

Supporting Information

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Synthesis and evaluation of antiproliferative and mPGES-1 inhibitory activities of novel carvacrol-triazole-acetanilide conjugates

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Table of Contents	Page
Figure S1: FTIR Spectrum of 5	5
Figure S2: ¹ H-NMR (300 MHz, DMSO) Spectrum of 5	5
Figure S3: FTIR Spectrum of 8	6
Figure S4: ¹ H-NMR (500 MHz, DMSO) Spectrum of 8	6
Figure S5: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 8	7
Figure S6: HPLC chromatogram of 8	7
Figure S7: ESI(-)-MS Spectrum of 8	8
Figure S8: FTIR Spectrum of 9	9
Figure S9: ¹ H-NMR (500 MHz, DMSO) Spectrum of 9	9
Figure S10: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 9	10
Figure S11: ESI(+)-MS Spectrum of 9	11
Figure S12: ESI(-)-MS Spectrum of 9	12
Figure S13: HPLC chromatogram of 9	12
Figure S14: FTIR Spectrum of 10	13
Figure S15: ¹ H-NMR (500 MHz, DMSO) Spectrum of 10	13
Figure S16: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 10	14
Figure S17: ESI(+)-MS Spectrum of 10	15

Figure S18: ESI(-)-MS Spectrum of 10	16
Figure S19: HPLC chromatogram of 10	16
Figure S20: FTIR Spectrum of 11	17
Figure S21: ¹H-NMR (500 MHz, DMSO) Spectrum of 11	17
Figure S22: ¹³C-NMR (125 MHz, DMSO) Spectrum of 11	18
Figure S23: ESI(+)-MS Spectrum of 11	19
Figure S24: ESI(-)-MS Spectrum of 11	20
Figure S25: HPLC chromatogram of 11	20
Figure S26: FTIR Spectrum of 12	21
Figure S27: ¹H-NMR (500 MHz, DMSO) Spectrum of 12	21
Figure S28: ¹³C-NMR (125 MHz, DMSO) Spectrum of 12	22
Figure S29: ESI(+)-MS Spectrum of 12	23
Figure S30: ESI(-)-MS Spectrum of 12	24
Figure S31: HPLC chromatogram of 12	24
Figure S32: FTIR Spectrum of 13	25
Figure S33: ¹H-NMR (500 MHz, DMSO) Spectrum of 13	25
Figure S34: ¹³C-NMR (125 MHz, DMSO) Spectrum of 13	26
Figure S35: ESI(+)-MS Spectrum of 13	27
Figure S36: ESI(-)-MS Spectrum of 13	28
Figure S37: HPLC chromatogram of 13	28
Figure S38: FTIR Spectrum of 14	29
Figure S39: ¹H-NMR (500 MHz, DMSO) Spectrum of 14	29
Figure S40: ¹³C-NMR (125 MHz, DMSO) Spectrum of 14	30
Figure S41: ESI(+)-MS Spectrum of 14	31
Figure S42: ESI(-)-MS Spectrum of 14	32
Figure S43: HPLC chromatogram of 14	32
Figure S44: FTIR Spectrum of 15	33
Figure S45: ¹H-NMR (500 MHz, DMSO) Spectrum of 15	33
Figure S46: ¹³C-NMR (125 MHz, DMSO) Spectrum of 15	34
Figure S47: ESI(+)-MS Spectrum of 15	35
Figure S48: ESI(-)-MS Spectrum of 15	36
Figure S49: HPLC chromatogram of 15	36
Figure S50: FTIR Spectrum of 16	37
Figure S51: ¹H-NMR (500 MHz, DMSO) Spectrum of 16	37
Figure S52: ¹³C-NMR (125 MHz, DMSO) Spectrum of 16	38
Figure S53: ESI(+)-MS Spectrum of 16	39
Figure S54: ESI(-)-MS Spectrum of 16	40
Figure S55: HPLC chromatogram of 16	40
Figure S56: FTIR Spectrum of 17	41
Figure S57: ¹H-NMR (500 MHz, DMSO) Spectrum of 17	41
Figure S58: ¹³C-NMR (125 MHz, DMSO) Spectrum of 17	42
Figure S59: ESI(+)-MS Spectrum of 17	43
Figure S60: ESI(-)-MS Spectrum of 17	44
Figure S61: HPLC chromatogram of 17	44
Figure S62: FTIR Spectrum of 19	45
Figure S63: ¹H-NMR (500 MHz, DMSO) Spectrum of 18	45

Figure S64: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 18	46
Figure S65: ESI(+)-MS Spectrum of 18	47
Figure S66: ESI(-)-MS Spectrum of 18	48
Figure S67: HPLC chromatogram of 18	48
Figure S68: FTIR Spectrum of 19	49
Figure S69: ^1H -NMR (500 MHz, DMSO) Spectrum of 19	49
Figure S70: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 19	50
Figure S71: ESI(+)-MS Spectrum of 19	51
Figure S72: ESI(-)-MS Spectrum of 19	52
Figure S73: HPLC chromatogram of 19	52
Figure S74: FTIR Spectrum of 20	53
Figure S75: ^1H -NMR (500 MHz, DMSO) Spectrum of 20	53
Figure S76: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 20	54
Figure S77: ESI(+)-MS Spectrum of 20	55
Figure S78: ESI(-)-MS Spectrum of 20	56
Figure S79: HPLC chromatogram of 20	56
Figure S80: FTIR Spectrum of 21	57
Figure S81: ^1H -NMR (500 MHz, DMSO) Spectrum of 21	57
Figure S82: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 21	58
Figure S83: ESI(+)-MS Spectrum of 21	59
Figure S84: ESI(-)-MS Spectrum of 21	60
Figure S85: HPLC chromatogram of 21	60
Figure S86: FTIR Spectrum of 22	61
Figure S87: ^1H -NMR (500 MHz, DMSO) Spectrum of 22	62
Figure S88: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 22	63
Figure S89: ESI(+)-MS Spectrum of 22	63
Figure S90: ESI(-)-MS Spectrum of 22	64
Figure S91: HPLC chromatogram of 22	64
Figure S92: FTIR Spectrum of 23	65
Figure S93: ^1H -NMR (500 MHz, DMSO) Spectrum of 23	66
Figure S94: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 23	67
Figure S95: ESI(+)-MS Spectrum of 23	67
Figure S96: ESI(-)-MS Spectrum of 23	68
Figure S97: HPLC chromatogram of 23	68
Figure S98: FTIR Spectrum of 24	69
Figure S99: ^1H -NMR (500 MHz, DMSO) Spectrum of 24	69
Figure S100: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 24	70
Figure S101: ESI(+)-MS Spectrum of 24	71
Figure S102: ESI(-)-MS Spectrum of 24	72
Figure S103: HPLC chromatogram of 24	72
Figure S104: FTIR Spectrum of 25	73
Figure S105: ^1H -NMR (500 MHz, DMSO) Spectrum of 25	73
Figure S106: ^{13}C -NMR (125 MHz, DMSO) Spectrum of 25	74
Figure S107: ESI(+)-MS Spectrum of 25	75
Figure S108: ESI(-)-MS Spectrum of 25	76
Figure S109: HPLC chromatogram of 25	76

Figure S110: FTIR Spectrum of 26	77
Figure S111: ¹ H-NMR (500 MHz, DMSO) Spectrum of 26	77
Figure S112: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 26	78
Figure S113: ESI(+)-MS Spectrum of 26	79
Figure S114: ESI(-)-MS Spectrum of 26	80
Figure S115: HPLC chromatogram of 26	80
Table S1. ADMET profiles of compounds 9-26 .	81

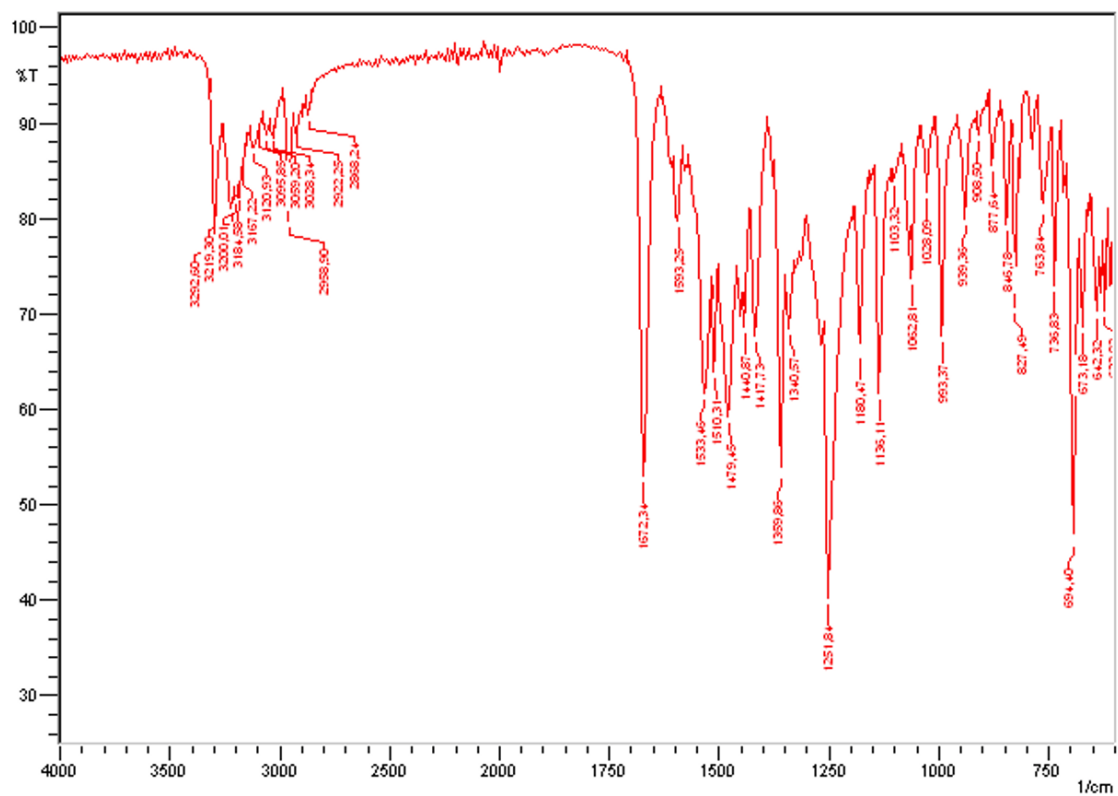


Figure S1: FTIR Spectrum of 5

ID8-TSC_1H

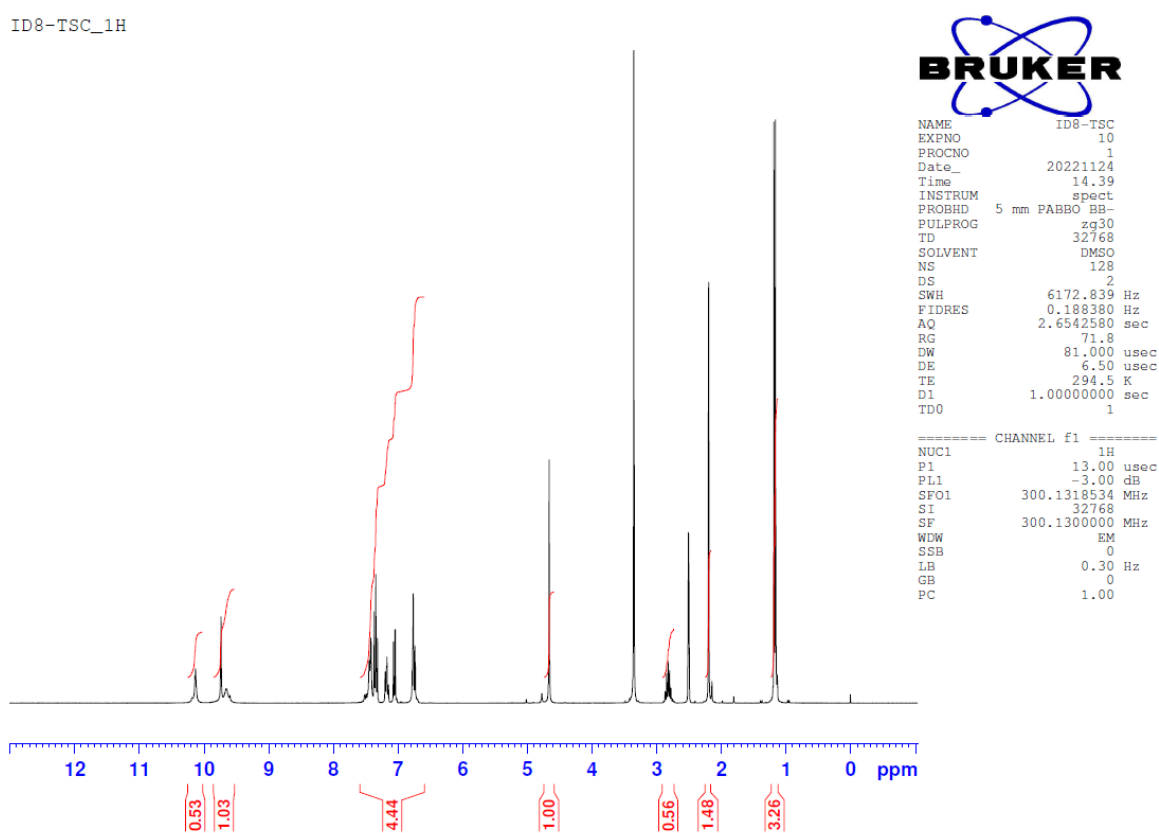


Figure S2: ¹H-NMR (300 MHz, DMSO) Spectrum of 5

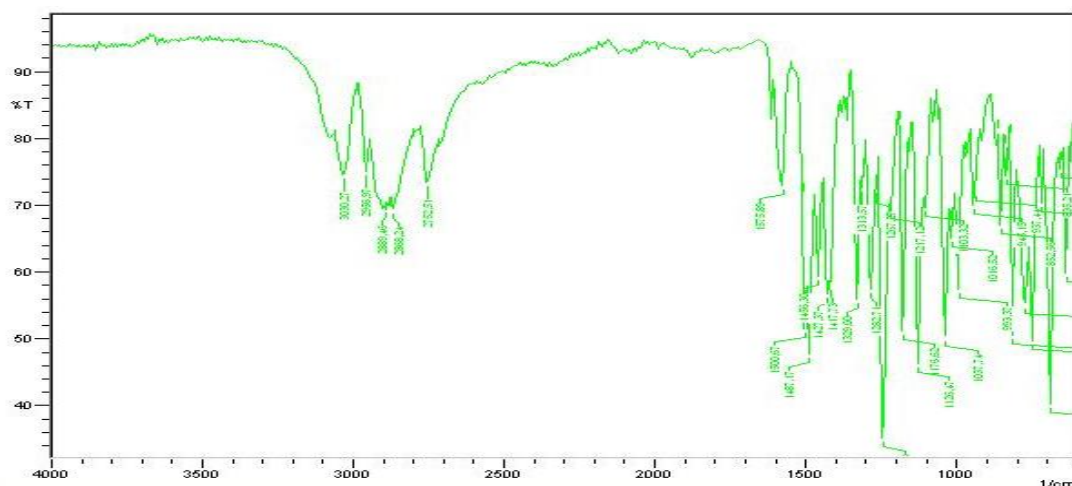


Figure S3: FTIR Spectrum of 8

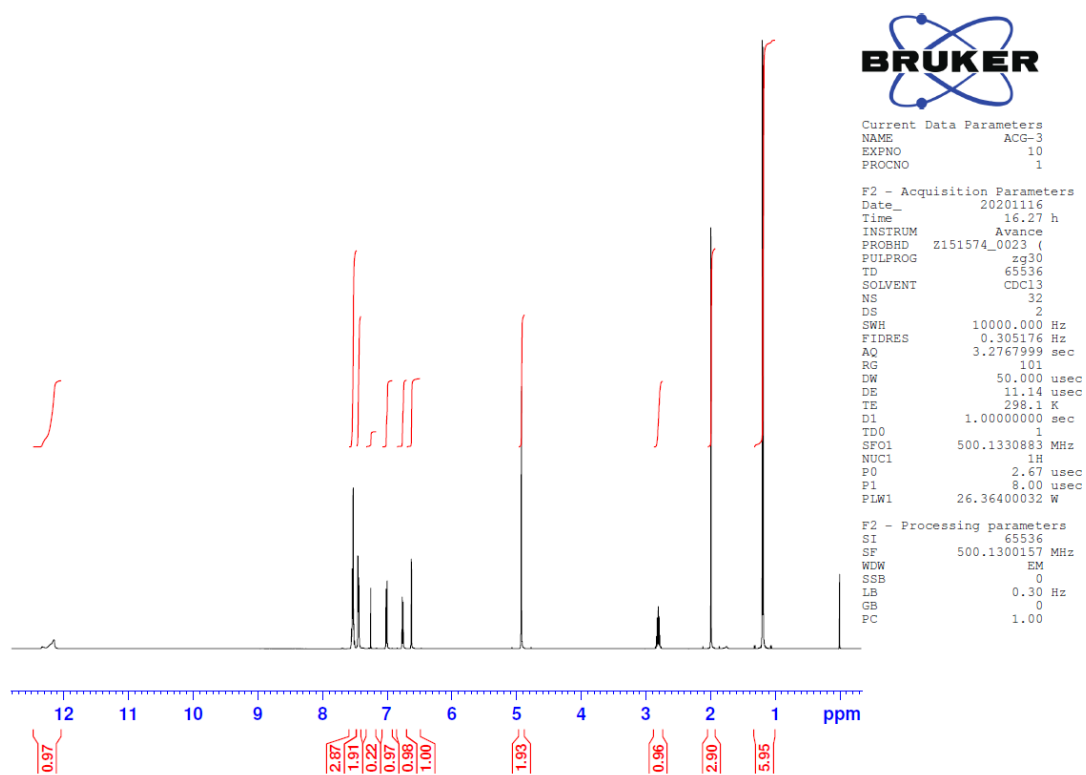


Figure S4: ¹H-NMR (500 MHz, DMSO) Spectrum of 8



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EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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Time 2.26 h
INSTRUM Avance
PROBHD z151574_0023 (zpg30)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SF01 125.7703643 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 85.85099792 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 26.36400032 W
PLW12 0.26363999 W
PLW13 0.13260999 W

F2 - Processing parameters
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SF 125.7577916 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

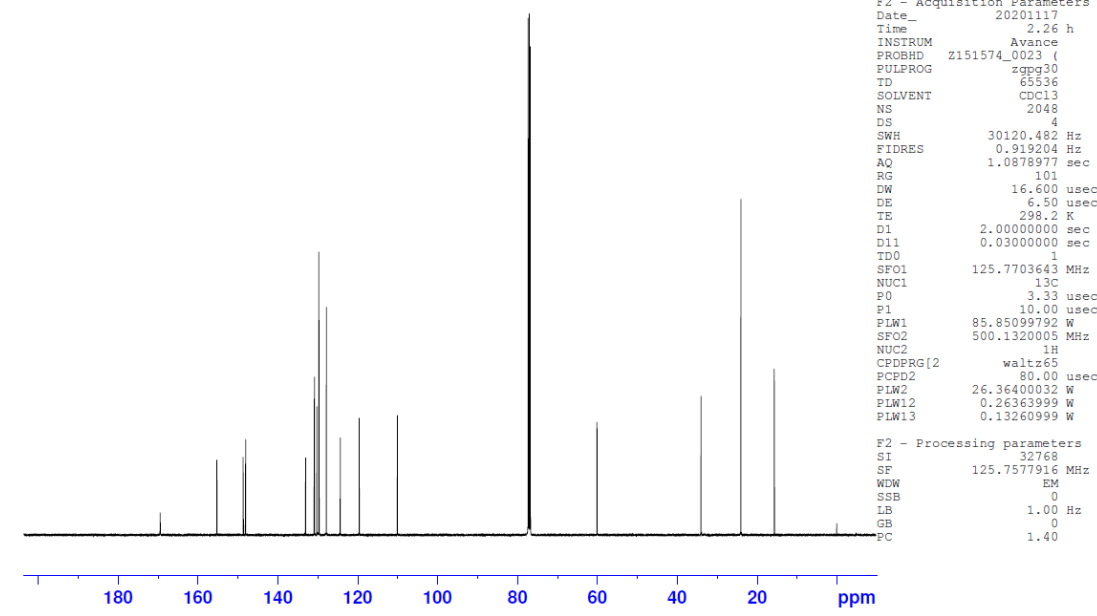


Figure S5: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **8**

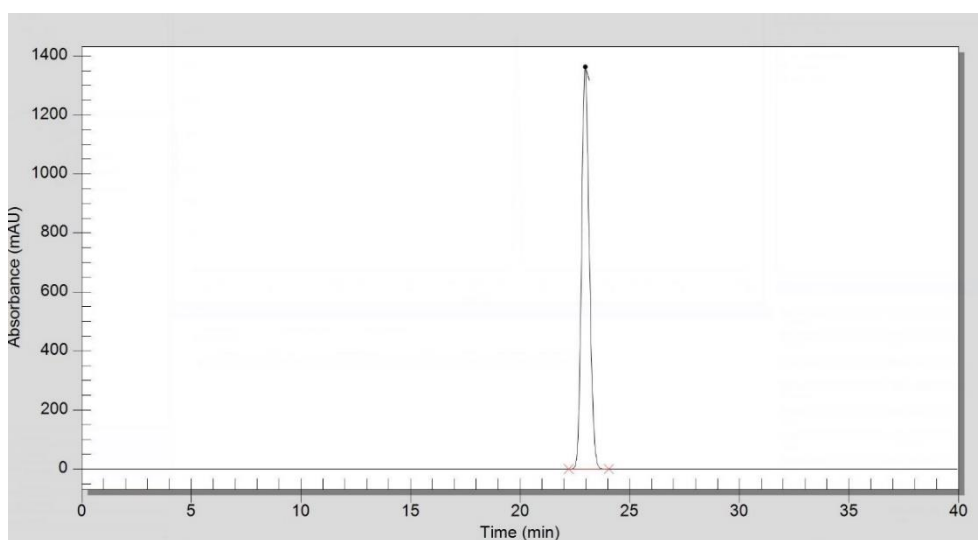


Figure S6: HPLC chromatogram of **8**

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MassPeaks:5 BasePeak:338.15(20000000)
Spectrum Mode:Single 0.186(12)
BG Mode:None Polarity:Negative Segment 1 - Event 2

