

Electronic Supplementary Information

A synthetically benign one-pot construction of enamino-xanthene dyes

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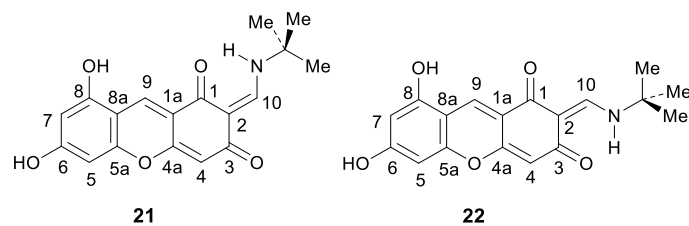
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ENERGY DATA (TABLES AND FIGURES)

Table S1. Energy barrier to interconversion of **21/22**.



Signal	Assignment	$\Delta\delta^a$	$\Delta\vartheta^b$	T_c^c	T_c^d	$\Delta G^{\ddagger e}$
NH	Enamine	0,055	27,5	87	360	18,1
=CH	C10	0,029	14,5	87	360	18,5
CH	C9	0,020	10,0	77	350	18,2
CH	C7	0,044	22,0	97	370	18,7

^a In ppm; ^b In Hz; ^c In °C; ^d In K; ^e In kcal·mol⁻¹ (1 cal = 4.184 J).

Table S2. Relative electronic energy, enthalpy, and Gibbs energy in gas phase.^a

Compound	Enamine			TS [‡]				Imine		
	ΔE	ΔH	ΔG	ΔE^{\ddagger}	ΔH^{\ddagger}	ΔG^{\ddagger}	$\tilde{\nu}^{\ddagger b}$	ΔE	ΔH	ΔG
21/49	0.0	0.0	0.6	7.3	3.7	4.6	-1074.6	5.9	5.2	6.4
22/50	0.0	0.0	0.0	6.4	3.1	4.4	-1025.5	5.3	4.4	5.3

^a In kcal·mol⁻¹, ^b In cm⁻¹.

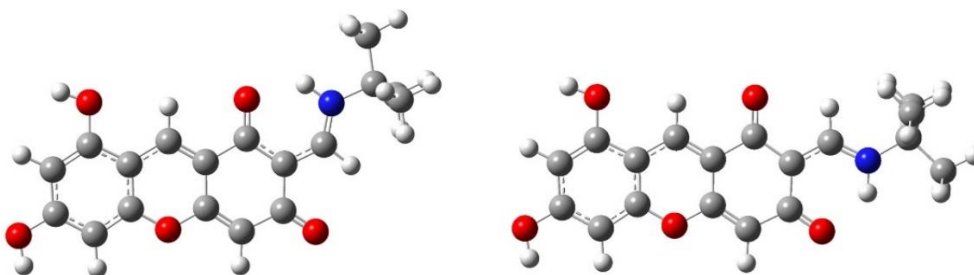


Figure S1. Optimized structures of ketoenamines **21** and **22** in the gas phase.

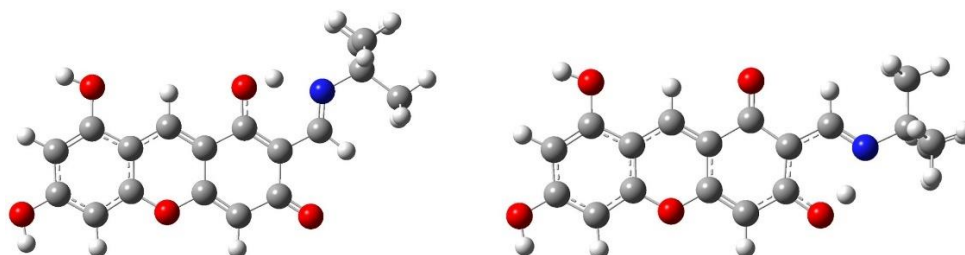


Figure S2. Optimized structures of phenolimines **49** and **50** in the gas phase.

Table S3. Relative electronic energy, enthalpy, and Gibbs energy in DMSO.^a

Compound	Enamine			TS [‡]				Imine		
	ΔE	ΔH	ΔG	ΔE^{\ddagger}	ΔH^{\ddagger}	ΔG^{\ddagger}	$\tilde{\nu}^{\ddagger b}$	ΔE	ΔH	ΔG
21/49	0.0	0.0	0.6	8.8	5.1	6.0	-896.9	8.3	7.1	8.0
22/50	0.3	0.3	0.0	8.3	4.9	5.9	-861.4	7.9	6.6	7.5

^a In kcal·mol⁻¹, ^b In cm⁻¹.**Table S4.** Relative electronic energy, enthalpy, and Gibbs energy in DMSO, ethanol and water.^a

Compound	DMSO			Ethanol			Water		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
21	0.0	0.0	0.6	0.0	0.0	0.3	0.0	0.0	0.0
49	8.3	7.1	8.0	9.1	7.6	8.6	9.8	8.2	8.8
50	7.9	6.6	7.5	8.8	7.3	8.5	9.5	8.1	8.6
22	0.3	0.3	0.0	0.3	0.0	0.0	0.5	0.2	0.0

^a In kcal·mol⁻¹.

MASS SPECTROMETRY

Note: Signals around m/z 157.0357 correspond to dimethylsulfoxide $[M_2+H]^+$, used as solvent.

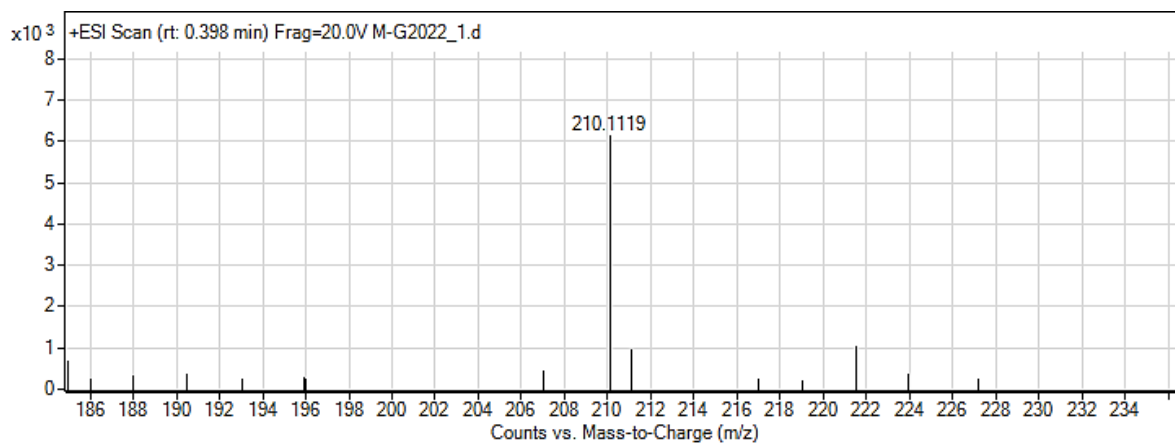


Figure S3. LC-MS of **18** - $C_{11}H_{15}NO_3$ $[M+H]^+$ m/z calcd. 210.1125.

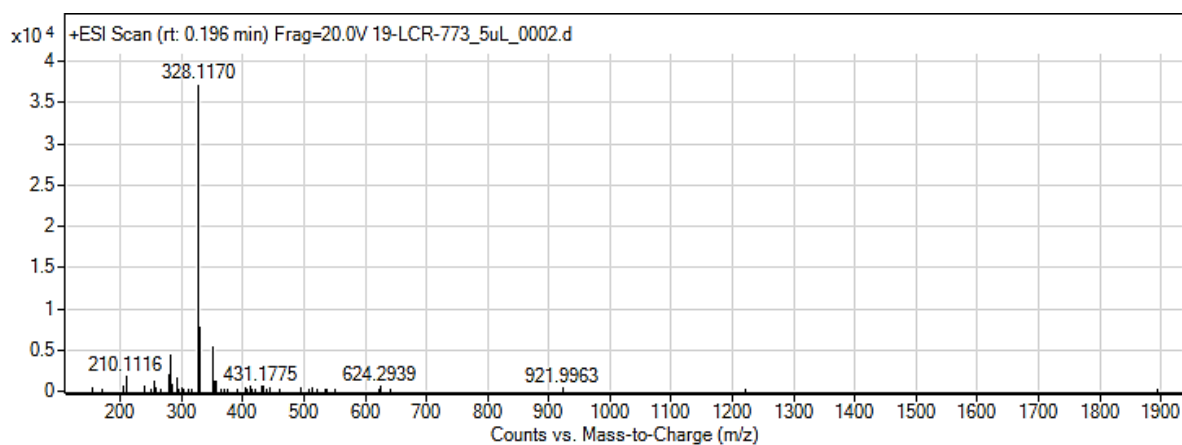


Figure S4. LC-MS of **19** - $C_{18}H_{17}NO_5$ $[M+H]^+$ m/z calcd. 328.1180.

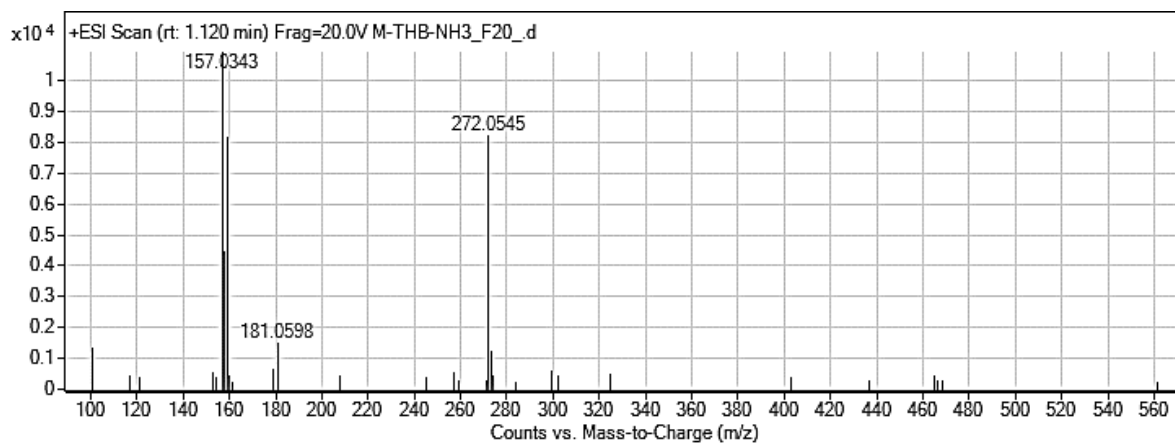


Figure S5. LC-MS of **23** - $C_{14}H_9NO_5$ $[M+H]^+$ m/z calcd. 272.0554.

