy)benzo[b]thiophen-2-yl)methanone (11c).

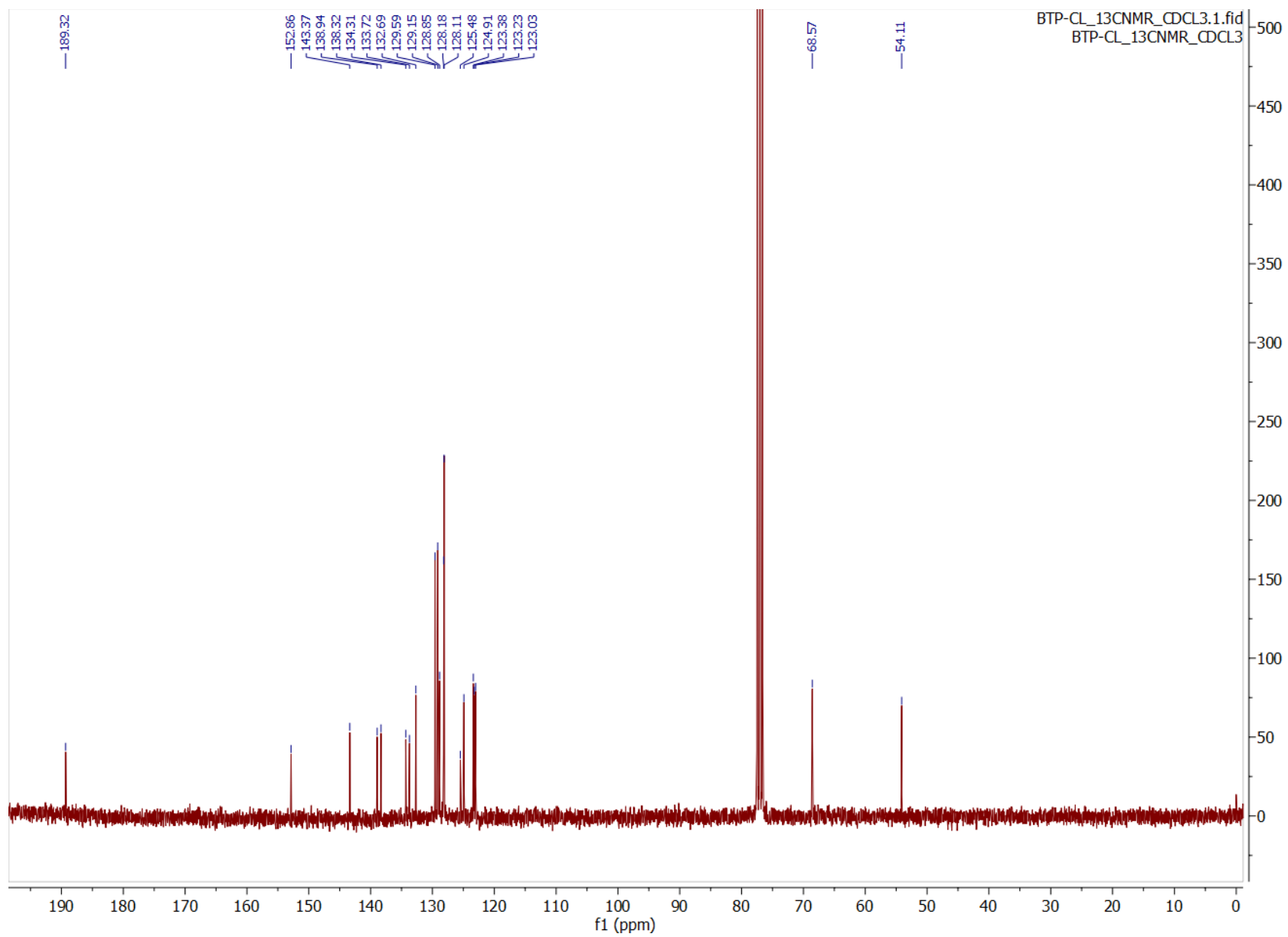


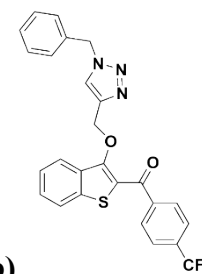




