

**Isolation and characterization of novel degradation products in Fenoverine by LC-QTOF-MS/MS, LC-MSⁿ
and 2D-NMR**

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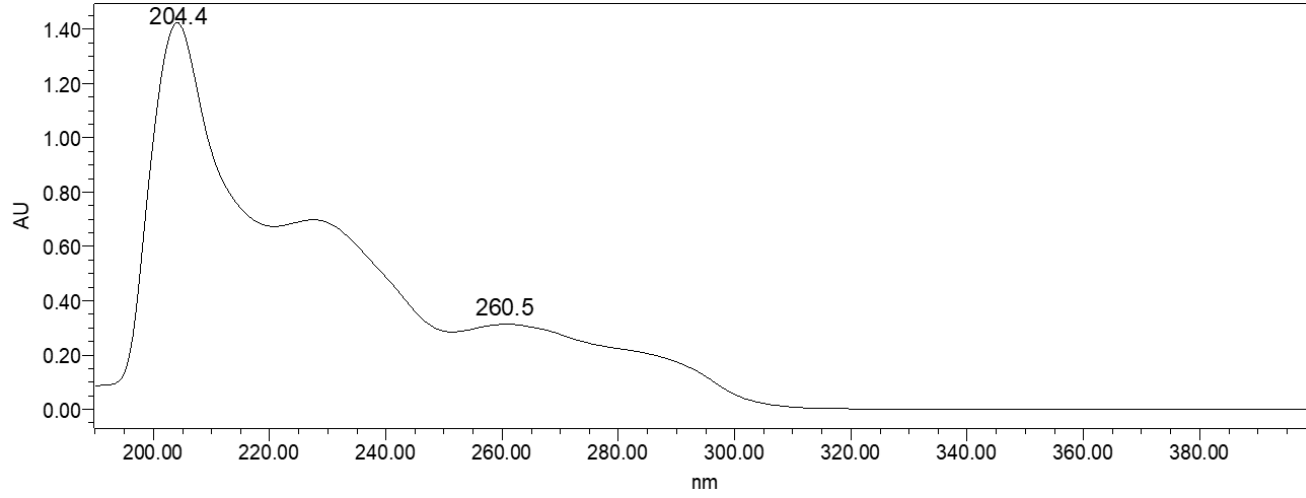


Figure 1: UV Spectra of FEN.

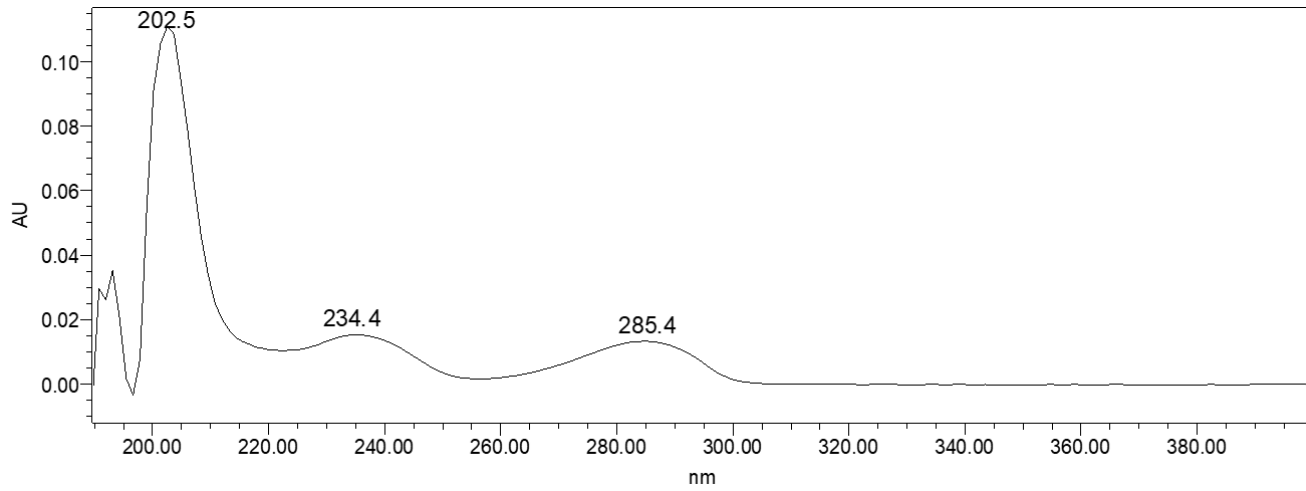


Figure 2: UV Spectra of FAD1.

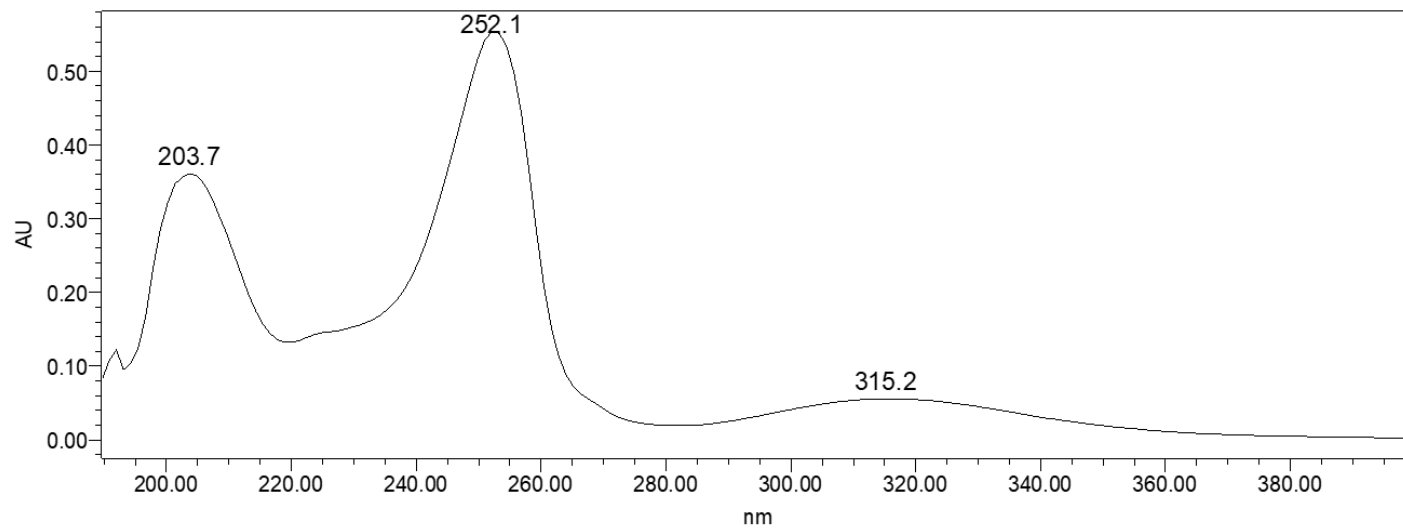


Figure 3: UV Spectra of FAD2.

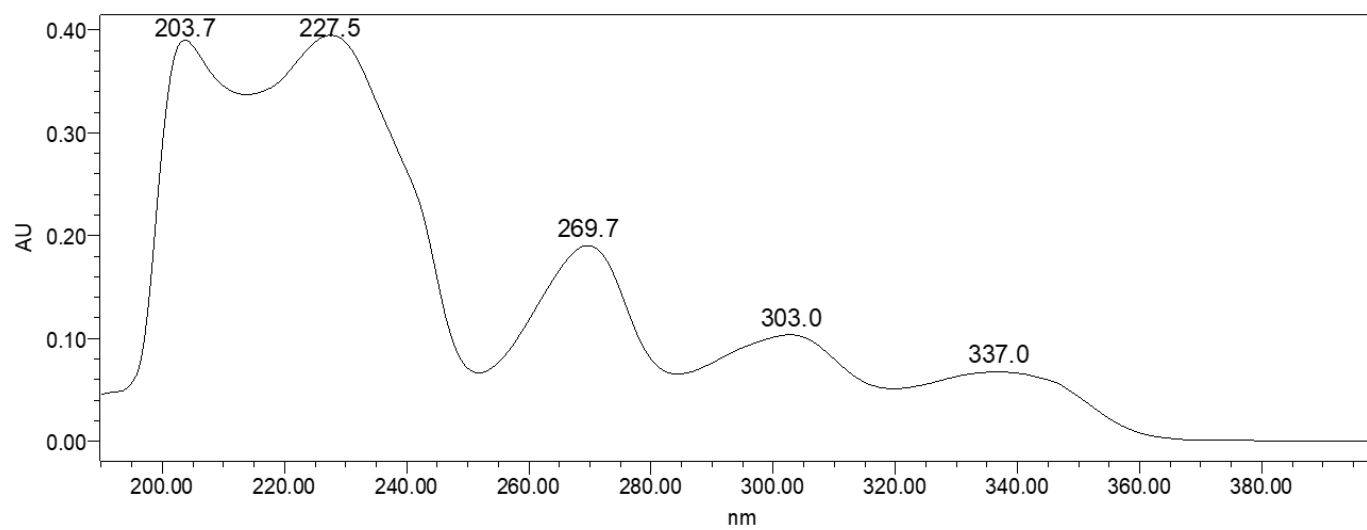


Figure 4: UV Spectra of FOD1.

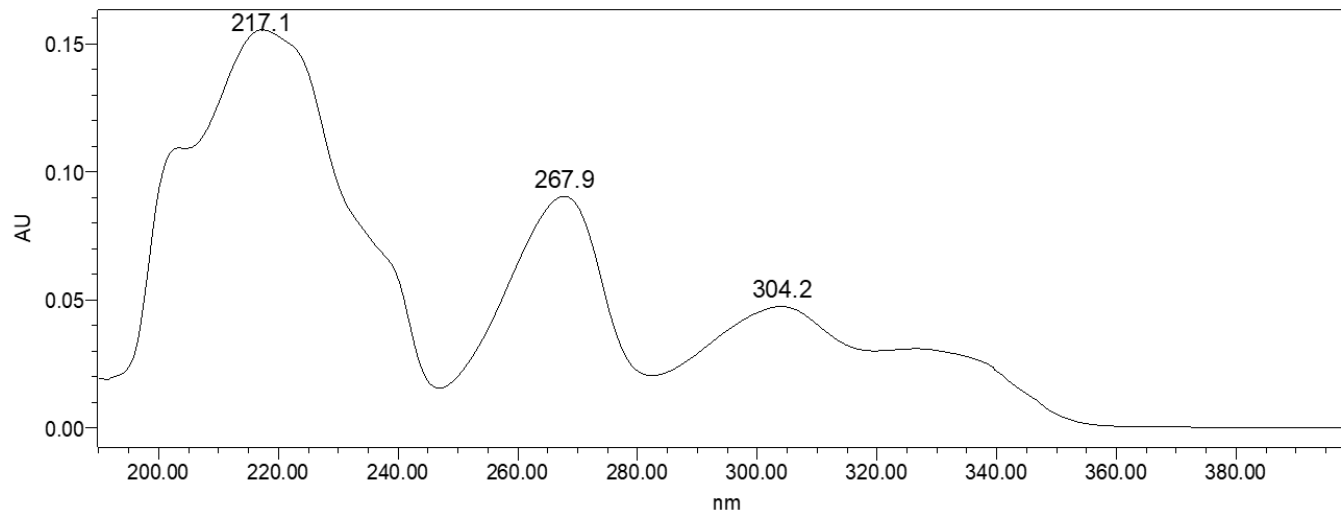


Figure 5: UV Spectra of FOD2.

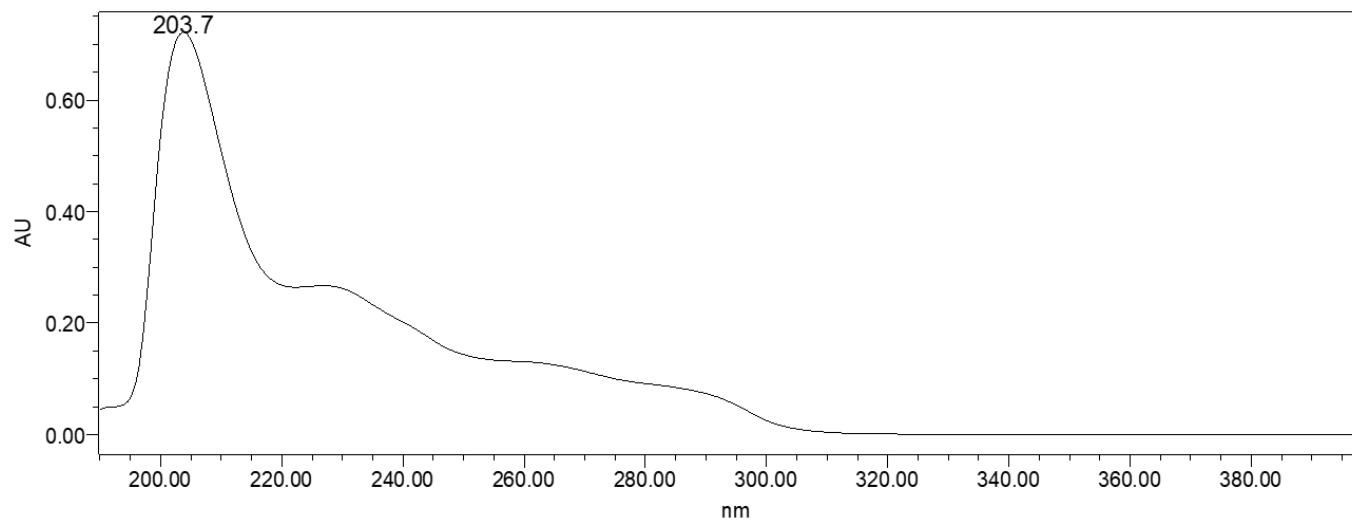


Figure 6: UV Spectra of FOD3.

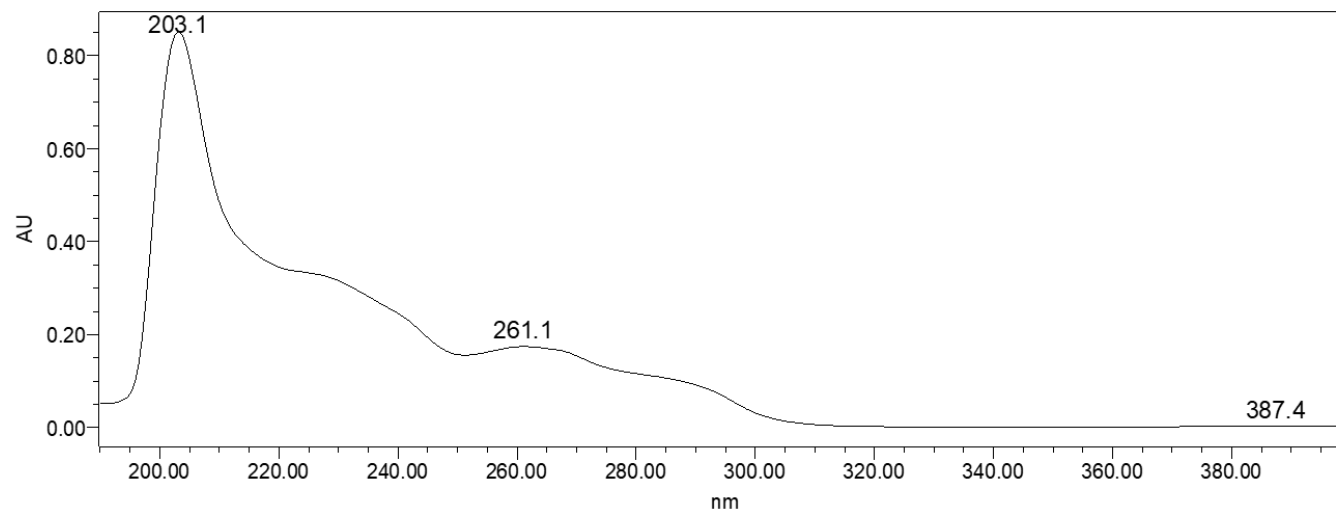


Figure 7: UV Spectra of FOD4

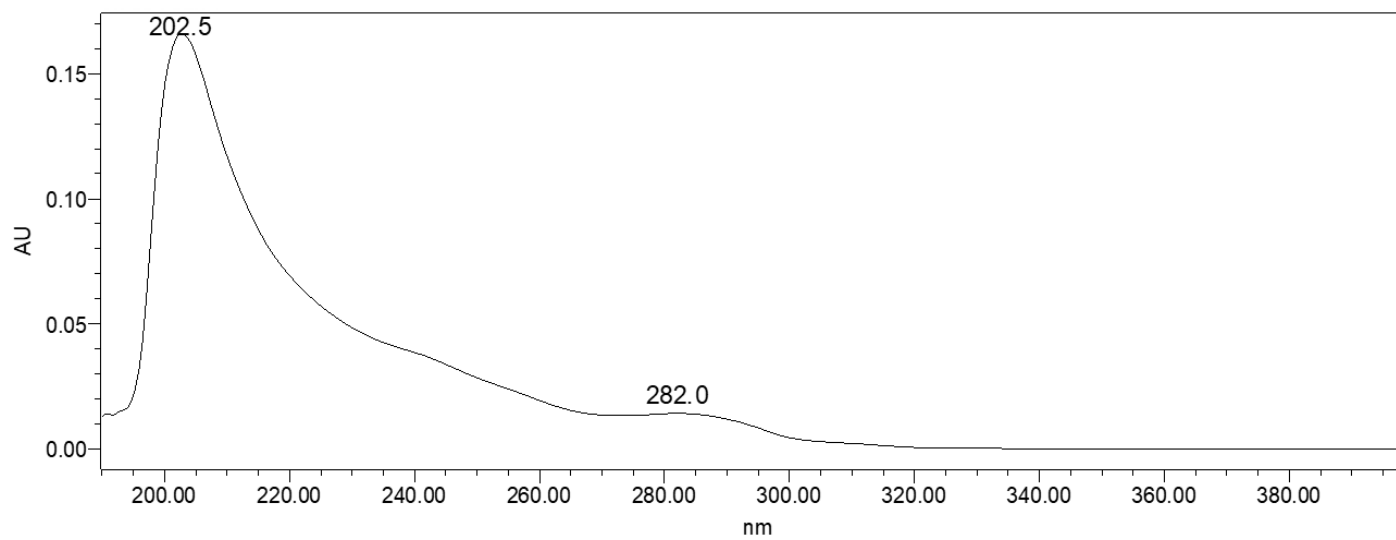


Figure 8: UV Spectra of FOD5

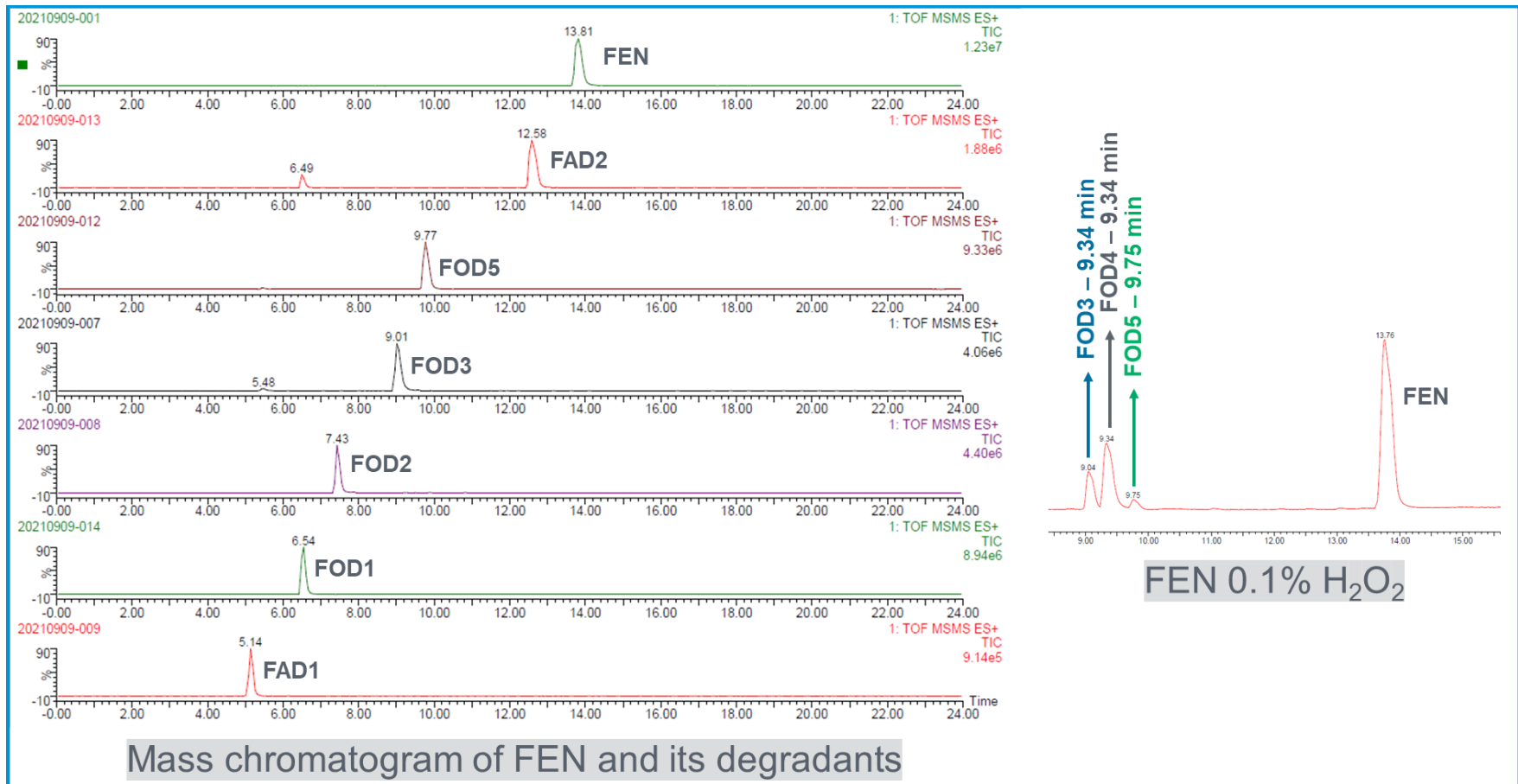


Figure 9: Mass chromatograms of FEN and its degradation products FAD1, FAD2, FOD1 to FOD5

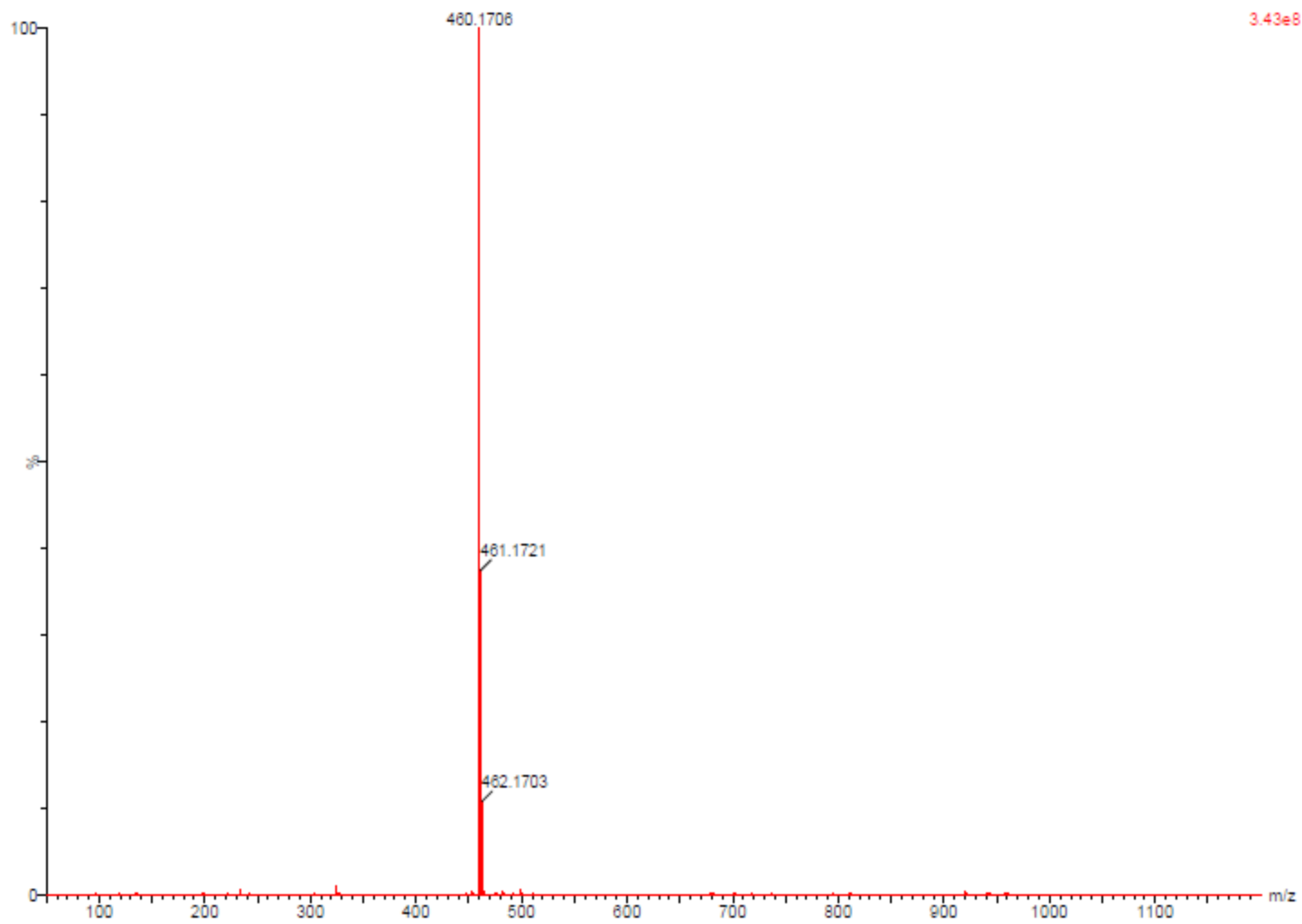


Figure 10: High resolution mass spectrum of FEN

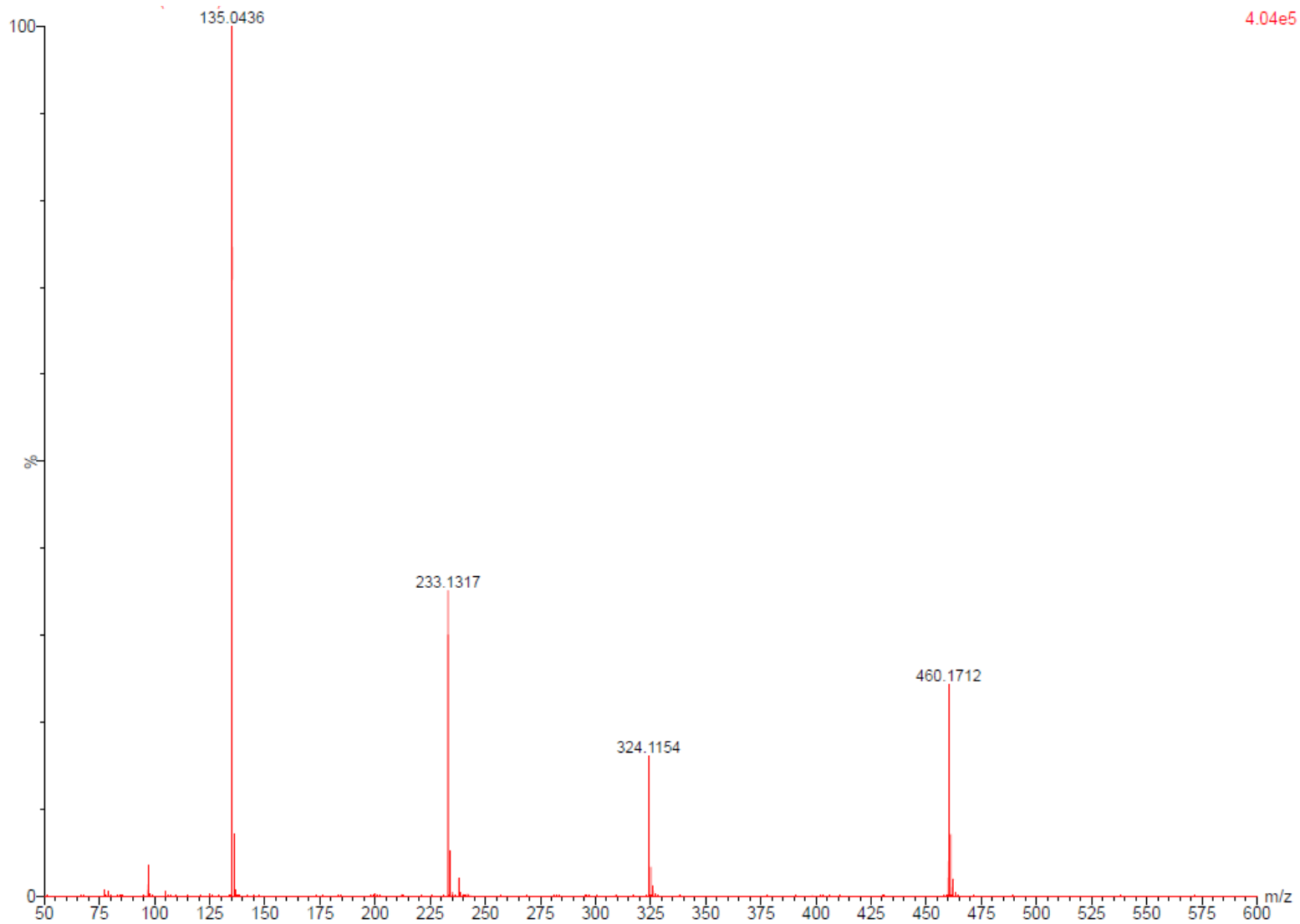
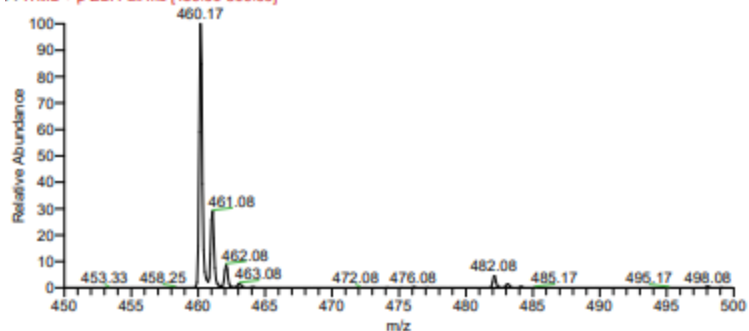
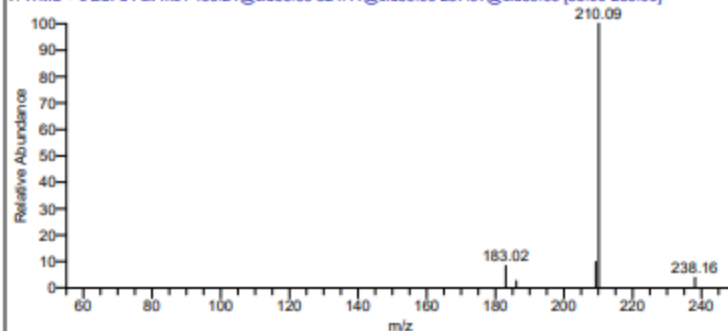


Figure 11: High resolution MSMS Spectrum of FEN

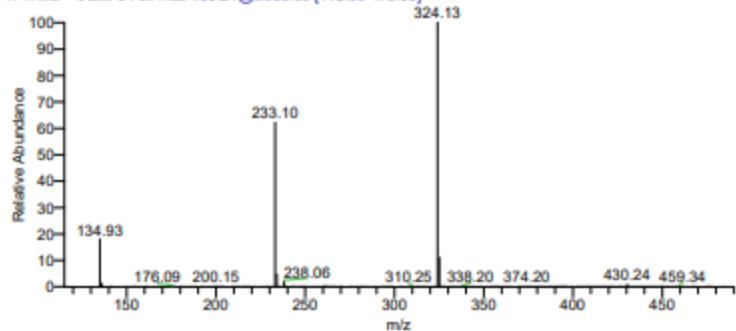
FEN-13-11 #296 RT: 1.13 AV: 1 NL: 2.01E6
F: ITMS + p ESI Full ms [450.00-500.00]



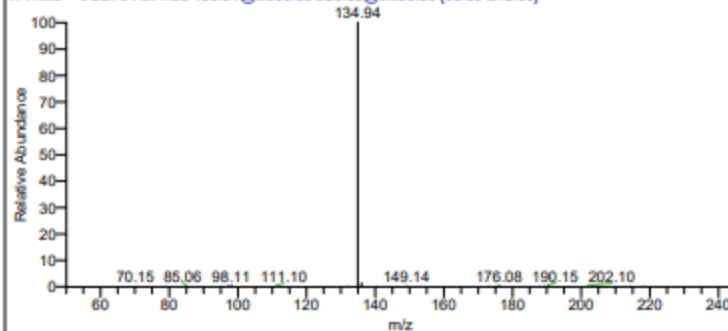
FEN-13-11 #97-538 RT: 0.37-1.85 AV: 4 NL: 5.29E3
T: ITMS + c ESI d Full ms4 460.21@cid60.00 324.11@cid60.00 237.97@cid60.00 [55.00-250.00]



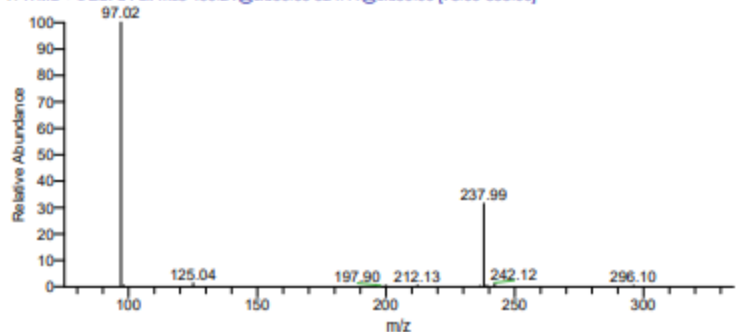
FEN-13-11 #3-507 RT: 0.02-1.77 AV: 14 NL: 2.98E5
T: ITMS + c ESI d Full ms2 460.21@cid60.00 [115.00-475.00]



FEN-13-11 #72-513 RT: 0.30-1.78 AV: 4 NL: 5.62E5
T: ITMS + c ESI d Full ms3 460.21@cid60.00 233.09@cid60.00 [50.00-245.00]



FEN-13-11 #71-512 RT: 0.30-1.78 AV: 4 NL: 1.62E5
T: ITMS + c ESI d Full ms3 460.21@cid60.00 324.11@cid60.00 [75.00-335.00]



FEN-13-11 #73-514 RT: 0.30-1.78 AV: 4 NL: 2.18E2
T: Average spectrum MS3 460.29,134.94 (73-514)