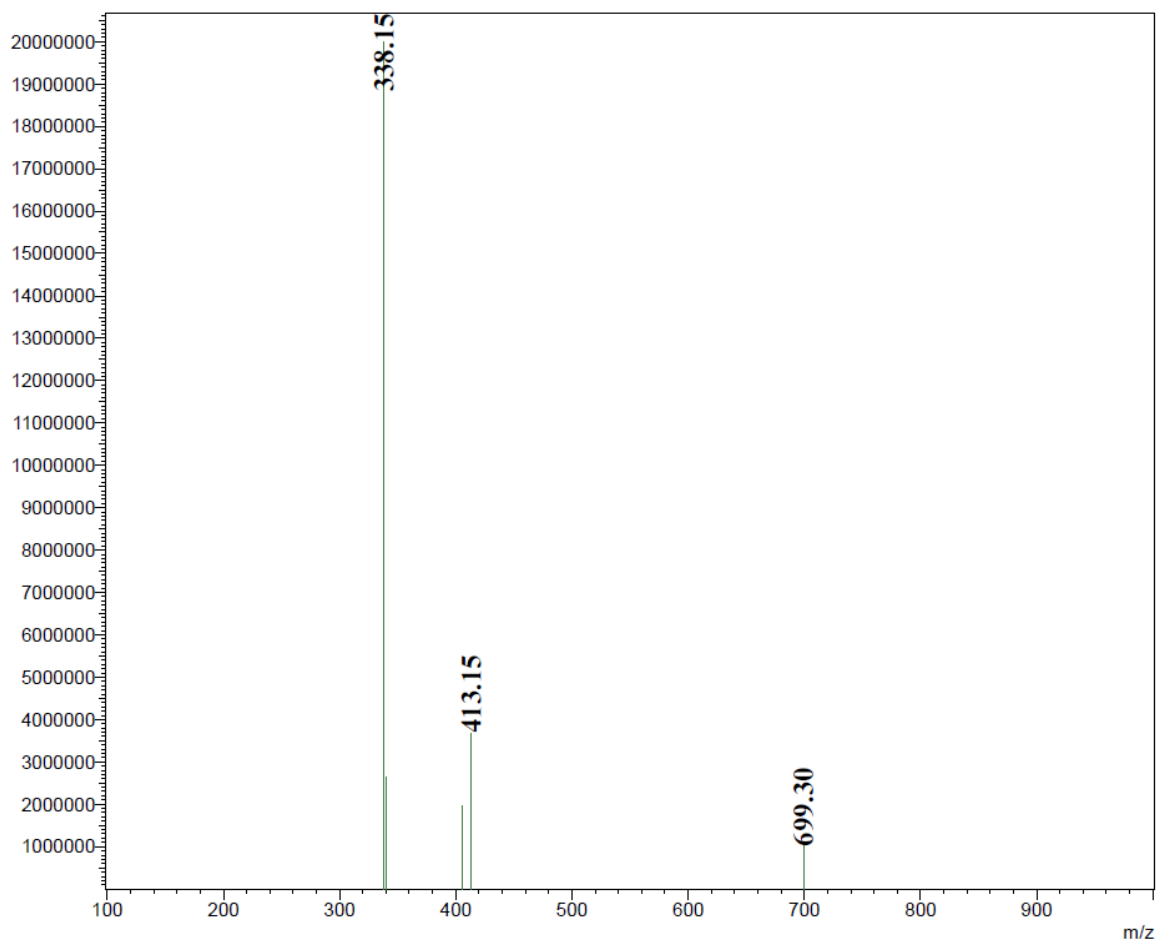


Figure S7: ESI(-)-MS Spectrum of 8

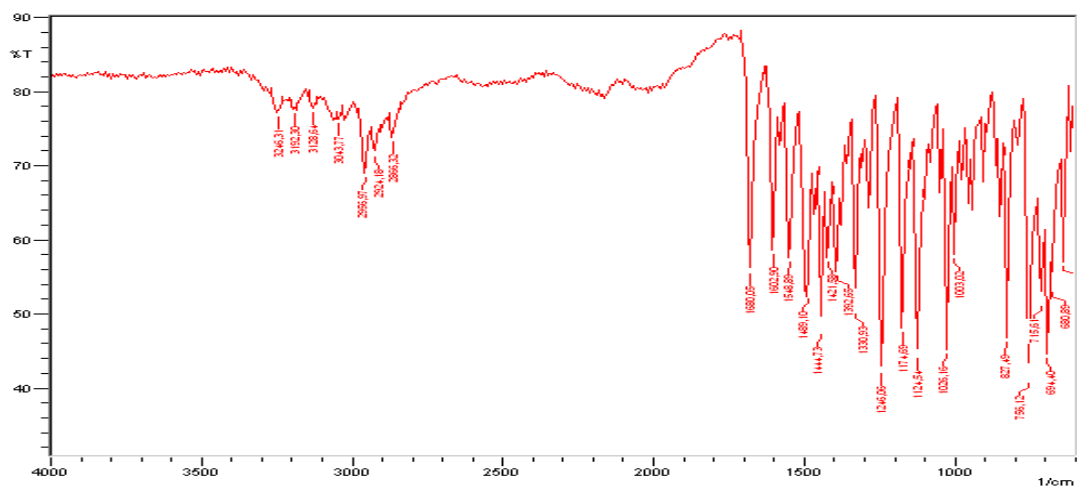


Figure S8: FTIR Spectrum of **9**

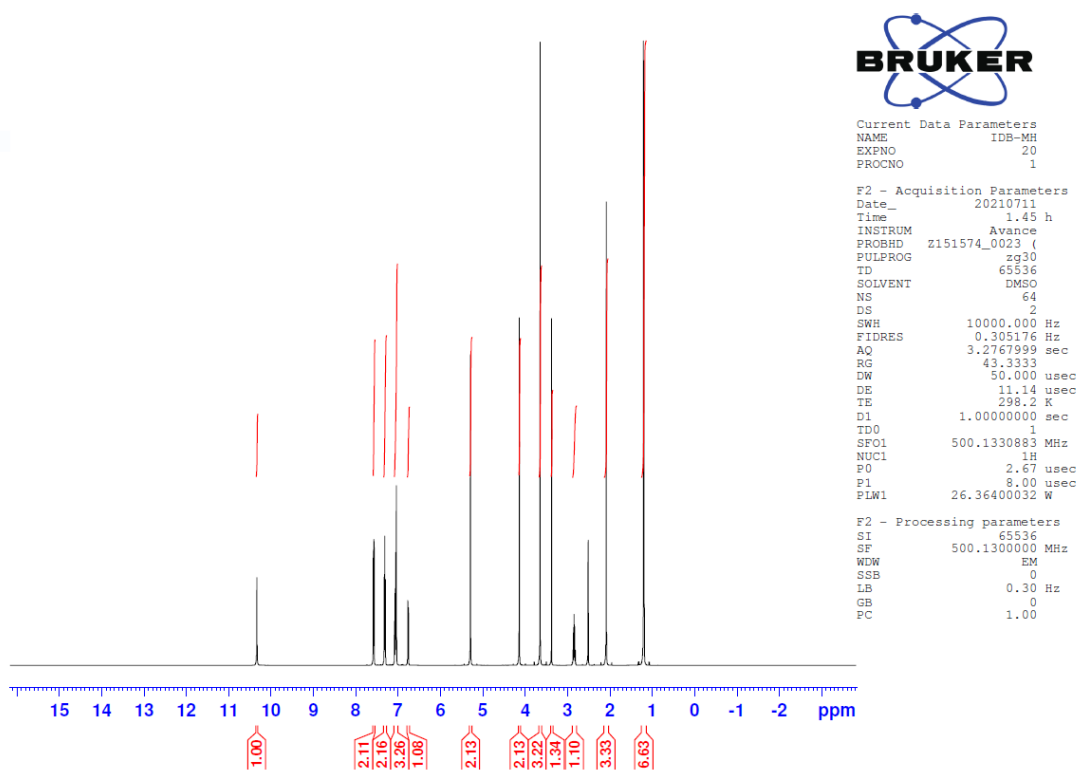


Figure S9: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of **9**

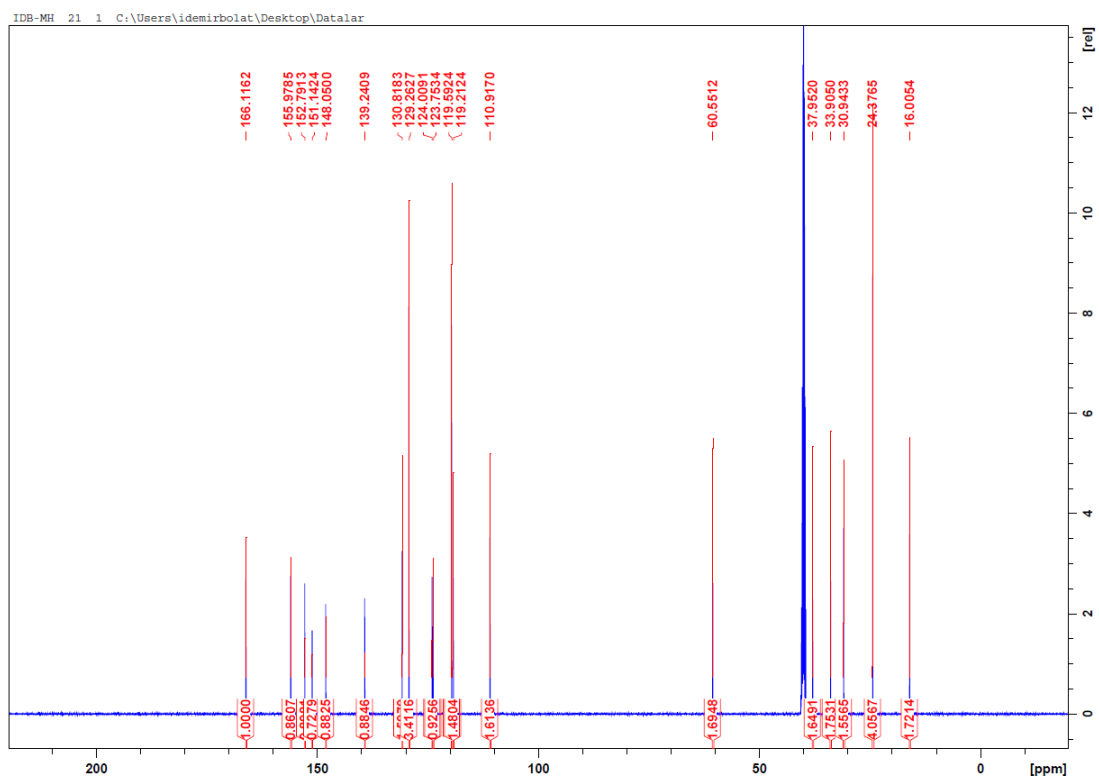


Figure S10: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **9**

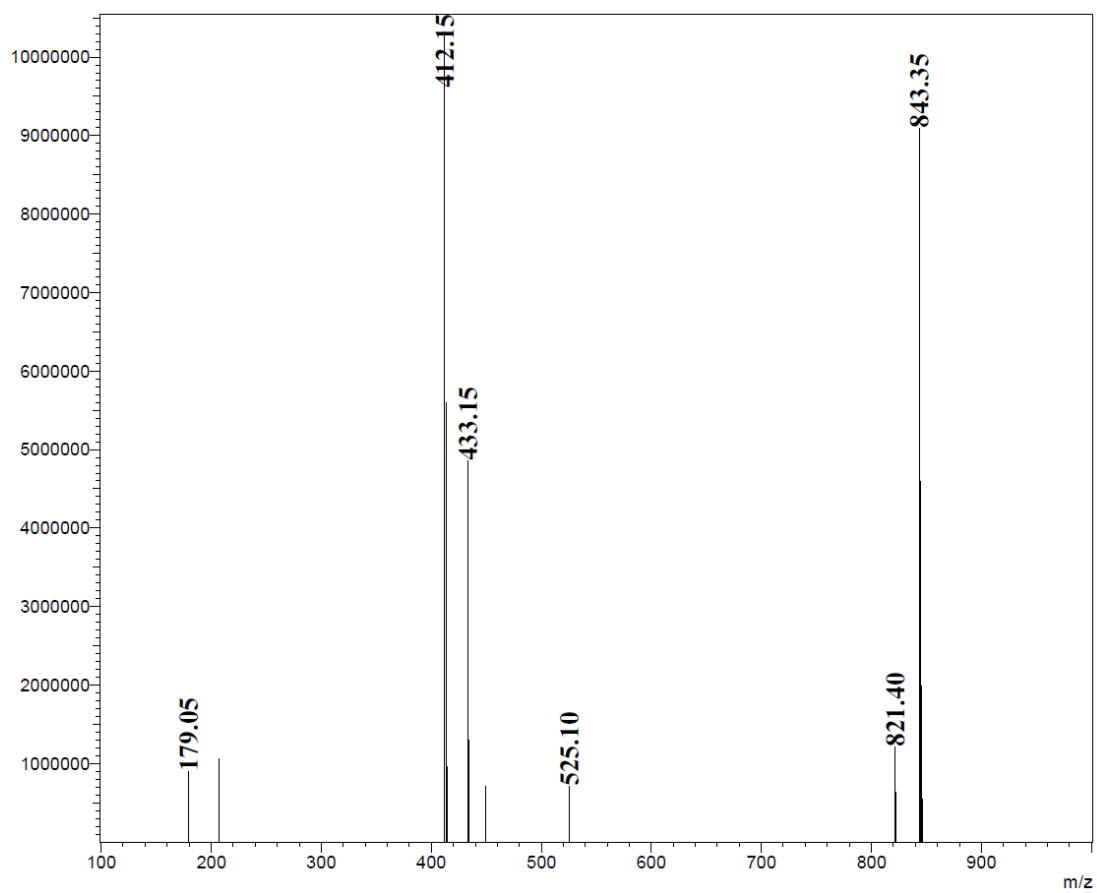


Figure S11: ESI(+)-MS Spectrum of 9

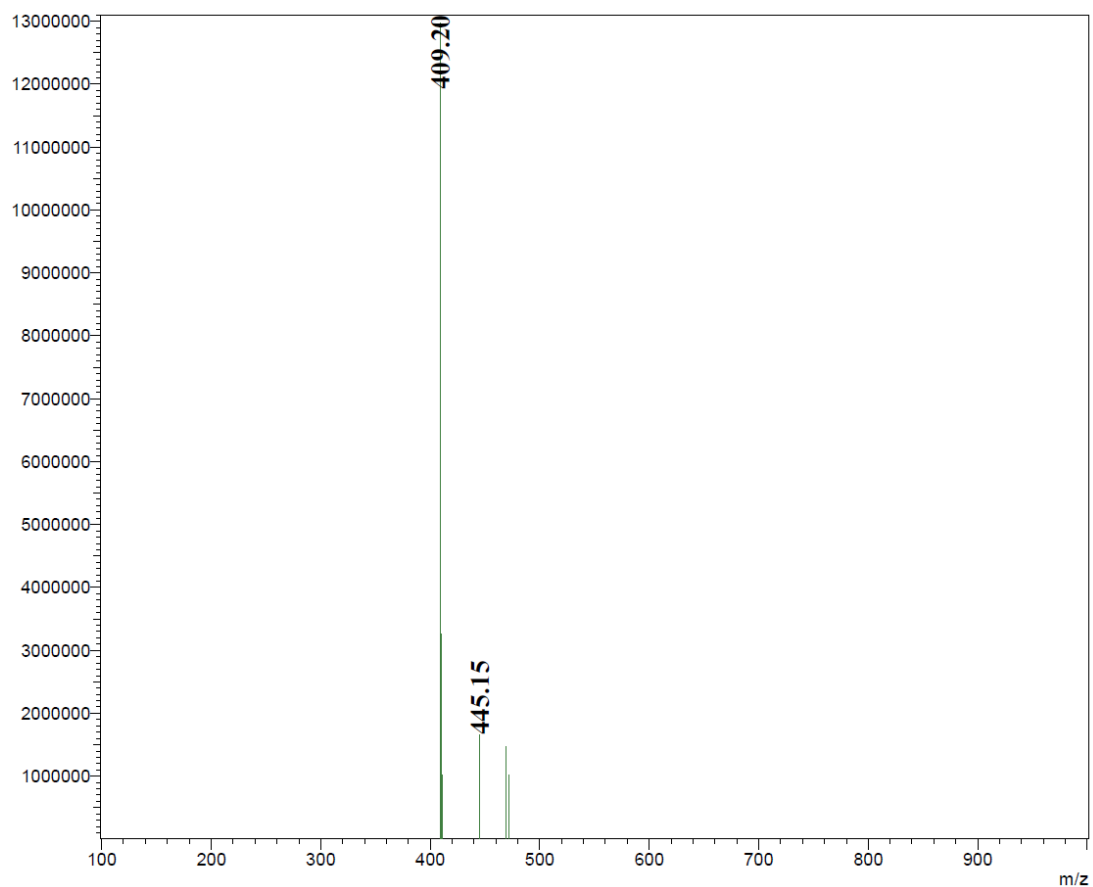


Figure S12: ESI(-)-MS Spectrum of 9

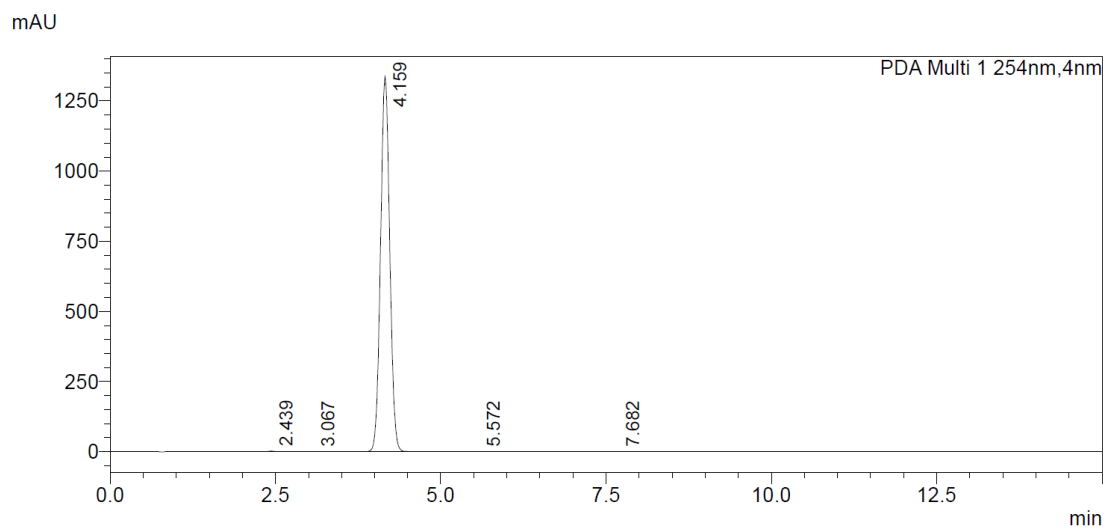


Figure S13: HPLC chromatogram of 9

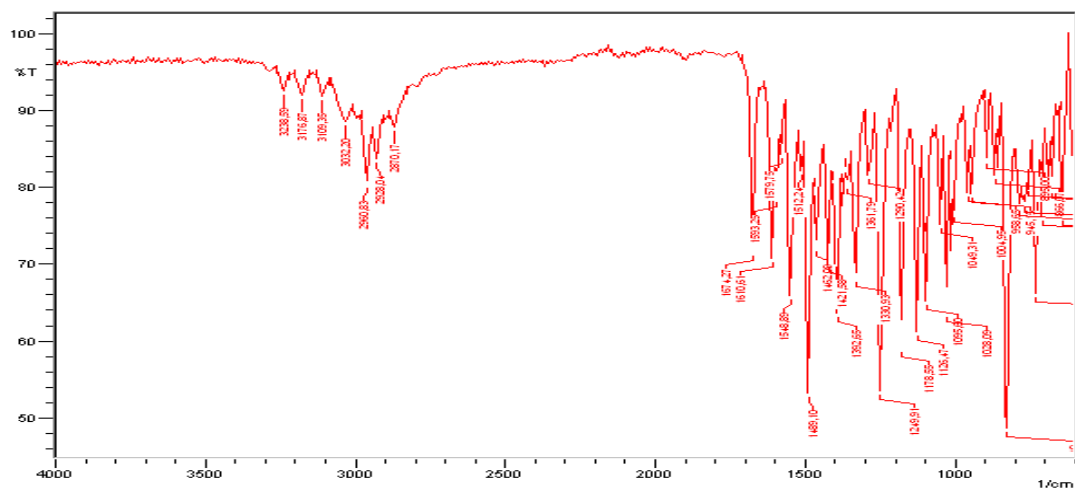


Figure S14: HFTIR spectrum of 10

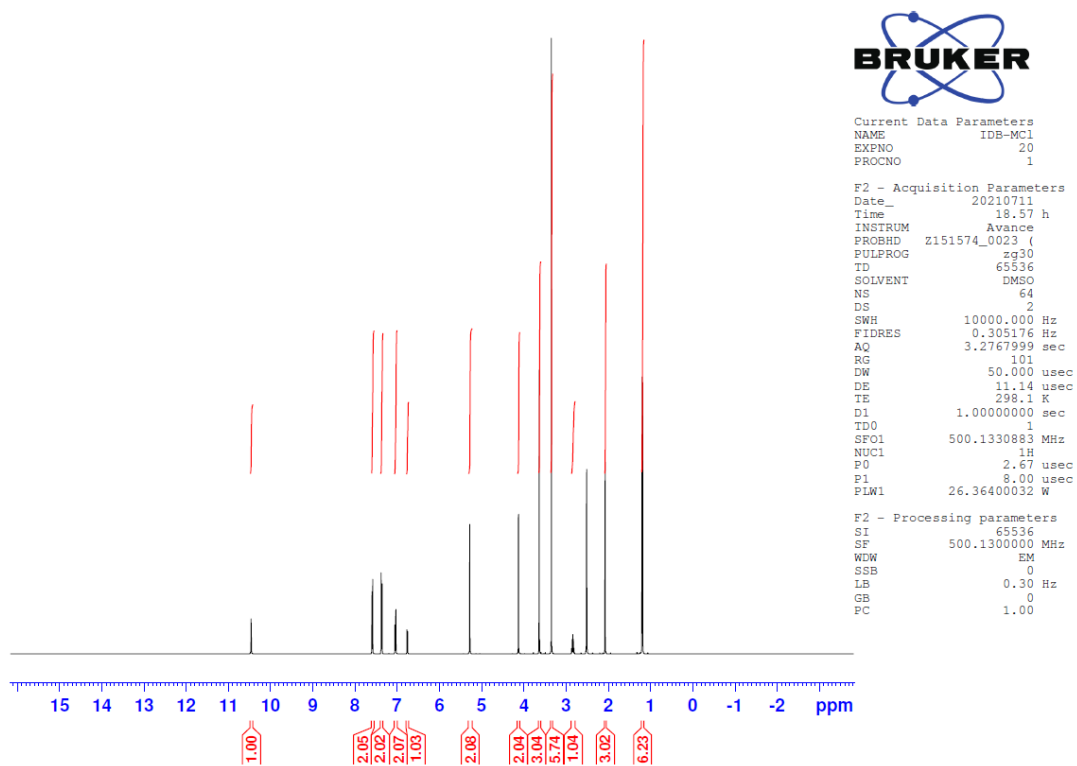


Figure S15: ^1H -NMR (500 MHz, DMSO) Spectrum of 10

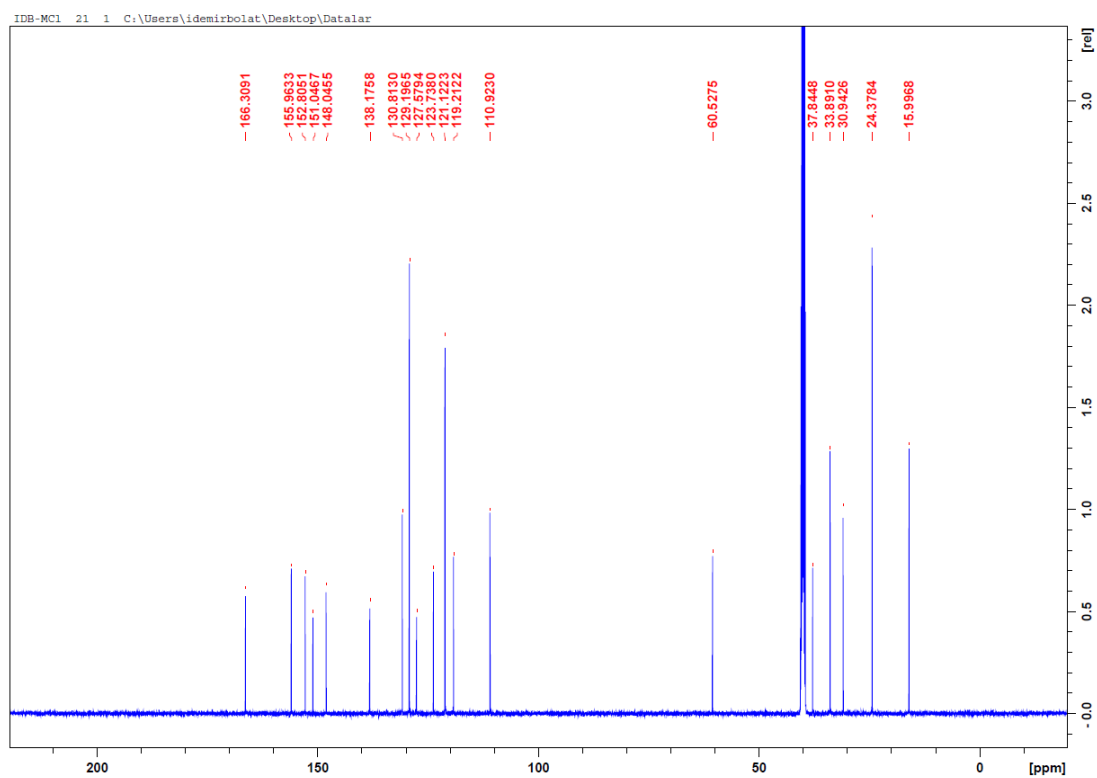


Figure S16: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **10**

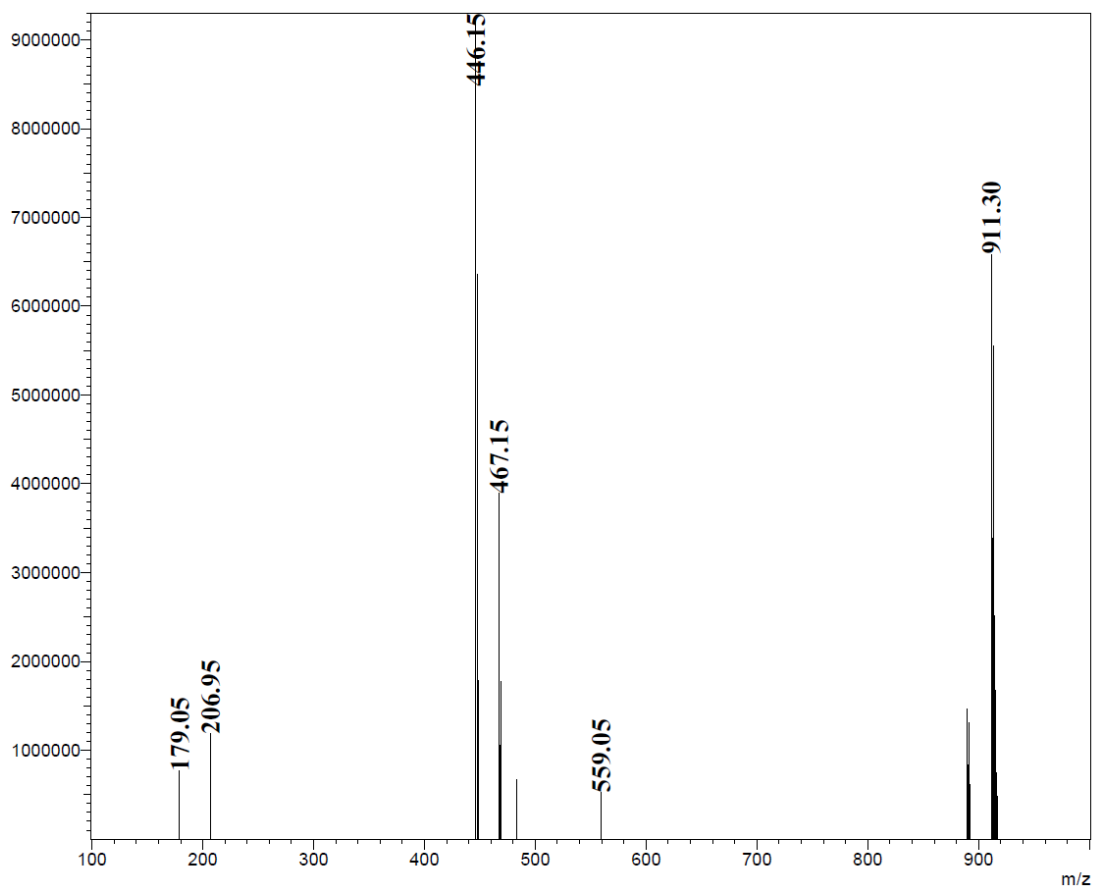


Figure S17: ESI(+)-MS Spectrum of 10

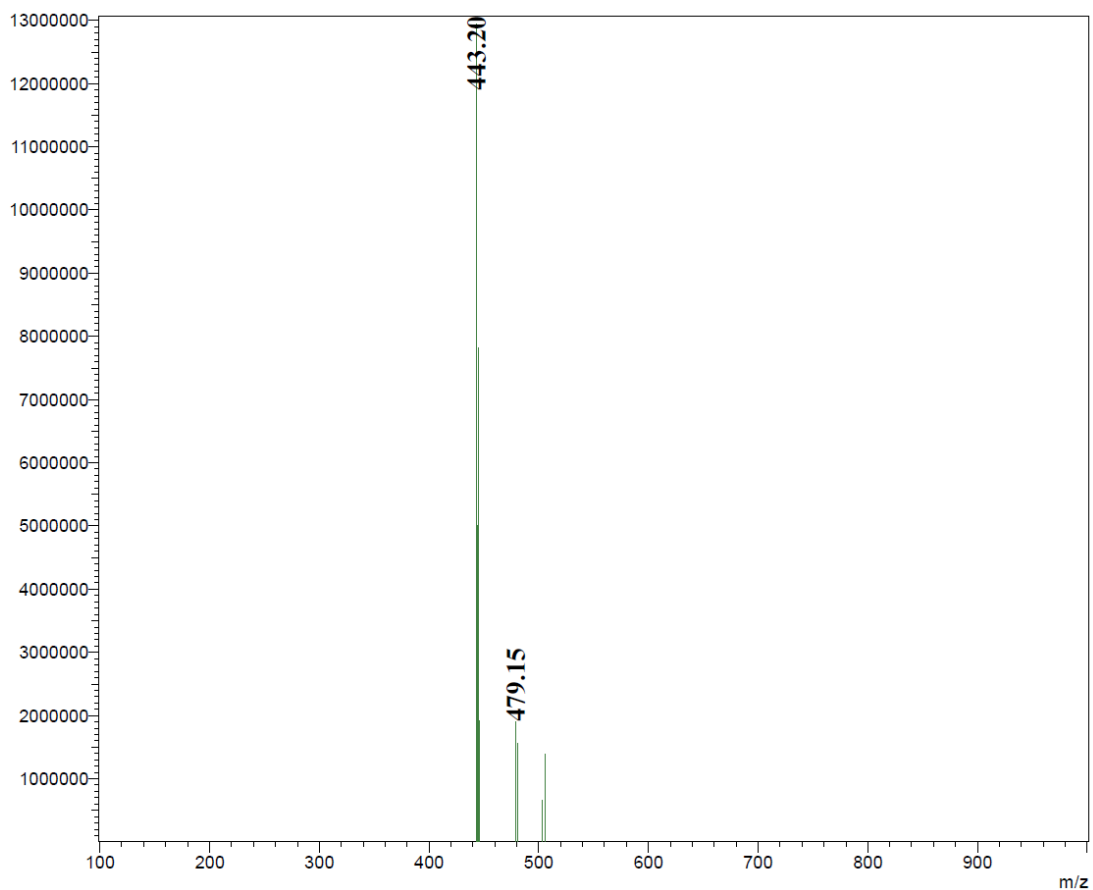


Figure S18: ESI(-)-MS Spectrum of 10

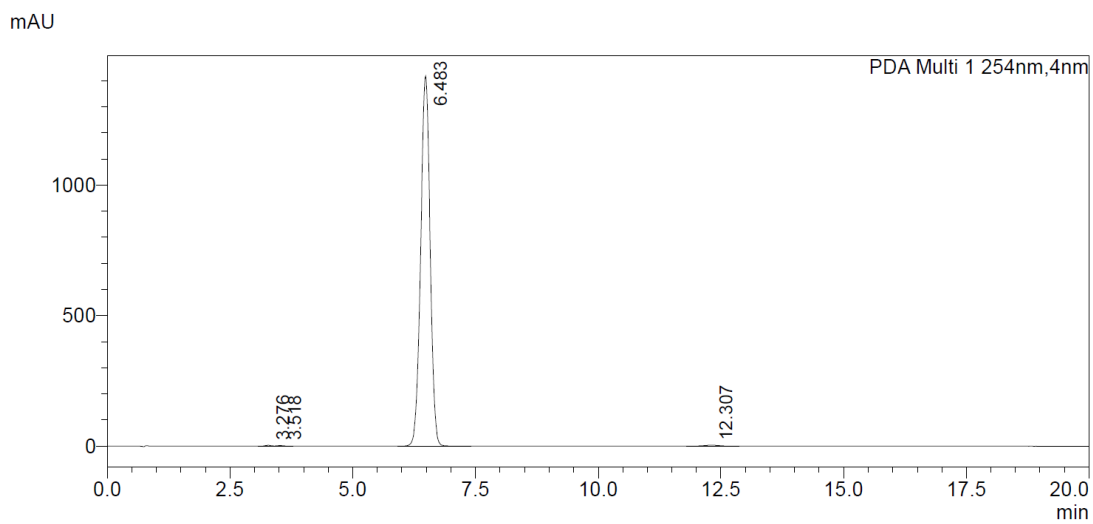


Figure S19: HPLC chromatogram of 10

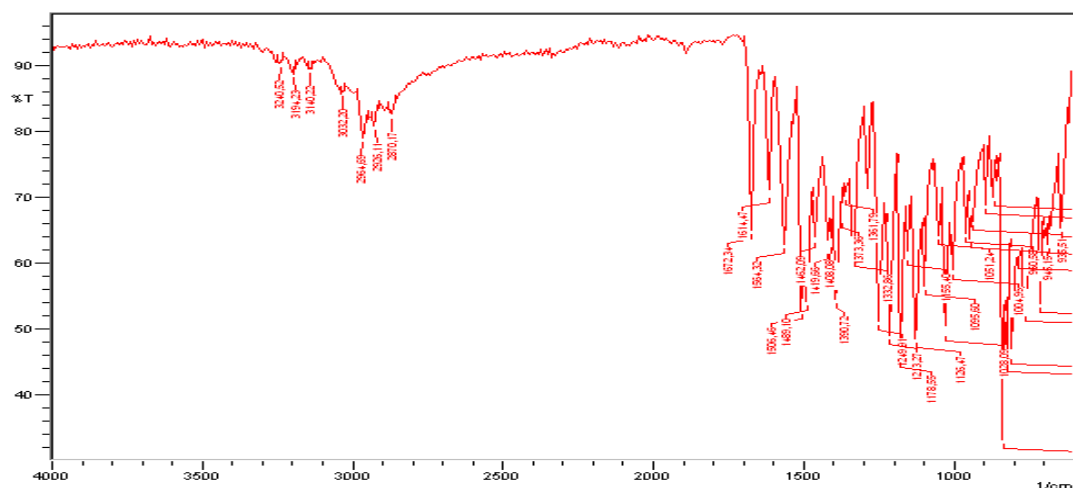


Figure S20: FTIR spectrum of 11

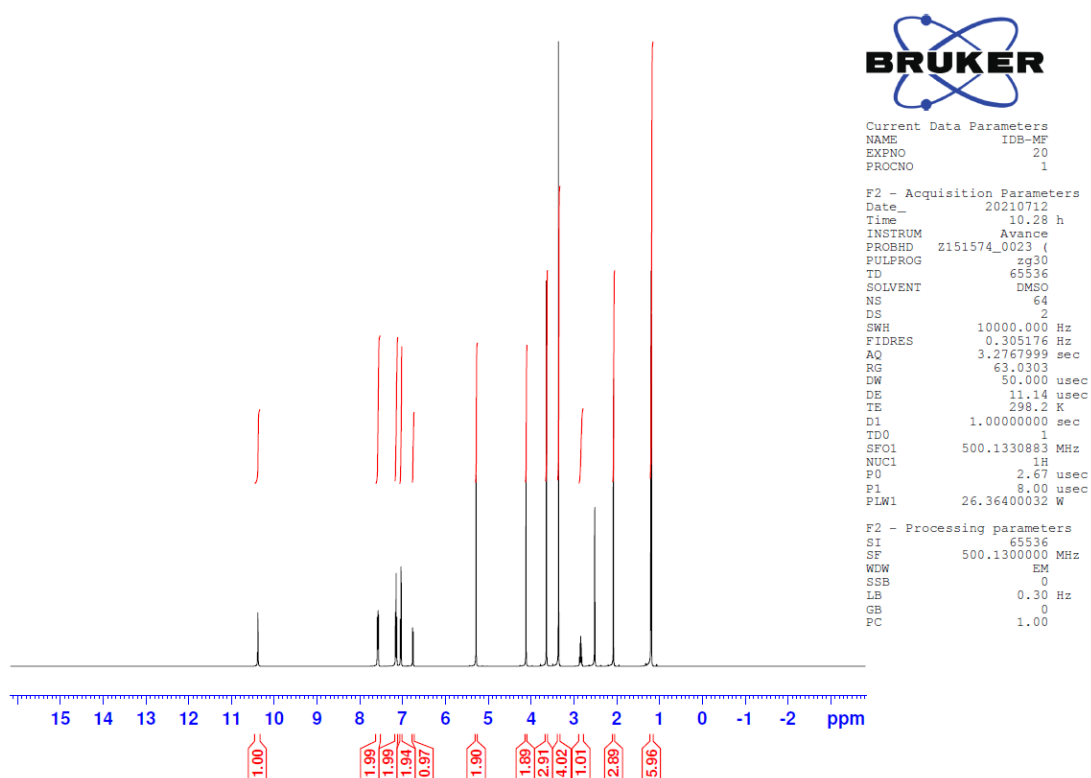


Figure S21: ¹H-NMR (500 MHz, DMSO) Spectrum of 11

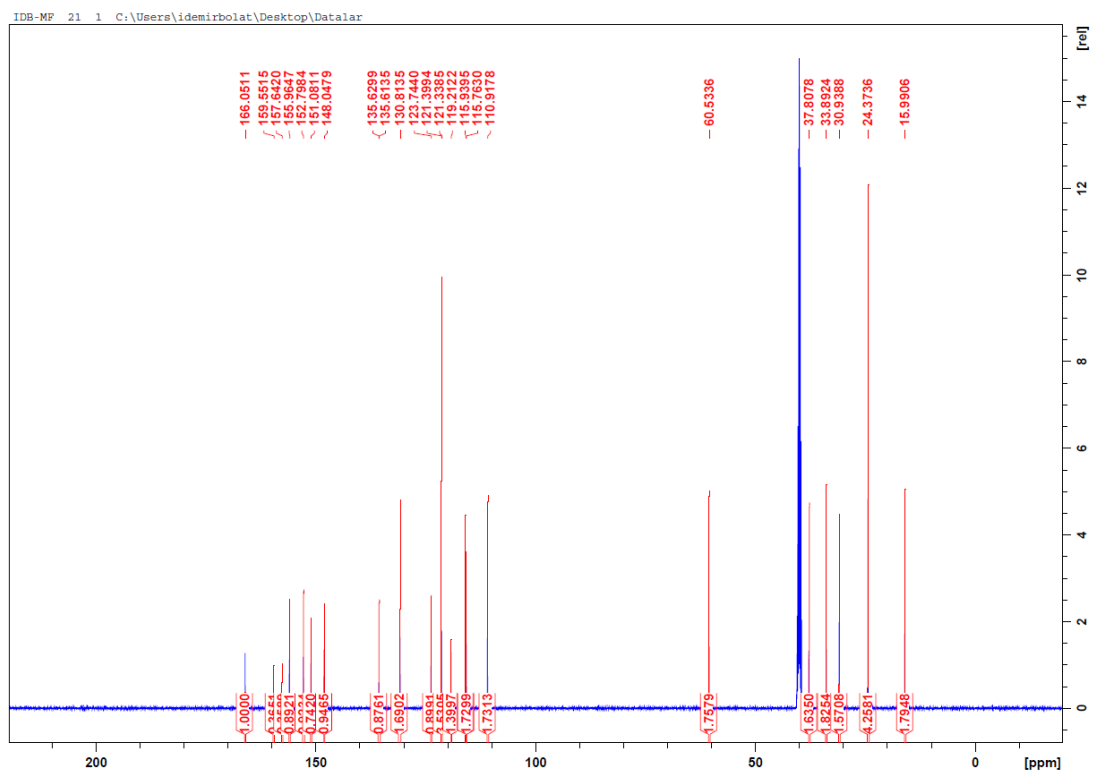