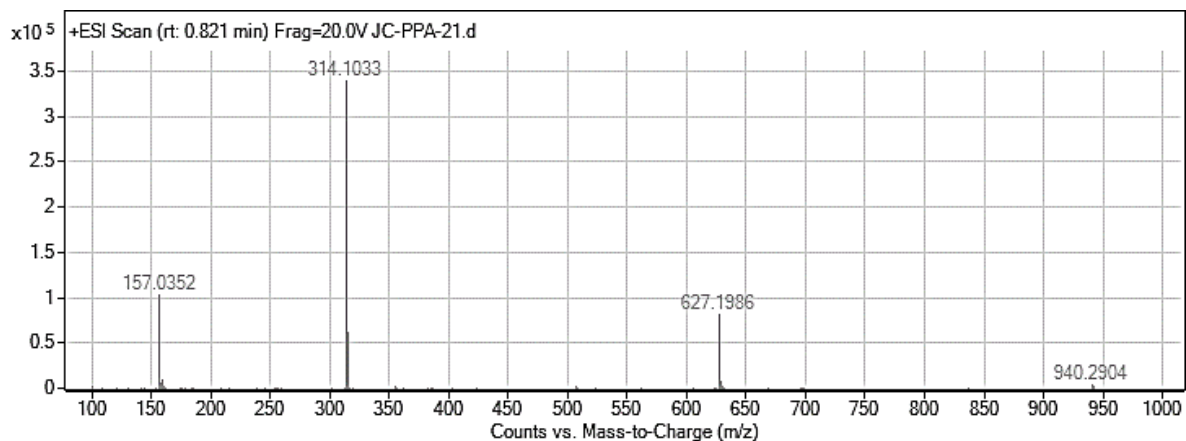


Figure S6. LC-MS of **24** - C₁₇H₁₅NO₅ [M+H]⁺ m/z calcd. 314.1023; [M₂+H]⁺ m/z calcd. 627.1973; [M₃+H]⁺ m/z calcd. 940.2923.

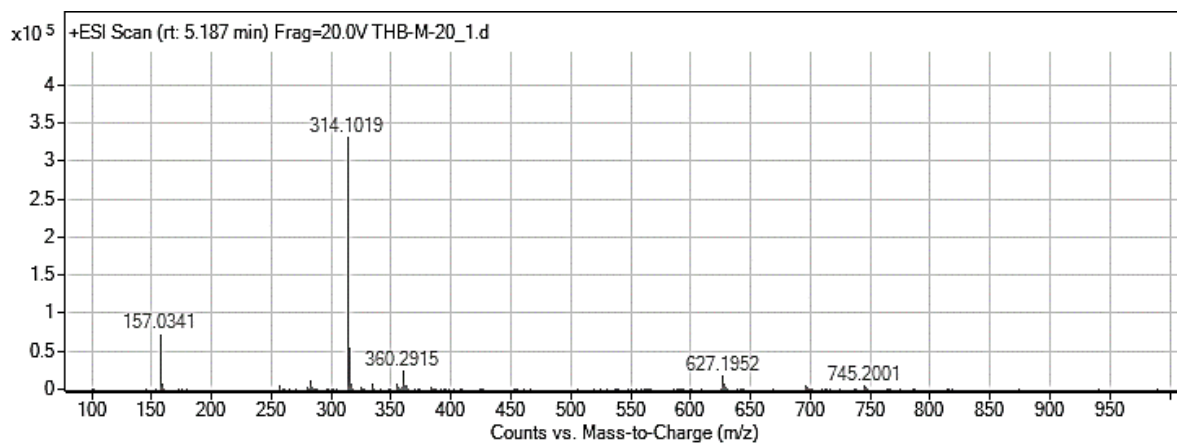


Figure S7. LC-MS of **25** C₁₇H₁₅NO₅ [M+H]⁺ m/z calcd. 314.1023; [M₂+H]⁺ m/z calcd. 627.1973.

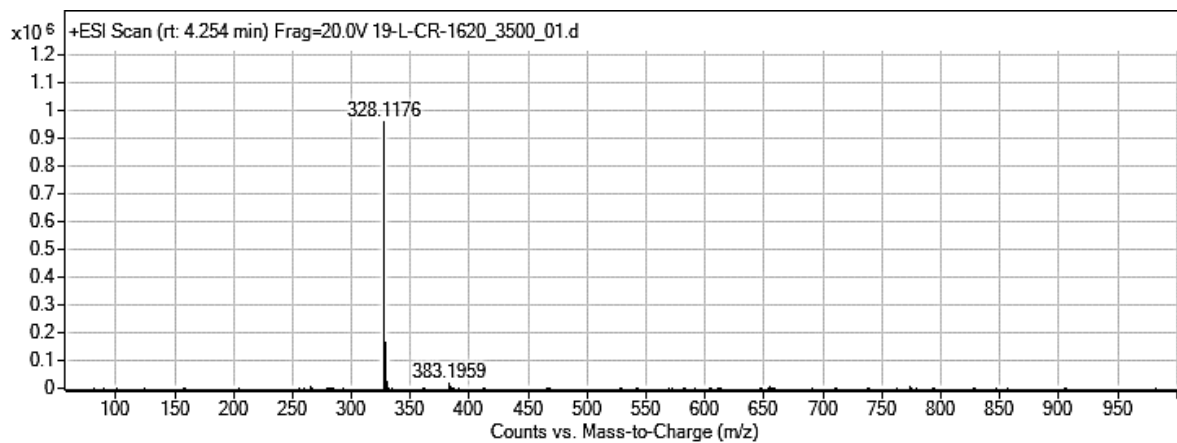


Figure S8. LC-MS of **26** - C₁₈H₁₇NO₅ [M+H]⁺ m/z calcd. 328.1180.

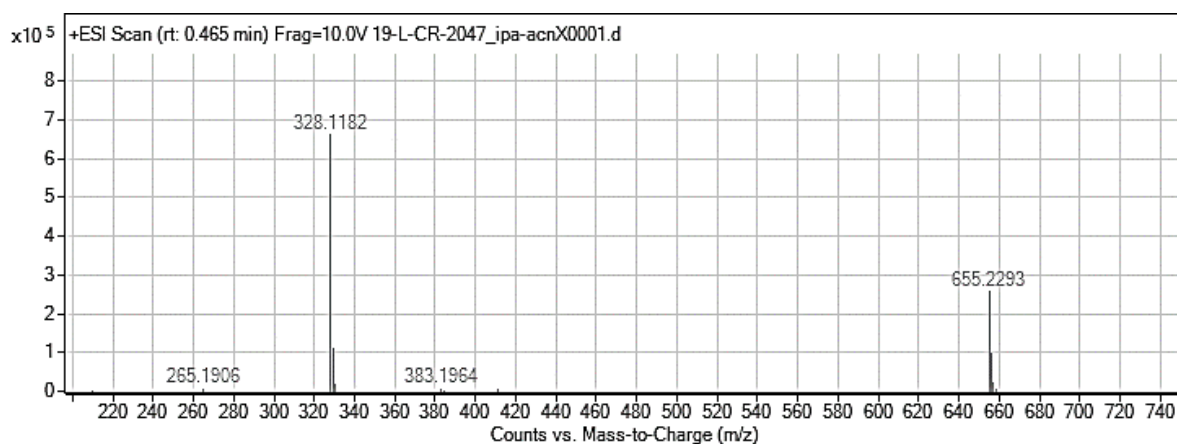


Figure S9. LC-MS of **27** - $C_{18}H_{17}NO_5$ $[M+H]^+$ m/z calcd. 328.1180; $[M_2+H]^+$ m/z calcd. 655.2286.

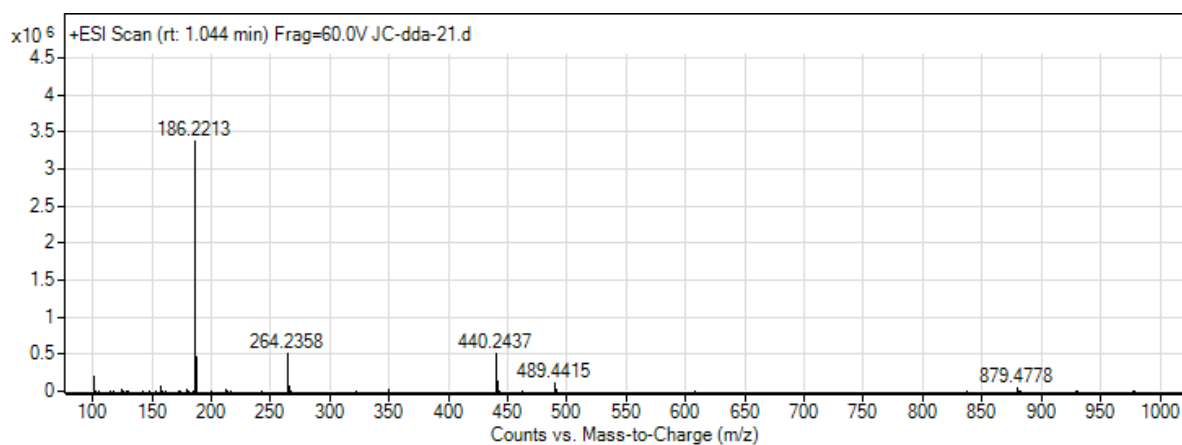


Figure S10. LC-MS of **28** - $C_{26}H_{33}NO_5$ $[M+H]^+$ m/z calcd. 440.2432; $[M_2+H]^+$ m/z calcd. 879.4790.

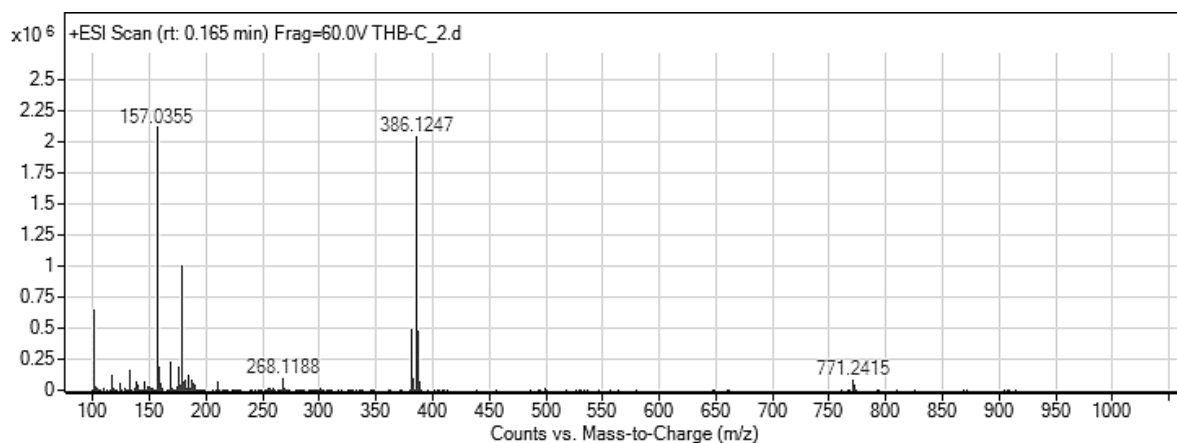


Figure S11. LC-MS of **29** - $C_{20}H_{19}NO_7$ $[M+H]^+$ m/z calcd. 386.1234; $[M_2+H]^+$ m/z calcd. 771.2401.