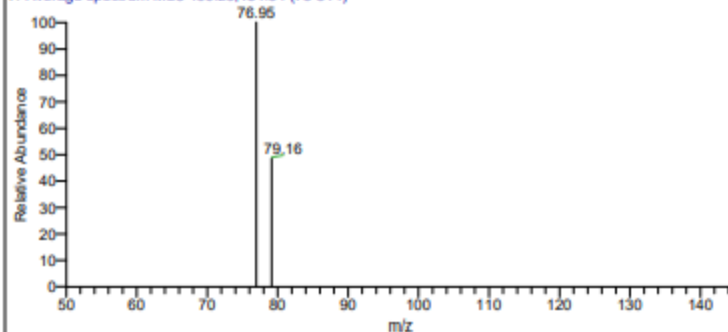


Figure 12: MSⁿ spectrum of FEN

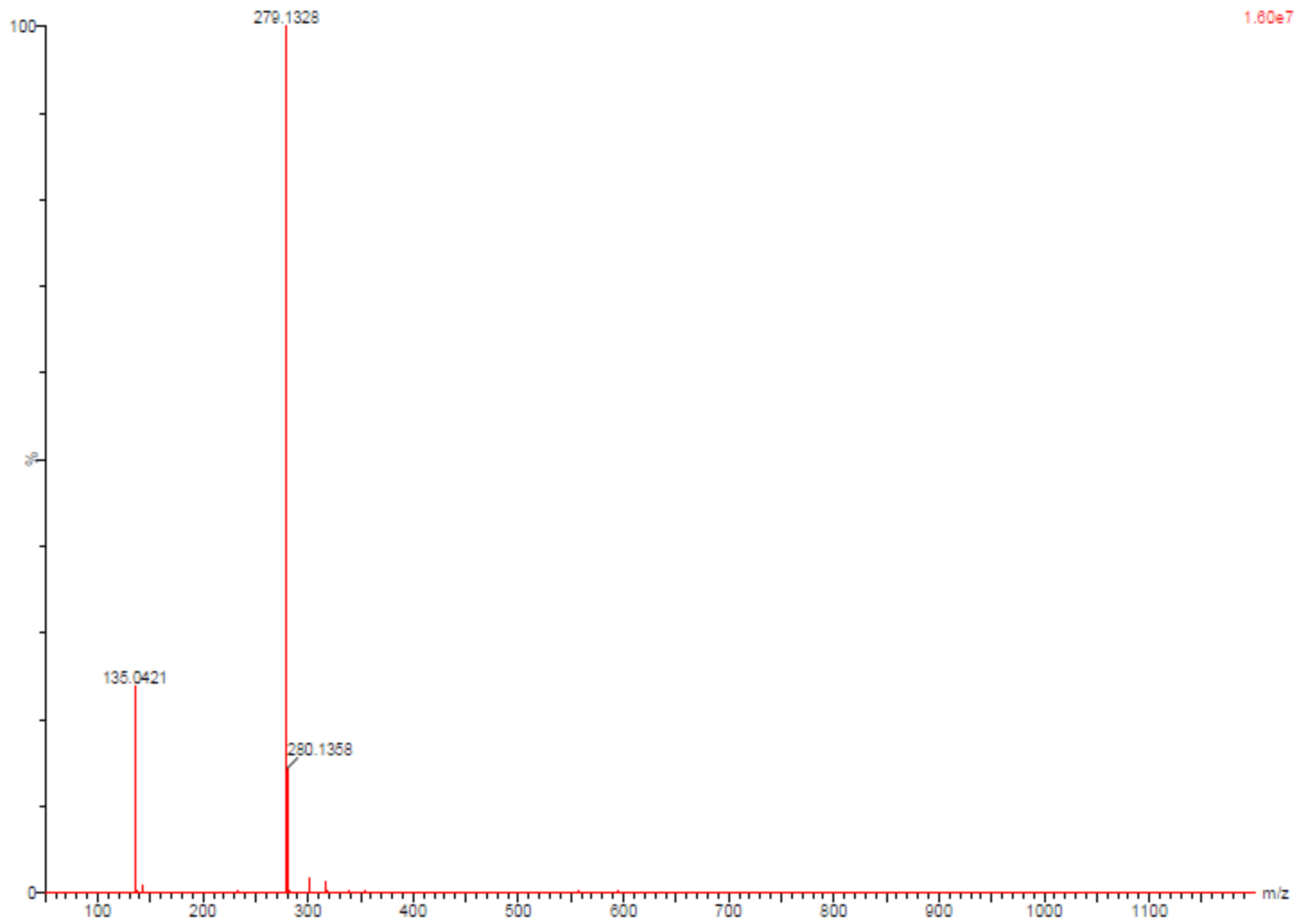


Figure 13: High resolution mass spectrum of FAD1

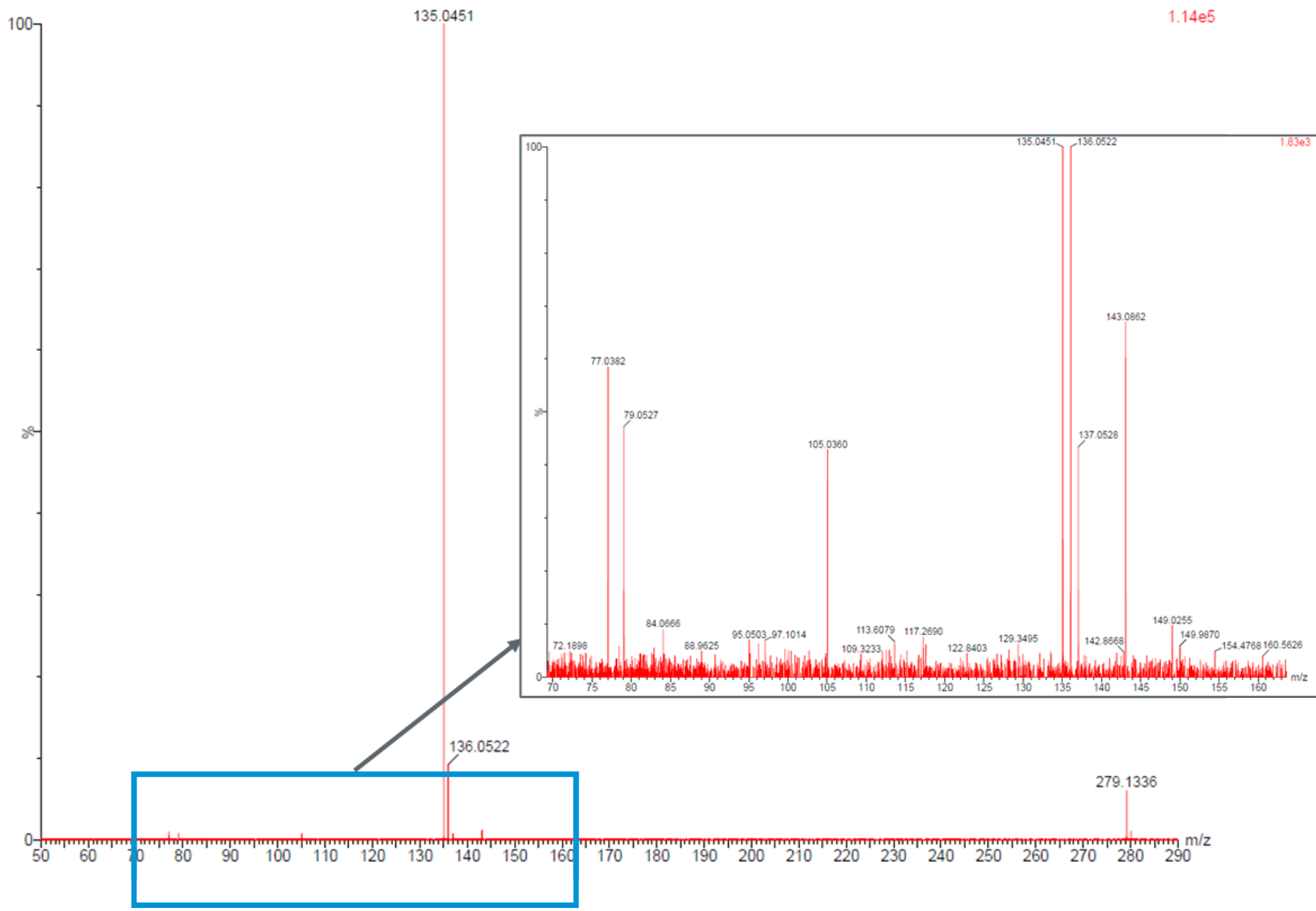


Figure 14: High resolution MSMS Spectrum of FAD1

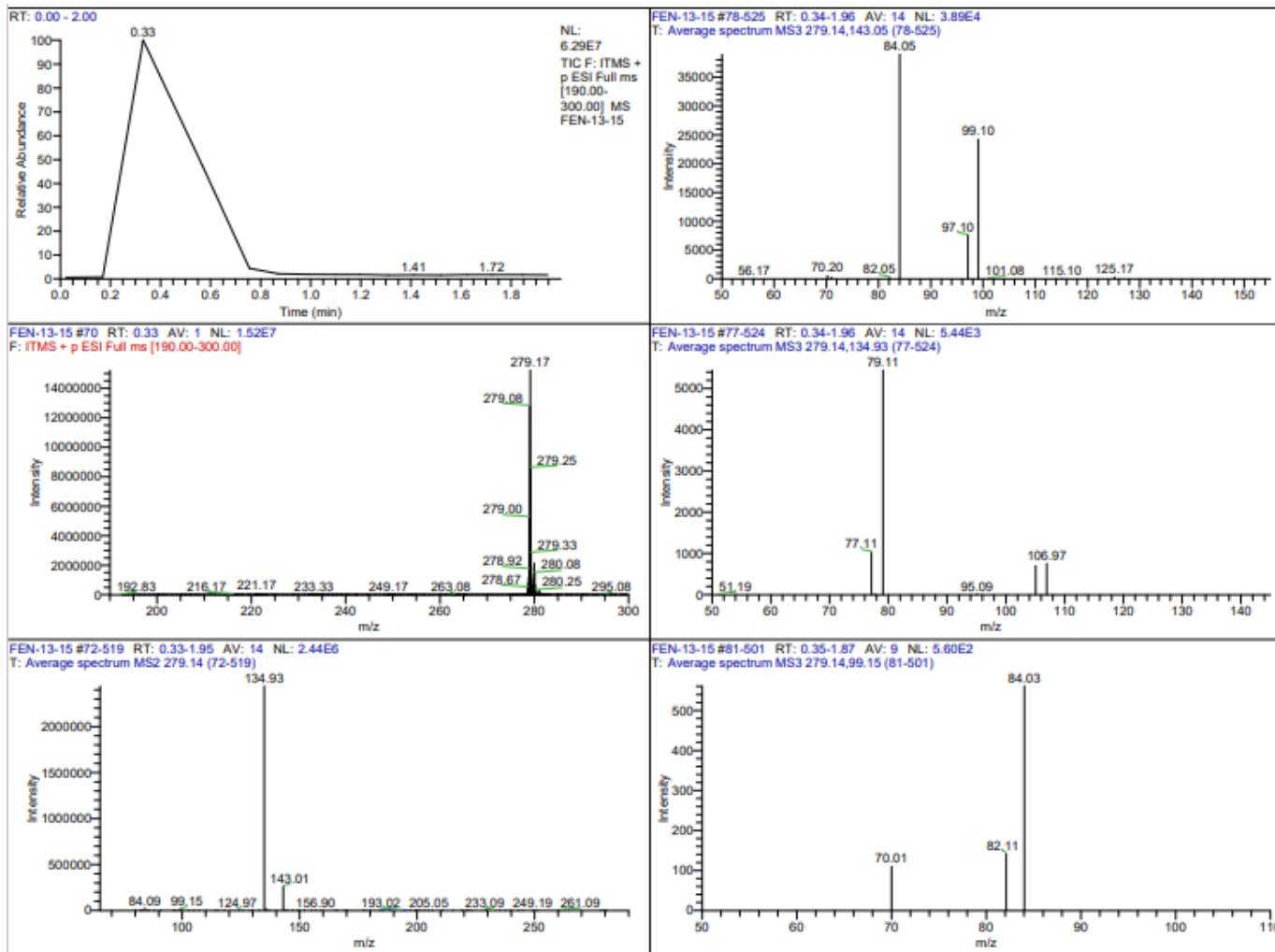


Figure 15: MSⁿ Spectrum of FAD1

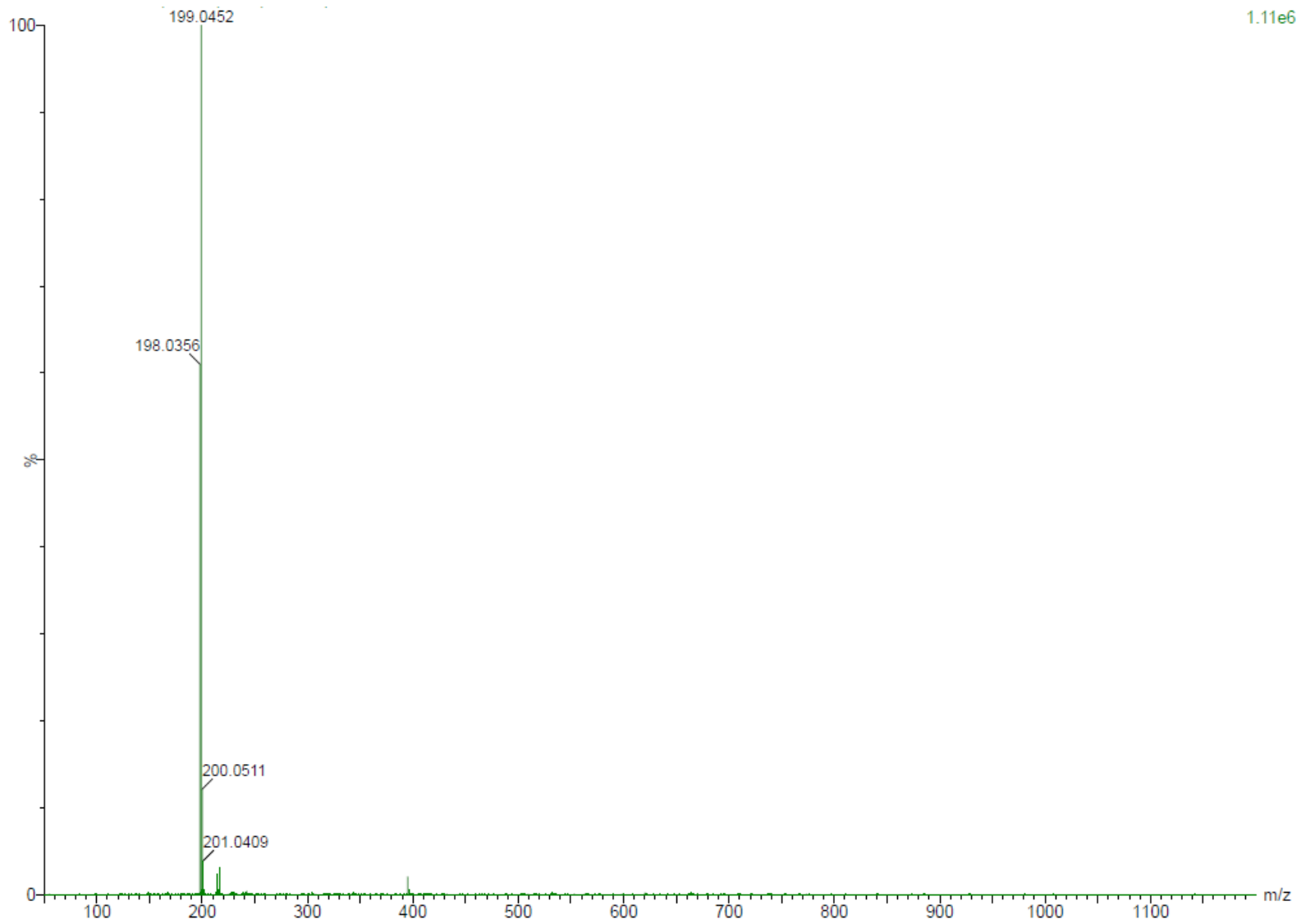


Figure 16: High resolution mass spectrum of FAD2

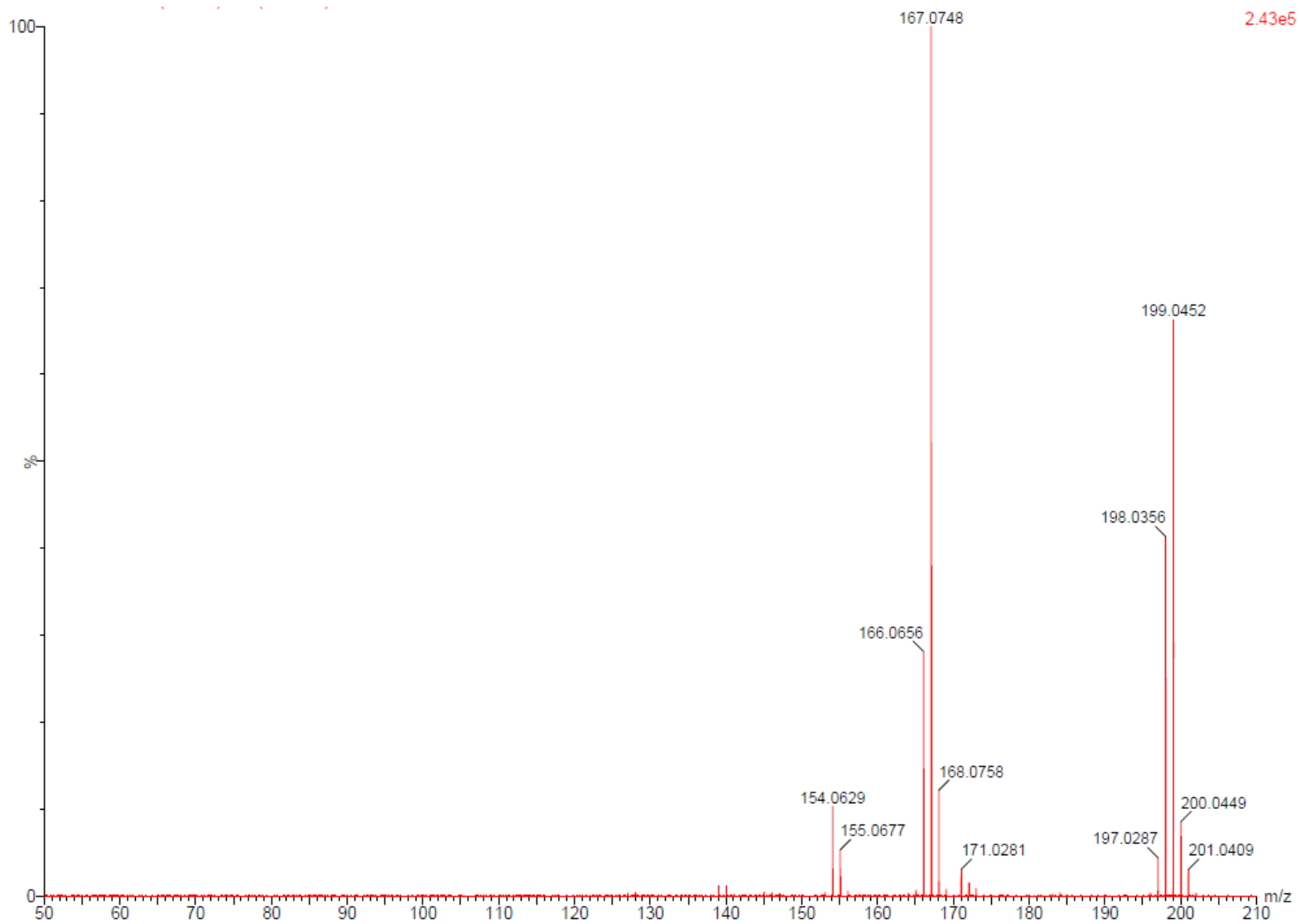


Figure 17: High resolution MSMS Spectrum of FAD2

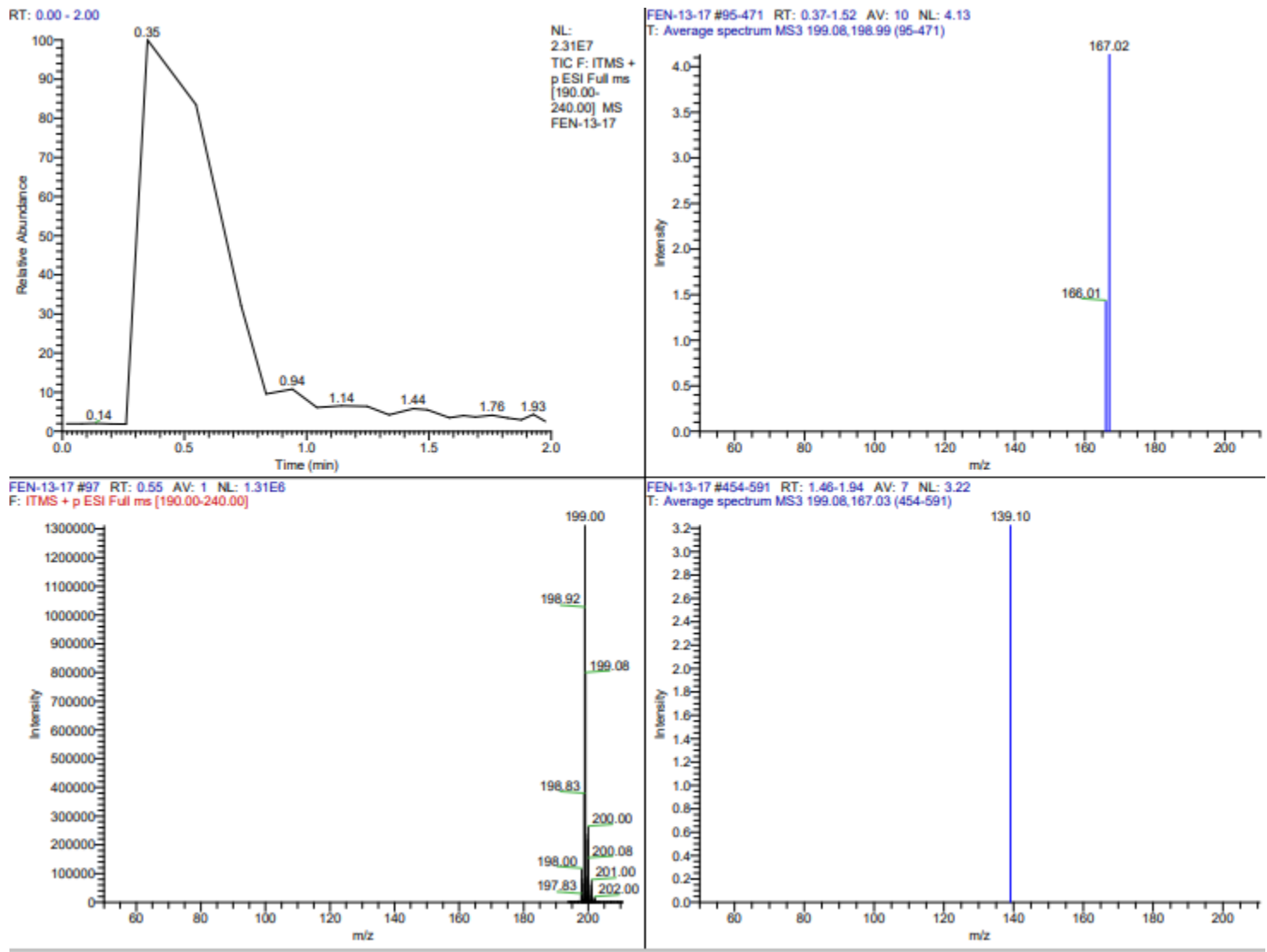


Figure 18: MSⁿ Spectrum of FAD2

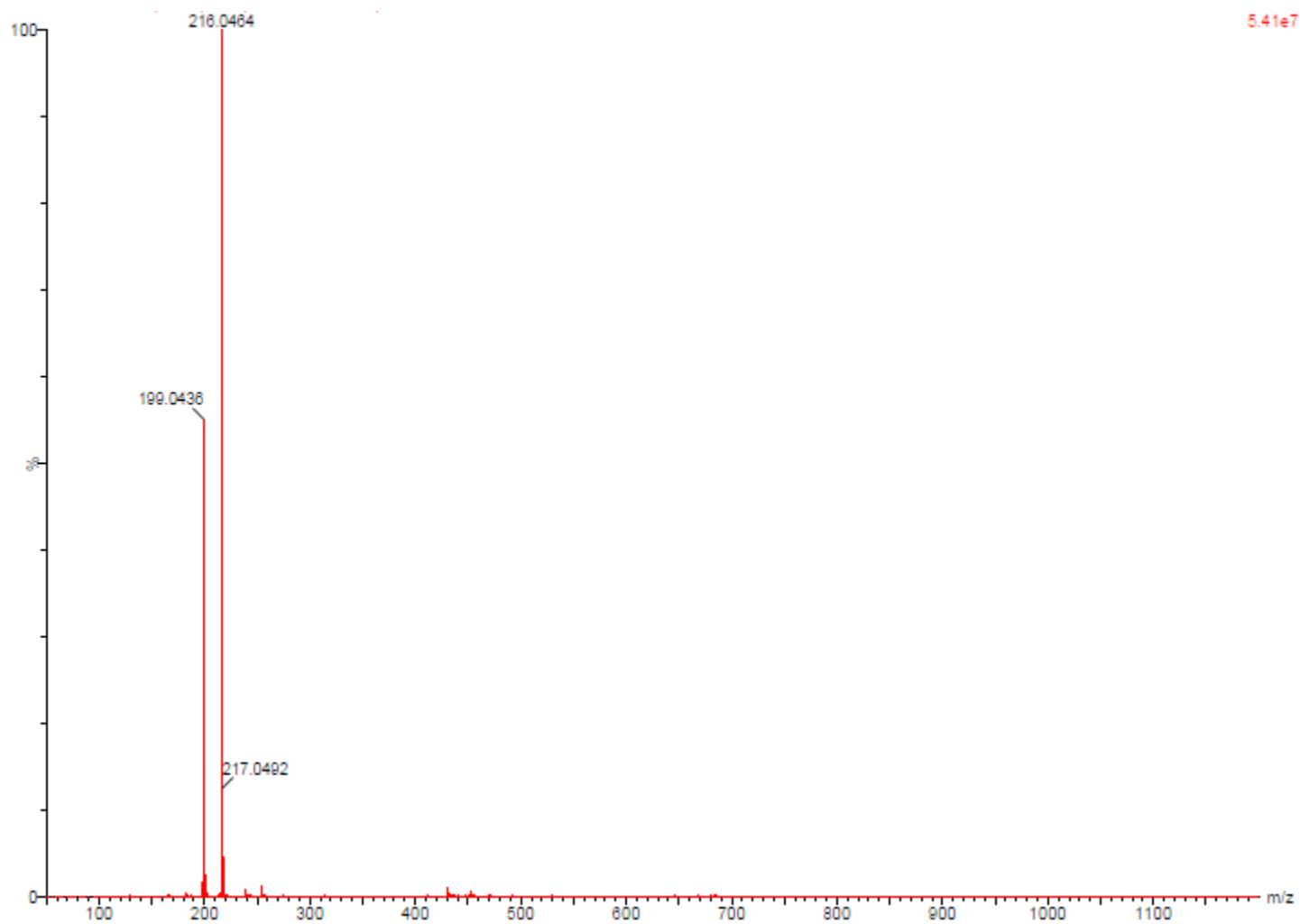


Figure 19: High resolution mass spectrum of FOD1

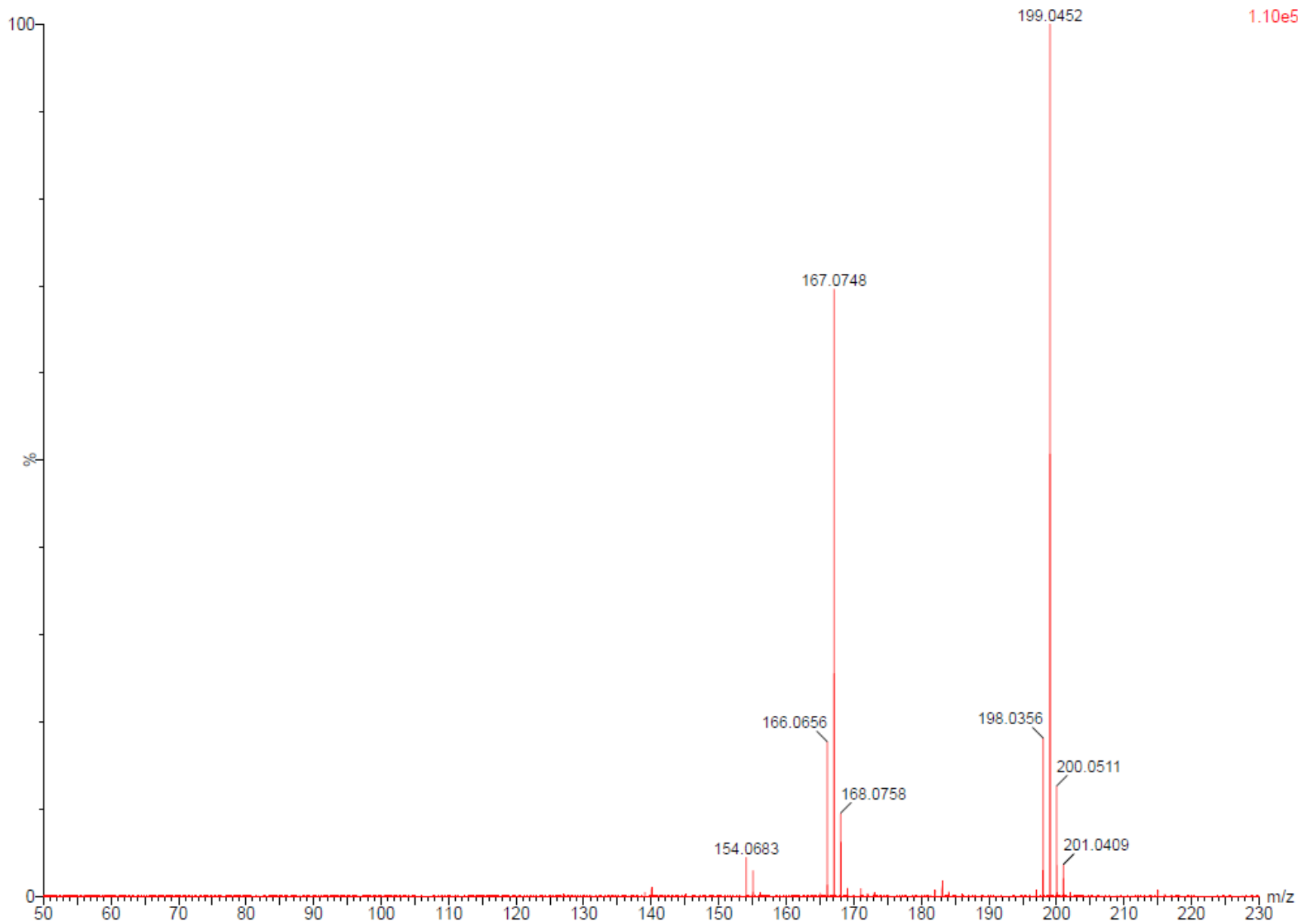


Figure 20: High resolution MSMS Spectrum of FOD1

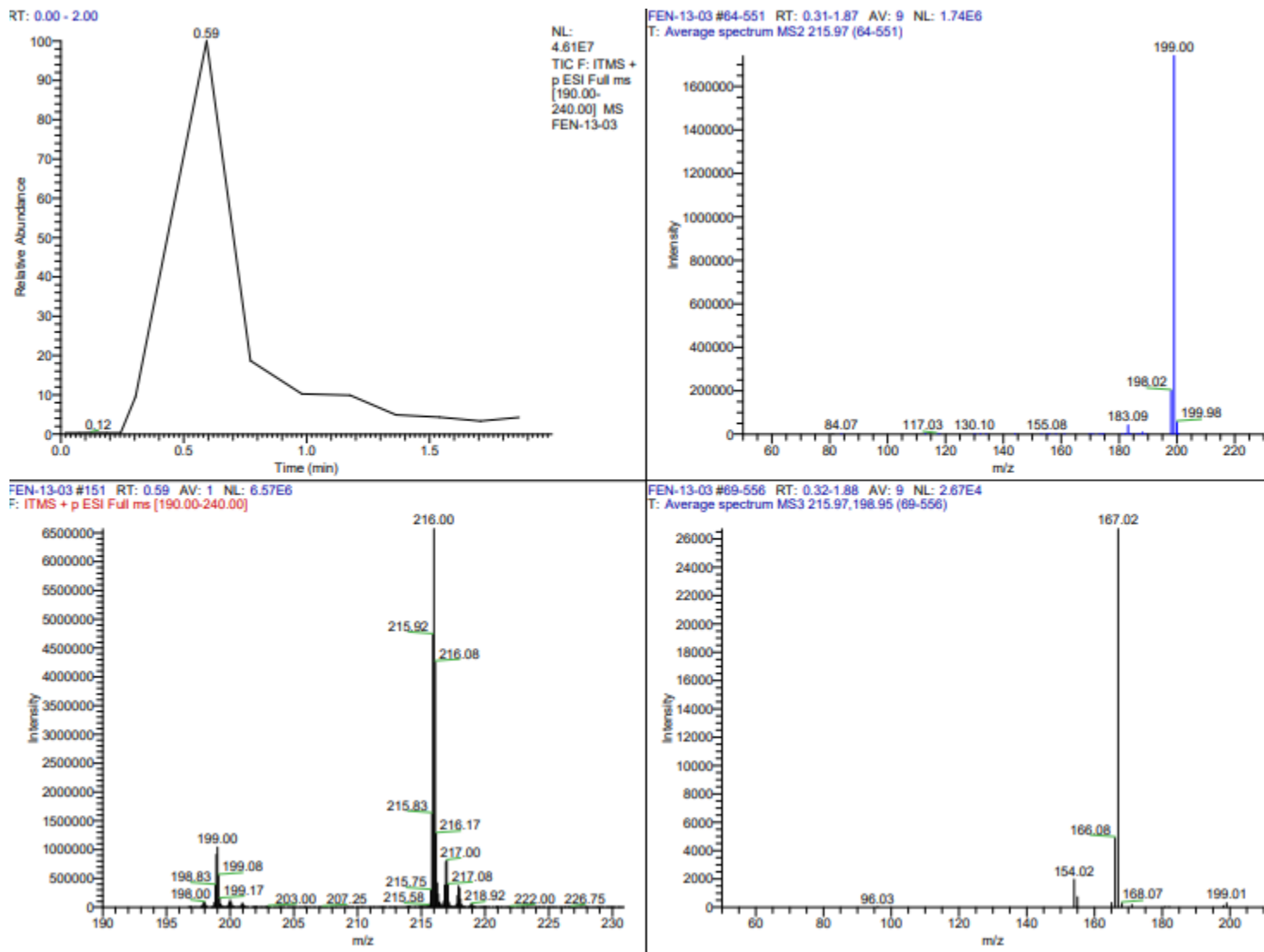


Figure 21: MSⁿ Spectrum of FOD1

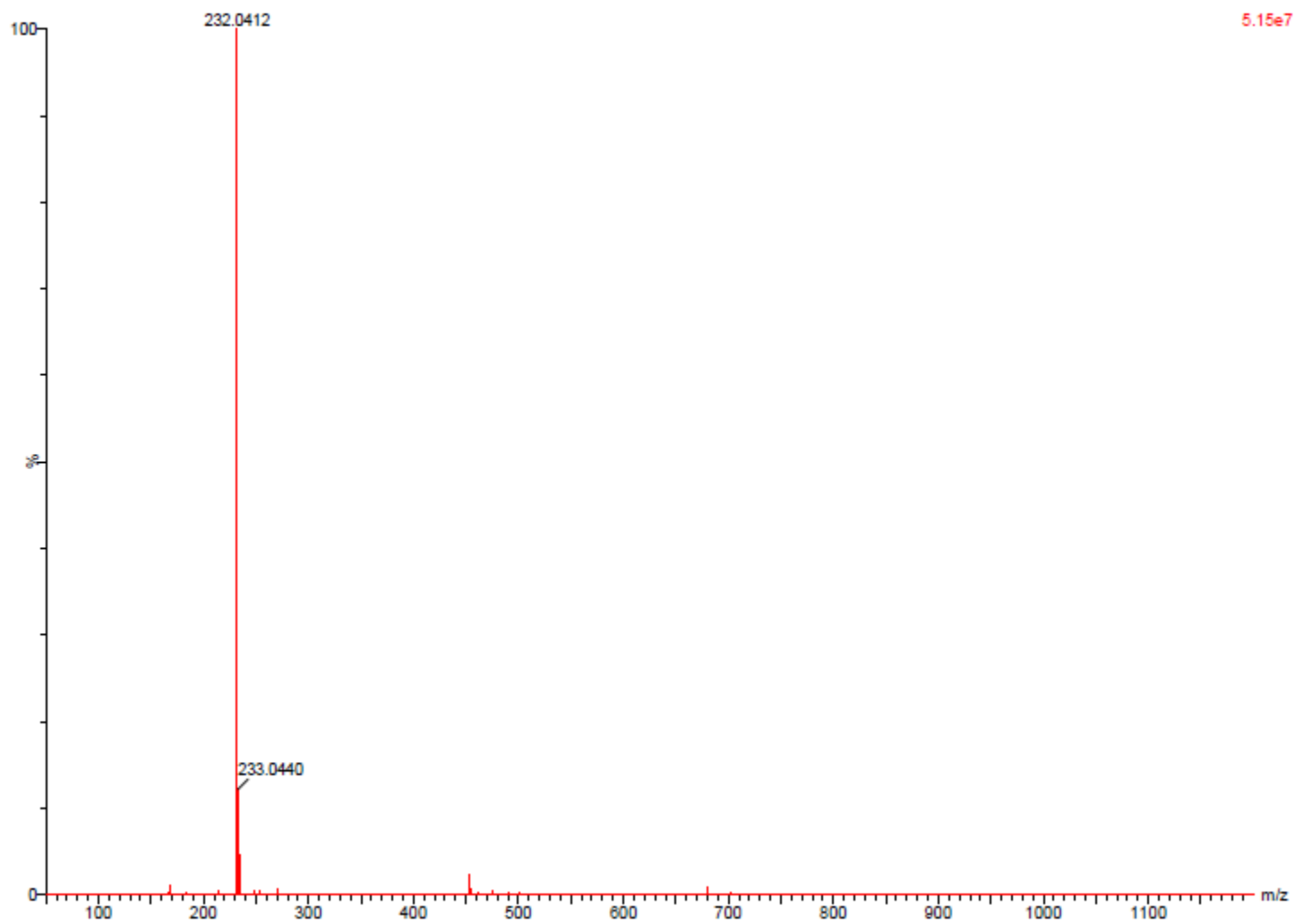


Figure 22: High resolution mass Spectrum of FOD2

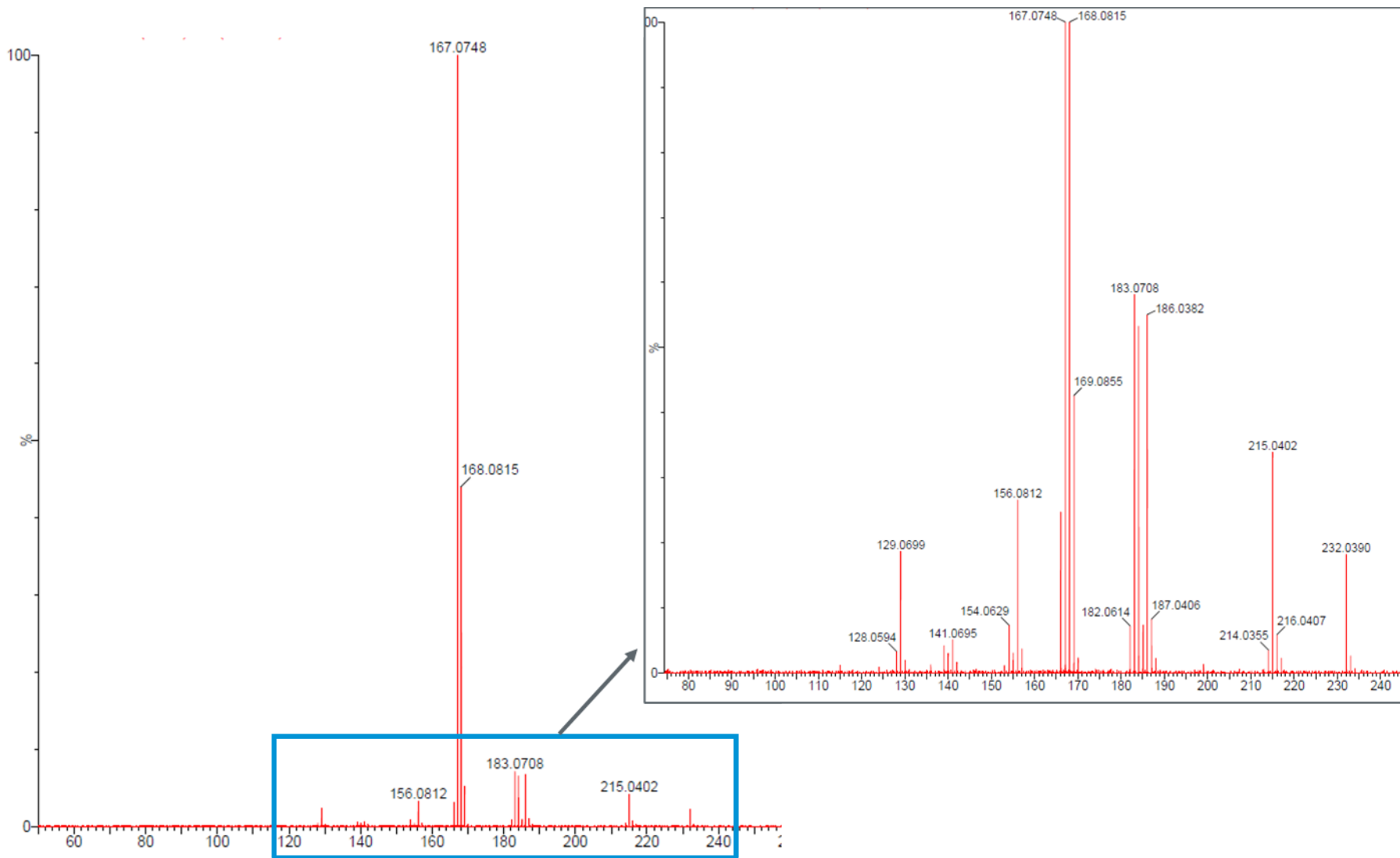