Figure S22: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **11**

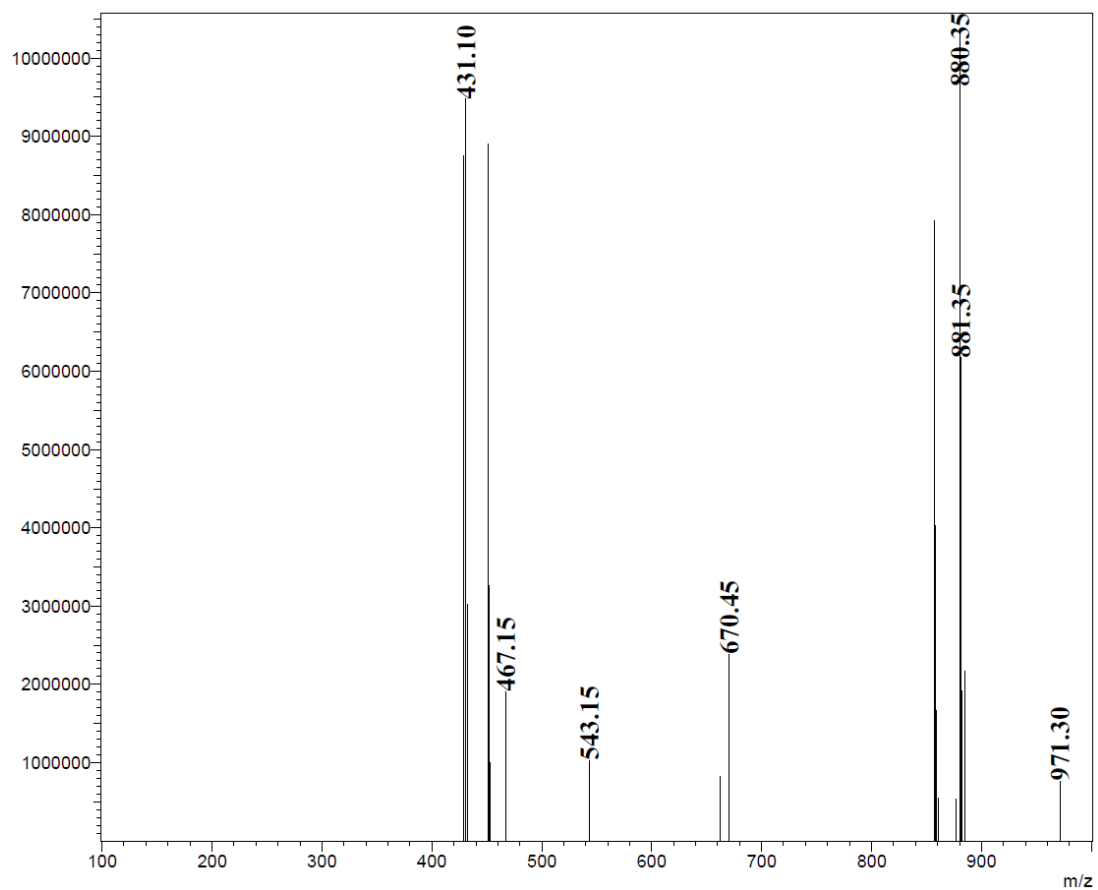


Figure S23: ESI(+)-MS Spectrum of **11**

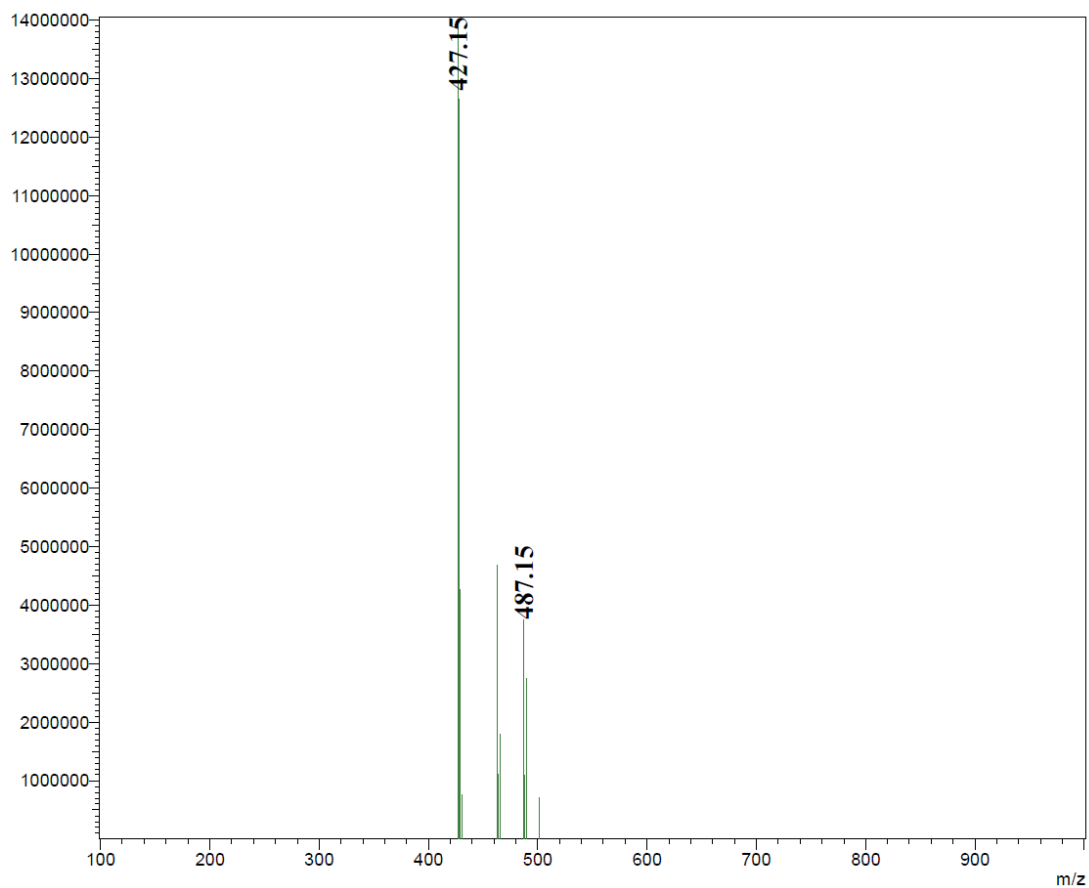


Figure S24: ESI(-)-MS Spectrum of 11

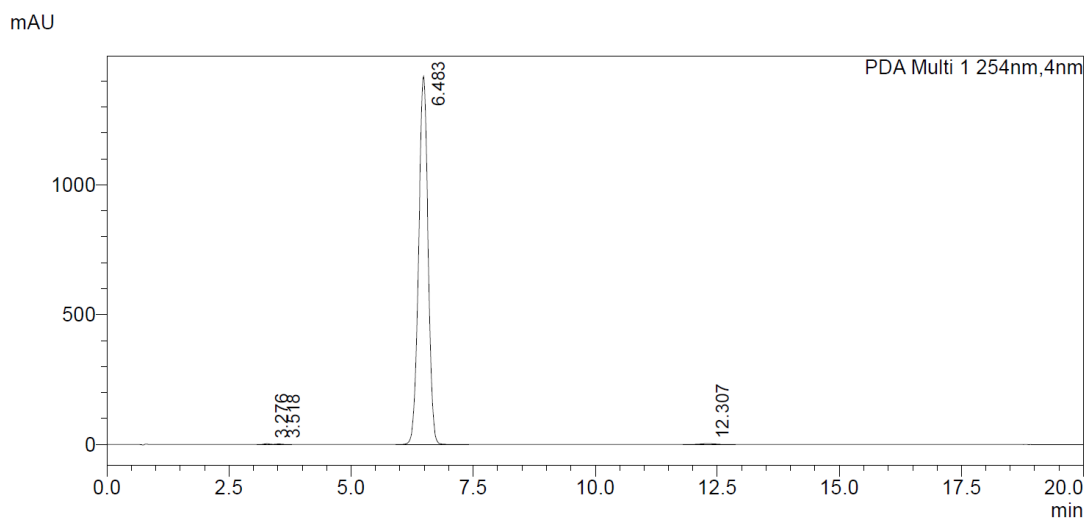


Figure S25: HPLC chromatogram of 11

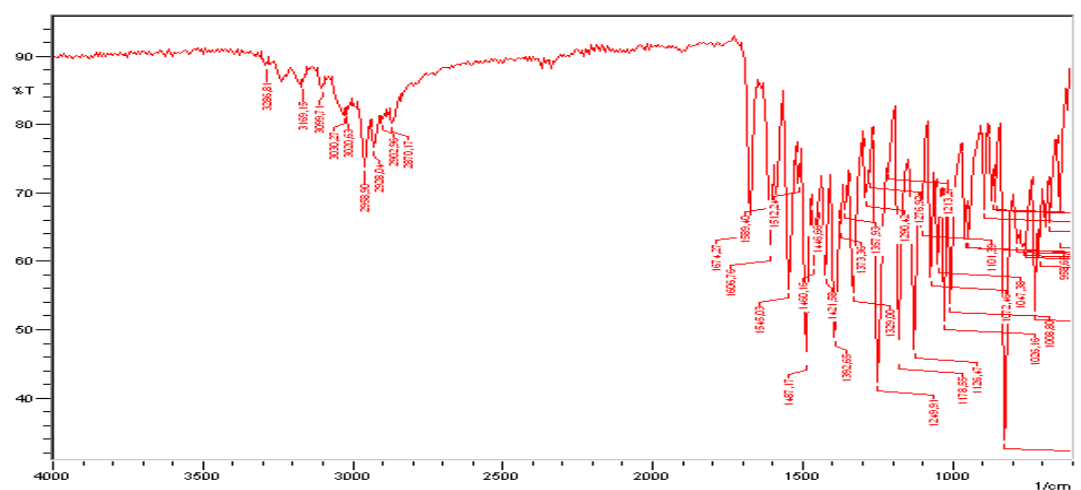


Figure S26: FTIR spectrum of 12

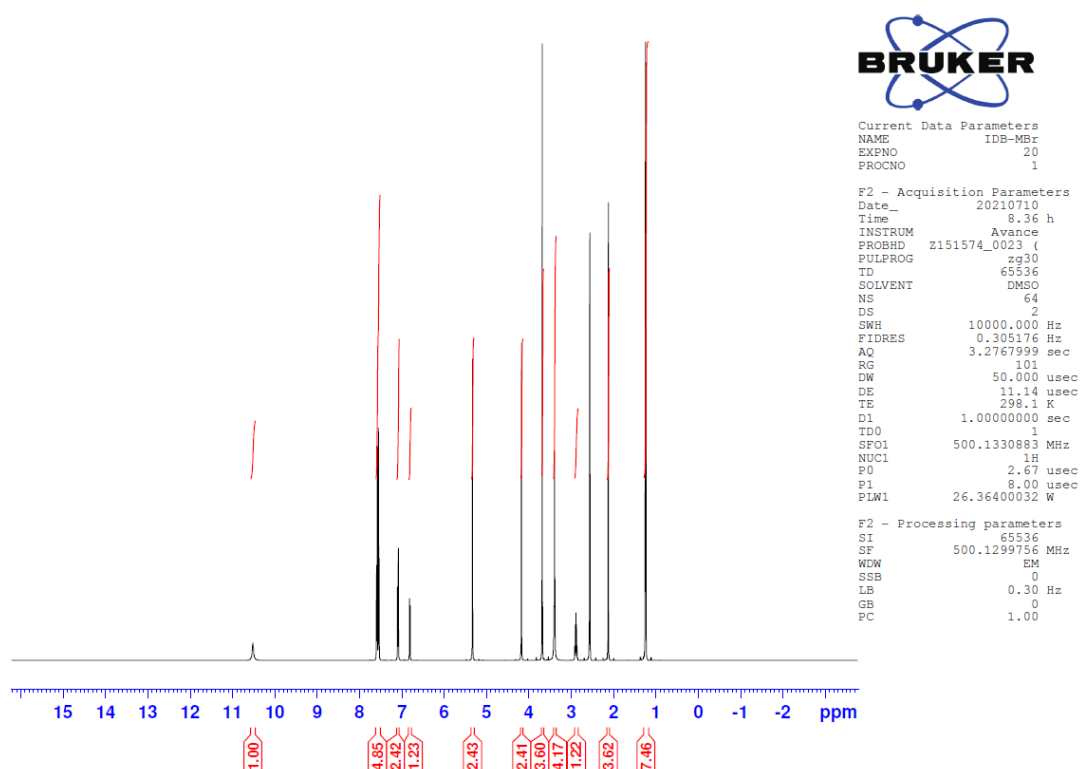


Figure S27: ¹H-NMR (500 MHz, DMSO) Spectrum of 12

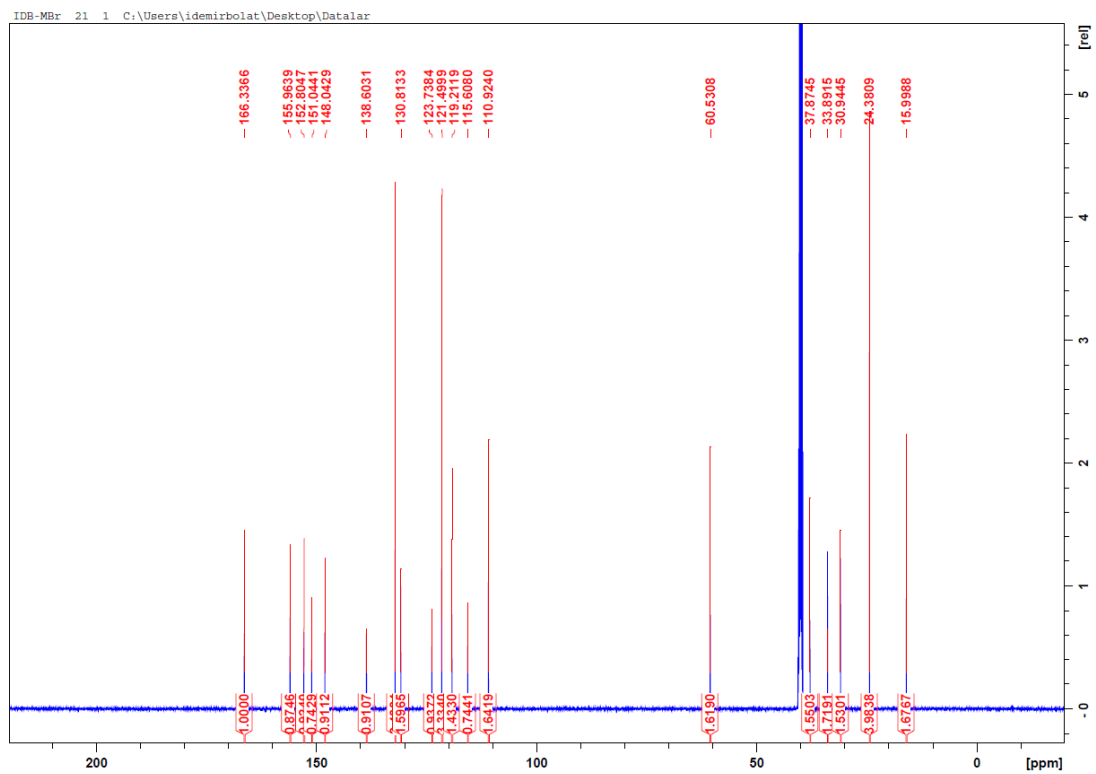


Figure S28: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **12**

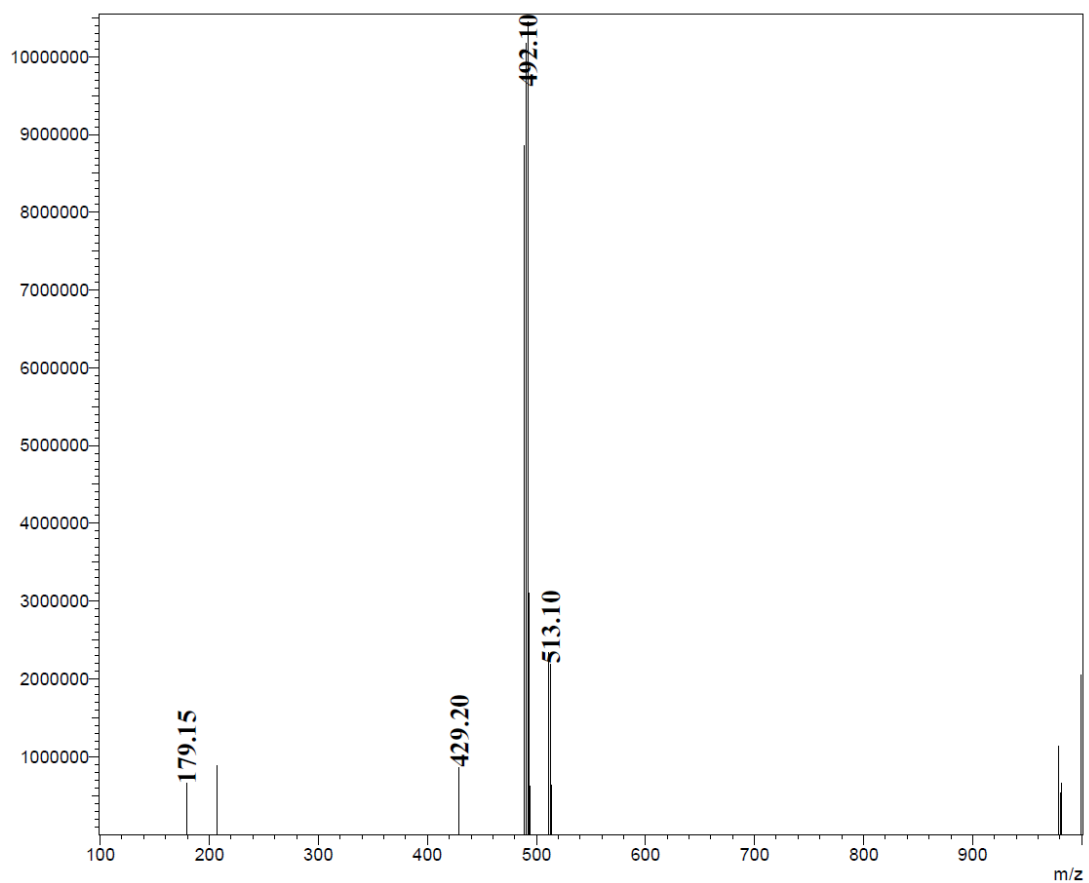


Figure S29: ESI(+)-MS Spectrum of 12

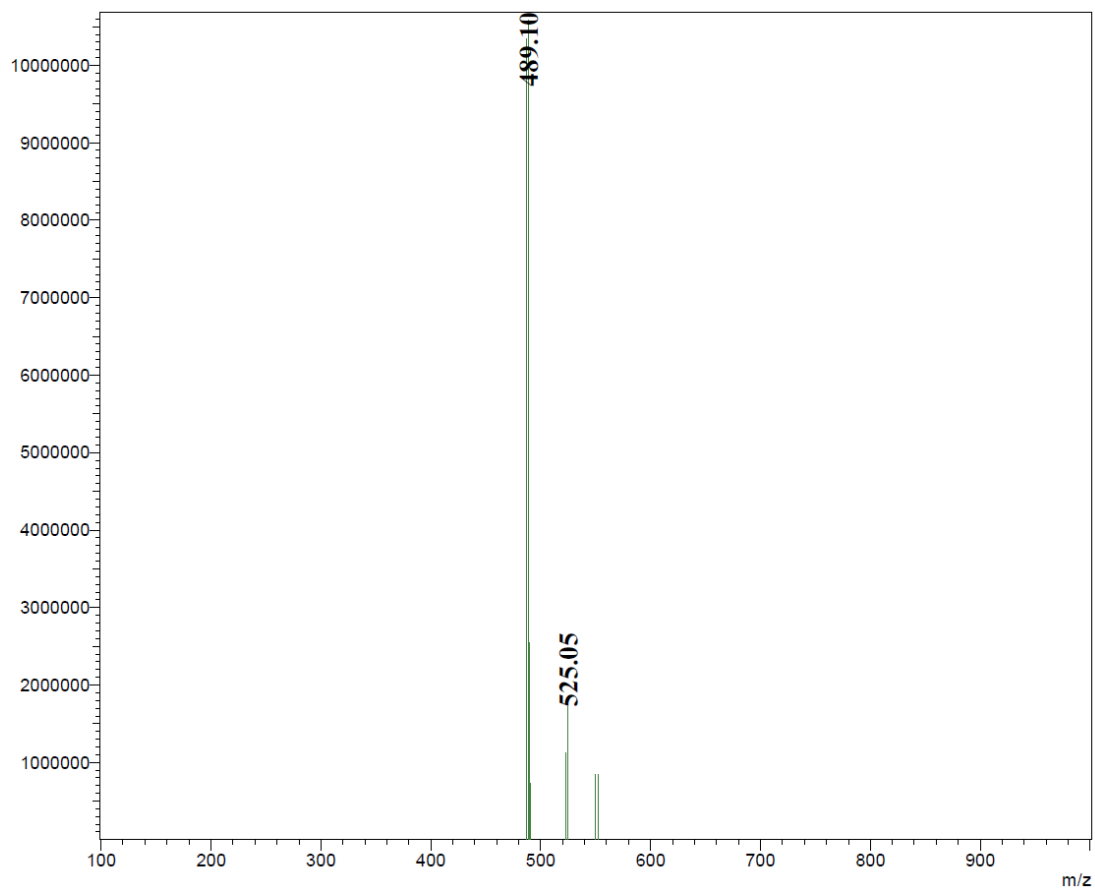


Figure S30: ESI(-)-MS Spectrum of 12

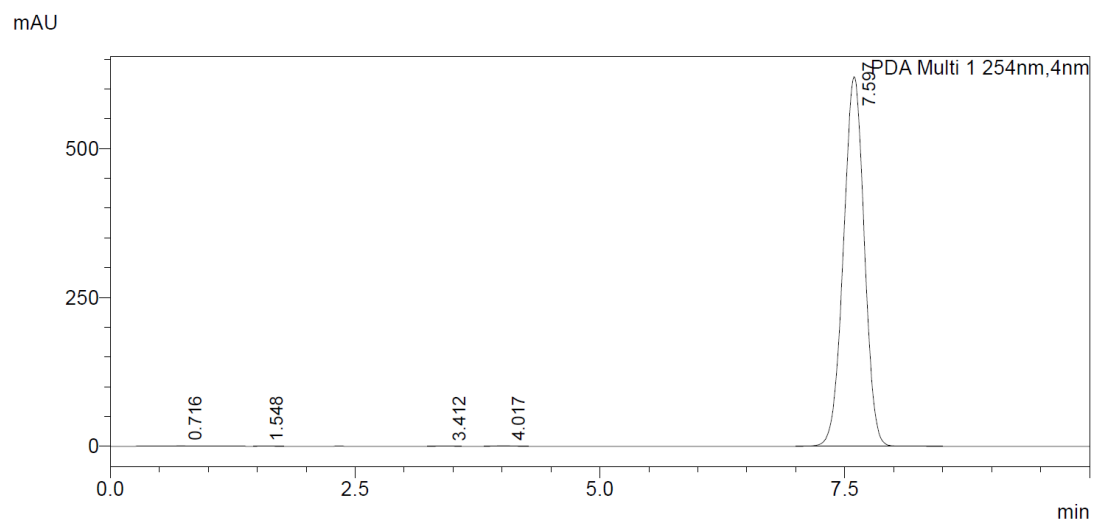


Figure S31: HPLC chromatogram of 12

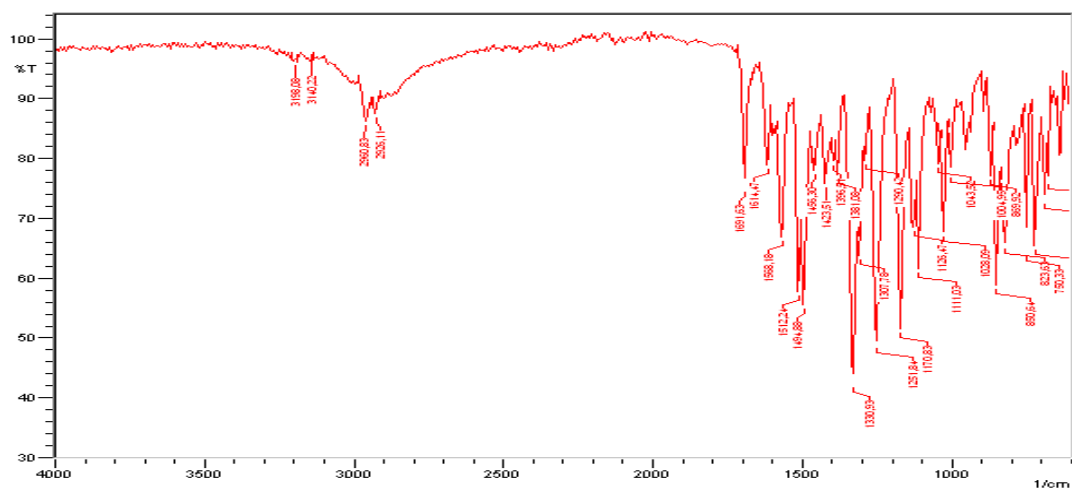


Figure S32: FTIR spectrum of 13

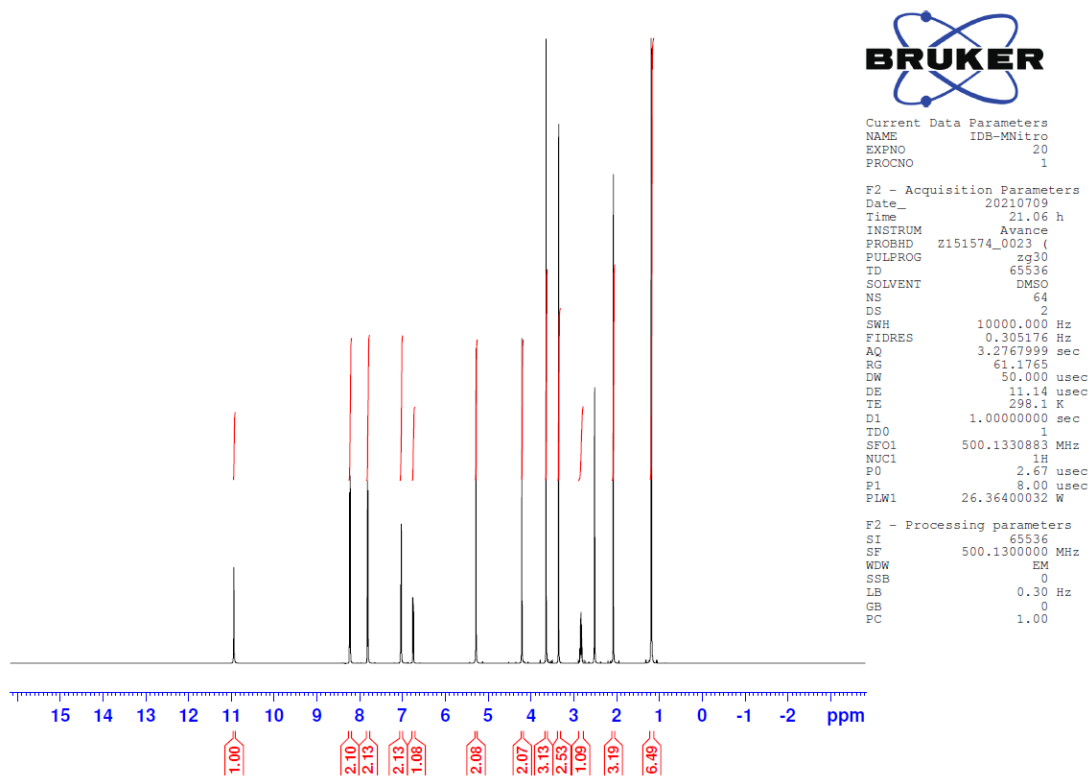


Figure S33: ¹H-NMR (500 MHz, DMSO) Spectrum of 13

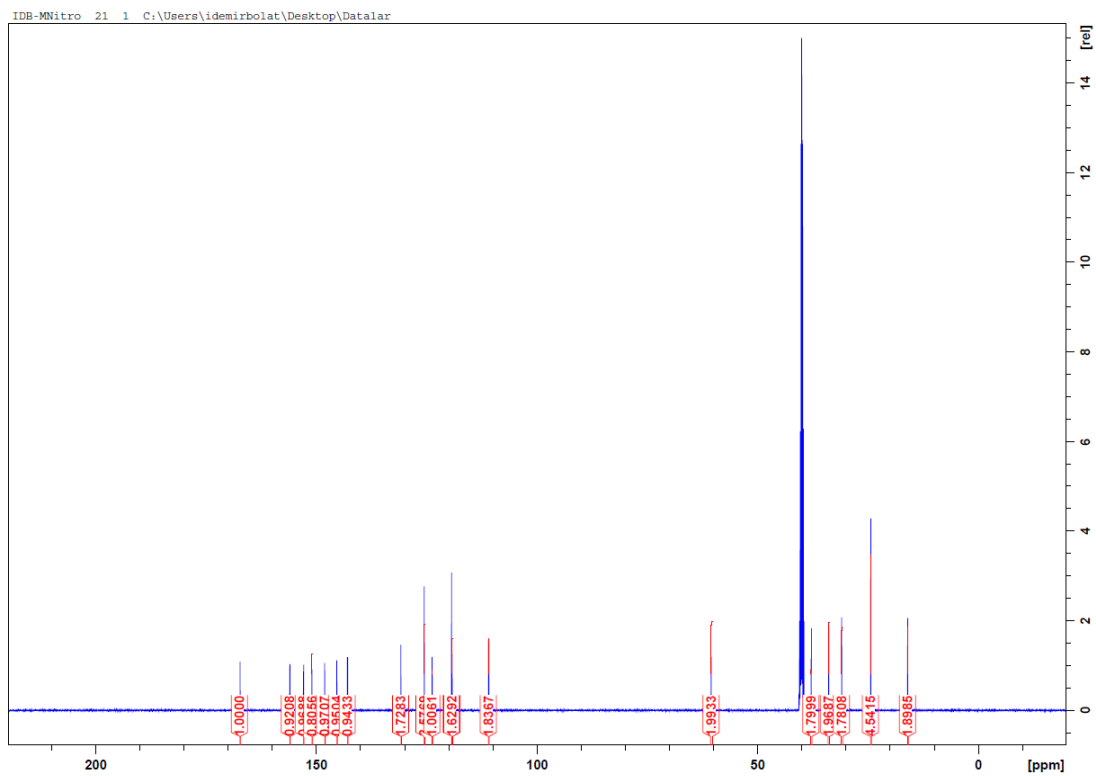


Figure S34: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **13**

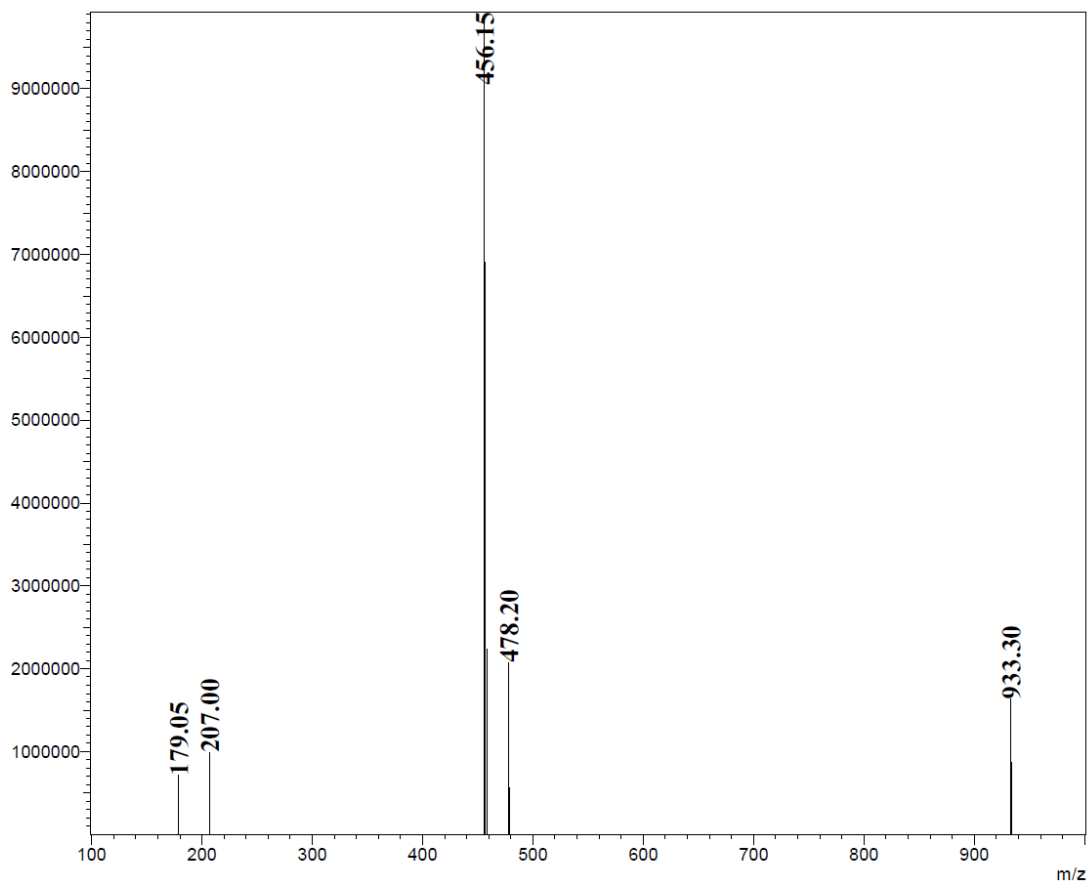


Figure S35: ESI(+)-MS Spectrum of 13

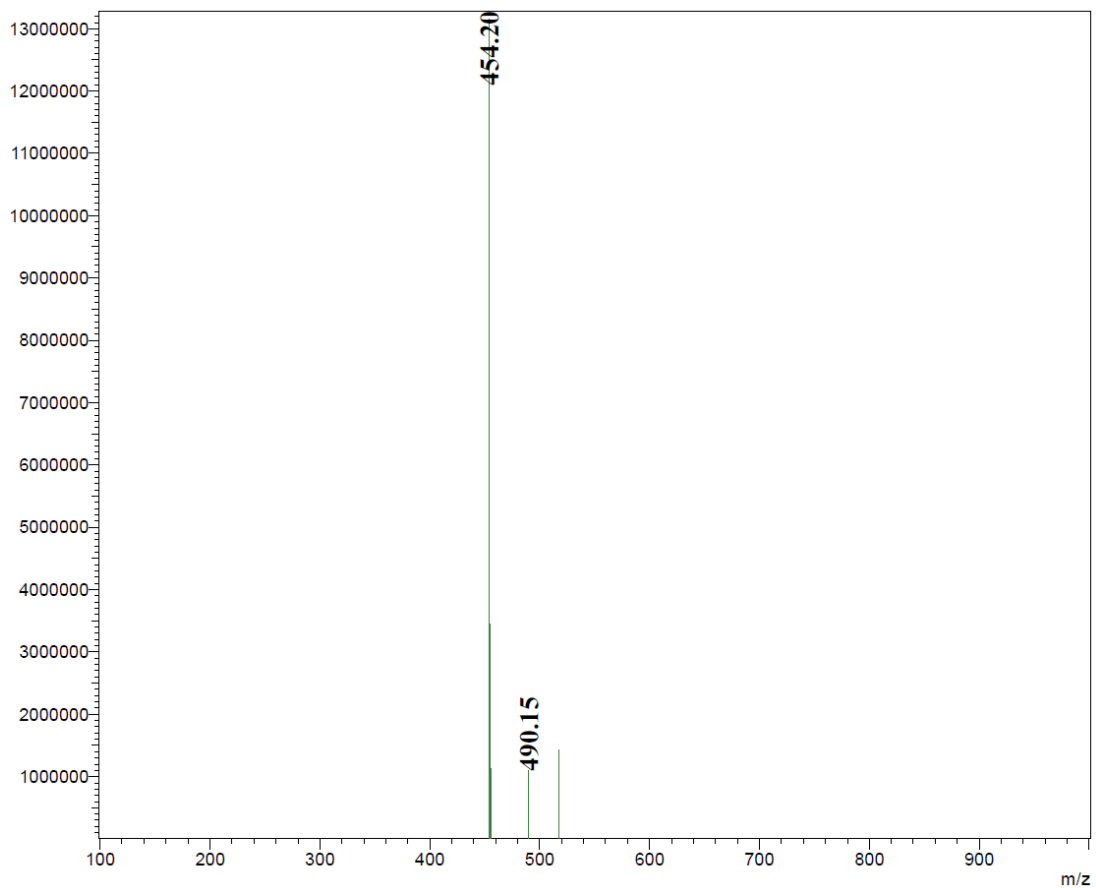


Figure S36: ESI(-)-MS Spectrum of 13

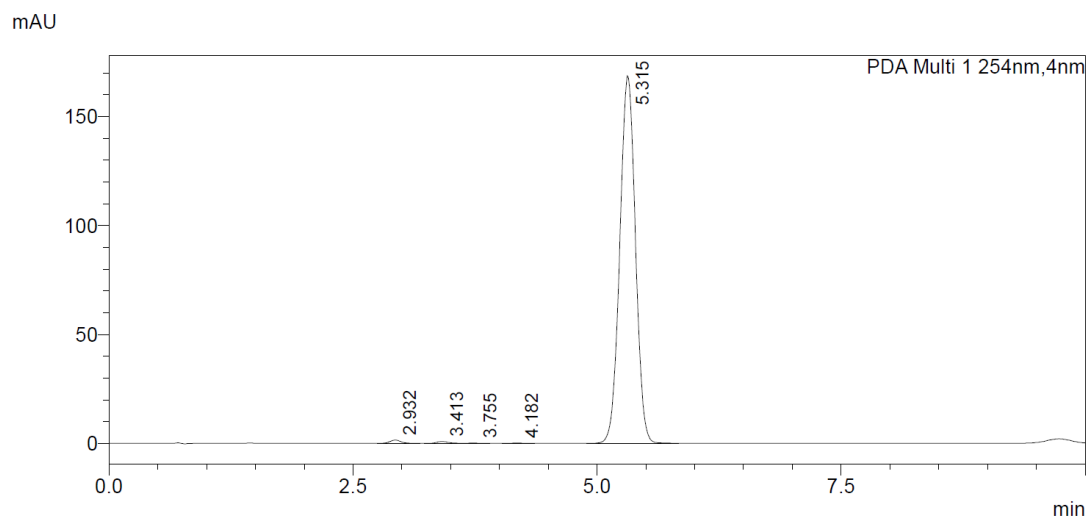


Figure S37: HPLC chromatogram of 13

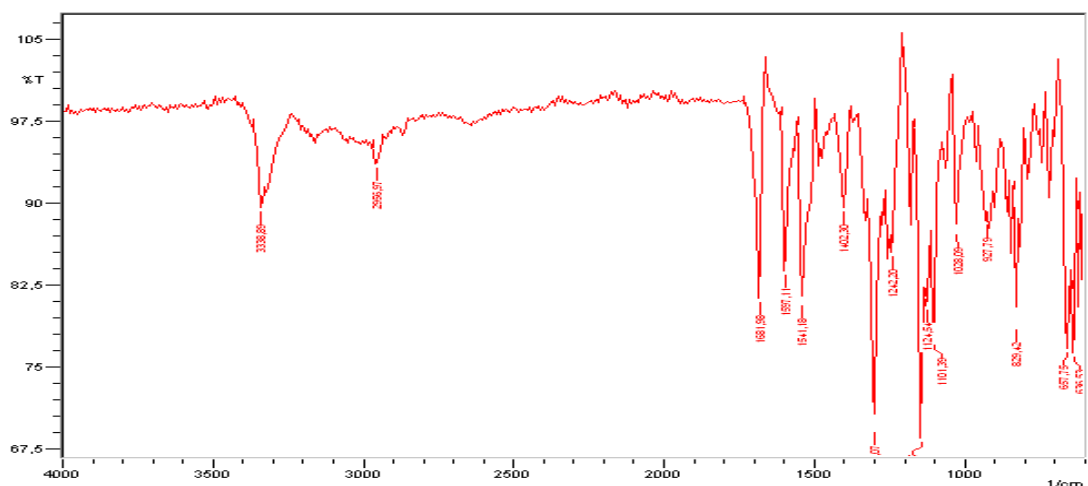


