

Supplementary Materials

New aspects of the reaction of thioacetamide and N-arylmaleimides

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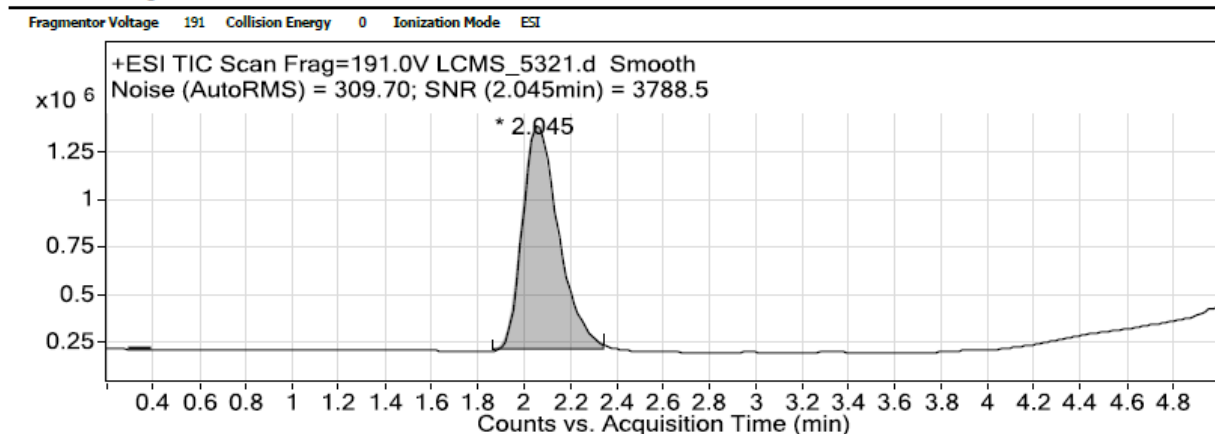
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User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.863	2.045	2.343	1173307.92	12879644.72	100	3788.5

Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Auto-RMS	Height	1	309.7027588

User Spectra

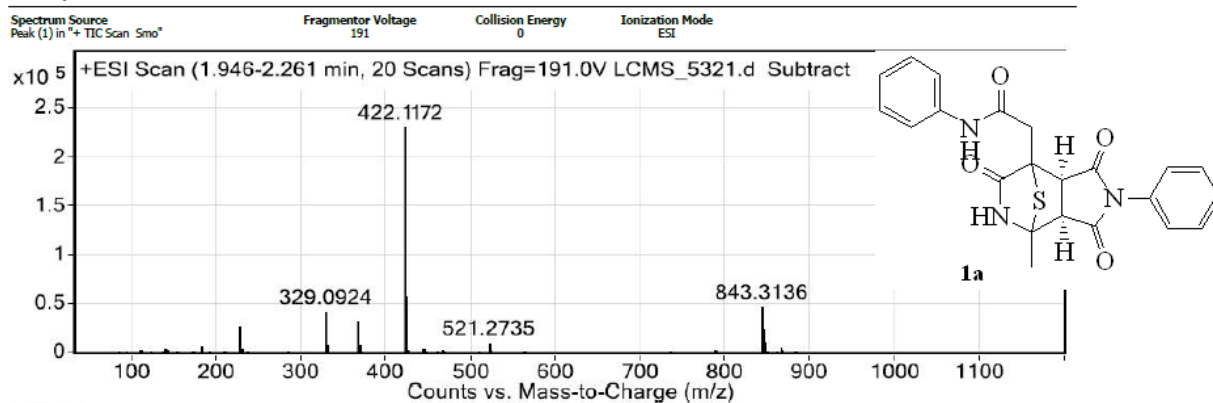


Figure S1: Data HPLC of compound **1a**

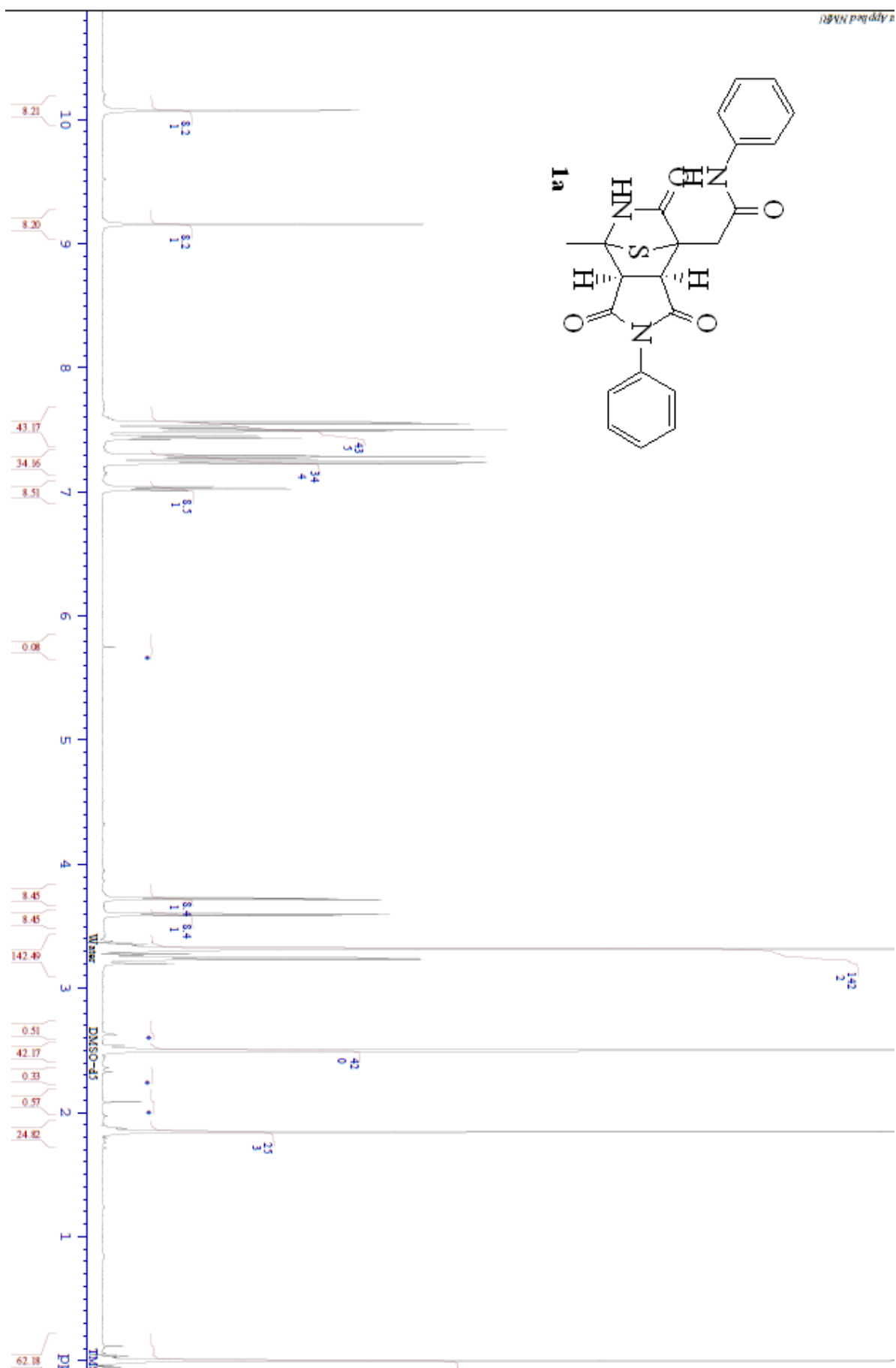
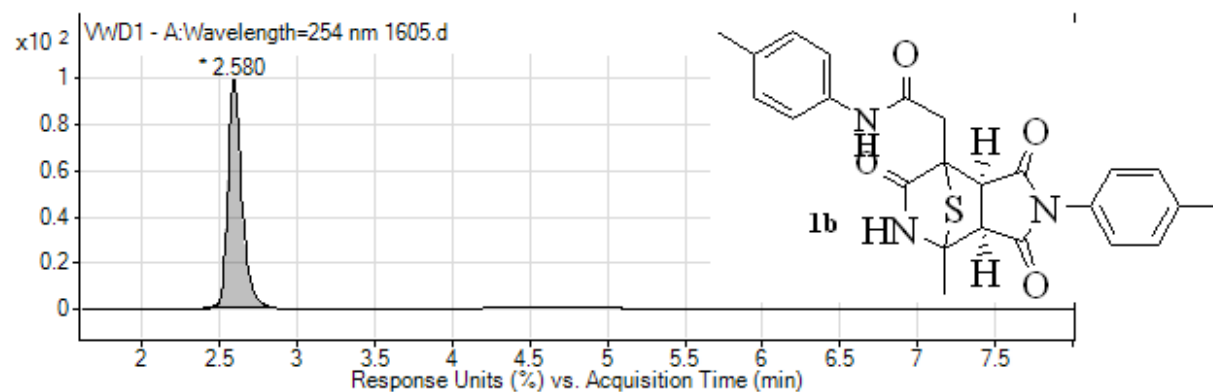


Figure S2: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **1a**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2,393	2,58	2,847	594,36	3743,44	100

User Spectra

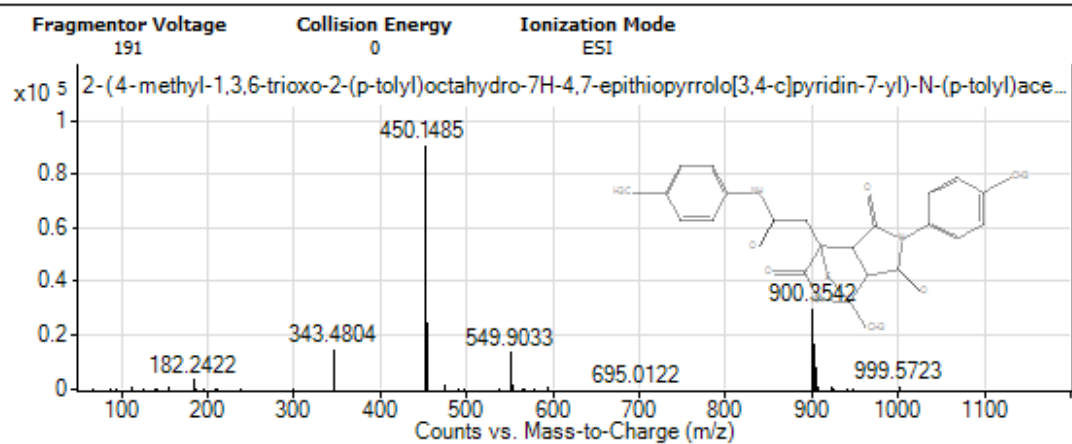


Figure S3: Data HPLC of compound **1b**

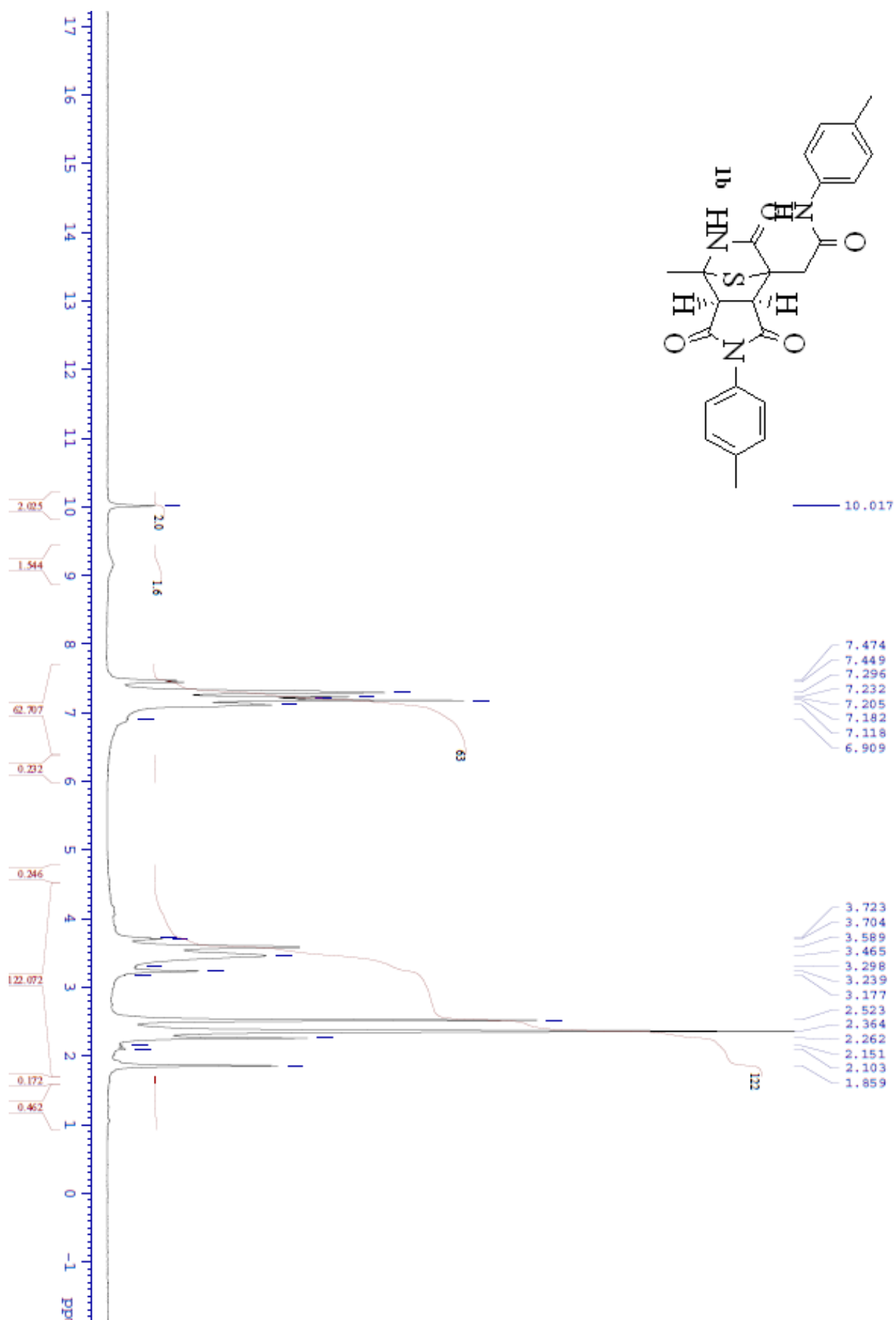


Figure S4: ^1H NMR spectrum (500 MHz, DMSO- d_6) of compound **1b**

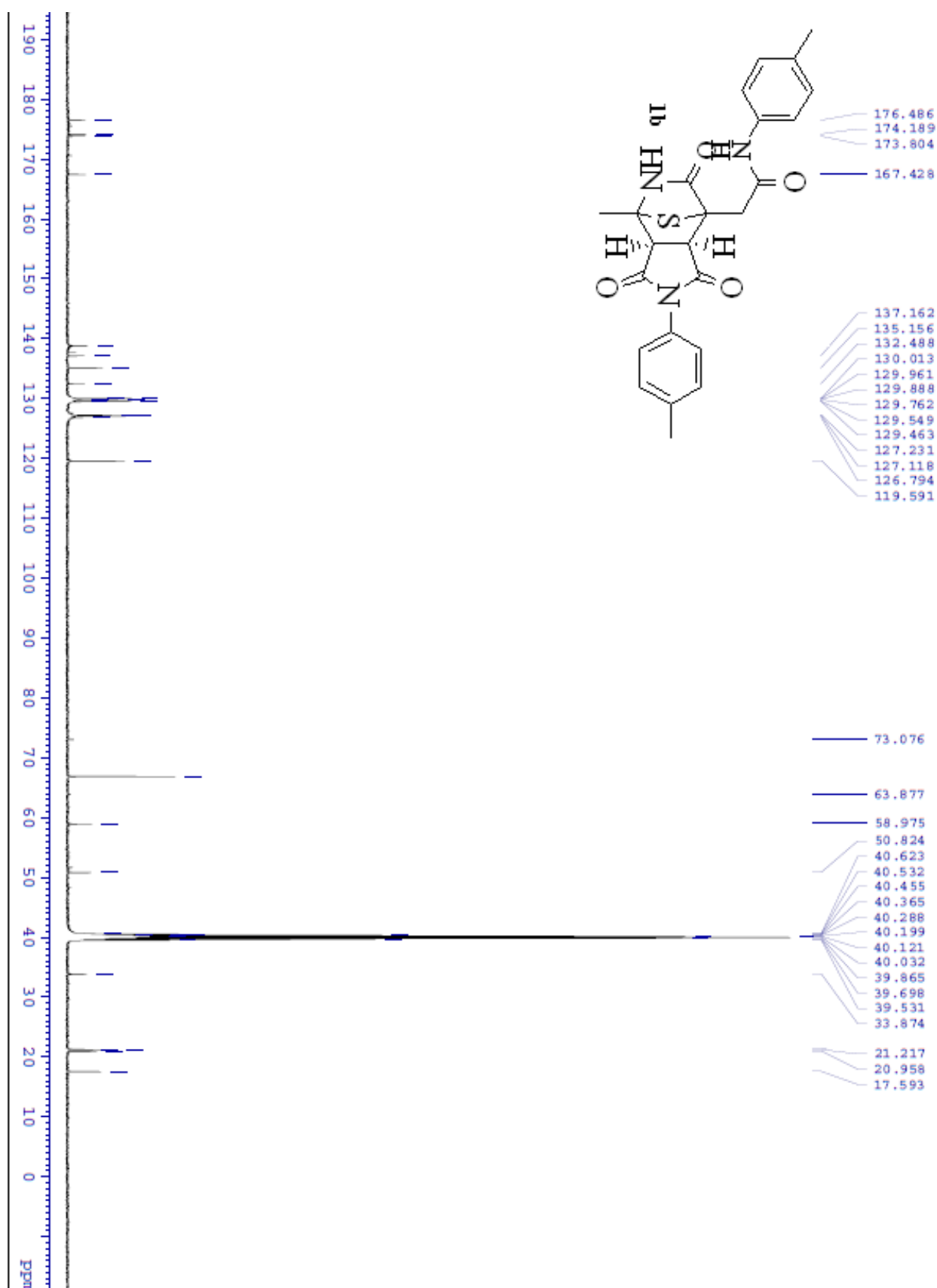
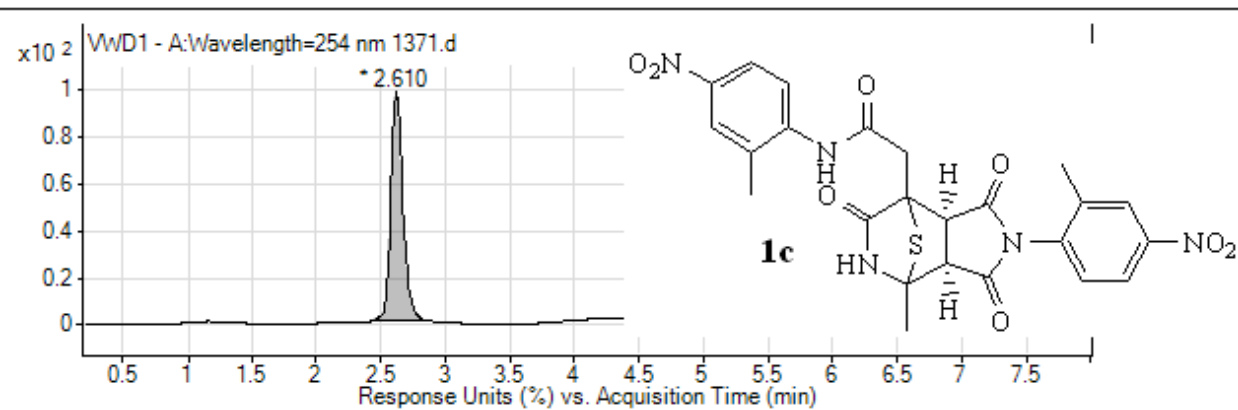


Figure S5: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **1b**



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2,42	2,61	2,863	186,8	1237,52	100