Figure 23: High resolution MSMS Spectrum of FOD2

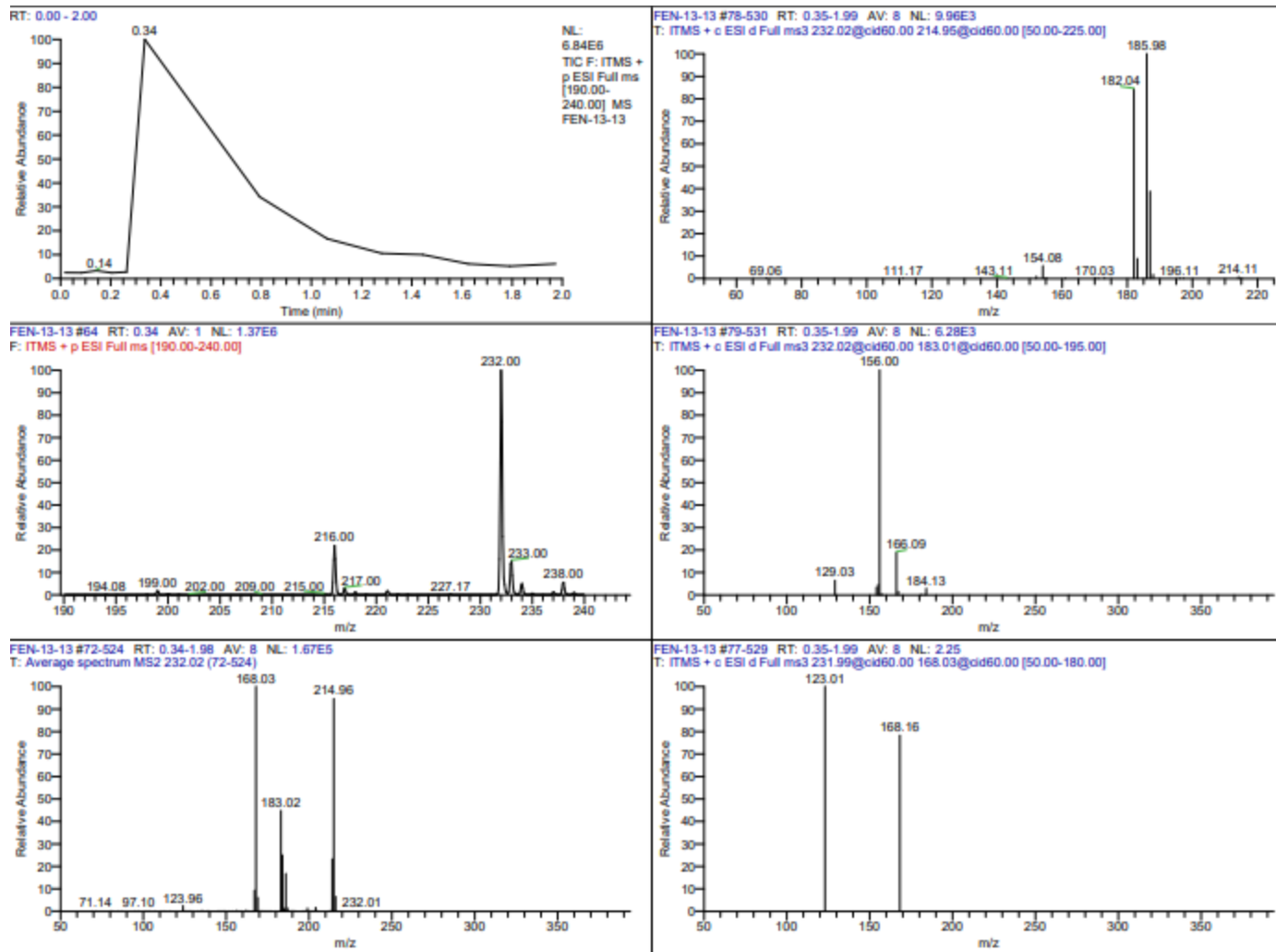


Figure 24: MSⁿ spectrum of FOD2

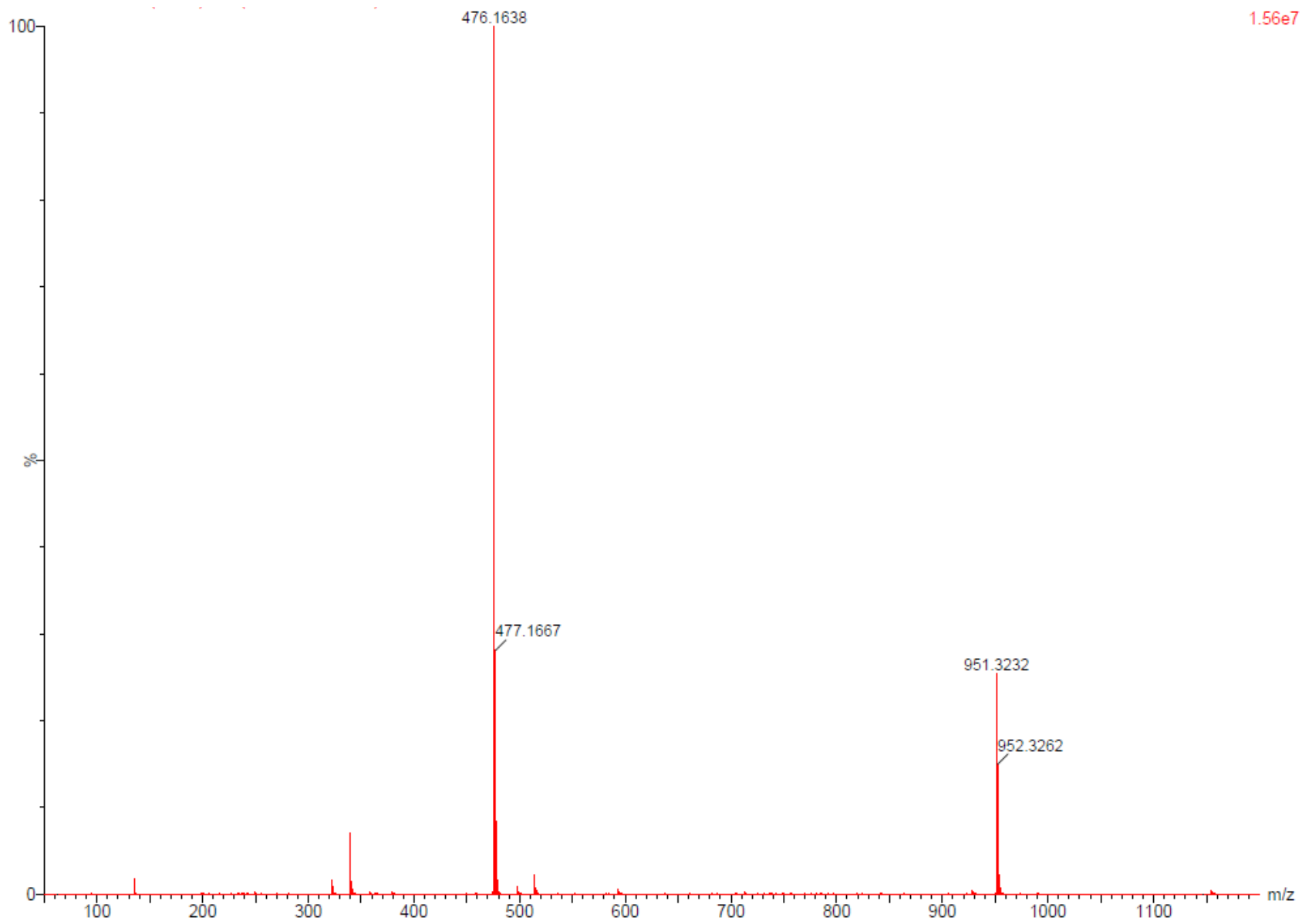


Figure 25: High resolution mass Spectrum of FOD3

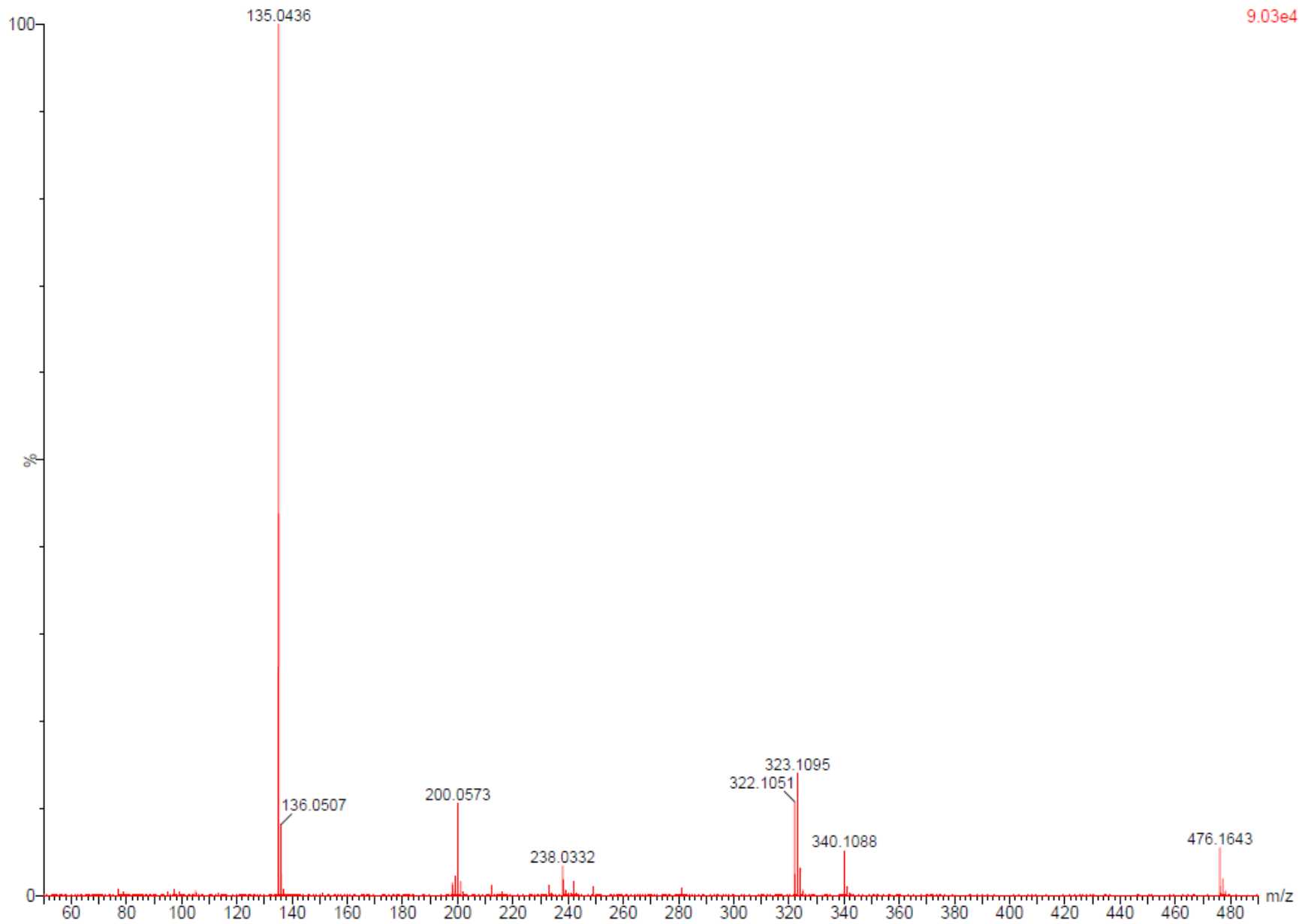


Figure 26: High resolution MSMS Spectrum of FOD3

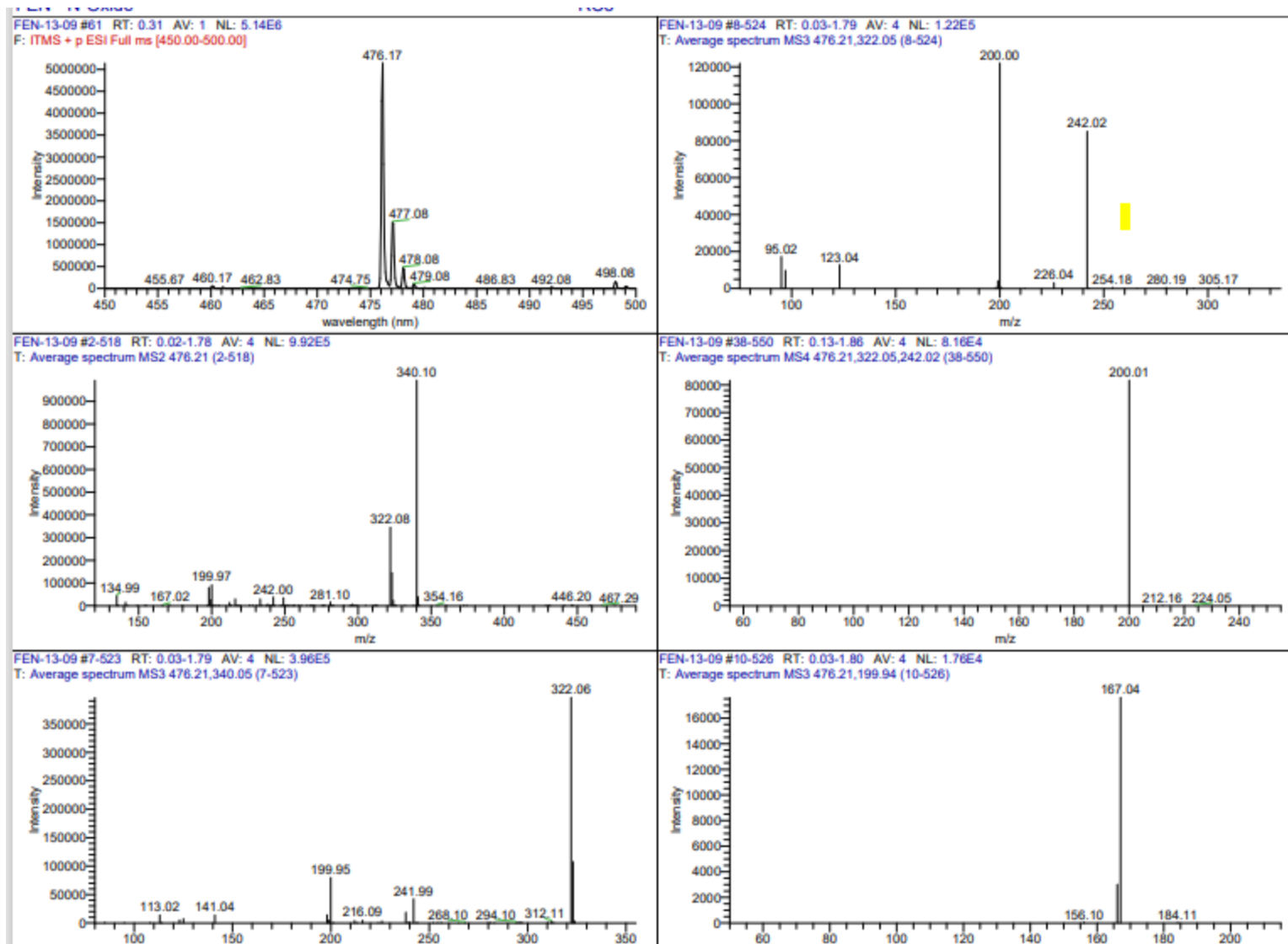


Figure 27: MSⁿ spectrum of FOD3

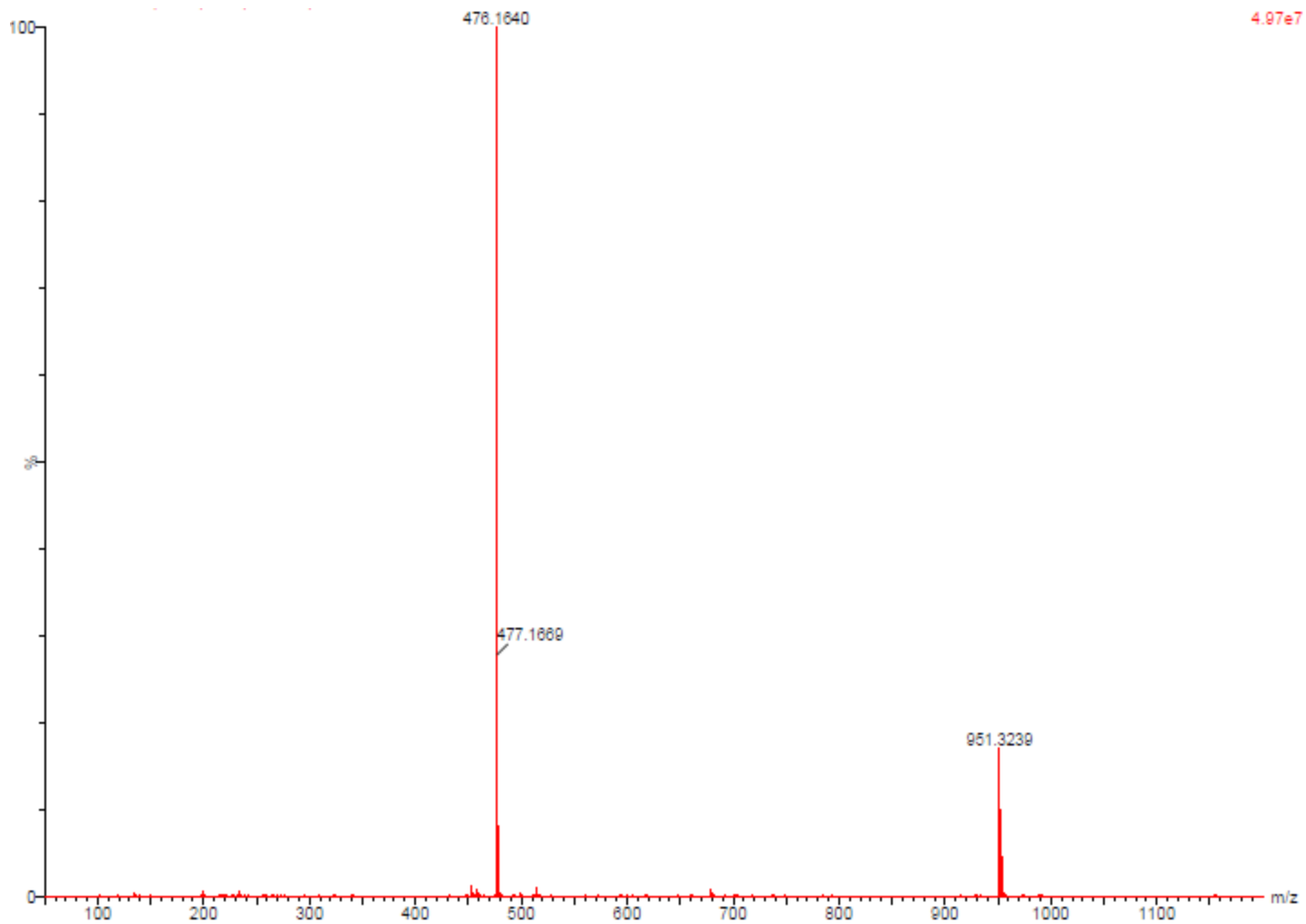


Figure 28: High resolution mass Spectrum of FOD4

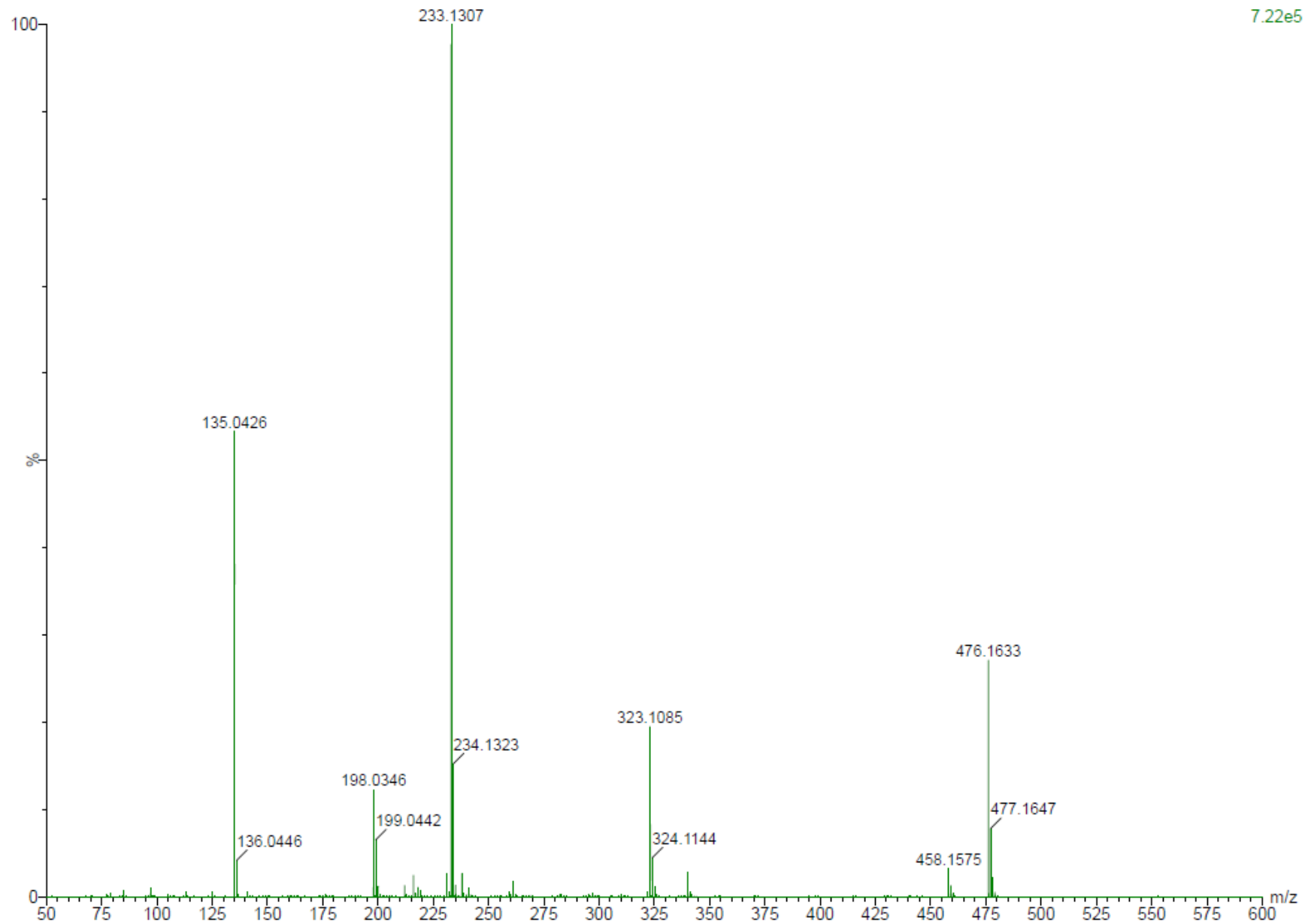


Figure 29: High resolution MSMS Spectrum of FOD4

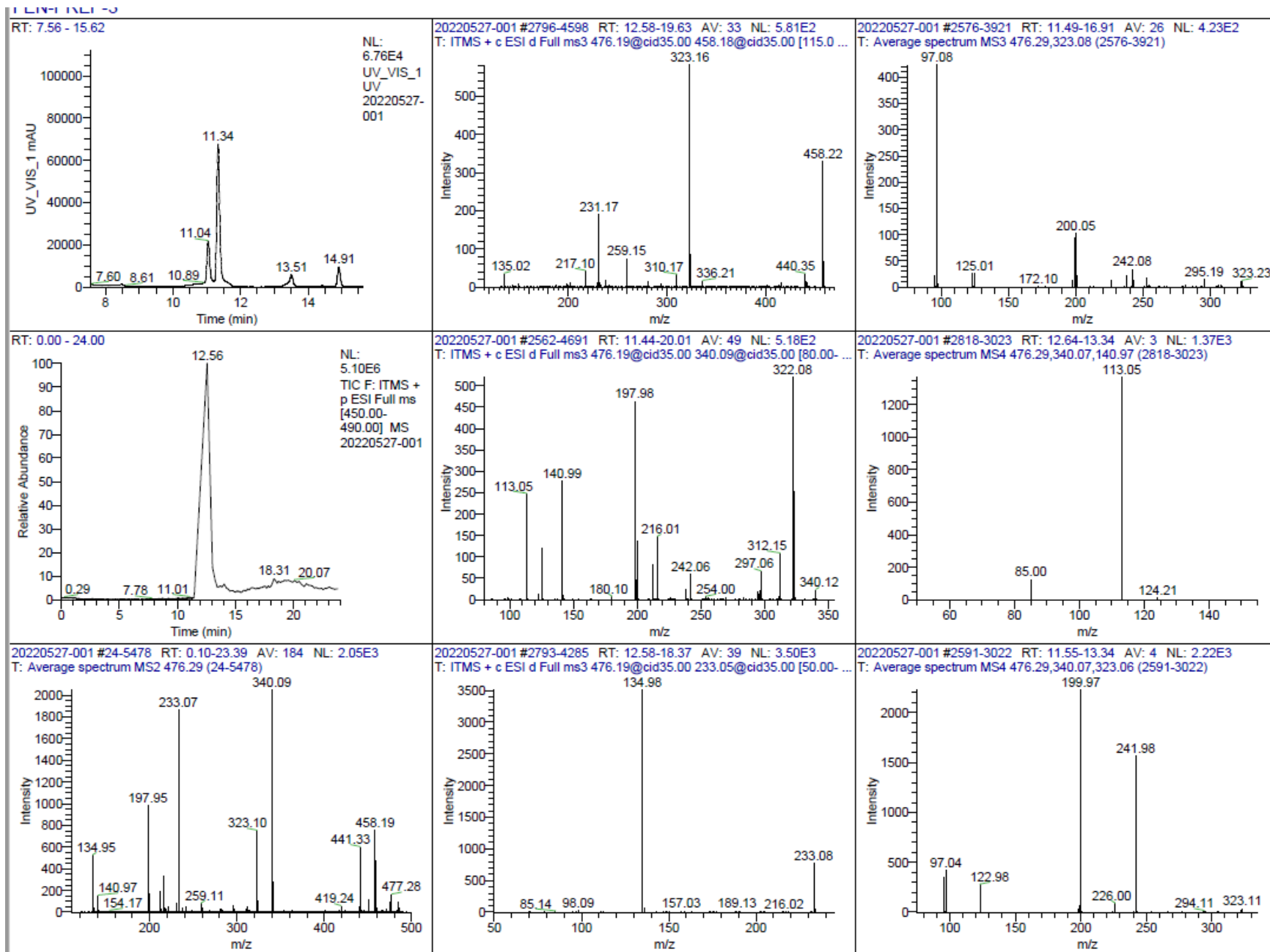


Figure 30: MSⁿ spectrum of FOD4

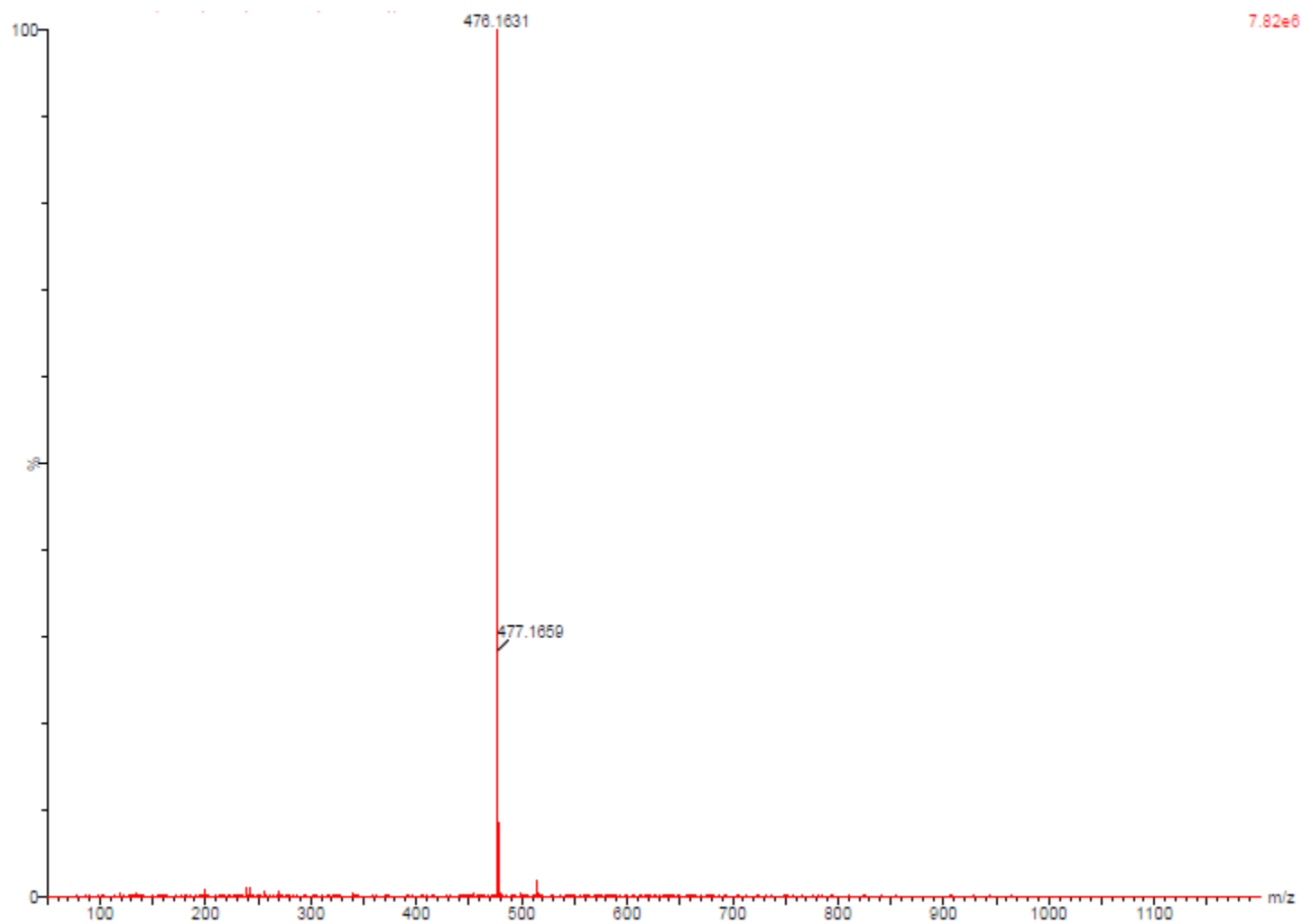


Figure 31: High resolution mass Spectrum of FOD5

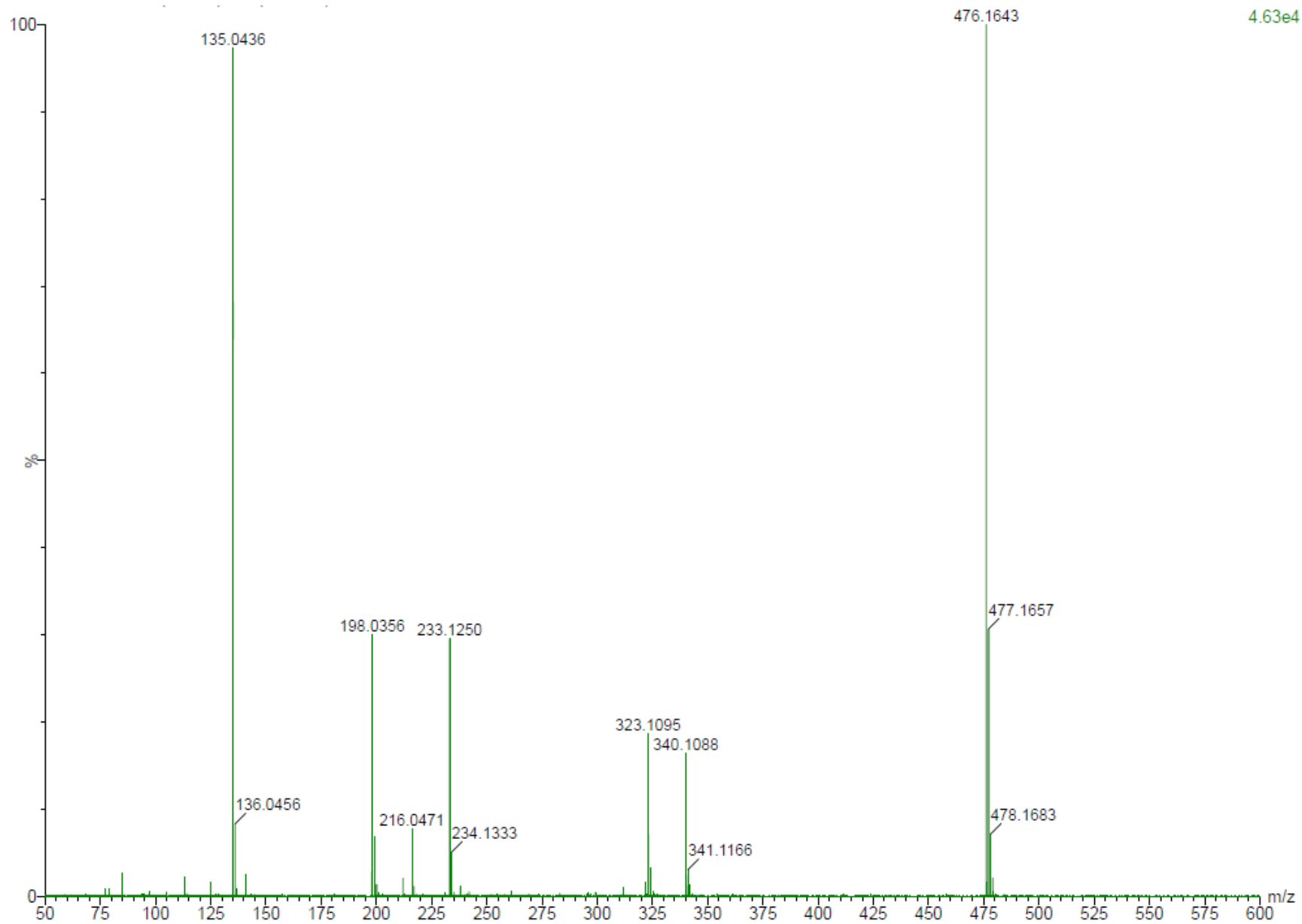


Figure 32: High resolution MSMS Spectrum of FOD5

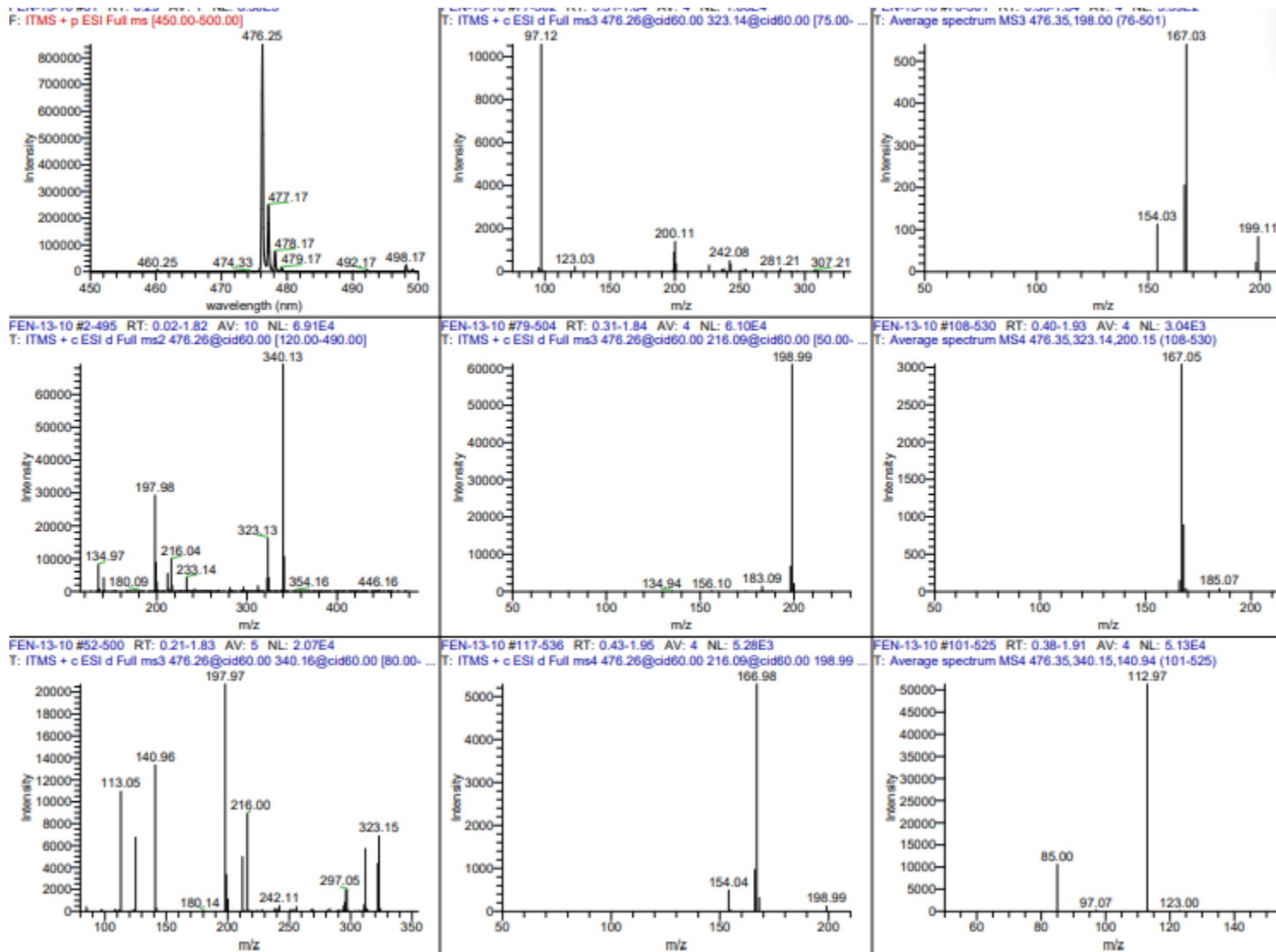


Figure 33: MSⁿ spectrum of FOD5

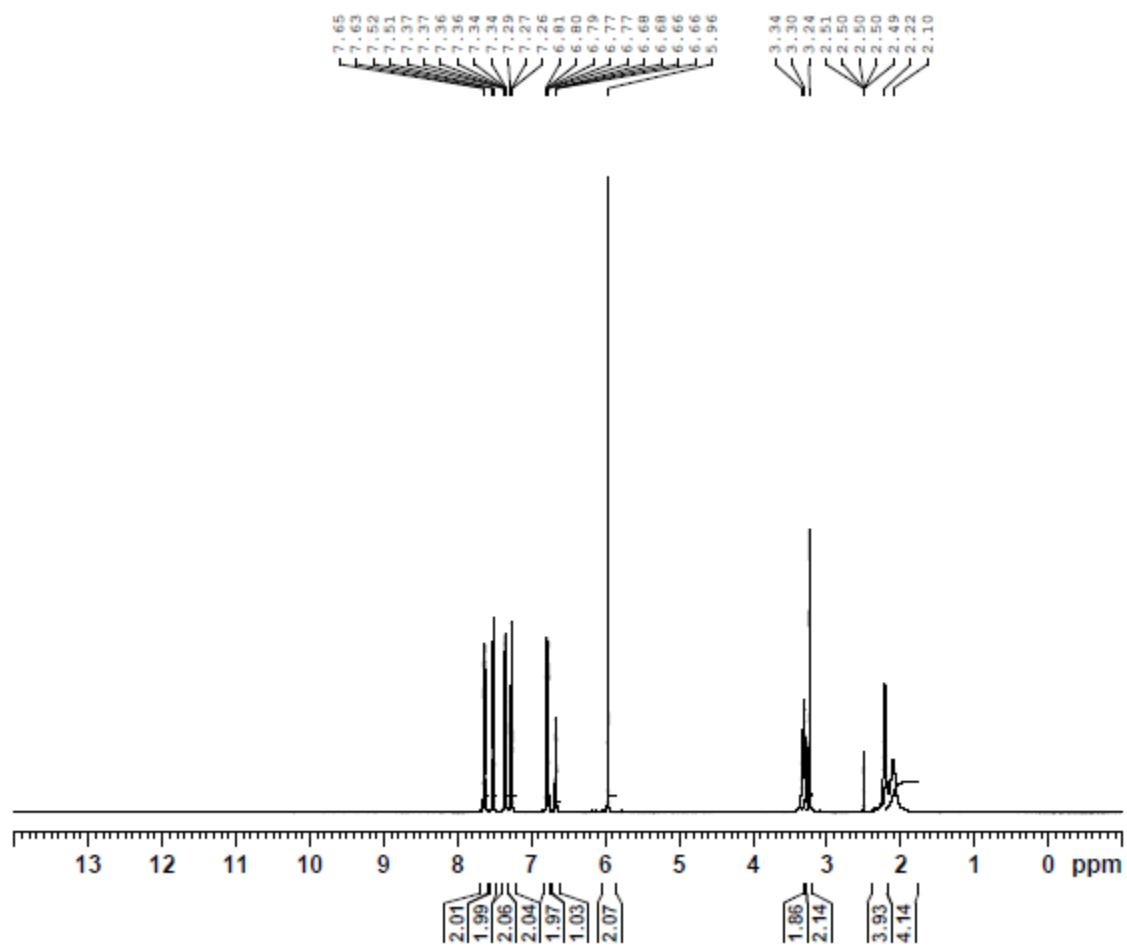


Figure 34: ¹H NMR Spectrum of FEN (500 MHz, DMSO-*d*₆, 300K)