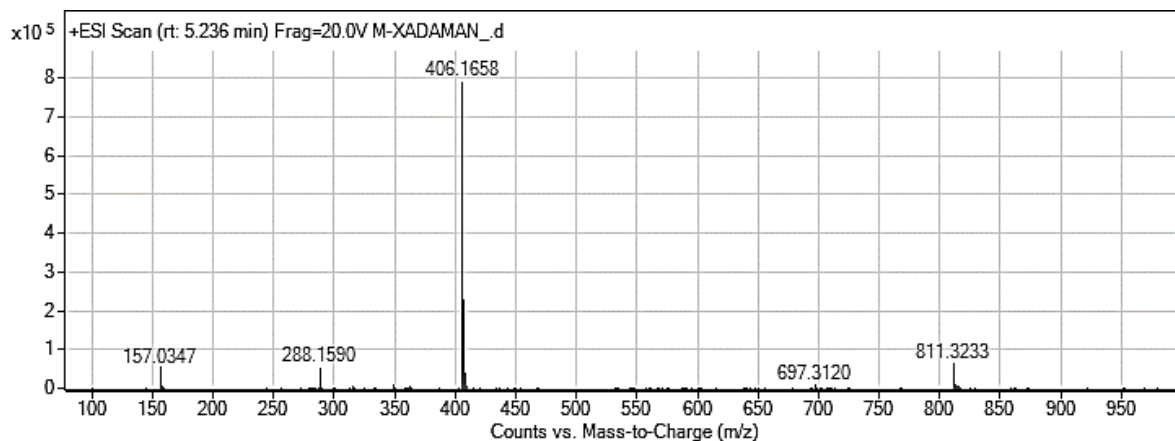


Figure S12. LC-MS of **30** - $C_{24}H_{23}NO_5$ $[M+H]^+$ m/z calcd. 406.1649; $[M_2+H]^+$ m/z calcd. 811.3225.

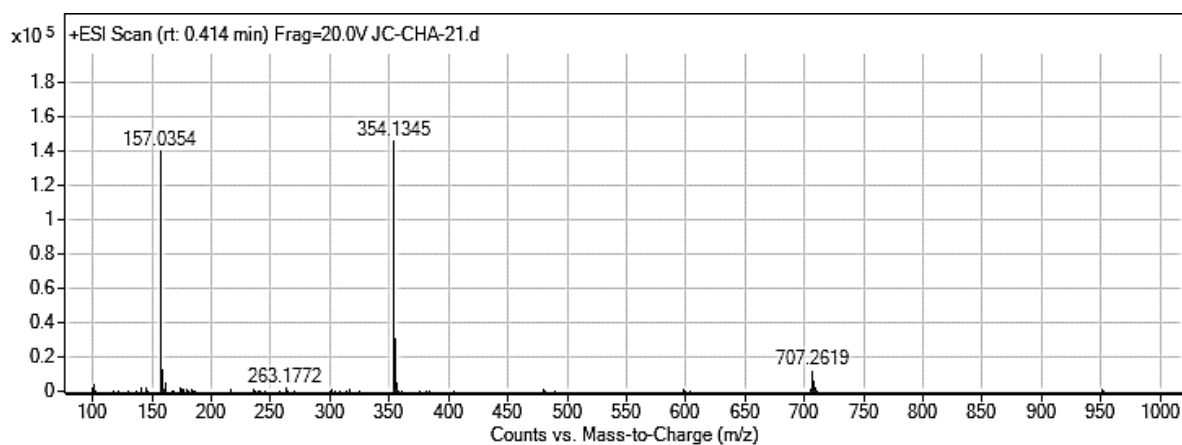


Figure S13. LC-MS of **31** - $C_{20}H_{19}NO_5$ $[M+H]^+$ m/z calcd. 354.1336; $[M_2+H]^+$ m/z calcd. 707.2599.

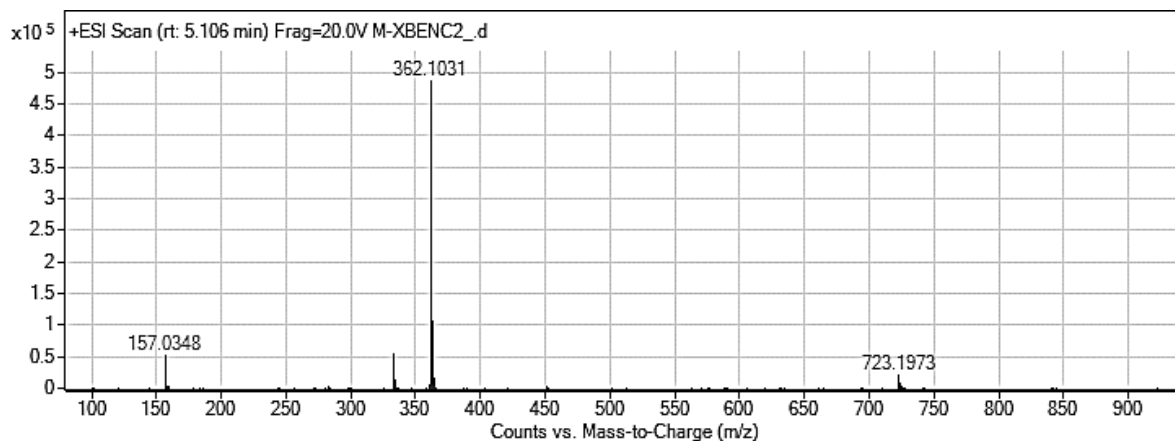


Figure S14. LC-MS of **32** - $C_{21}H_{15}NO_5$ $[M+H]^+$ m/z calcd. 362.1023; $[M_2+H]^+$ m/z calcd. 723.1973.

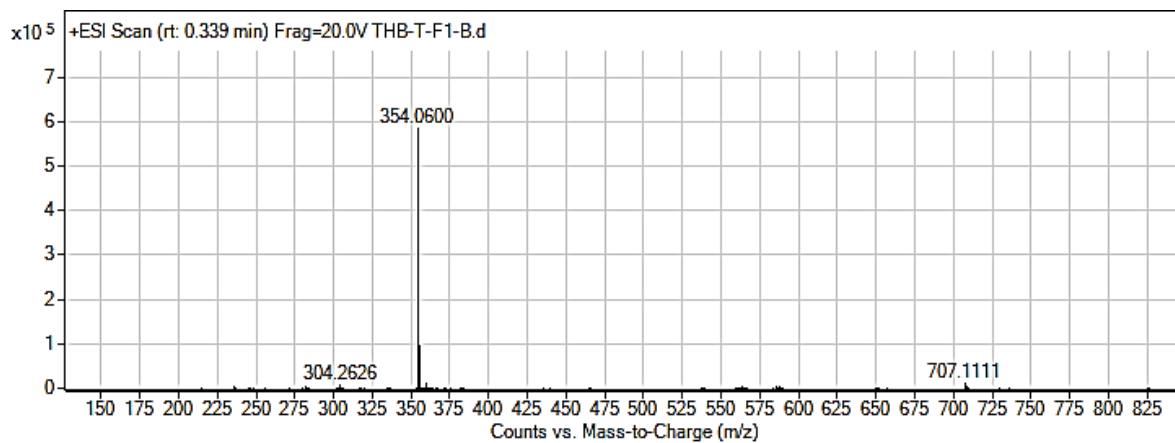


Figure S15. LC-MS of **33** - $C_{16}H_{10}F_3NO_5$ $[M+H]^+$ m/z calcd. 354.0584; $[M_2+H]^+$ m/z calcd. 707.1095.

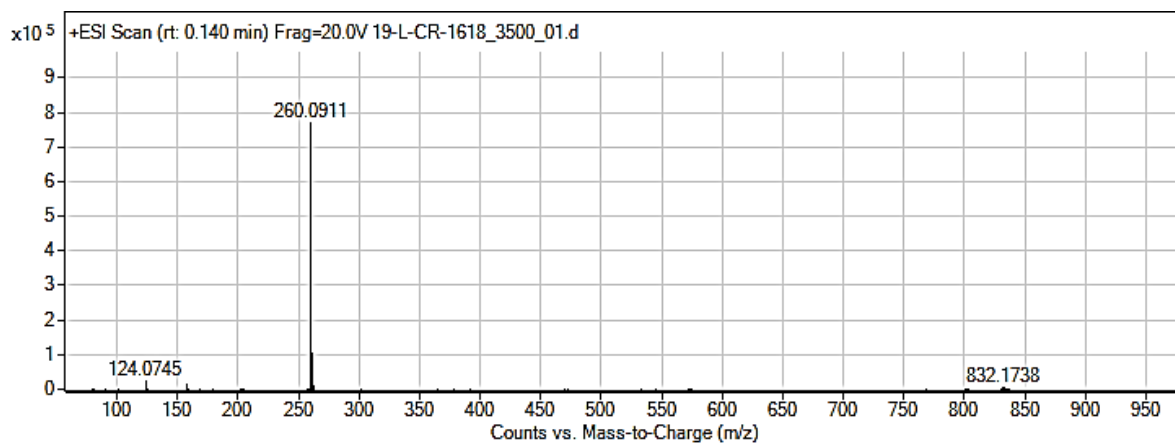


Figure S16. LC-MS of **51** - $C_{14}H_{13}NO_4$ $[M+H]^+$ m/z calcd. 260.0917.

INFRARED SPECTROSCOPY

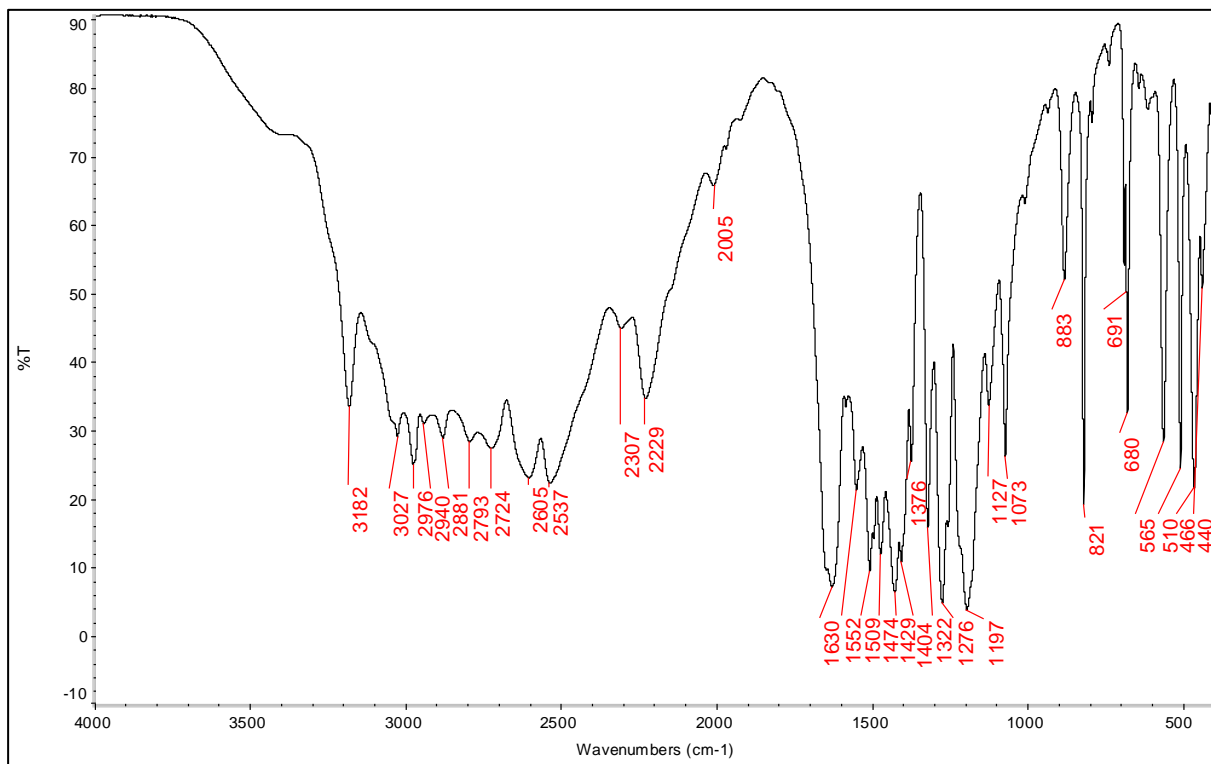


Figure S17. FTIR spectrum of 18.