Figure S38: FTIR spectrum of 14

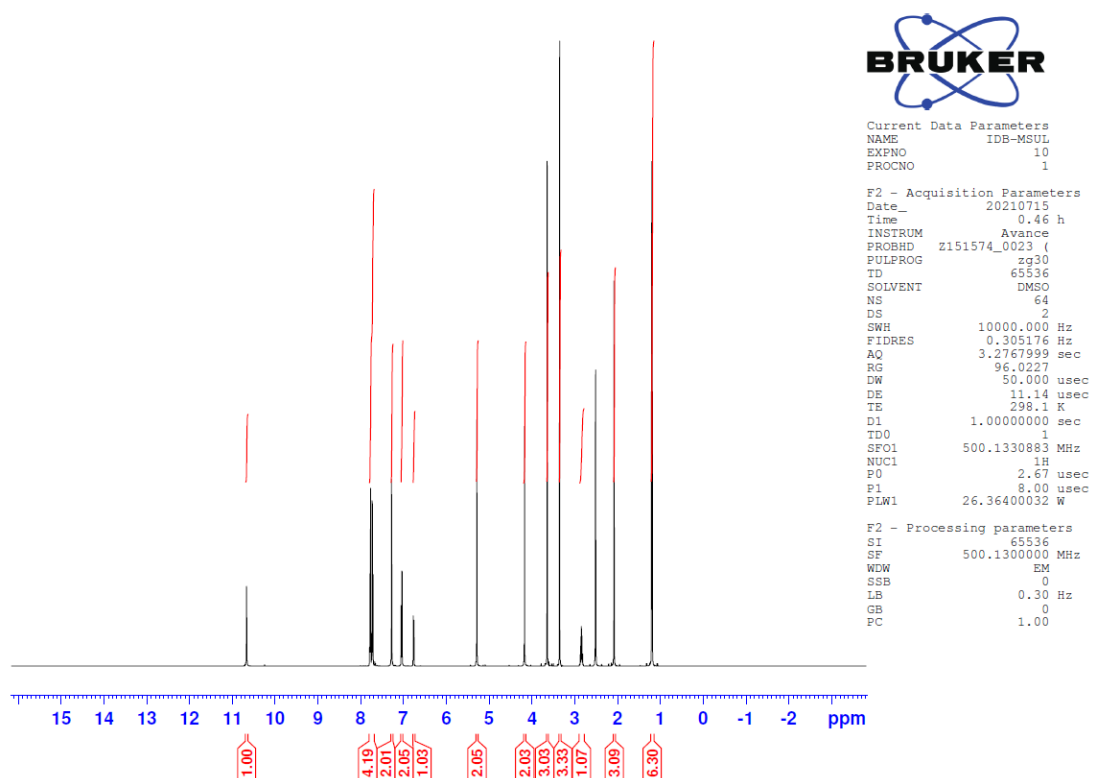


Figure S39: ¹H-NMR (500 MHz, DMSO) Spectrum of 14

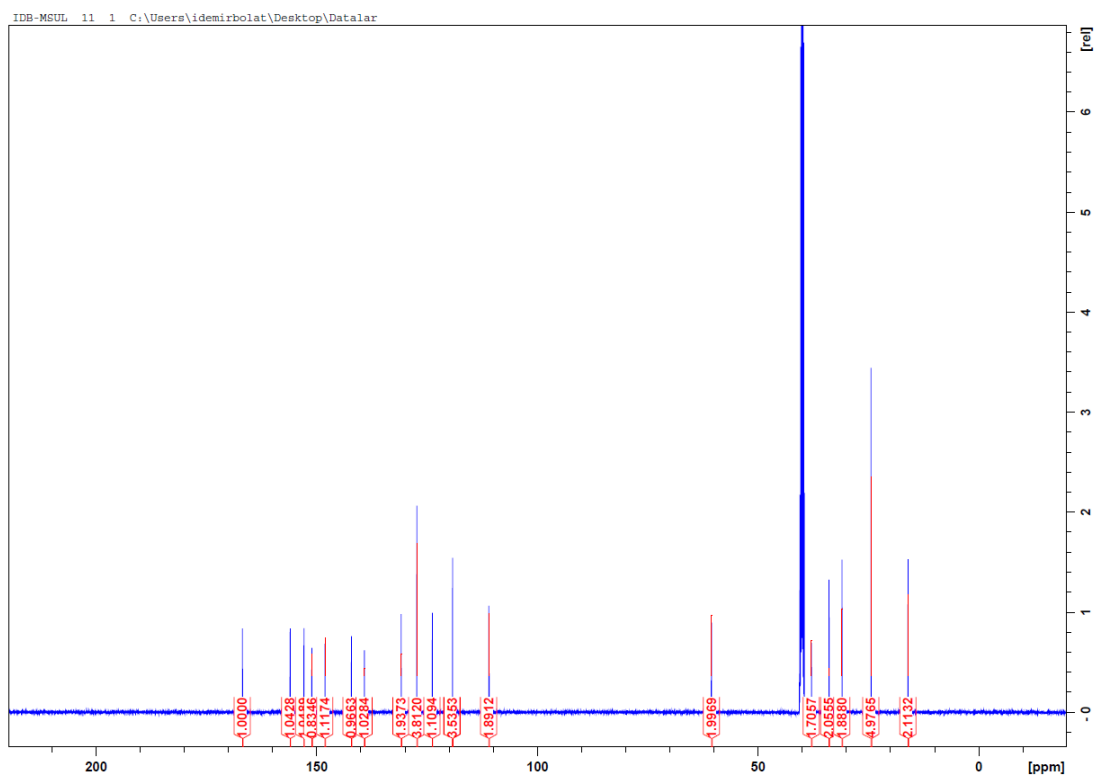


Figure S40: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **14**

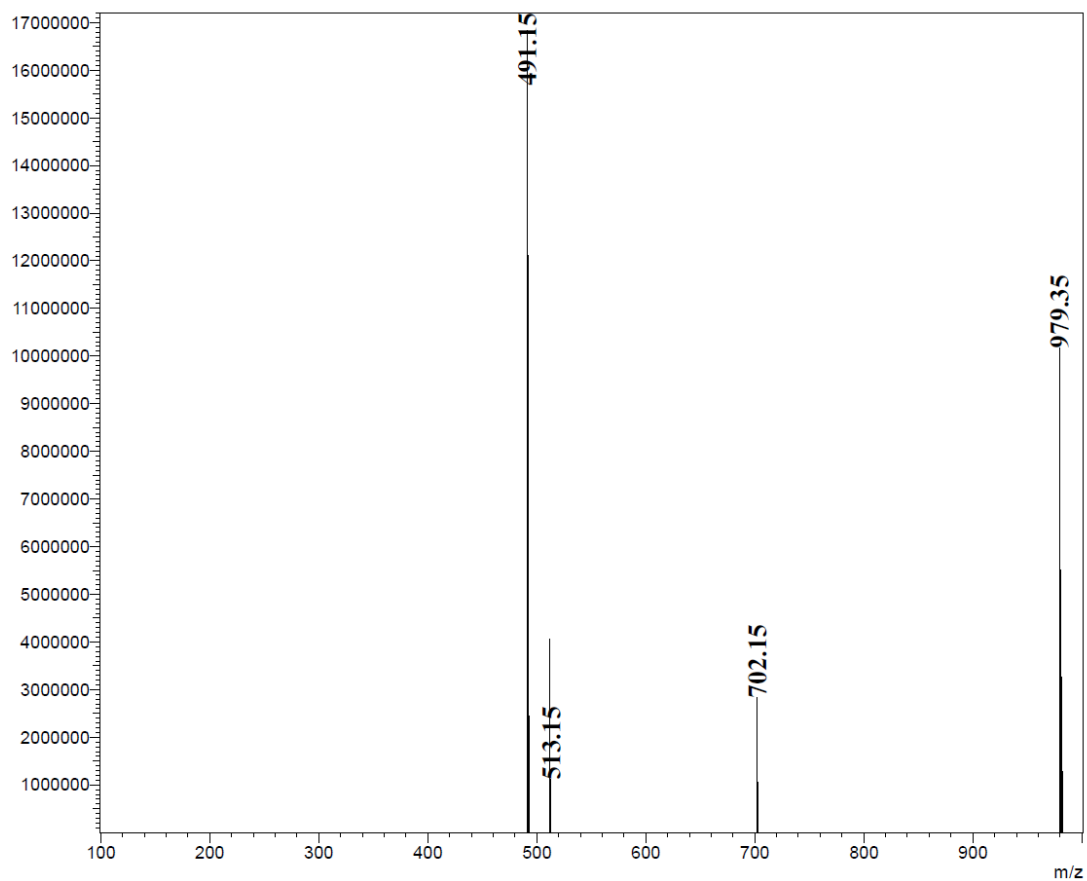


Figure S41: ESI(+)-MS Spectrum of **14**

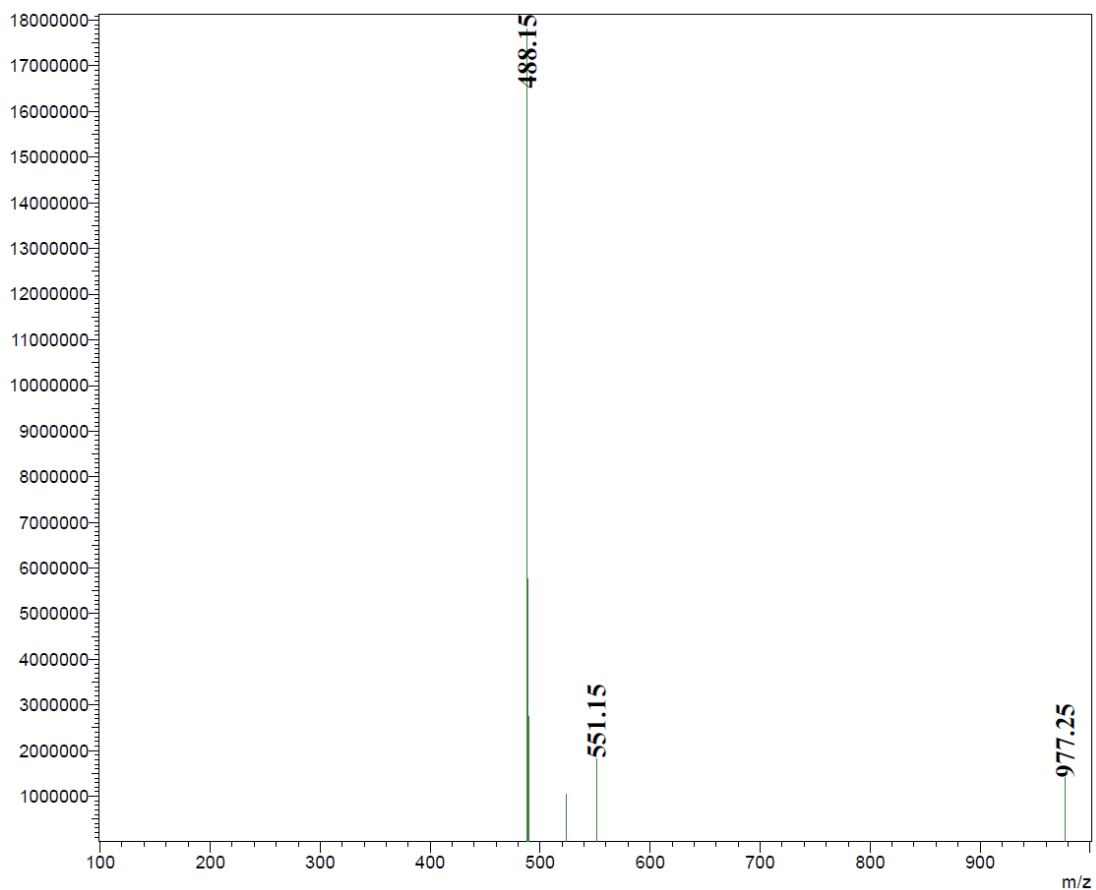


Figure S42: ESI(-)-MS Spectrum of 14

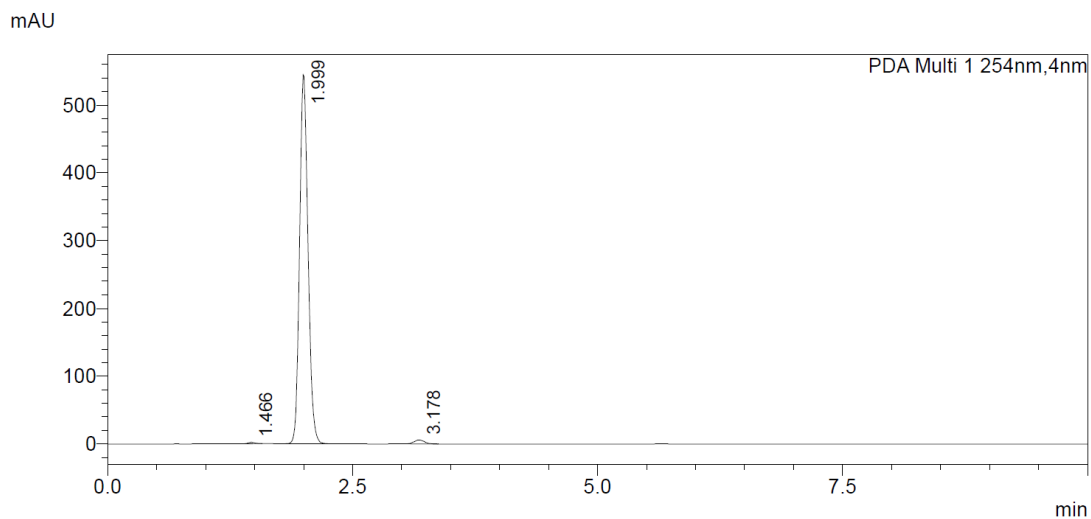


Figure S43: HPLC chromatogram of 14

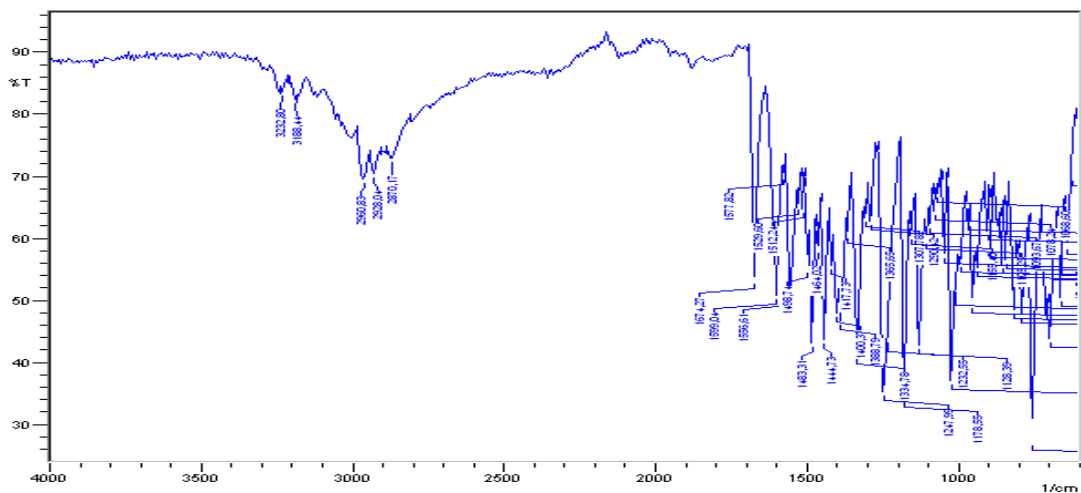


Figure S44: HPLC chromatogram of 15

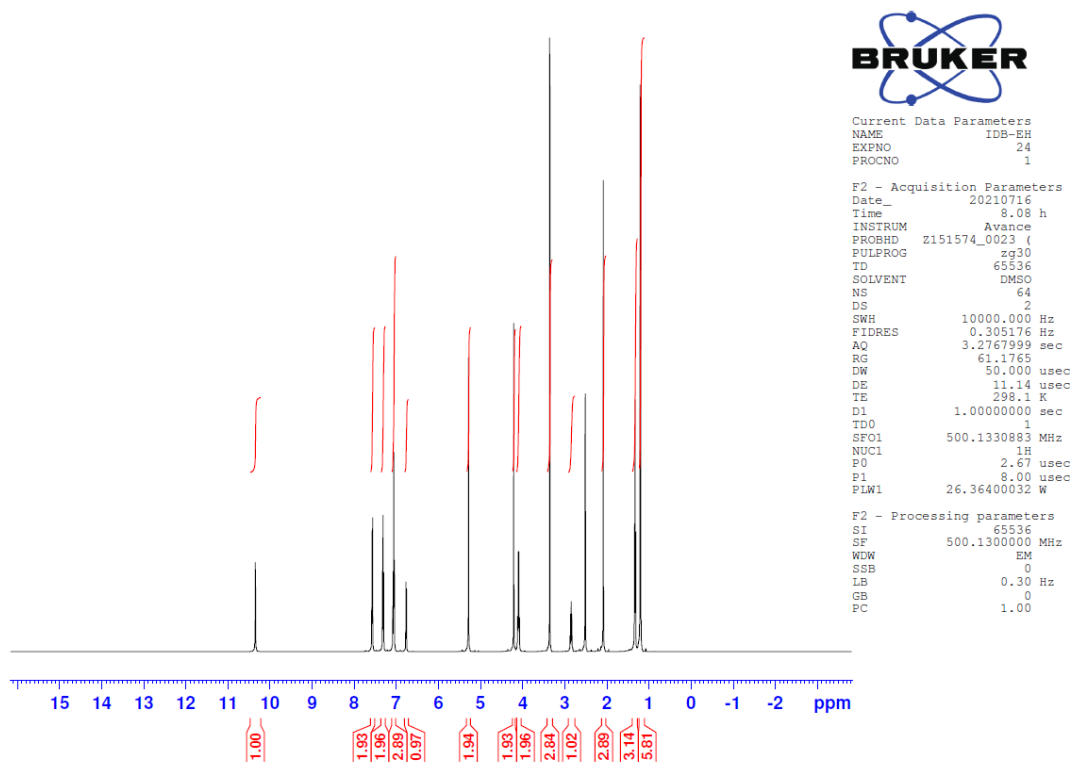


Figure S45: ¹H-NMR (500 MHz, DMSO) Spectrum of 15

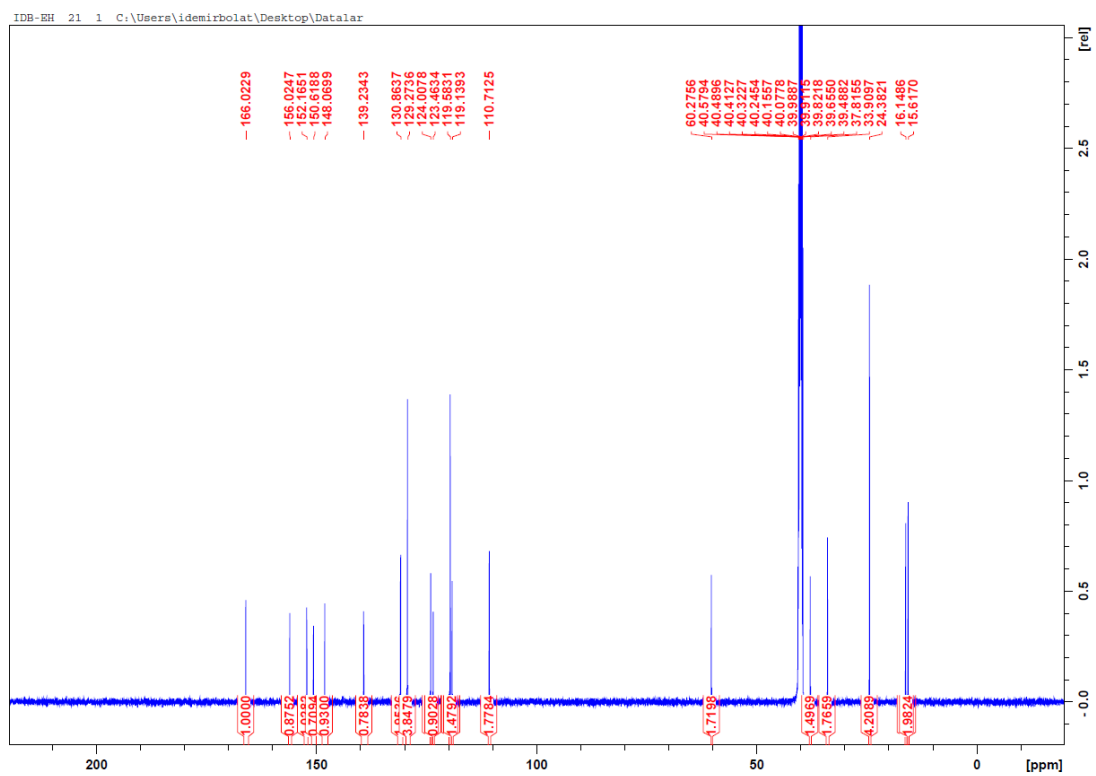


Figure S46: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **15**

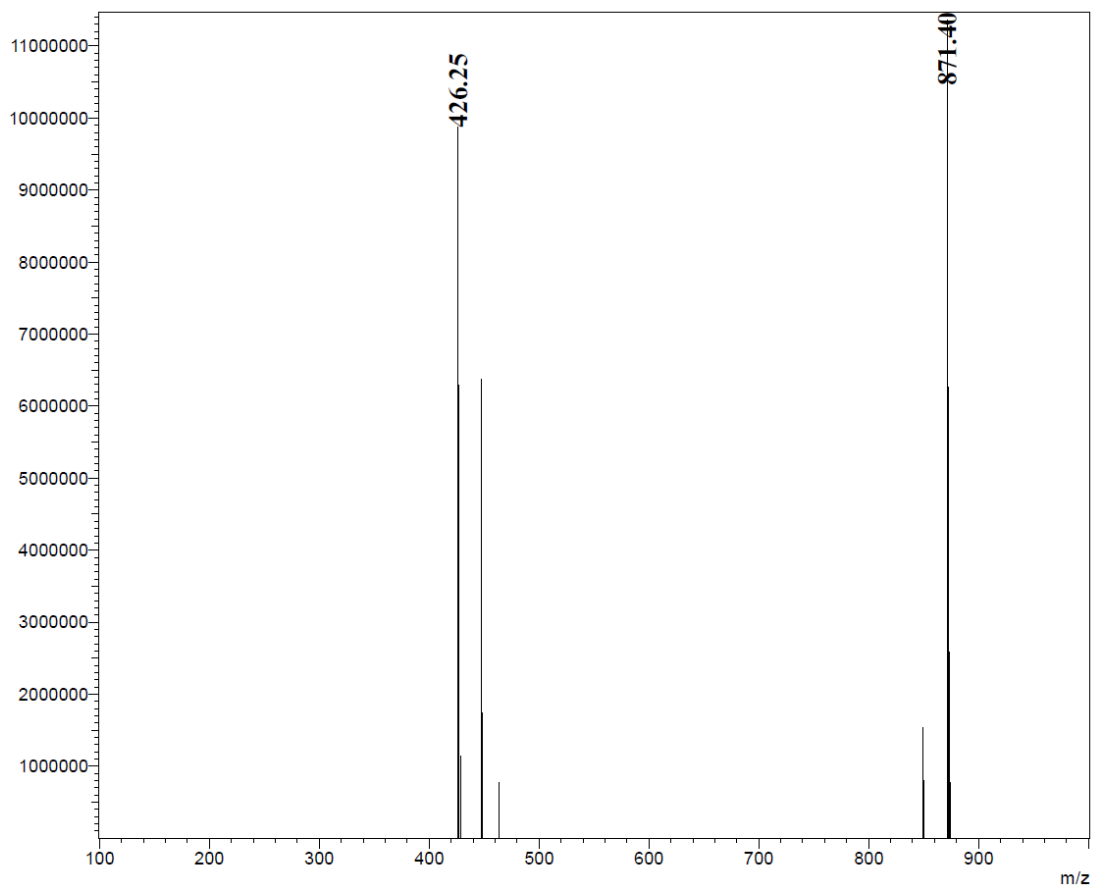


Figure S47: ESI(+)-MS Spectrum of **15**

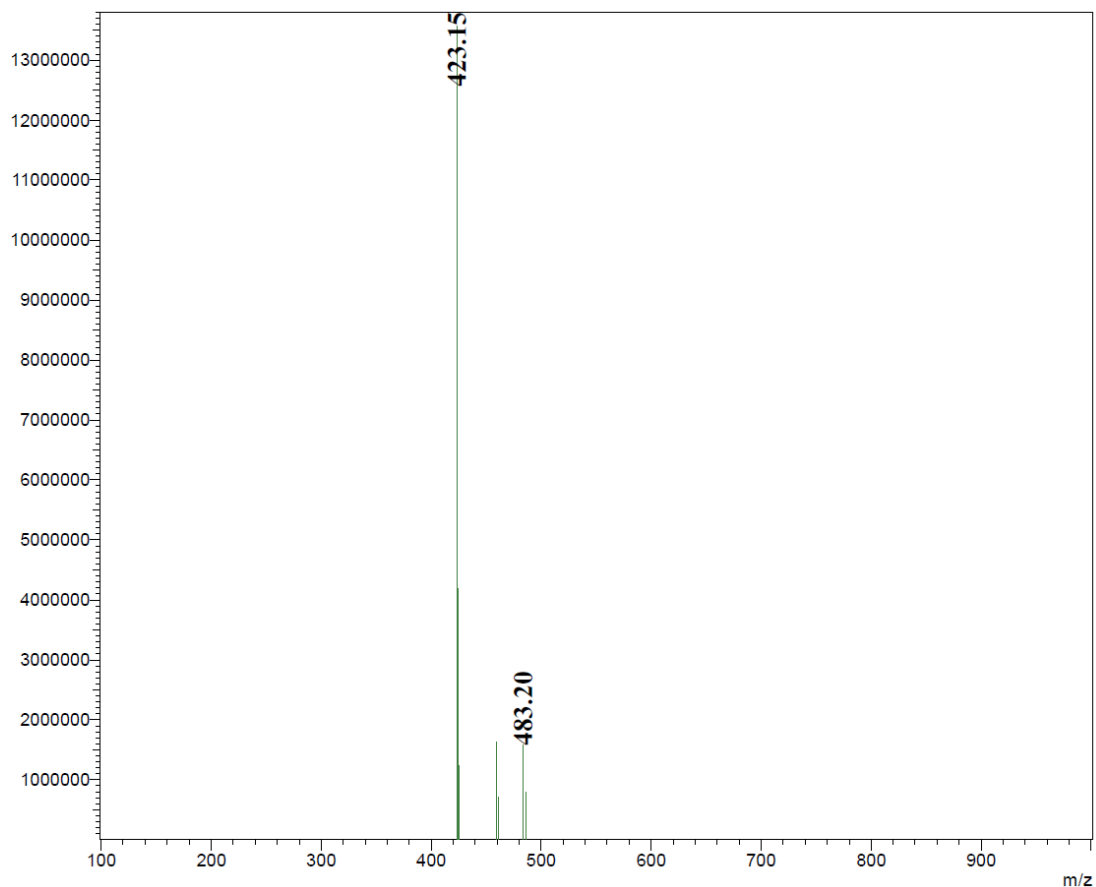


Figure S48: ESI(-)-MS Spectrum of **15**

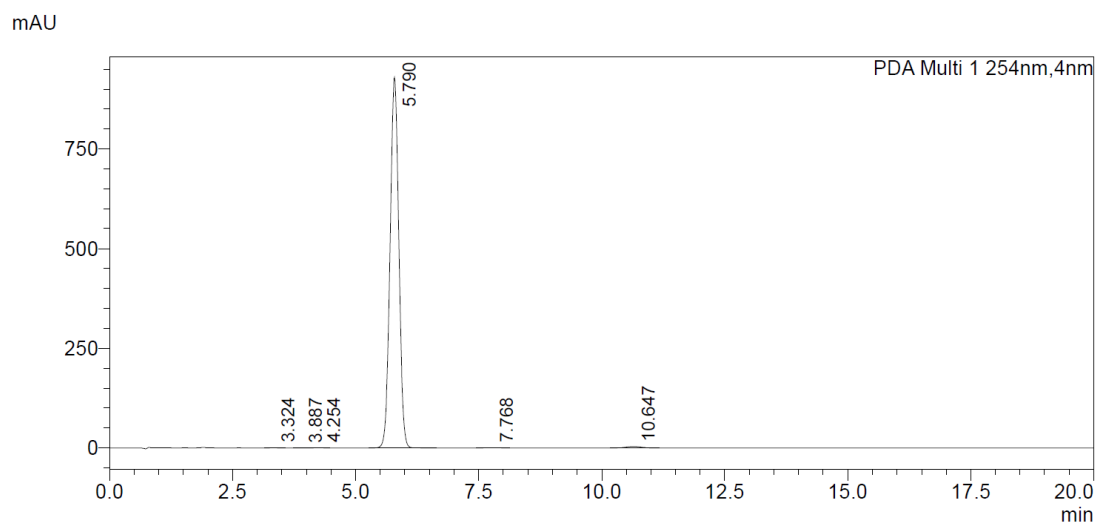


Figure S49: HPLC chromatogram of **15**

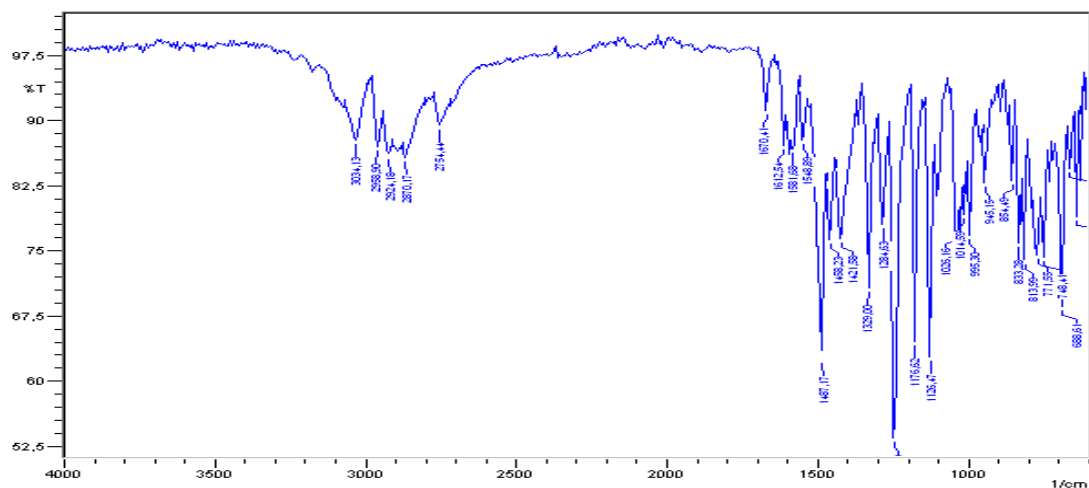


Figure S50: FTIR spectrum of 16

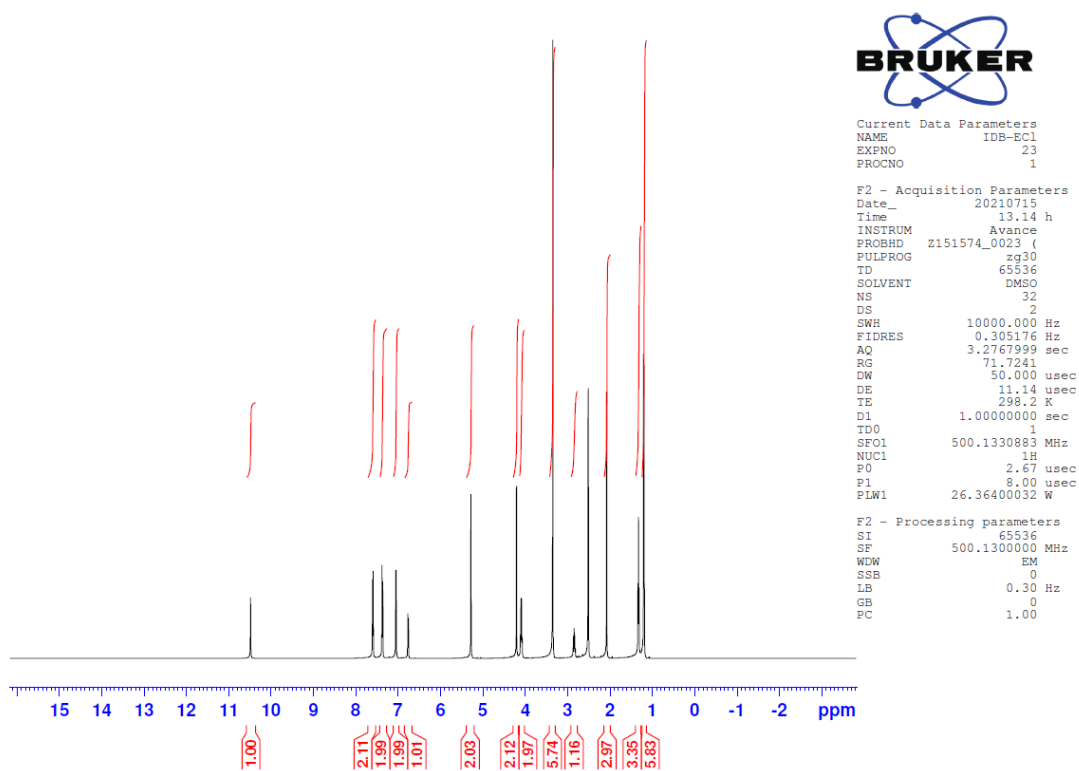


Figure S51: ¹H-NMR (500 MHz, DMSO) Spectrum of 16

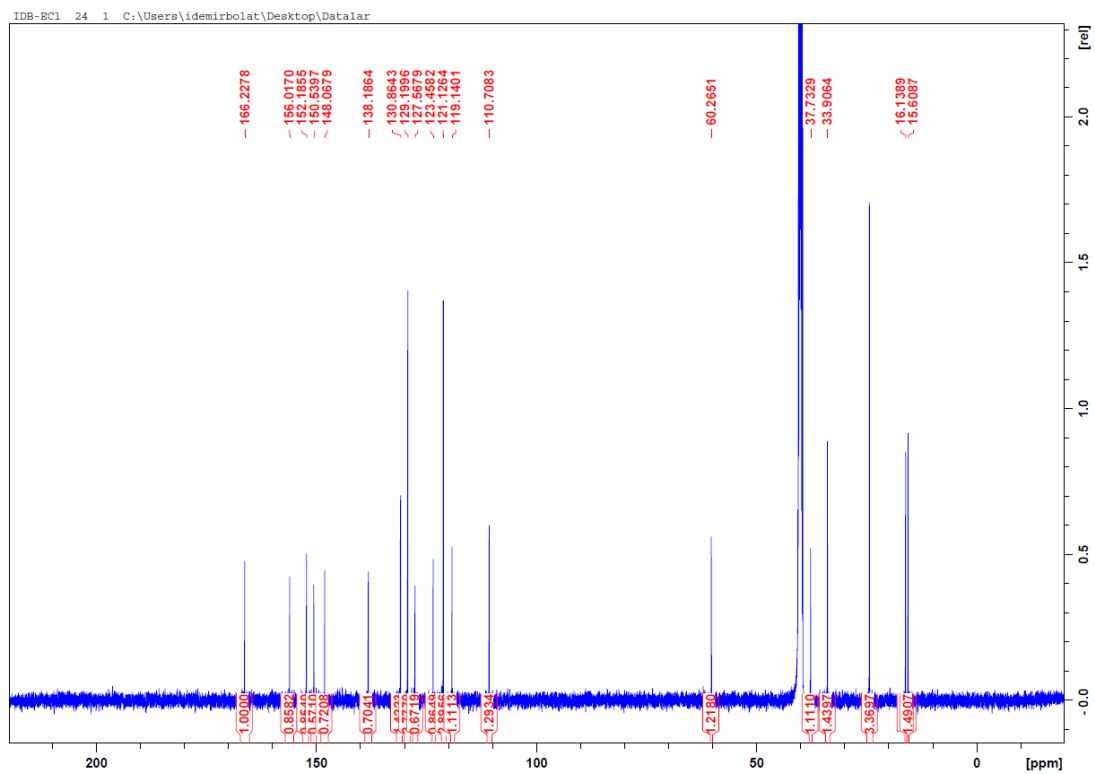


Figure S52: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **16**

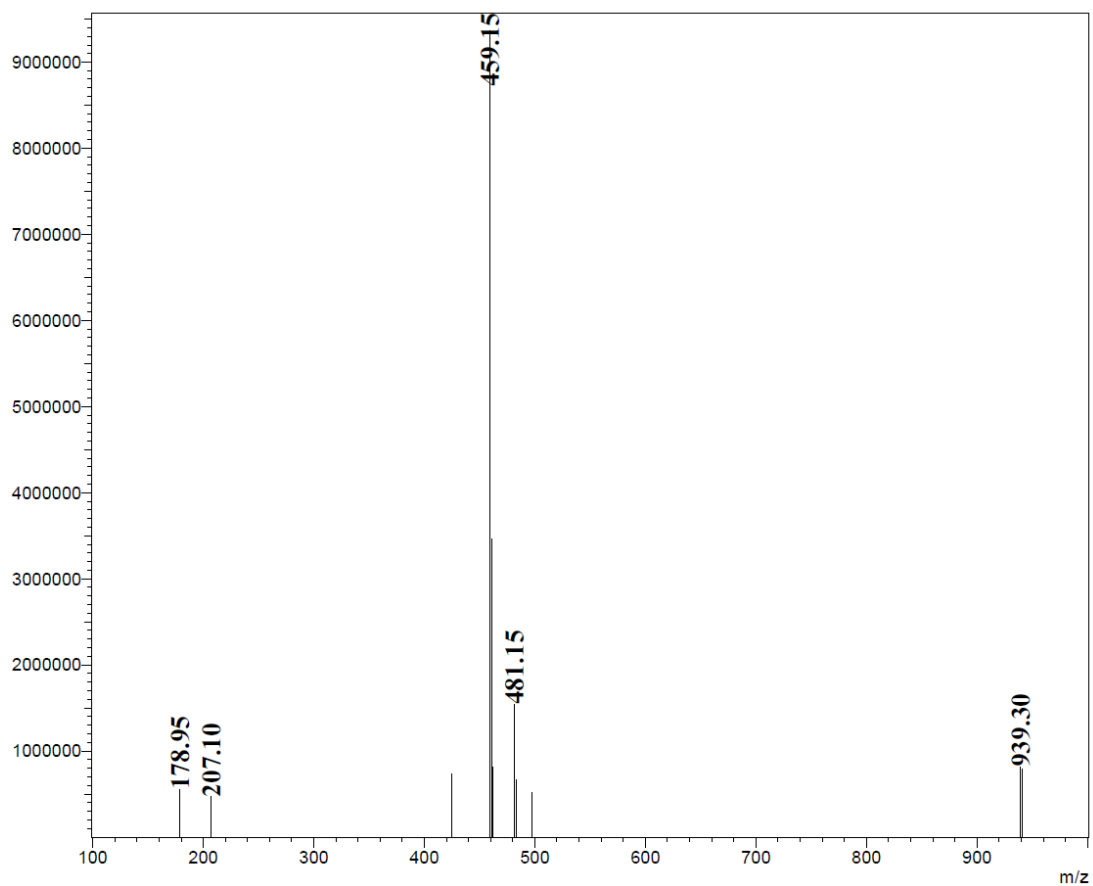