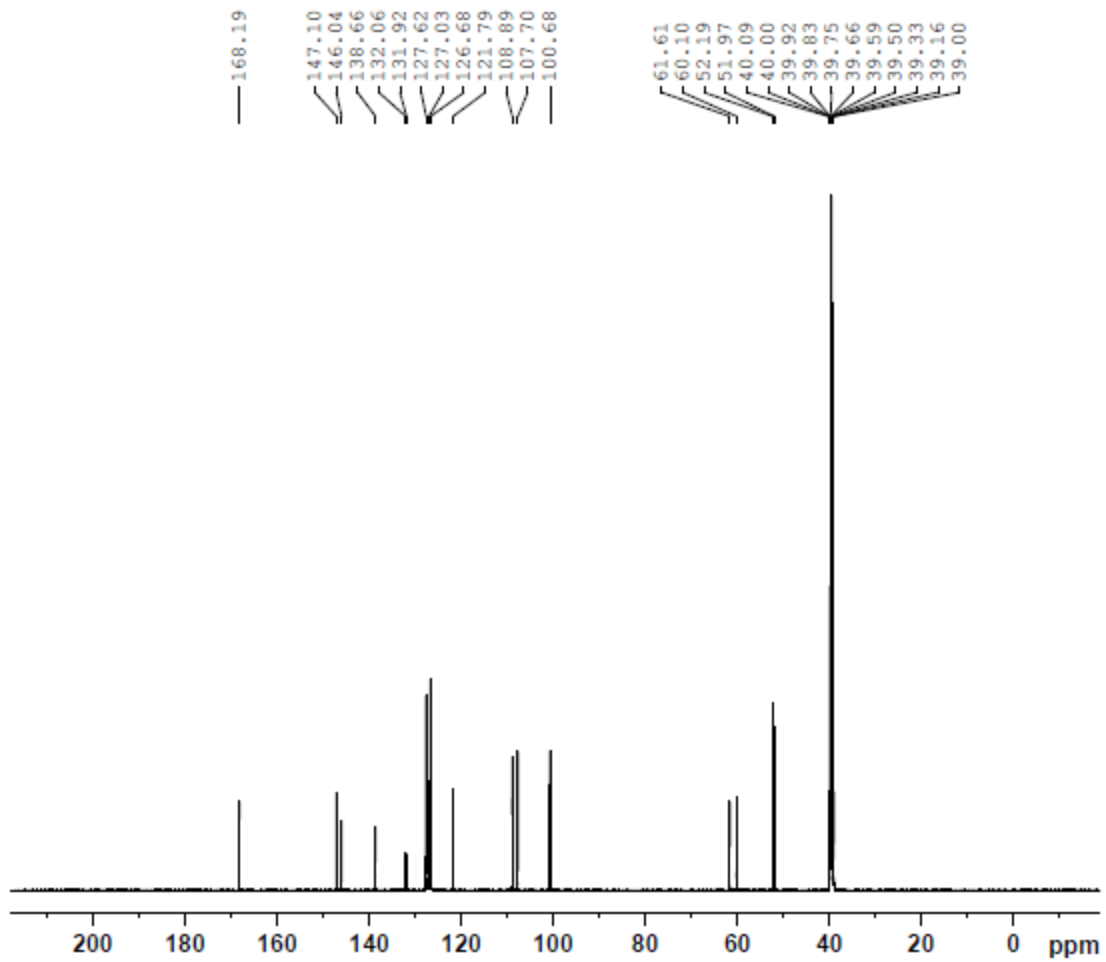


Figure 35: ^{13}C NMR Spectrum of FEN (126 MHz, DMSO-d₆, 300K)

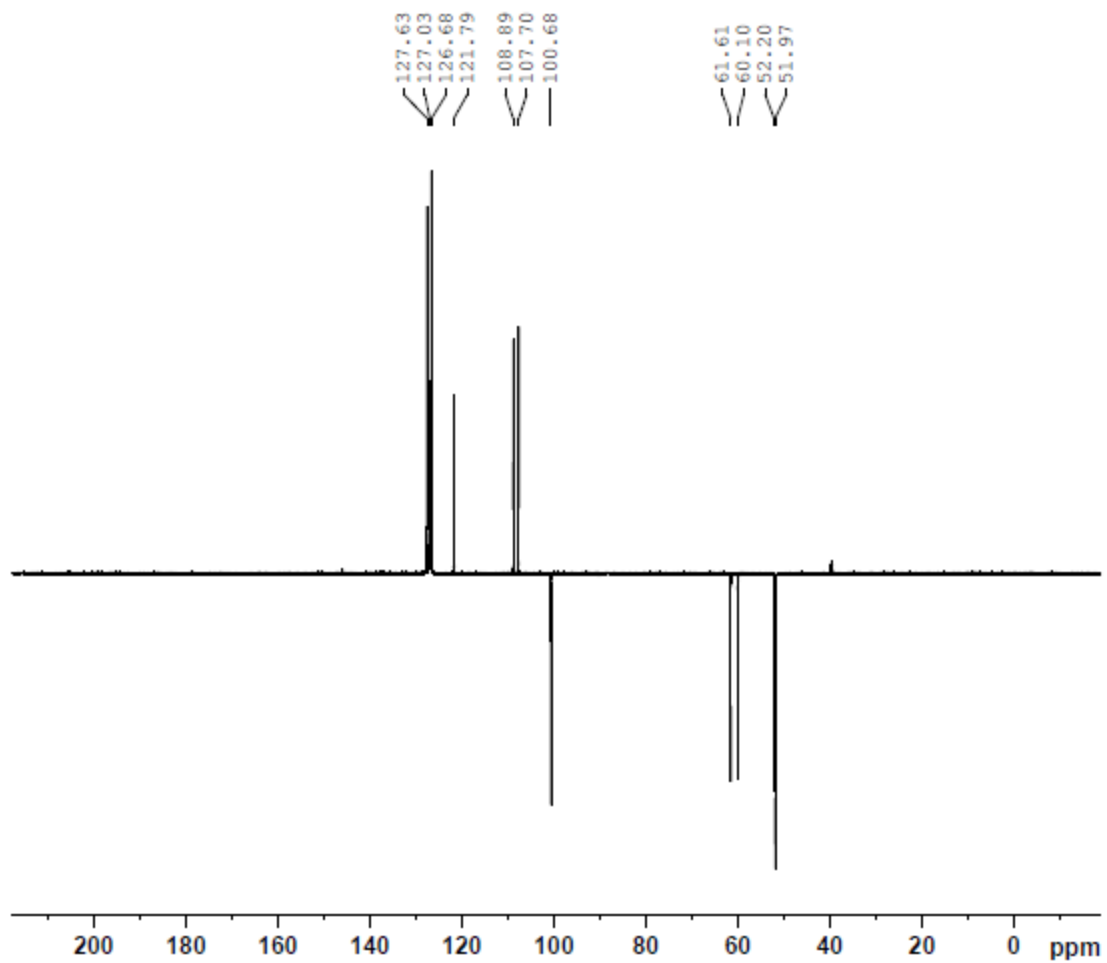


Figure 36: DEPT135 NMR Spectrum of FEN (126 MHz, DMSO-d₆, 300K)

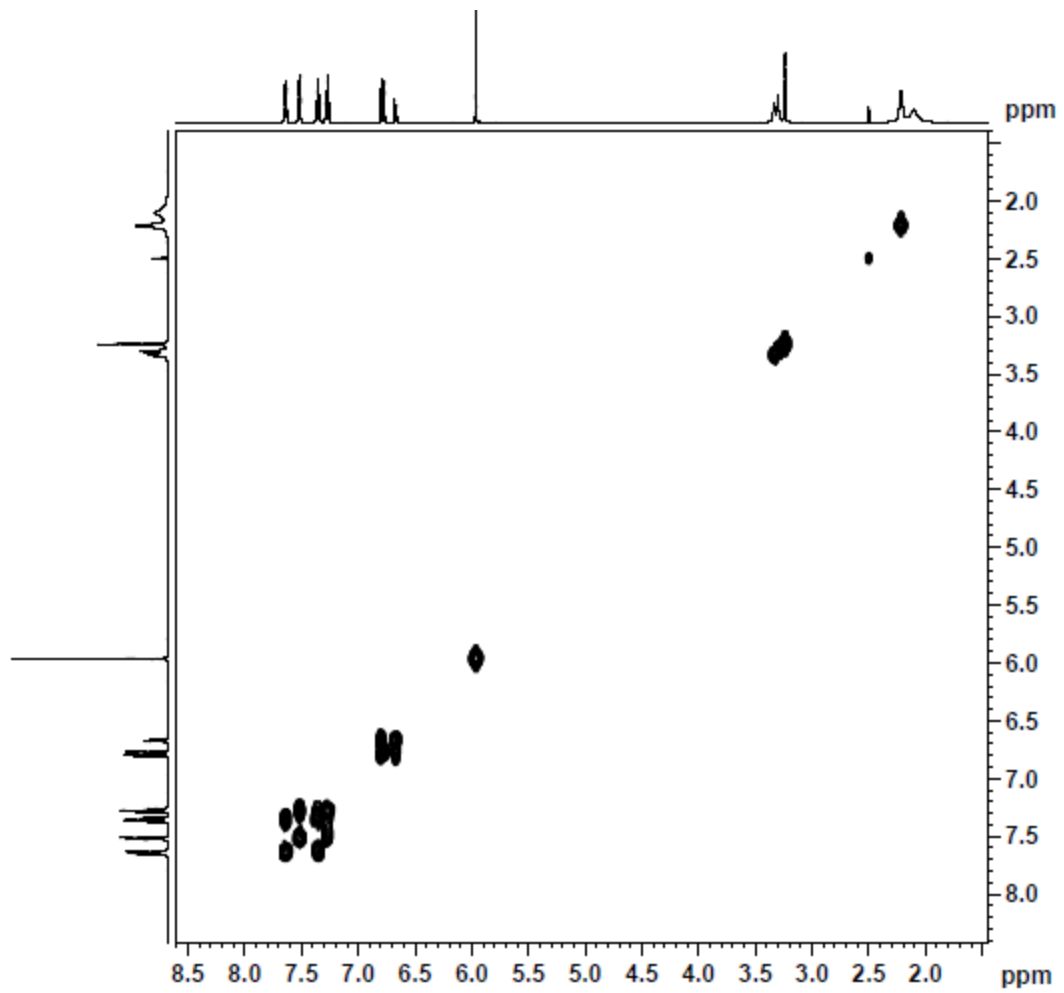


Figure 37: COSY NMR Spectrum of FEN (500 MHz, DMSO-d₆, 300K)

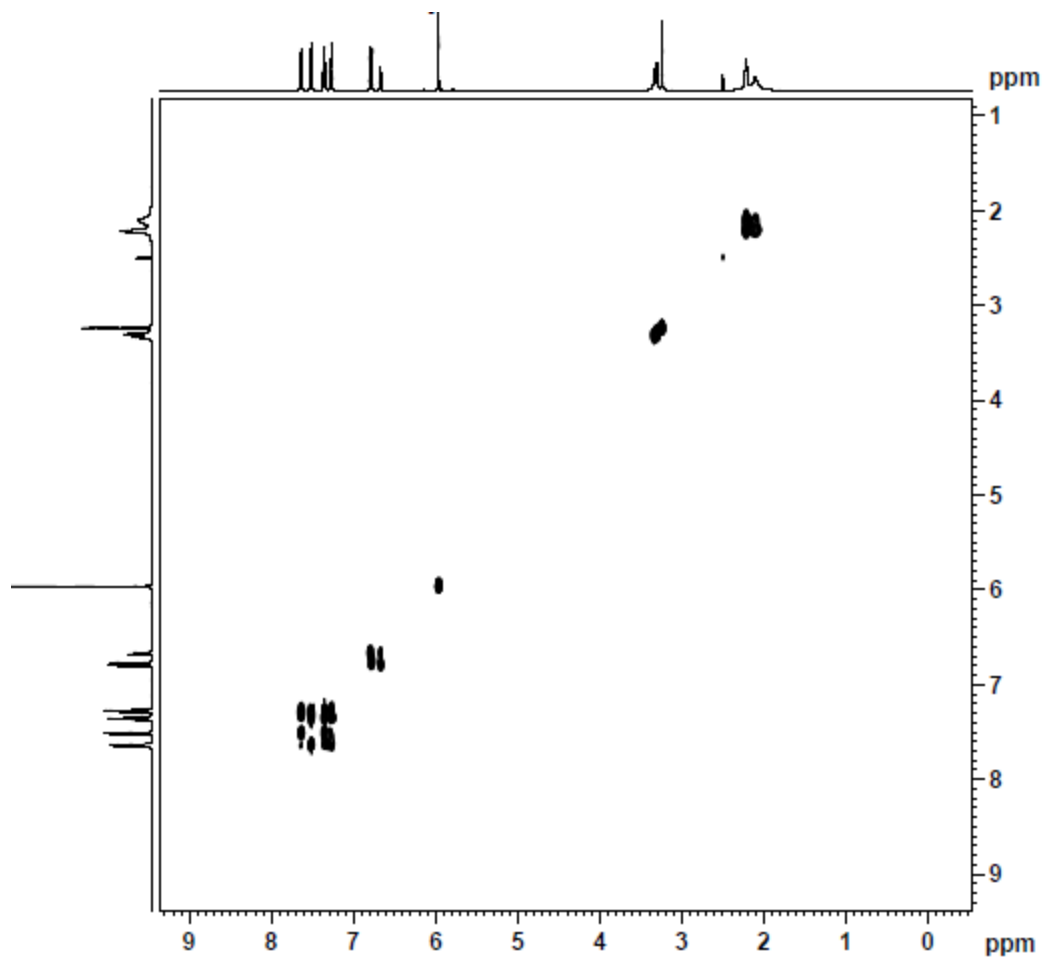


Figure 38: TOCSY NMR Spectrum of FEN (500 MHz, DMSO-d₆, 300K)

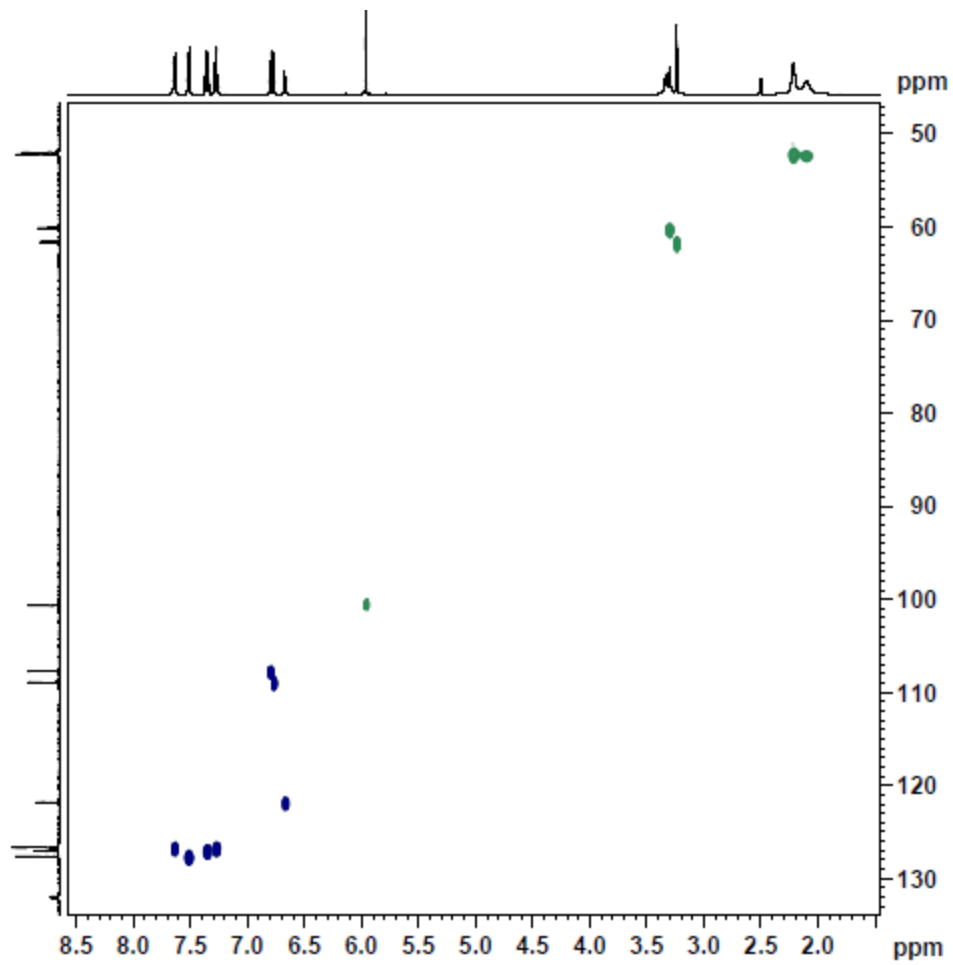


Figure 39: HSQC NMR Spectrum of FEN (500 MHz, DMSO-d₆, 300K)

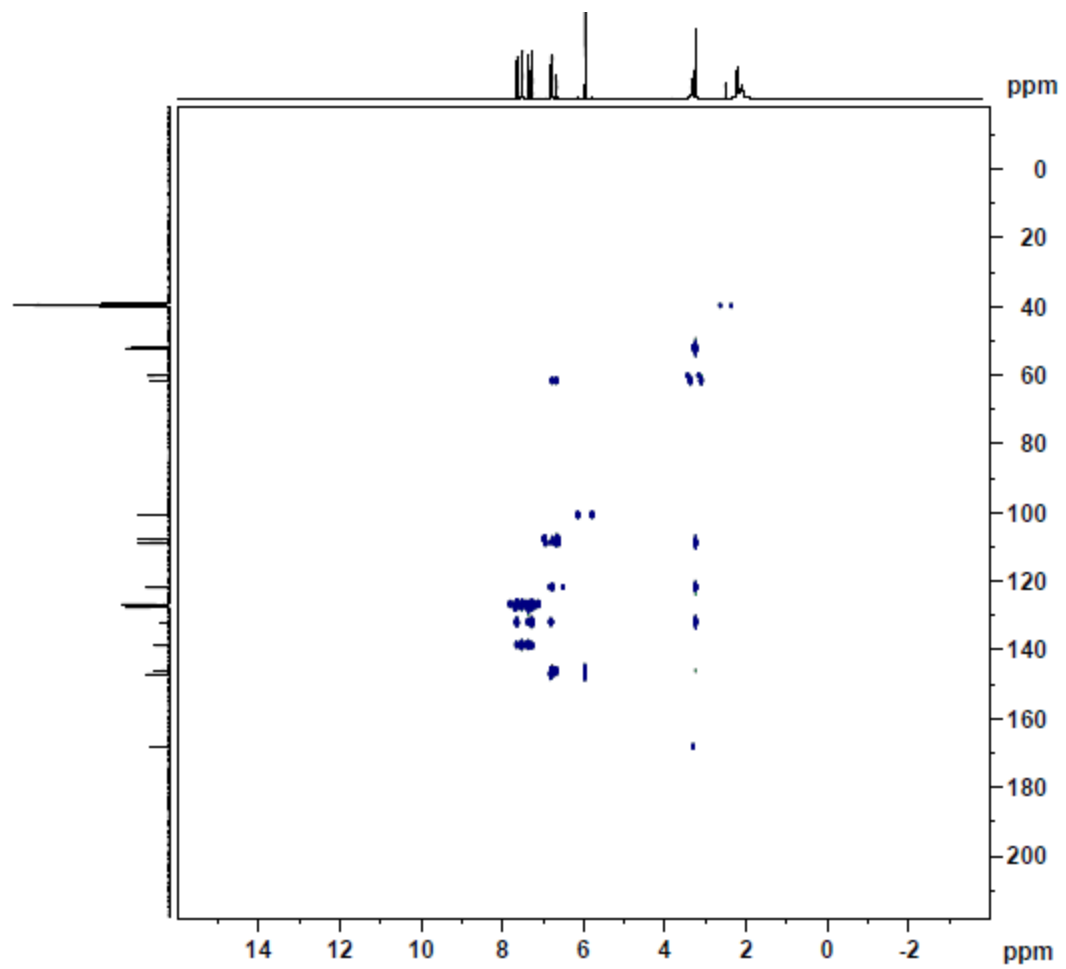


Figure 40: HMBC NMR Spectrum of FEN (500 MHz, DMSO-d₆, 300K)

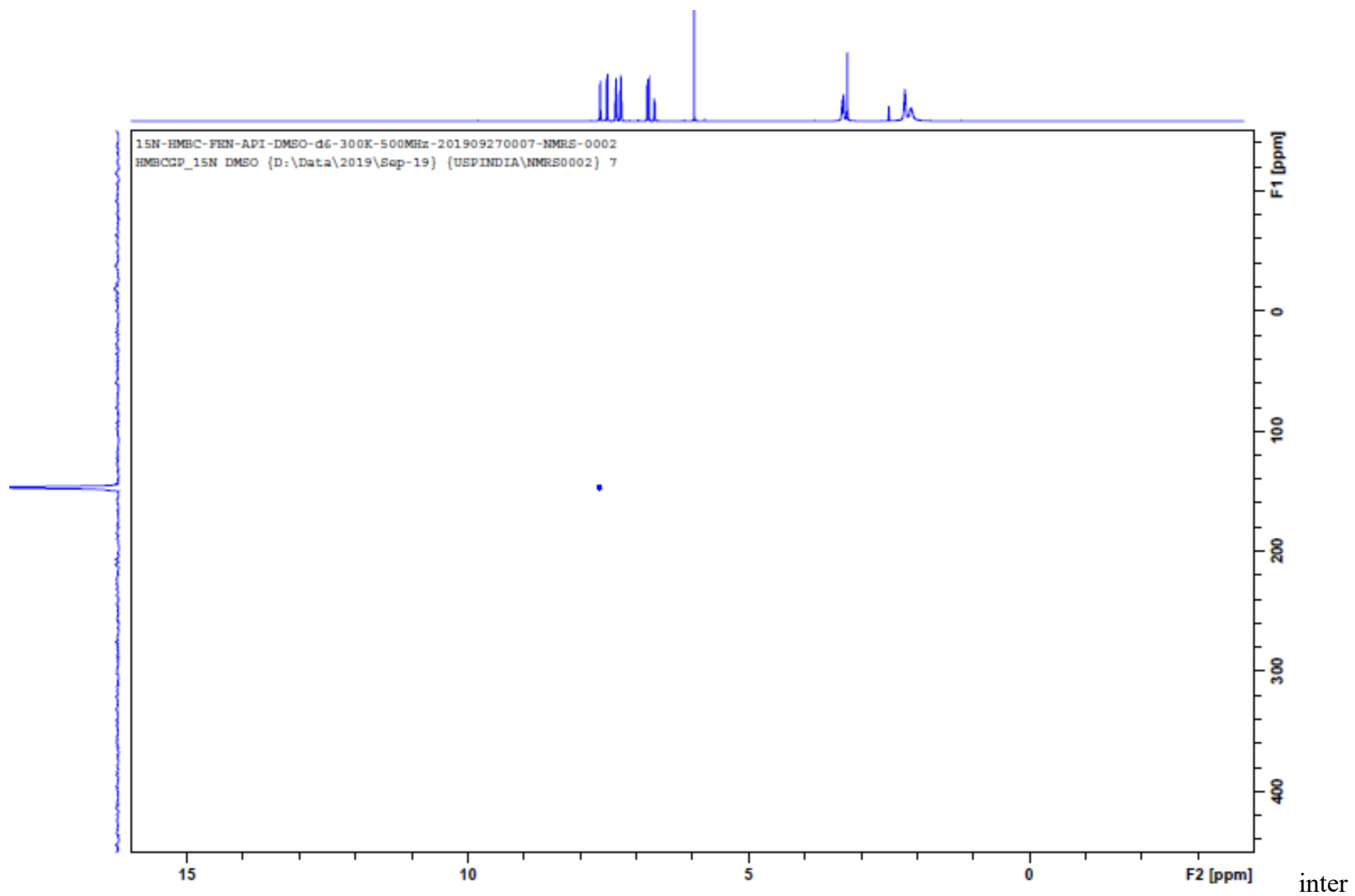


Figure 41: ^{15}N -HMBC NMR Spectrum of FEN (500 MHz, DMSO-d₆, 300K)

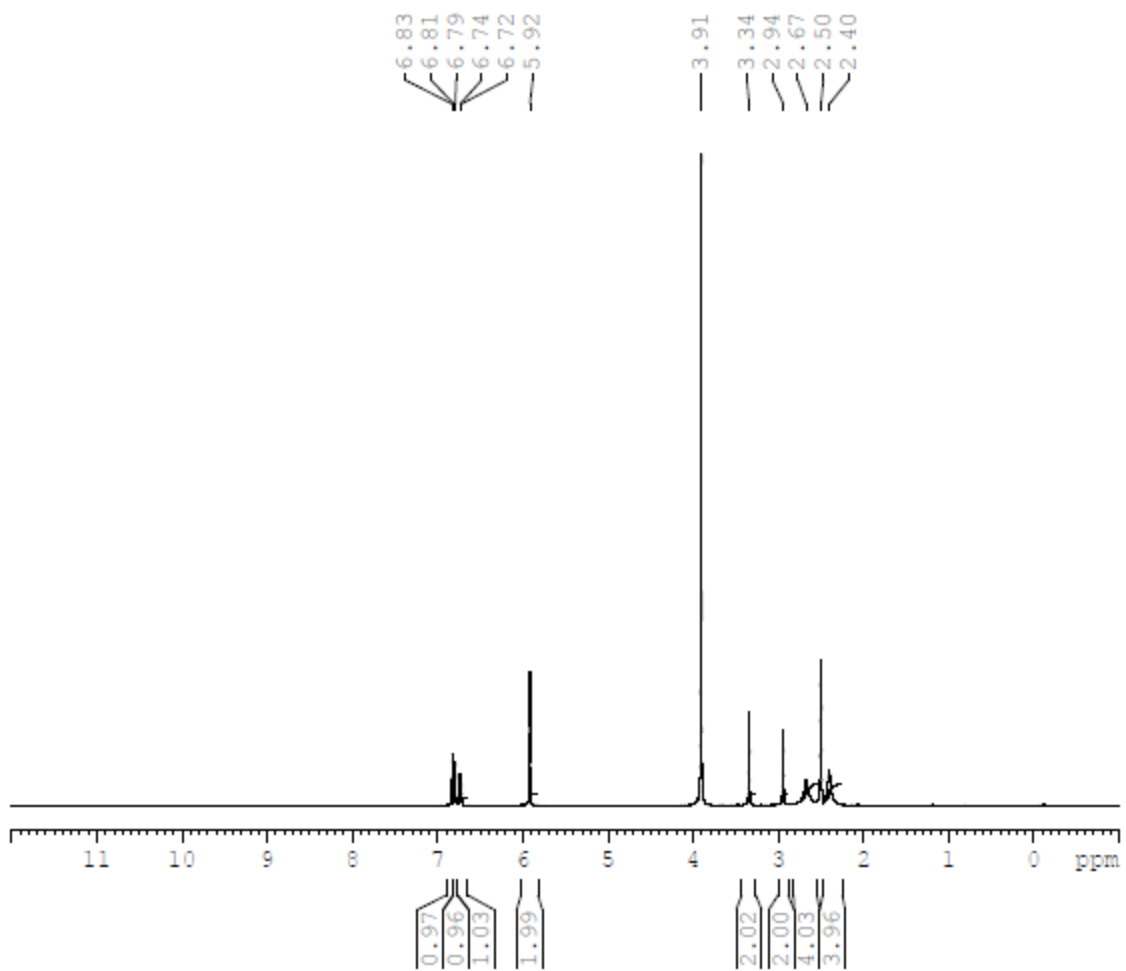


Figure 42: ^1H NMR Spectrum of FAD1 (500 MHz, $\text{DMSO-}d_6$, 300K)

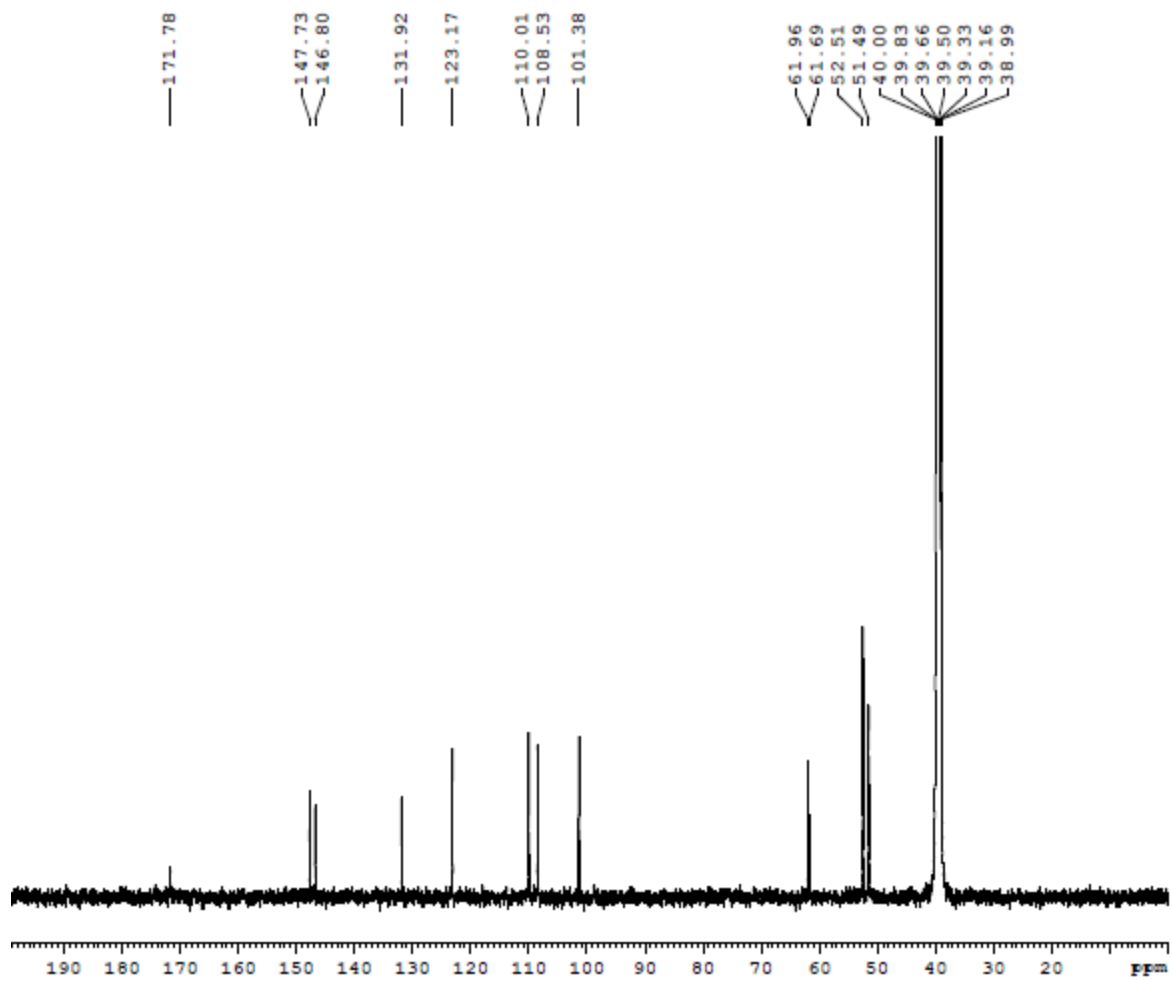


Figure 43: ^{13}C NMR Spectrum of FAD1 (126 MHz, DMSO- d_6 , 300K)

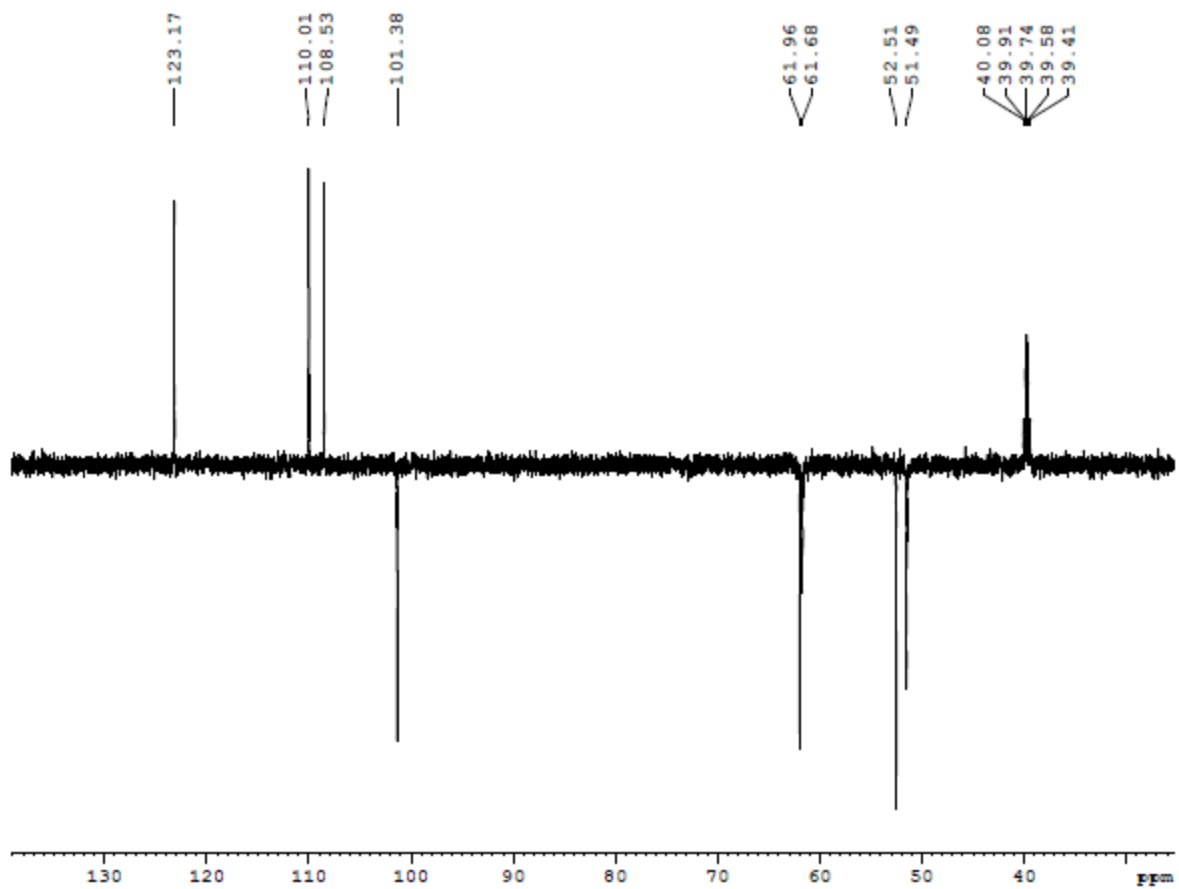


Figure 44: DEPT135 NMR Spectrum of CD1 (126 MHz, DMSO-d6, 300K)

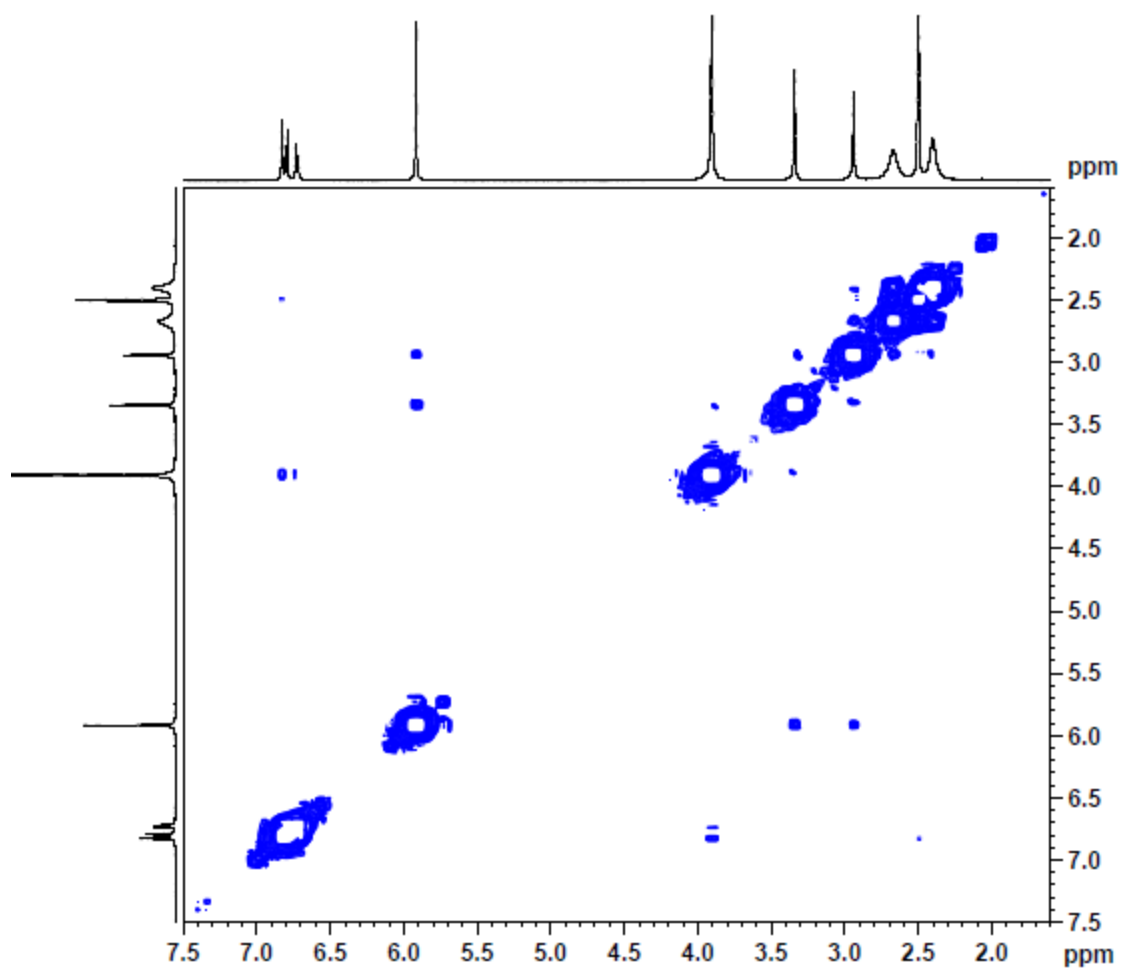


Figure 45: COSY NMR Spectrum of FAD1 (500 MHz, DMSO-d6, 300K)

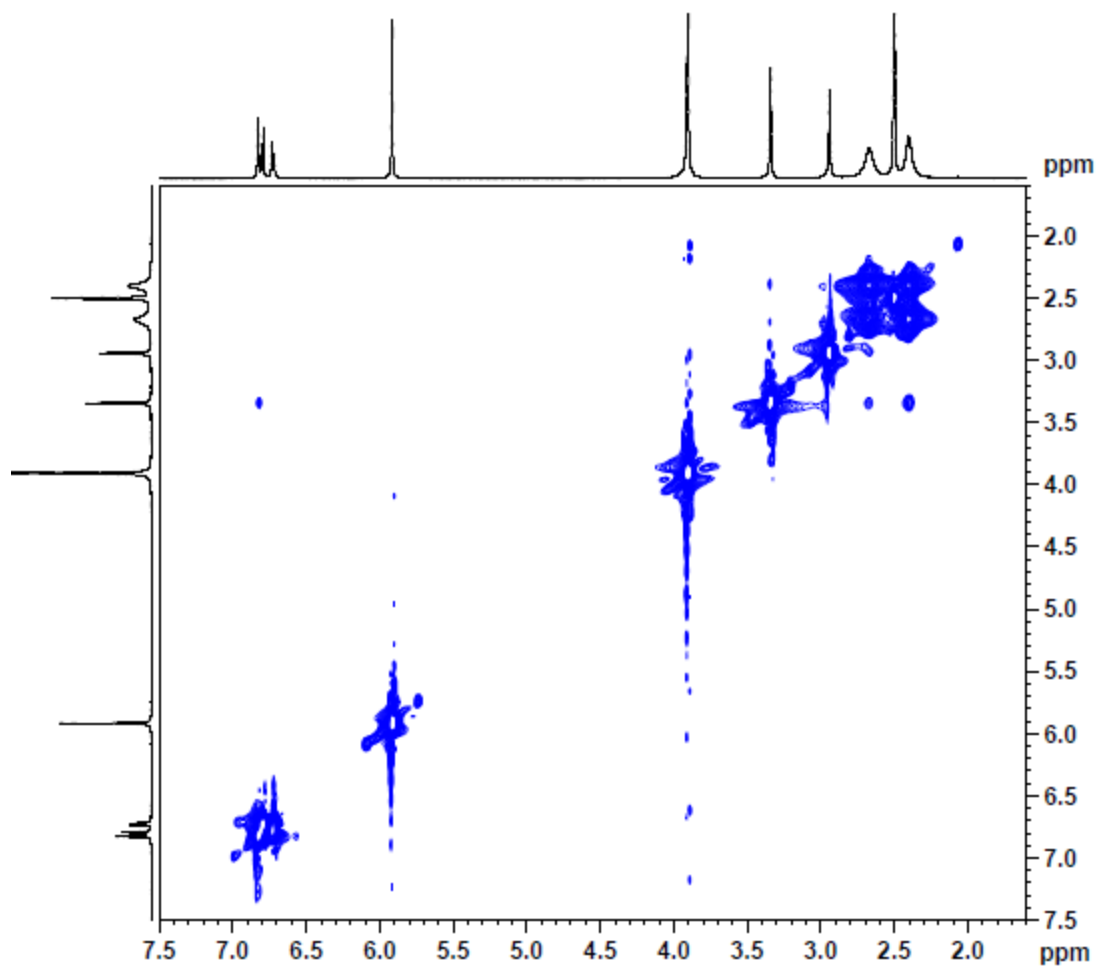


Figure 46: TOCSY NMR Spectrum of FAD1 (500 MHz, DMSO-d₆, 300K)