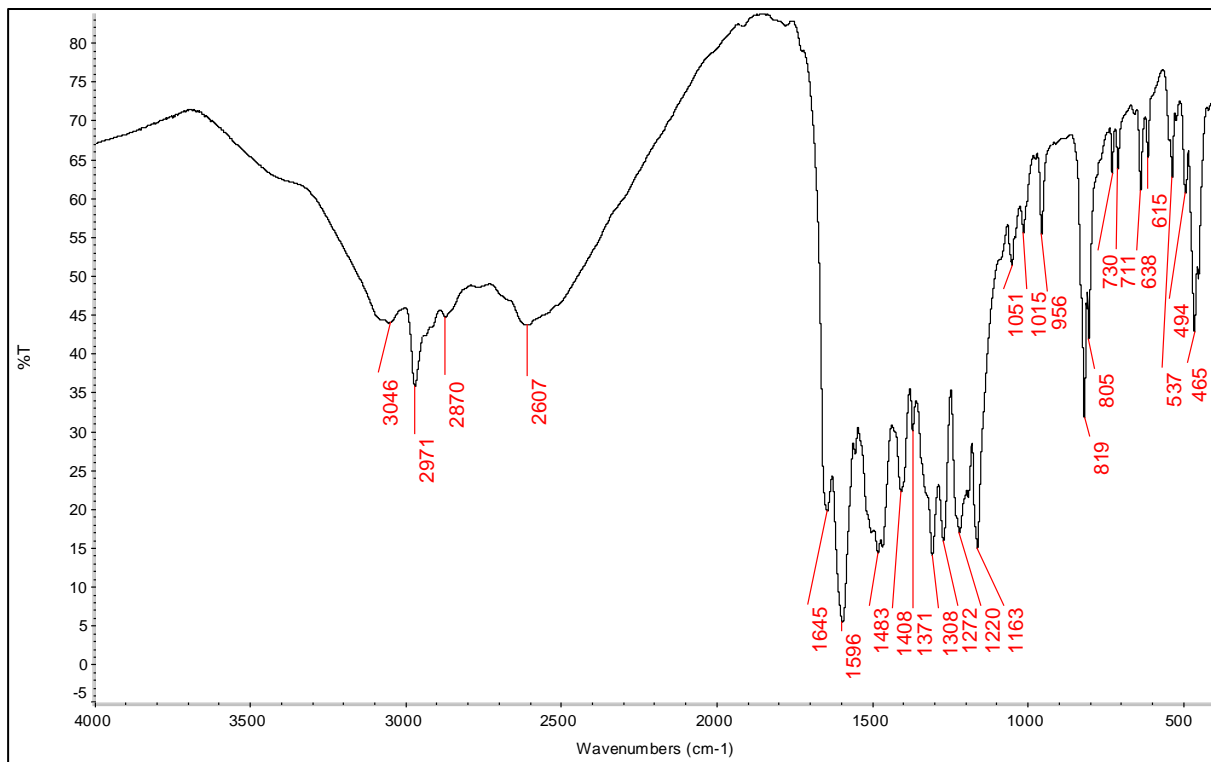


Figure S18. FTIR spectrum of 19.

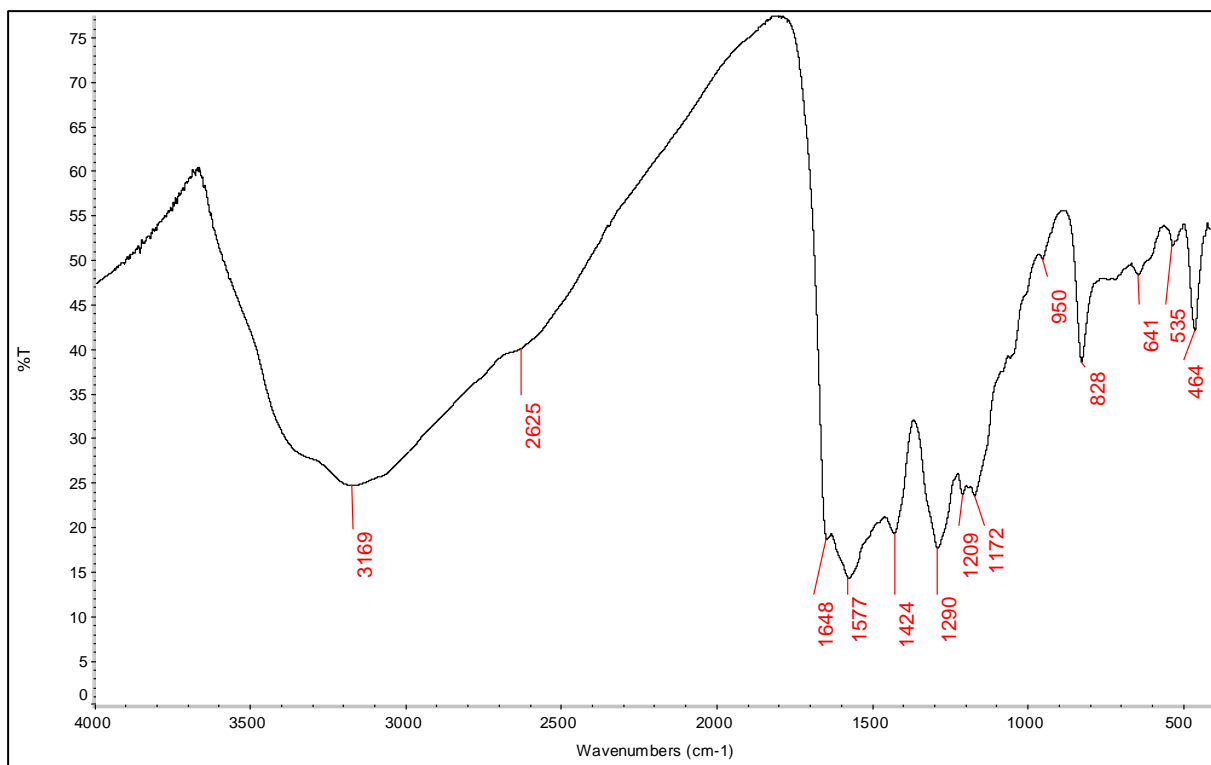


Figure S19. FTIR spectrum of 23.

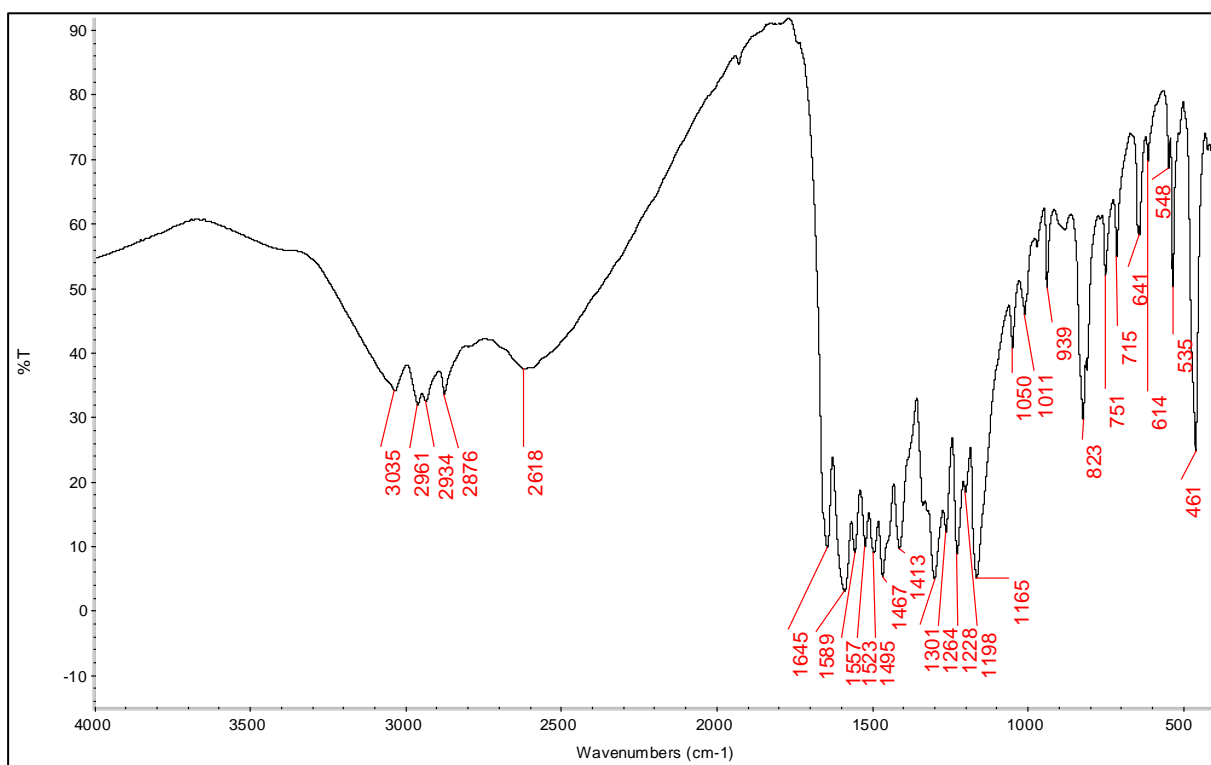


Figure S20. FTIR spectrum of 24.