User Spectra

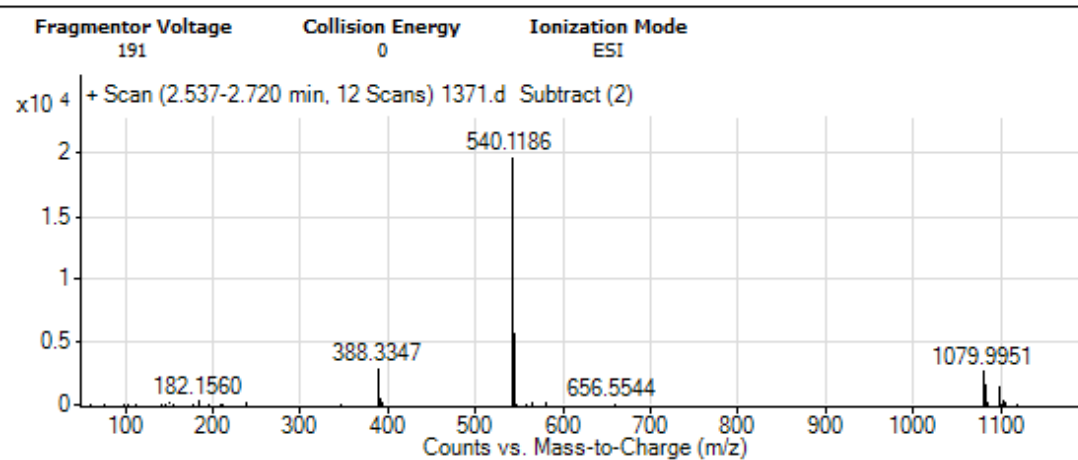


Figure S6: Data HPLC of compound **1c**

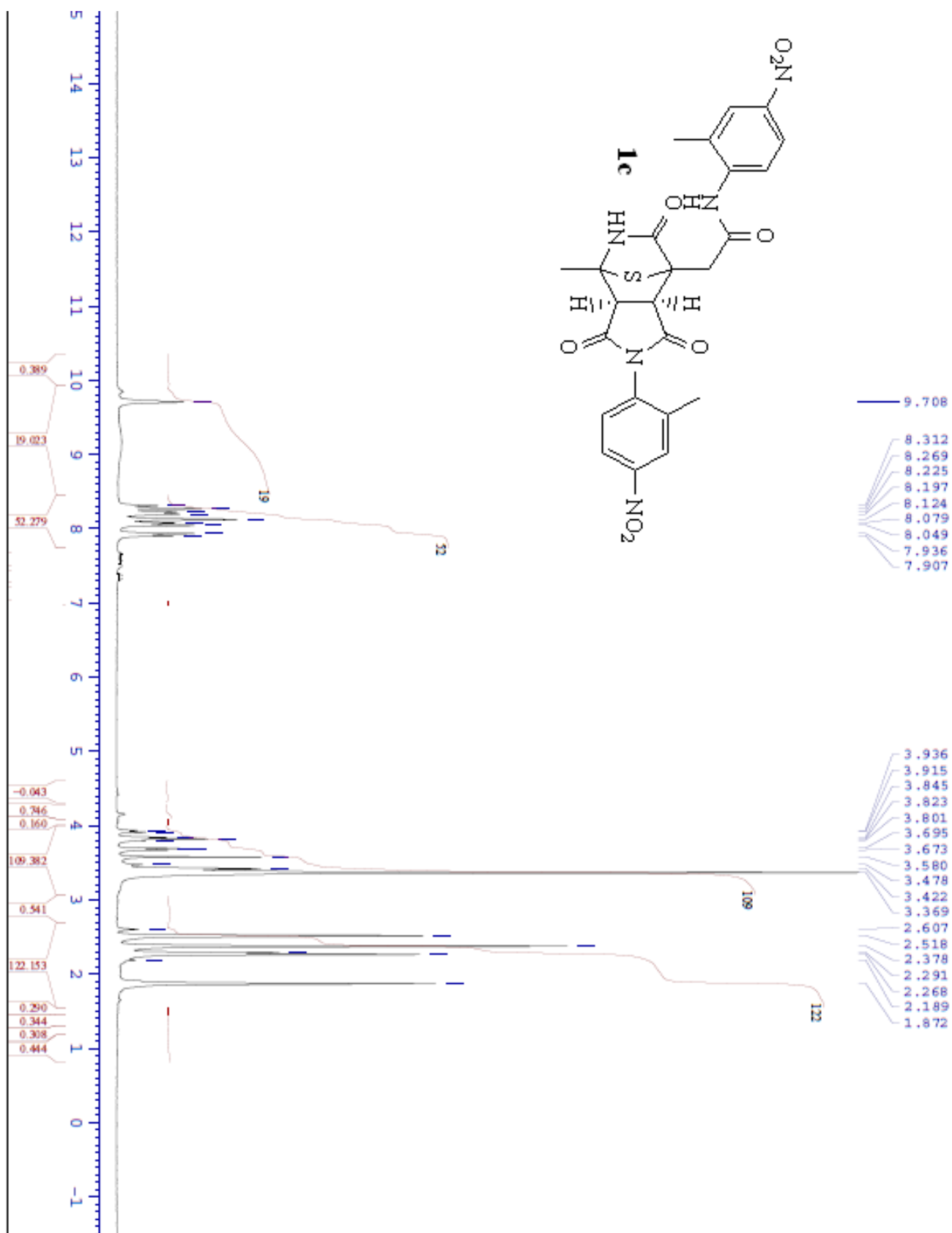


Figure S7: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **1c**

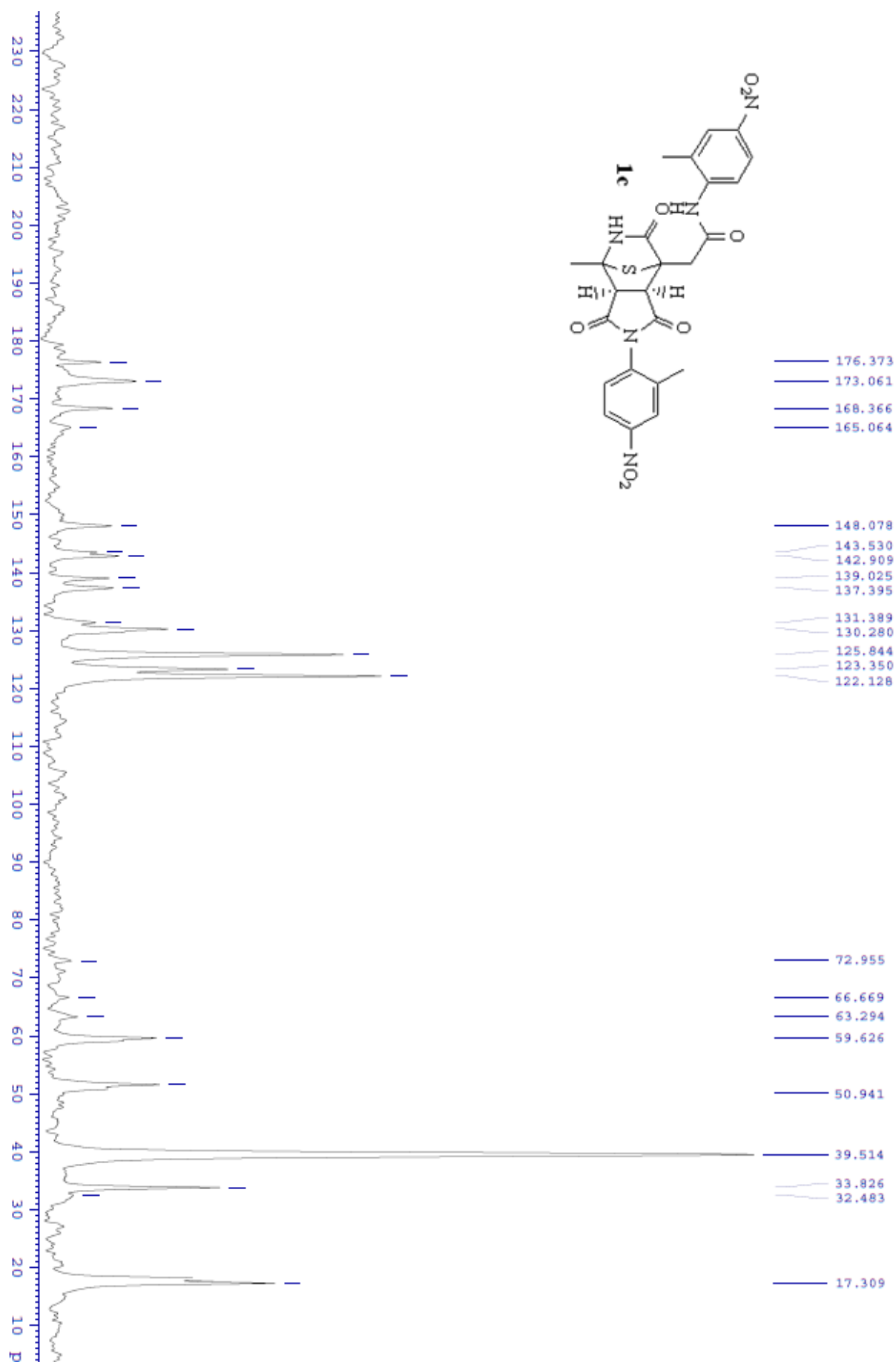
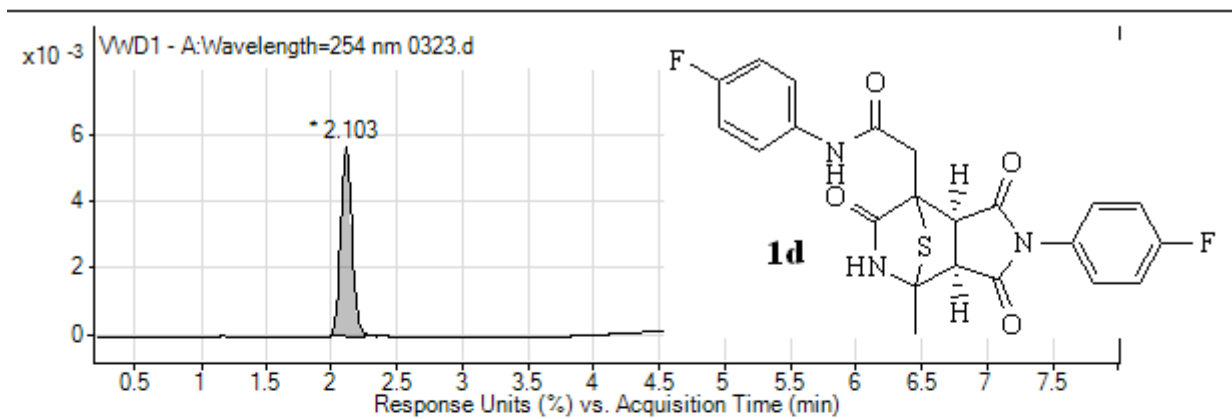


Figure S8: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **1c**



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1,983	2,103	2,247	330,89	1957,57	100

User Spectra

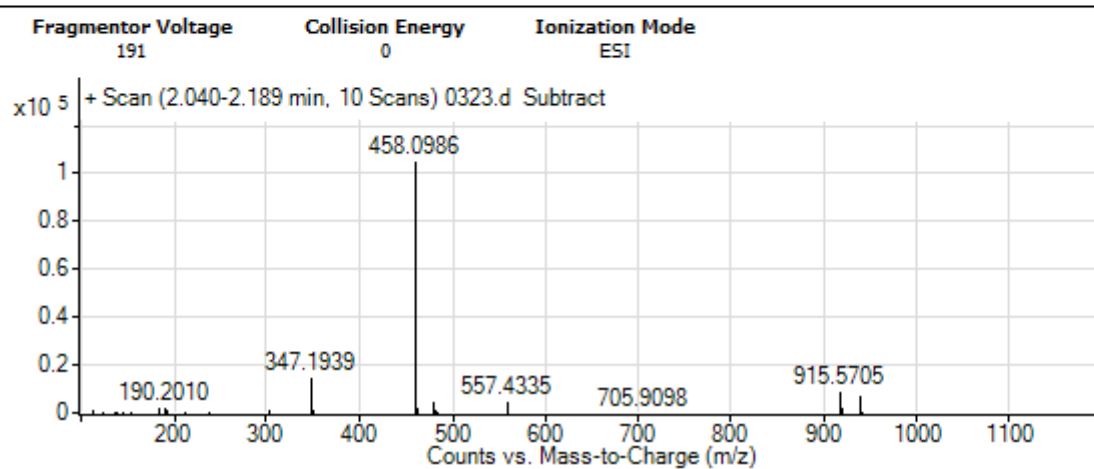


Figure S9: Data HPLC of compound **1d**

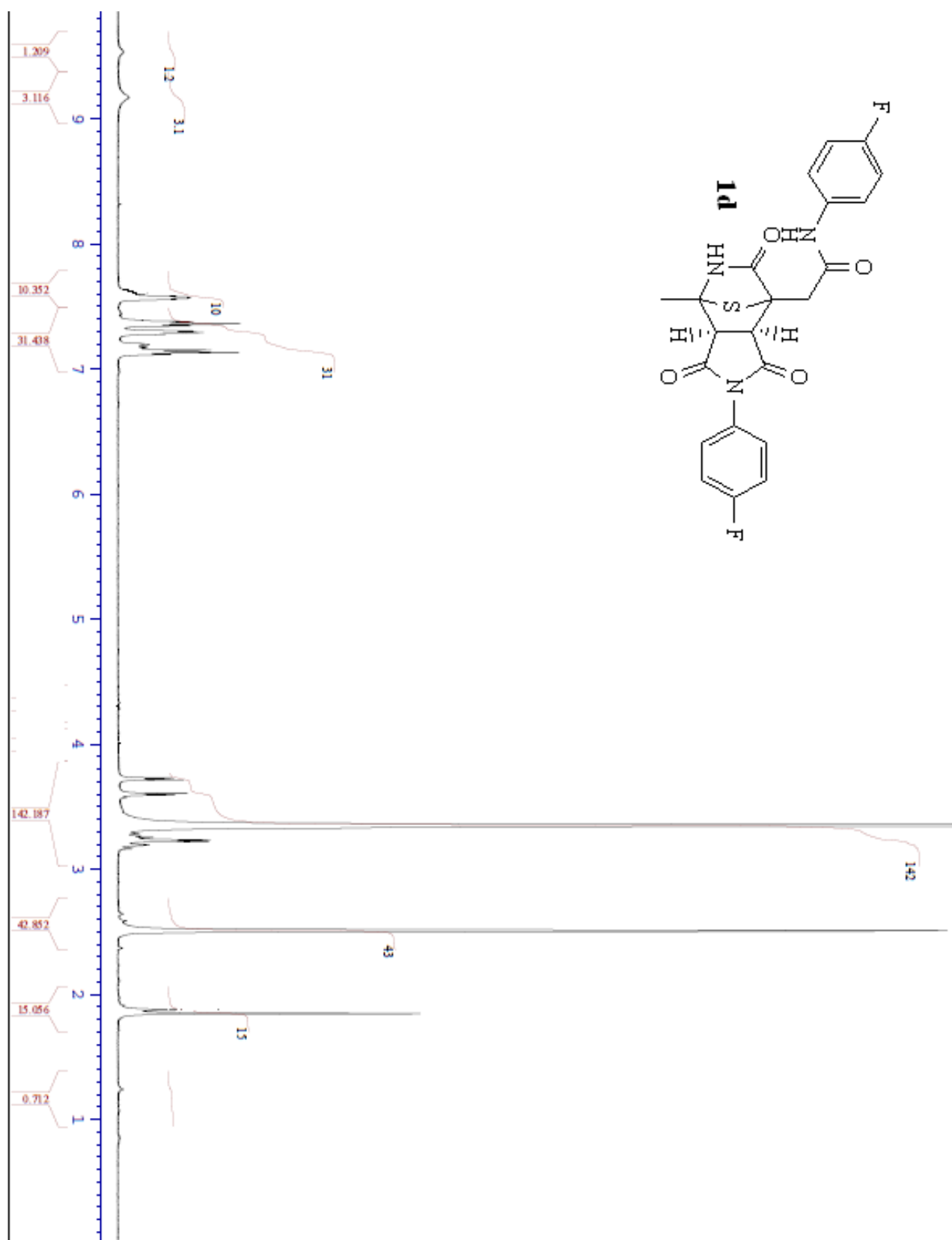


Figure S10: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **1d**

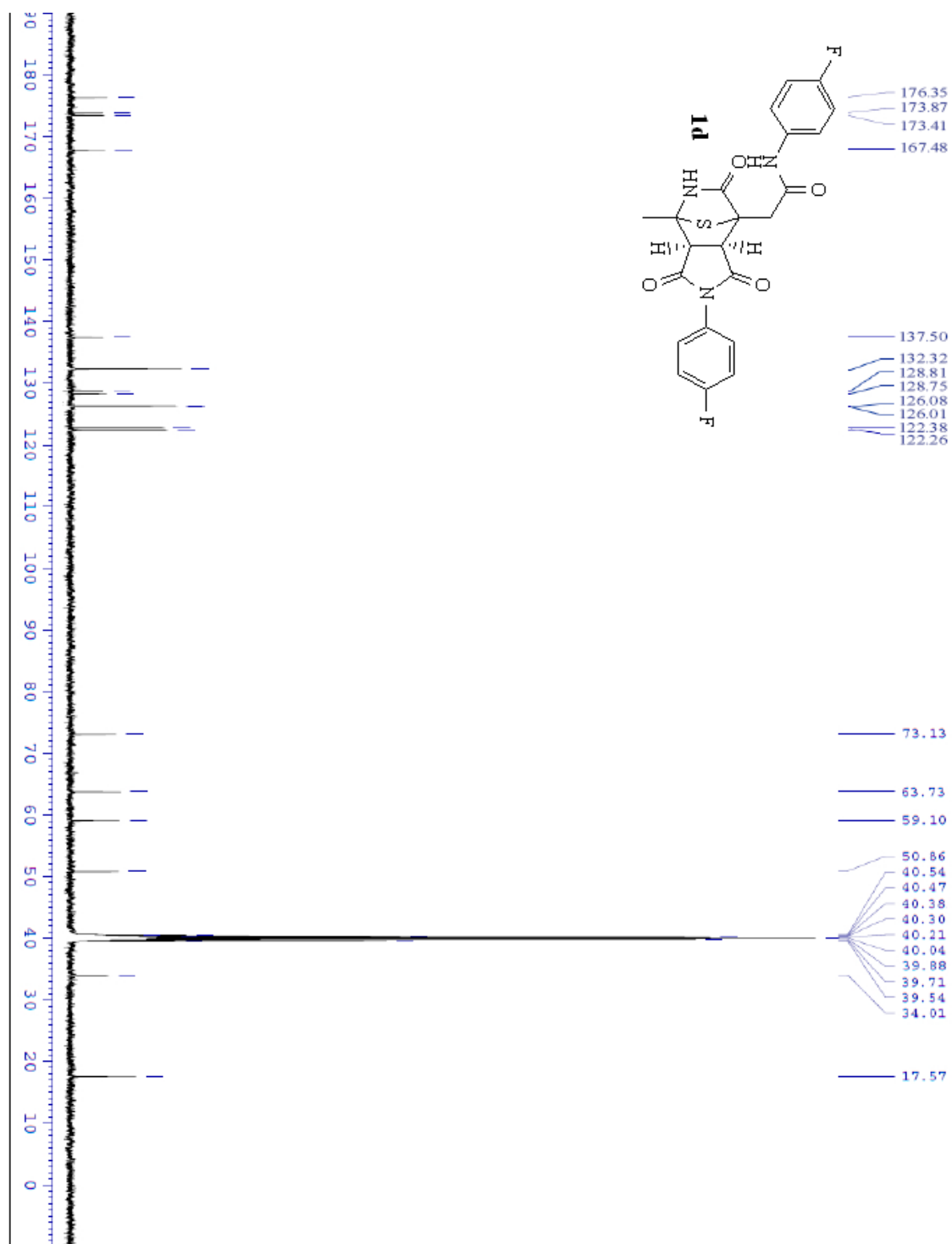
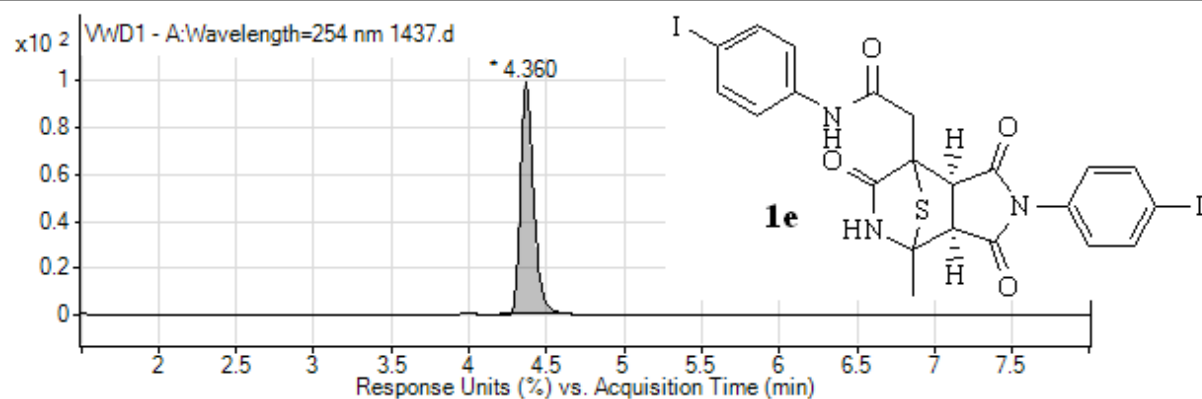


Figure S11: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **1d**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4,2	4,36	4,637	921,53	5377,5	100

User Spectra

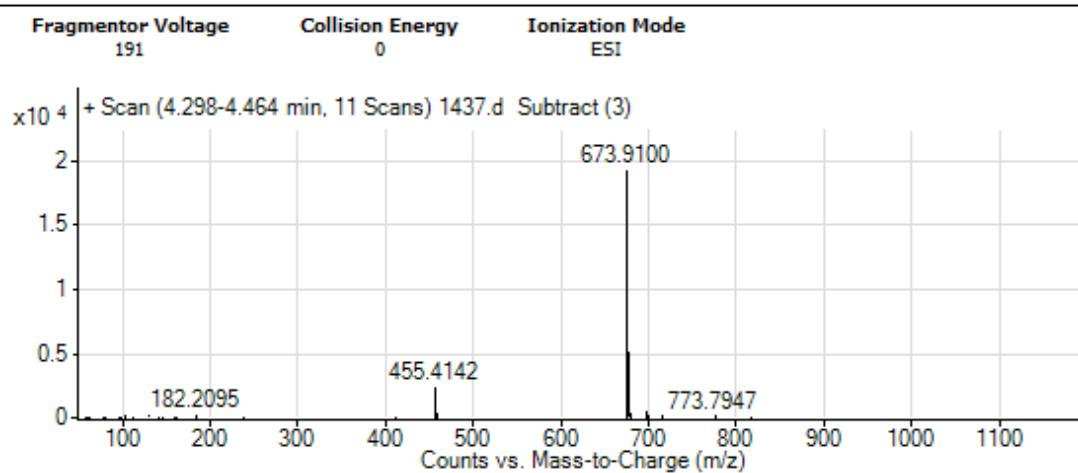


Figure S12: Data HPLC of compound **1e**

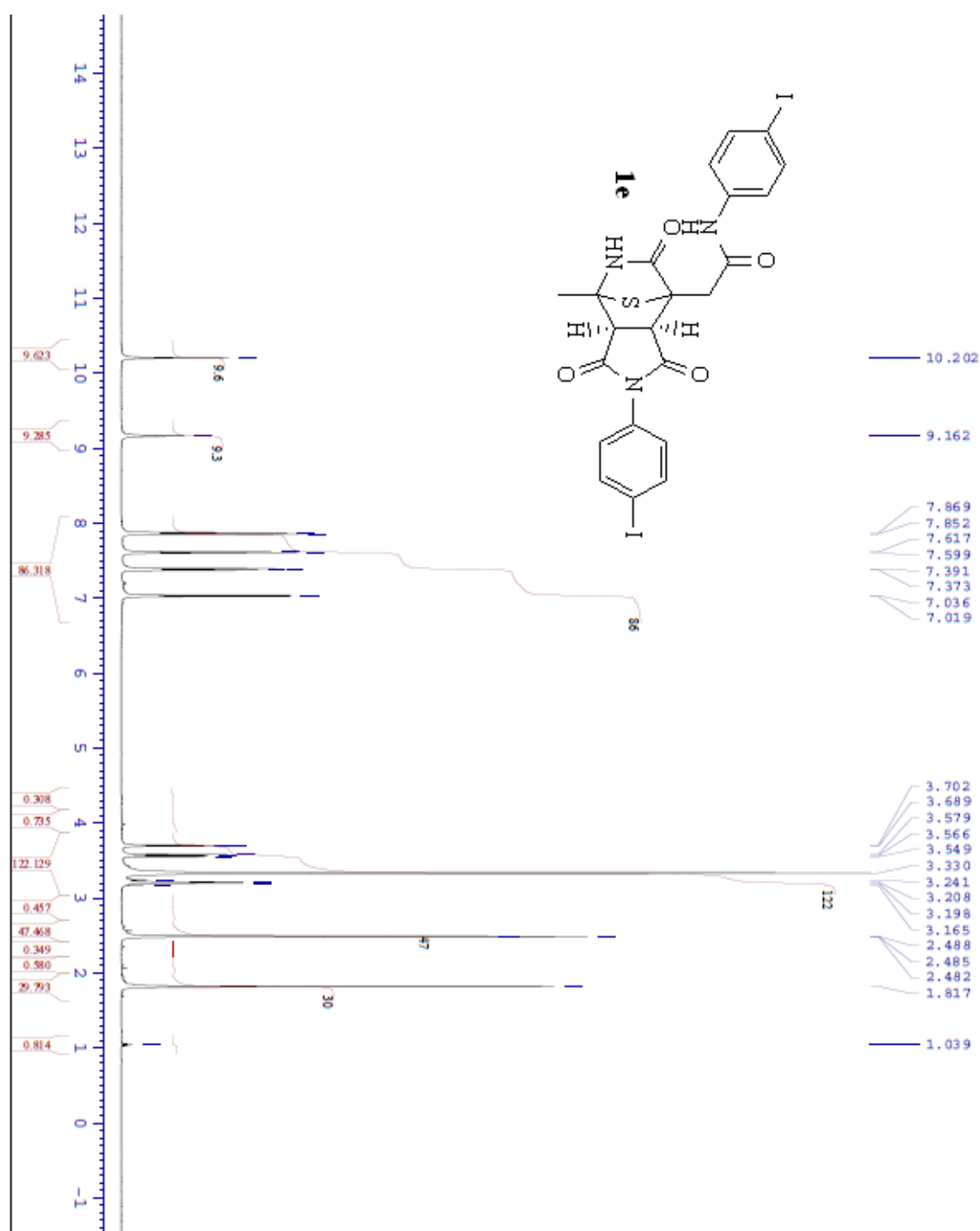


Figure S13: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **1e**

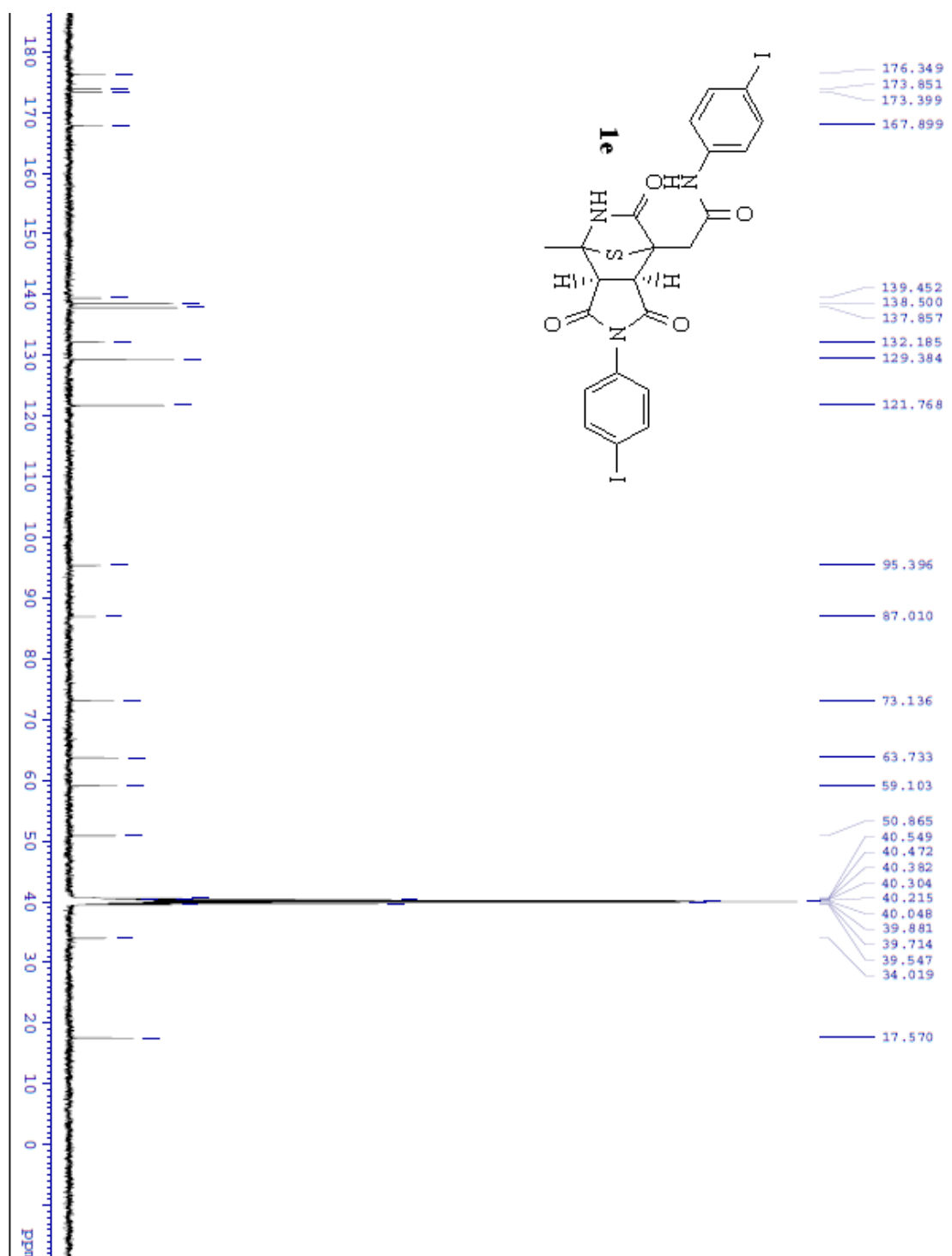
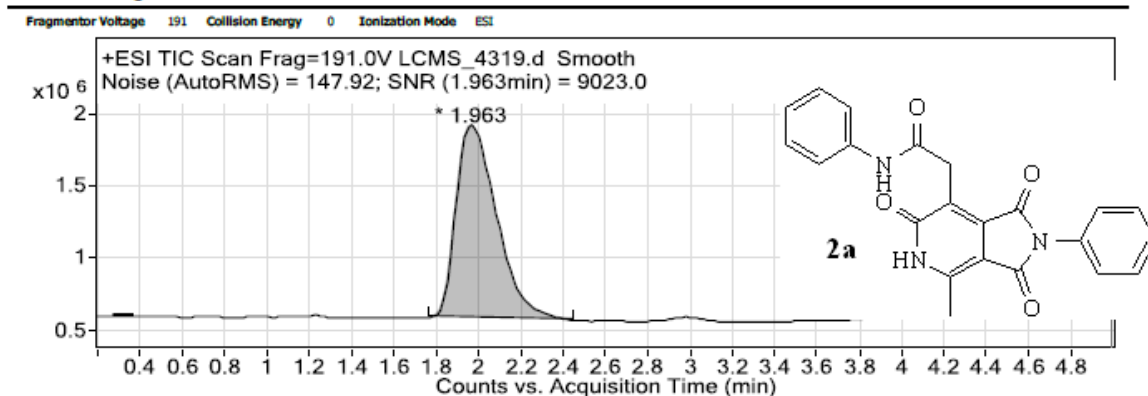