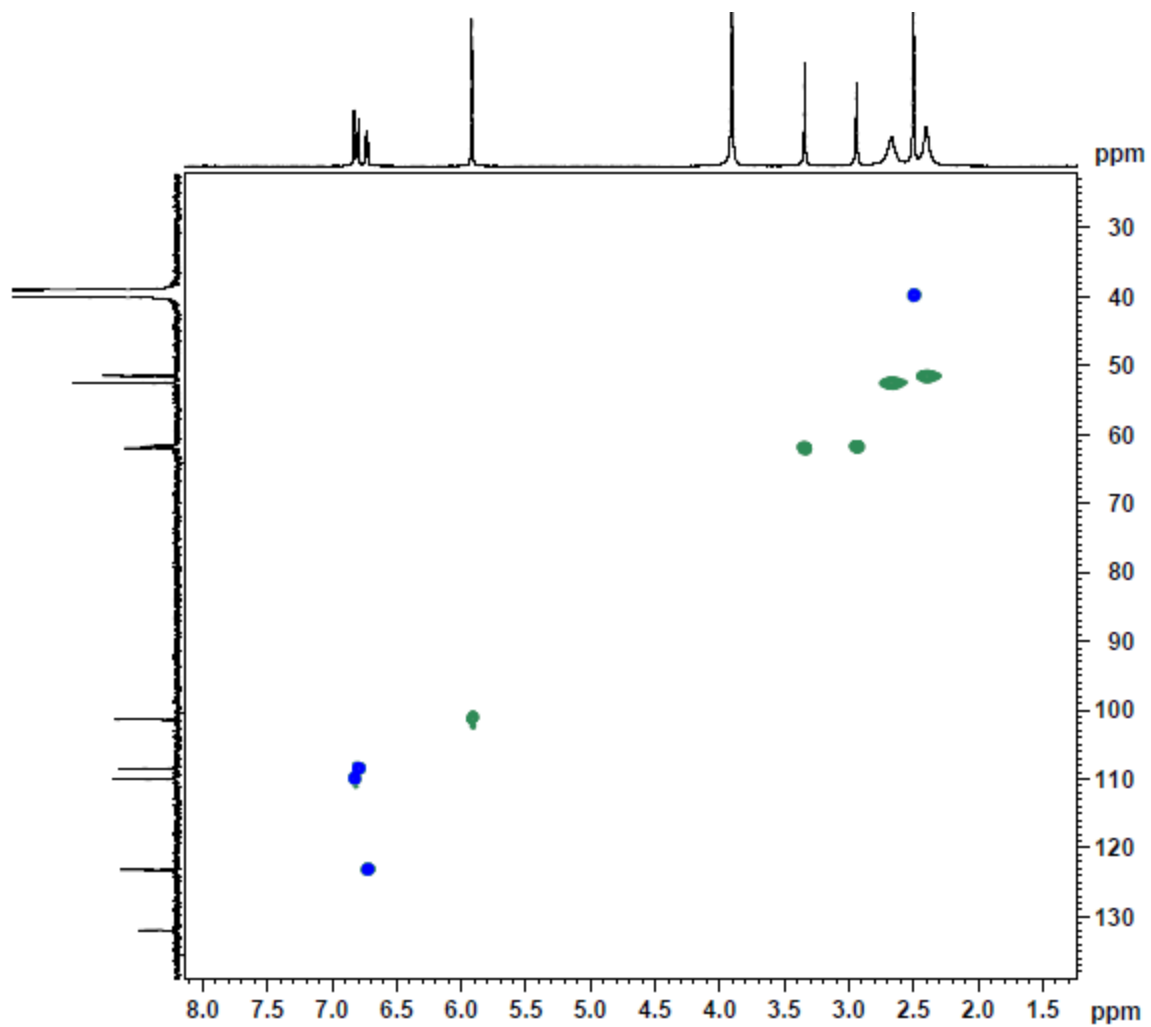


Figure 47: HSQC NMR Spectrum of FAD1 (500 MHz, DMSO-d₆, 300K)

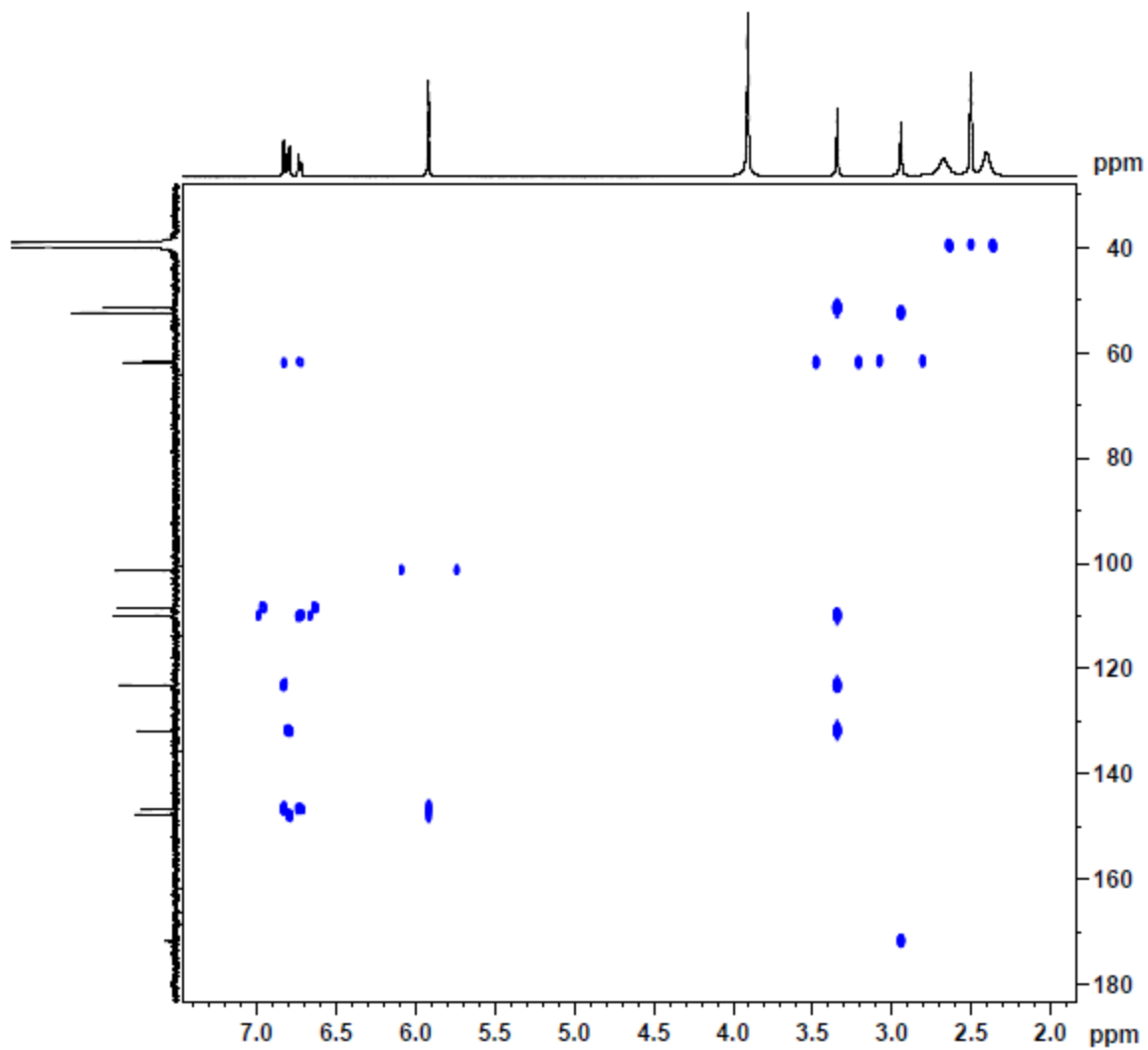


Figure 48: HMBC NMR Spectrum of FAD1 (500 MHz, DMSO-d₆, 300K)

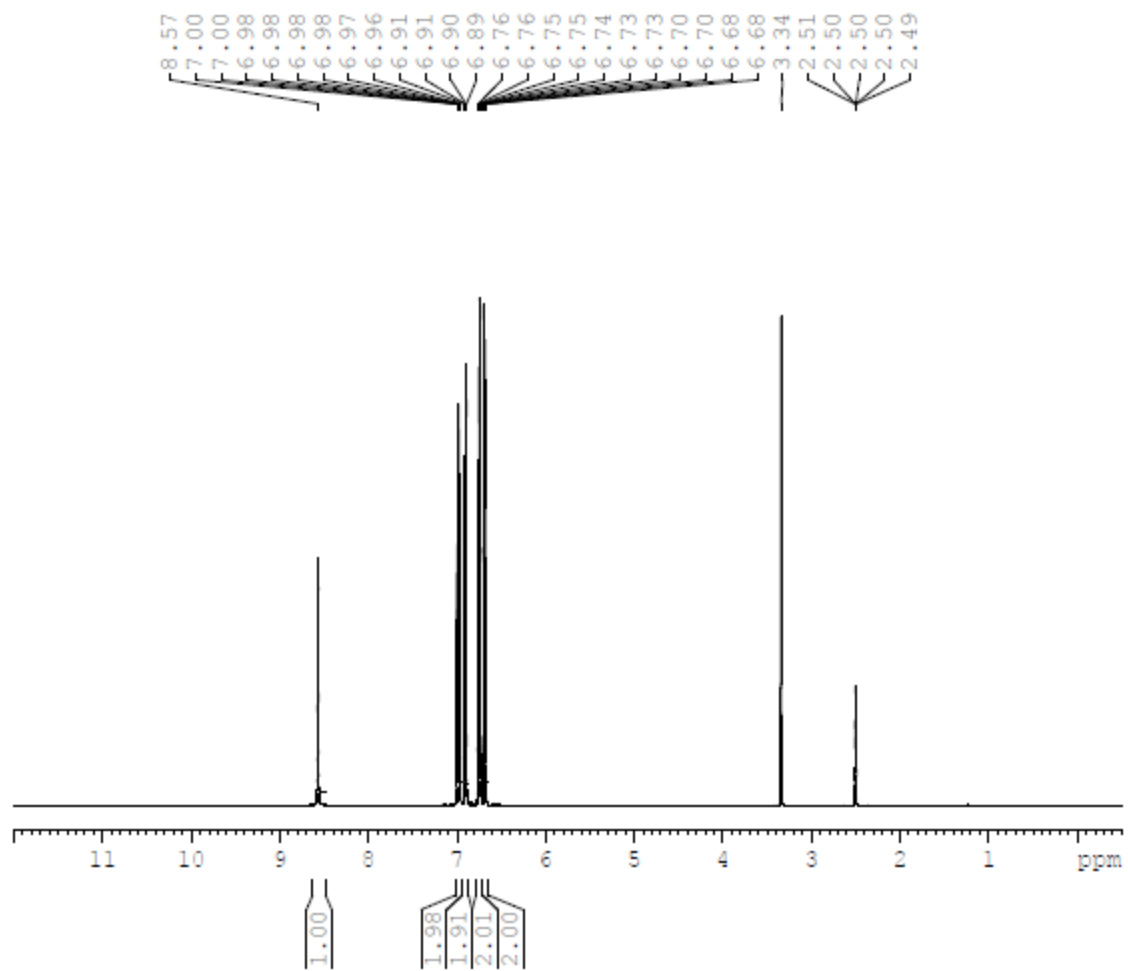


Figure 49: ^1H NMR Spectrum of FAD2 (500 MHz, $\text{DMSO-}d_6$, 300K)

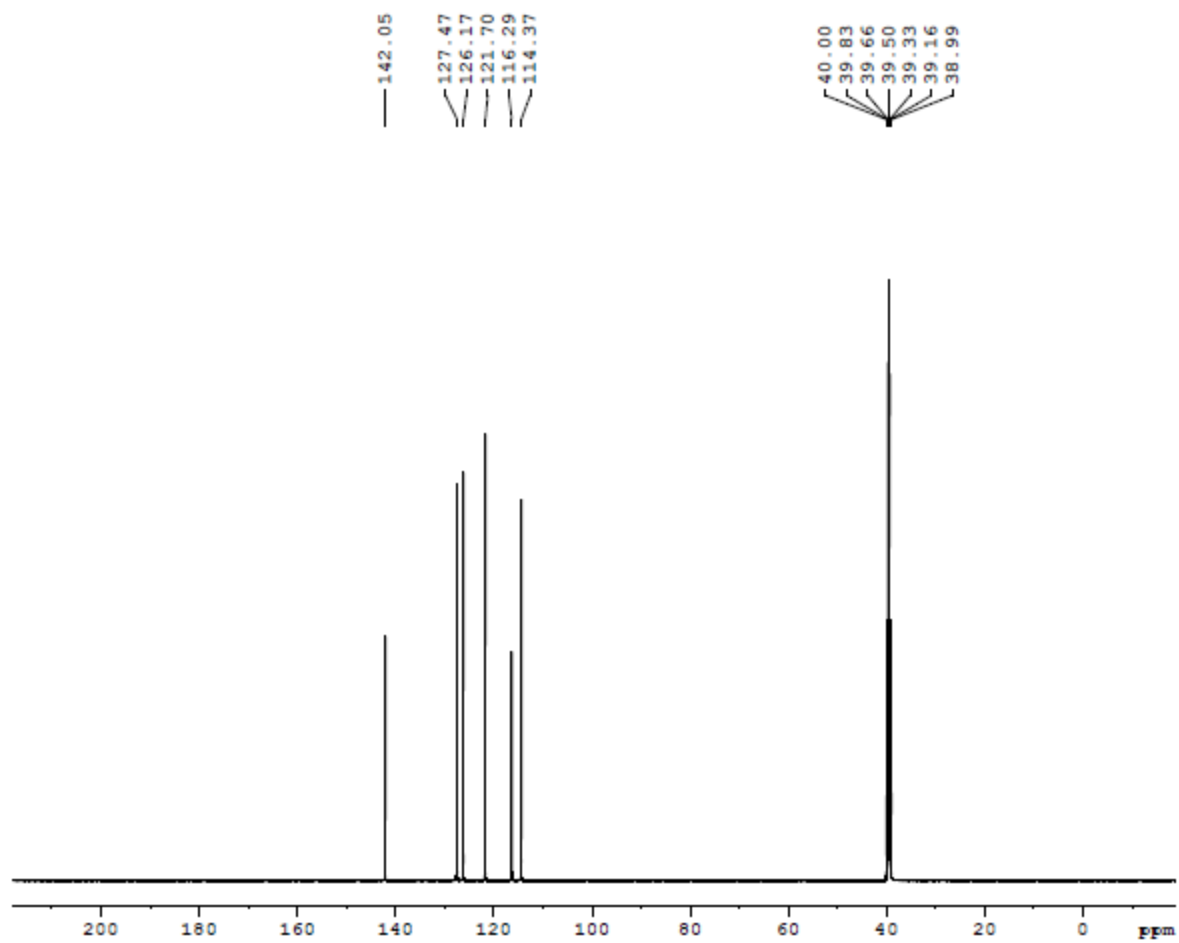


Figure 50: ^{13}C NMR Spectrum of FAD2 (126 MHz, DMSO-d₆, 300K)

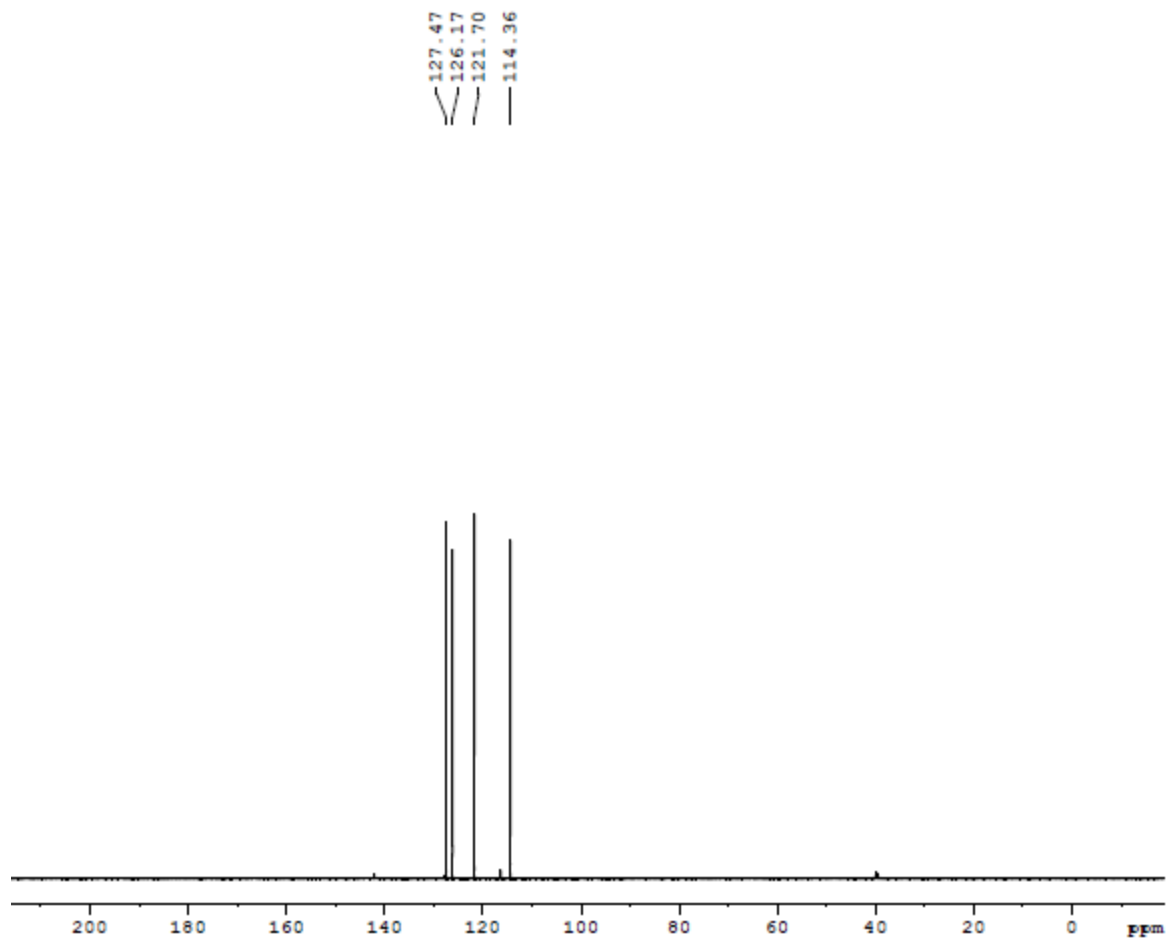


Figure 51: DEPT90 NMR Spectrum of FAD2 (126 MHz, DMSO-d6, 300K)

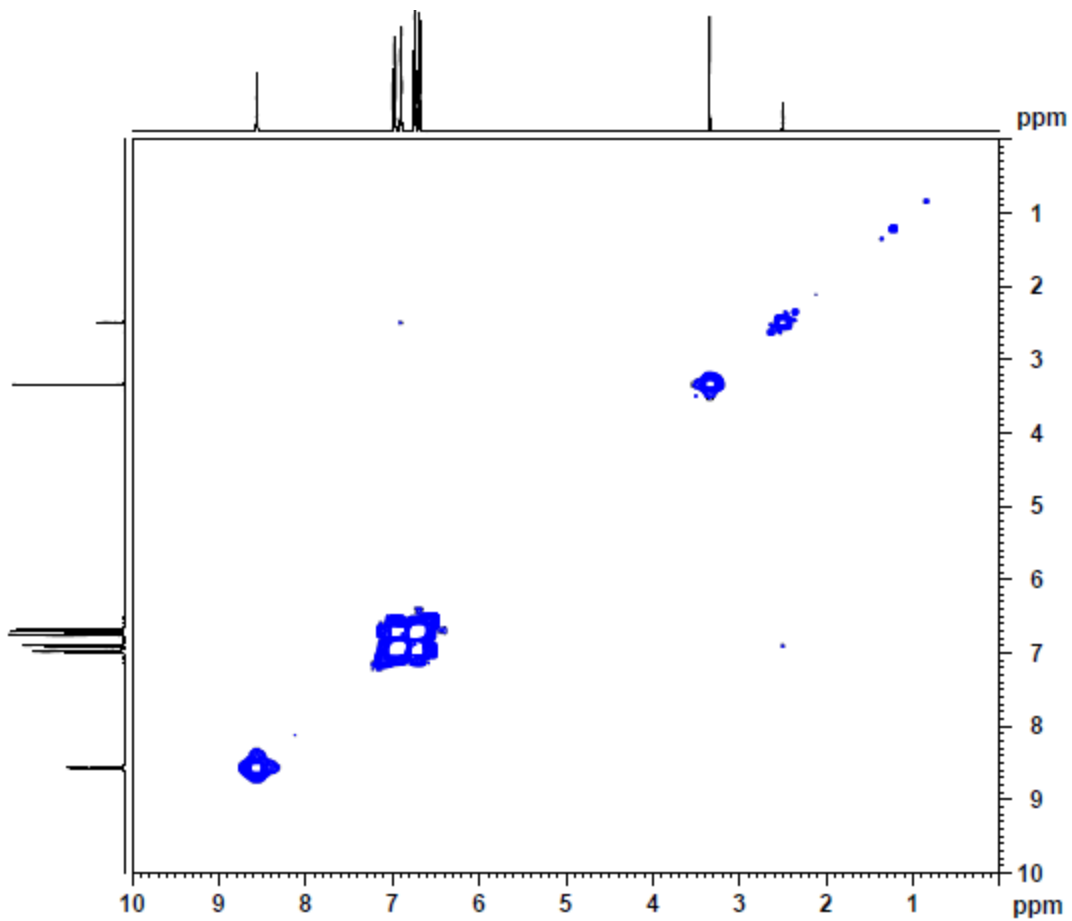


Figure 52: COSY NMR Spectrum of FAD2 (500 MHz, DMSO-d₆, 300K)

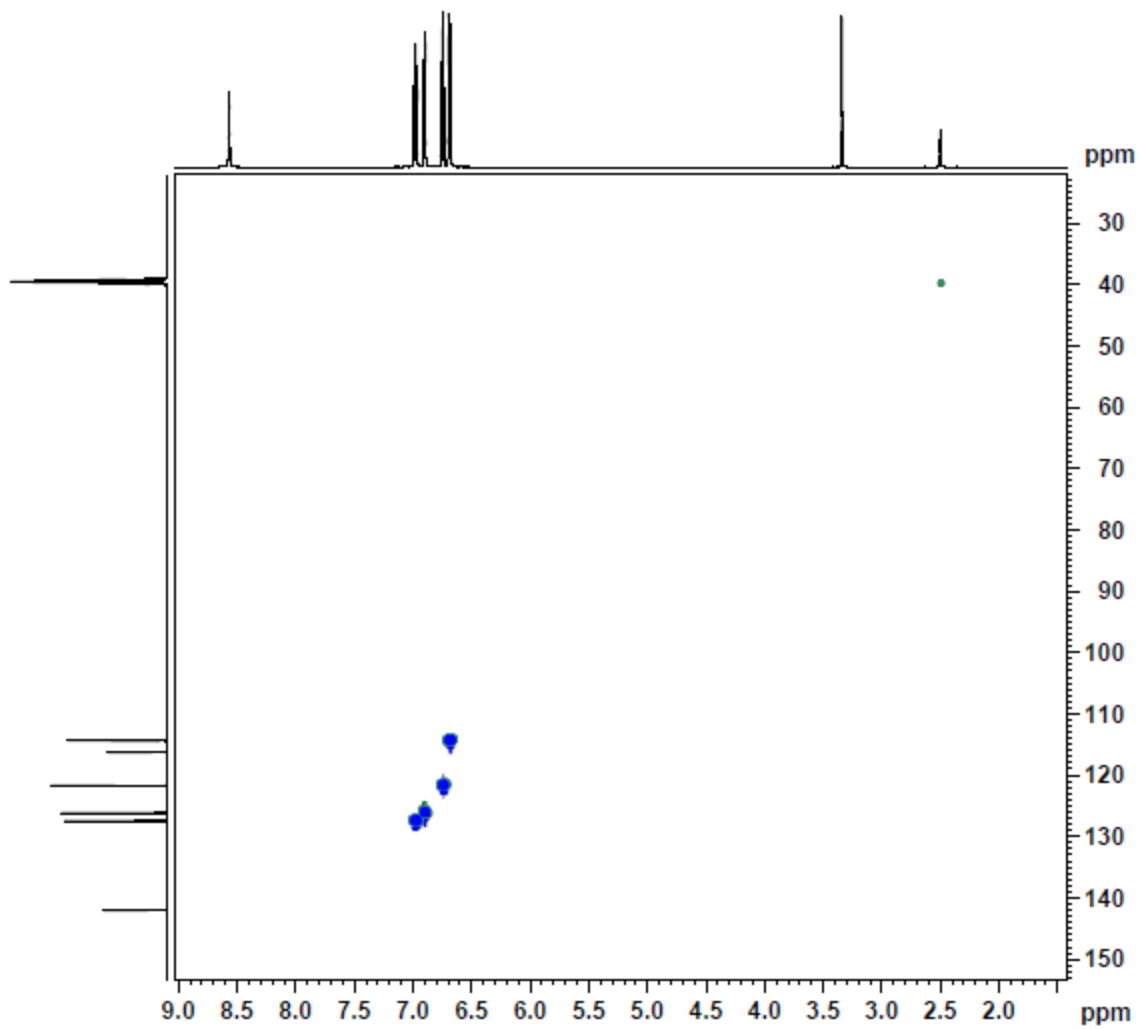


Figure 53: HSQC NMR Spectrum of FAD2 (500 MHz, DMSO-d6, 300K)

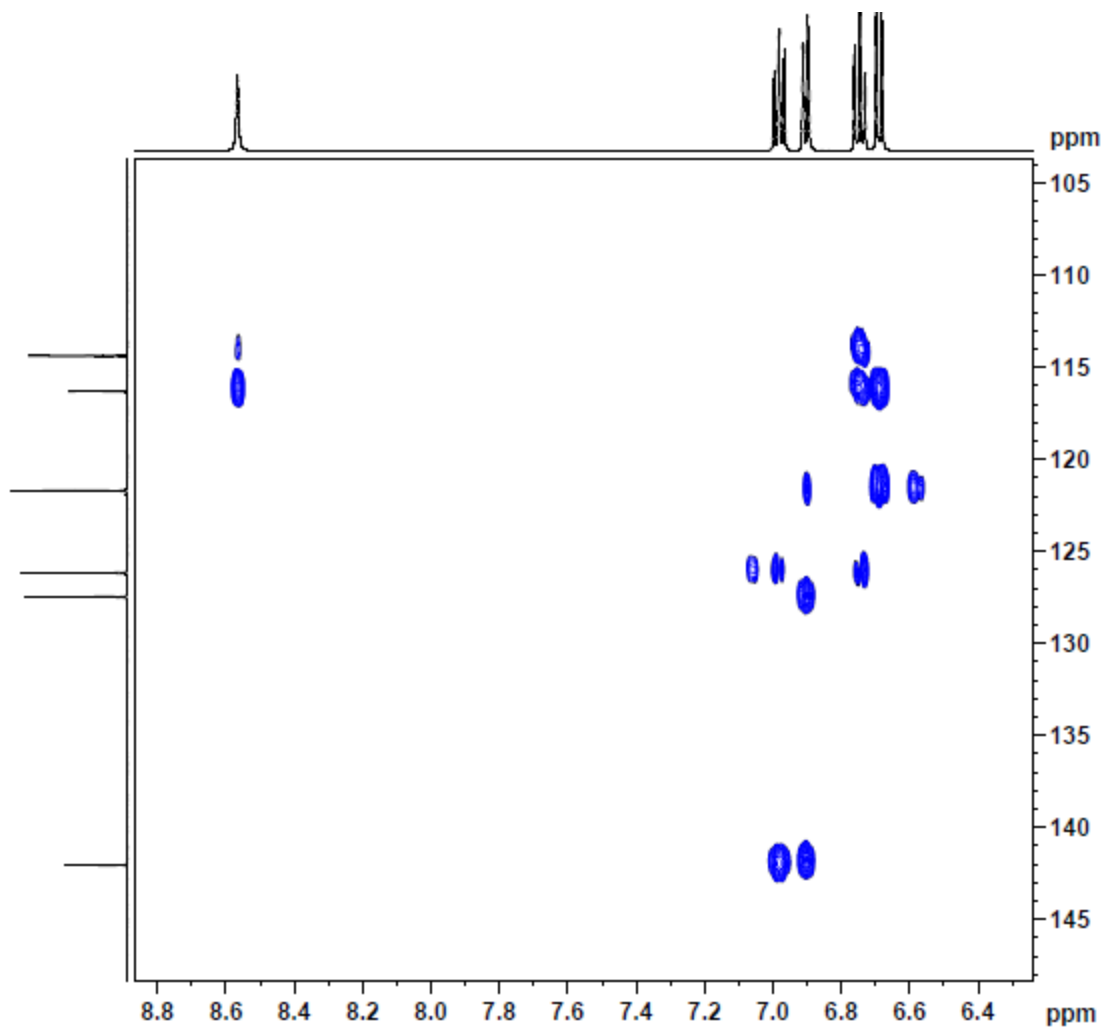


Figure 54: HMBC NMR Spectrum of FAD2 (500 MHz, DMSO-d₆, 300K)

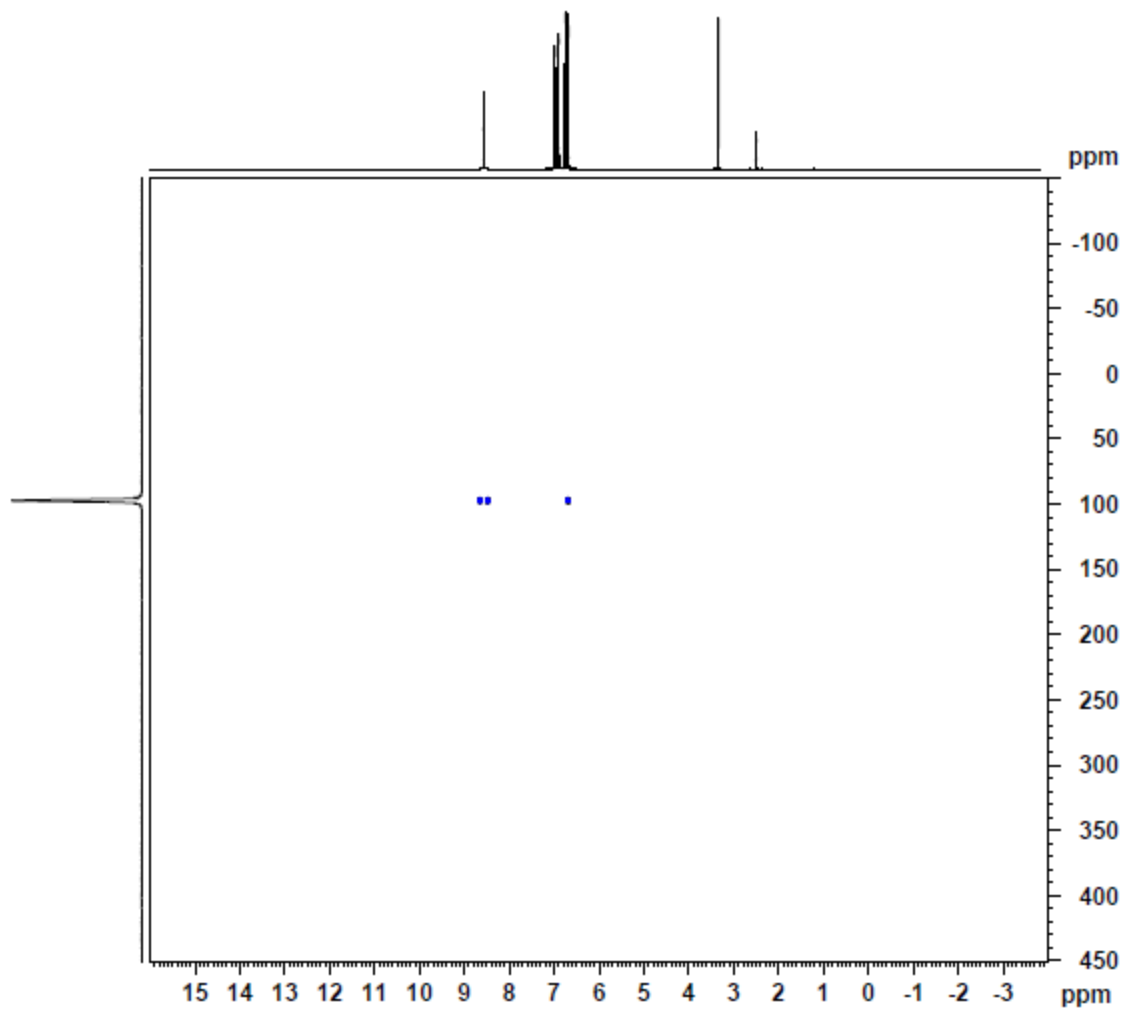


Figure 55: ^{15}N -HMBC NMR Spectrum of FAD2 (500 MHz, DMSO- d_6 , 300K)

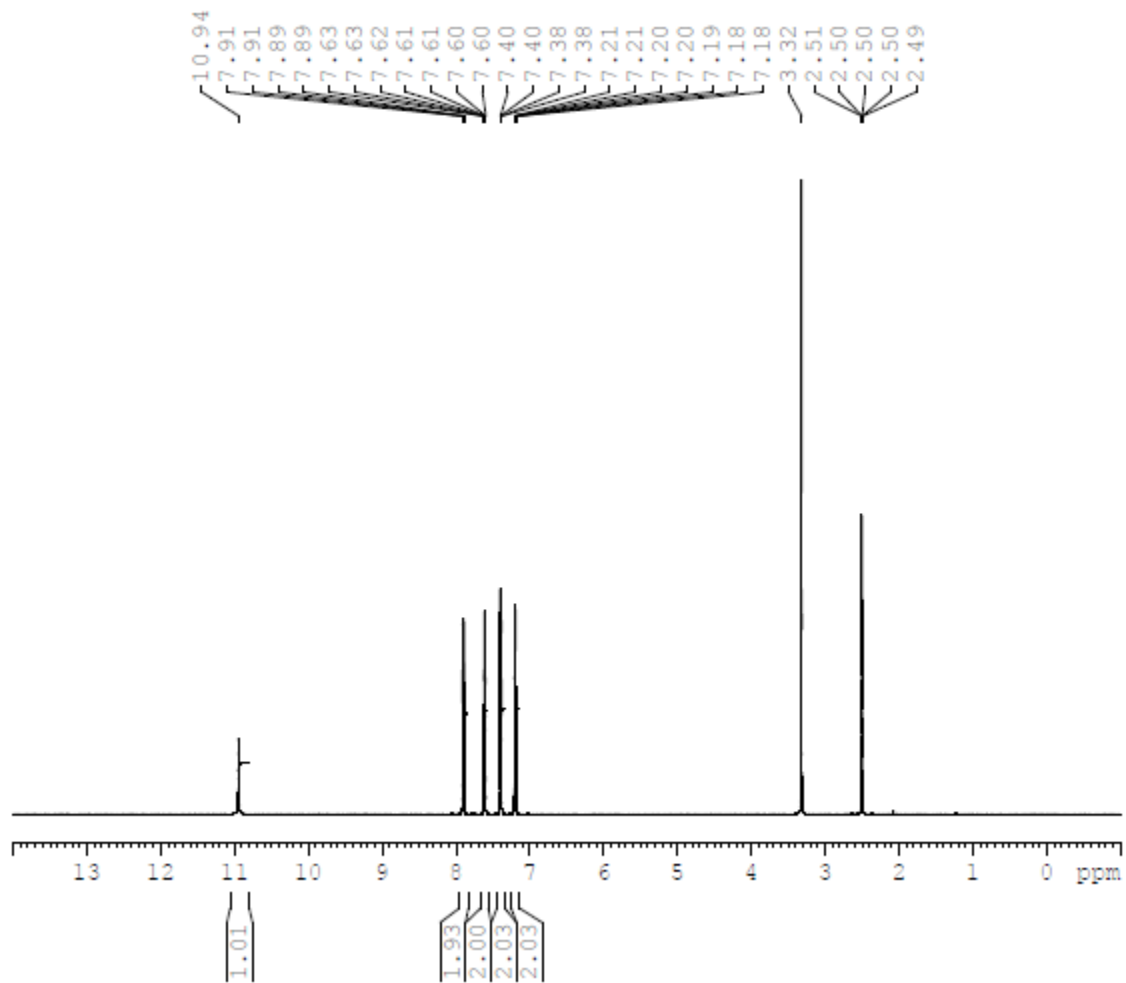


Figure 56: ¹H NMR Spectrum of FOD1 (500 MHz, DMSO-*d*₆, 300K)

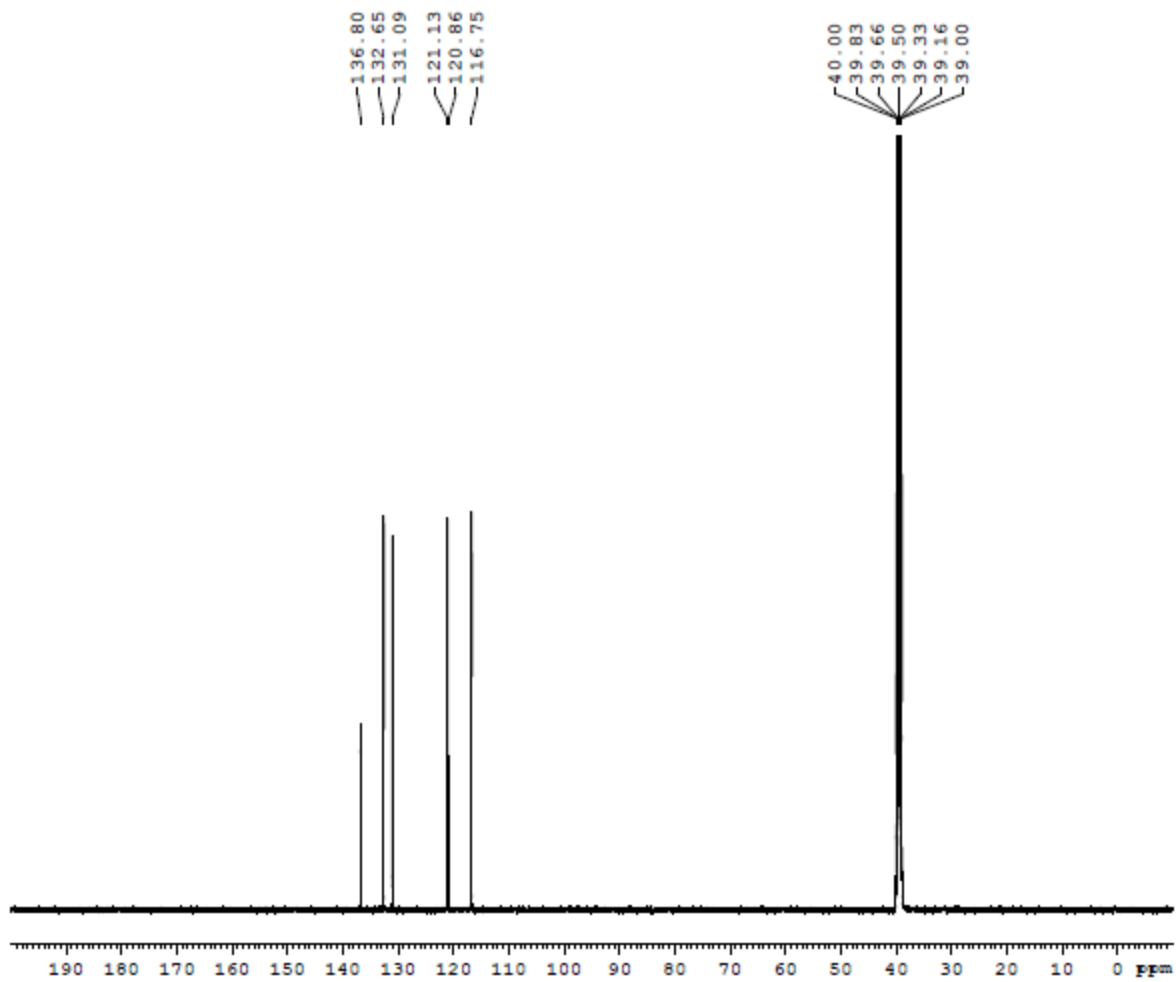


Figure 57: ¹³C NMR Spectrum of FOD1 (126 MHz, DMSO-d₆, 300K)