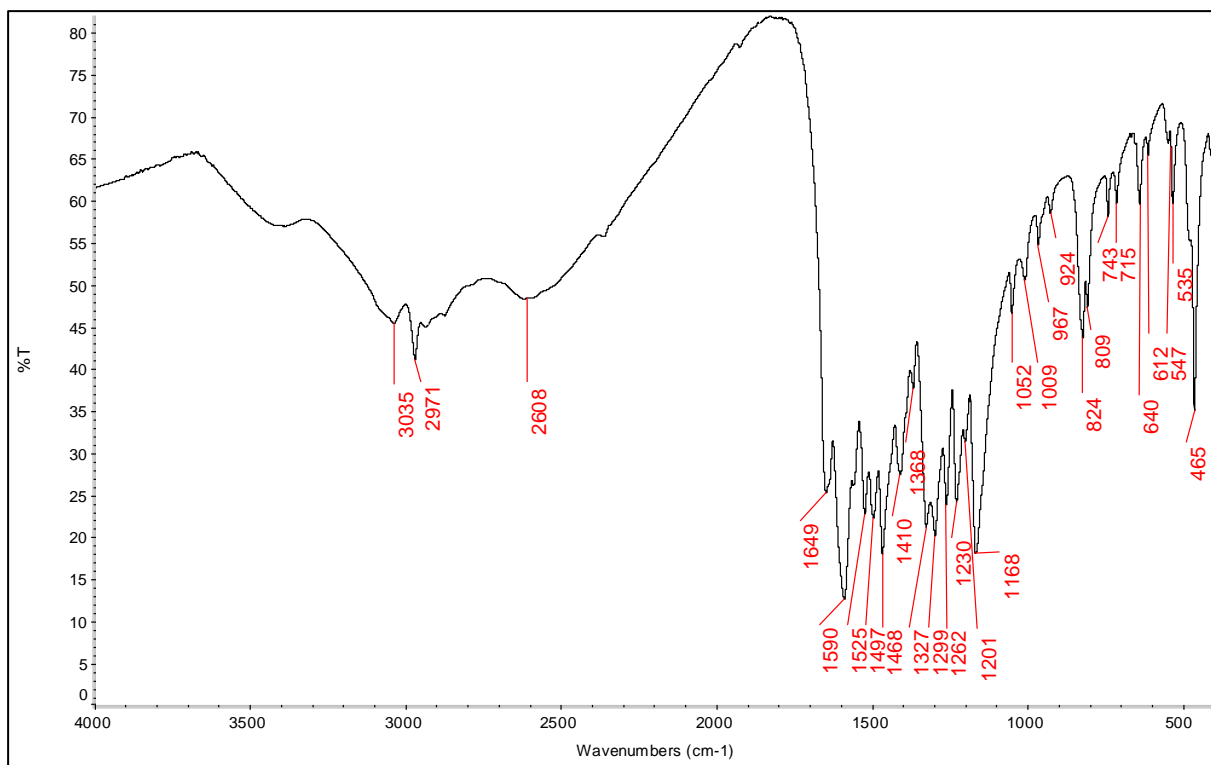


Figure S21. FTIR spectrum of 25.

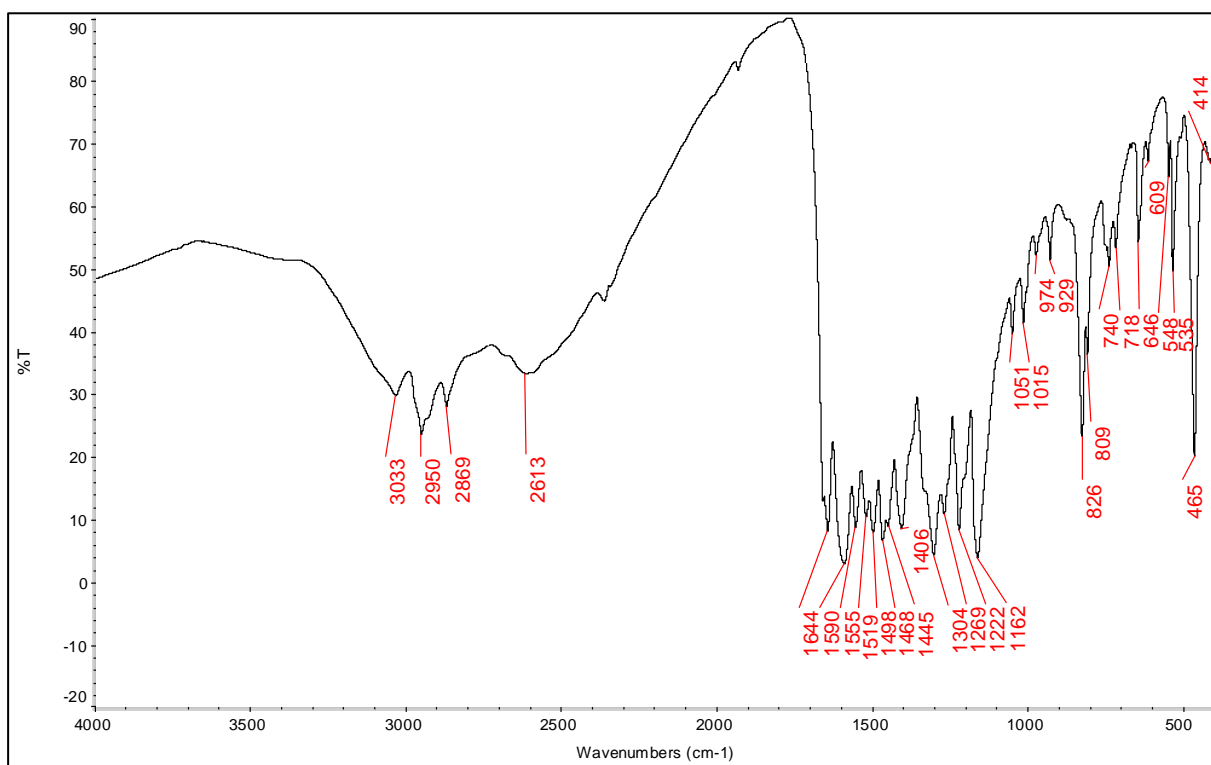


Figure S22. FTIR spectrum of 26.

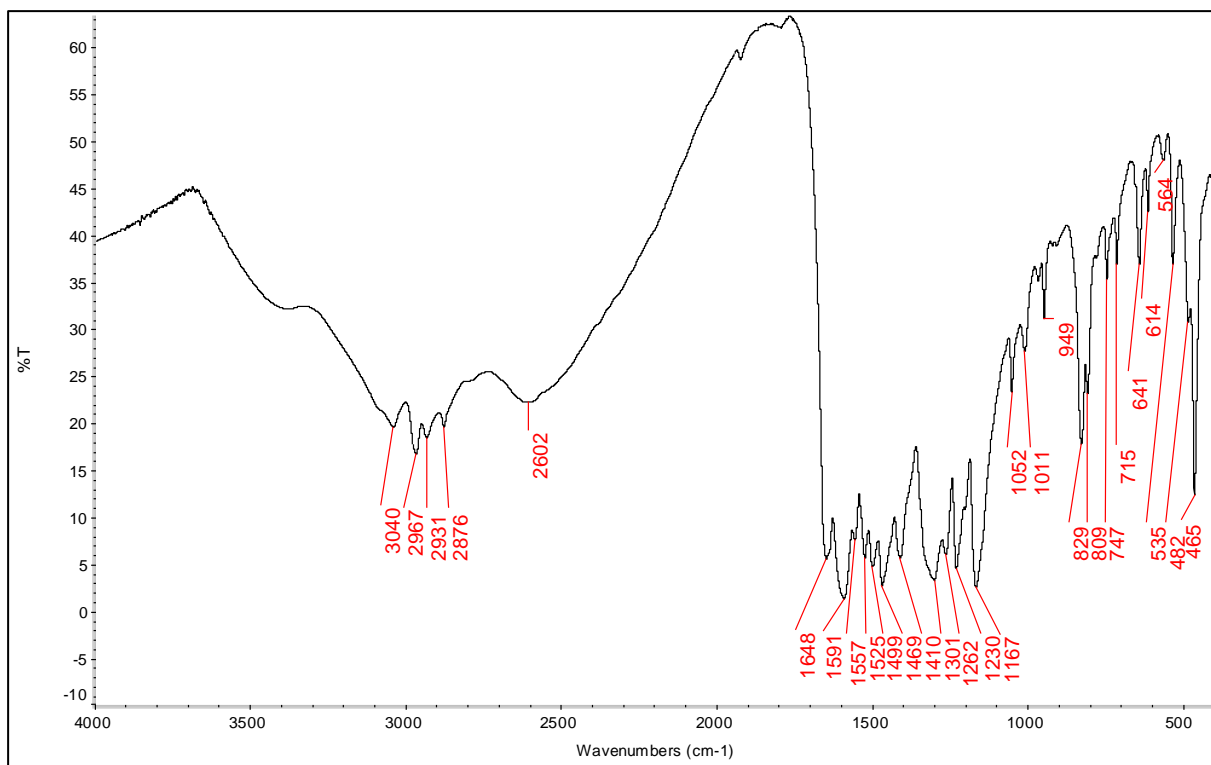


Figure S23. FTIR spectrum of 27.

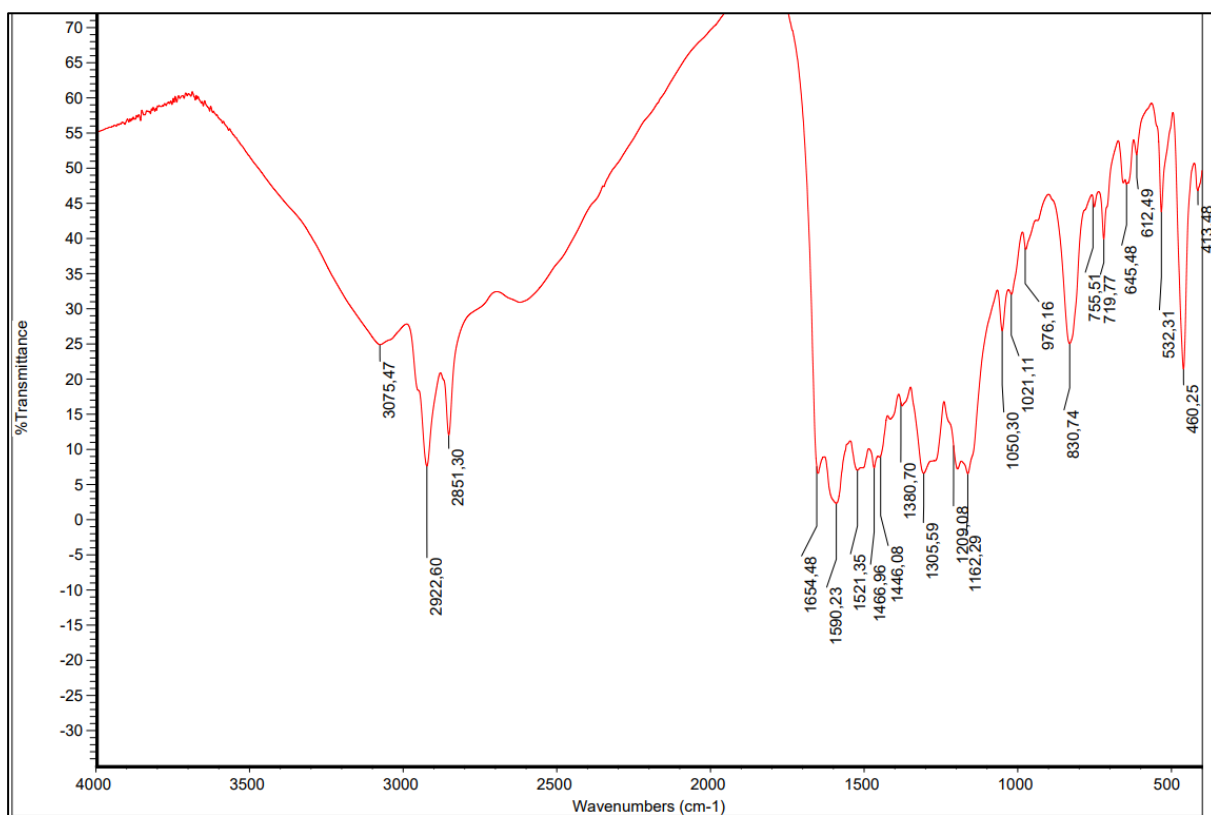


Figure S24. FTIR spectrum of 28.