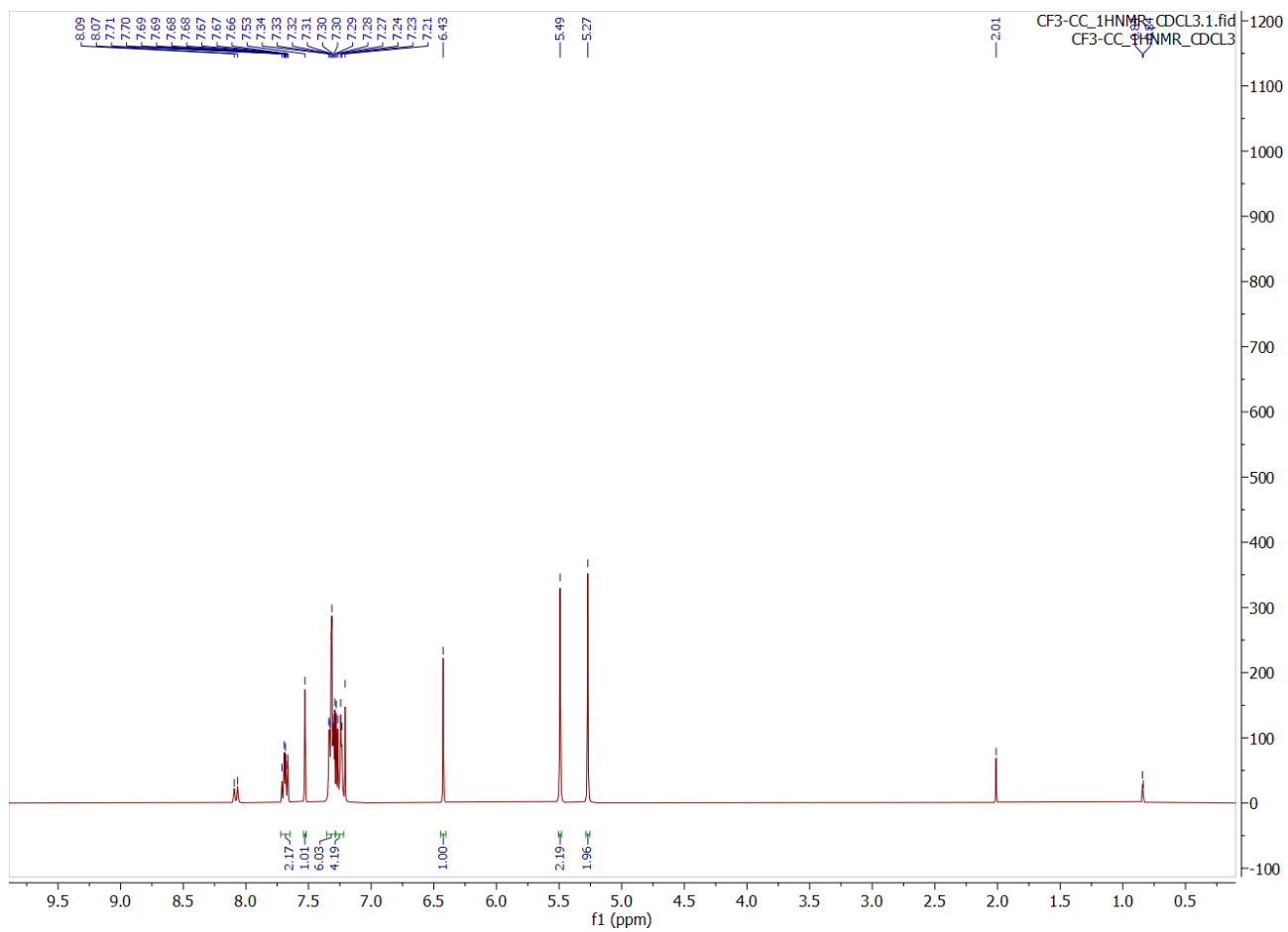
(3-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzo[b]thiophen-2-yl)(phenyl)methanone (14a)