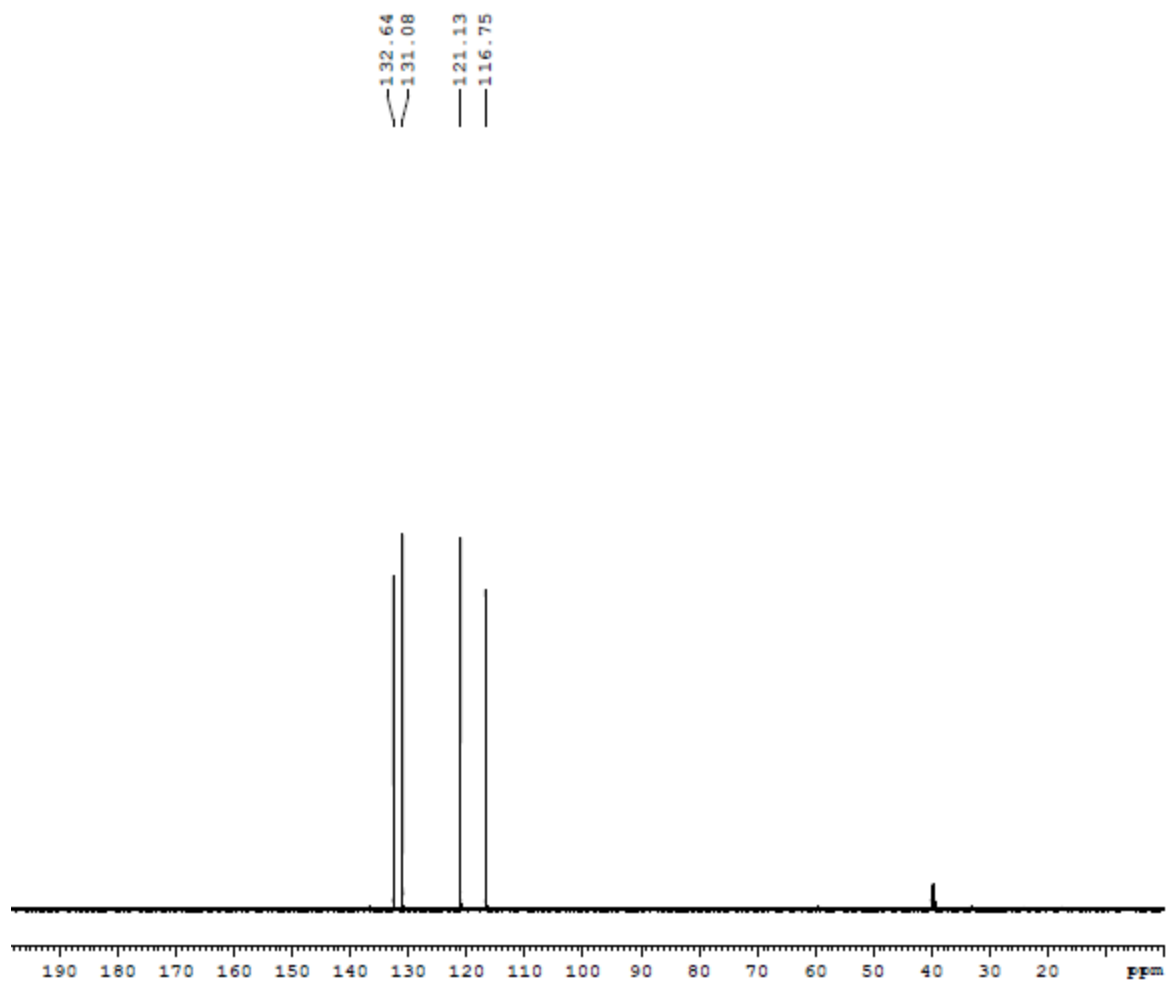


Figure 58: DEPT90 NMR Spectrum of FOD1 (126 MHz, DMSO-d₆, 300K)

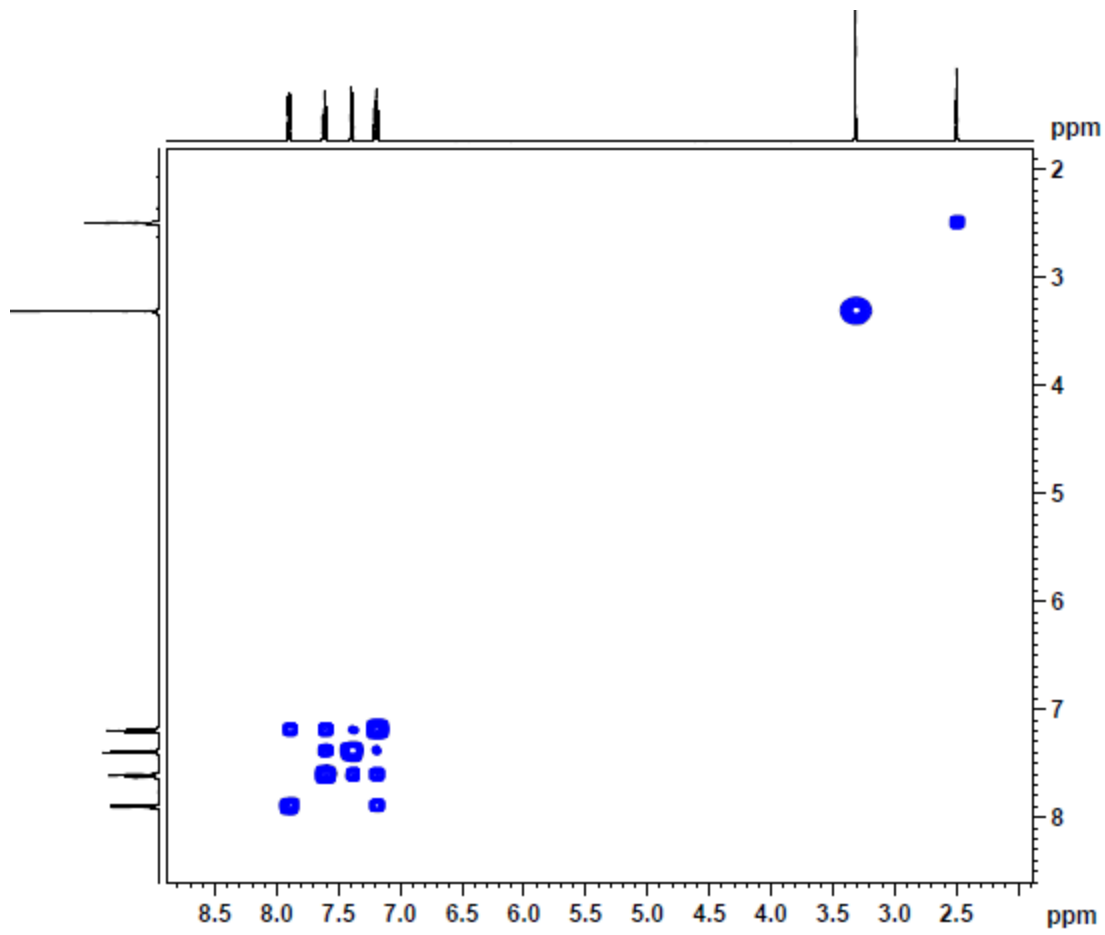


Figure 59: COSY NMR Spectrum of FOD1 (500 MHz, DMSO-d₆, 300K)

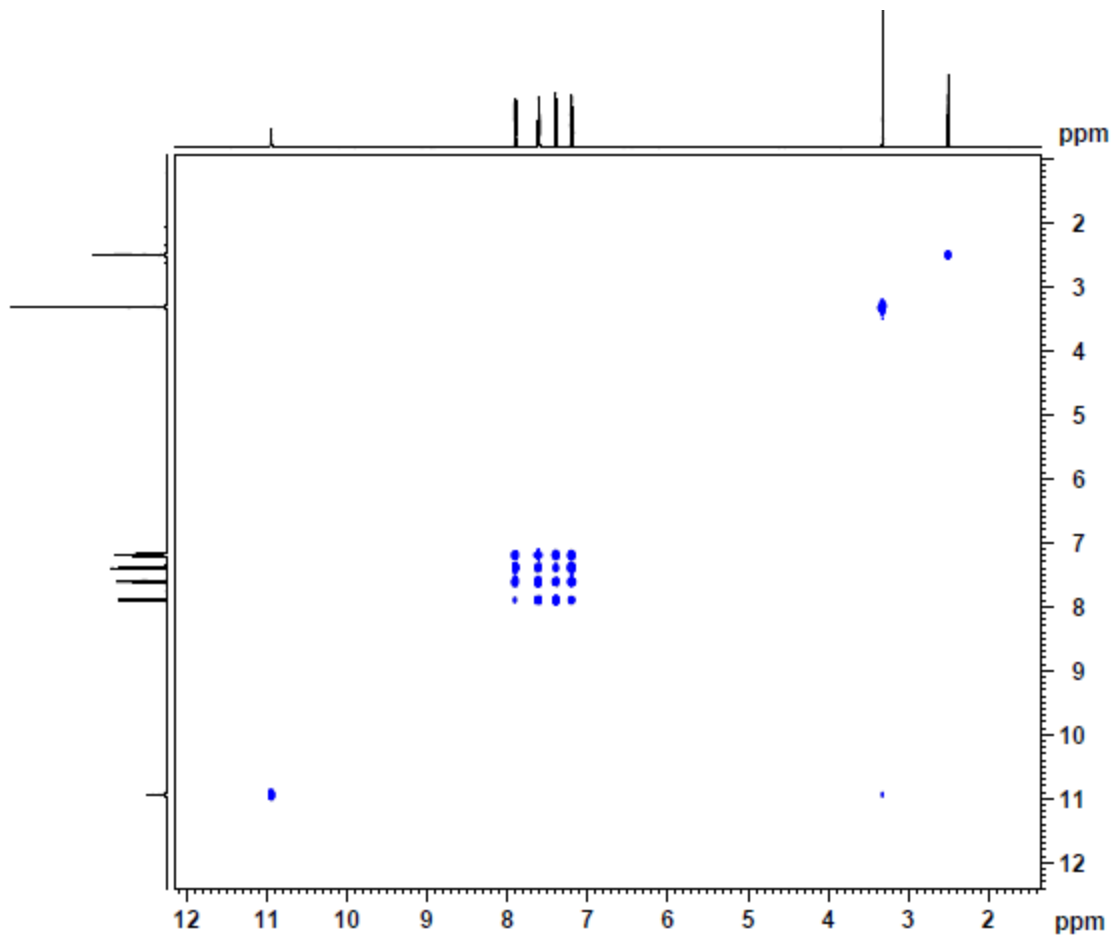


Figure 60: TOCSY NMR Spectrum of FOD1 (500 MHz, DMSO-d₆, 300K)

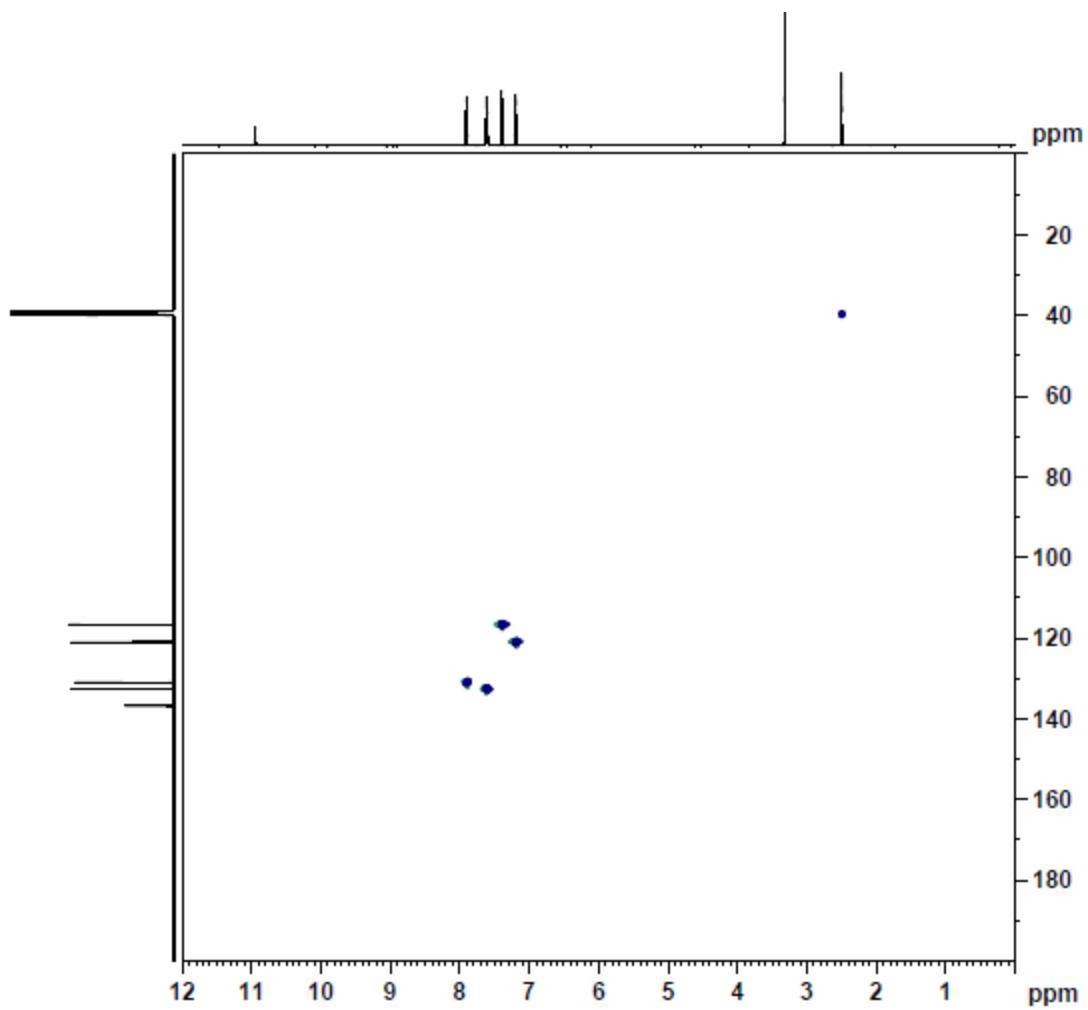


Figure 61: HSQC NMR Spectrum of FOD1 (500 MHz, DMSO-d₆, 300K)

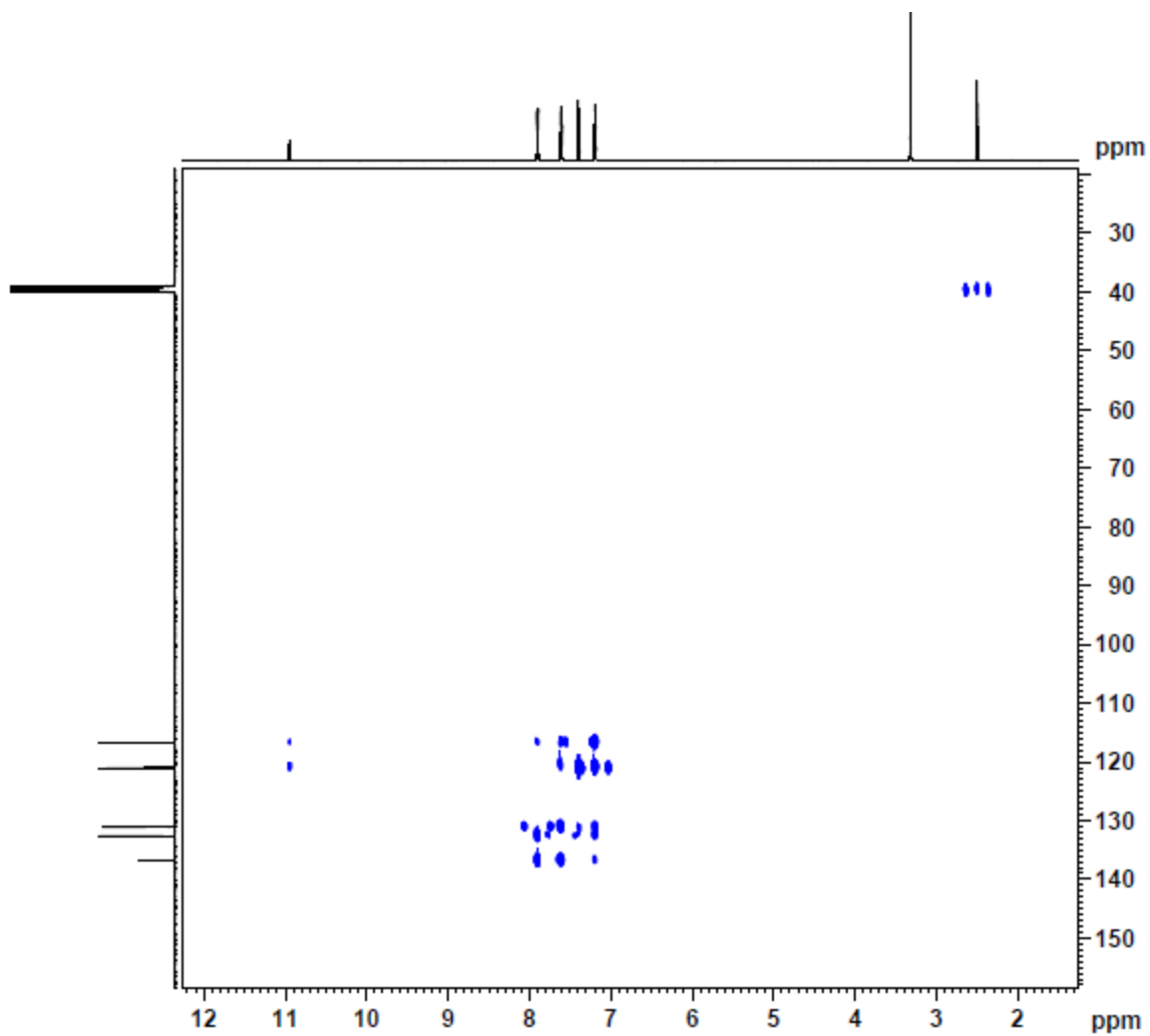


Figure 62: HMBC NMR Spectrum of FOD1 (500 MHz, DMSO-d₆, 300K)

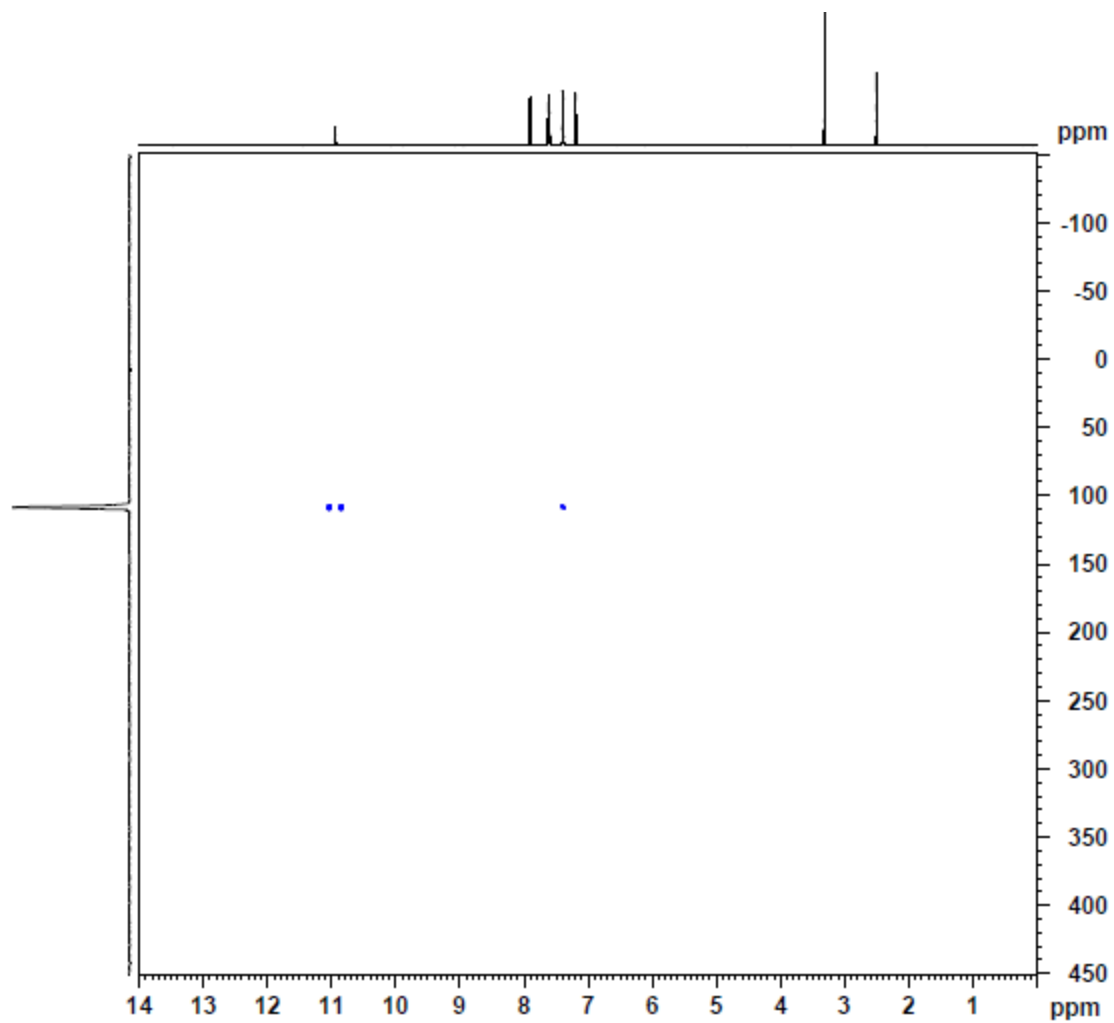


Figure 63: ^{15}N -HMBC NMR Spectrum of FOD1 (500 MHz, DMSO- d_6 , 300K)

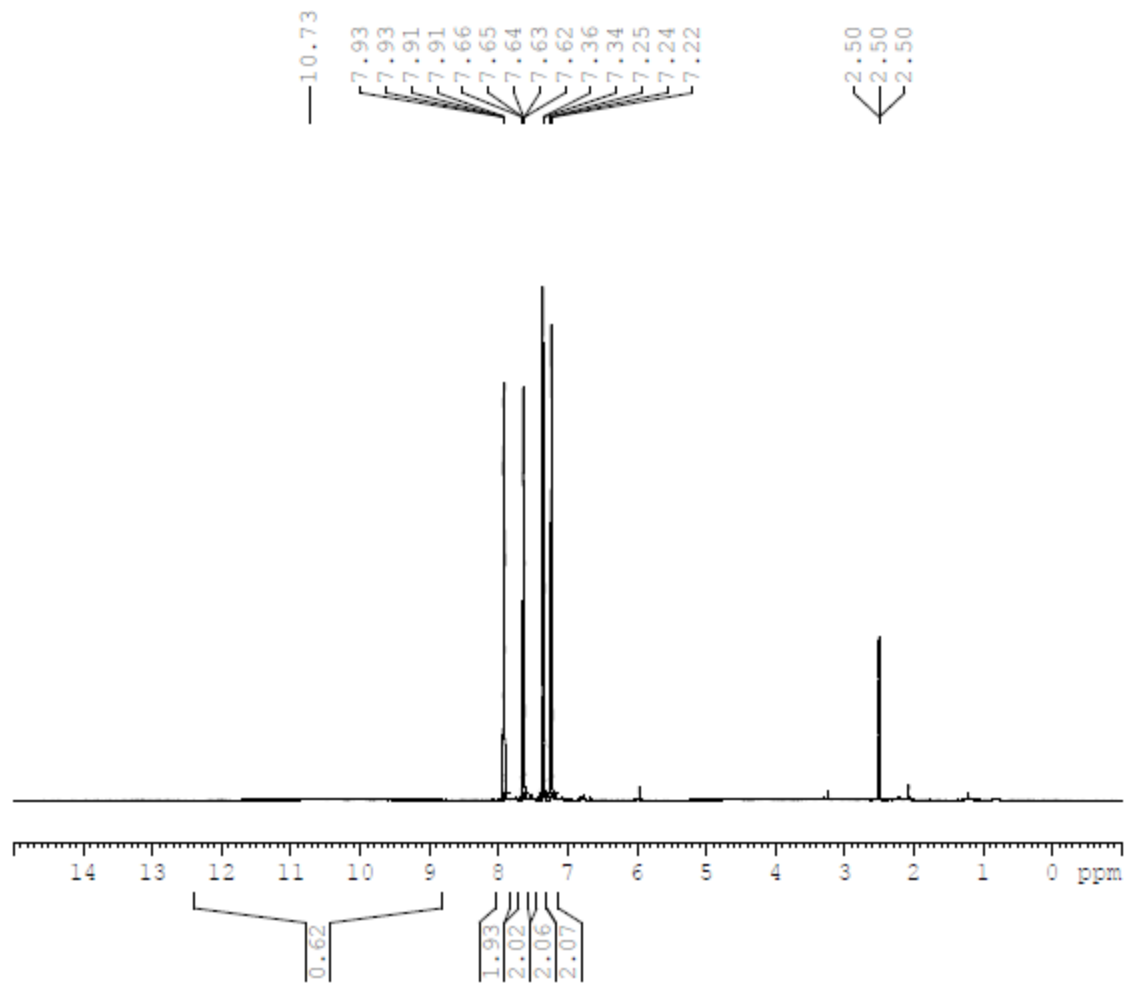


Figure 64: ^1H NMR Spectrum of FOD2 (500 MHz, $\text{DMSO-}d_6$, 300K)

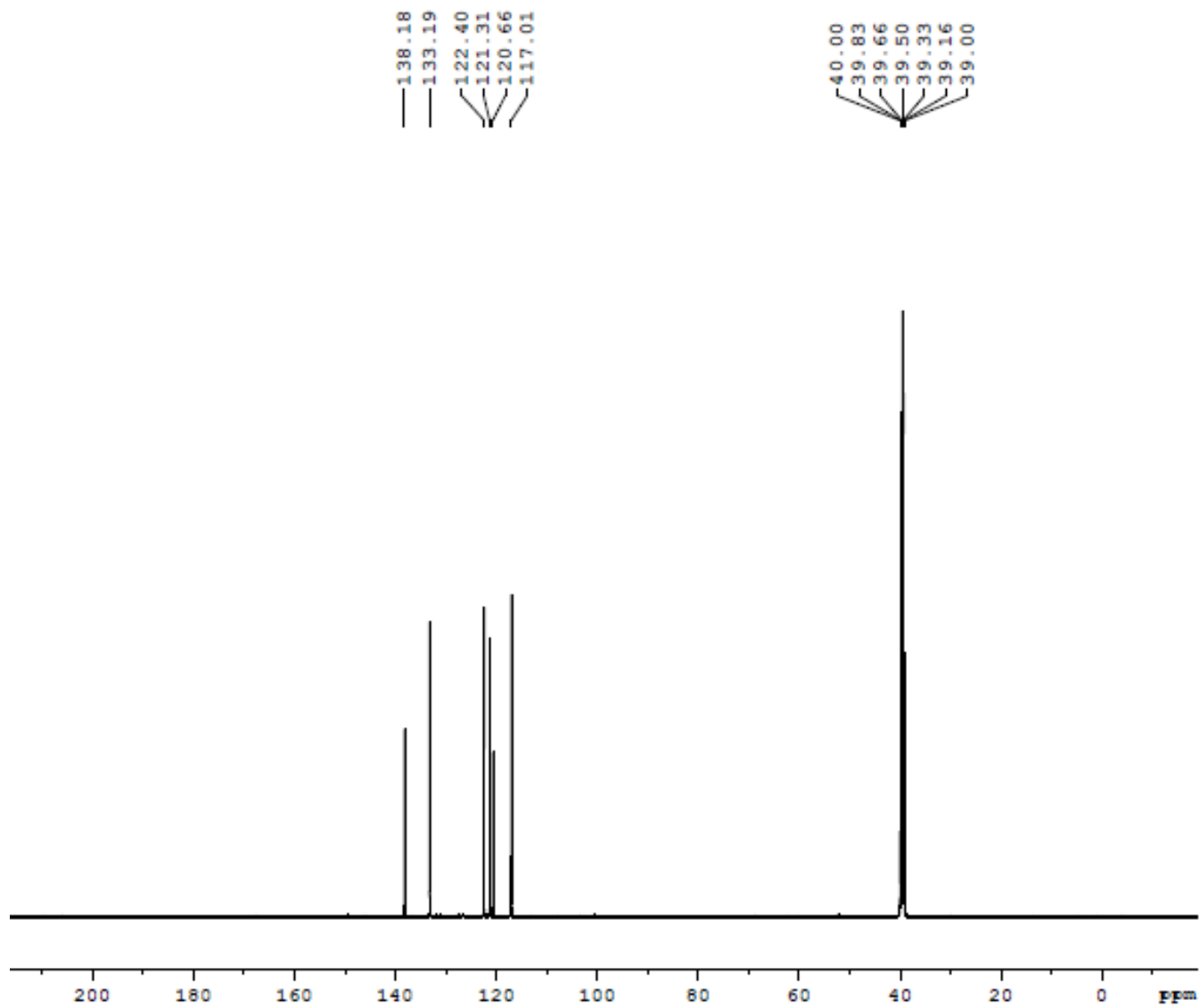


Figure 65: ¹³C NMR Spectrum of FOD2 (126 MHz, DMSO-d₆, 300K)

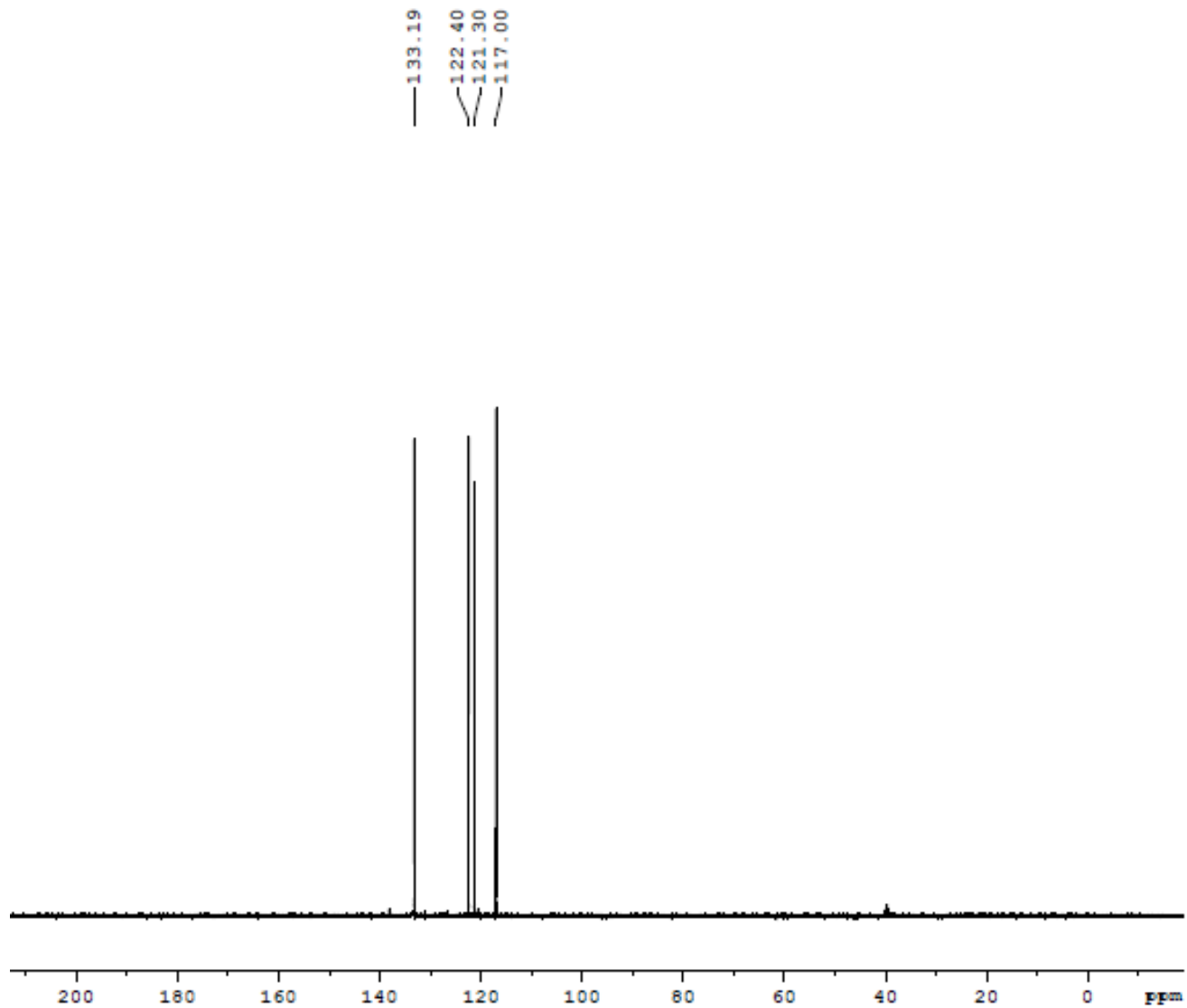


Figure 66: DEPT135 NMR Spectrum of FOD2 (126 MHz, DMSO-d6, 300K)

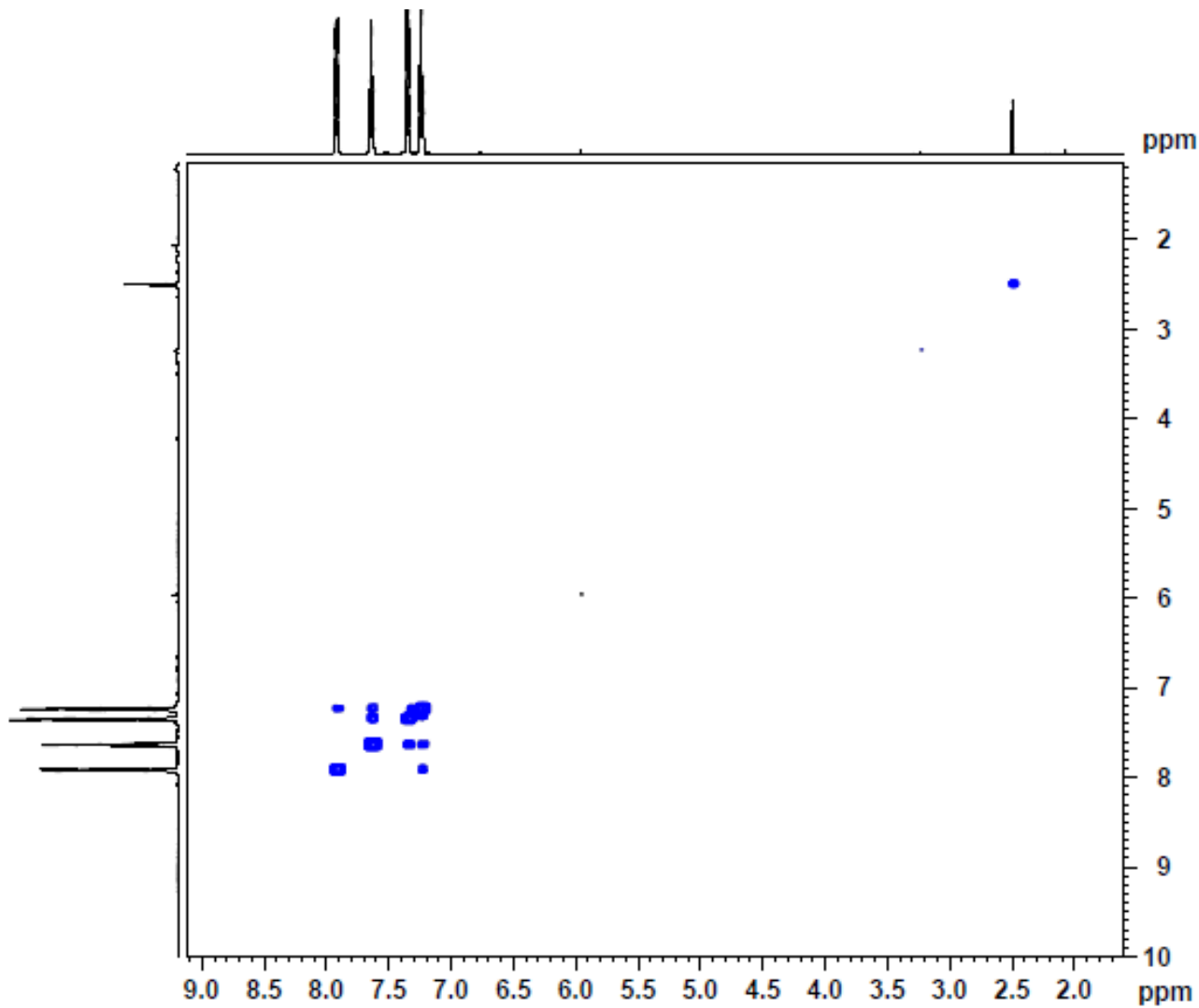


Figure 67: COSY NMR Spectrum of FOD2 (500 MHz, DMSO-d₆, 300K)