Figure S14: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **1e**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	1.764	1.963	2.444	1334703.11	17856755.04	100	9023

Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Auto-RMS	Height	1	147.9220123

Noise Regions

Start	End
0.273183333	0.373183333

User Spectra

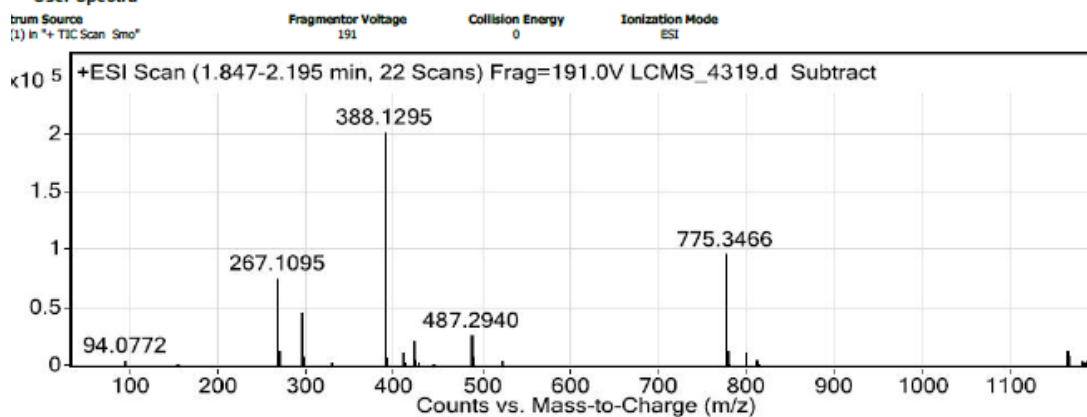


Figure S15: Data HPLC of compound 2a

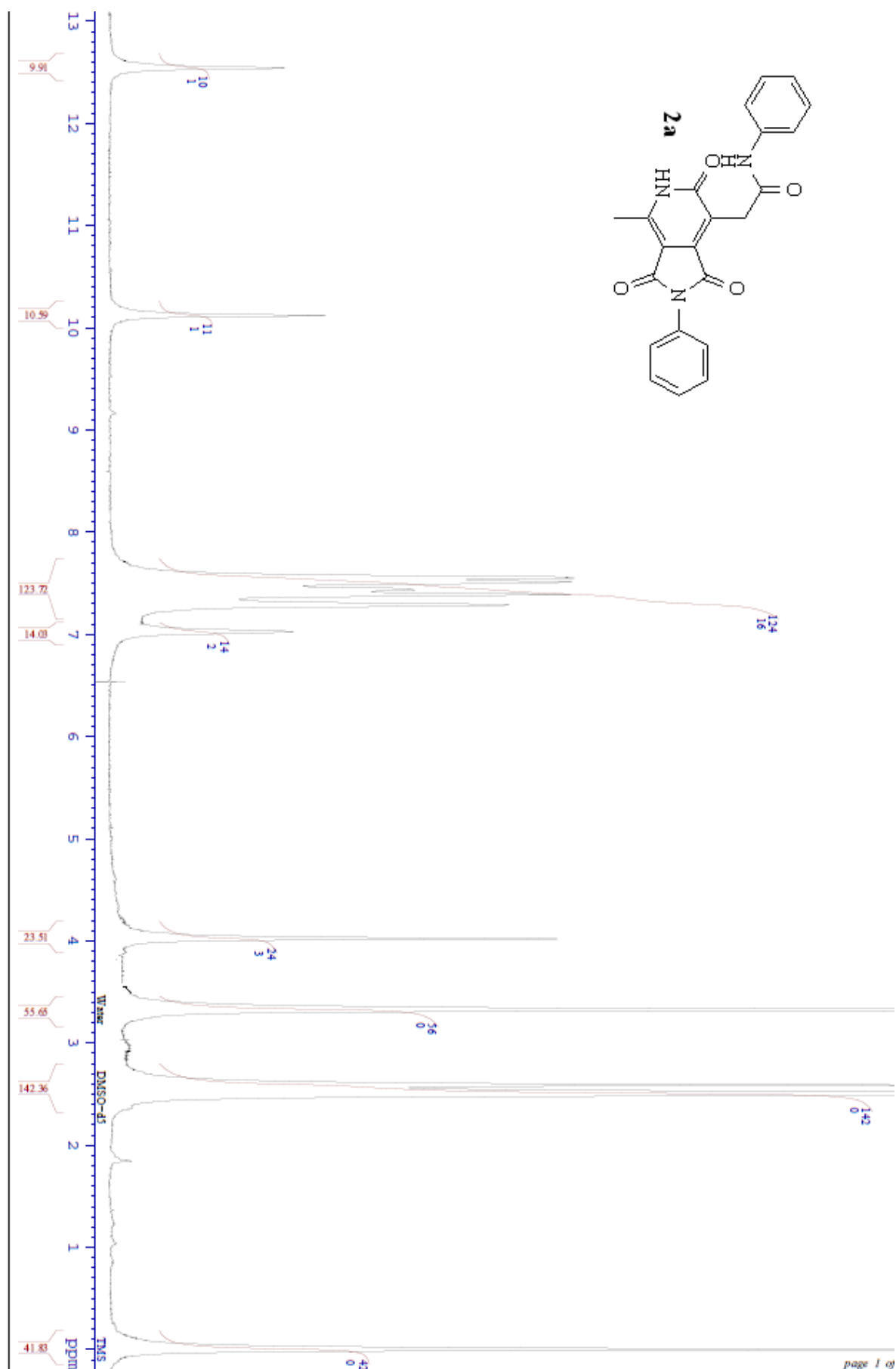


Figure S16: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **2a**

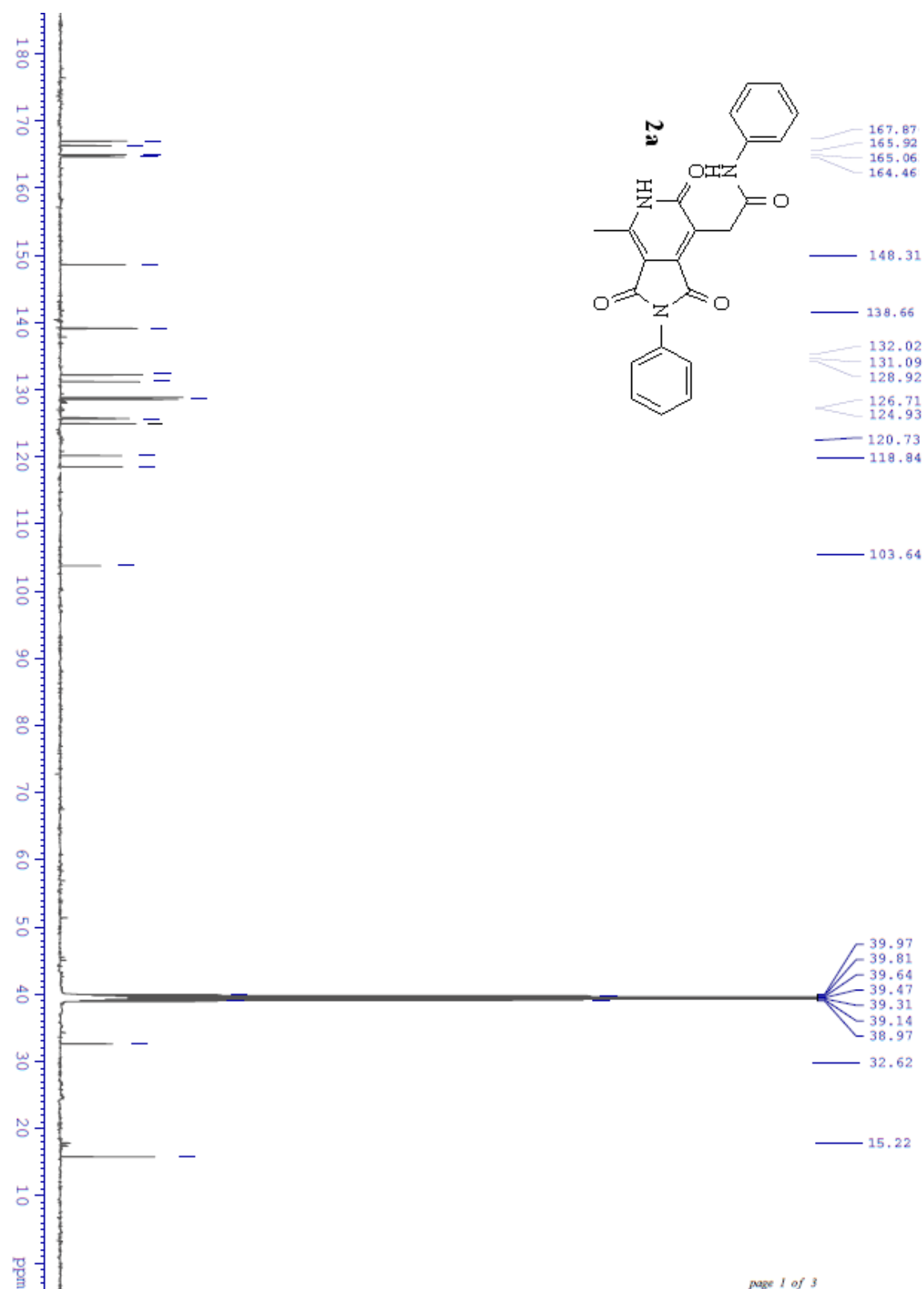


Figure S17: ¹³C NMR spectrum (125 MHz, DMSO-d₆) of compound **2a**

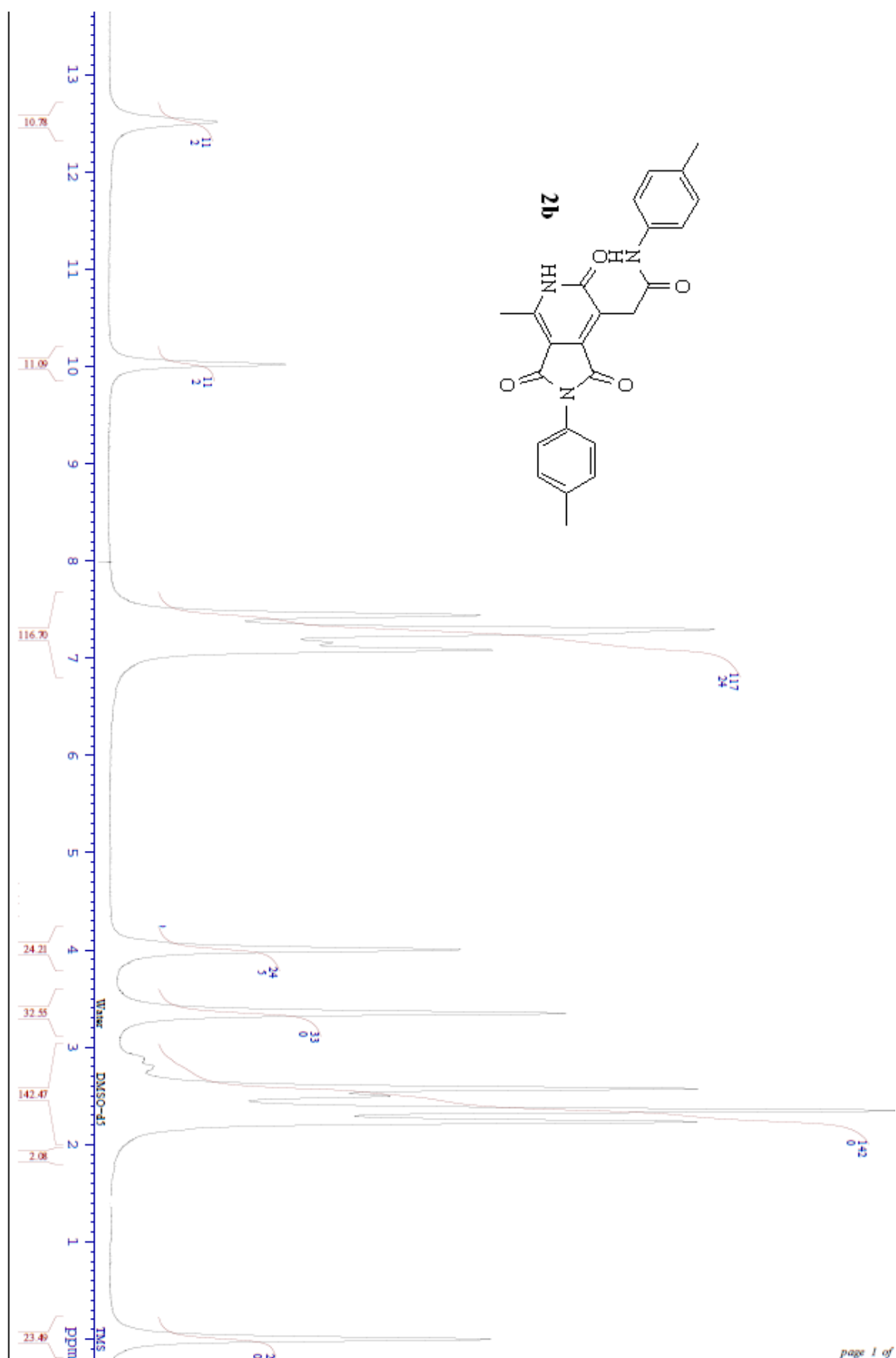
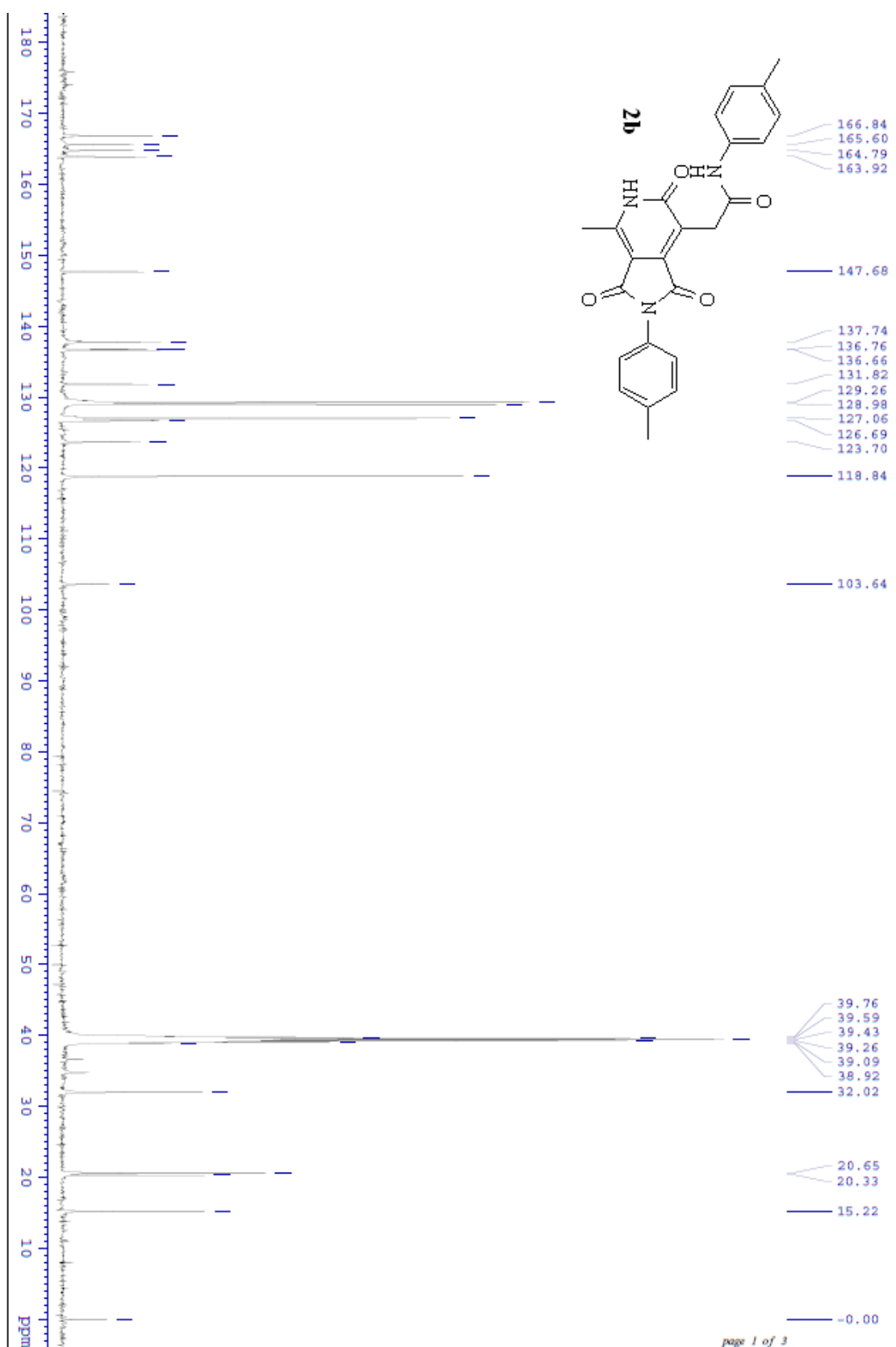
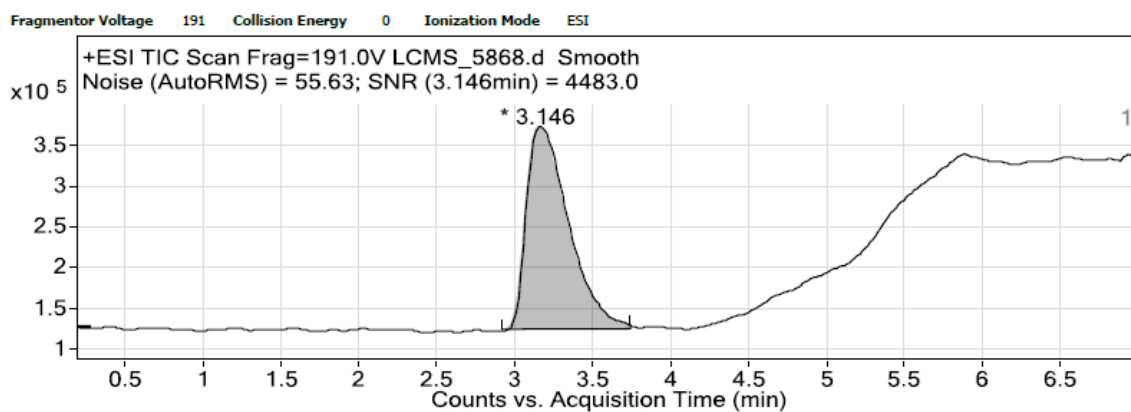


Figure S19: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **2b**





User Chromatogram Peak List

RT	Height	Height %	Area	Area %	Area Sum %	S/N	Symmetry	Width
3.146	249392.82	100	4749675.21	100	100	4483	2.82	0.829