Figure S25. FTIR spectrum of 29.

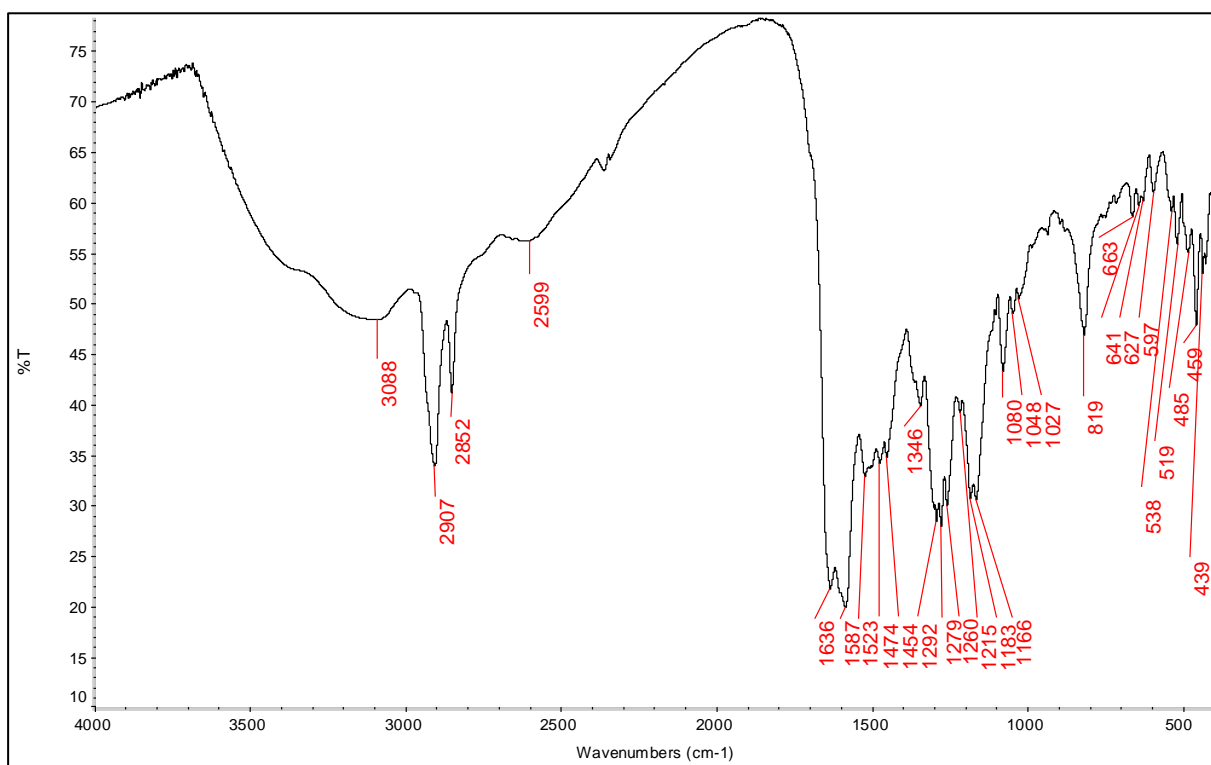


Figure S26. FTIR spectrum of 30.

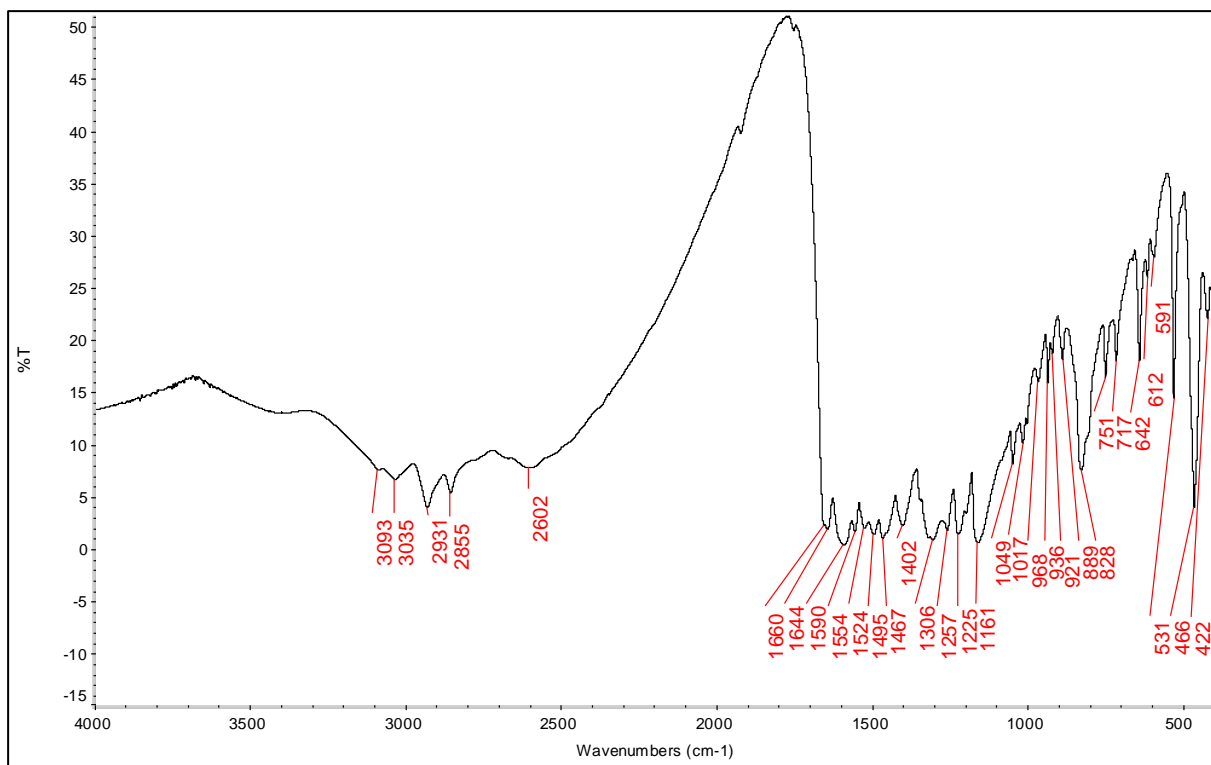


Figure S27. FTIR spectrum of 31.

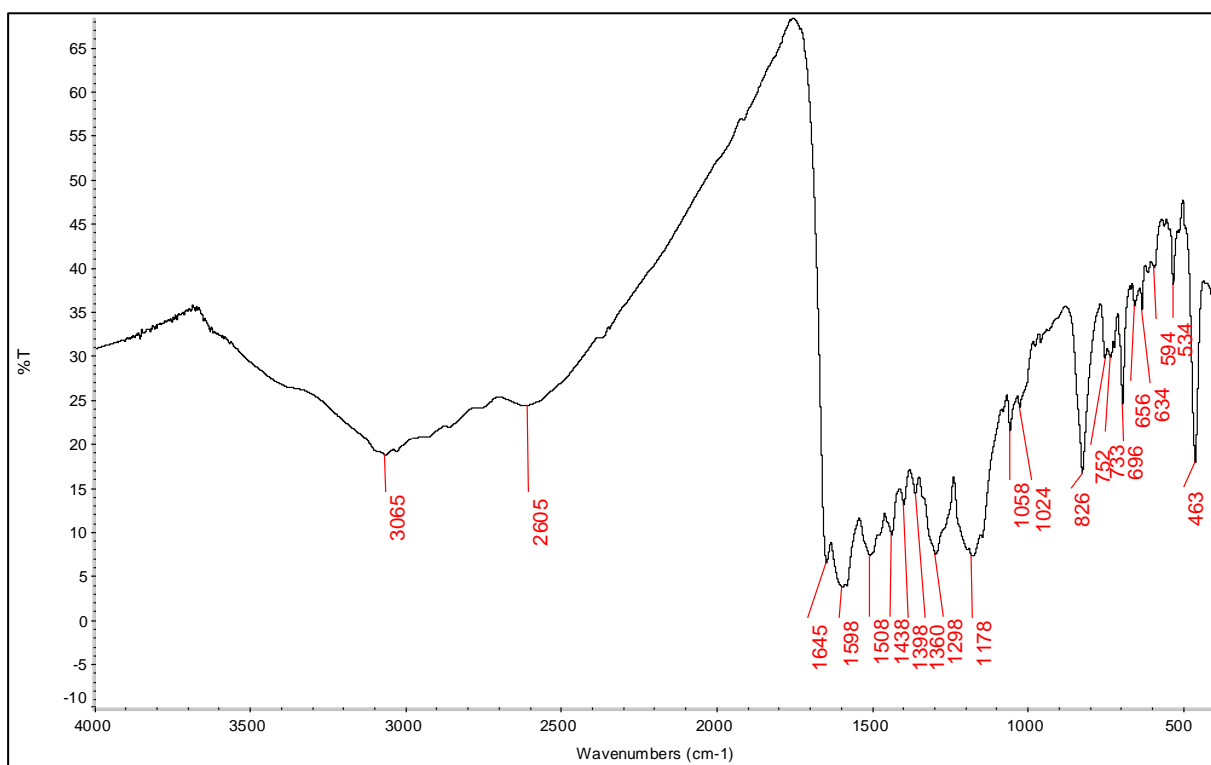


Figure S28. FTIR spectrum of 32.