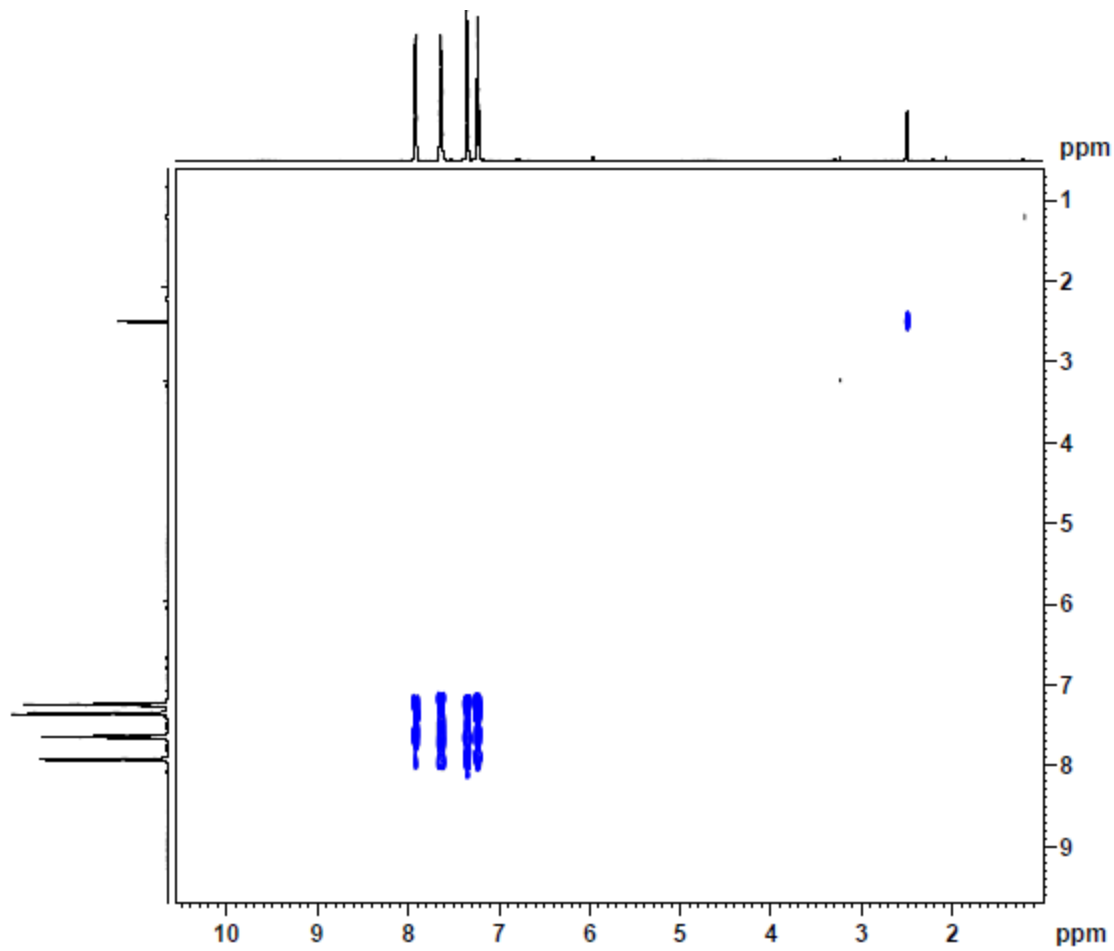


Figure 68: TOCSY NMR Spectrum of FOD2 (500 MHz, DMSO-d₆, 300K)

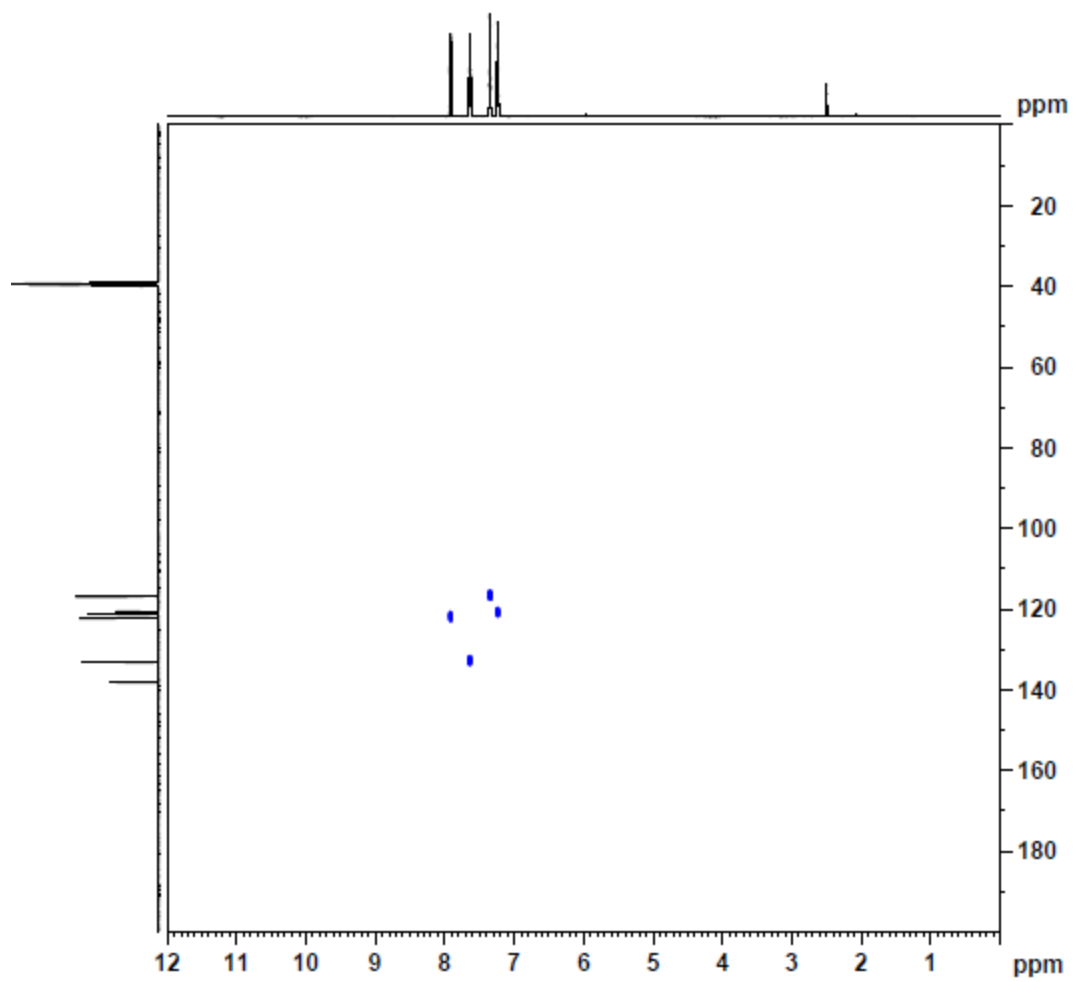


Figure 69: HSQC NMR Spectrum of FOD2 (500 MHz, DMSO-d₆, 300K)

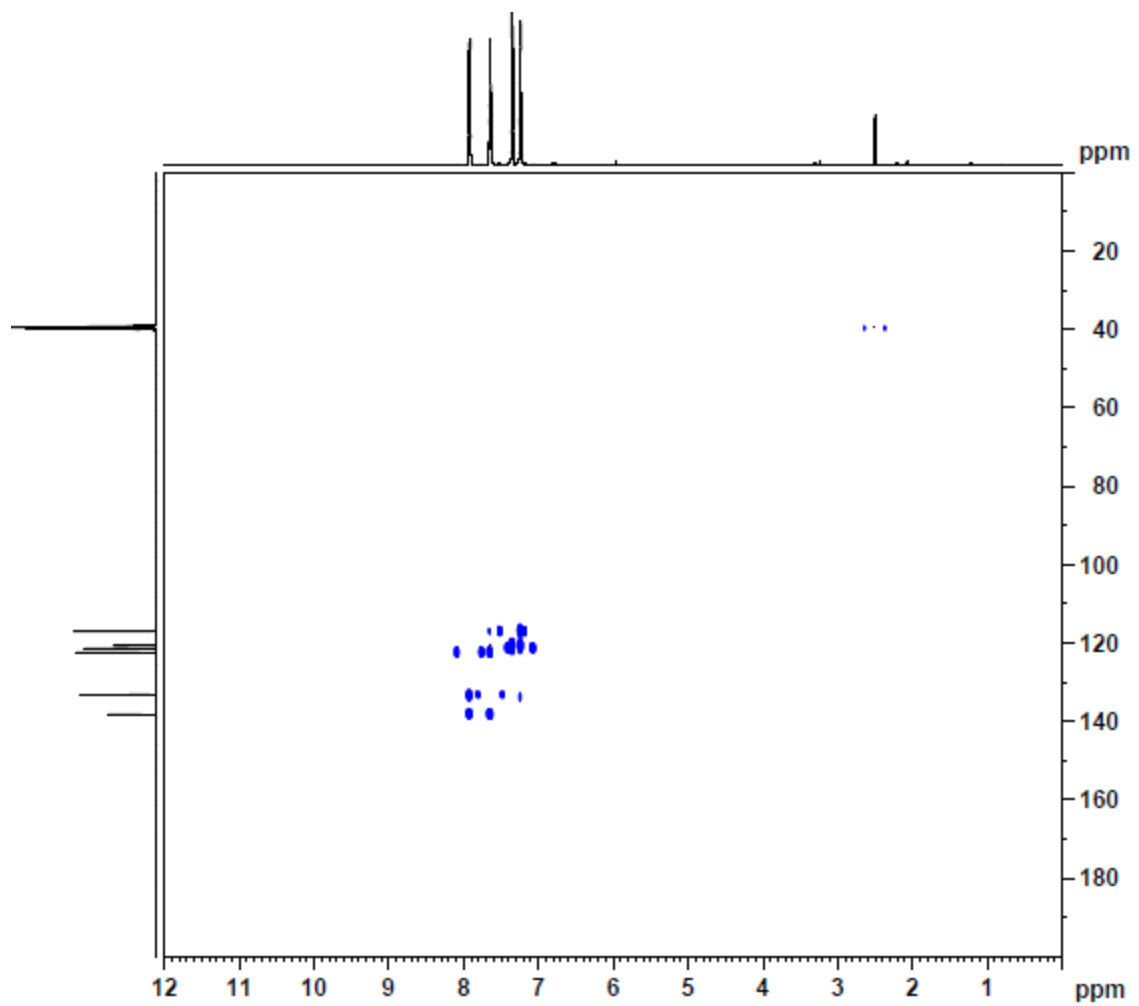


Figure 70: HMBC NMR Spectrum of FOD2 (500 MHz, DMSO-d₆, 300K)

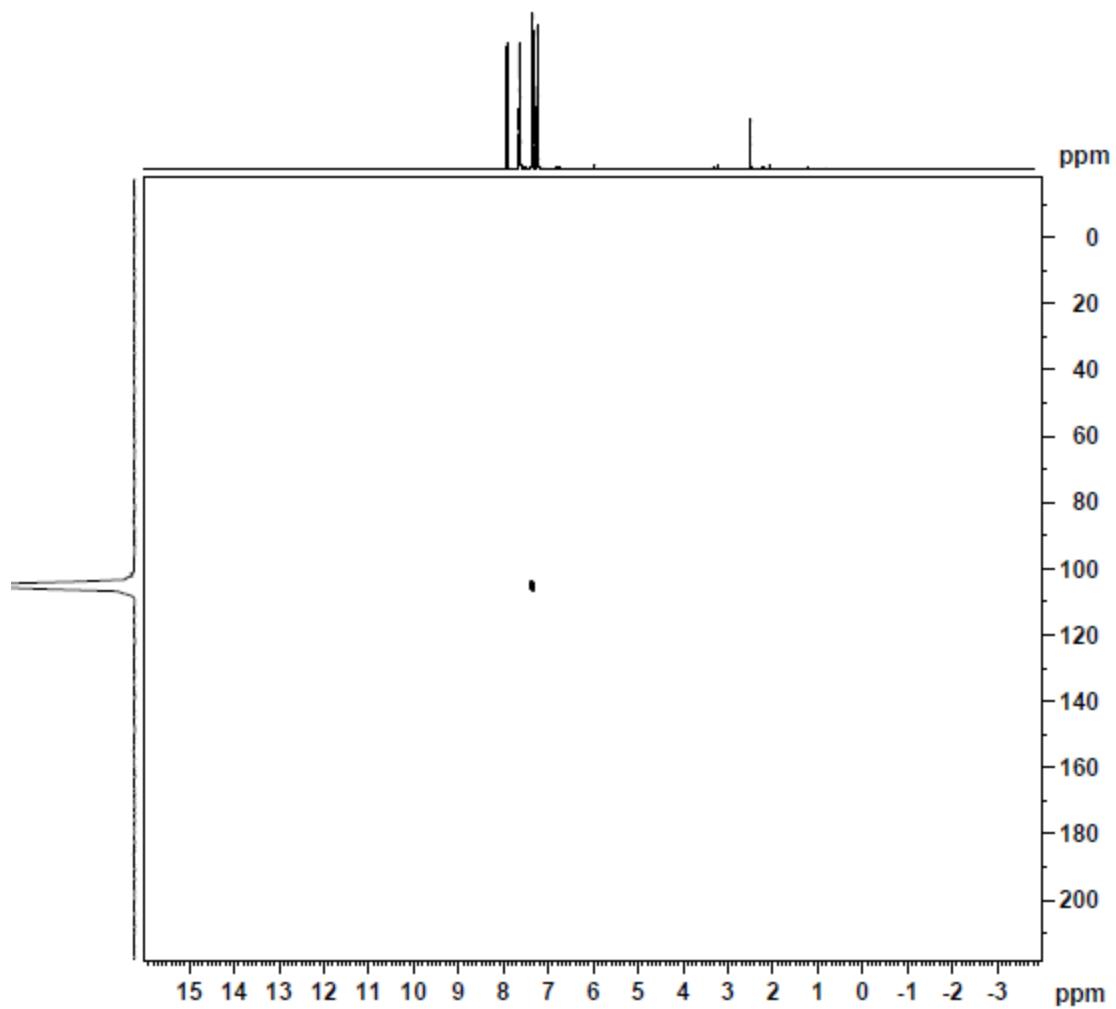


Figure 71: ^{15}N -HMBC NMR Spectrum of FOD2 (500 MHz, DMSO- d_6 , 300K)

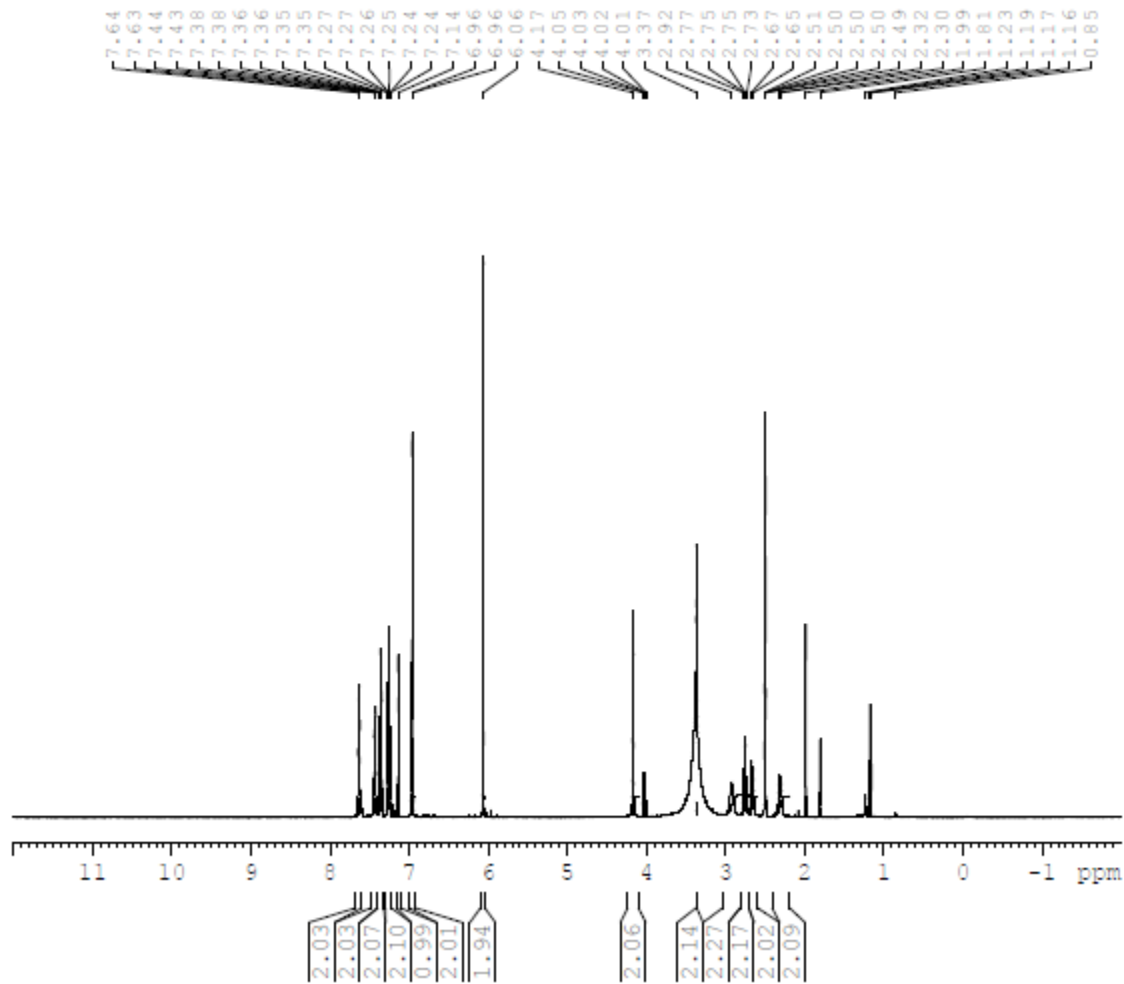


Figure 72: ^1H NMR Spectrum of FOD3 (500 MHz, $\text{DMSO-}d_6$, 300K)

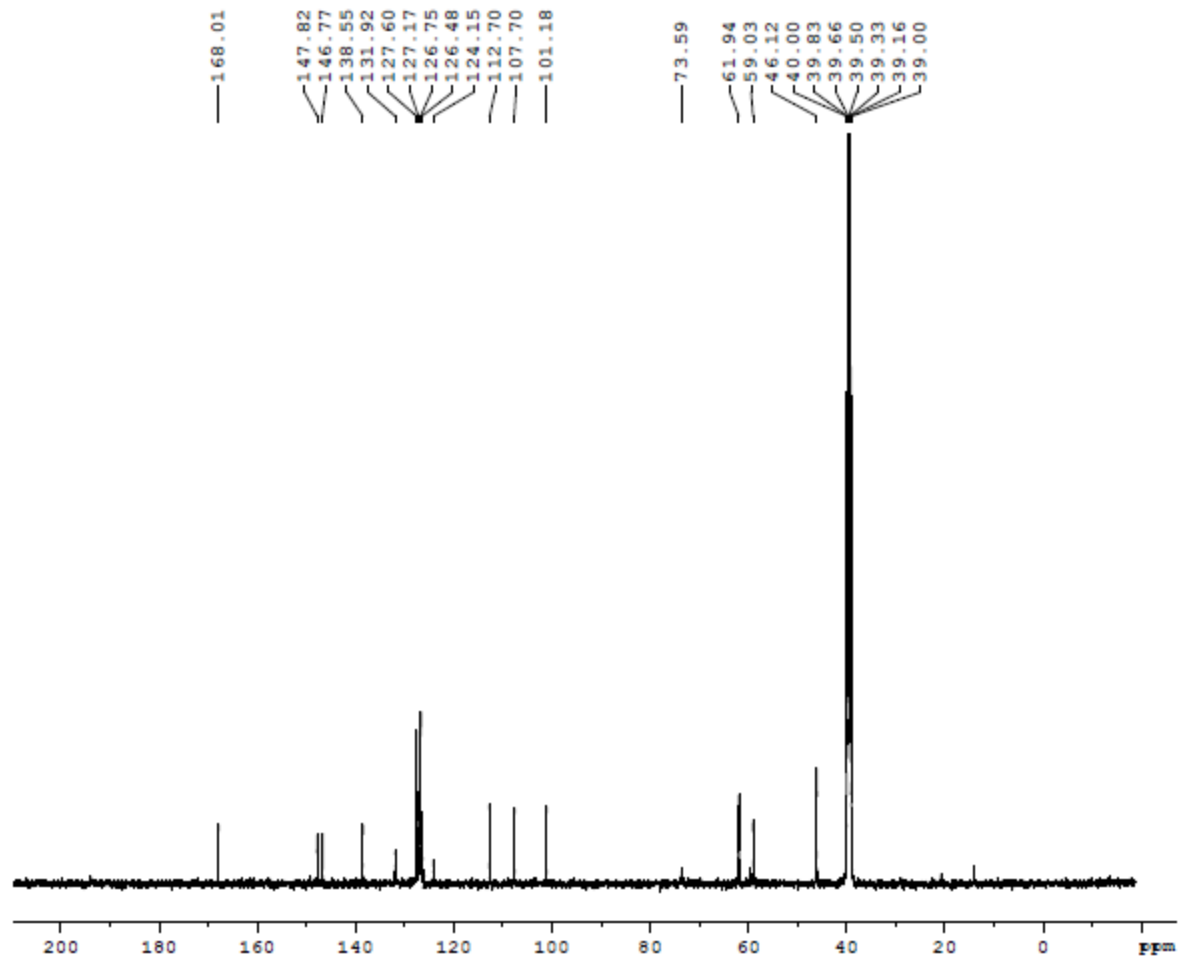


Figure 73: ^{13}C NMR Spectrum of FOD3 (126 MHz, DMSO-d_6 , 300K)

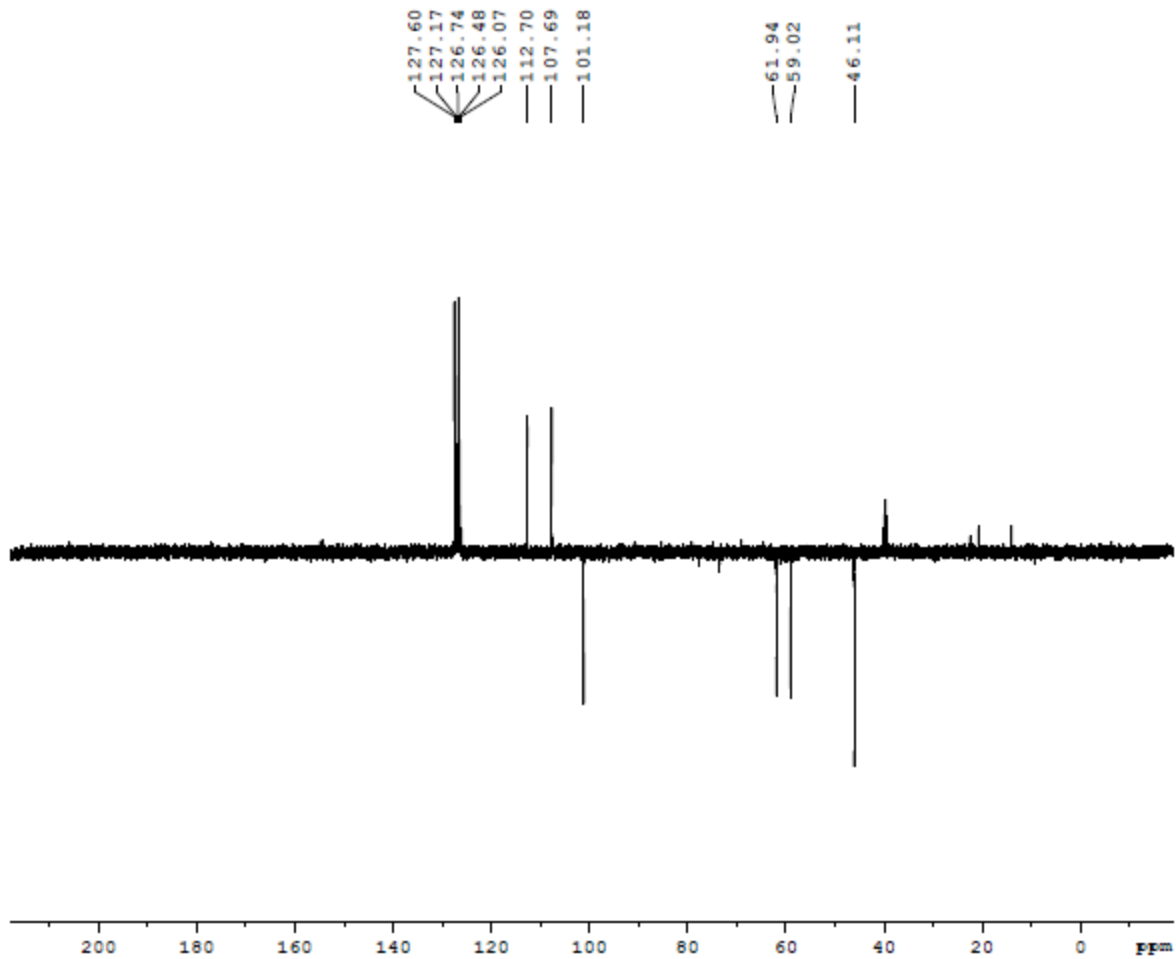


Figure 74: DEPT135 NMR Spectrum of FOD3 (126 MHz, DMSO-d₆, 300K)

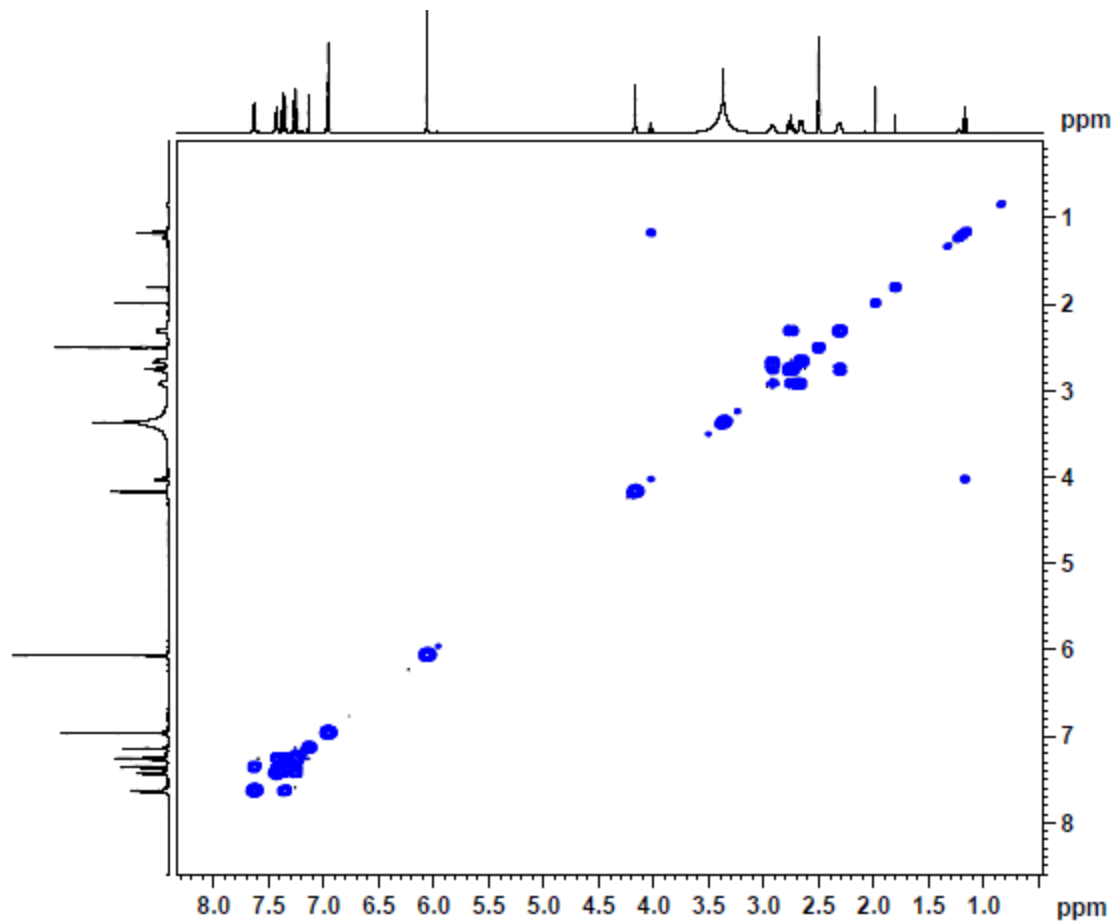


Figure 75: COSY NMR Spectrum of FOD3 (500 MHz, DMSO-d₆, 300K)

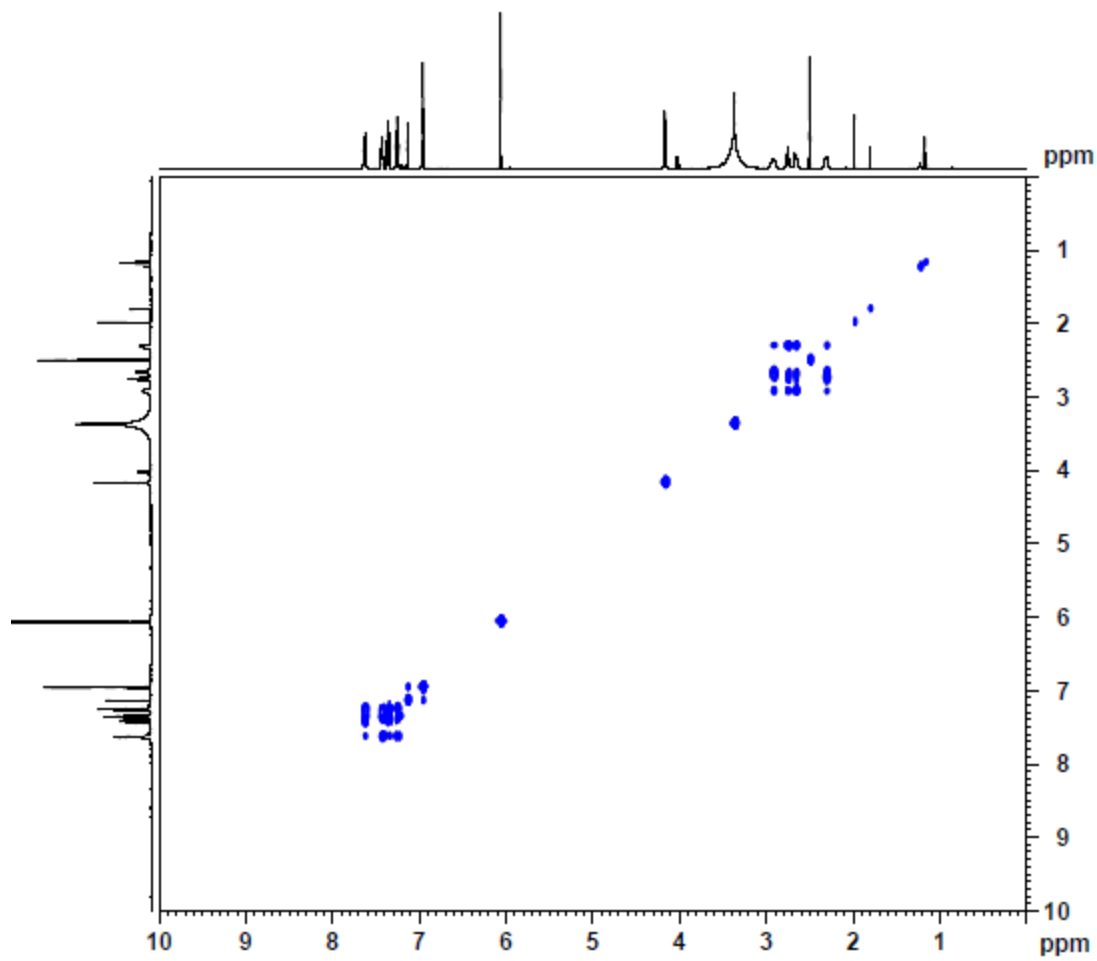


Figure 76: TOCSY NMR Spectrum of FOD3 (500 MHz, DMSO-d₆, 300K)

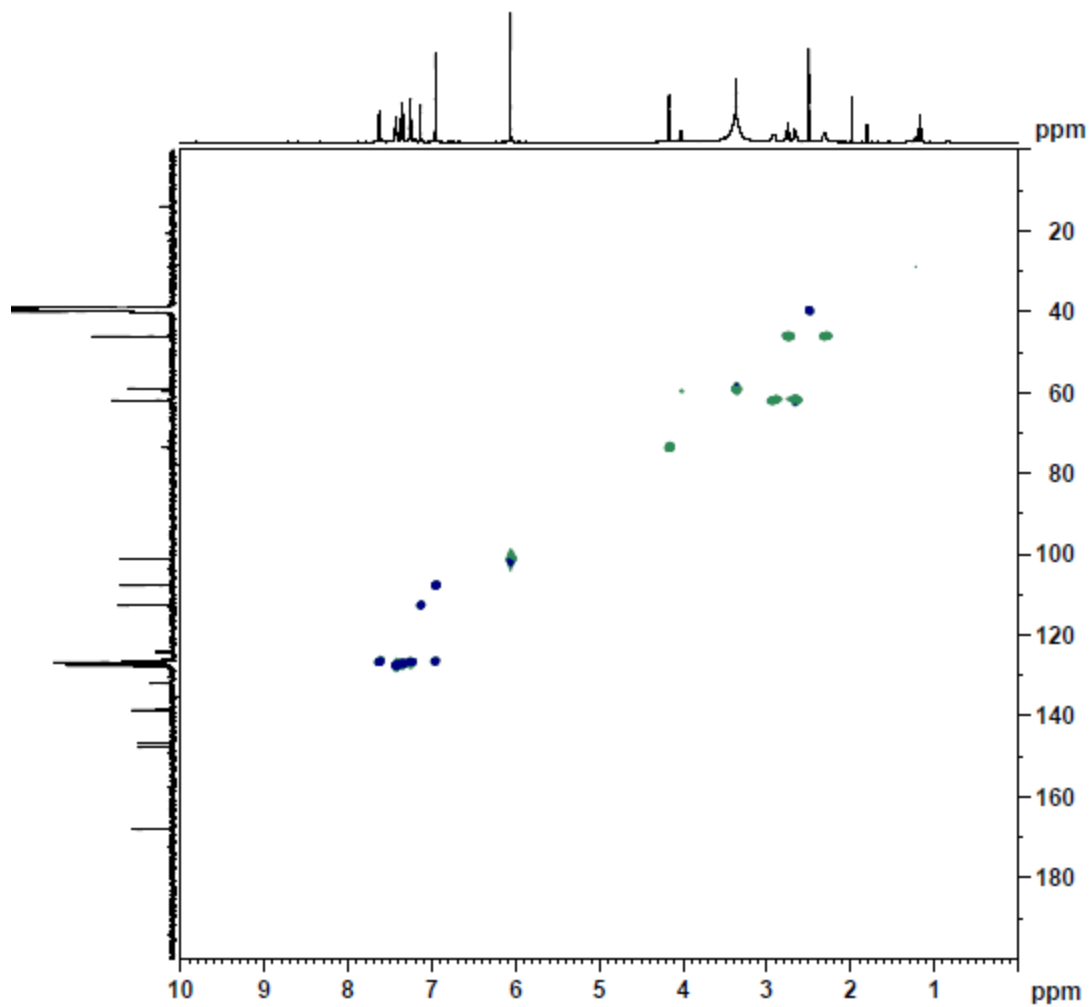


Figure 77: HSQC NMR Spectrum of FOD3 (500 MHz, DMSO-d₆, 300K)

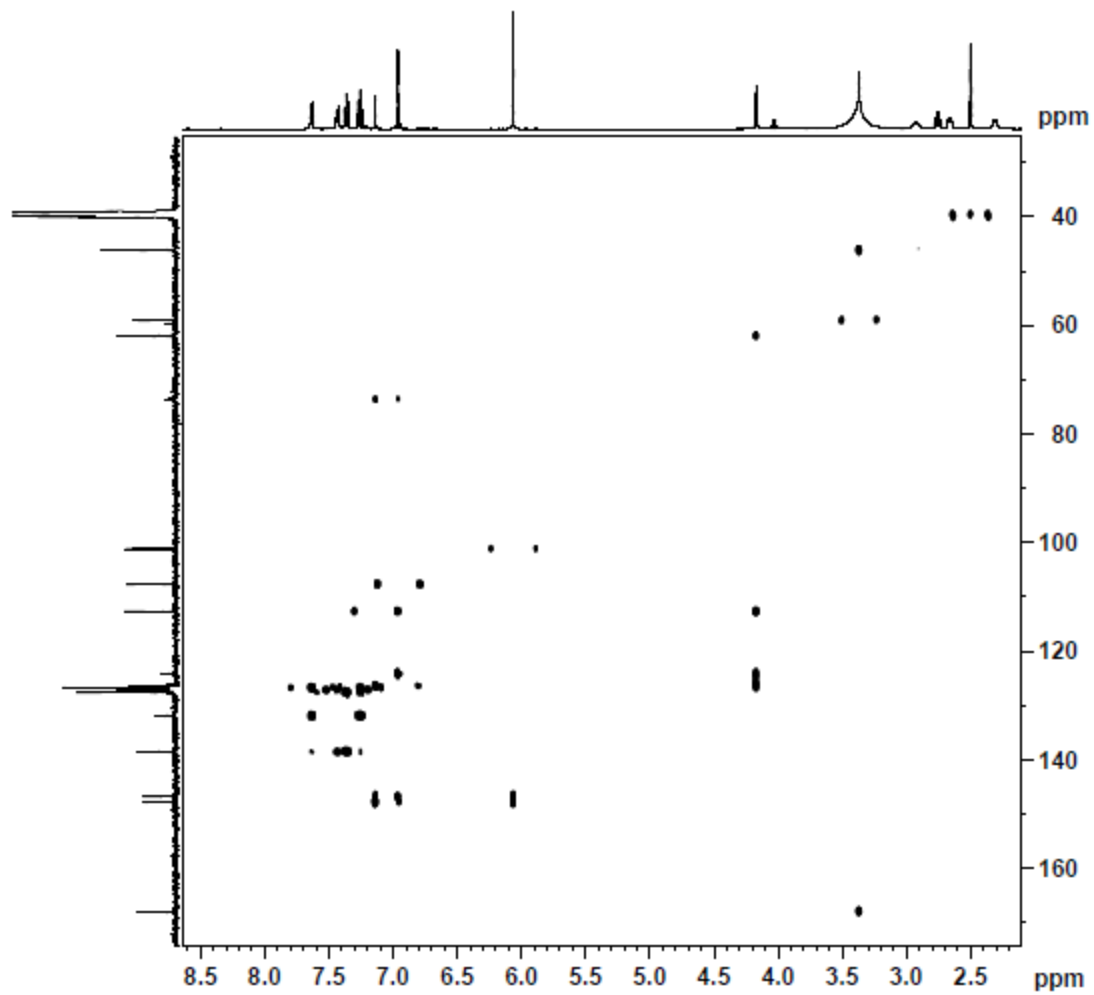


Figure 78: HMBC NMR Spectrum of FOD3 (500 MHz, DMSO-d6, 300K)

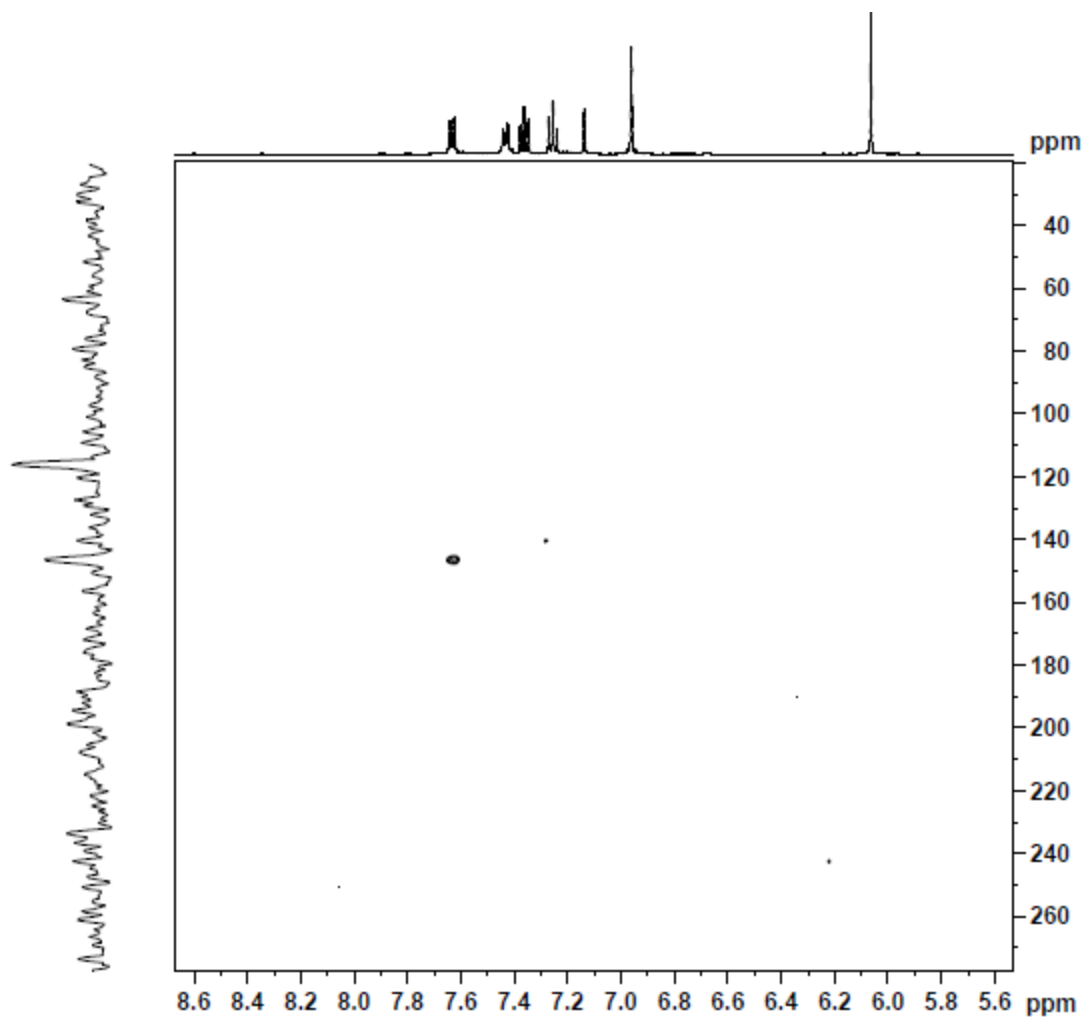


Figure 79: ^{15}N -HMBC NMR Spectrum of FOD3 (500 MHz, DMSO- d_6 , 300K)