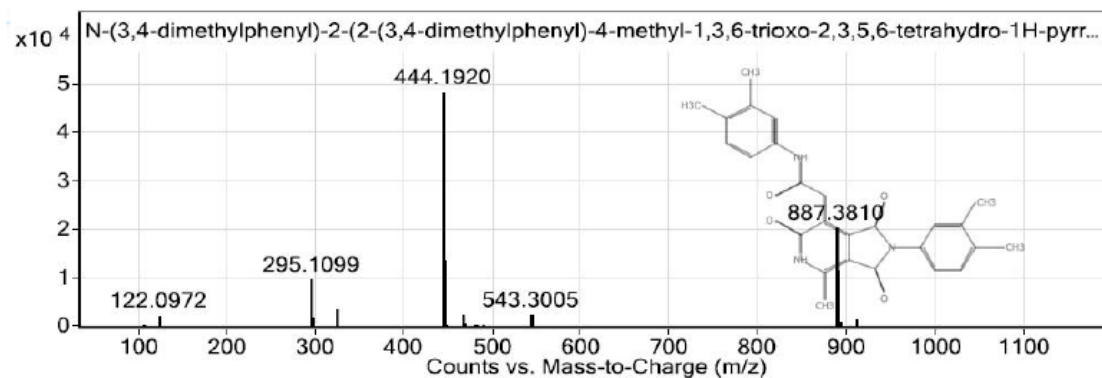


Figure S21: Data HPLC of compound 2c

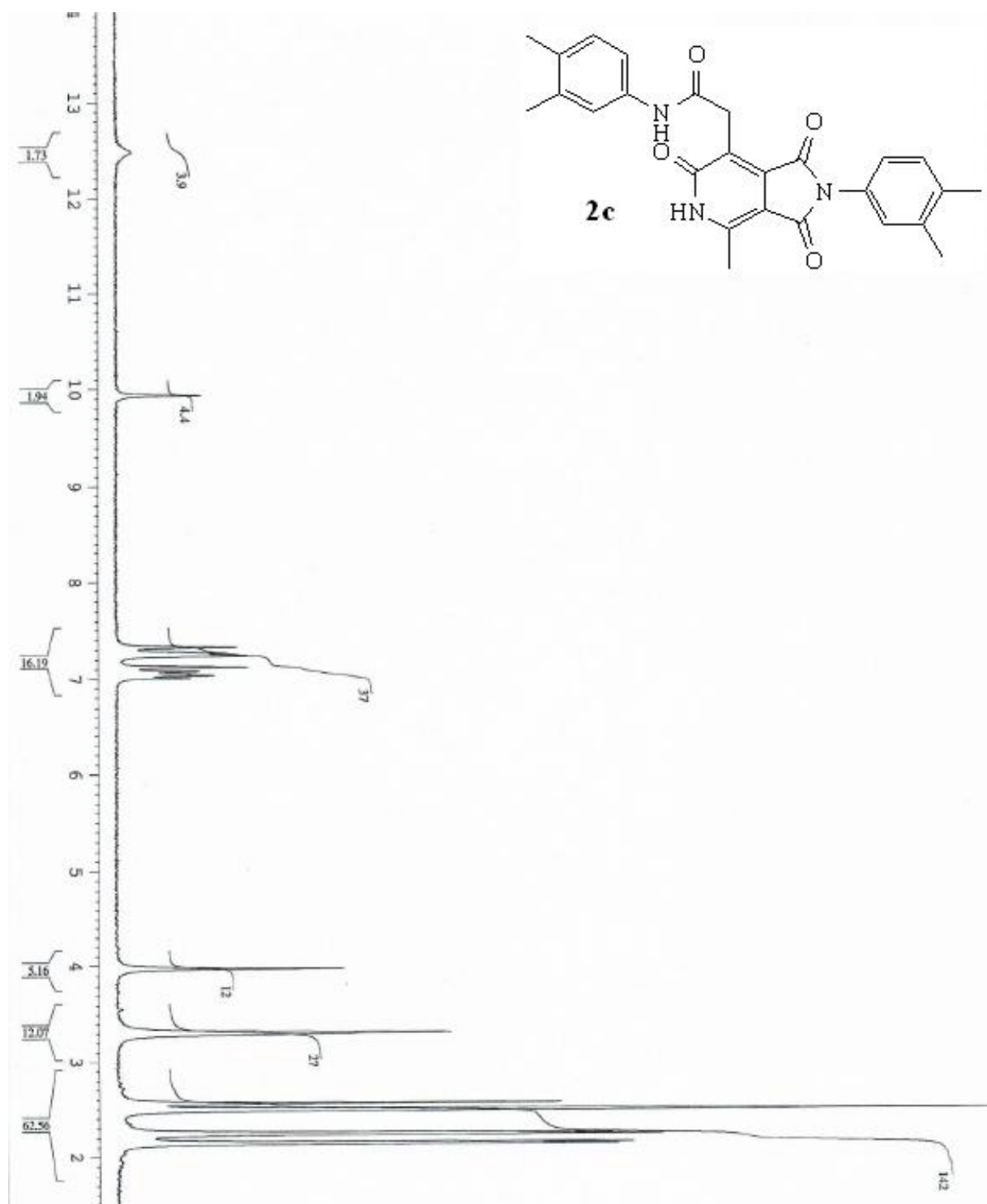


Figure S22: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **2c**

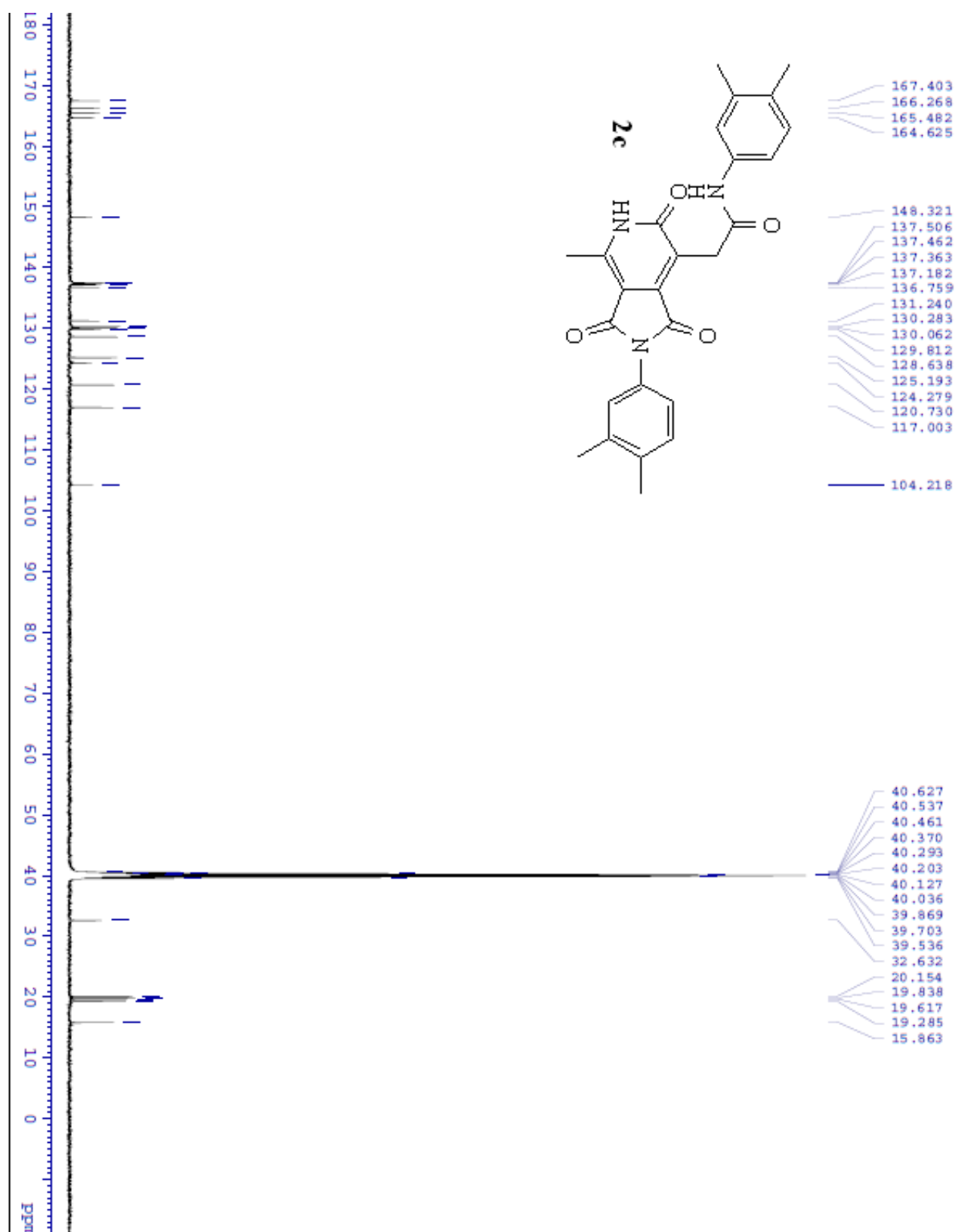
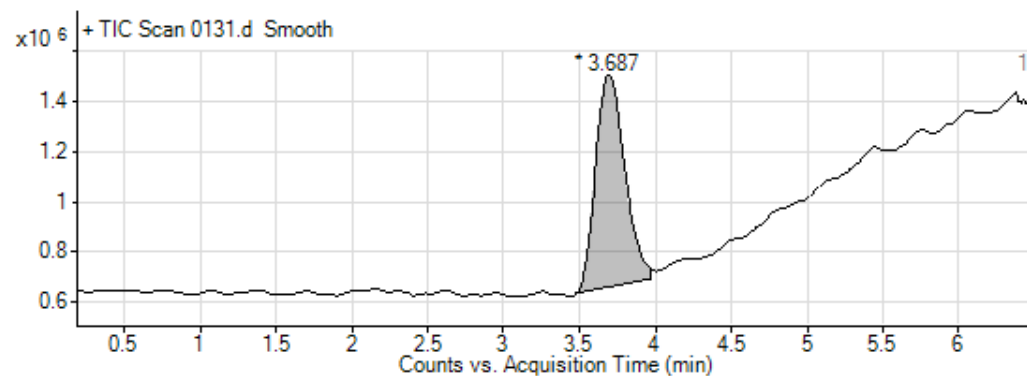


Figure S23: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **2c**

User Chromatograms

Fragmentor Voltage 191 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,472	3,687	3,969	854435,71	11440062,31	100

User Spectra

Fragmentor Voltage 191 Collision Energy 0 Ionization Mode ESI

+ Scan (3.538-3.902 min, 23 Scans) 0131.d Subtract

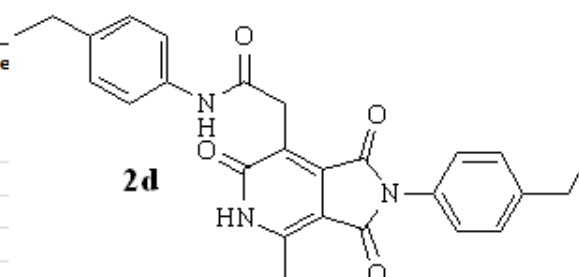
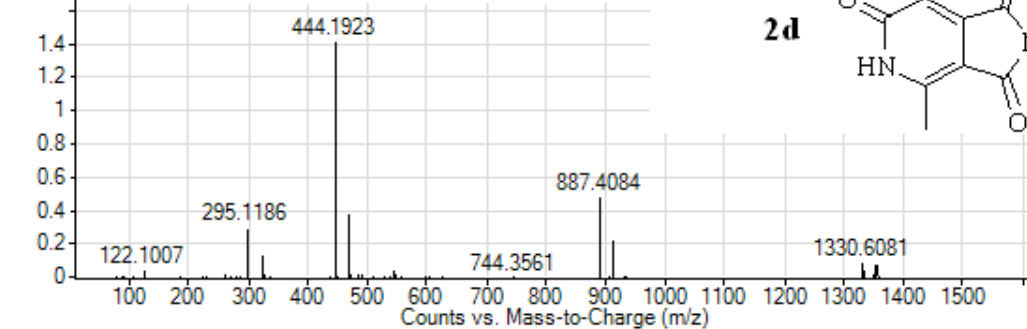


Figure S24: Data HPLC of compound **2d**

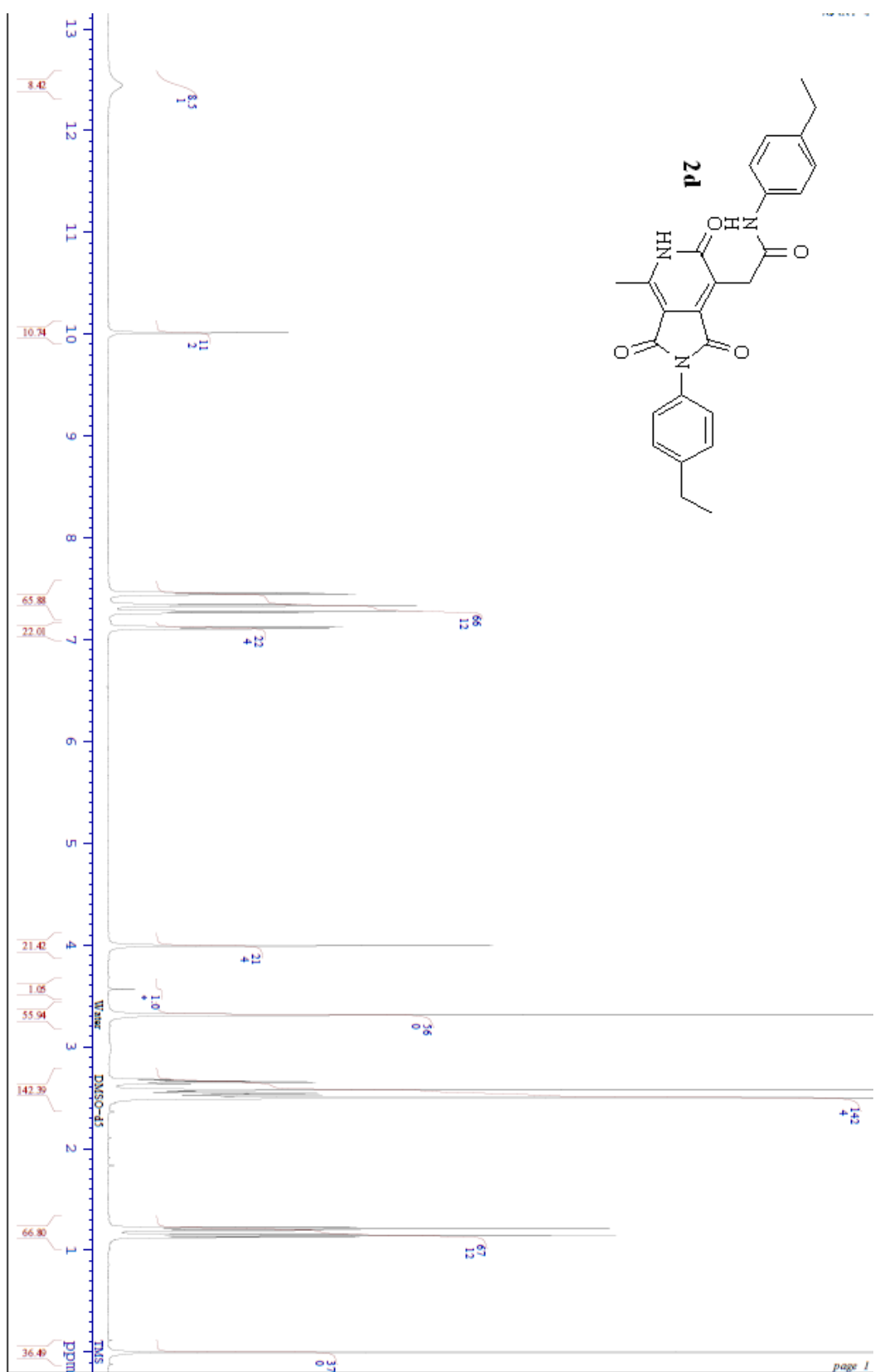


Figure S25: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **2d**

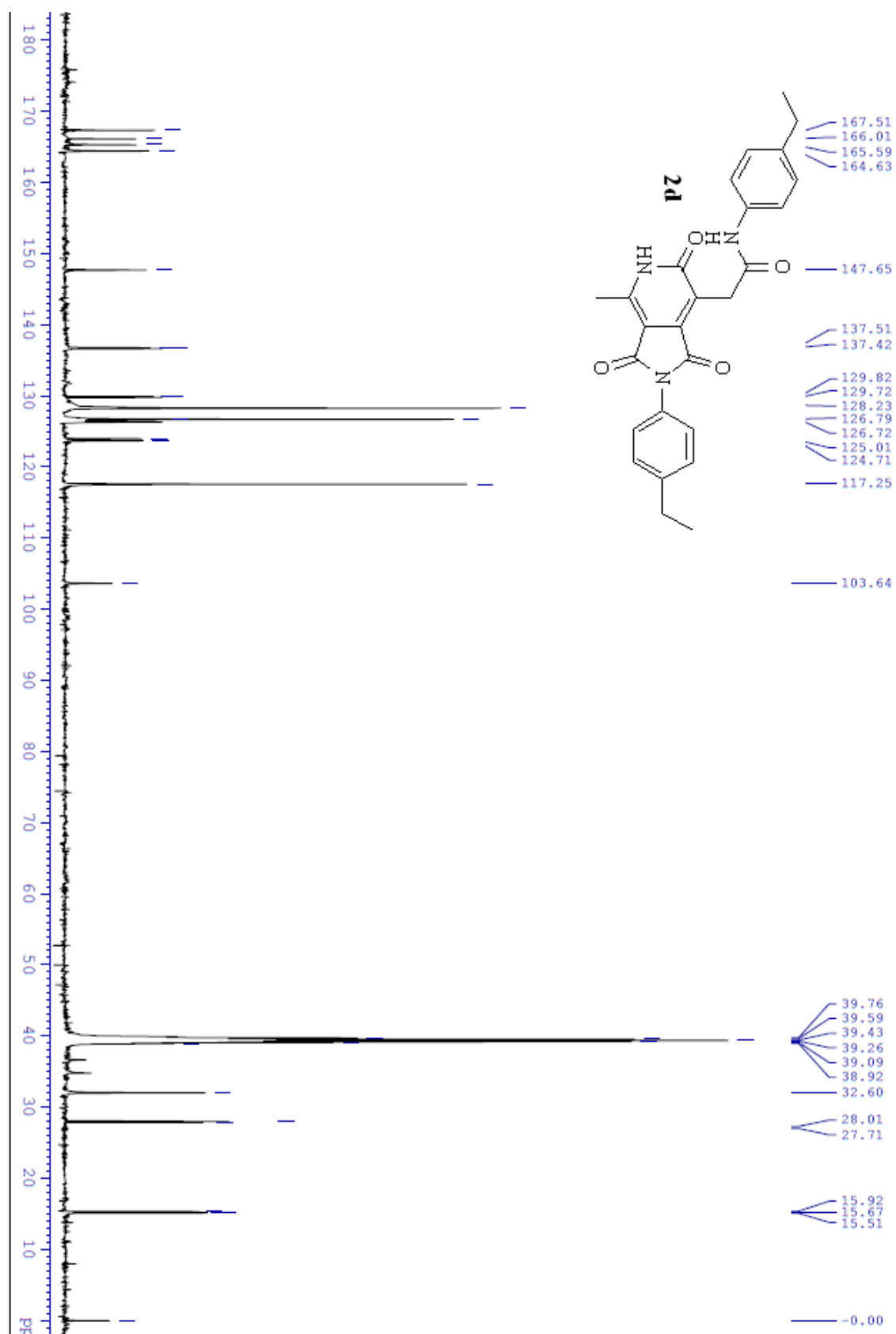
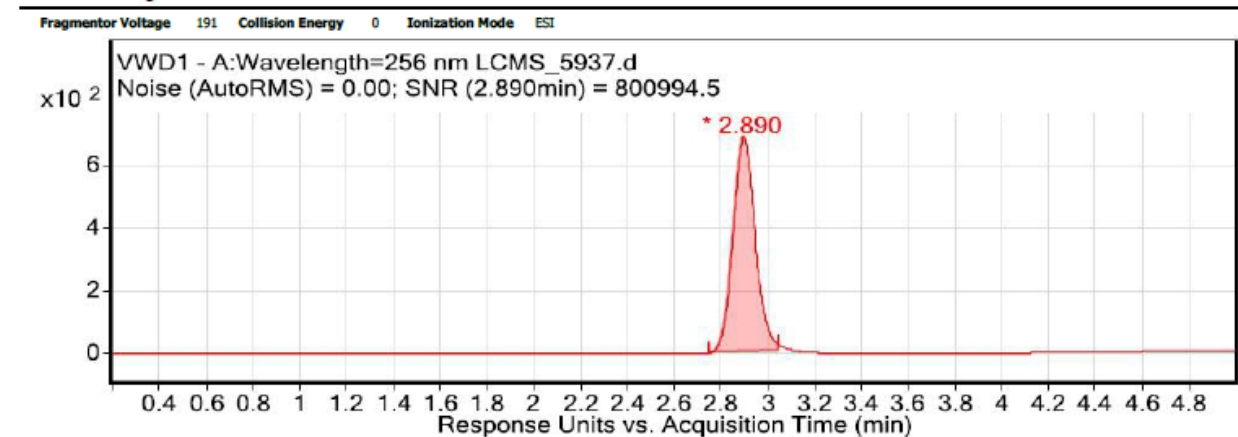


Figure S26: ¹³C NMR spectrum (125 MHz, DMSO-d₆) of compound **2d**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	2.75	2.89	3.043	692.29	4583.64	100	800994.5

Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Auto-RMS	Height	1	0.000864285