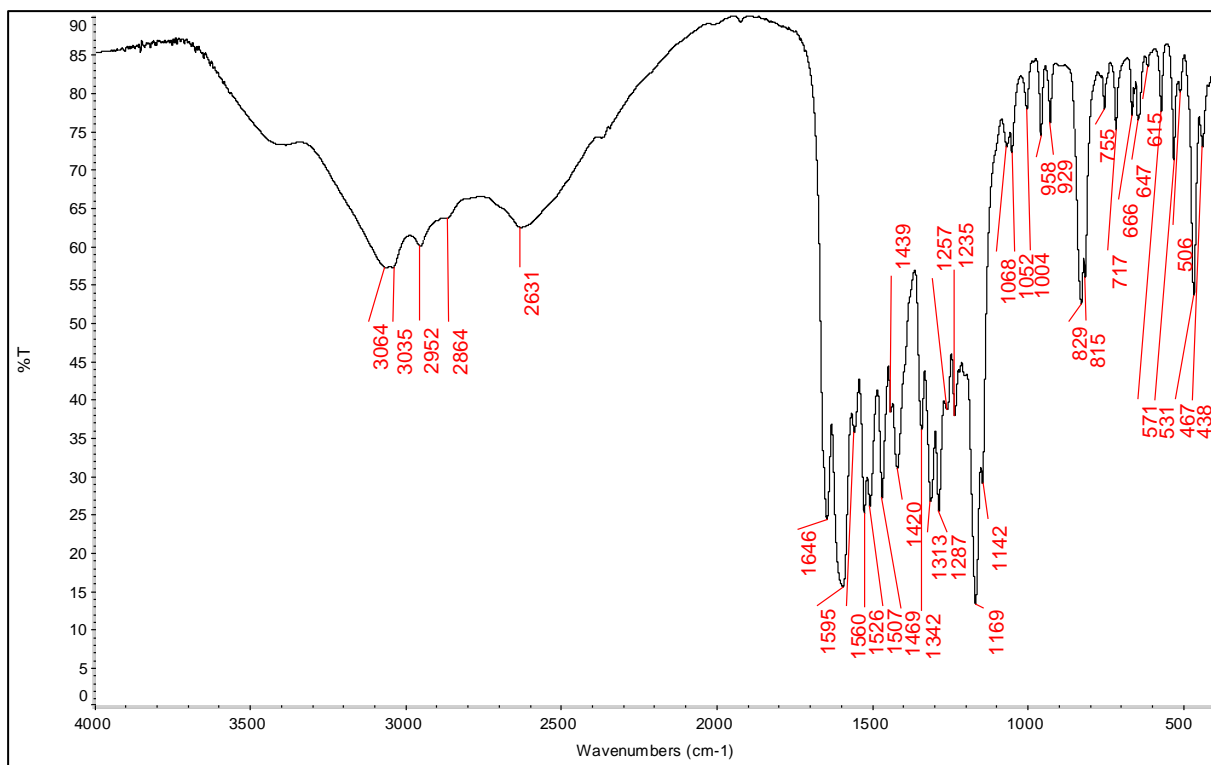


Figure S29. FTIR spectrum of 33.

Compound 51. IR (KBr) spectrum

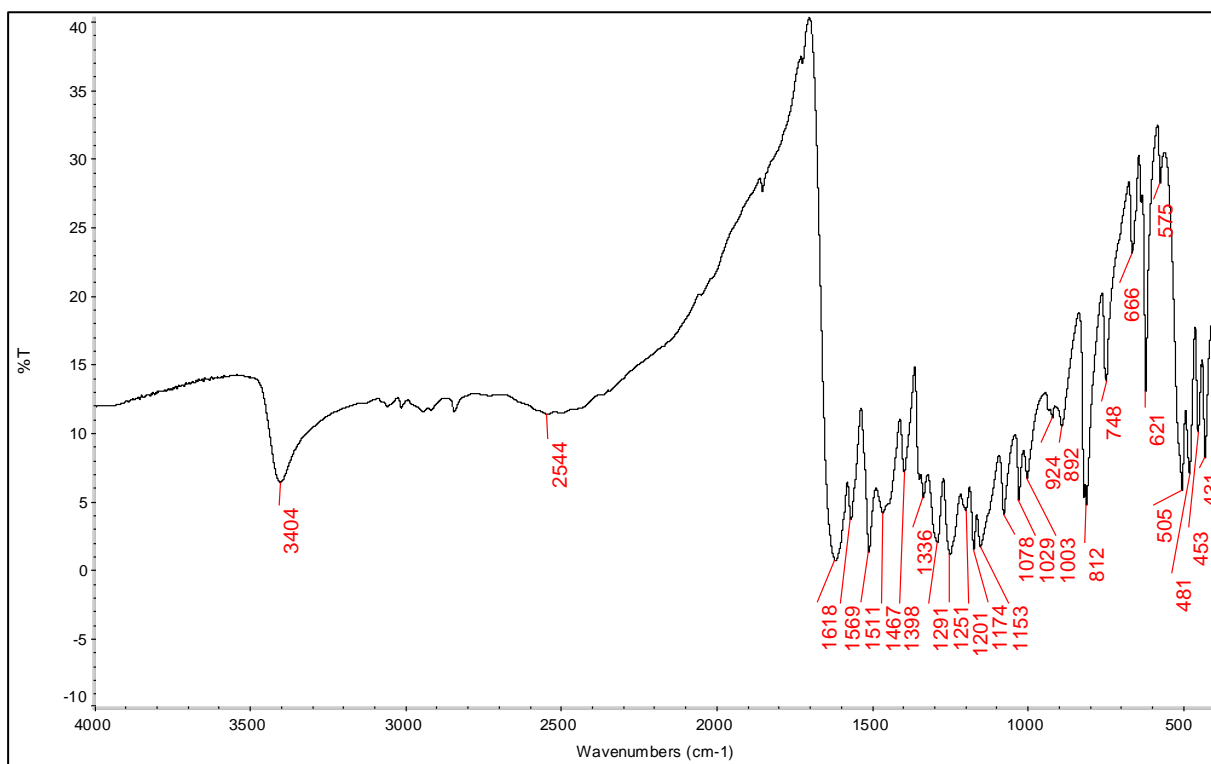


Figure S30. FTIR spectrum of 51.

¹H NMR, ¹³C NMR AND DEPT SPECTRA

(18) H-NMR in DMSO-d₆ / 500 MHz

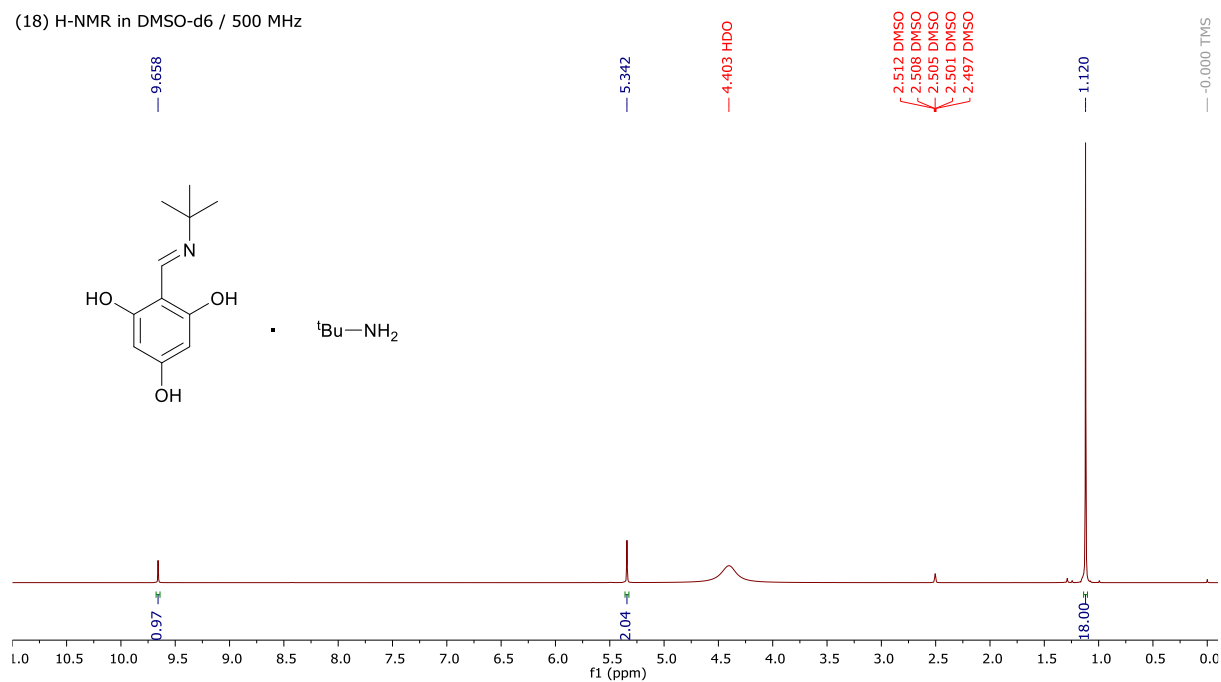


Figure S31. ¹H NMR spectrum of **18** in DMSO-d₆ / 500 MHz.

(18) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

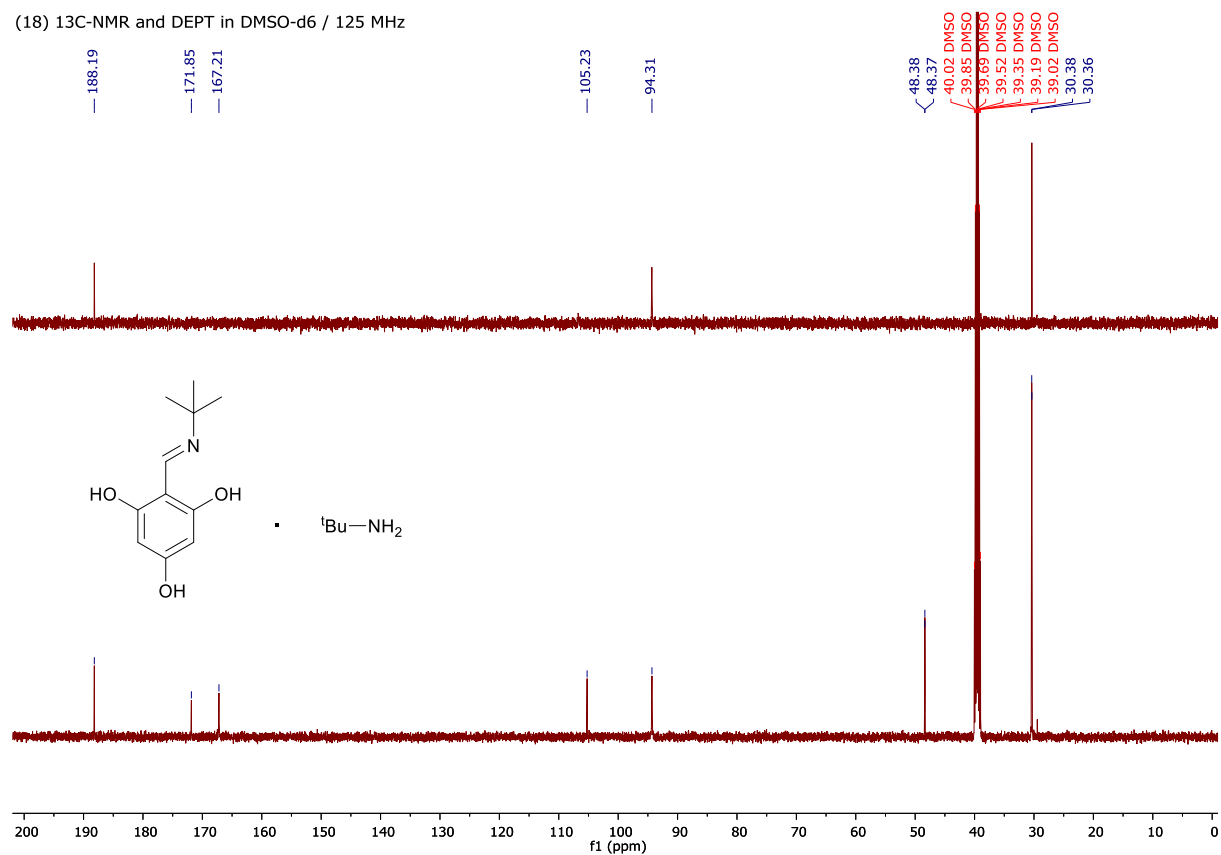


Figure S32. ¹³C NMR and DEPT spectra of **18** in DMSO-d₆ / 125 MHz.