Figure S53: ESI(+)-MS Spectrum of 16

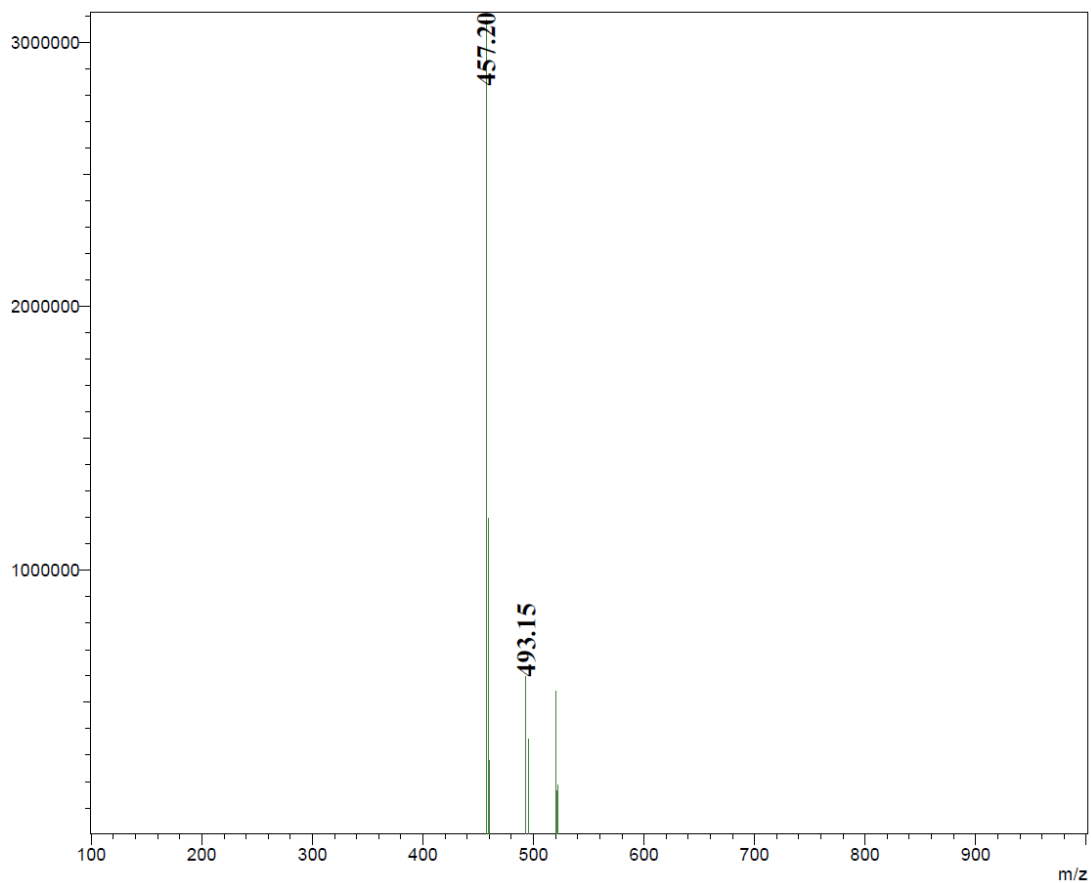


Figure S54: ESI(-)-MS Spectrum of 16

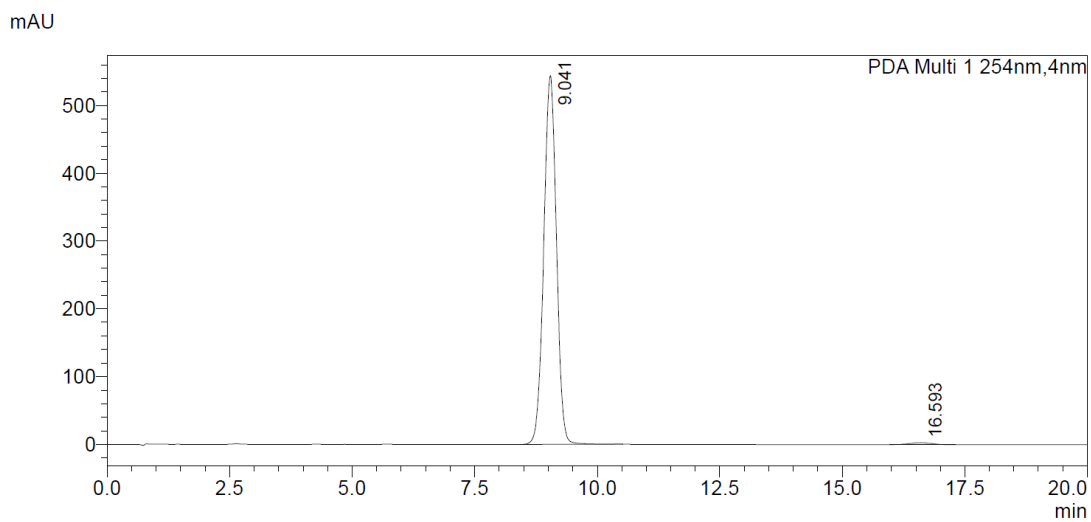


Figure S55: HPLC chromatogram of 16

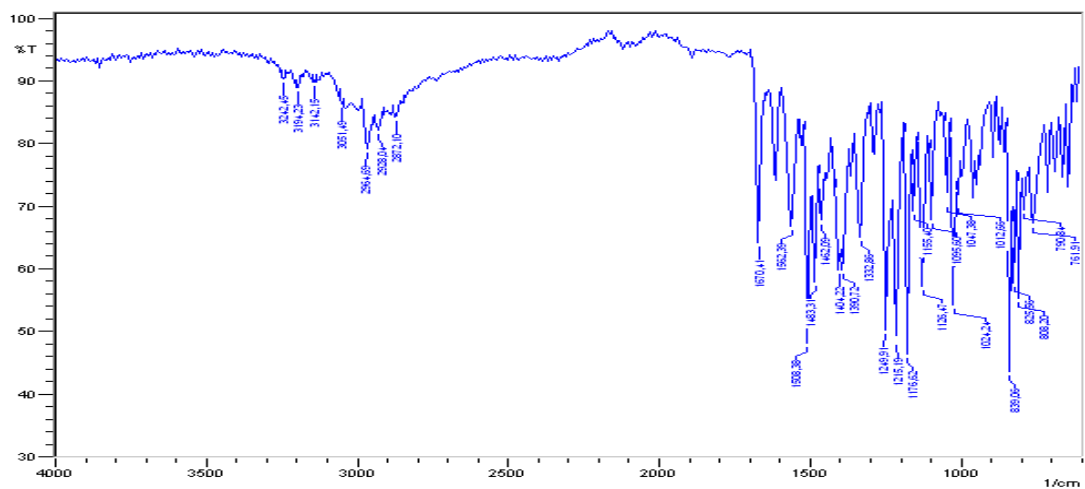


Figure S56: HPLC chromatogram of 17

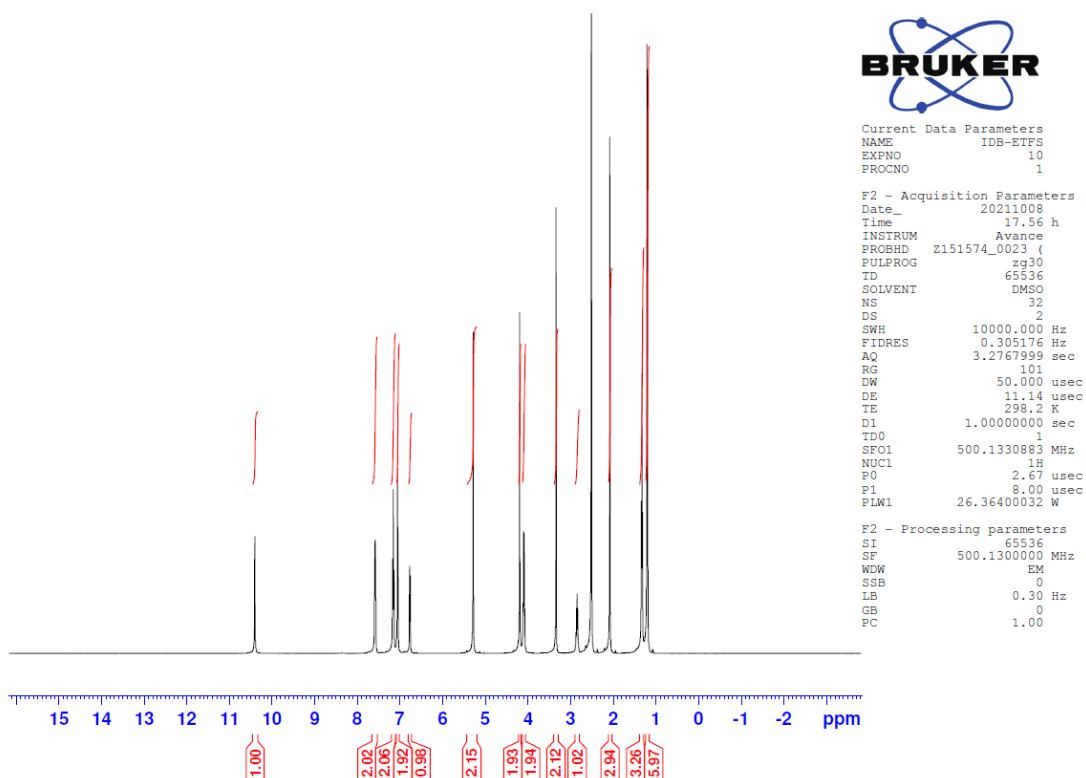


Figure S57: ¹H-NMR (500 MHz, DMSO) Spectrum of 17

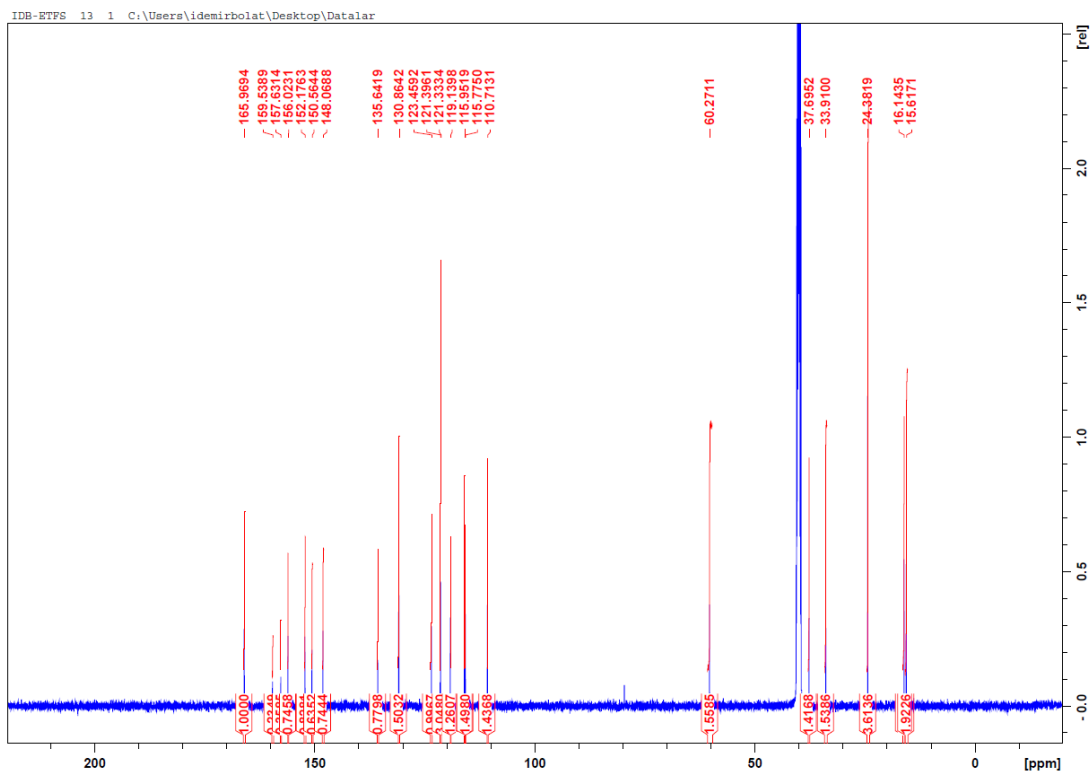


Figure S58: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **17**

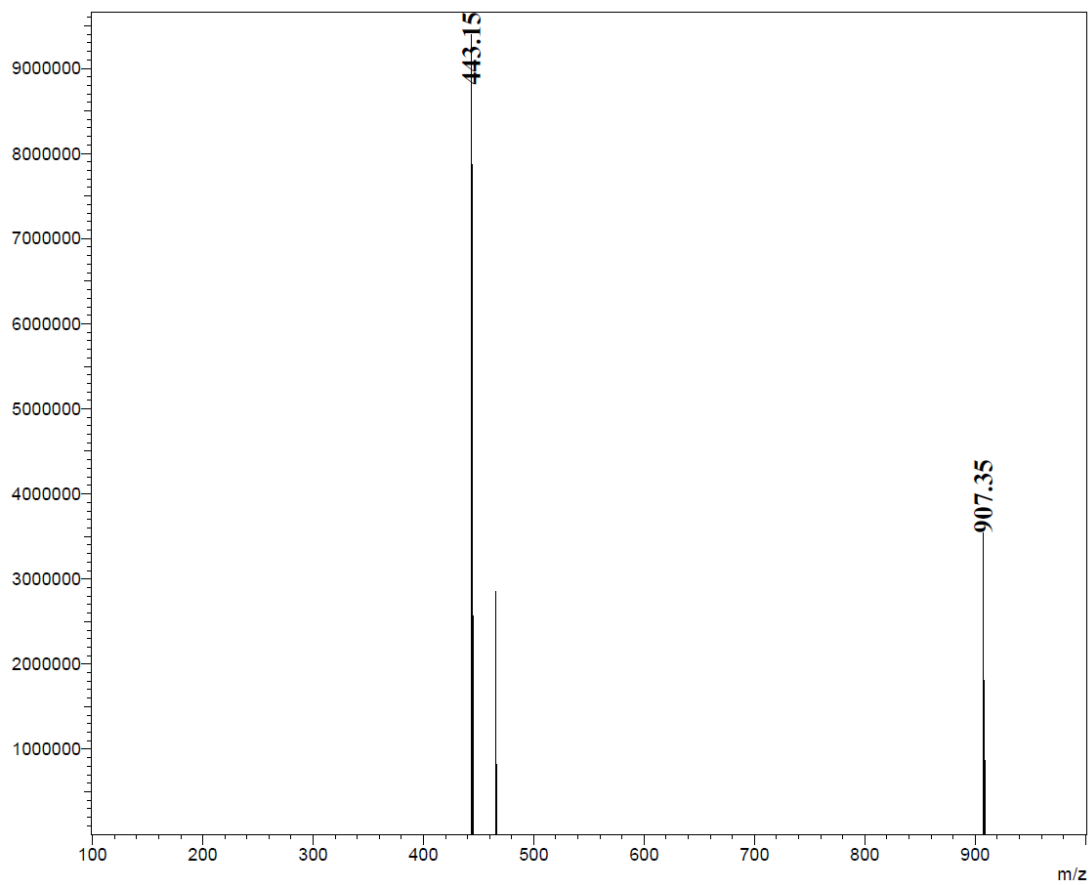


Figure S59: ESI(+)-MS Spectrum of **17**

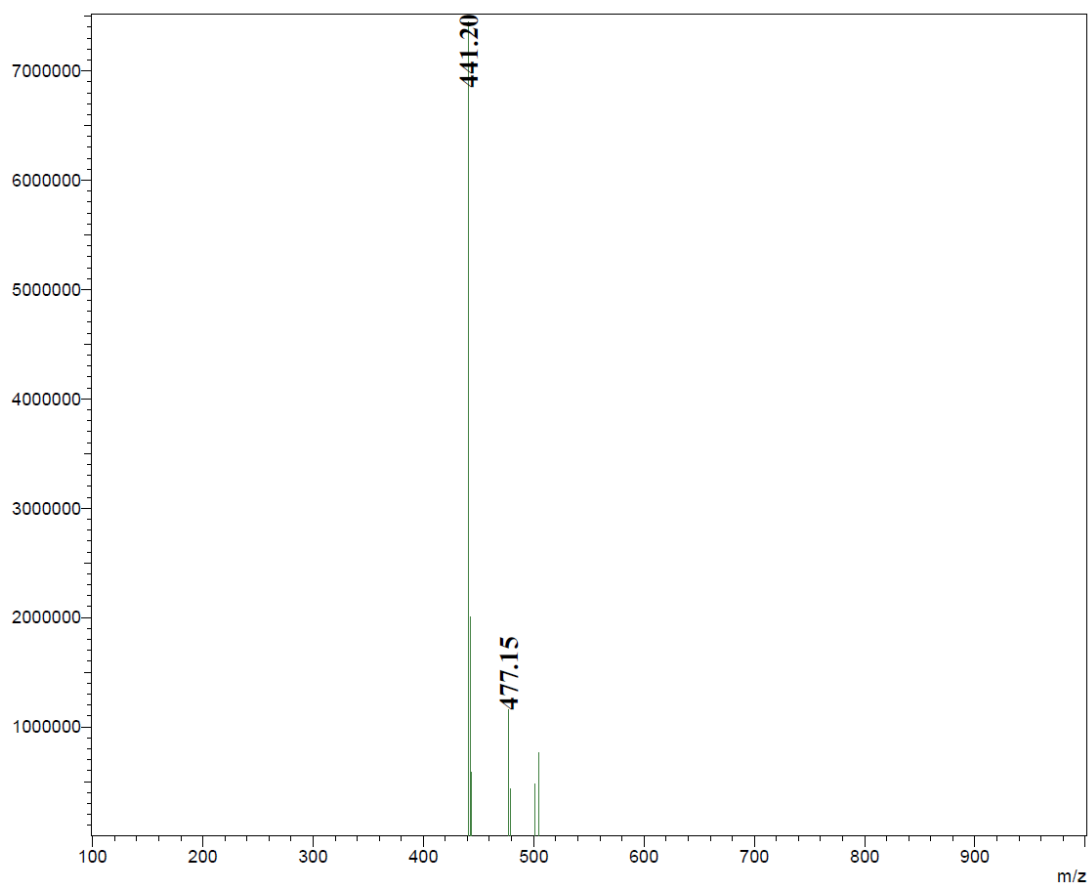


Figure S60: ESI(-)-MS Spectrum of 17

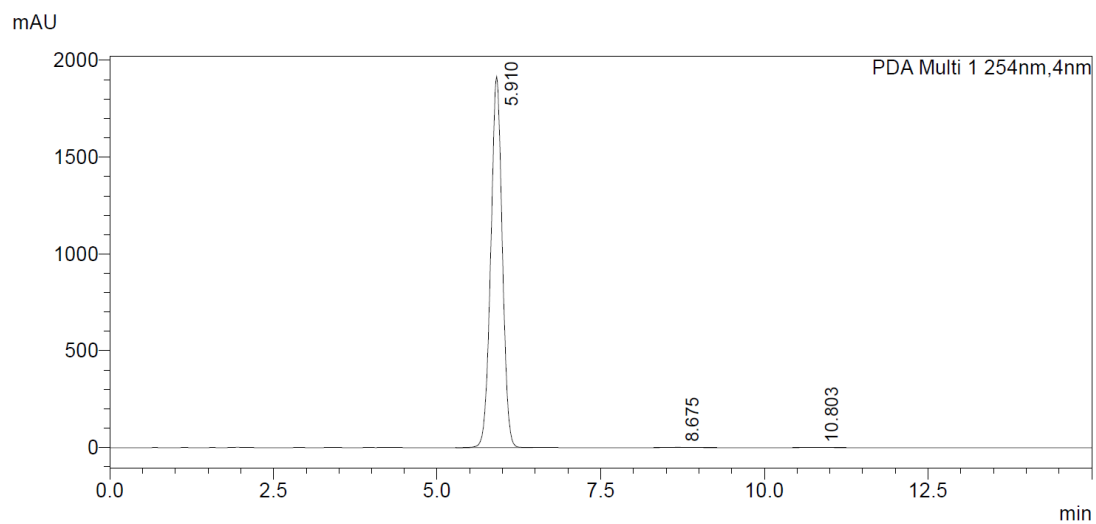


Figure S61: HPLC chromatogram of 17

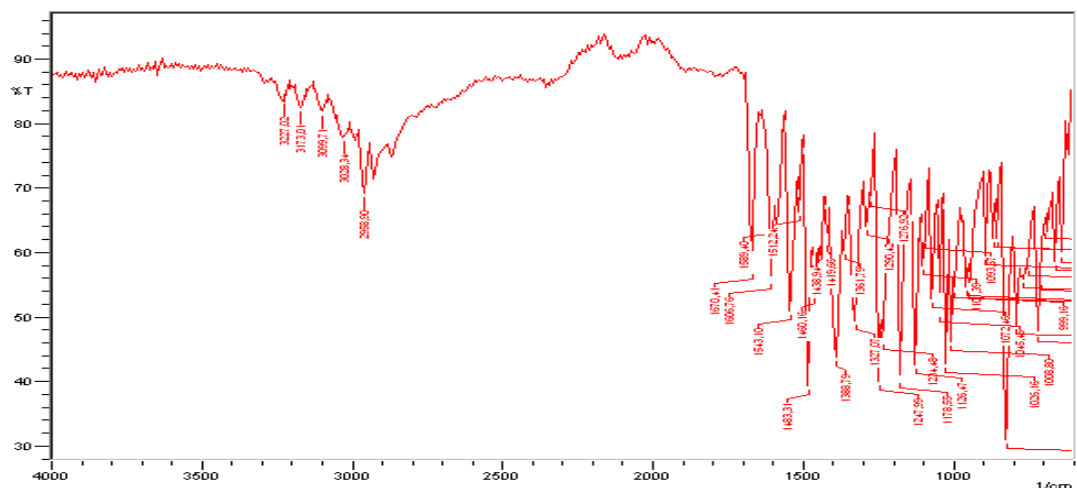


Figure S62: HPLC chromatogram of 18

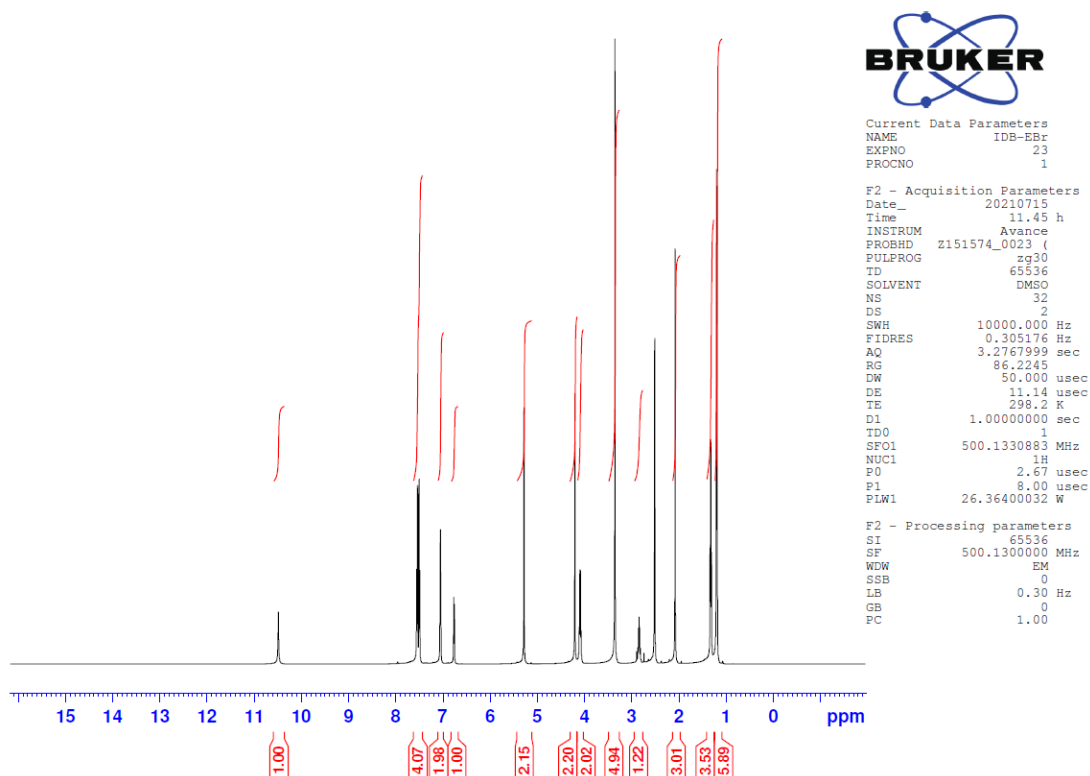


Figure S63: ¹H-NMR (500 MHz, DMSO) Spectrum of 18

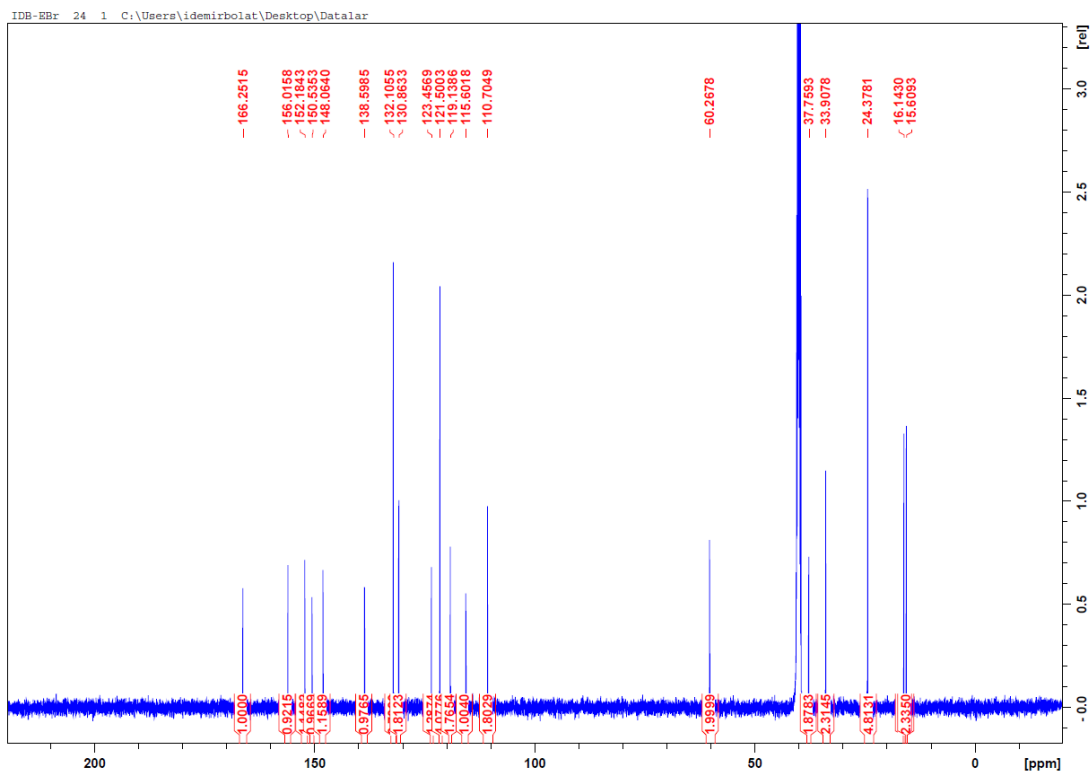


Figure S64: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **18**

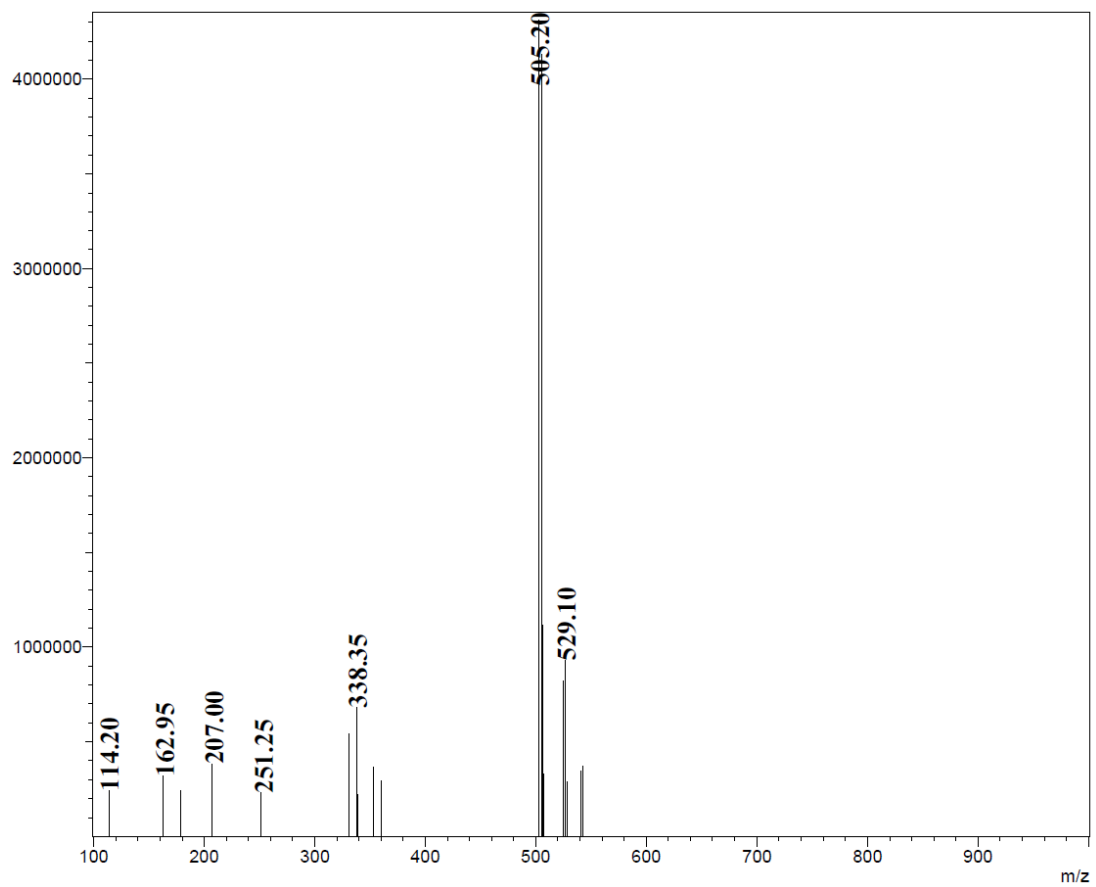


Figure S65: ESI(+)-MS Spectrum of 18

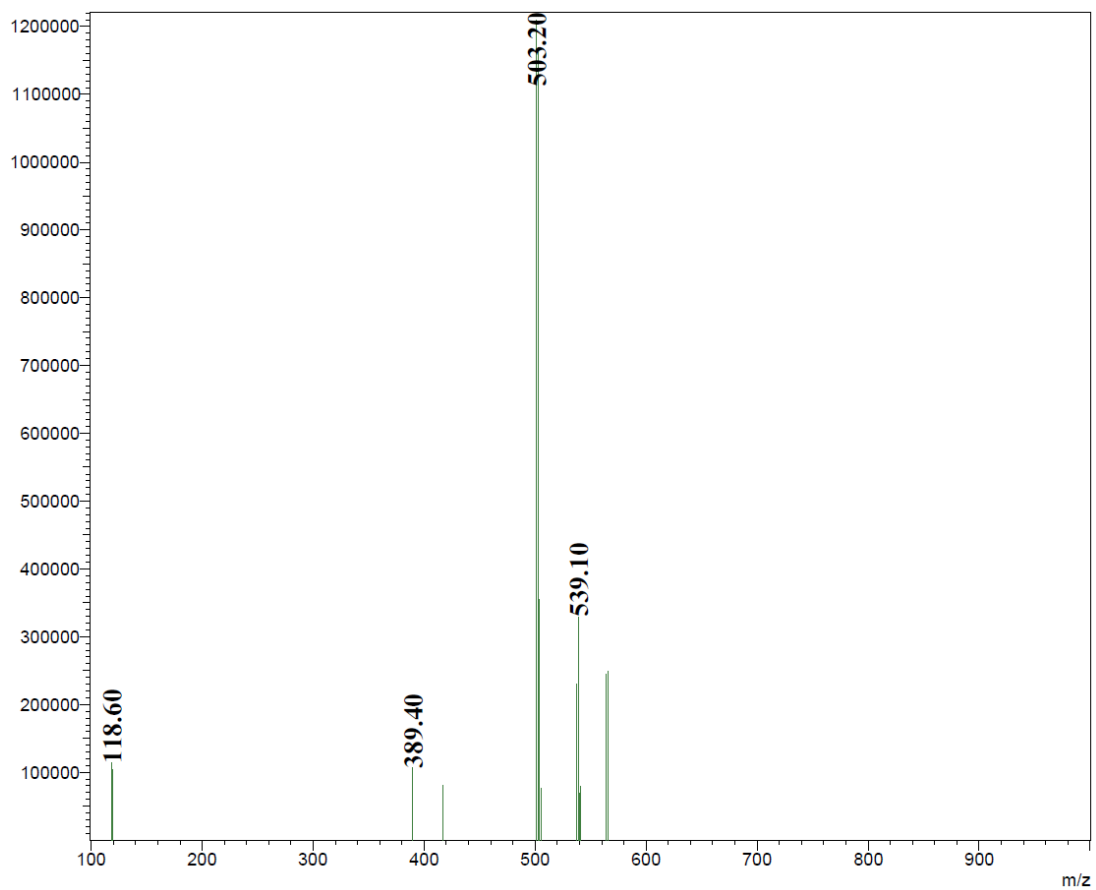


Figure S66: ESI(-)-MS Spectrum of **18**

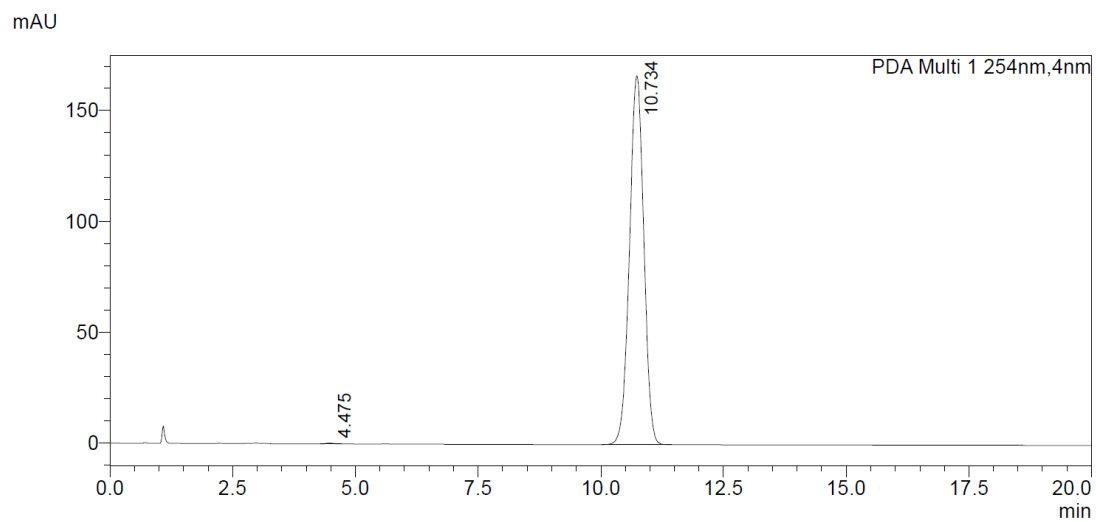


Figure S67: HPLC chromatogram of **18**

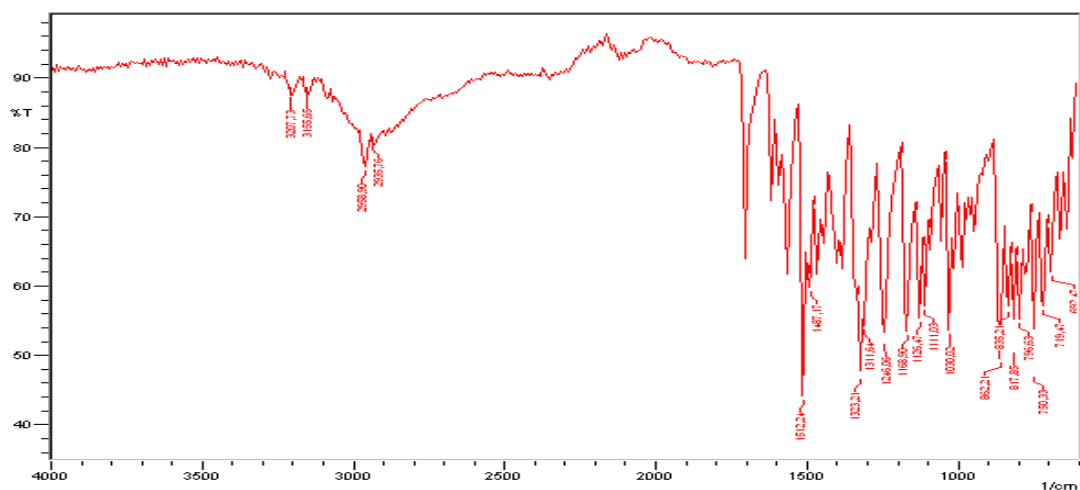


Figure S68: FTIR spectrum of 19

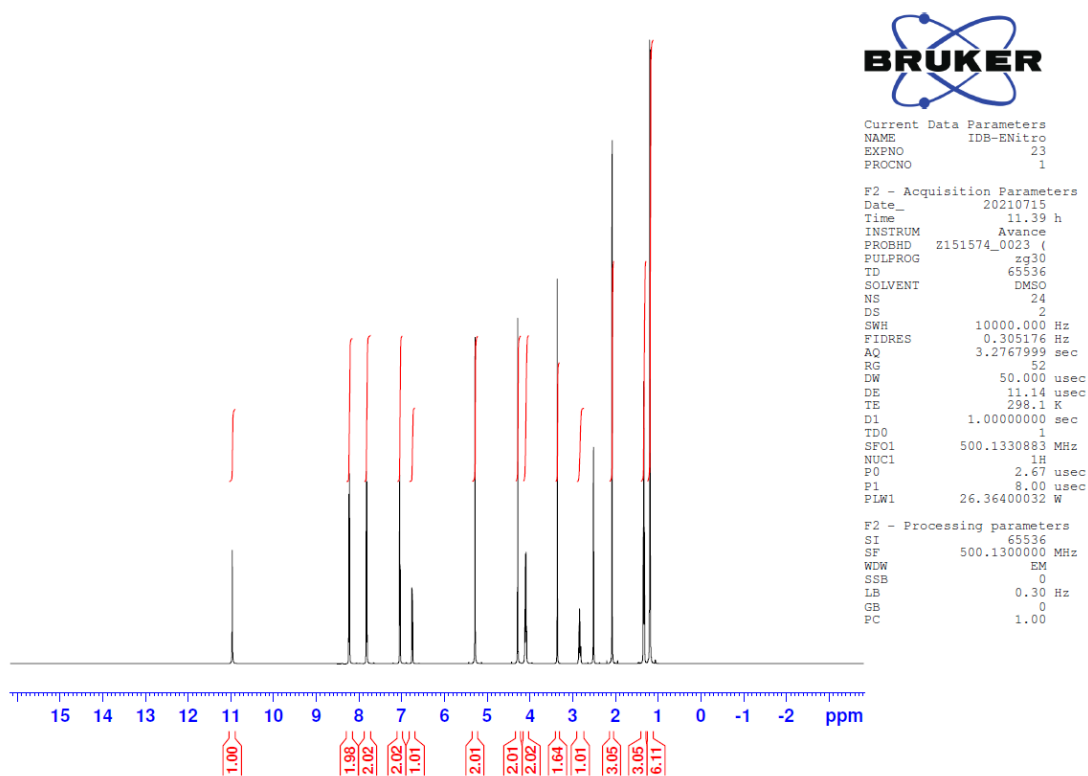