User Spectra

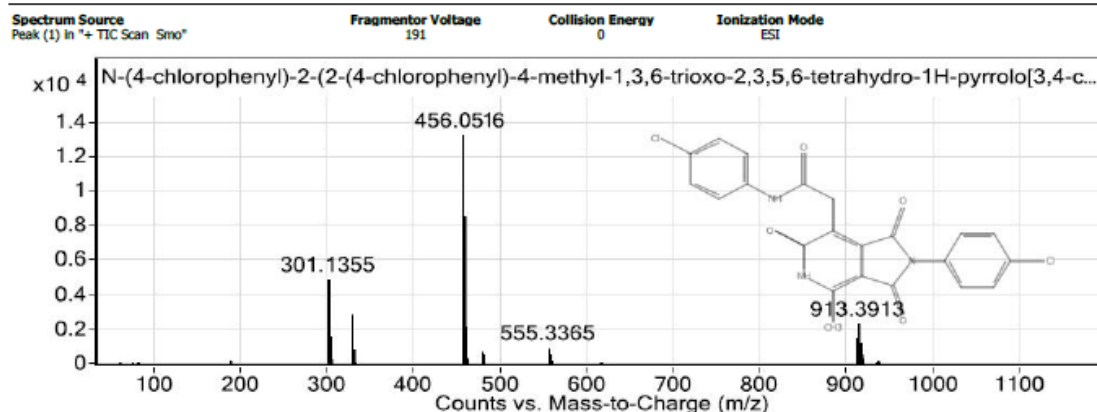


Figure S27: Data HPLC of compound 2e

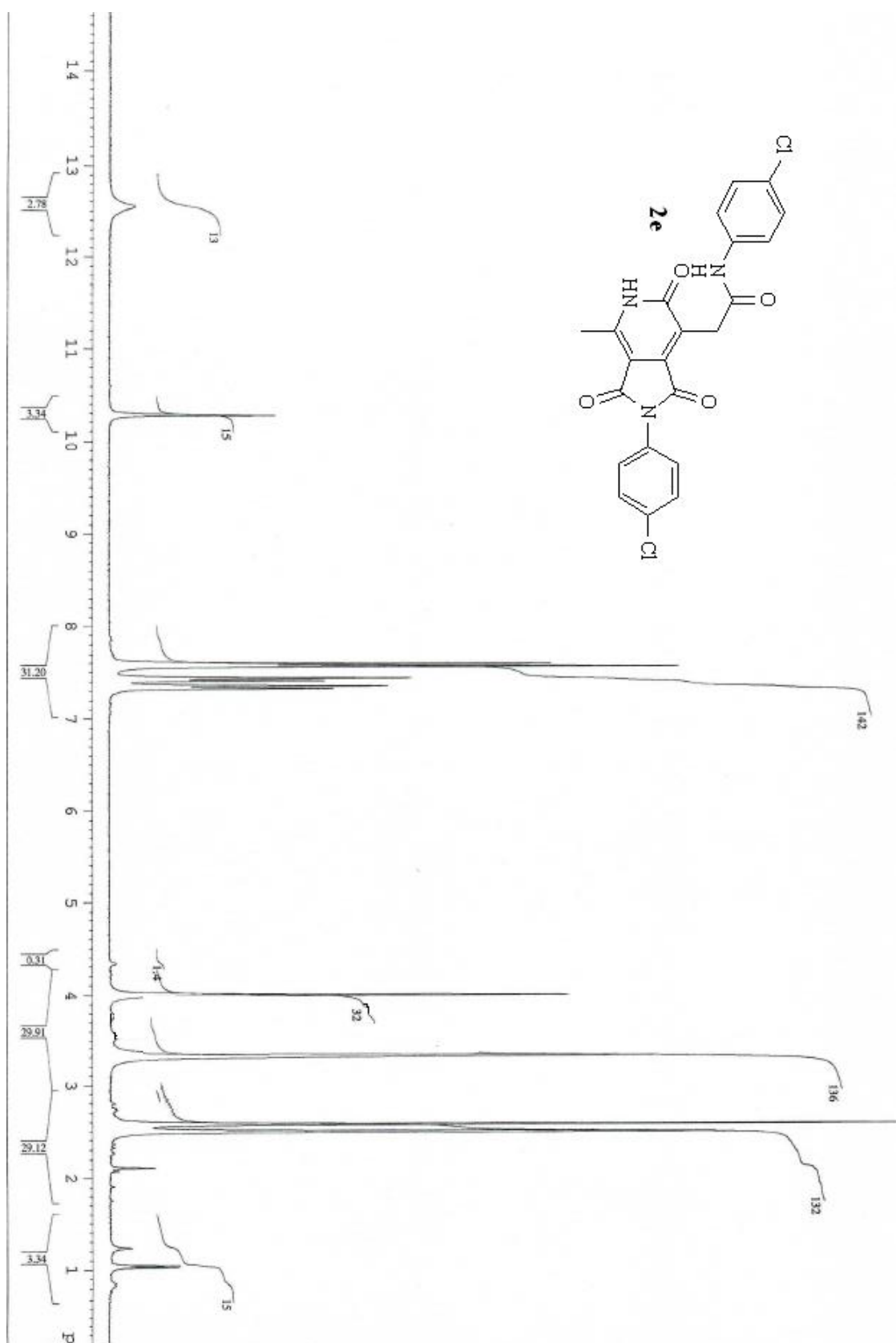


Figure S28: ^1H NMR spectrum (500 MHz, DMSO- d_6) of compound **2e**

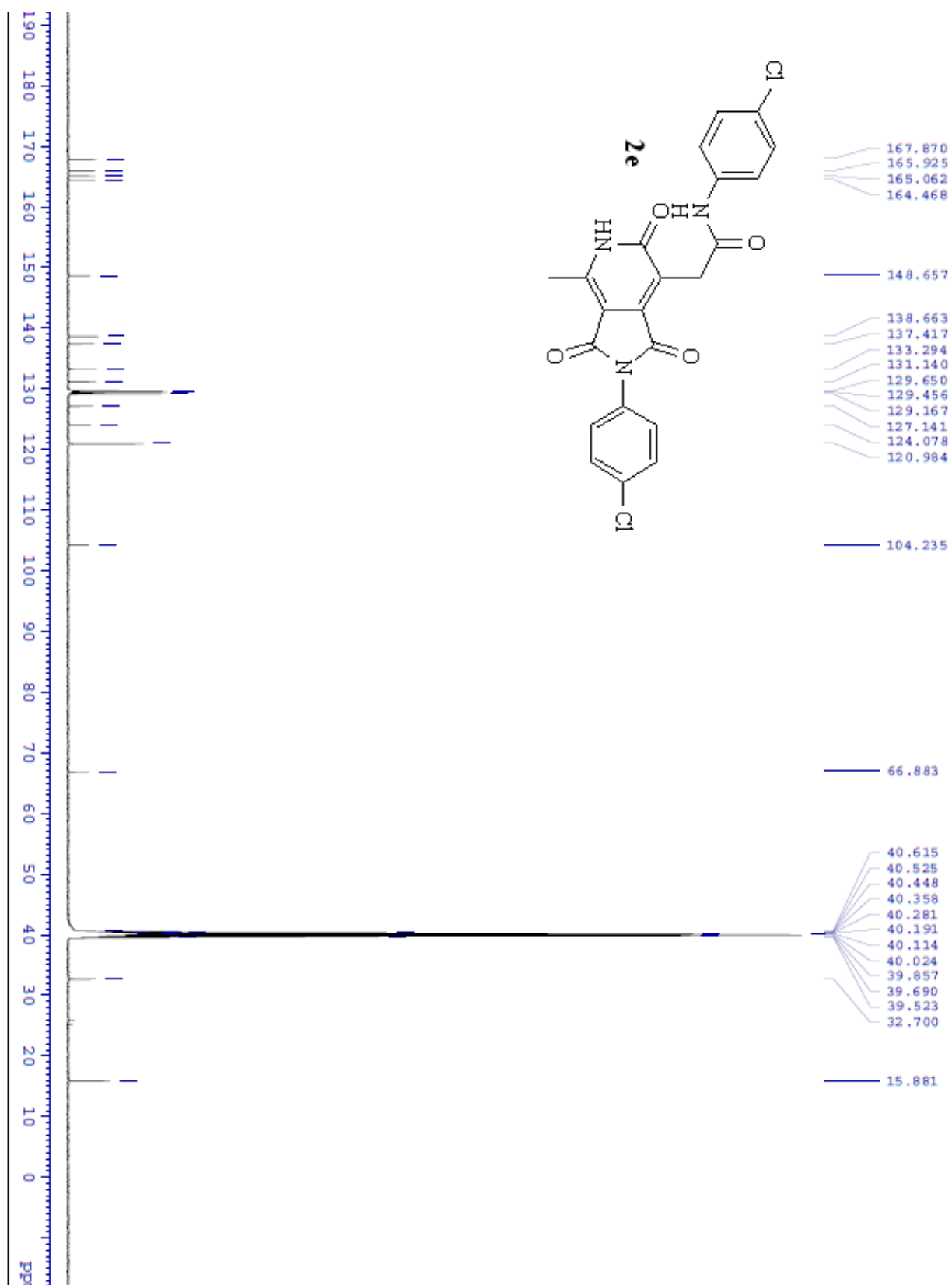
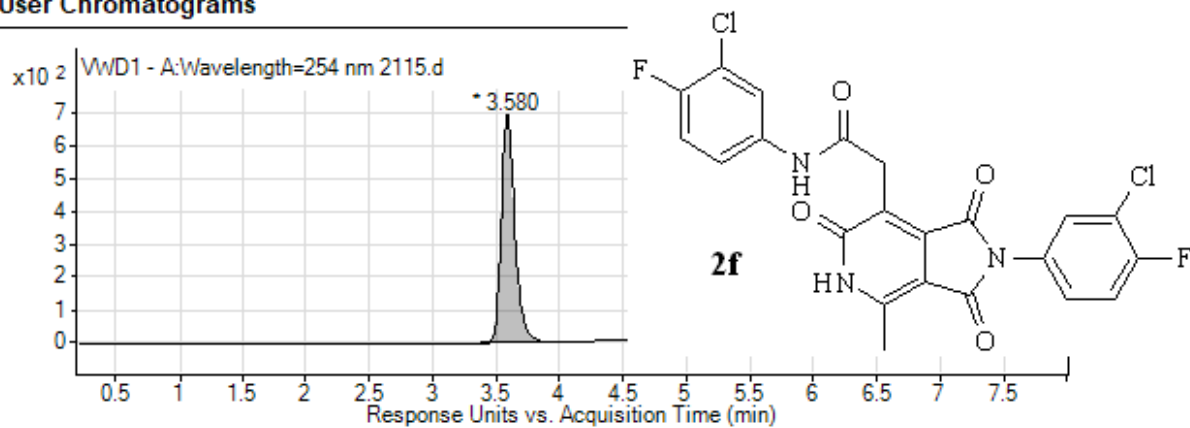


Figure S29: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **2e**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,377	3,58	3,977	696,92	5138,01	100

User Spectra

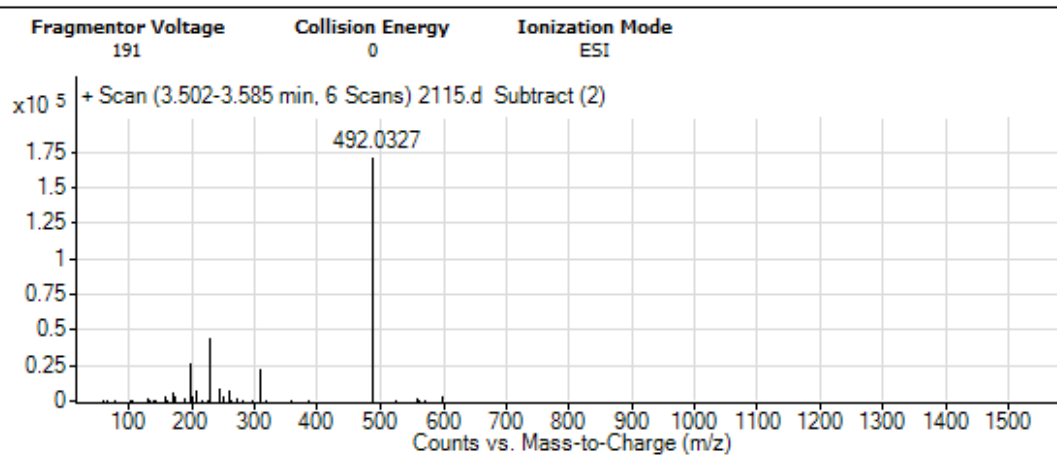


Figure S30: Data HPLC of compound **2f**

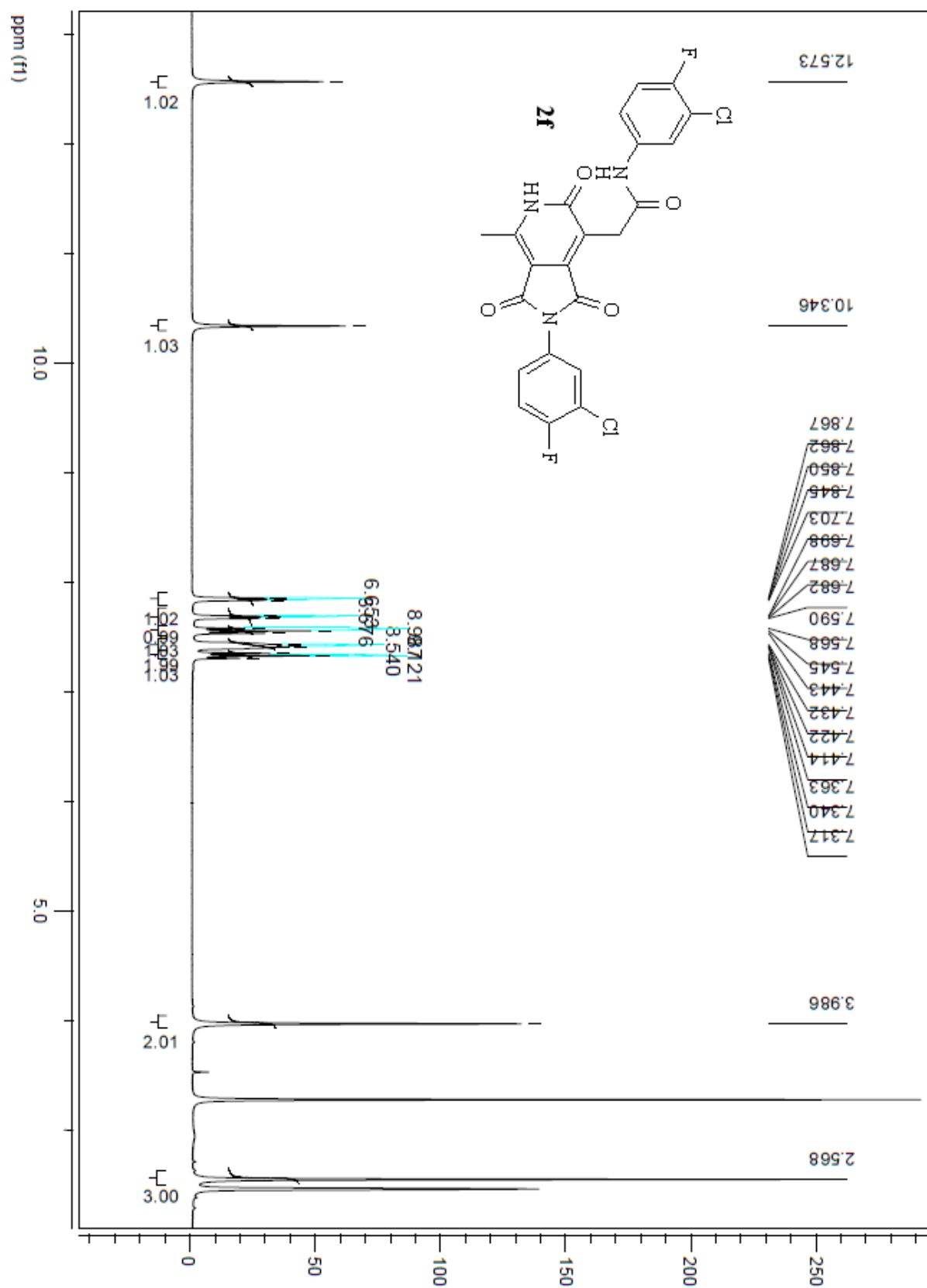


Figure S31: ^1H NMR spectrum (500 MHz, DMSO- d_6) of compound **2f**

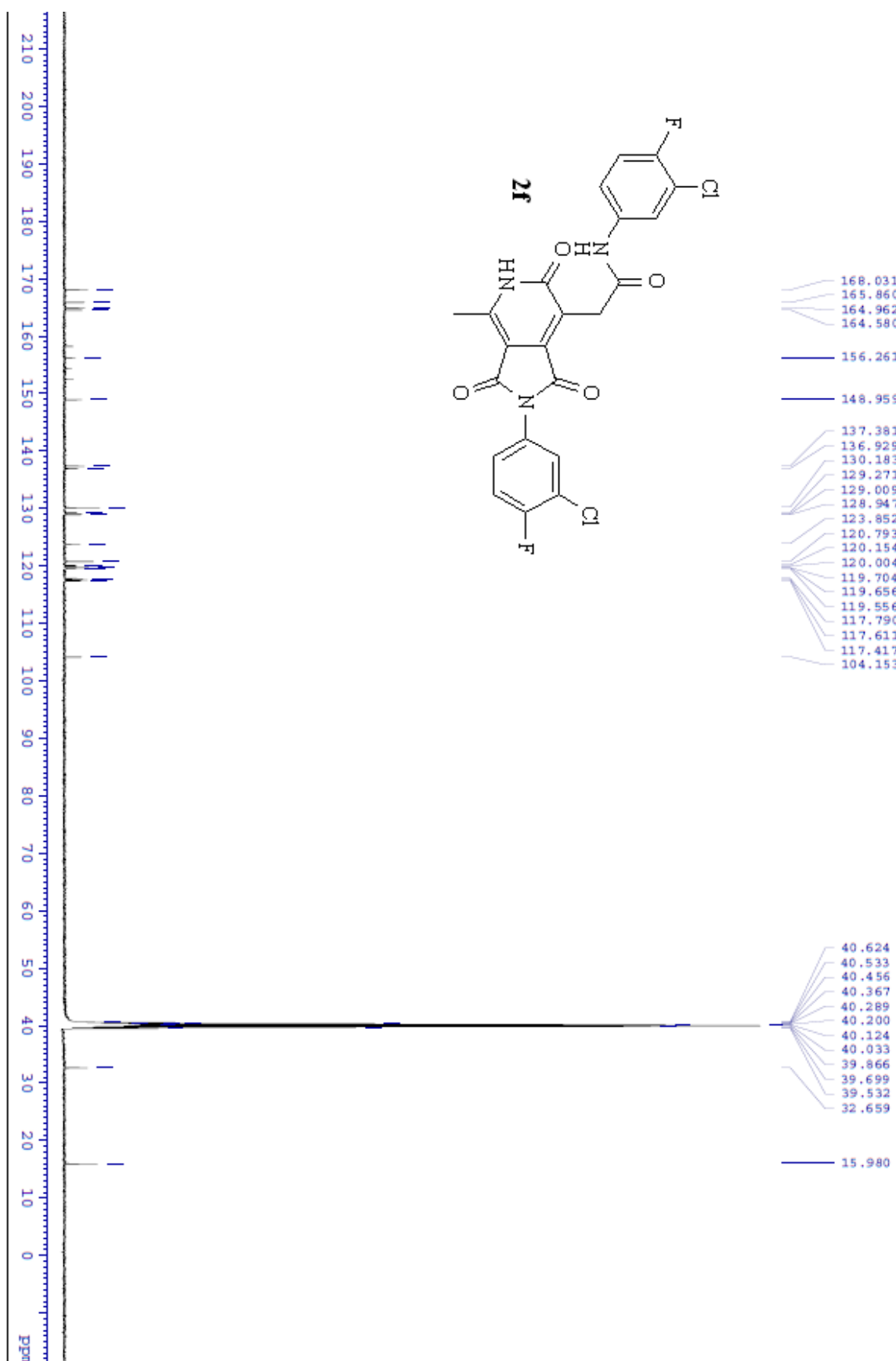
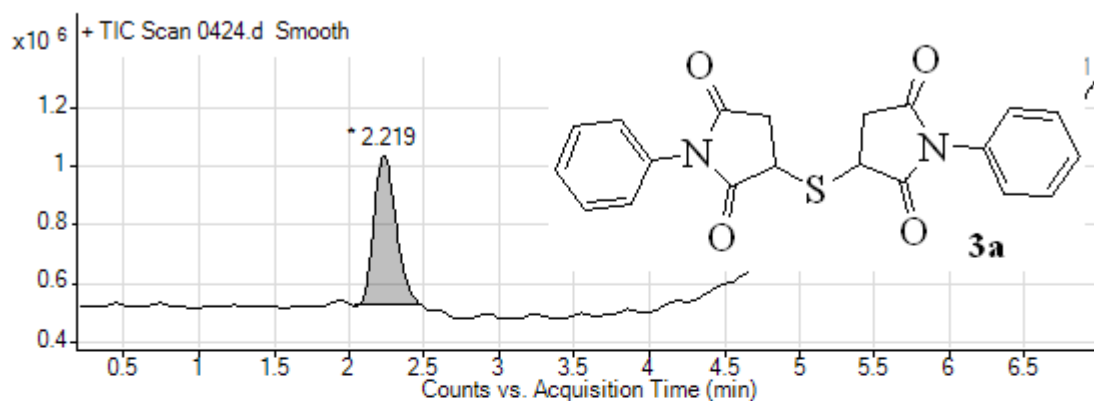


Figure S32: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **2f**

User Chromatograms

Fragmentor Voltage 191 Collision Energy 0 Ionization Mode ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2,037	2,219	2,468	511906,16	5209411,17	100

User Spectra

Fragmentor Voltage 191 Collision Energy 0 Ionization Mode ESI

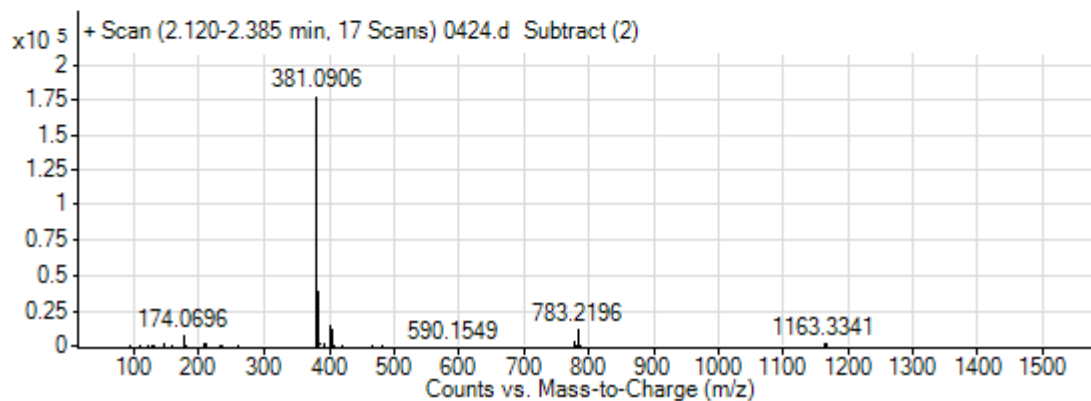


Figure S33: Data HPLC of compound 3a

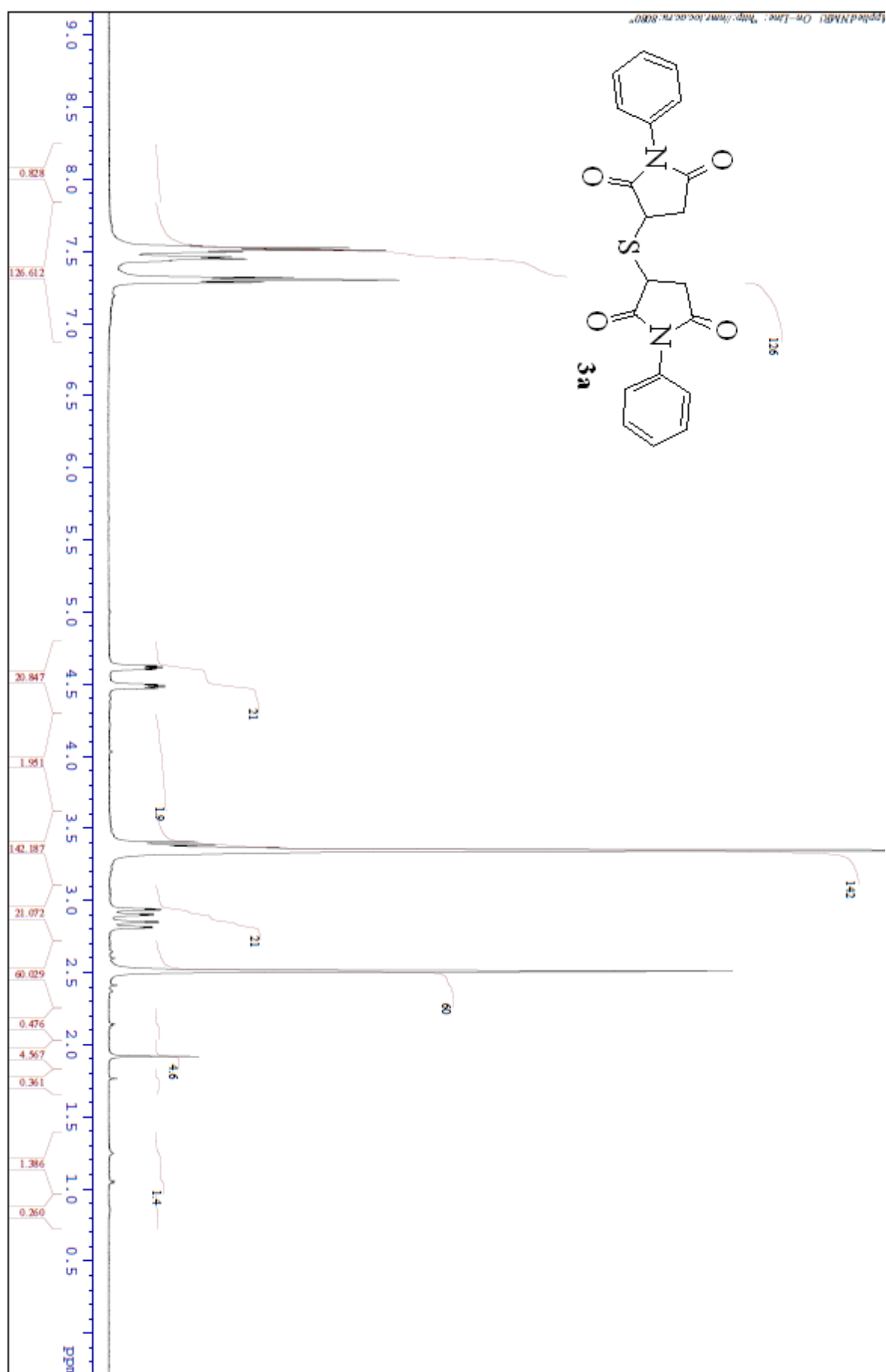


Figure S35: ^1H NMR spectrum (500 MHz, DMSO- d_6) of compound **3a**

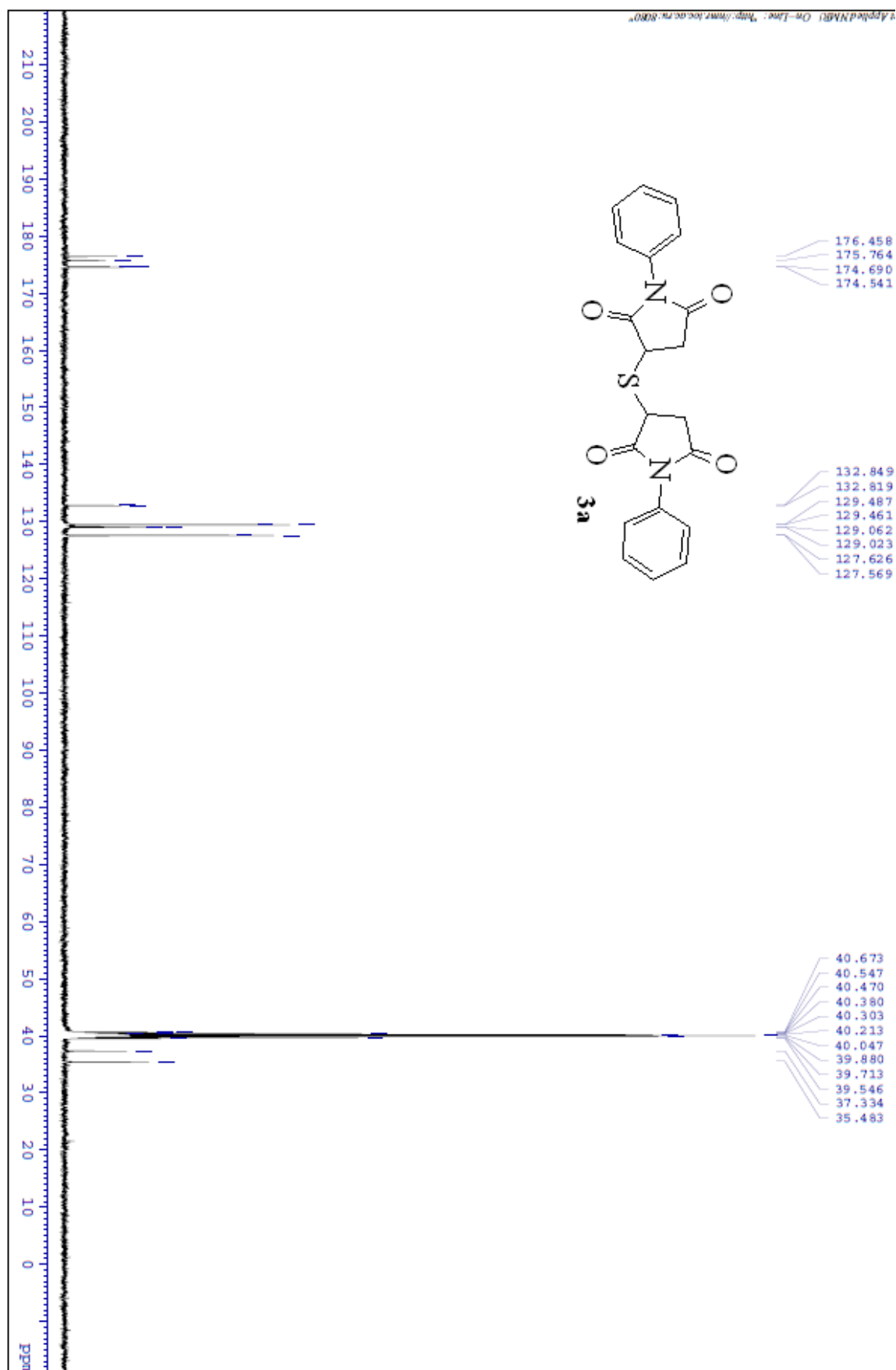


Figure S36: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **3a**

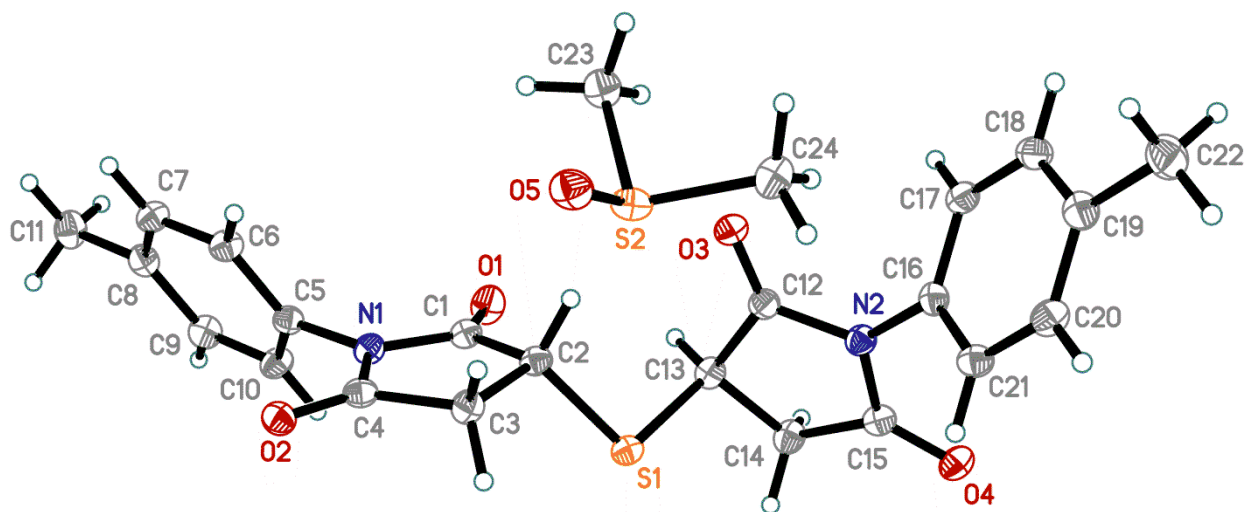


Figure S37: Molecular structure of **3b**•DMSO. A probability level for atomic displacement parameters for non-H atoms is set to 50%.