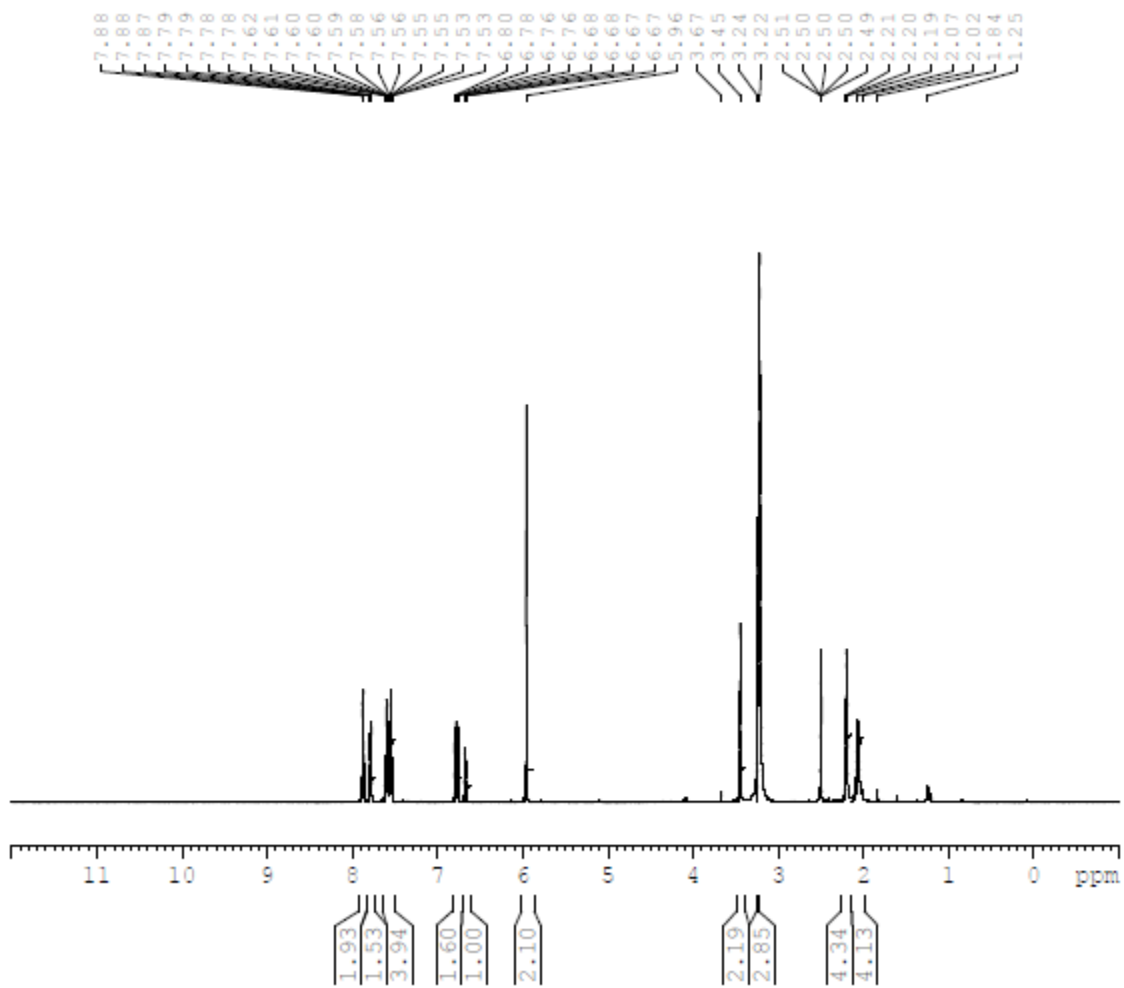


Figure 80: ¹H NMR Spectrum of FOD5 (500 MHz, DMSO-*d*₆, 300K)

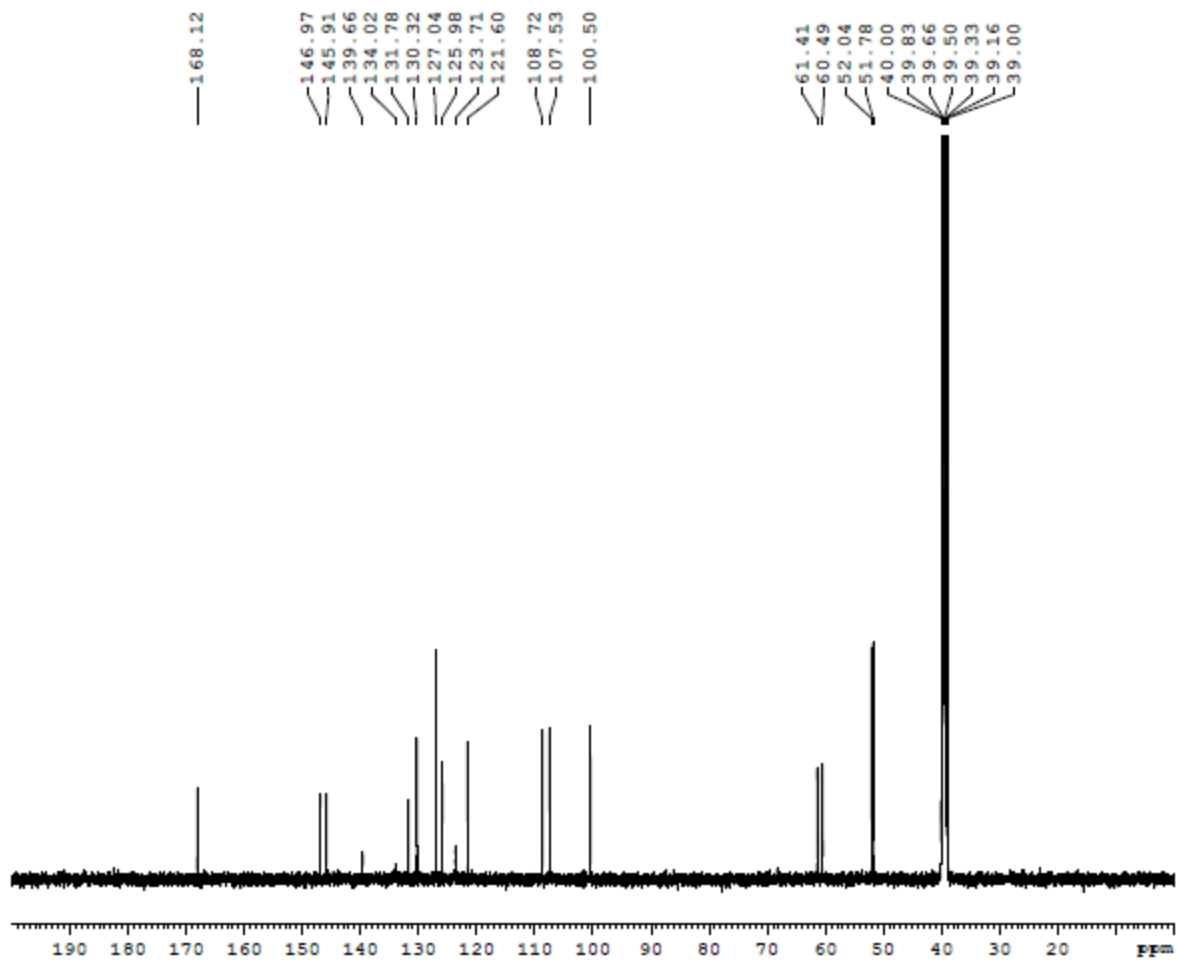


Figure 81: ^{13}C NMR Spectrum of FOD5 (126 MHz, DMSO-d_6 , 300K)

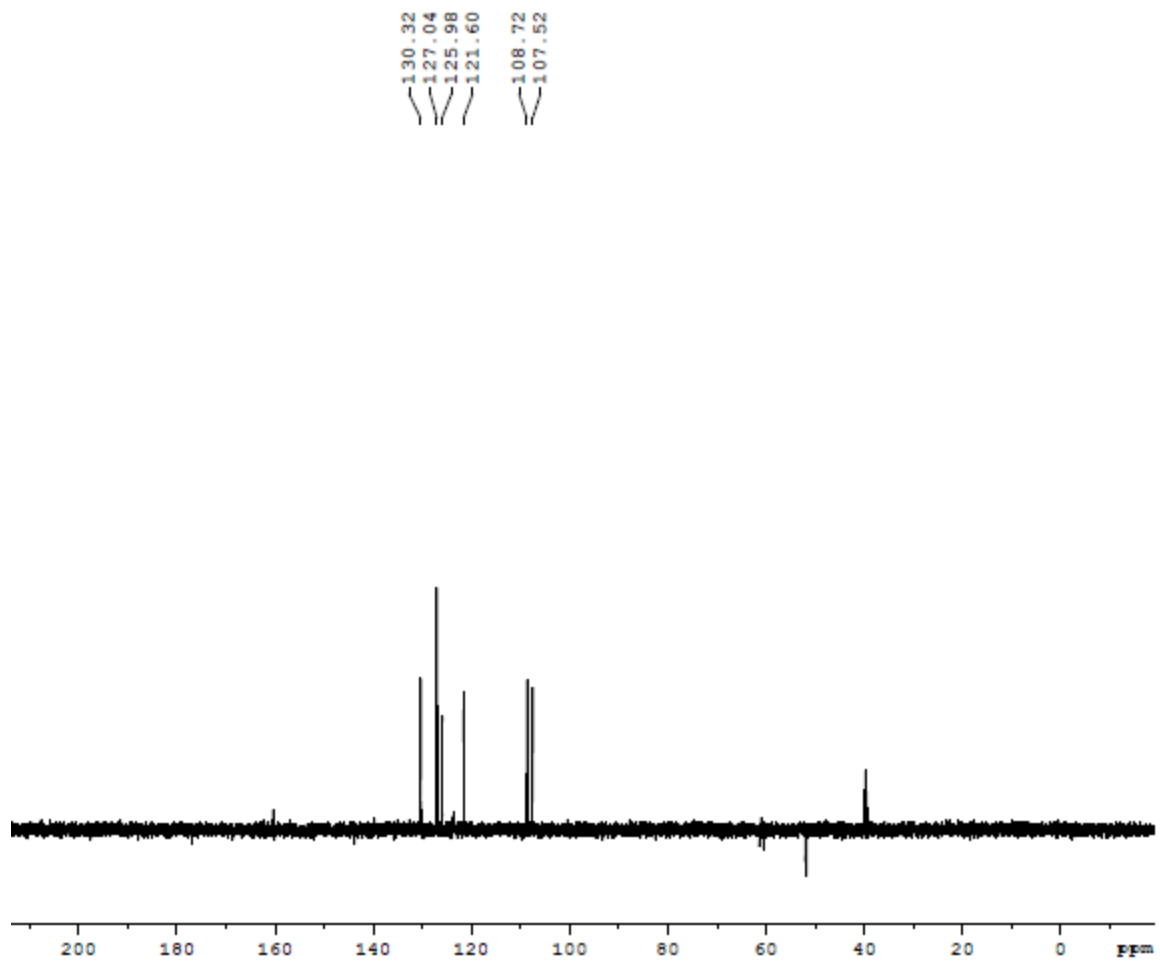


Figure 82: DEPT90 NMR Spectrum of FOD5 (126 MHz, DMSO-d6, 300K)

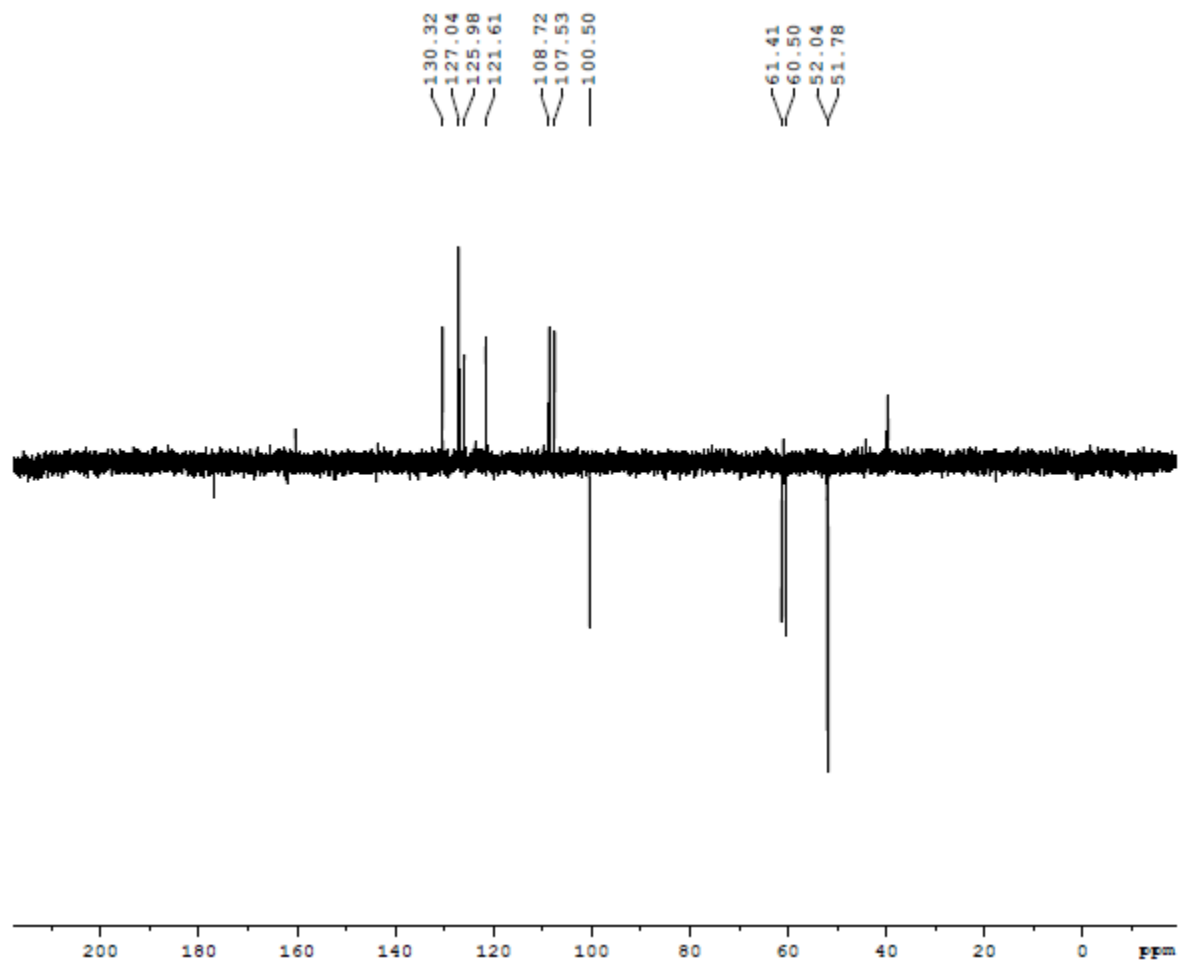


Figure 83: DEPT135 NMR Spectrum of FOD5 (126 MHz, DMSO-d6, 300K)

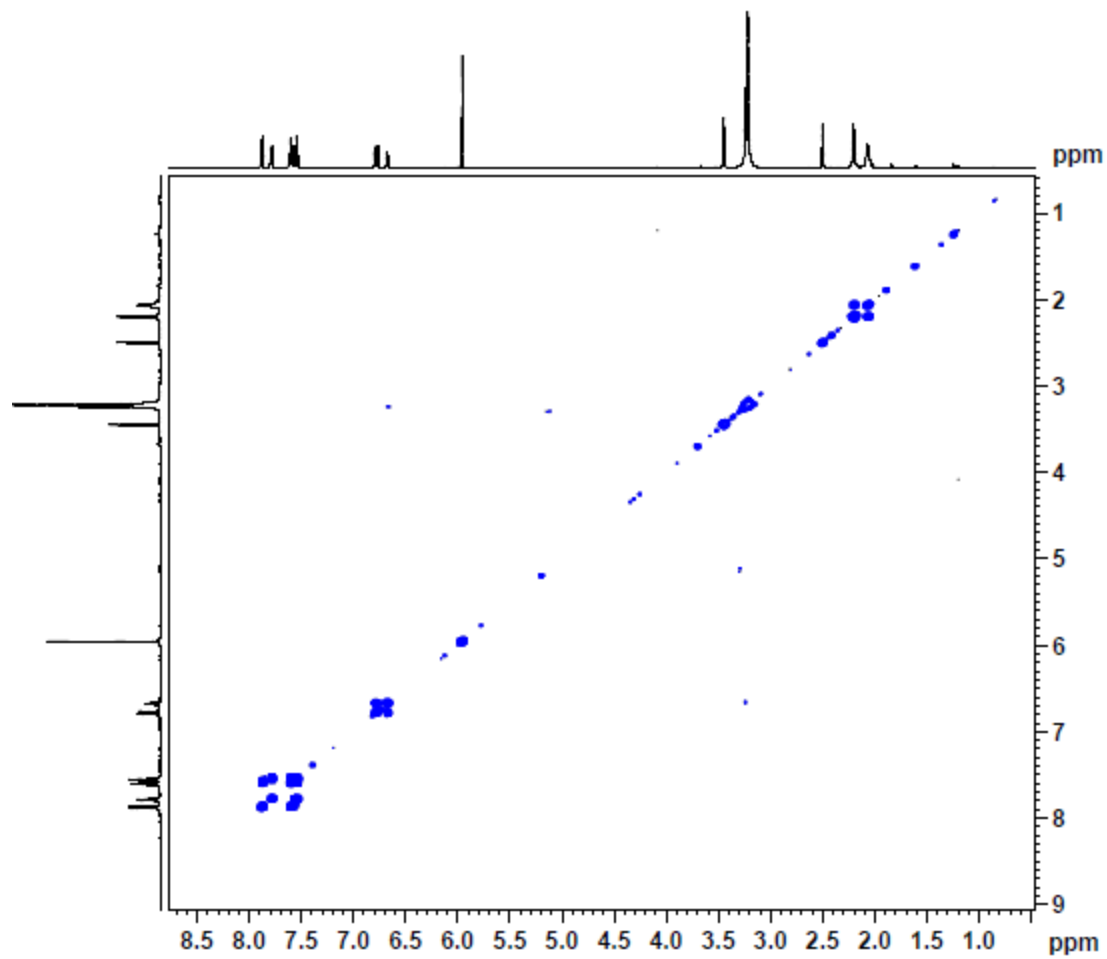


Figure 84: COSY NMR Spectrum of FOD5 (500 MHz, DMSO-d₆, 300K)

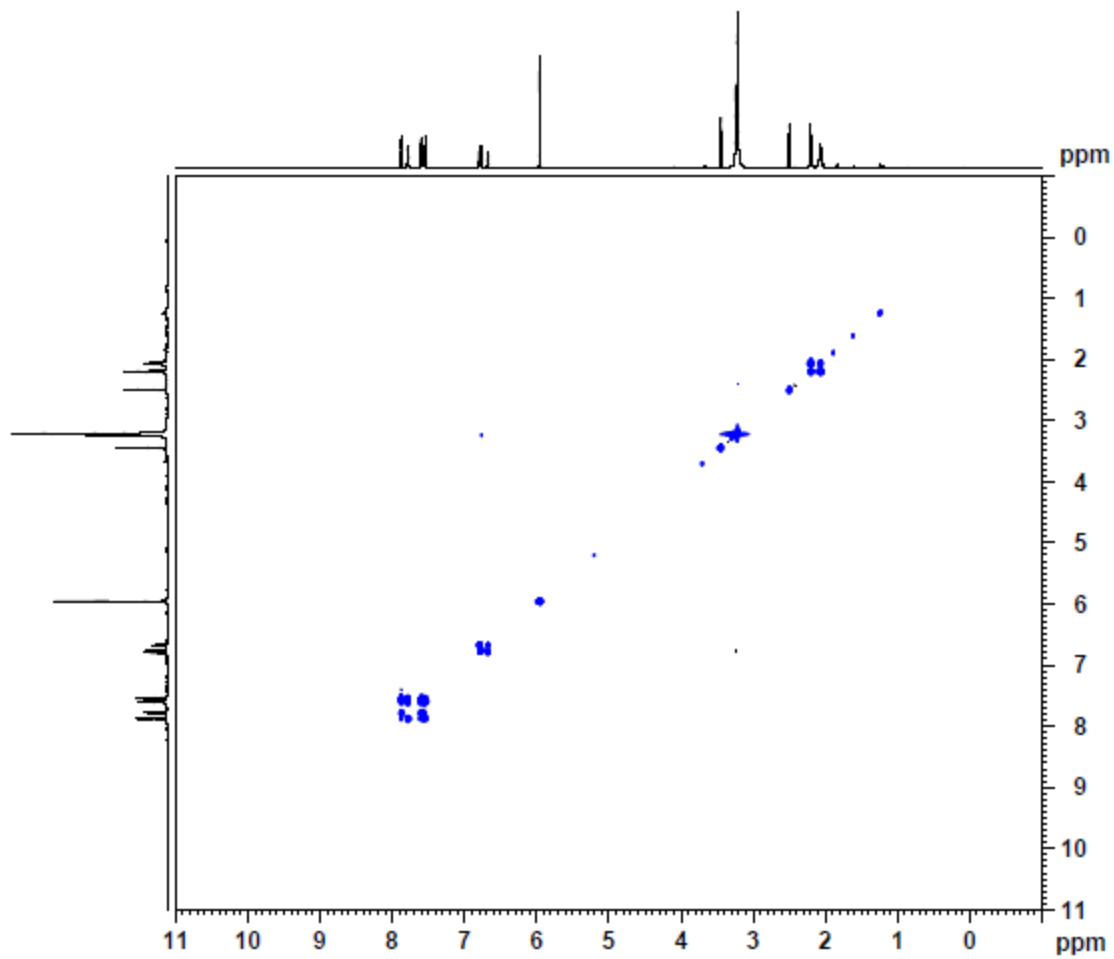


Figure 85: TOCSY NMR Spectrum of FOD5 (500 MHz, DMSO-d6, 300K)

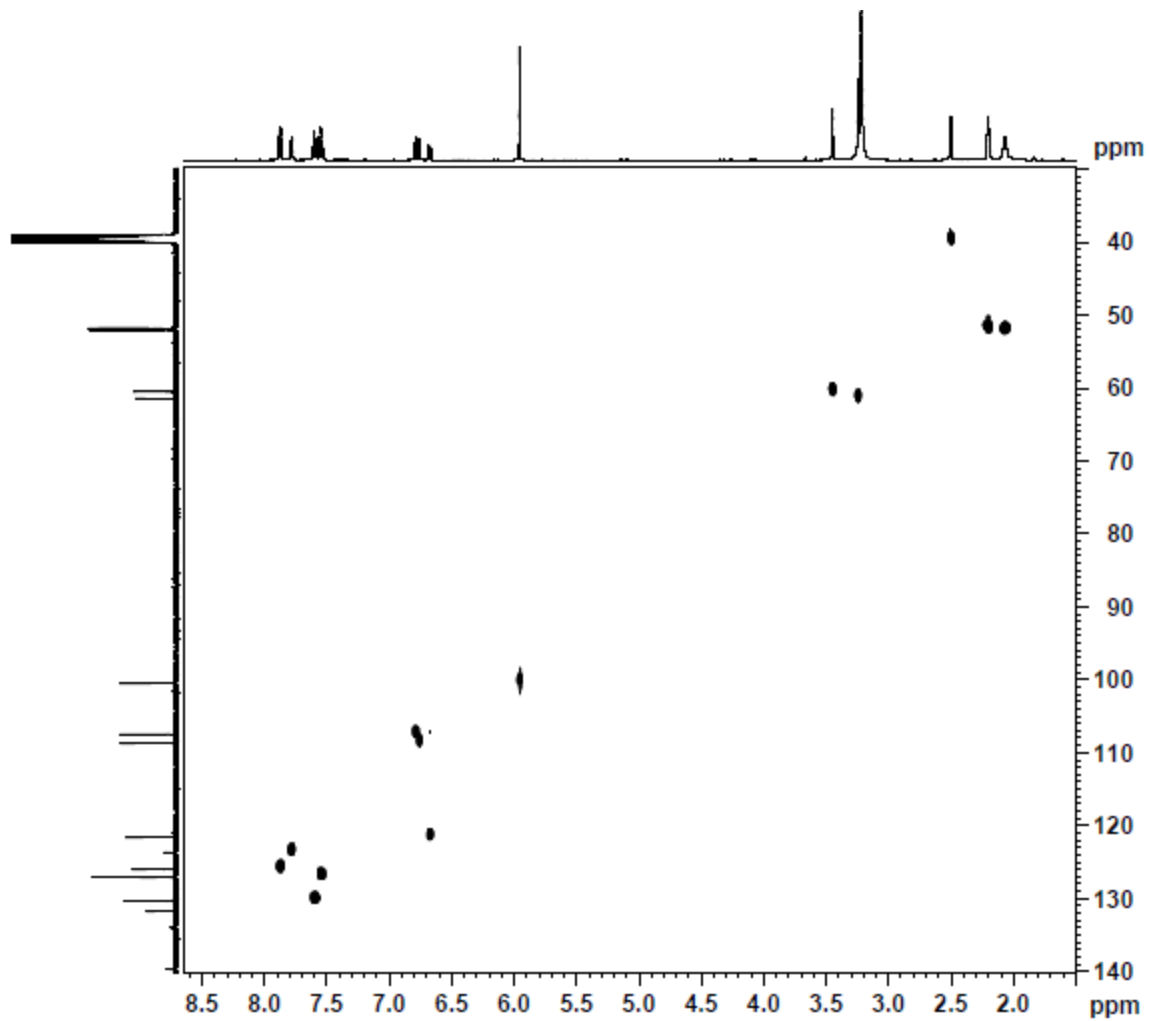


Figure 86: HSQC NMR Spectrum of FOD5 (500 MHz, DMSO-d₆, 300K)

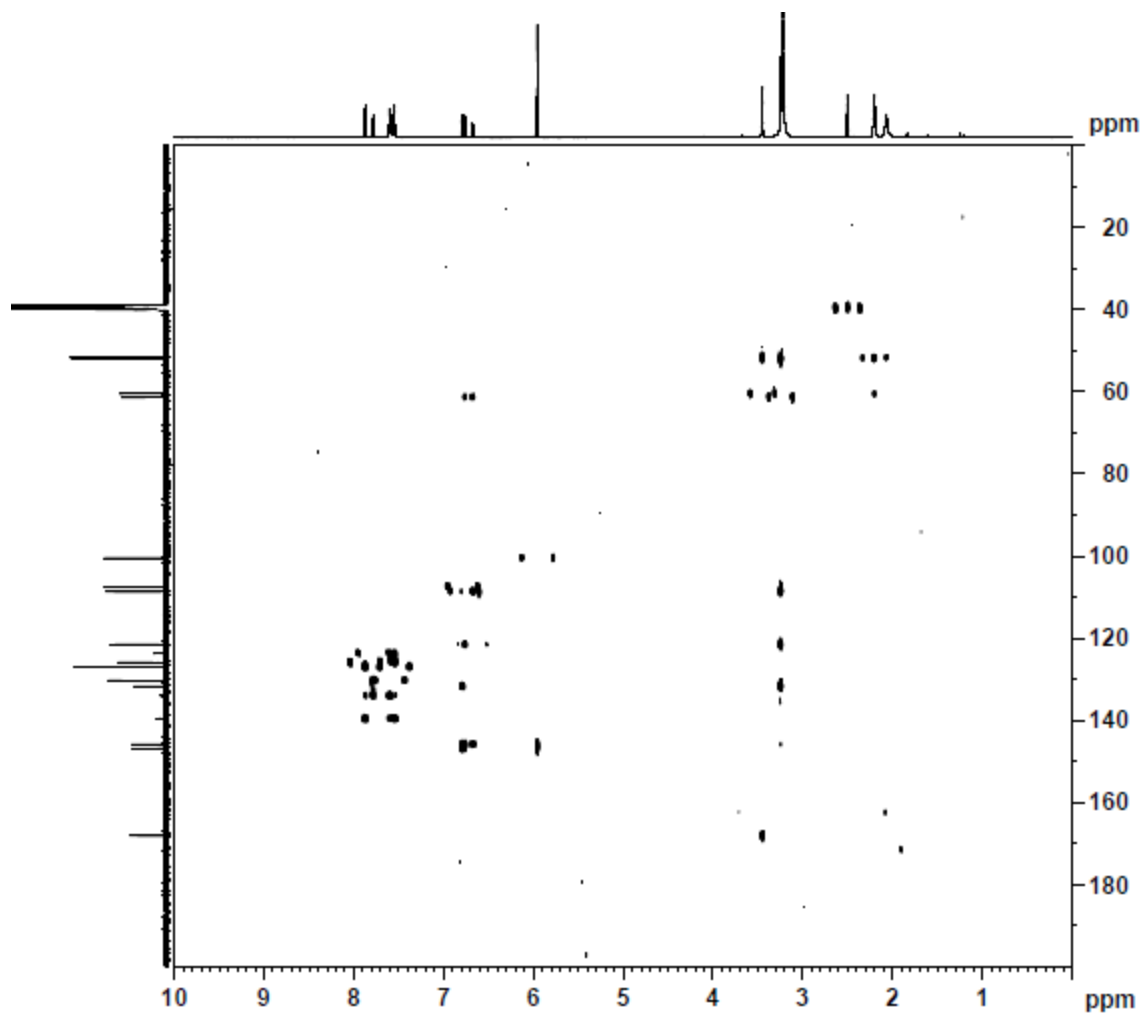
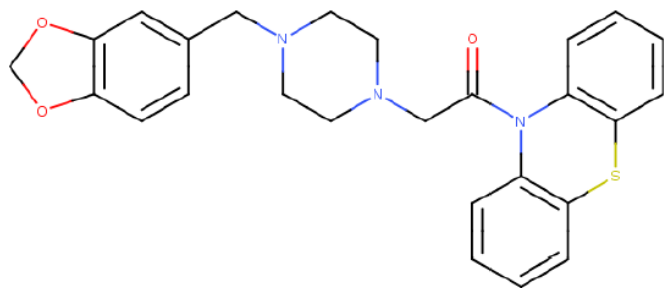


Figure 87: HMBC NMR Spectrum of FOD5 (500 MHz, DMSO-d₆, 300K)

Prediction Summary - FEN

Derek: Inactive

Sarah: Negative



Smiles:

O=C(CN3CCN(CC2=CC=1OCOC=1C=C2)CC3)N5C=CC=CC=C5SC6=CC=CC=C6

Average Mol Mass:	459.56
Exact Mol Mass:	459.1617
Log Kp:	-1.99
Log P:	4.97

Figure 88: In-silico prediction report for FEN

ACD/MS Fragmenter data

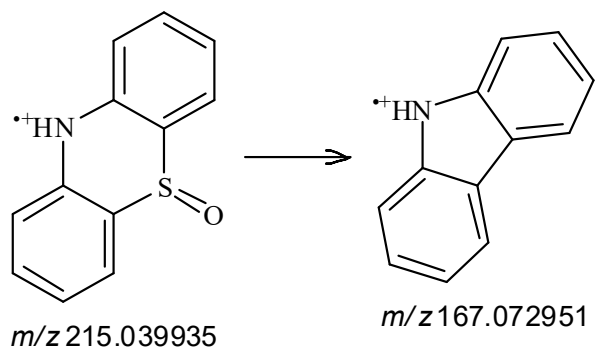
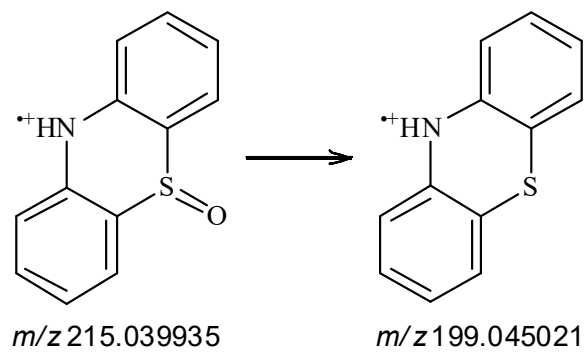


Figure 89: Fragment structures of FOD1 by ACD-MS Fragmentor

ACD/MS Fragmenter data

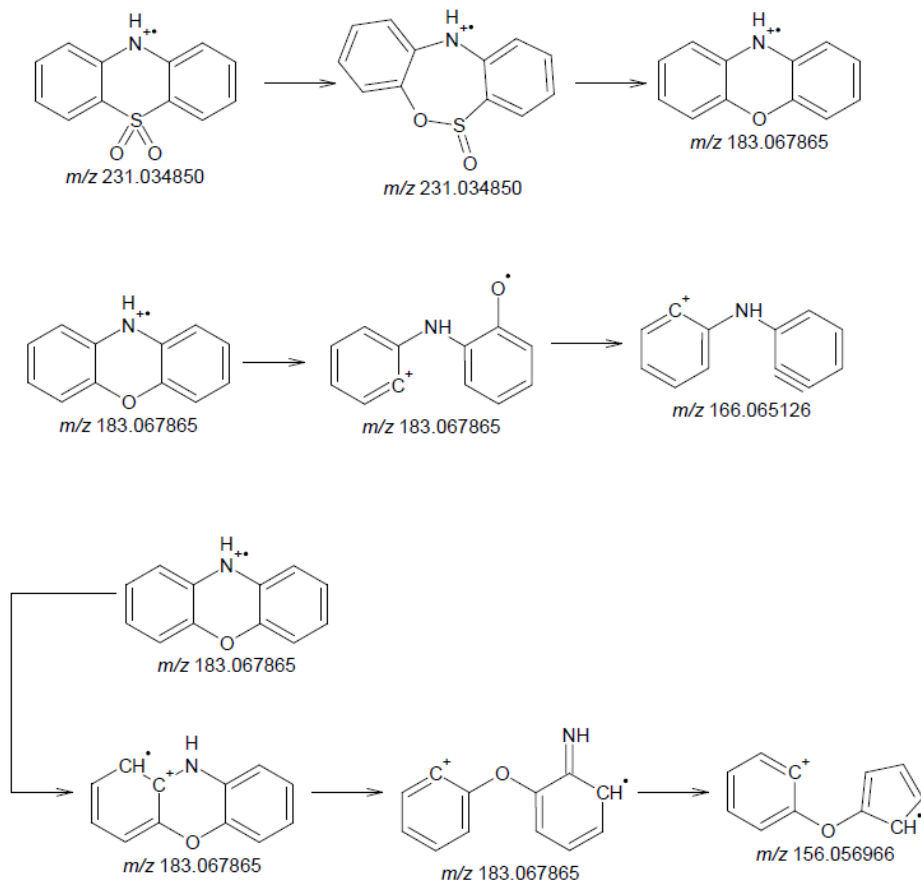


Figure 90: Fragment structures of FOD2 by ACD-MS Fragmentor

Table S-1: HRMS fragmentation data of Fenoverine (FEN) and its degradation products FAD1, FAD2, FOD1 to FOD5.

	HRMS data				
	Accurate mass	Obtained m/z values of fragments	Proposed chemical formula	Calculated m/z value	Error in ppm
[FEN + H] ⁺	460.1706	324.1154	C ₁₈ H ₁₈ N ₃ OS ⁺	324.1165	-3.4
		233.1317	C ₁₃ H ₁₇ N ₂ O ₂ ⁺	233.1285	13.7
		135.0436	C ₈ H ₇ O ₂ ⁺	135.0441	-3.7
[FAD1 + H] ⁺	279.1328	143.0862	C ₆ H ₁₁ N ₂ O ₂ ⁺	143.0815	32.8
		135.0451	C ₈ H ₇ O ₂ ⁺	135.0441	7.4
		105.0360	C ₇ H ₅ O ⁺	105.0335	23.8
		79.0527	C ₆ H ₇ ⁺	79.0542	-19.0
		77.0382	C ₆ H ₅ ⁺	77.0386	-5.2
[FOD1 + H] ⁺	216.0464	199.0452	C ₁₂ H ₉ NS ⁺	199.0450	1.0
		167.0748	C ₁₂ H ₉ N ⁺	167.0730	10.8
		154.0683	C ₁₁ H ₈ N ⁺	154.0651	20.8
[FOD2 + H] ⁺	232.0412	215.0402	C ₁₂ H ₉ NOS ⁺	215.0399	1.4
		183.0708	C ₁₂ H ₉ NO ⁺	183.0679	15.8
		167.0748	C ₁₂ H ₉ N ⁺	167.0730	10.8
		156.0812	C ₁₁ H ₁₀ N ⁺	156.0808	2.6
		129.0699	C ₁₀ H ₉ ⁺	129.0699	0.0
[FOD3 + H] ⁺	476.1638	340.1088	C ₁₈ H ₁₈ N ₃ O ₂ S ⁺	340.1114	-7.6
		322.1051	C ₁₈ H ₁₆ N ₃ OS ⁺	322.1009	13.0
		200.0573	C ₁₂ H ₁₀ NS ⁺	200.0528	22.5
		135.0436	C ₈ H ₇ O ₂ ⁺	135.0441	-3.7
[FOD4 + H] ⁺	476.1640	458.1575	C ₂₆ H ₂₄ N ₃ O ₃ S ⁺	458.1533	9.2
		323.1085	C ₁₈ H ₁₇ N ₃ OS ⁺	323.1087	-0.6
		233.1307	C ₁₃ H ₁₇ N ₂ O ₂ ⁺	233.1285	9.4
		198.0346	C ₁₂ H ₈ NS ⁺	198.0372	-13.1
		135.0426	C ₈ H ₇ O ₂ ⁺	135.0441	-11.1
[FOD5 + H] ⁺	476.1631	340.1088	C ₁₈ H ₁₈ N ₃ O ₂ S ⁺	340.1114	-7.6
		323.1095	C ₁₈ H ₁₇ N ₃ OS ⁺	323.1087	2.5
		233.1250	C ₁₃ H ₁₇ N ₂ O ₂ ⁺	233.1285	-15.0
		216.0471	C ₁₂ H ₁₀ NOS ⁺	216.0478	-3.2
		198.0356	C ₁₂ H ₈ NS ⁺	198.0372	-8.1
		135.0436	C ₈ H ₇ O ₂ ⁺	135.0441	-3.7
[FAD2] ⁺	199.0452	167.0748	C ₁₂ H ₉ N ⁺	167.0730	10.8
		154.0629	C ₁₁ H ₈ N ⁺	154.0651	-14.3