Figure S69: ¹H-NMR (500 MHz, DMSO) Spectrum of 19

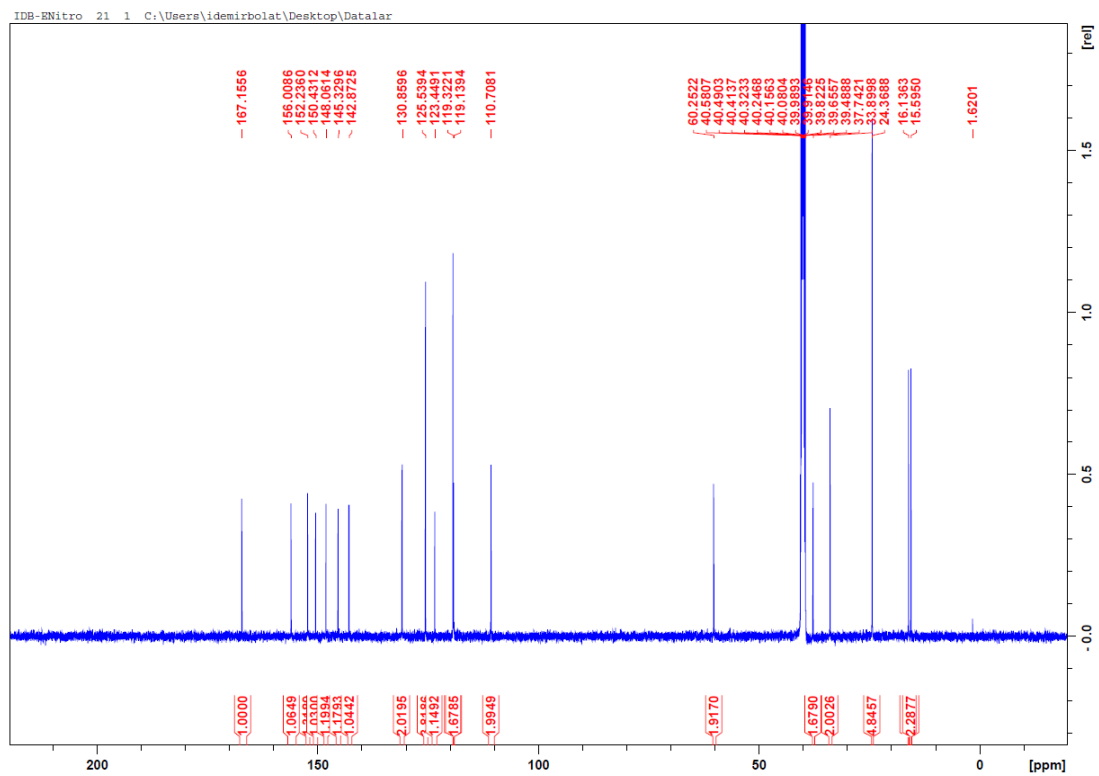


Figure S70: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **19**

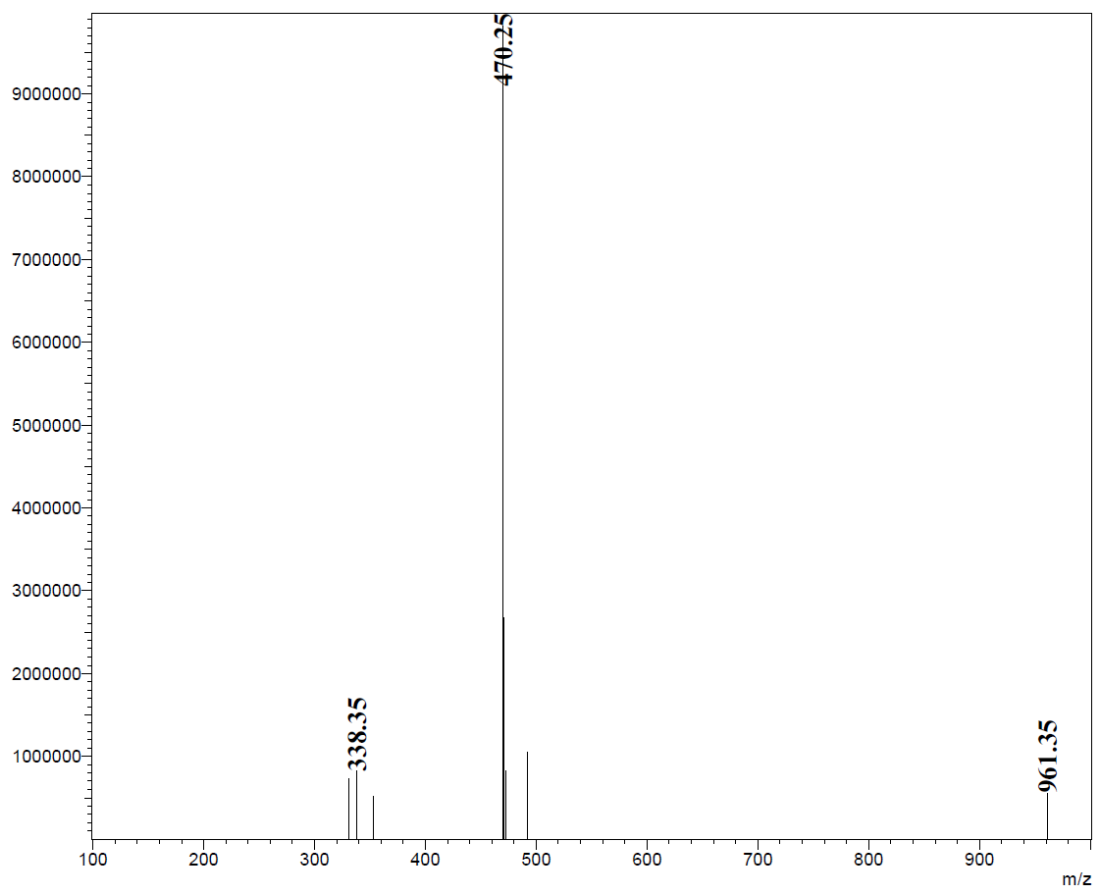


Figure S71: ESI(+)-MS Spectrum of 19

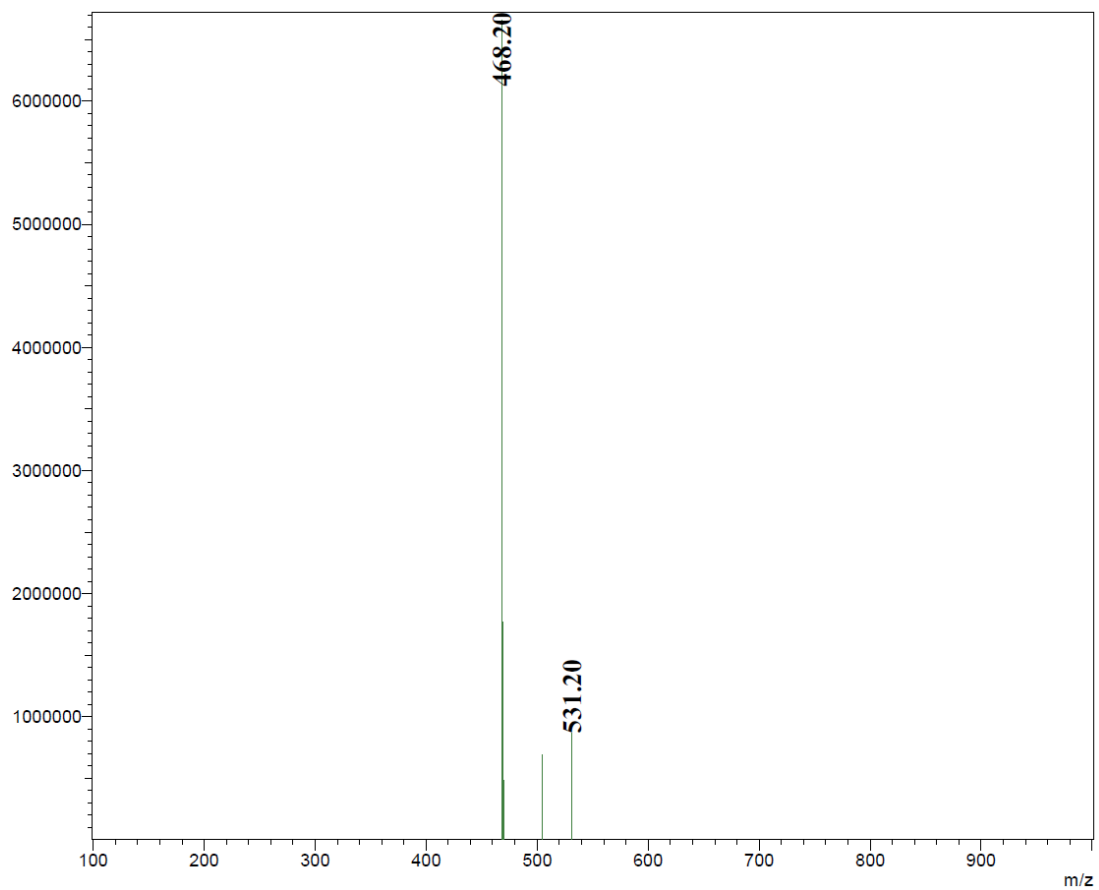


Figure S72: ESI(-)-MS Spectrum of 19

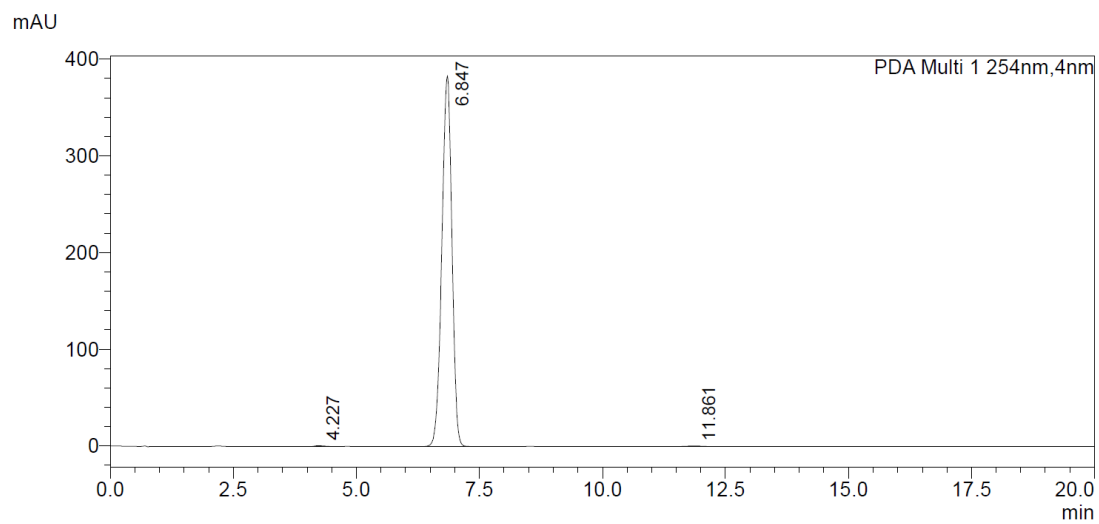


Figure S73: HPLC chromatogram of 19

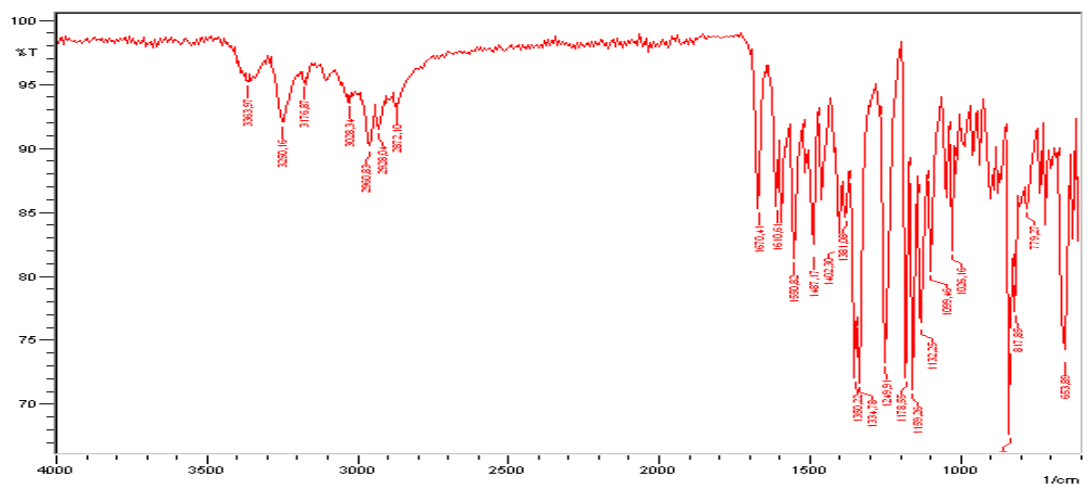


Figure S74 HPLC chromatogram of 20

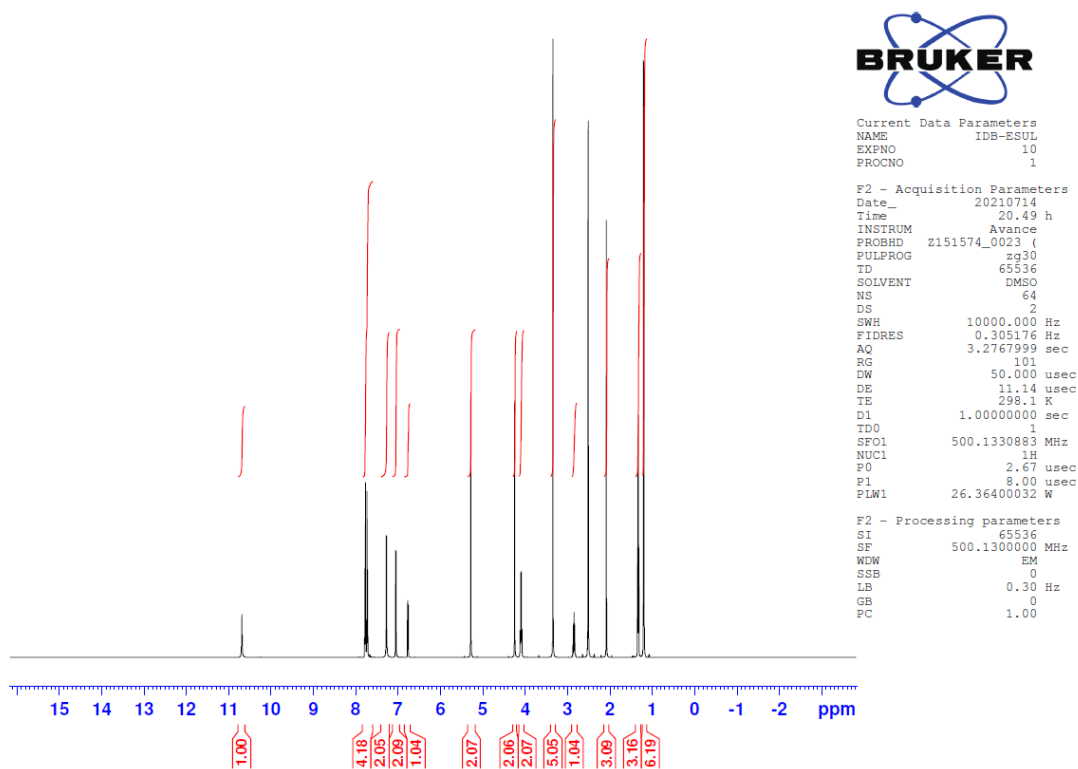


Figure S75: ¹H-NMR (500 MHz, DMSO) Spectrum of 20

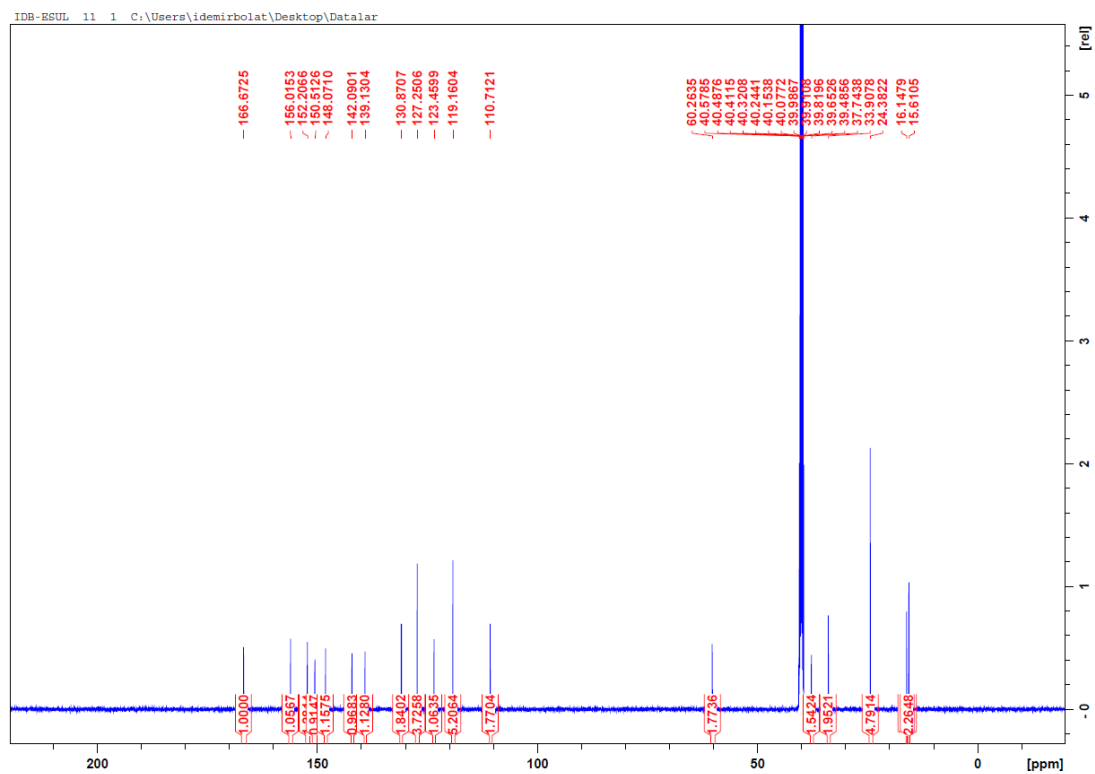


Figure S76: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **20**

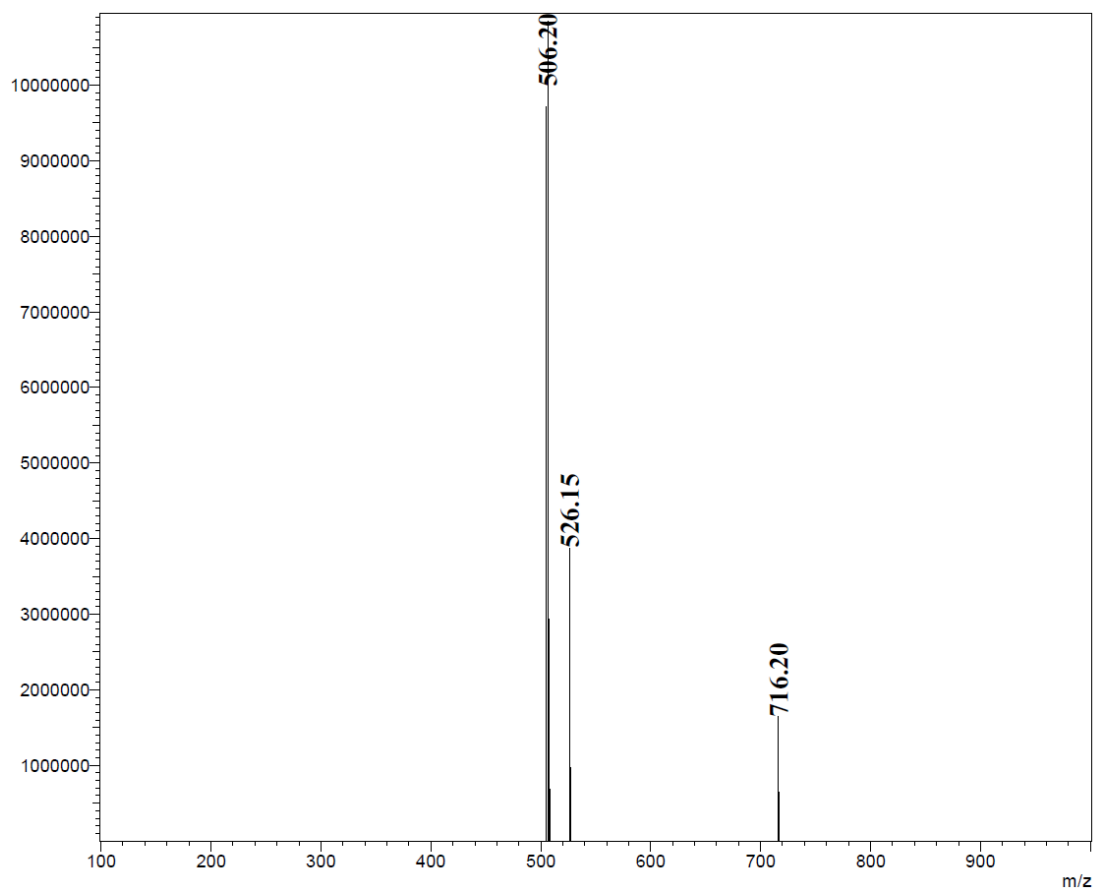


Figure S77: ESI(+)-MS Spectrum of **20**

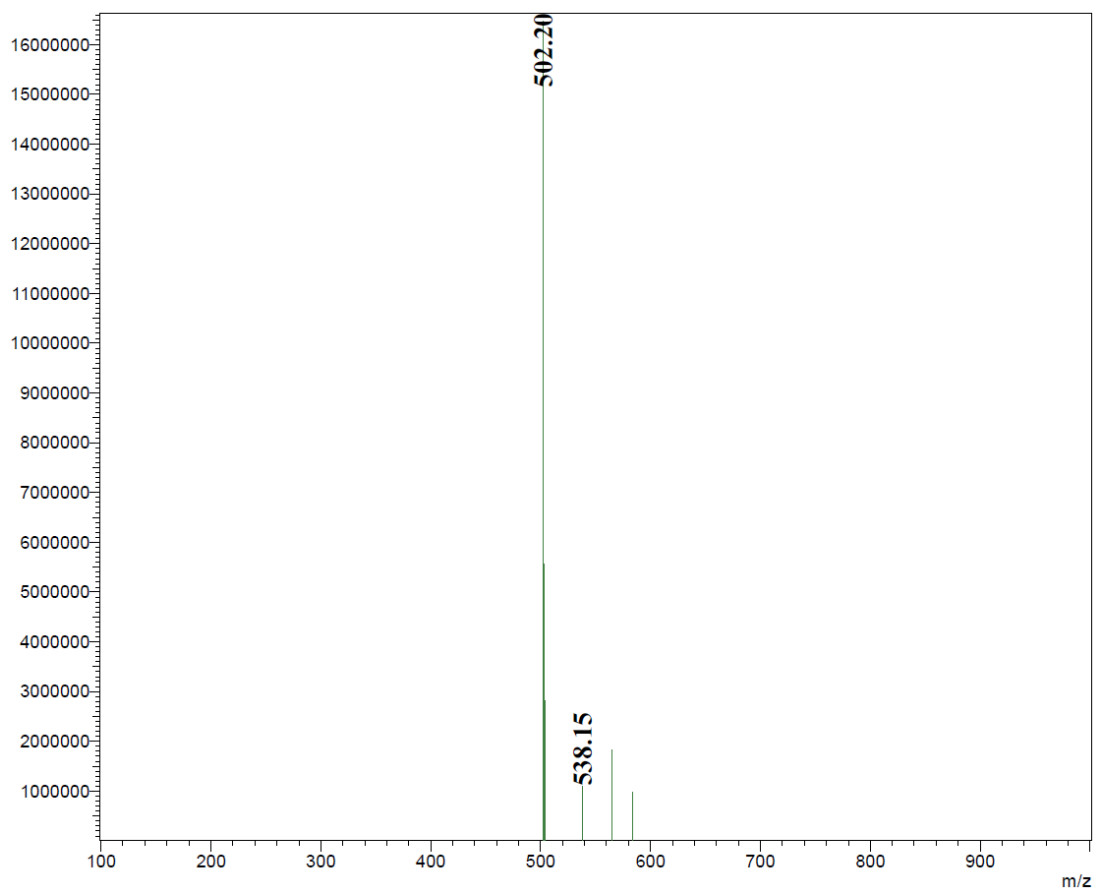


Figure S78: ESI(-)-MS Spectrum of **20**

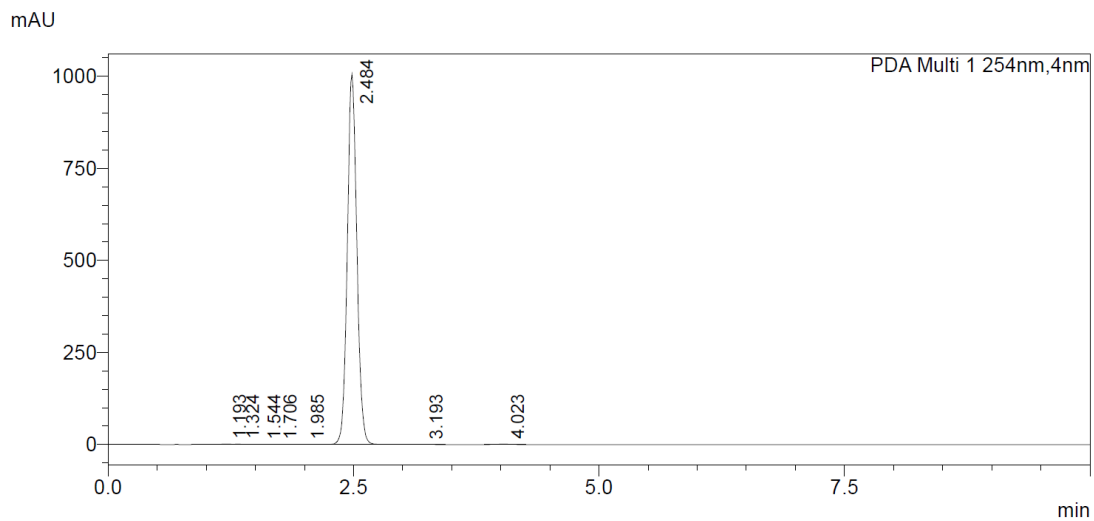


Figure S79: HPLC chromatogram of **20**

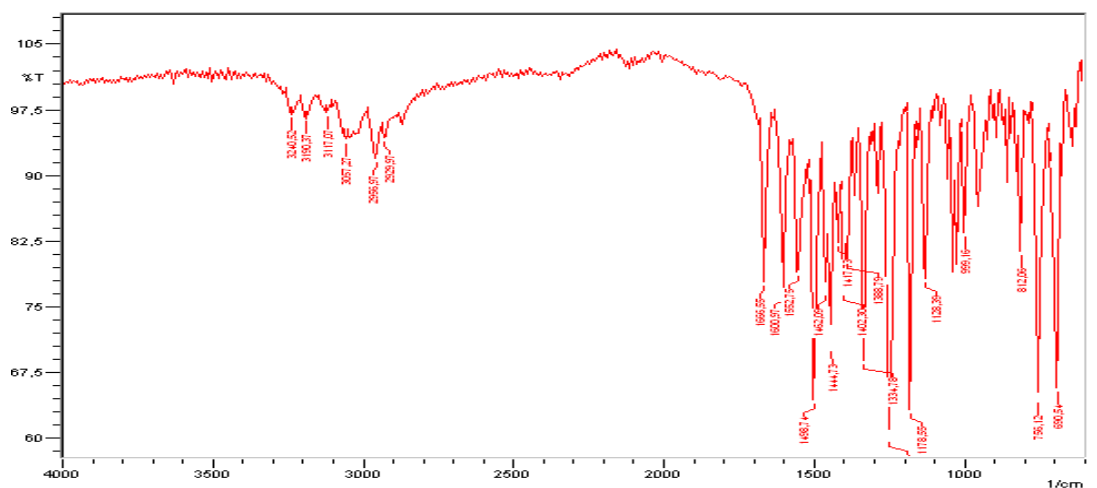


Figure S80: HPLC chromatogram of **21**

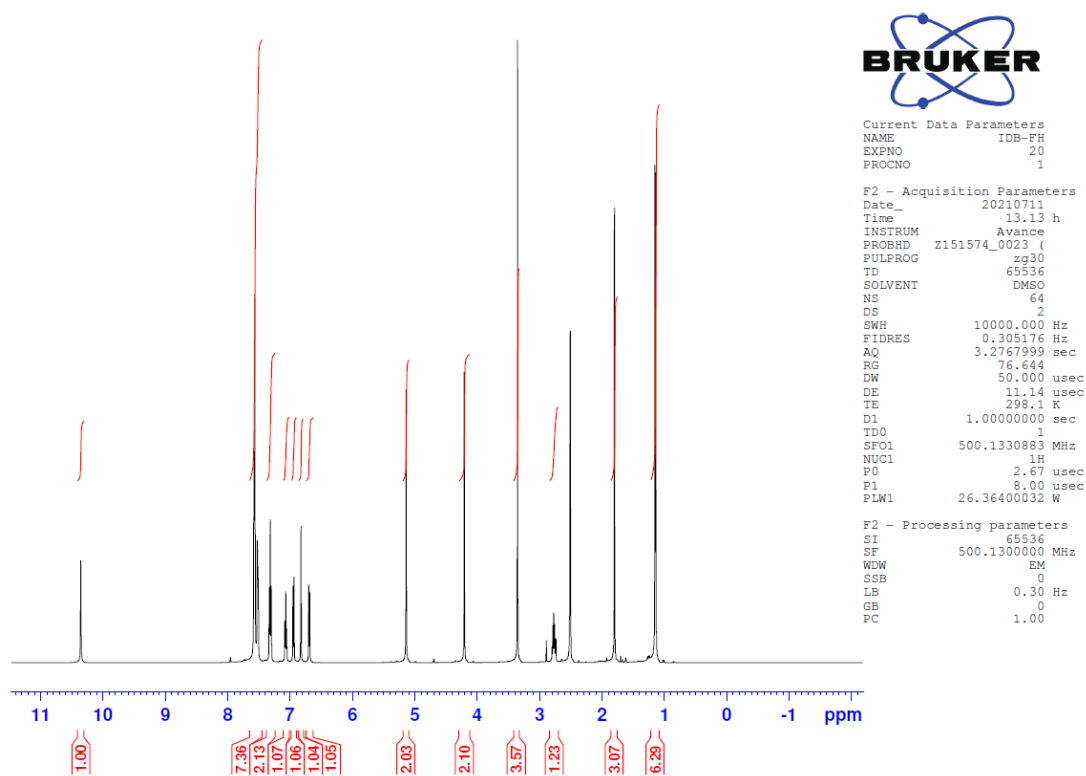


Figure S81: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of **21**

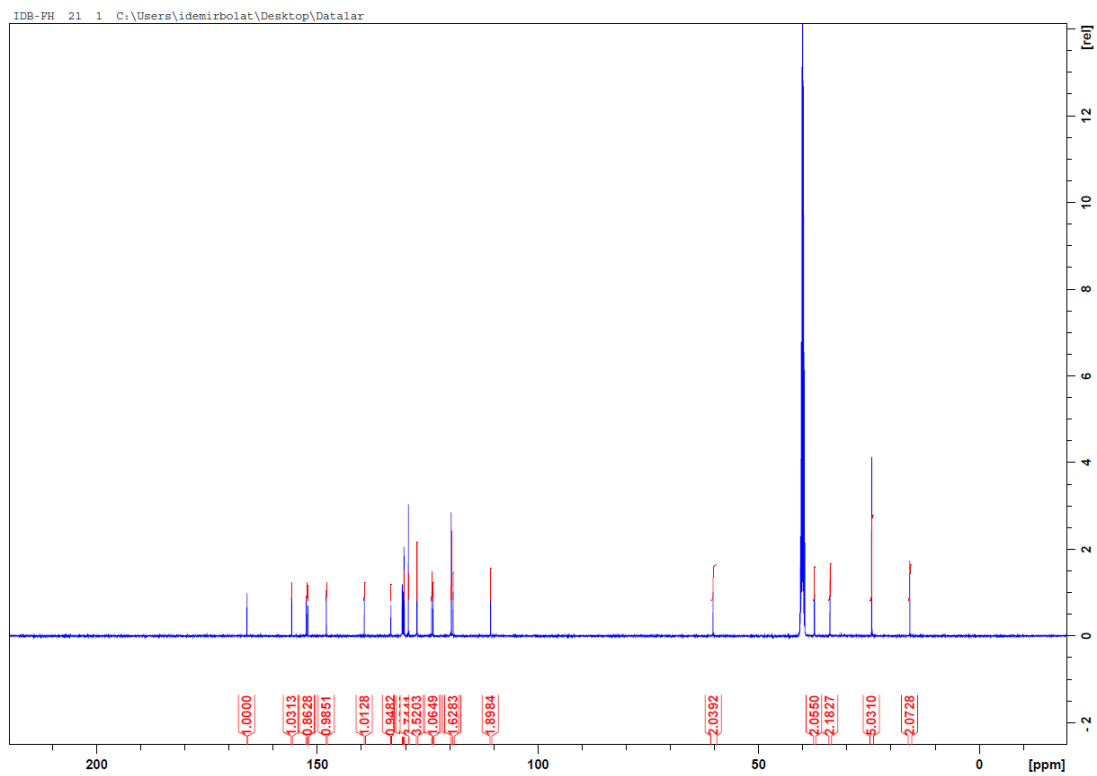


Figure S82: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **21**

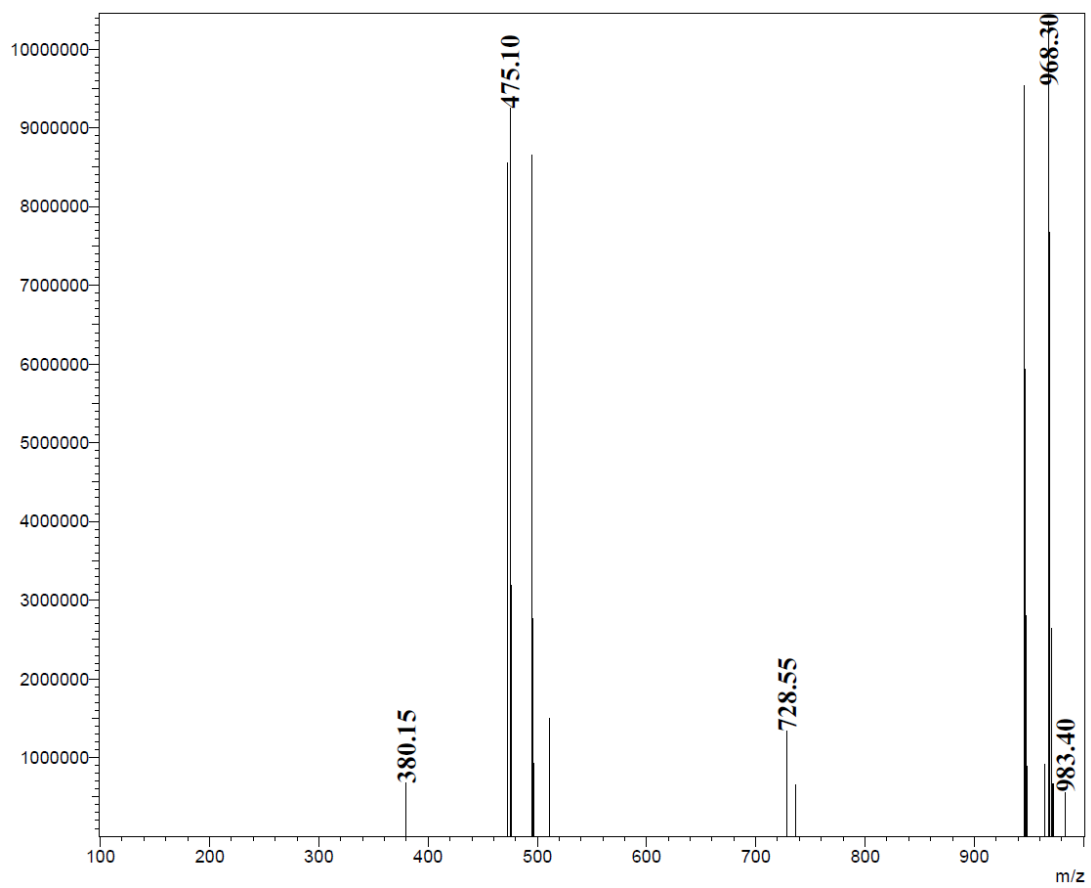


Figure S83: ESI(+)-MS Spectrum of **21**

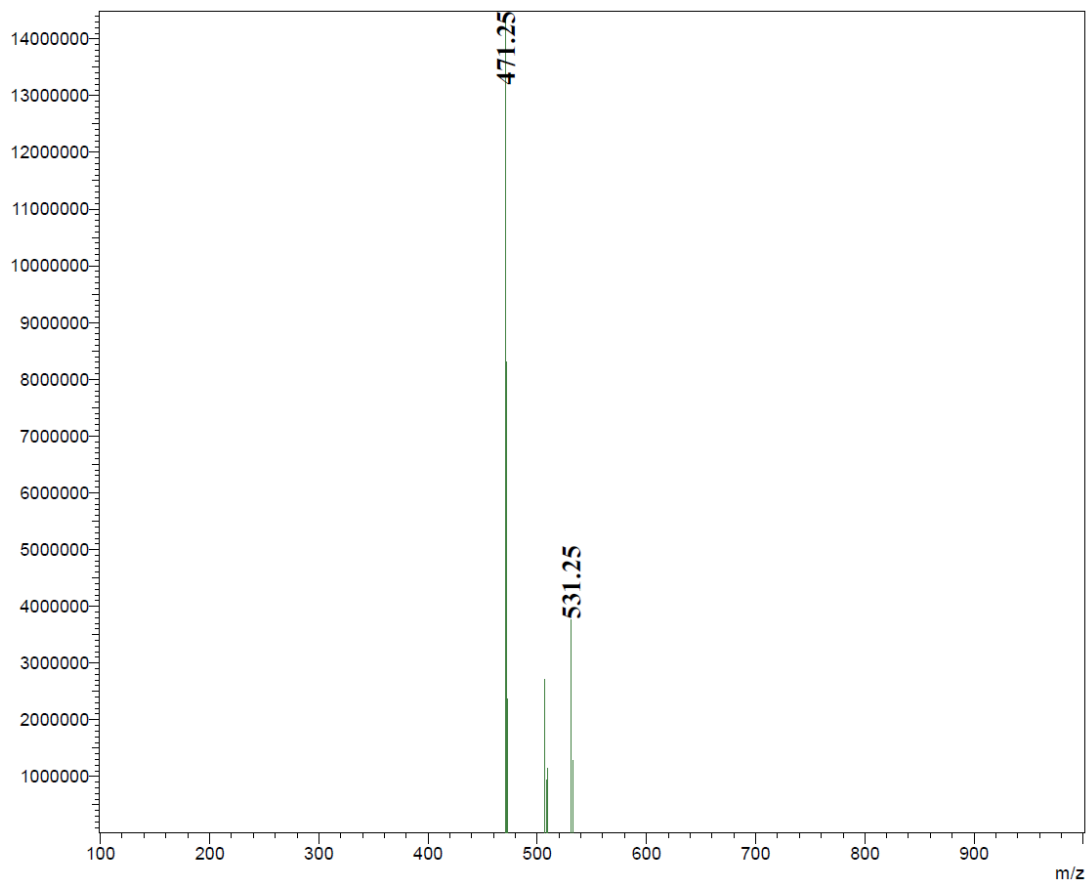