Table S1. Crystal data and structure refinement for **3b**.

Empirical formula	C ₂₂ H ₂₀ N ₂ O ₄ S•C ₂ H ₆ OS
Formula weight	486.59
Temperature, K	100(2)
Wavelength, Å	0.71073
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell dimensions	
a, Å	5.6417(2)
b, Å	13.7700(5)
c, Å	15.1459(6)
α , °	92.2380(10)
β , °	95.0400(10)
γ , °	95.8090(10)
Volume, Å ³	1164.69(8)
Z	2
Density (cald.), g•cm ⁻³	1.387
Absorption coefficient, mm ⁻¹	0.268
F(000)	512
Crystal size, mm	0.53×0.38×0.30
θ range for data collection, °	2.058–34.981
Index ranges	-9≤h≤9,
	-22≤k≤22,
	-24≤l≤24
Reflections	
Collected	60803
Independent [R _{int}]	10230 [0.1044]
Observed (with I>2σ(I))	6257

Completeness to $\theta_{\max} / \theta_{\text{full}}$	0.999 / 0.999
Data / restraints / parameters	10230 / 0 / 302
Goodness-of-fit on F^2	1.026
R1 / wR2 indices for $I > 2\sigma(I)$	0.0683 / 0.1208
R1 / wR2 indices (all data)	0.1329 / 0.1463
$\Delta\rho(\bar{e})_{\max} / \Delta\rho(\bar{e})_{\min}, \bar{e} \cdot \text{\AA}^{-3}$	0.501 / -0.674

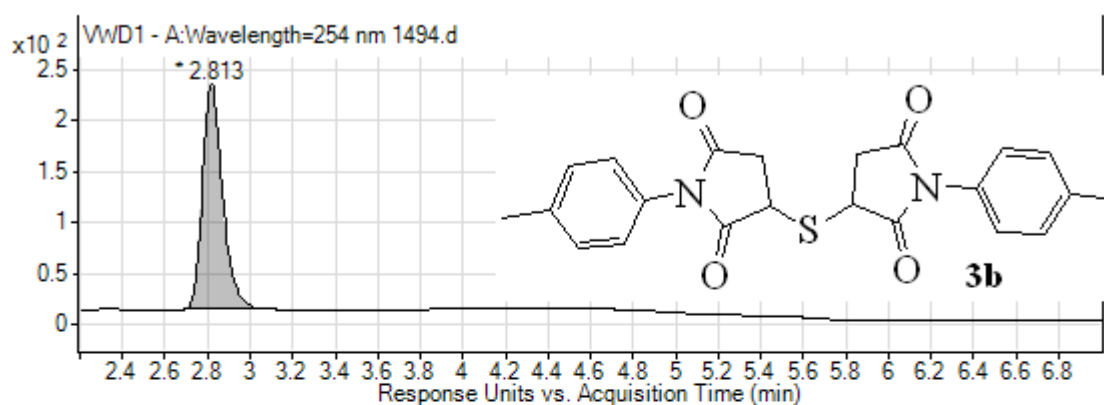
Table S2. Selected bond lengths for **3b**, Å.

S1-C2	1.8163(19)	N2-C16	1.432(2)	C12-C13	1.517(3)
S1-C13	1.827(2)	C1-C2	1.513(3)	C13-C14	1.535(3)
O1-C1	1.211(2)	C2-C3	1.529(3)	C14-C15	1.509(3)
O2-C4	1.208(2)	C3-C4	1.506(3)	C16-C21	1.387(3)
O3-C12	1.213(2)	C5-C6	1.385(3)	C16-C17	1.388(3)
O4-C15	1.204(2)	C5-C10	1.386(3)	C17-C18	1.383(3)
N1-C1	1.388(3)	C6-C7	1.391(3)	C18-C19	1.396(3)
N1-C4	1.401(2)	C7-C8	1.392(3)	C19-C20	1.388(3)
N1-C5	1.434(2)	C8-C9	1.393(3)	C19-C22	1.509(3)
N2-C12	1.393(2)	C8-C11	1.506(3)	C20-C21	1.389(3)
N2-C15	1.400(2)	C9-C10	1.390(3)		

Table S3. Selected angle values for **3b**, °.

C2-S1-C13	102.28(9)	N1-C4-C3	107.99(16)	C14-C13-S1	108.24(14)
C1-N1-C4	112.89(16)	C6-C5-C10	121.11(18)	C15-C14-C13	105.07(16)
C1-N1-C5	122.68(16)	C6-C5-N1	119.04(17)	O4-C15-N2	124.08(19)
C4-N1-C5	124.38(16)	C10-C5-N1	119.81(17)	O4-C15-C14	127.90(18)
C12-N2-C15	112.73(16)	C5-C6-C7	119.26(18)	N2-C15-C14	108.00(16)
C12-N2-C16	122.94(16)	C6-C7-C8	120.97(19)	C21-C16-C17	120.76(18)
C15-N2-C16	124.29(16)	C7-C8-C9	118.42(18)	C21-C16-N2	119.50(17)
O1-C1-N1	124.60(18)	C7-C8-C11	120.96(19)	C17-C16-N2	119.71(17)
O1-C1-C2	127.08(18)	C9-C8-C11	120.62(19)	C18-C17-C16	119.08(18)
N1-C1-C2	108.32(16)	C10-C9-C8	121.48(18)	C17-C18-C19	121.39(19)
C1-C2-C3	104.92(16)	C5-C10-C9	118.76(18)	C20-C19-C18	118.35(19)
C1-C2-S1	111.76(13)	O3-C12-N2	124.46(18)	C20-C19-C22	121.55(19)
C3-C2-S1	110.58(13)	O3-C12-C13	127.33(18)	C18-C19-C22	120.10(19)
C4-C3-C2	105.53(15)	N2-C12-C13	108.16(16)	C19-C20-C21	121.13(19)
O2-C4-N1	124.27(18)	C12-C13-C14	104.26(16)	C16-C21-C20	119.28(18)
O2-C4-C3	127.71(17)	C12-C13-S1	107.67(13)		

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	2,69	2,813	3,073	221,81	1456,45	100

User Spectra

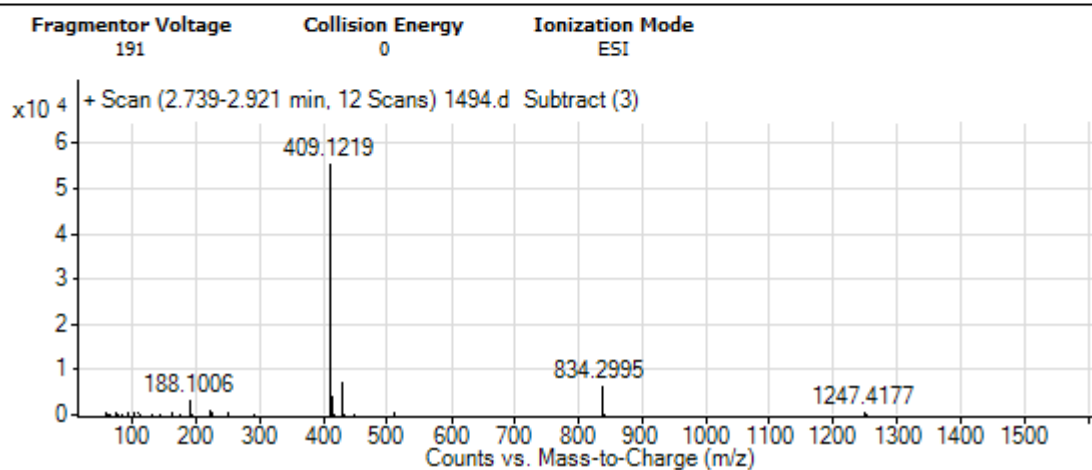


Figure S38: Data HPLC of compound **3b**

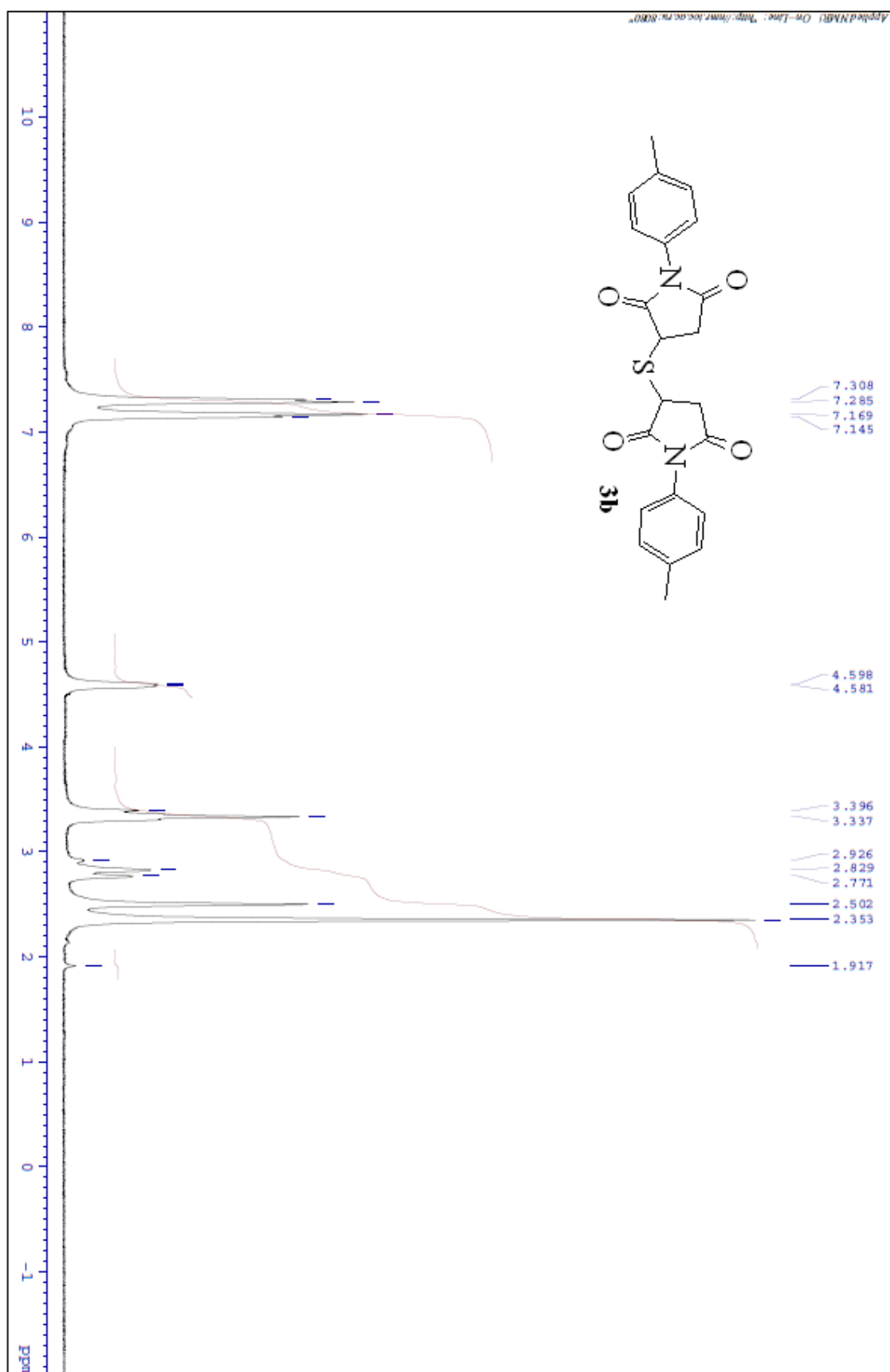


Figure S39: ^1H NMR spectrum (500 MHz, DMSO- d_6) of compound **3b**

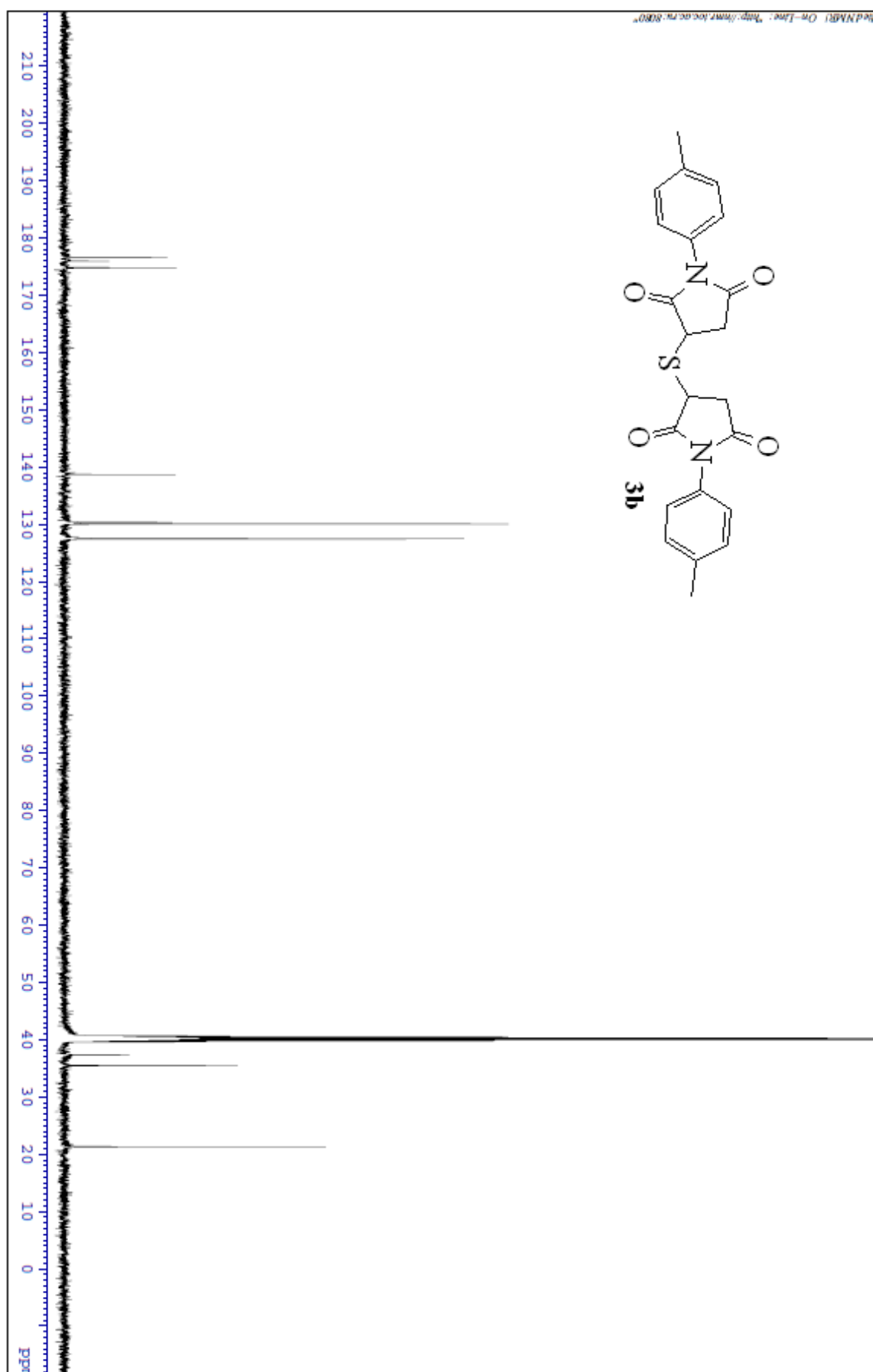
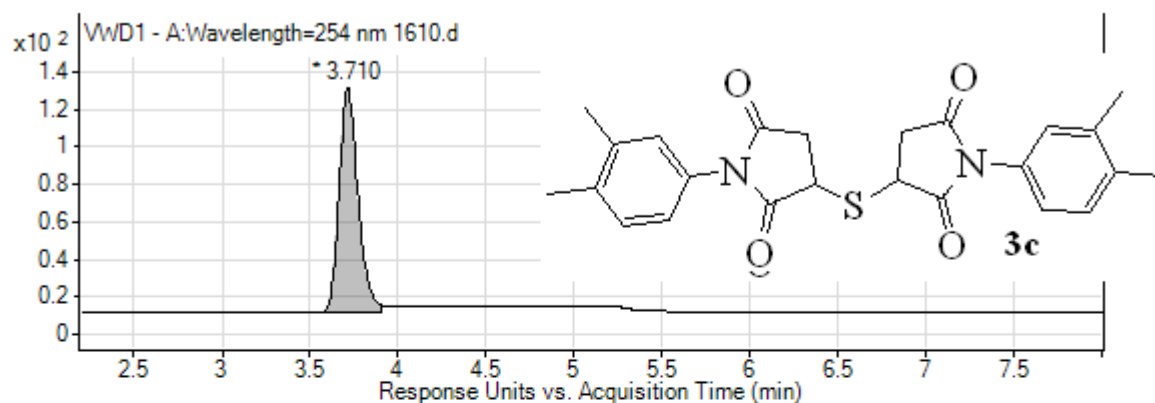


Figure S40: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **3b**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,577	3,71	3,903	119,74	895,67	100