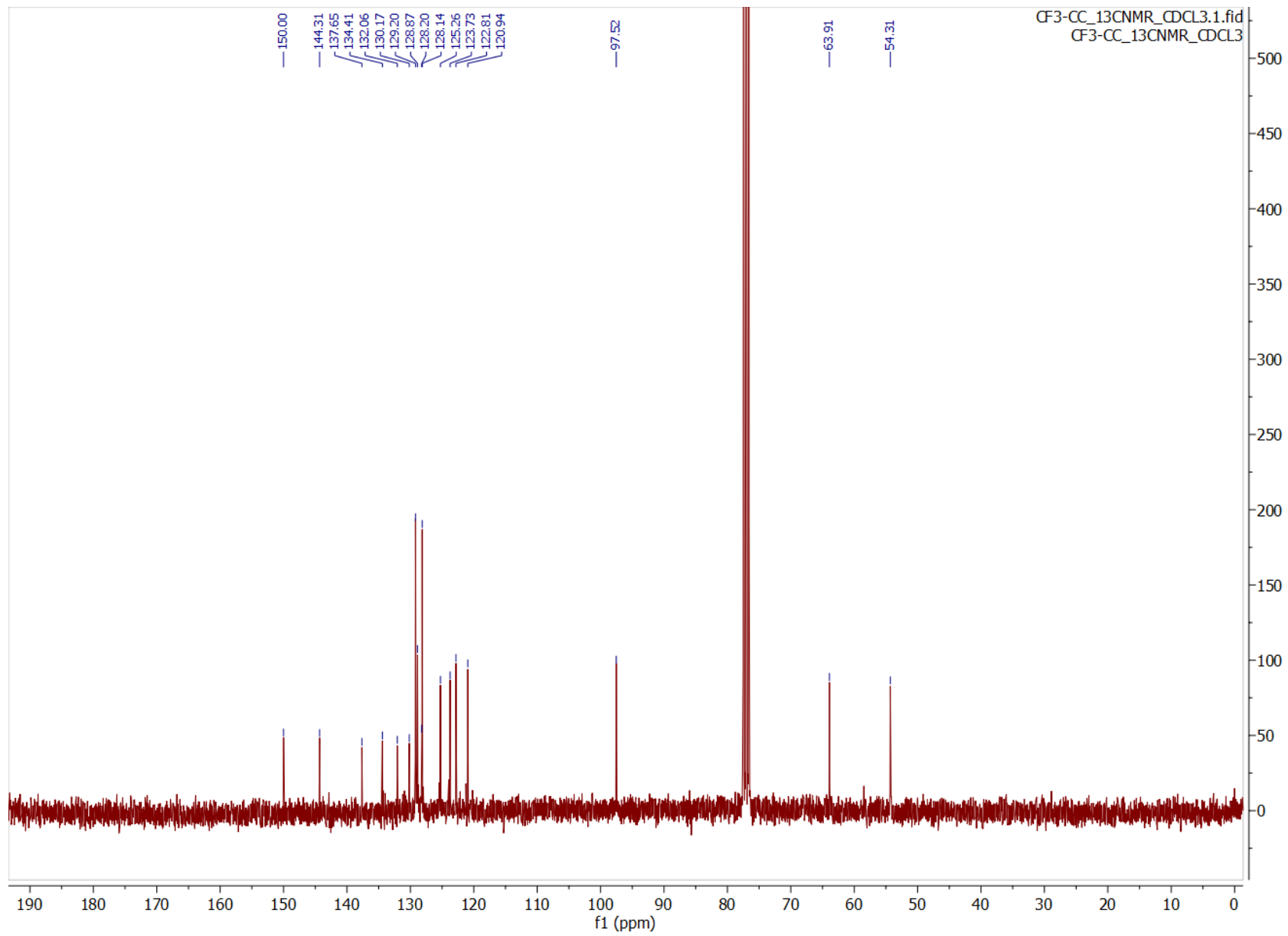


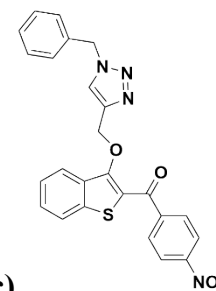




(3-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzo[b]thiophen-2-yl)(4-(trifluoromethyl)phenyl)methanone (14b)







(3-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzo[b]thiophen-2-yl)(4-nitrophenyl)methanone (14c)