Figure S84: ESI(-)-MS Spectrum of **21**

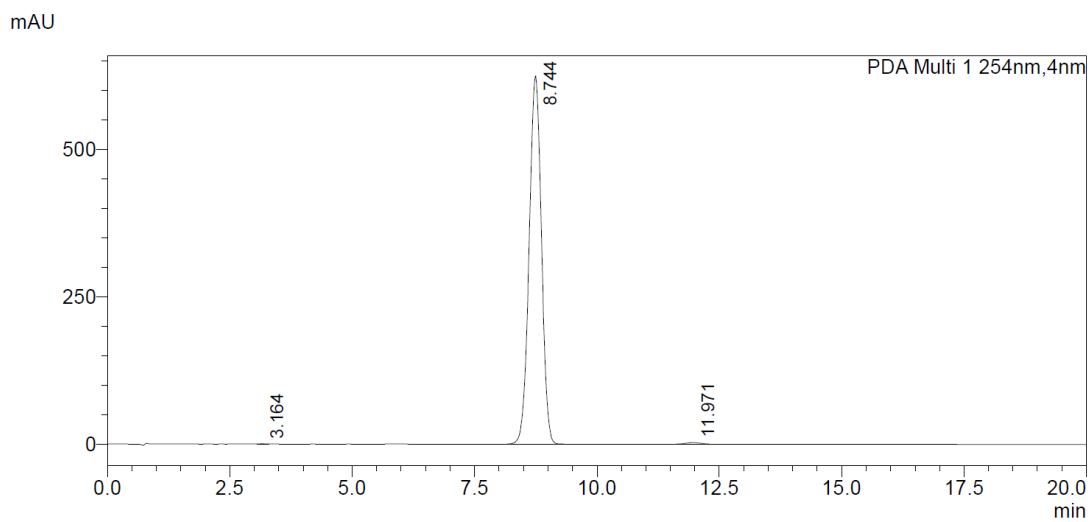


Figure S85: HPLC chromatogram of **21**

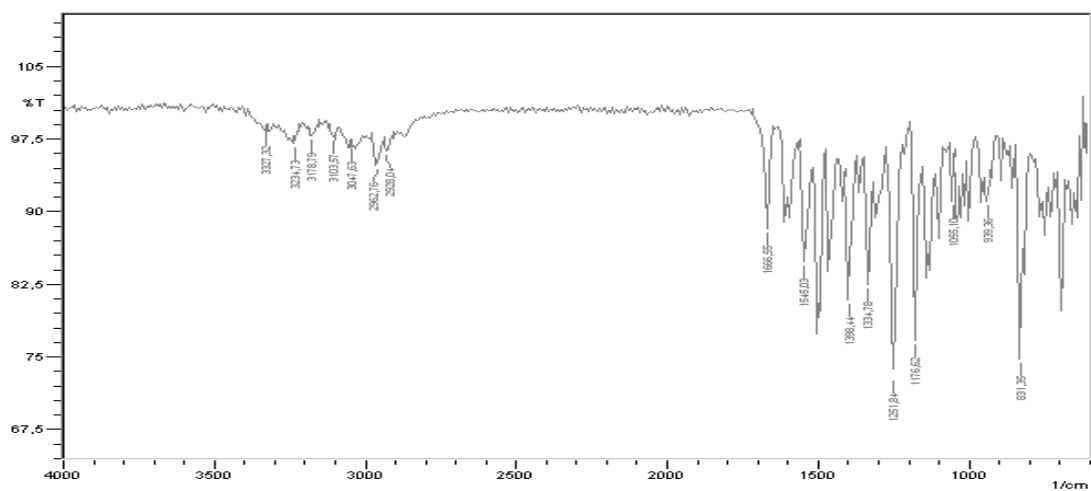


Figure S86: FTIR spectrum of 22

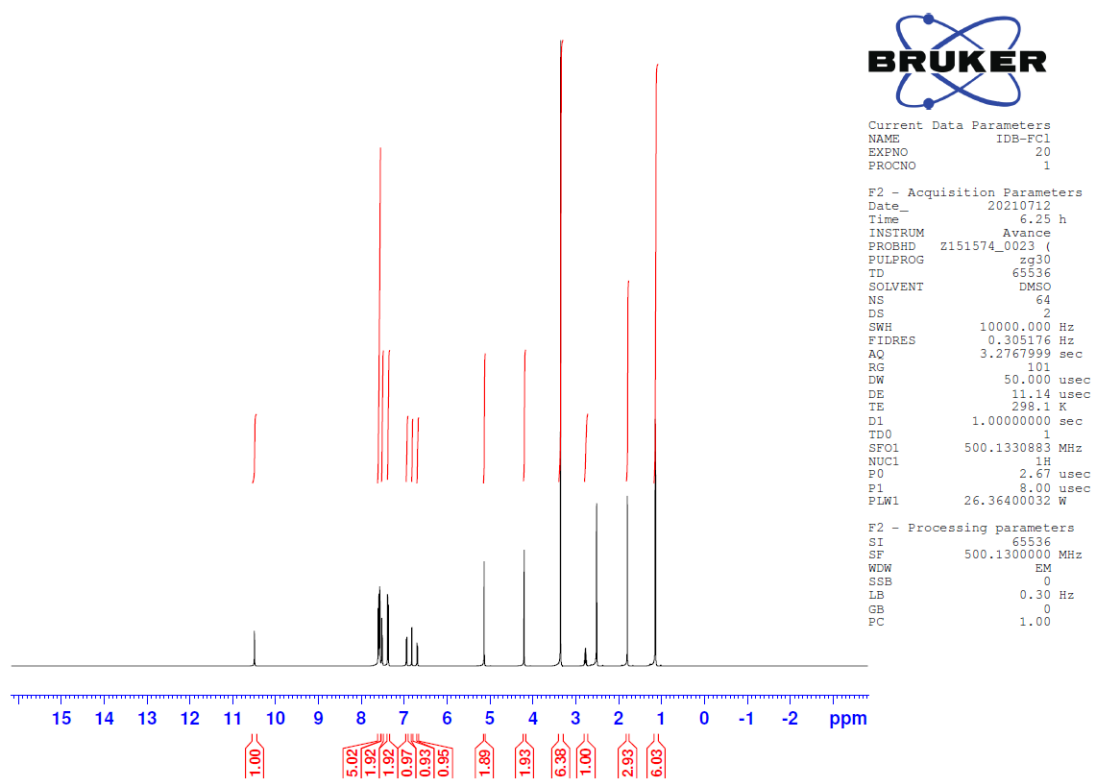


Figure S87: ¹H-NMR (500 MHz, DMSO) Spectrum of 22

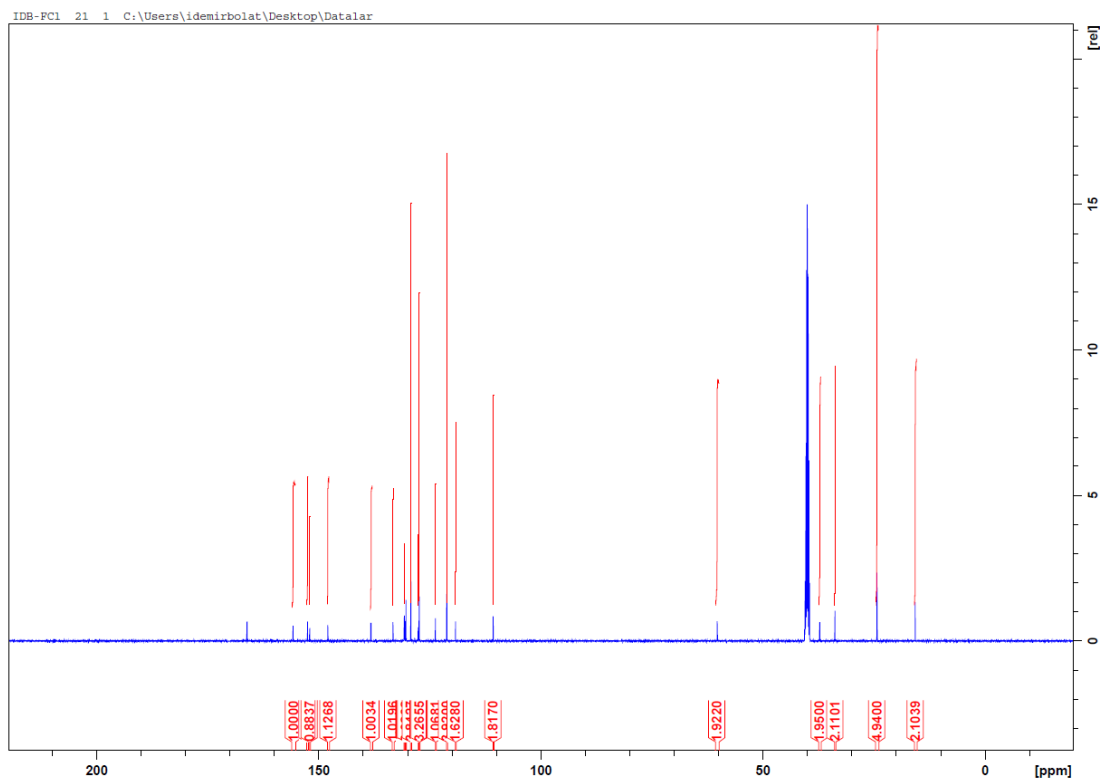


Figure S88: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **22**

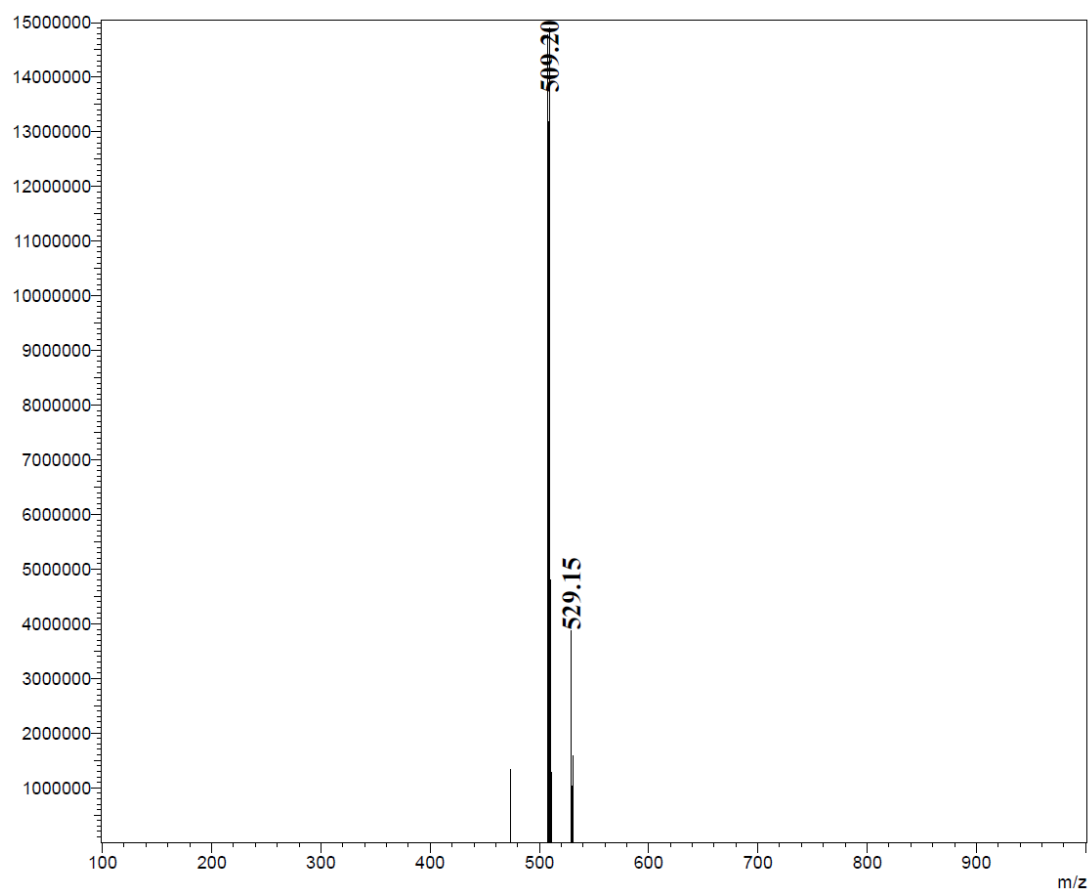


Figure S89: ESI(+)-MS Spectrum of **22**

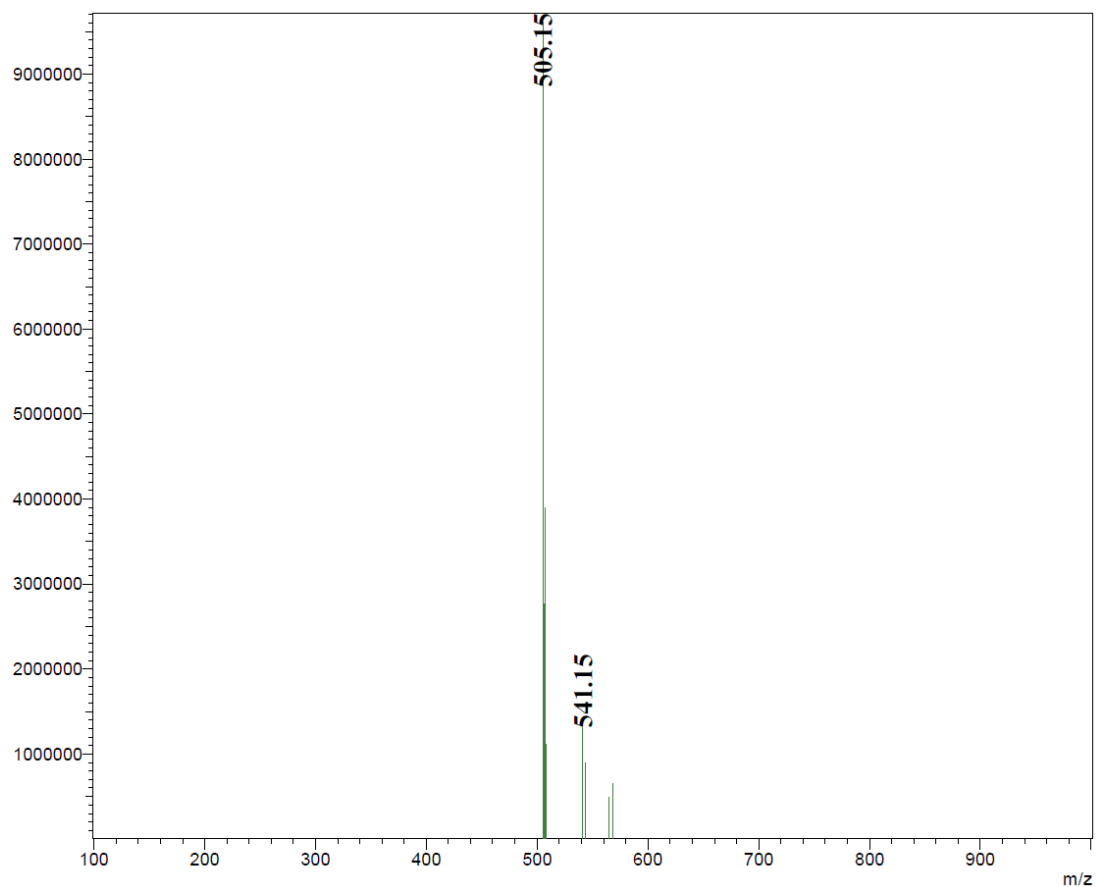


Figure S90: ESI(-)-MS Spectrum of **22**

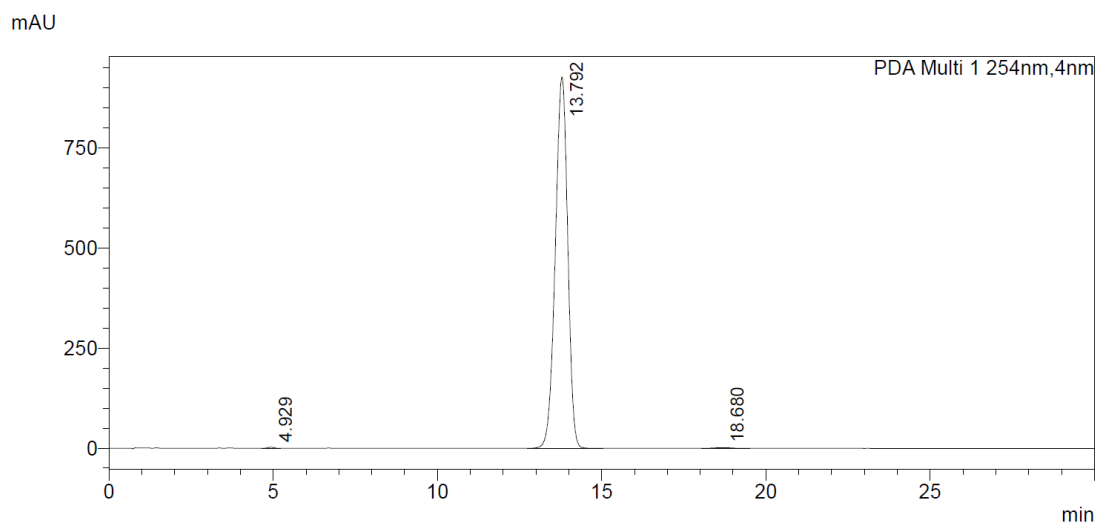


Figure S91: HPLC chromatogram of **22**

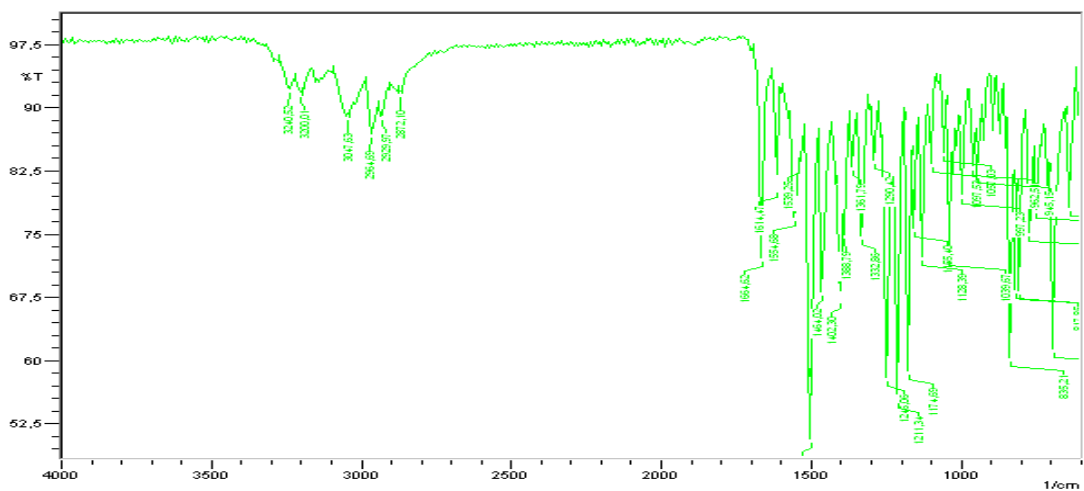


Figure S92: FTIR spectrum of 23

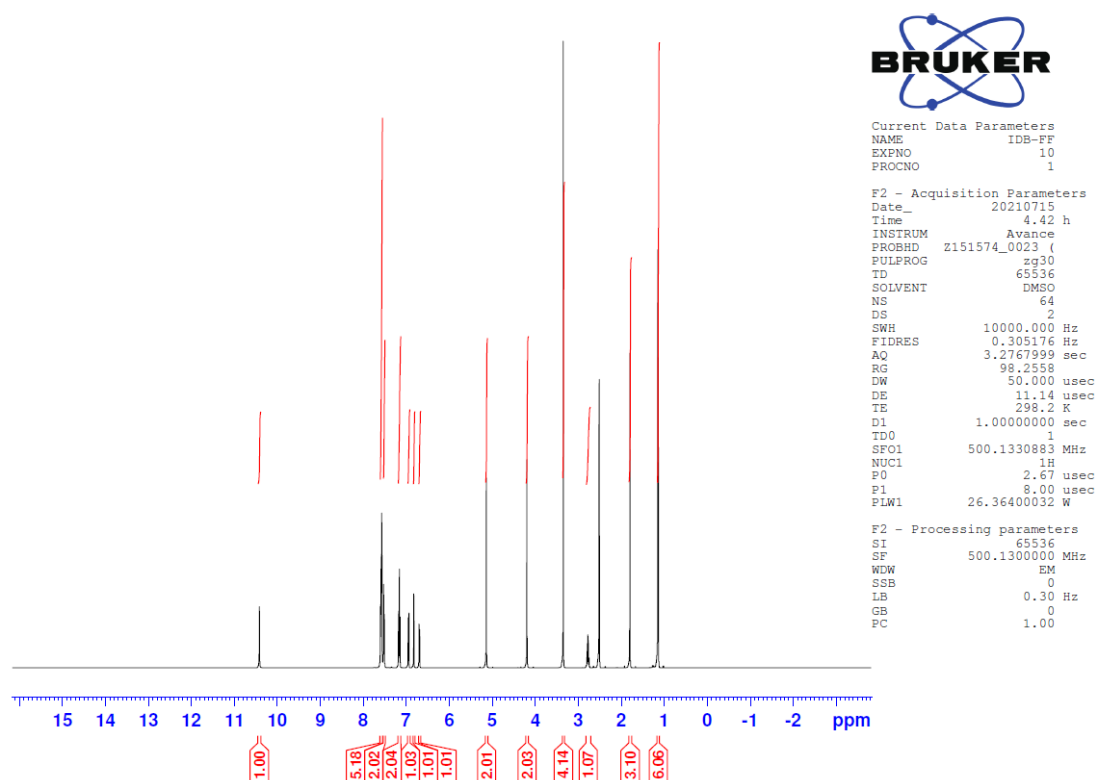


Figure S93: ¹H-NMR (500 MHz, DMSO) Spectrum of 23

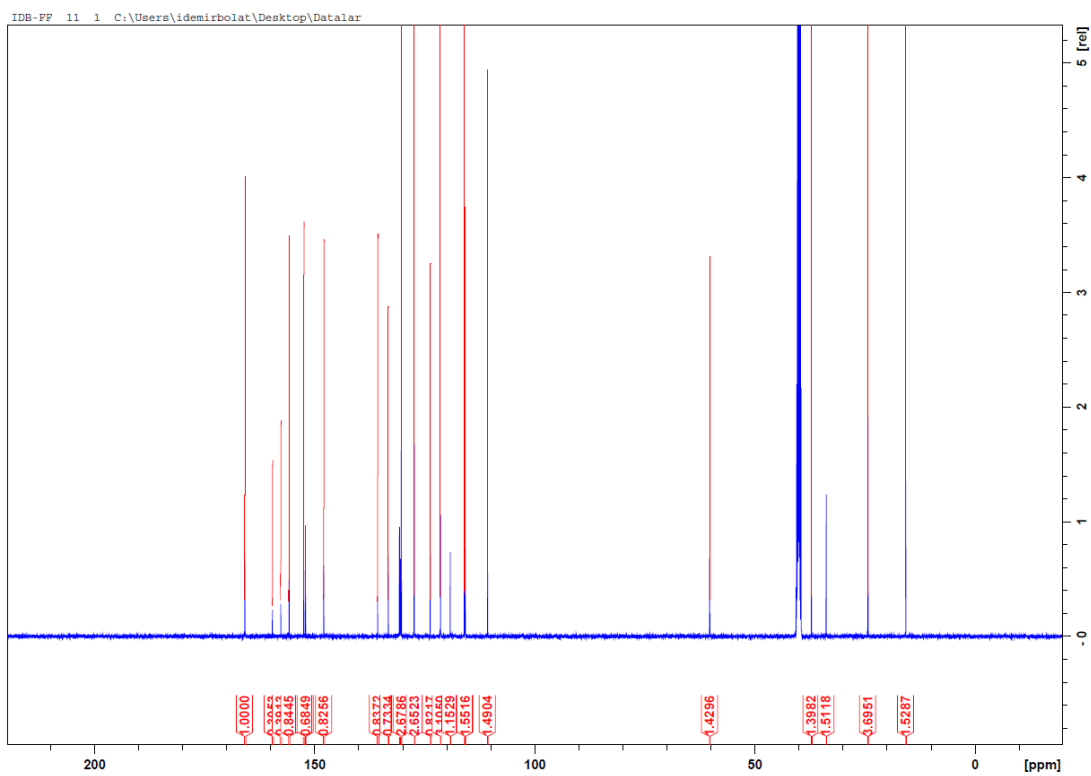


Figure S94: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **23**

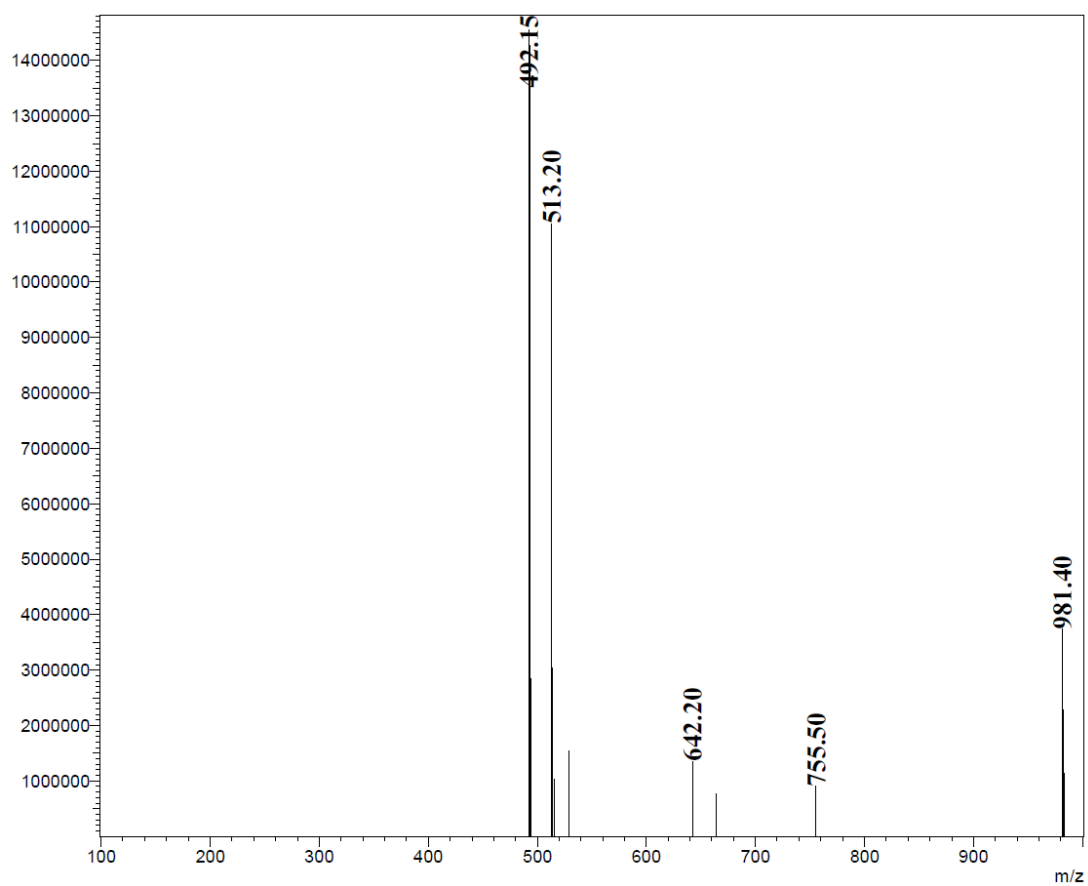


Figure S95: ESI(+)-MS Spectrum of **23**

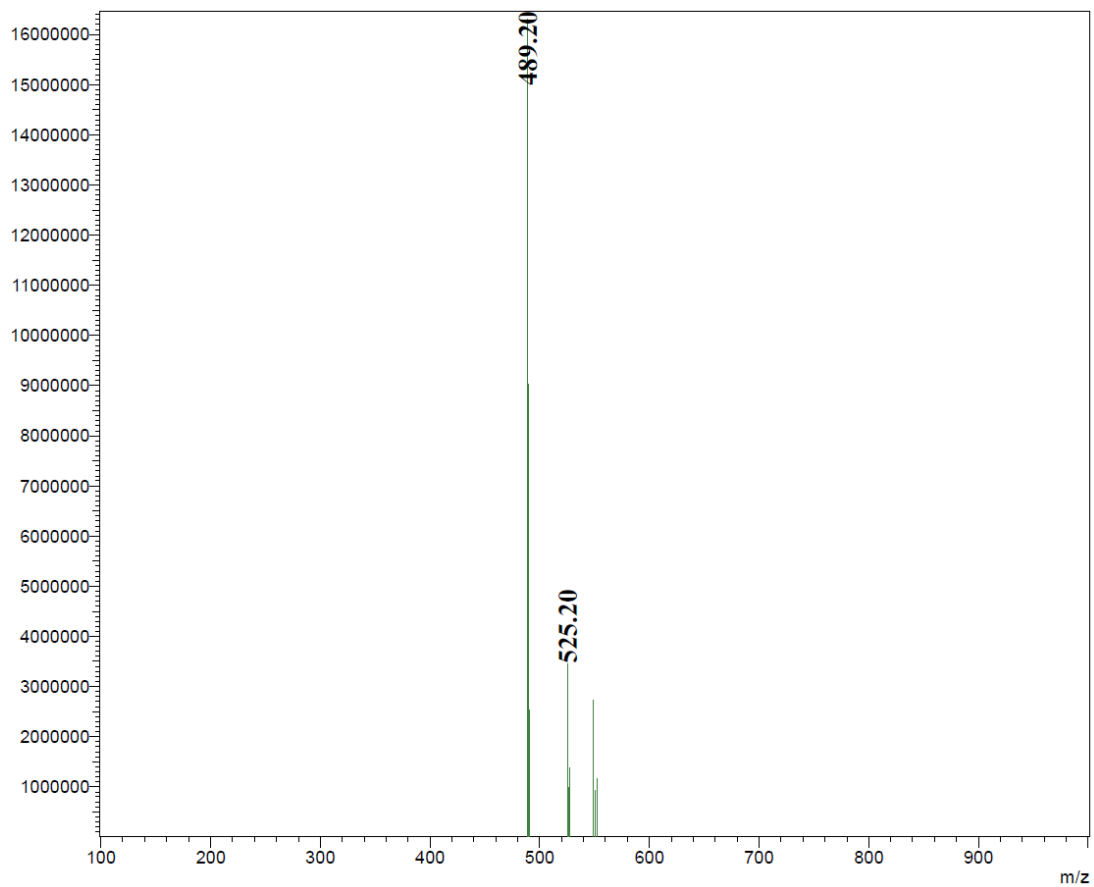


Figure S96: ESI(-)-MS Spectrum of **23**

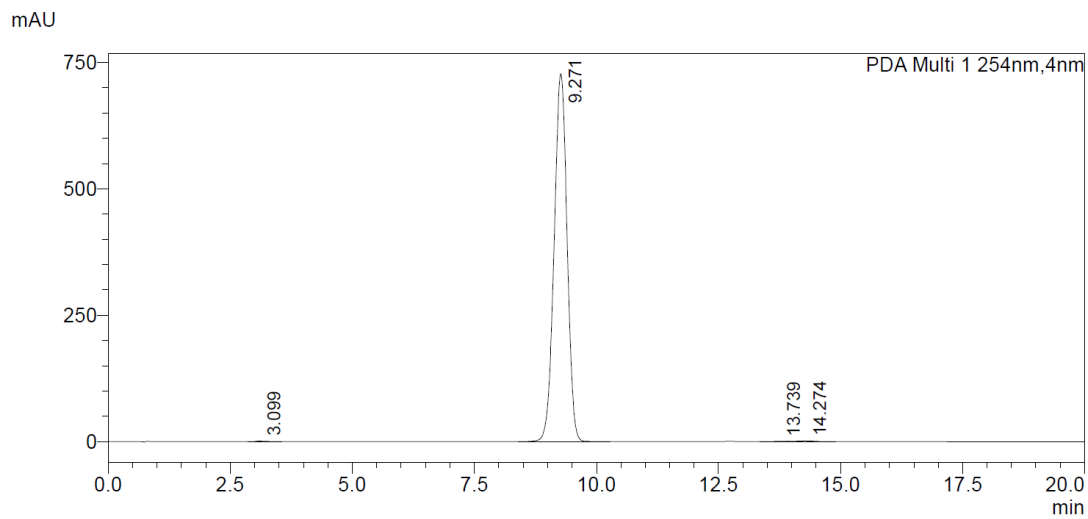


Figure S97: HPLC chromatogram of **23**

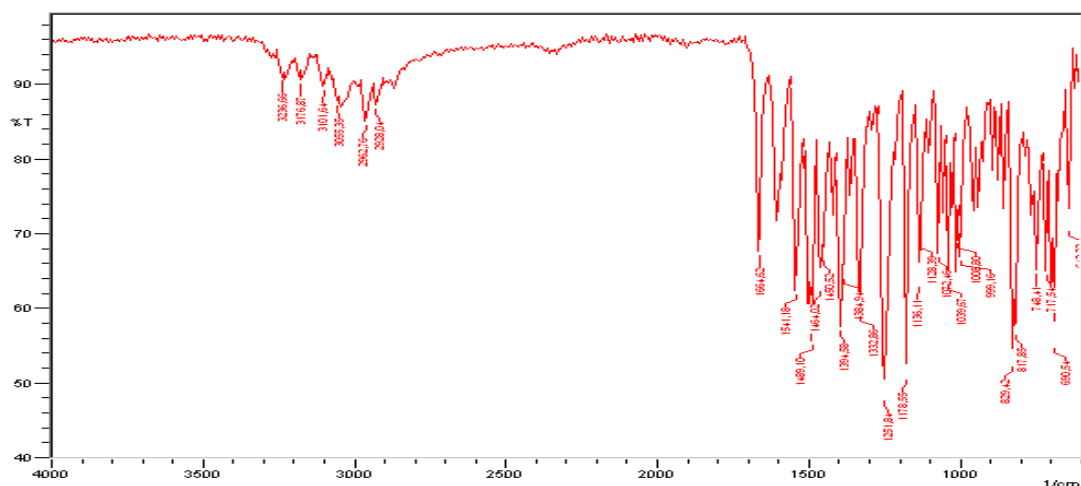


Figure S98: FTIR spectrum of 24

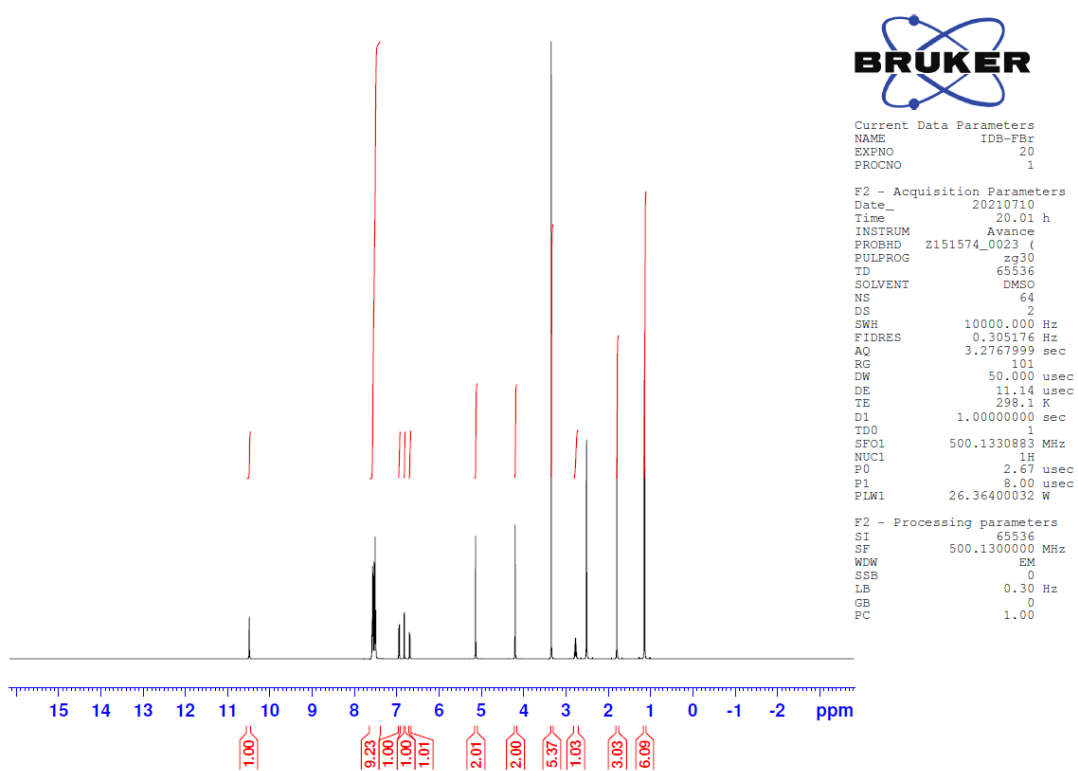
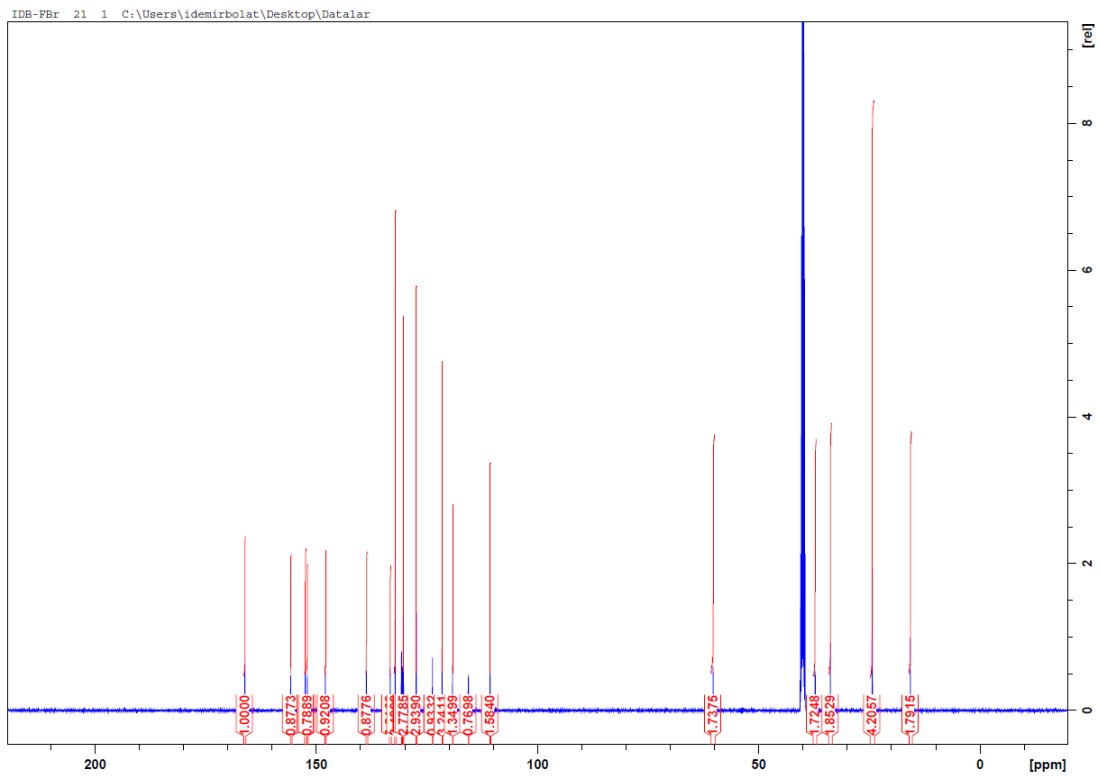