User Spectra

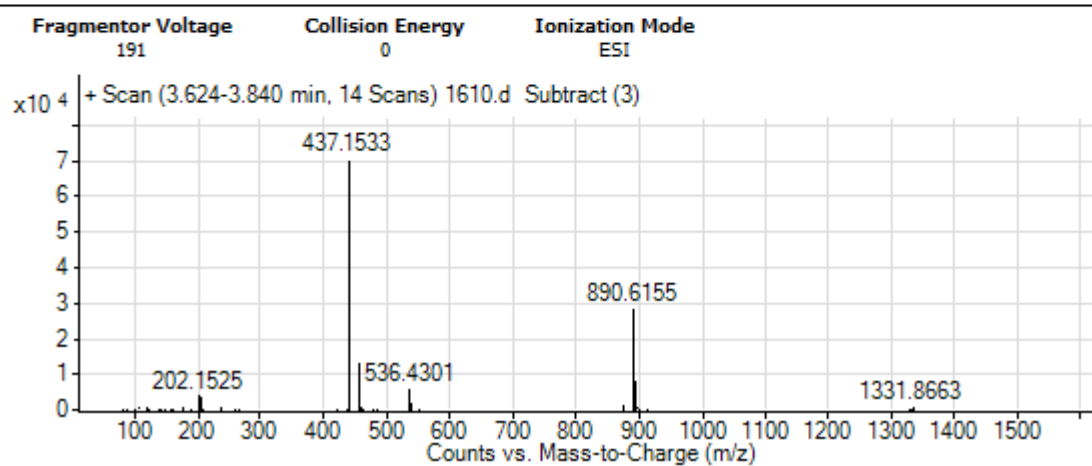


Figure S41: Data HPLC of compound 3c

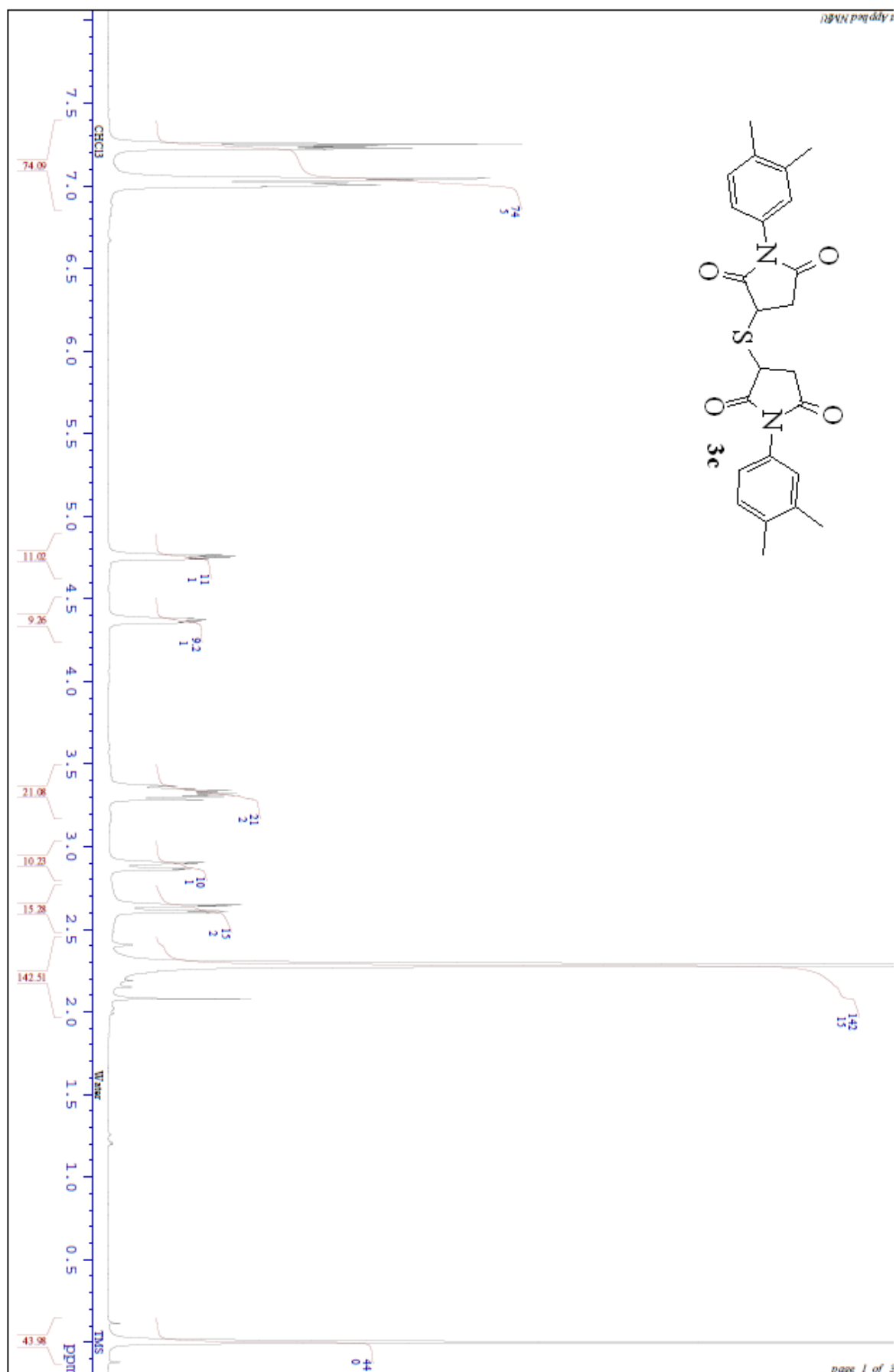


Figure S42: ¹H NMR spectrum (500 MHz, CDCl₃) of compound 3c

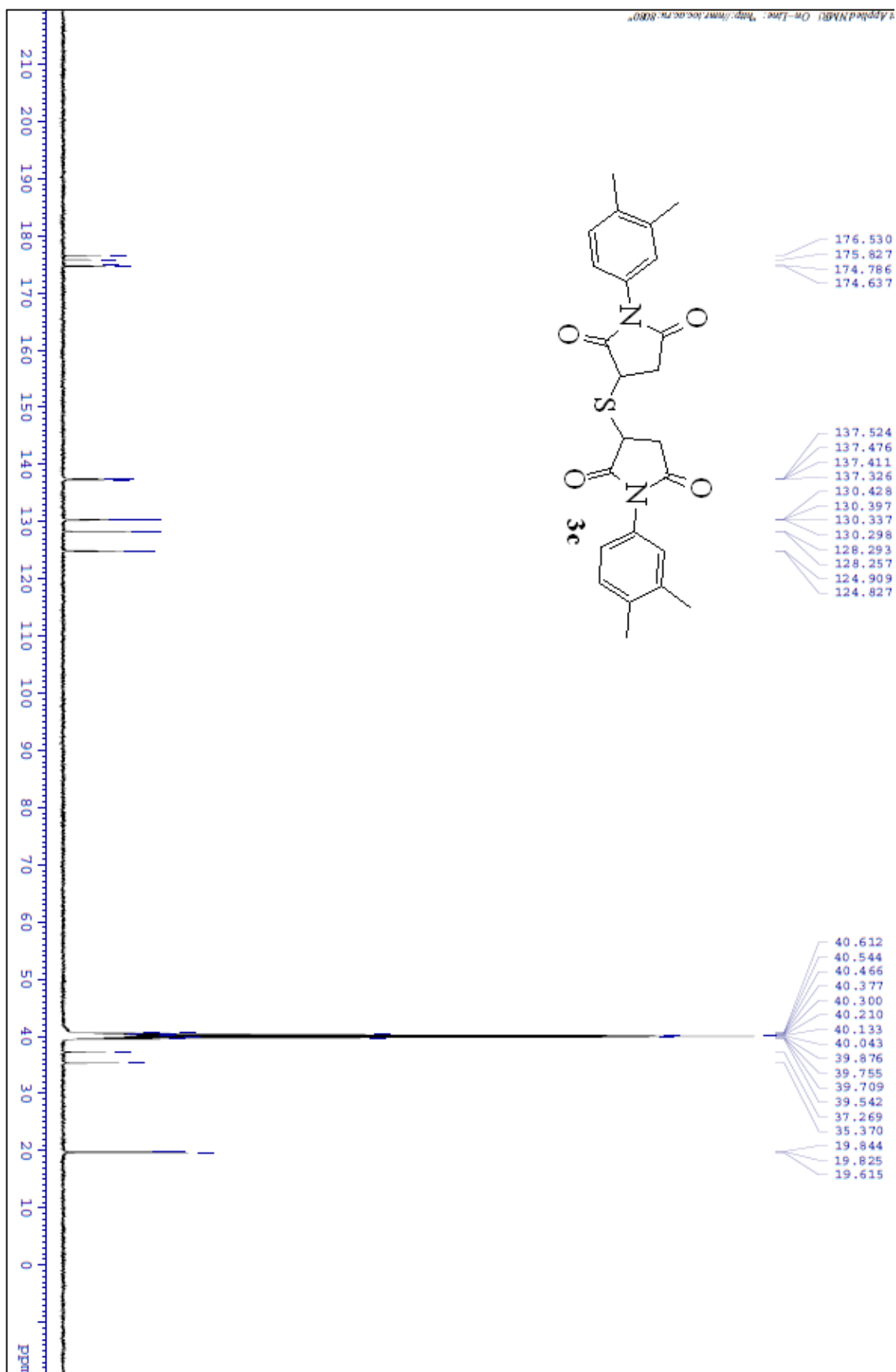
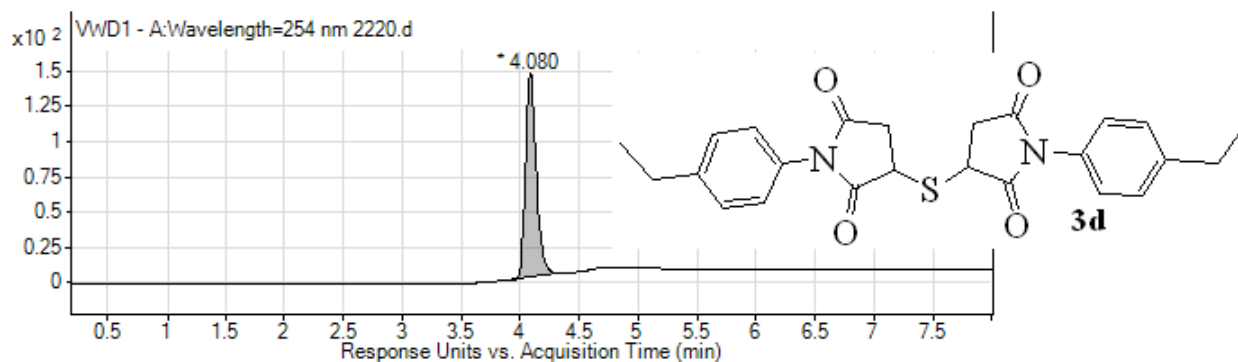


Figure S43: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **3c**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,91	4,08	4,337	144,21	918,31	100

User Spectra

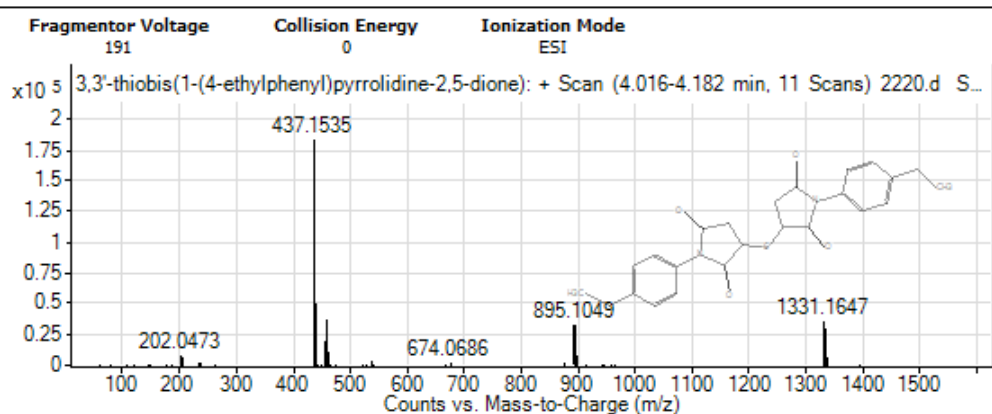


Figure S44: Data HPLC of compound **3d**



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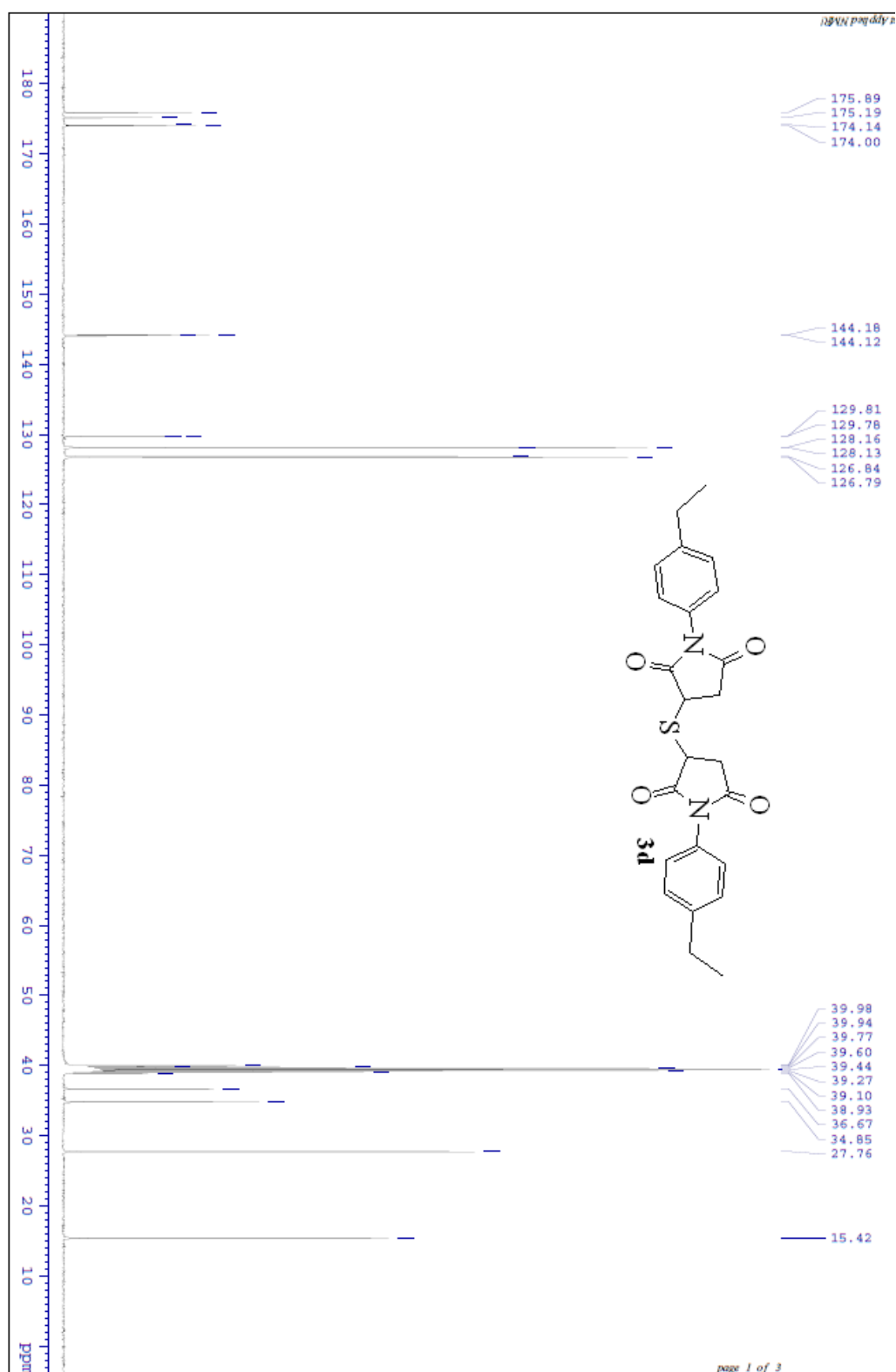
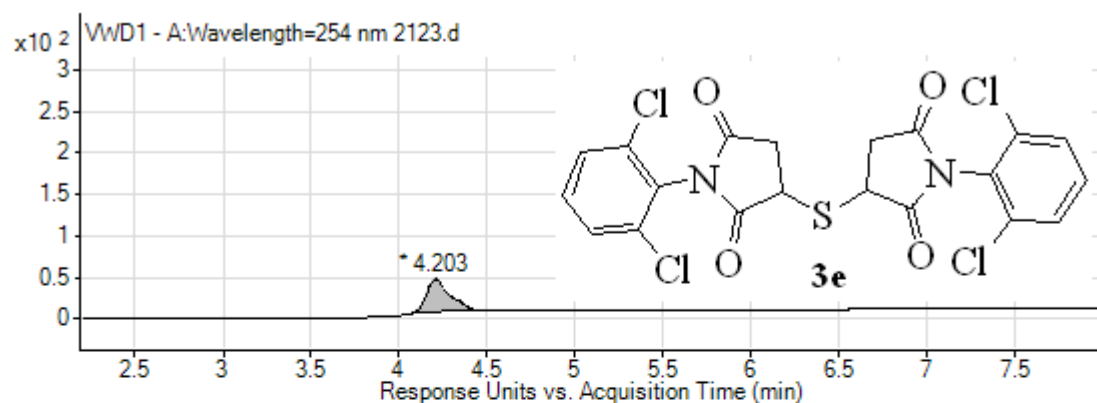


Figure S46: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **3d**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4,057	4,203	4,427	40,72	369,79	100

User Spectra

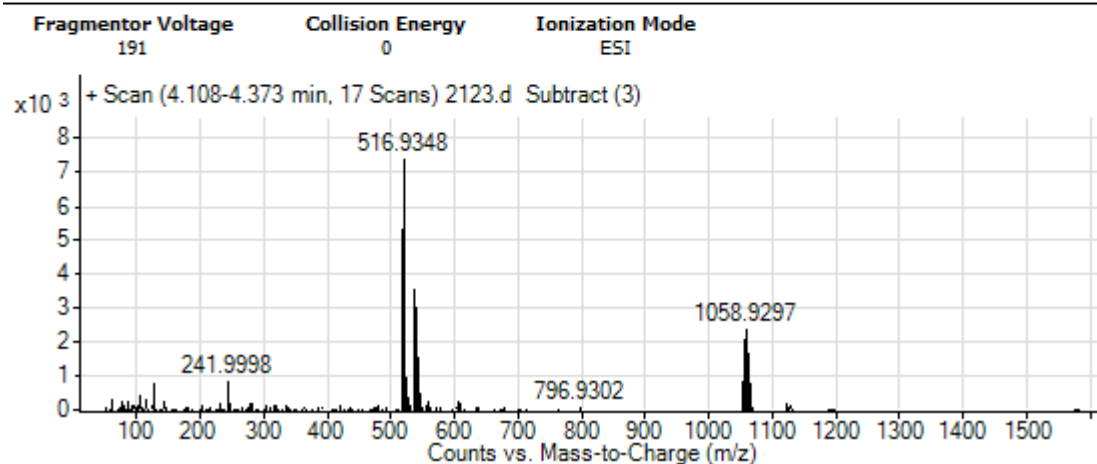


Figure S47: Data HPLC of compound **3e**

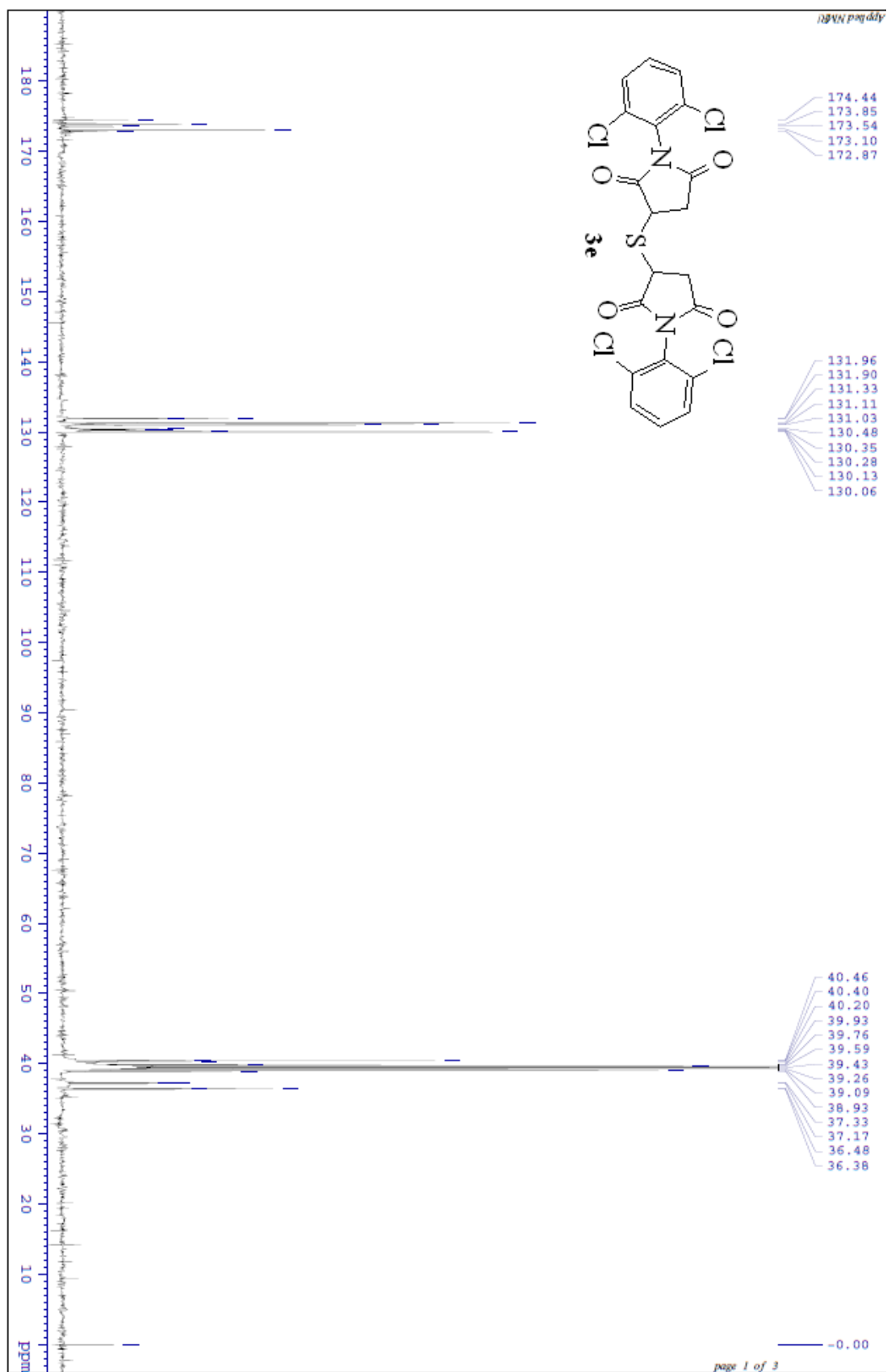
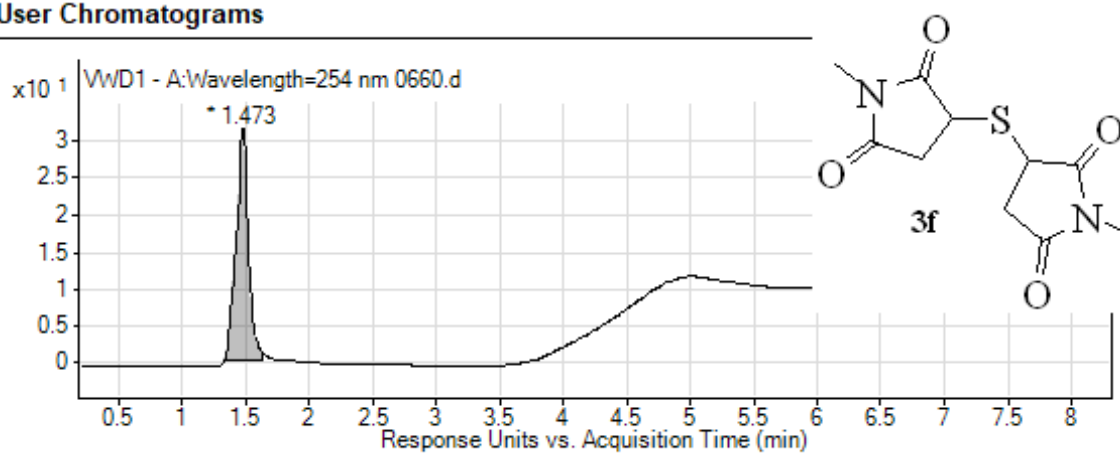


Figure S49: ¹³C NMR spectrum (125 MHz, DMSO-d₆) of compound **3e**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1,32	1,473	1,633	31,34	213,37	100