Figure S99: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of 24



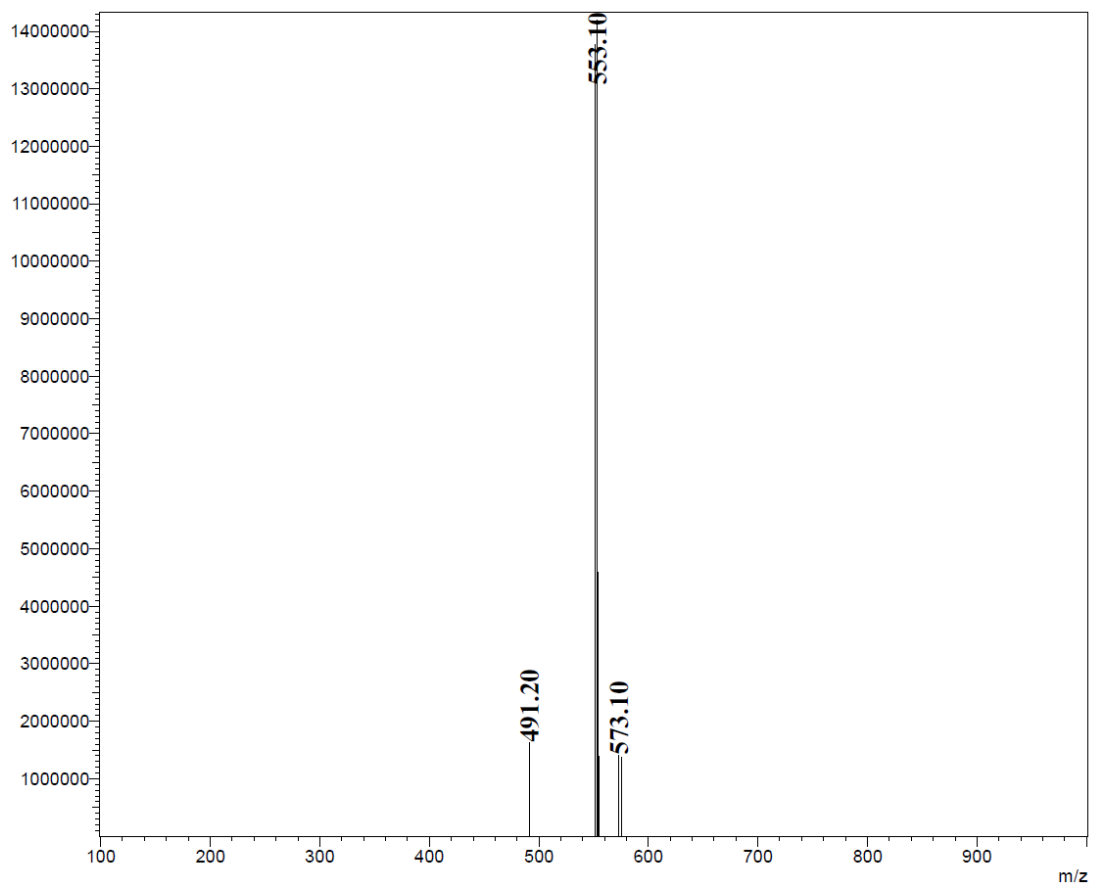


Figure S101: ESI(+)-MS Spectrum of 24

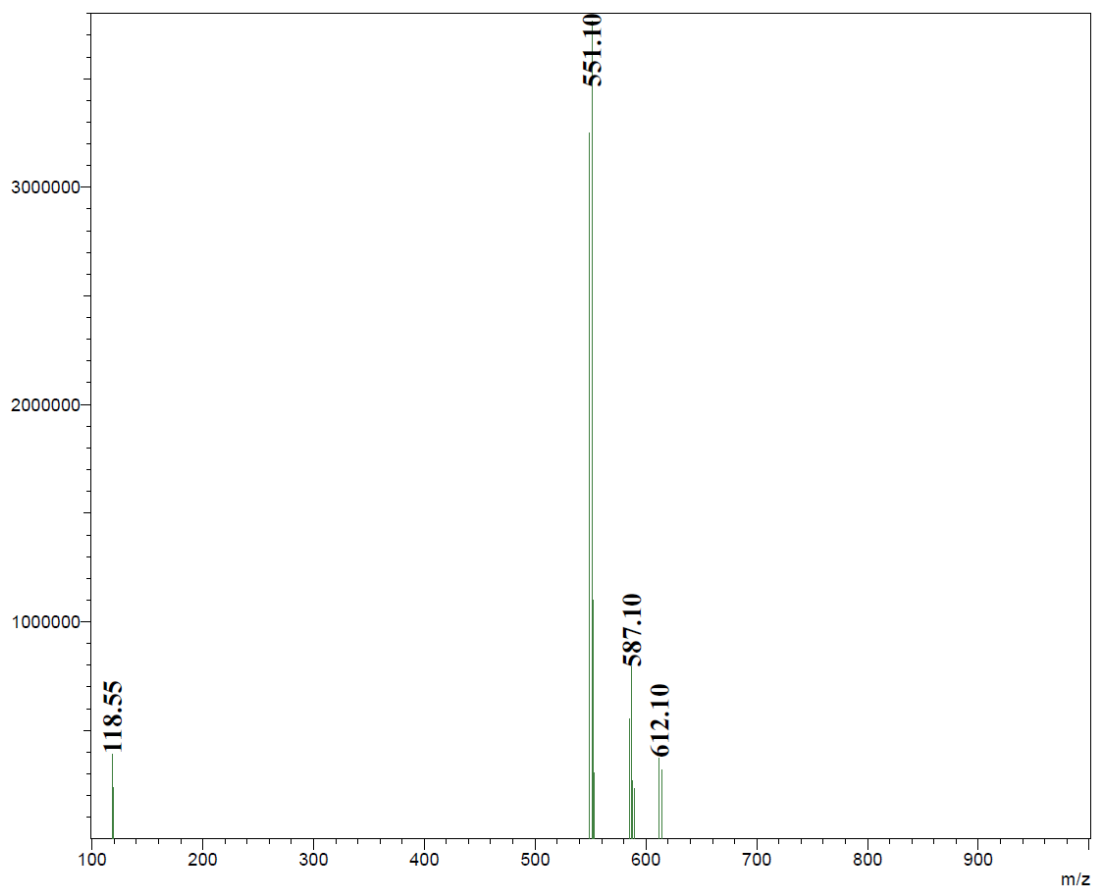


Figure S102: ESI(-)-MS Spectrum of 24

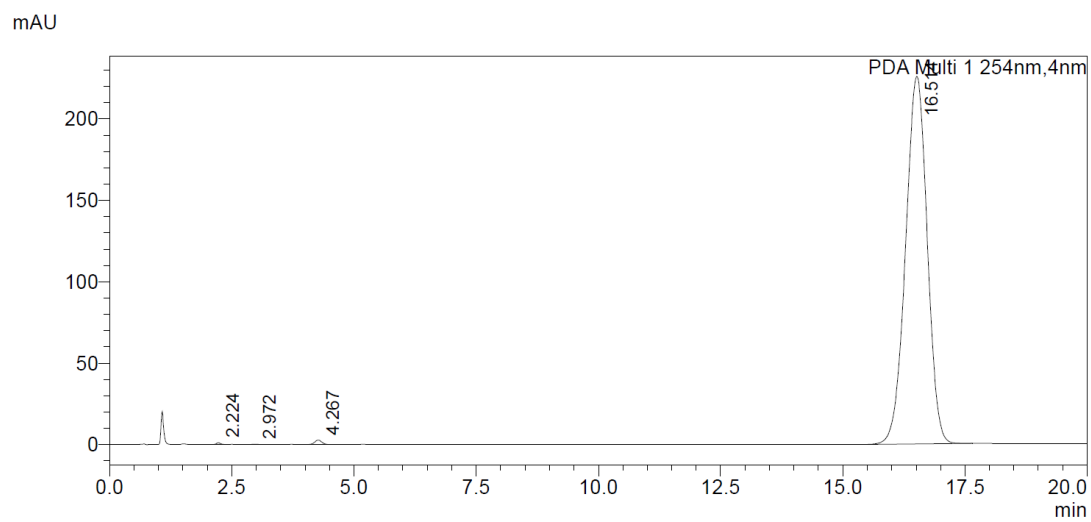


Figure S103: HPLC chromatogram of 24

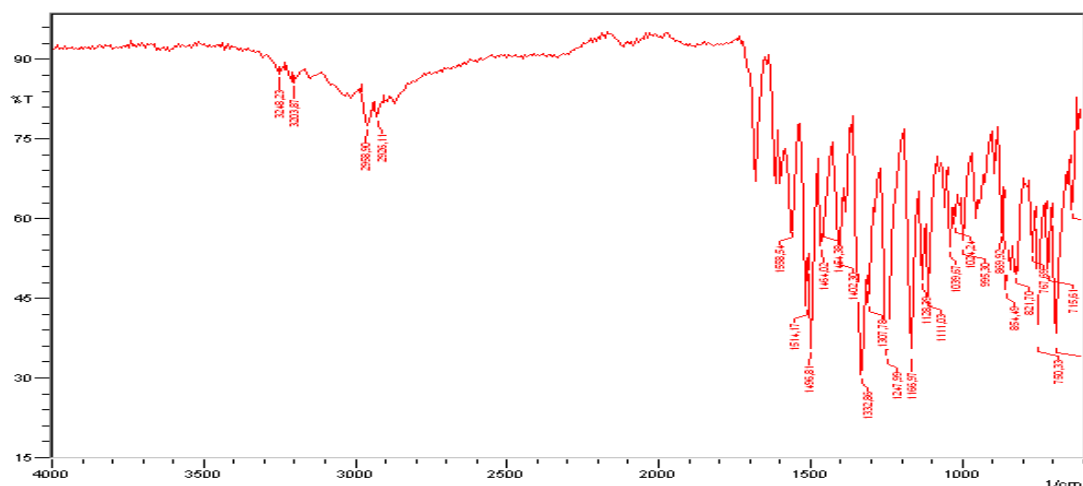


Figure S104: FTIR spectrum of **25**

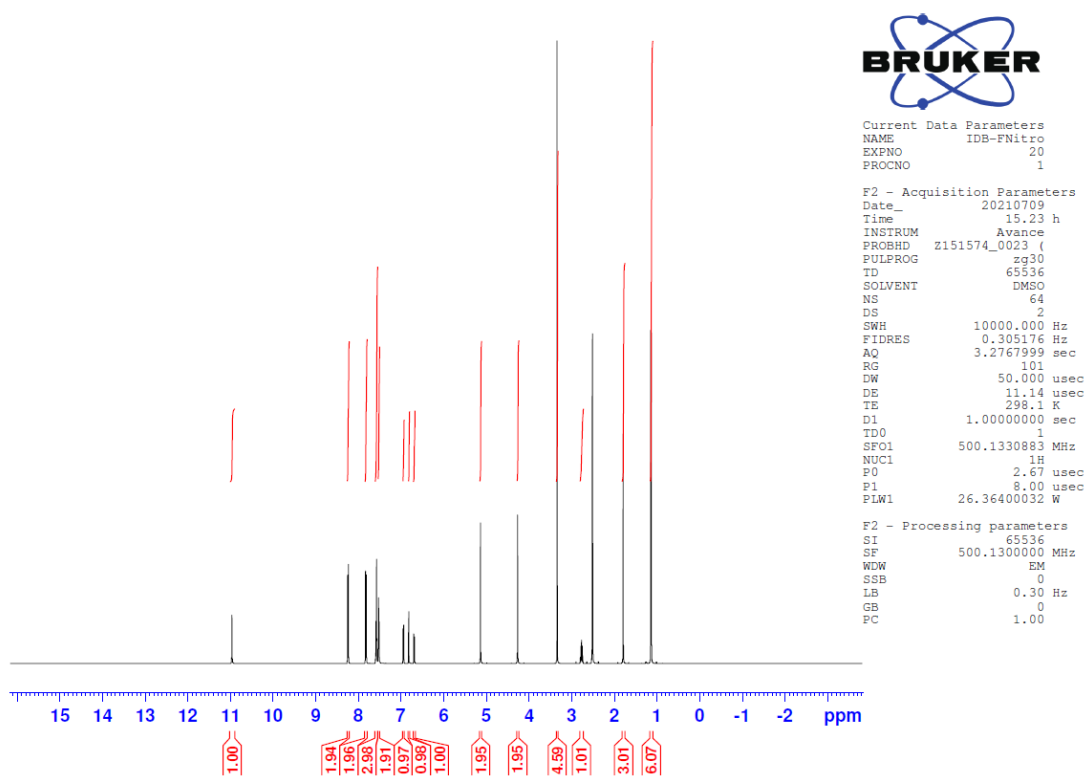


Figure S105: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of **25**

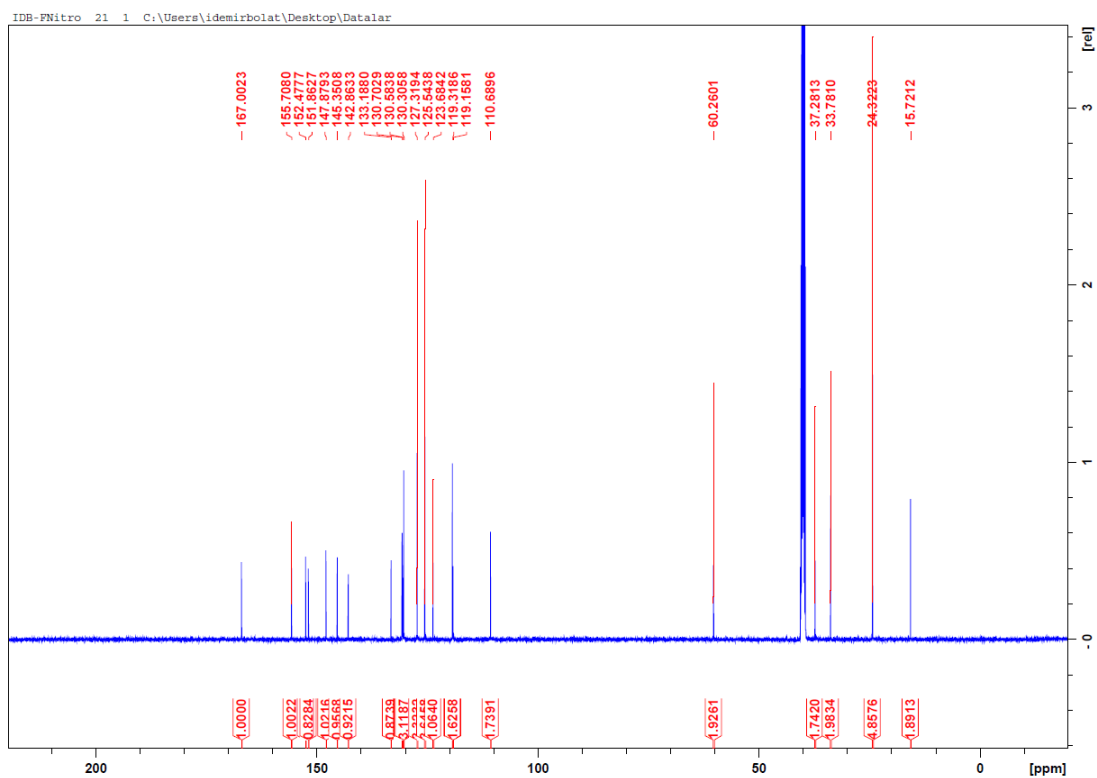


Figure S106: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **25**

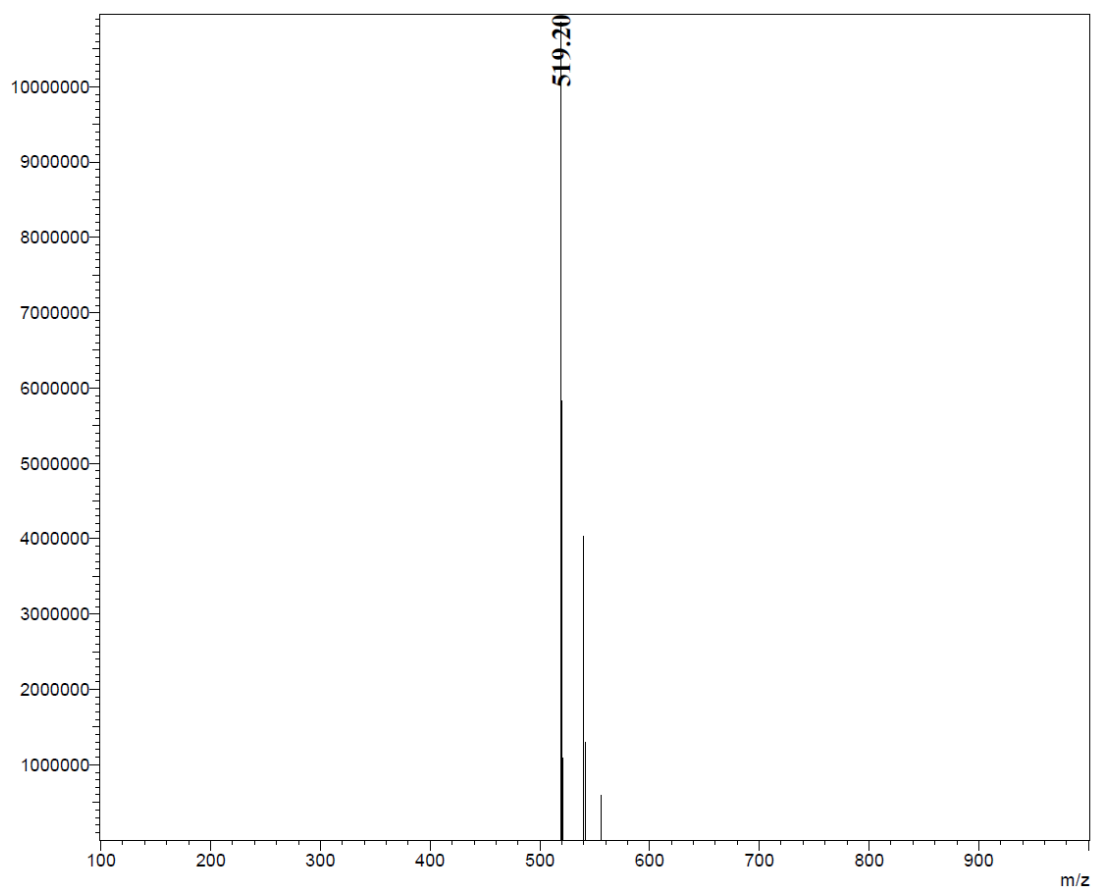


Figure S107: ESI(+)-MS Spectrum of 25

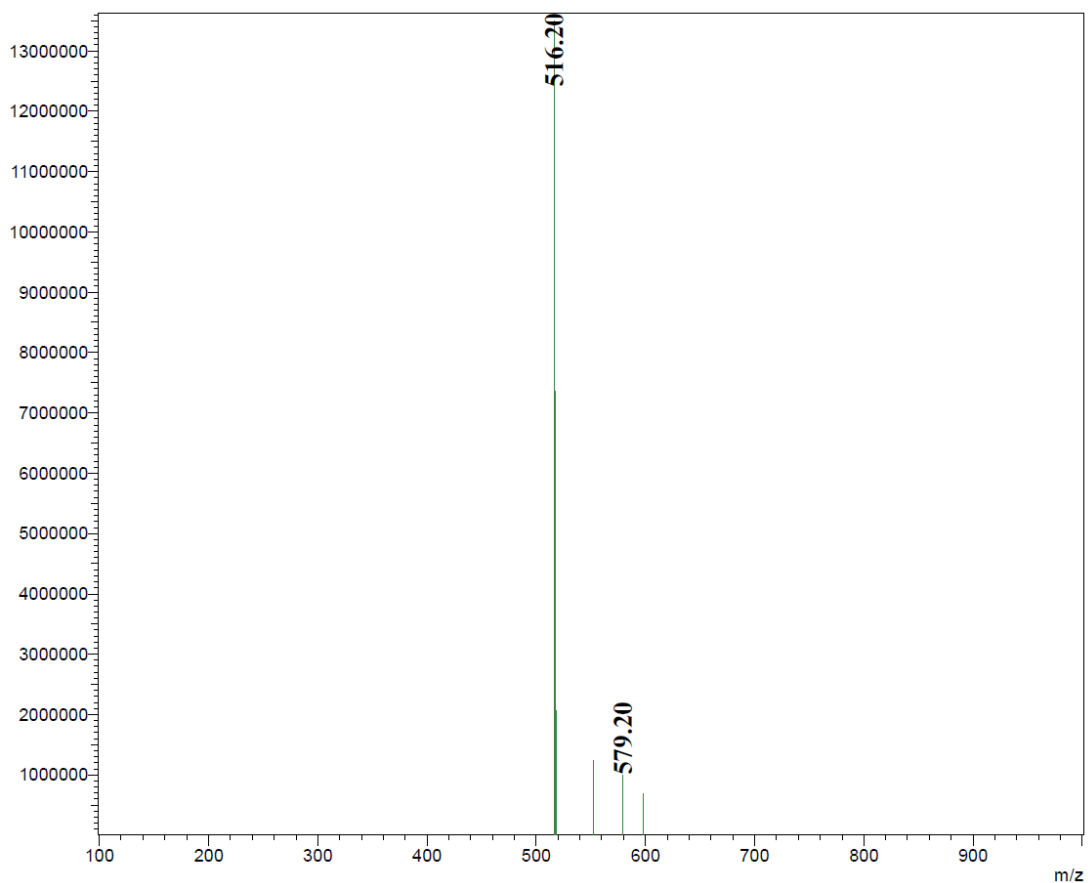


Figure S108: ESI(-)-MS Spectrum of 25

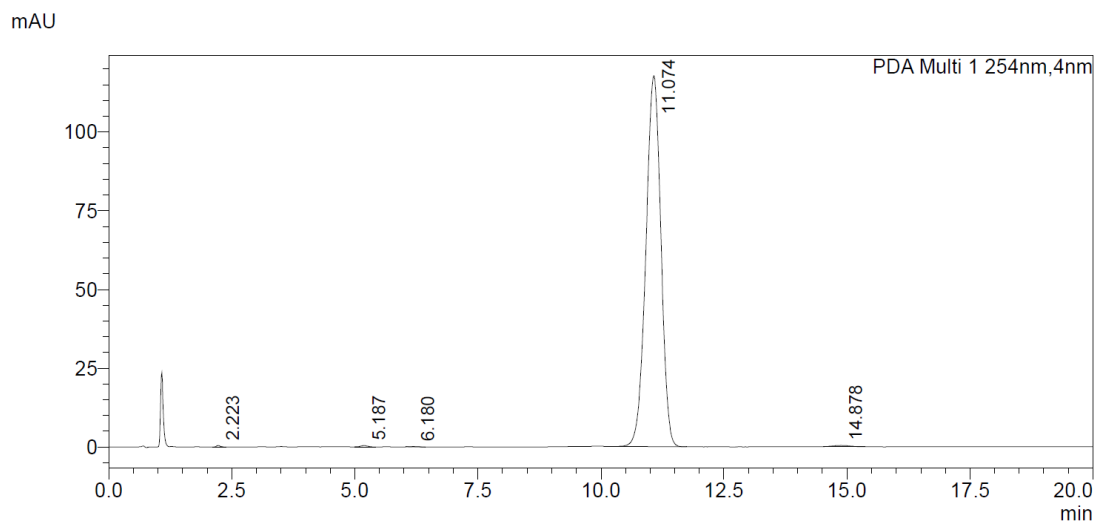


Figure S109: HPLC chromatogram of 25

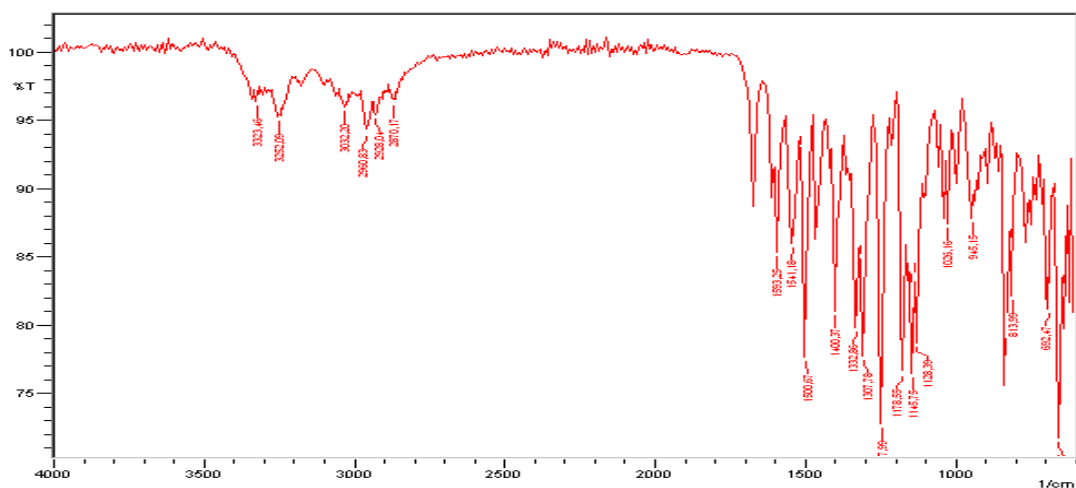


Figure S110: FTIR spectrum of **26**

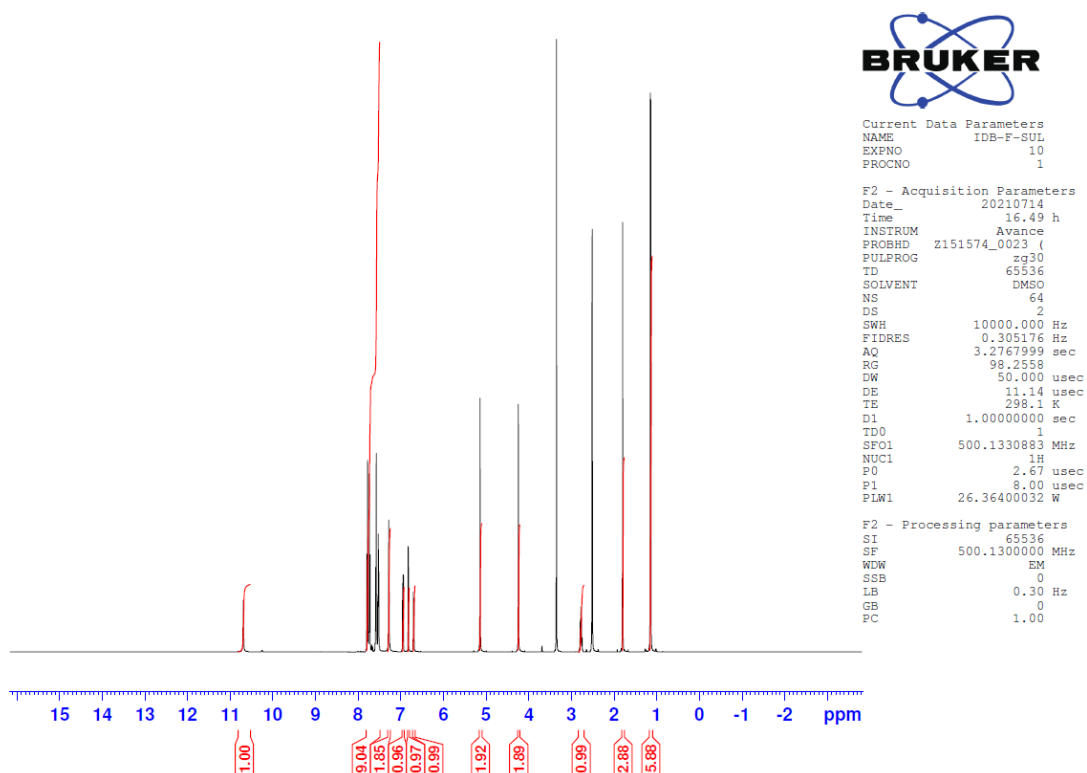


Figure S111: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of **26**

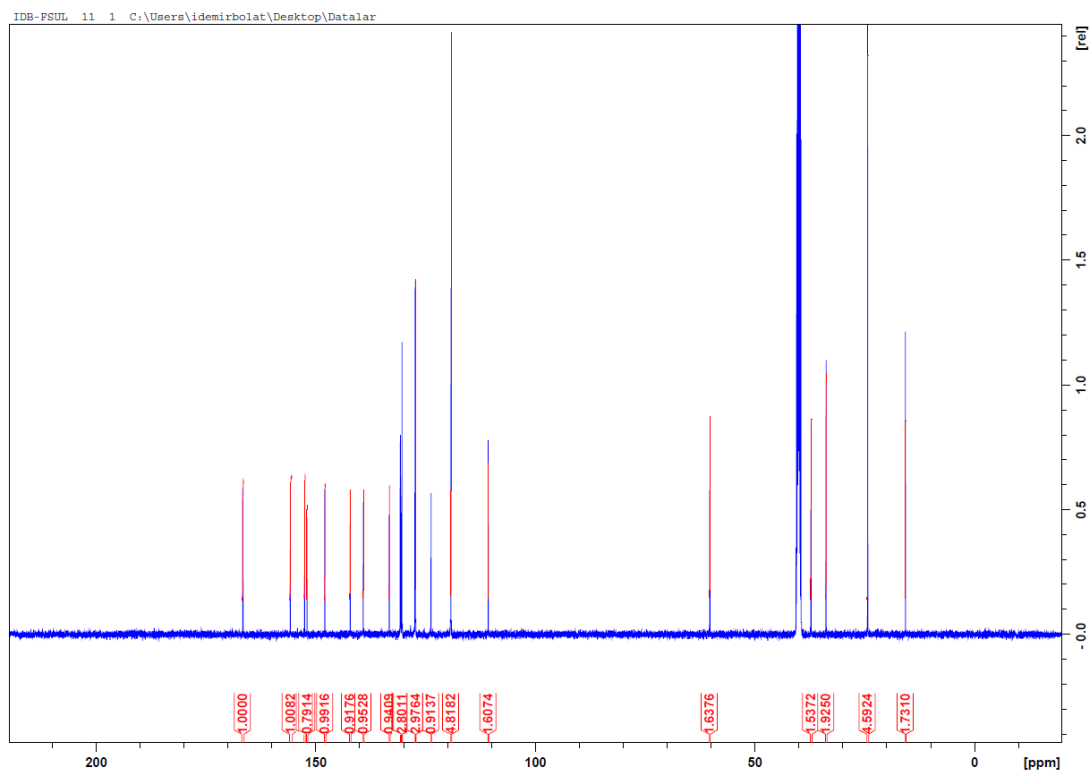


Figure S112: ^{13}C -NMR (125 MHz, DMSO) Spectrum of **26**

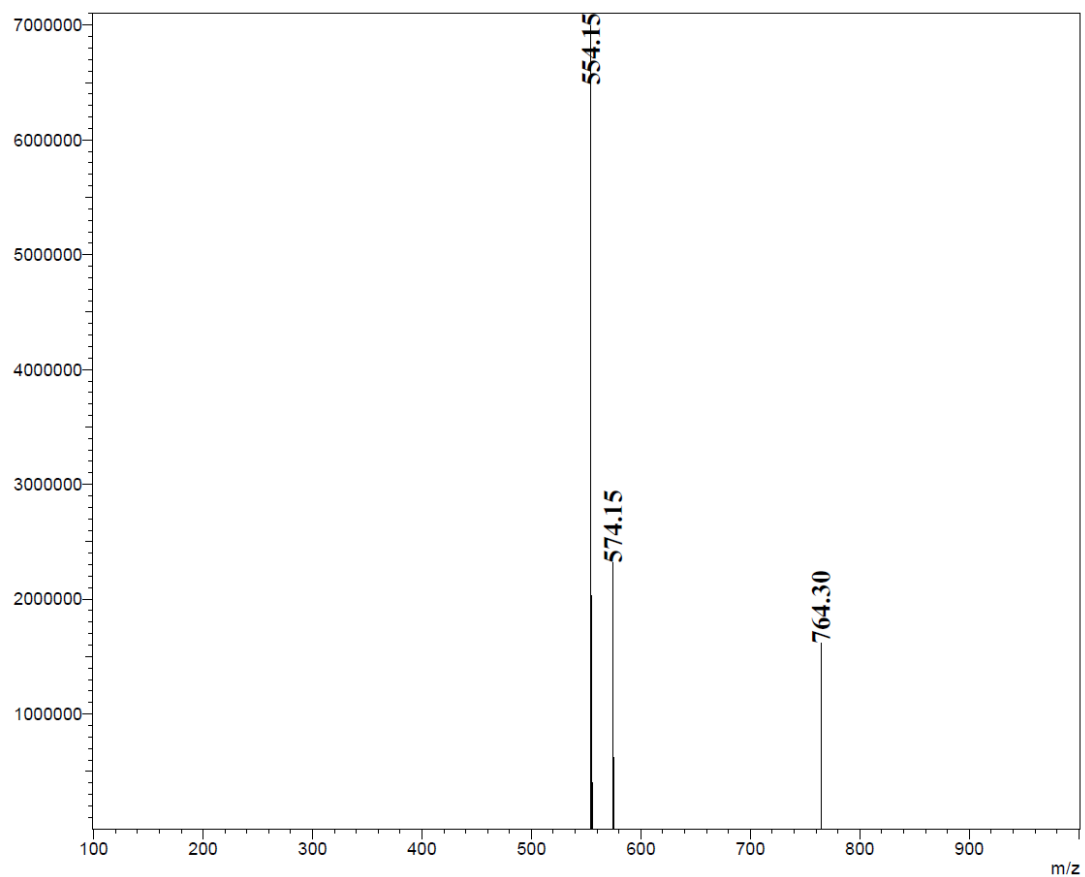


Figure S113: ESI(+)-MS Spectrum of 26

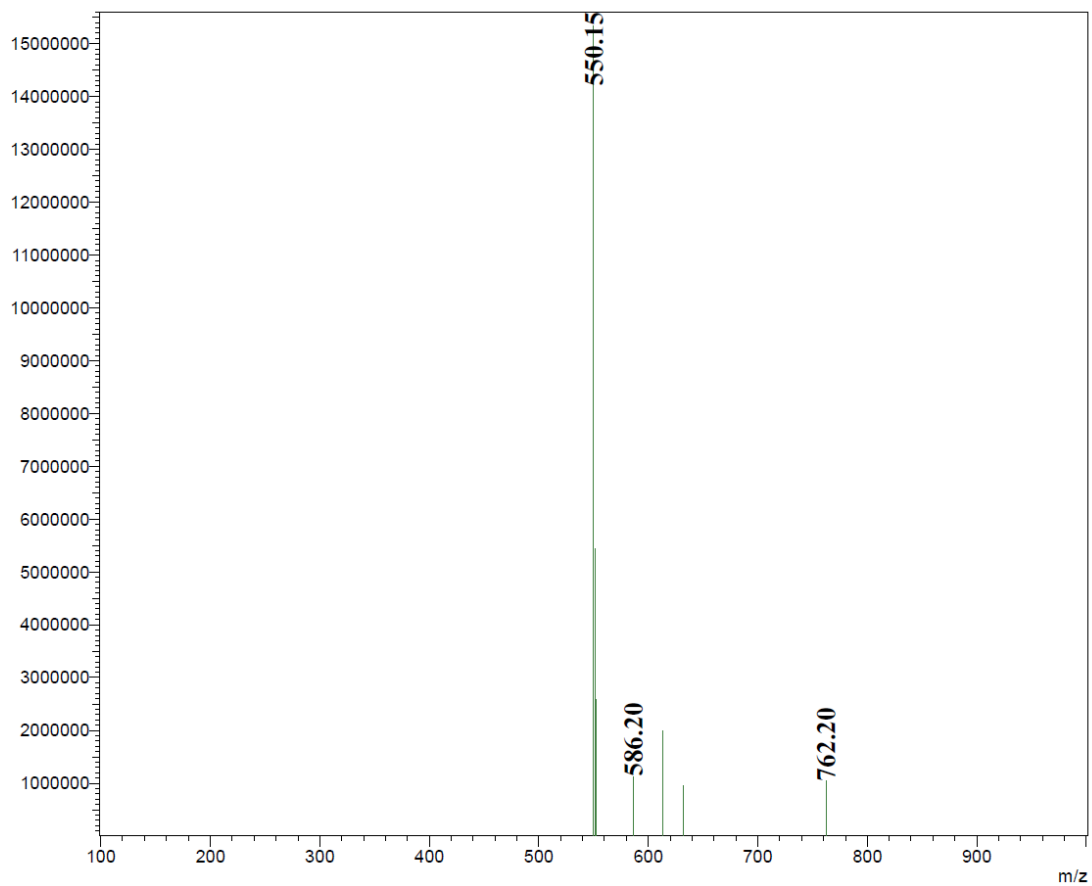


Figure S114: ESI(-)-MS Spectrum of 26

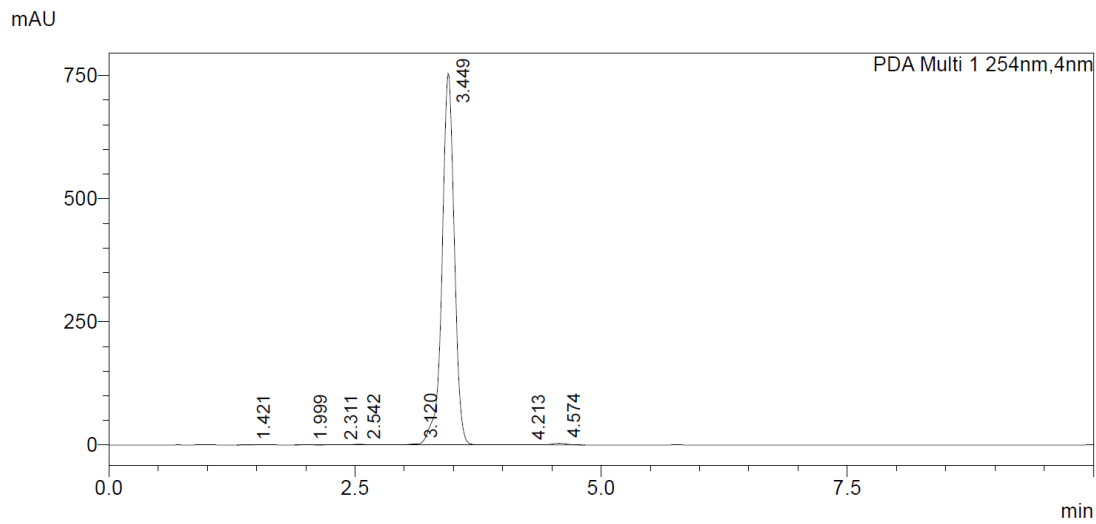


Figure S115: ESI(-)-MS Spectrum of 26

Table S1: ADMET profiles of compounds **9-26**.

Comp.	MW (g/mol)	LogP _{o/w}	LogS (ESOL)	<i>n</i> -ON	<i>n</i> -OHNH	<i>n</i> -ROTB	TPSA (Å ²)	%ABS*	<i>Lipinski's rule</i> <i>n</i> -violation	<i>Mutagenic</i>	<i>Tumorigenic</i>
9	410.53	3.76	-4.85	4	1	9	94.34	76.45	-	none	none
10	444.98	4.14	-5.44	4	1	9	94.34	76.45	-	none	none
11	428.52	3.95	-5.01	5	1	9	94.34	76.45	-	none	none
12	489.43	4.28	-5.76	4	1	9	94.34	76.45	-	none	high
13	455.53	3.04	-4.91	6	1	10	140.16	60.65	-	none	none
14	489.61	2.34	-4.32	7	2	10	162.88	52.81	-	none	none
15	424.56	3.99	-5.05	4	1	10	94.34	76.45	-	none	none
16	459.00	4.53	-5.64	4	1	10	94.34	76.45	-	none	none
17	442.55	4.32	-5.21	5	1	10	94.34	76.45	-	none	none
18	503.46	4.58	-5.96	4	1	10	94.34	76.45	1 (MW>500)	none	high
19	469.56	3.27	-5.12	6	1	11	140.16	60.65	-	none	none
20	503.64	2.87	-4.52	7	2	11	162.88	52.81	1 (MW>500)	none	none
21	472.60	4.95	-6.28	4	1	10	94.34	76.45	-	none	none
22	507.05	5.52	-6.87	4	1	10	94.34	76.45	2 (MW>500; logP>5)	none	none
23	490.59	5.26	-6.44	5	1	10	94.34	76.45	1 (logP>5)	none	none
24	551.50	5.61	-7.19	4	1	10	94.34	76.45	2 (MW>500; logP>5)	none	high
25	517.60	4.41	-6.34	6	1	11	140.16	60.65	1 (MW>500)	none	none
26	551.68	3.77	-5.75	7	2	11	162.88	52.81	1 (MW>500)	none	none