User Spectra

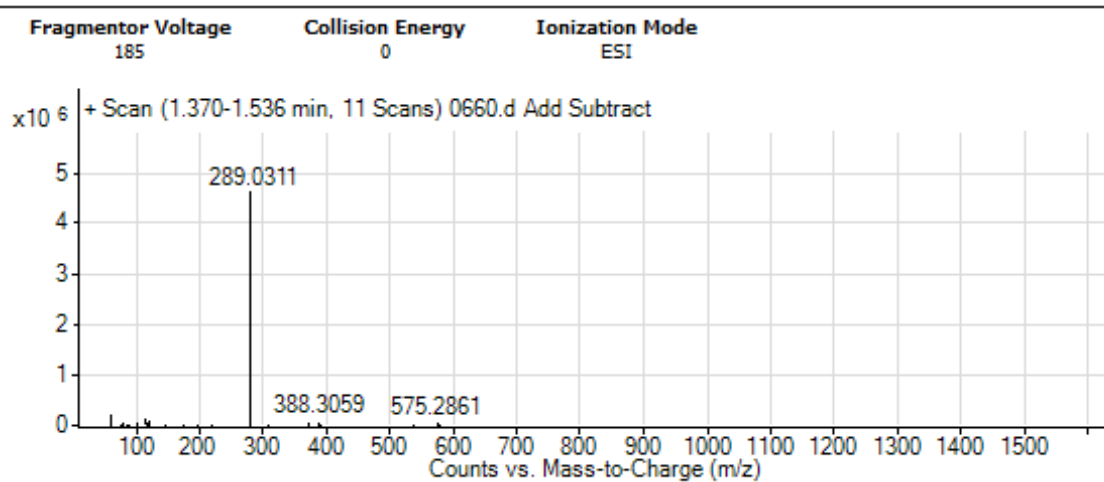


Figure S50: Data HPLC of compound 3f

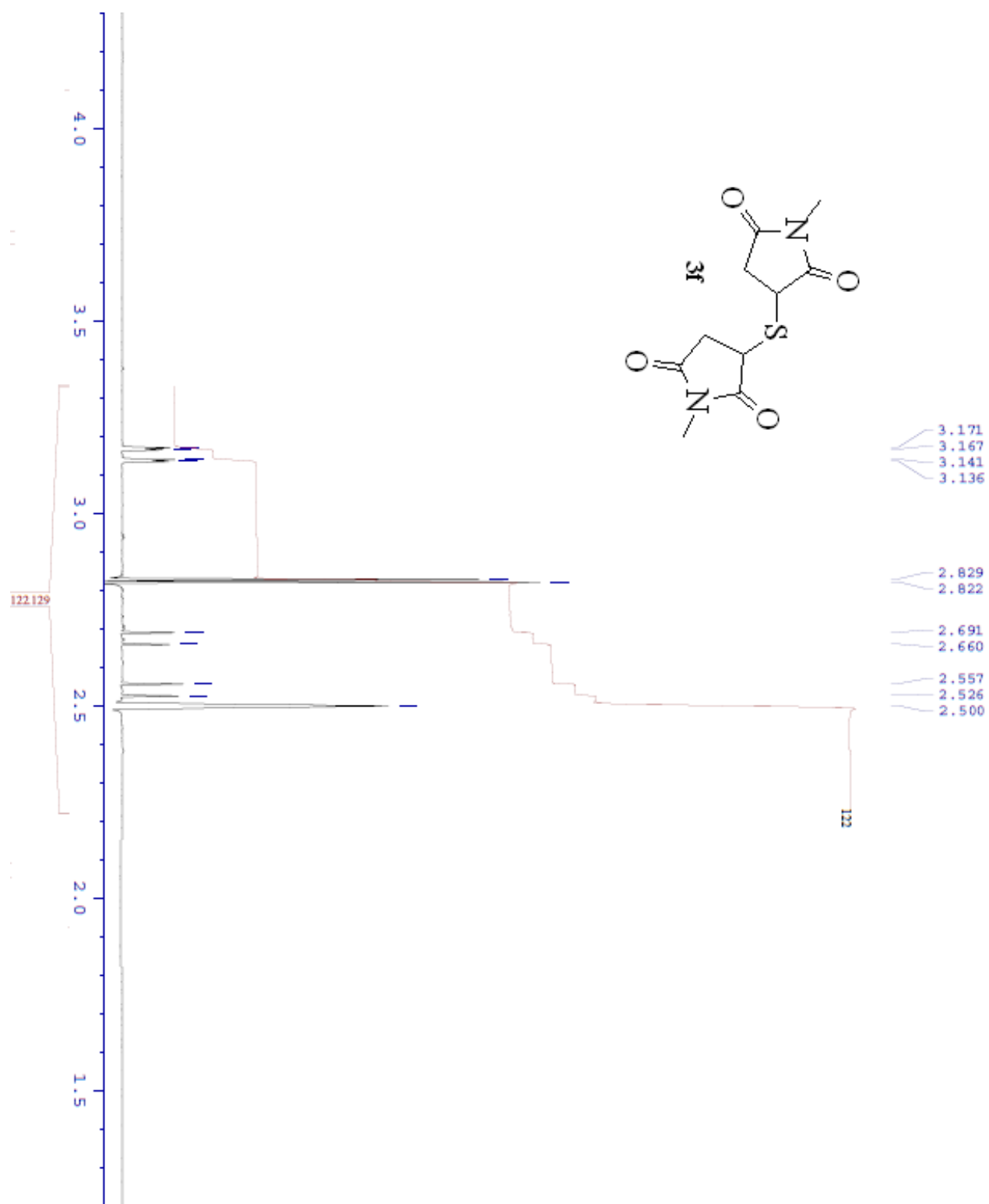


Figure S51: ^1H NMR spectrum (500 MHz, DMSO-d_6) of compound **3f**

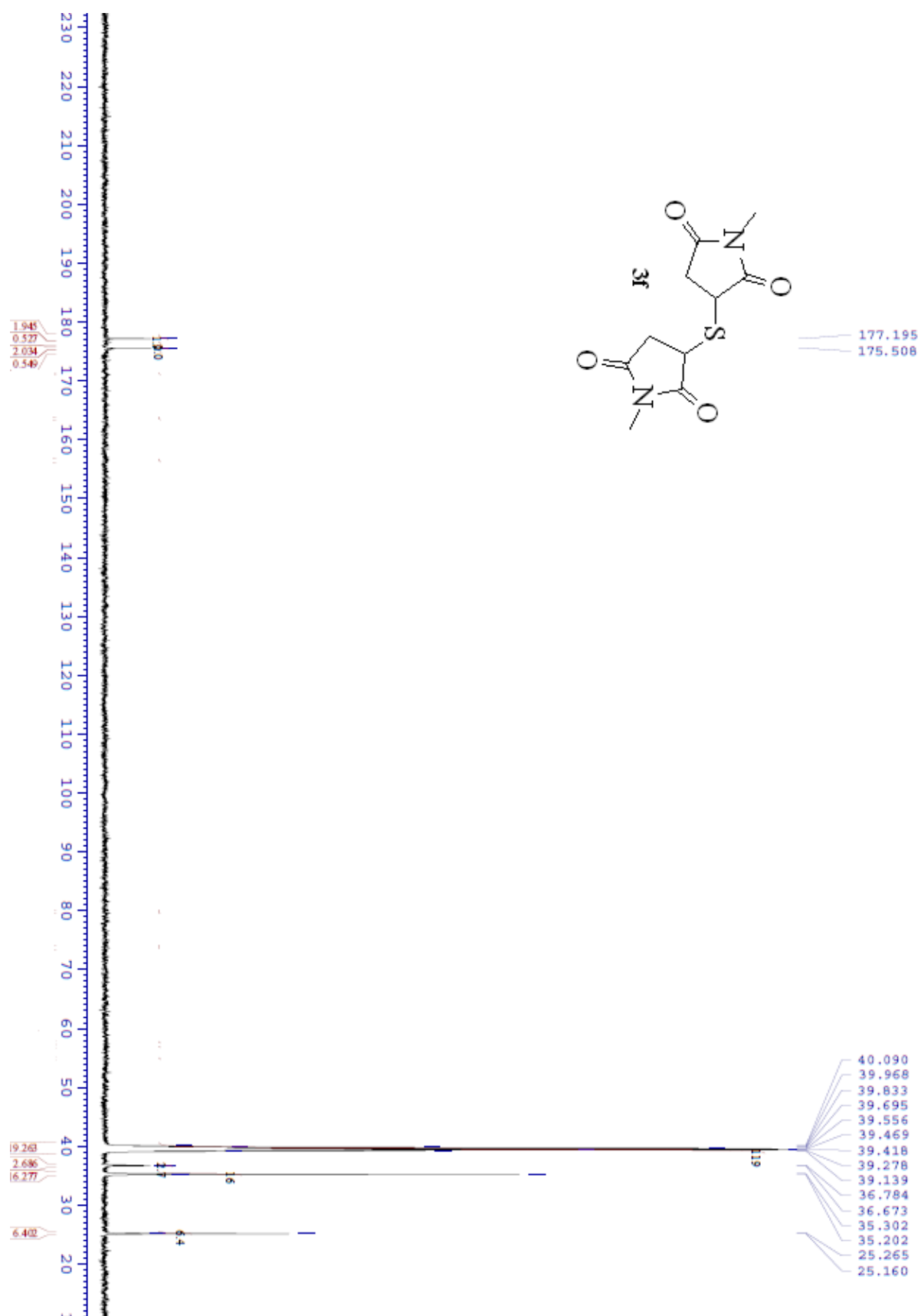
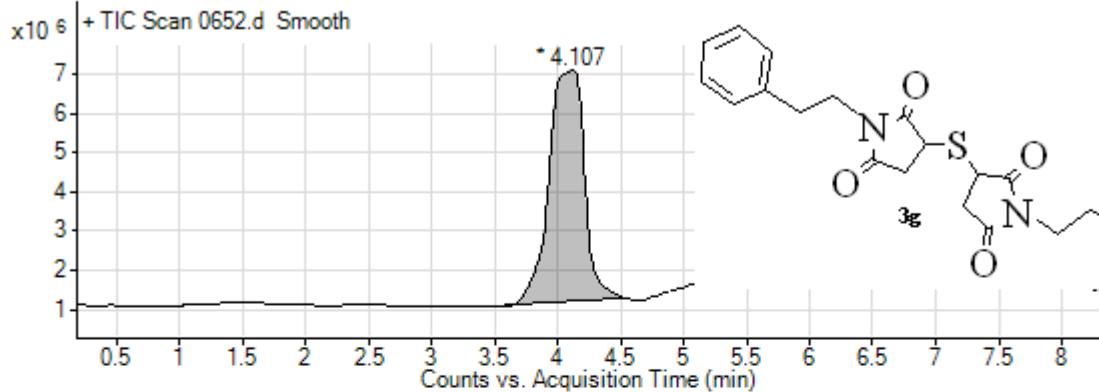


Figure S52: ¹³C NMR spectrum (125 MHz, DMSO-d₆) of compound **3f**

User Chromatograms

Fragmentor Voltage 185 Collision Energy 0 Ionization Mode ESI

x10⁶ + TIC Scan 0652.d Smooth



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,576	4,107	4,554	5909688,05	116224160,9	100

User Spectra

Fragmentor Voltage 185 Collision Energy 0 Ionization Mode ESI

x10⁵ + Scan (3.792-3.924, 4.206-4.305 min, 16 Scans) 0652.d Subtract

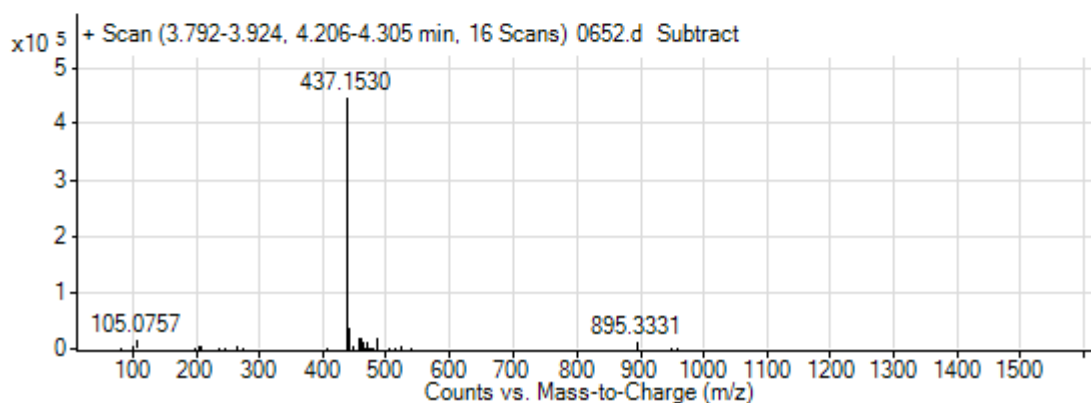


Figure S53: Data HPLC of compound **3g**

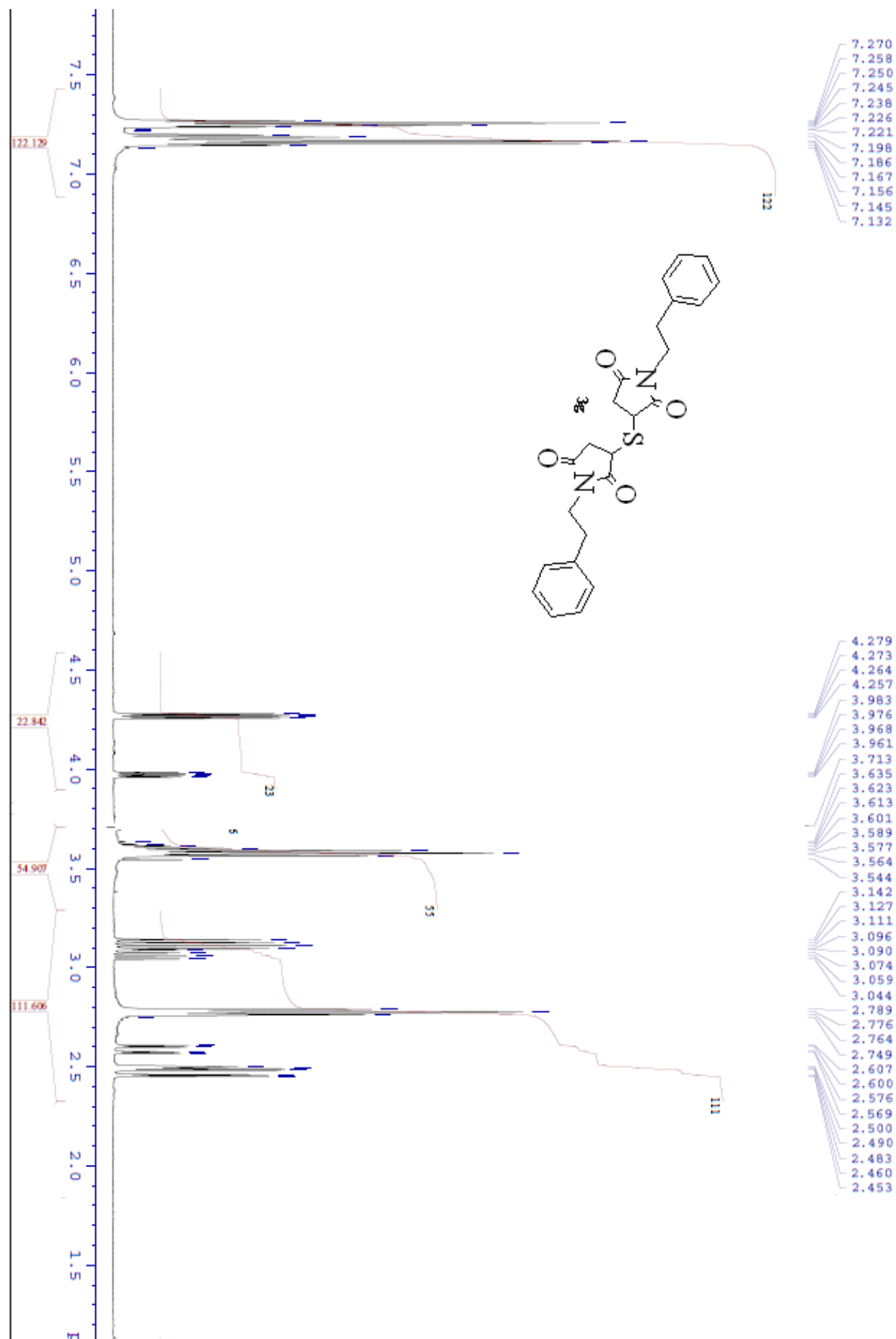


Figure S54: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound **3g**

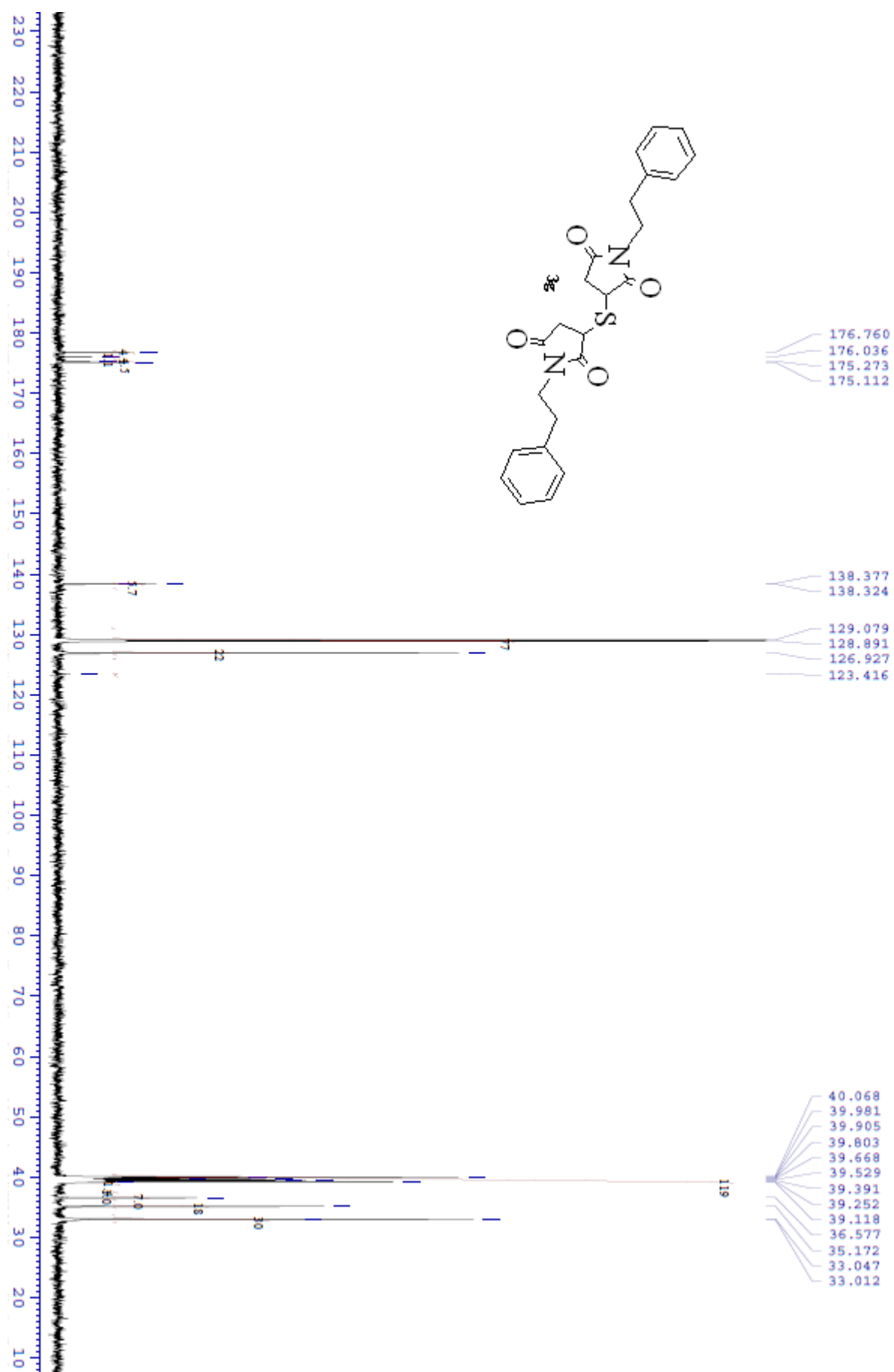
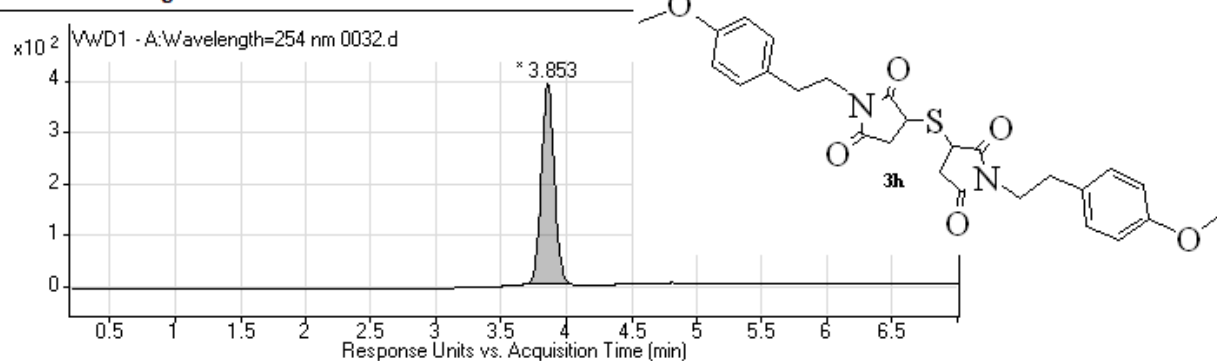


Figure S55: ¹³C NMR spectrum (125 MHz, DMSO-d₆) of compound **3g**

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3,66	3,853	4,05	391,5	2701,99	100

User Spectra

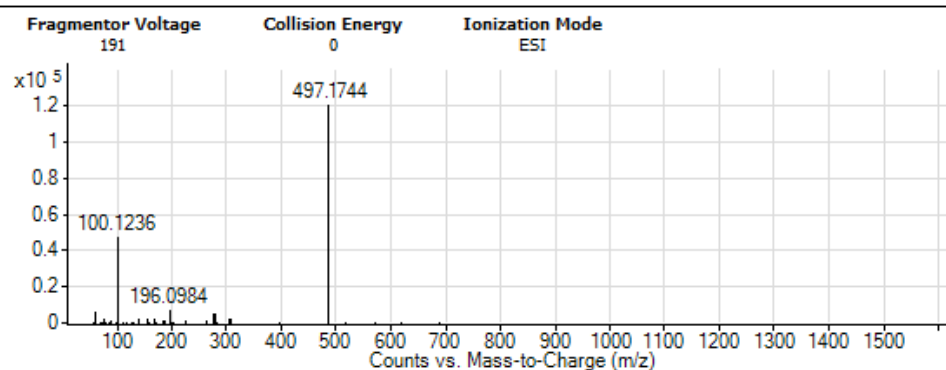


Figure S56: Data HPLC of compound 3h

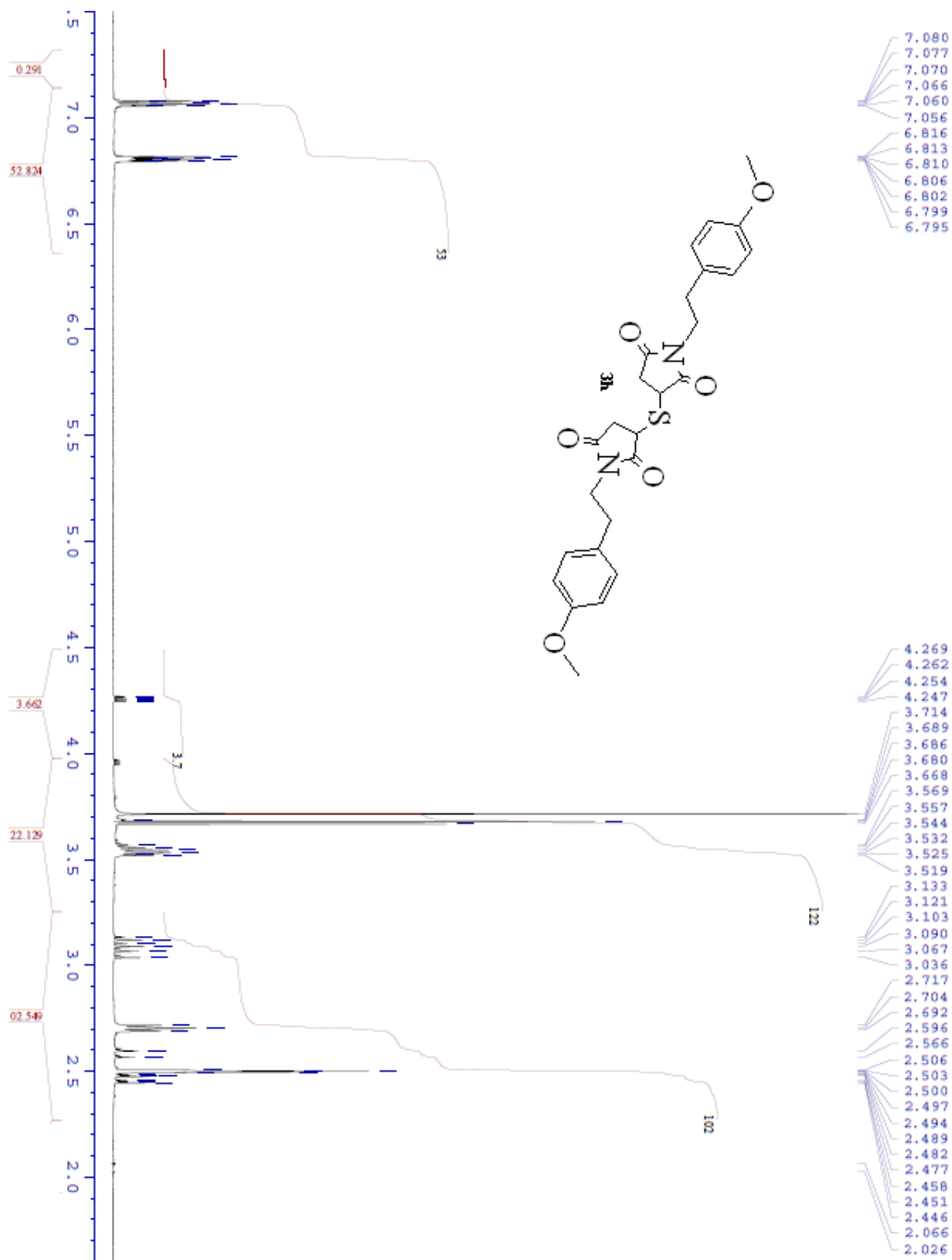


Figure S57: ¹H NMR spectrum (500 MHz, DMSO-d₆) of compound 3h

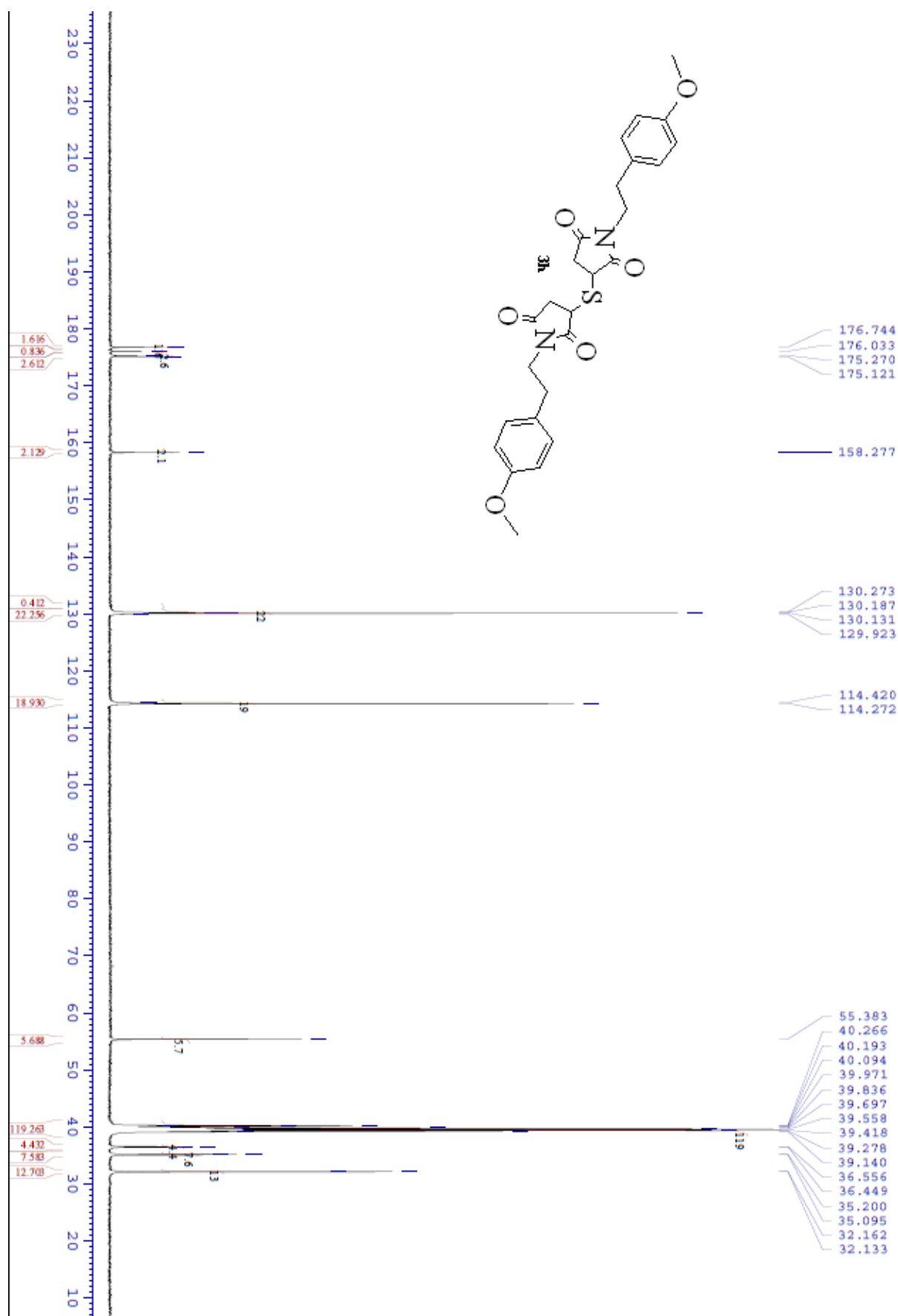


Figure S58: ^{13}C NMR spectrum (125 MHz, DMSO- d_6) of compound **3h**