(19) ¹H-NMR in DMSO-d₆ / 500 MHz

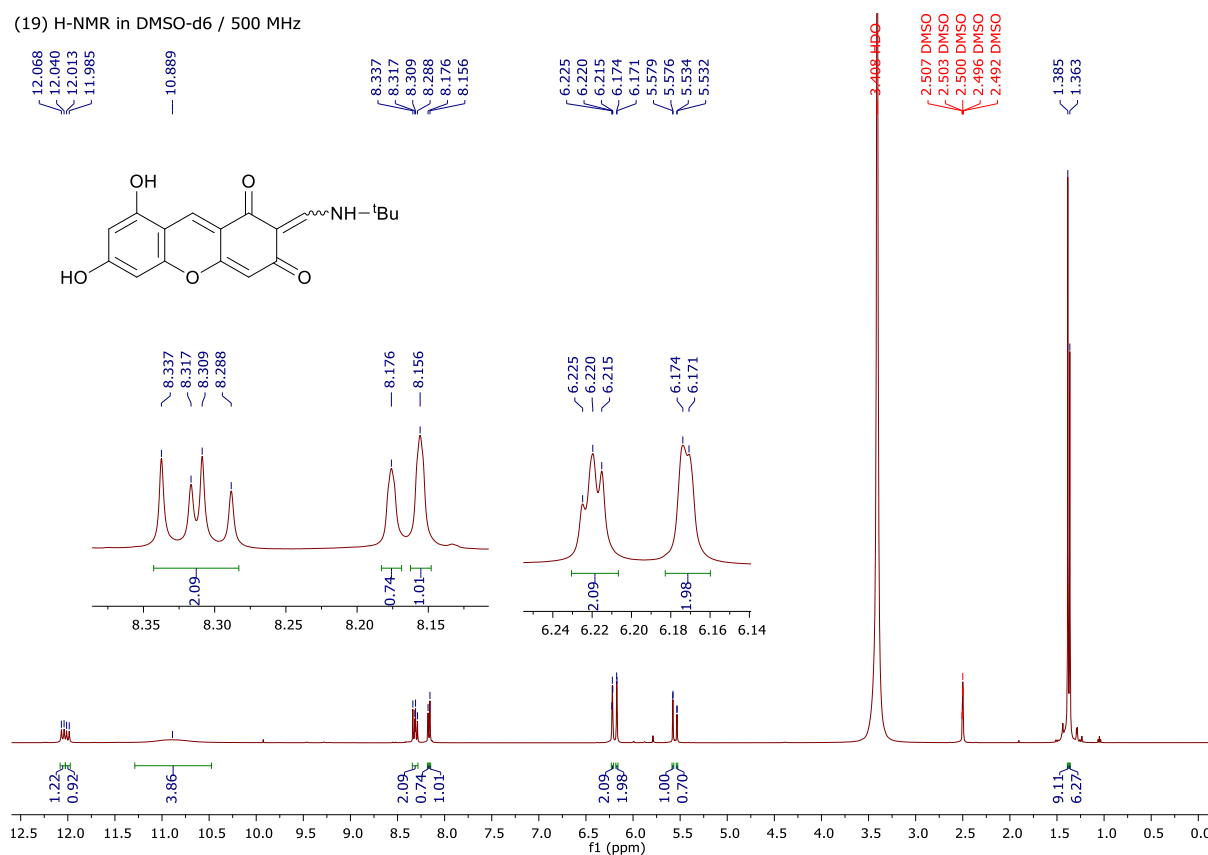


Figure S33. ¹H NMR spectrum of **19** in DMSO-d₆ / 500 MHz.

(19) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

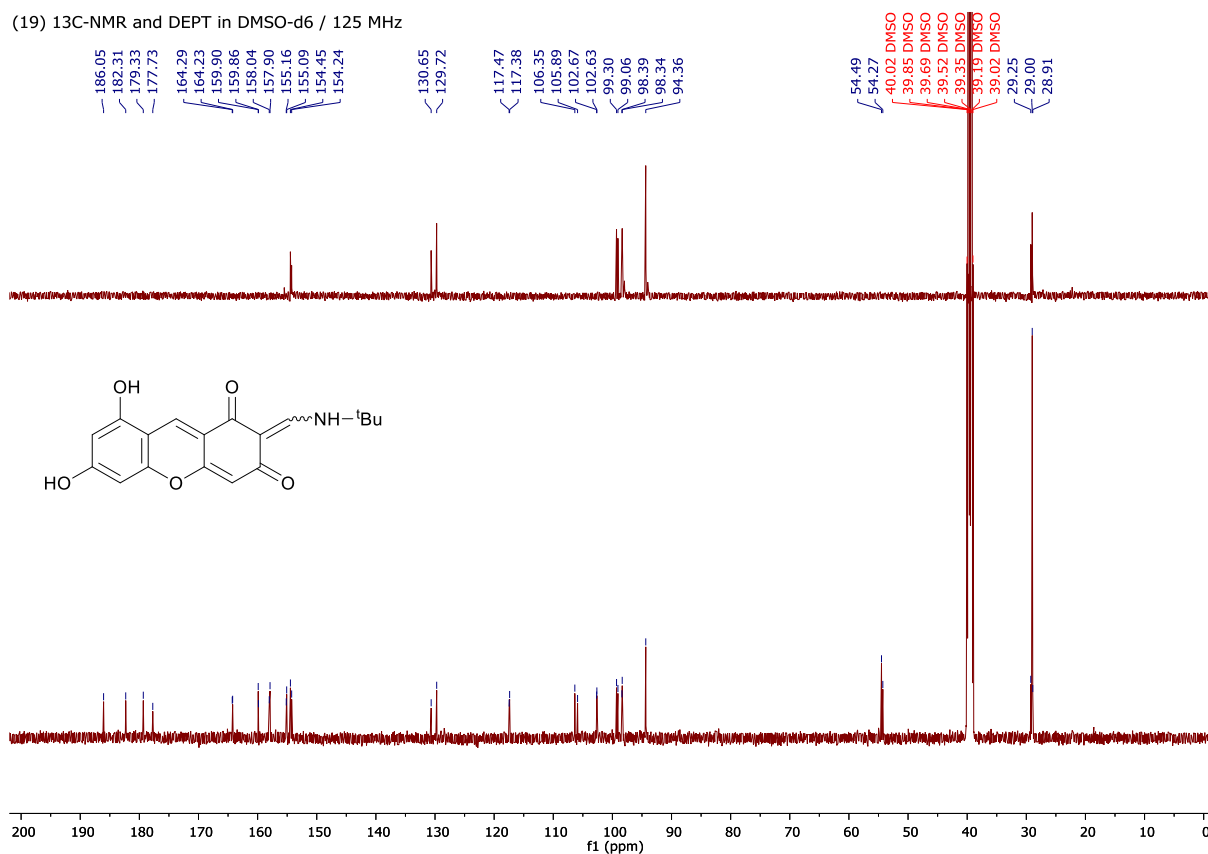


Figure S34. ¹³C NMR and DEPT spectra of **19** in DMSO-d₆ / 125 MHz.

(23) ¹H-NMR in DMSO-d₆ / 500 MHz

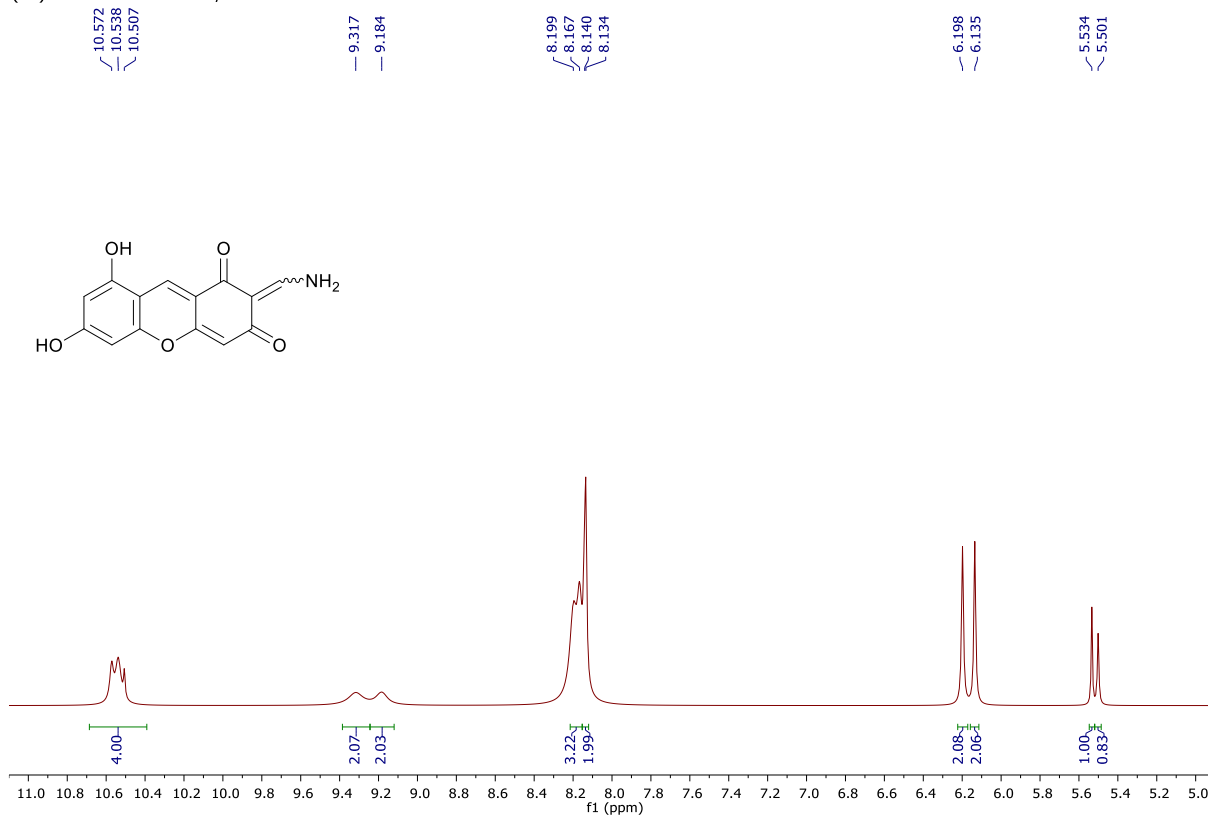


Figure S35. ¹H NMR spectrum of **23** in DMSO-d₆ / 500 MHz.

(24) ¹H-NMR in DMSO-d₆ / 500 MHz

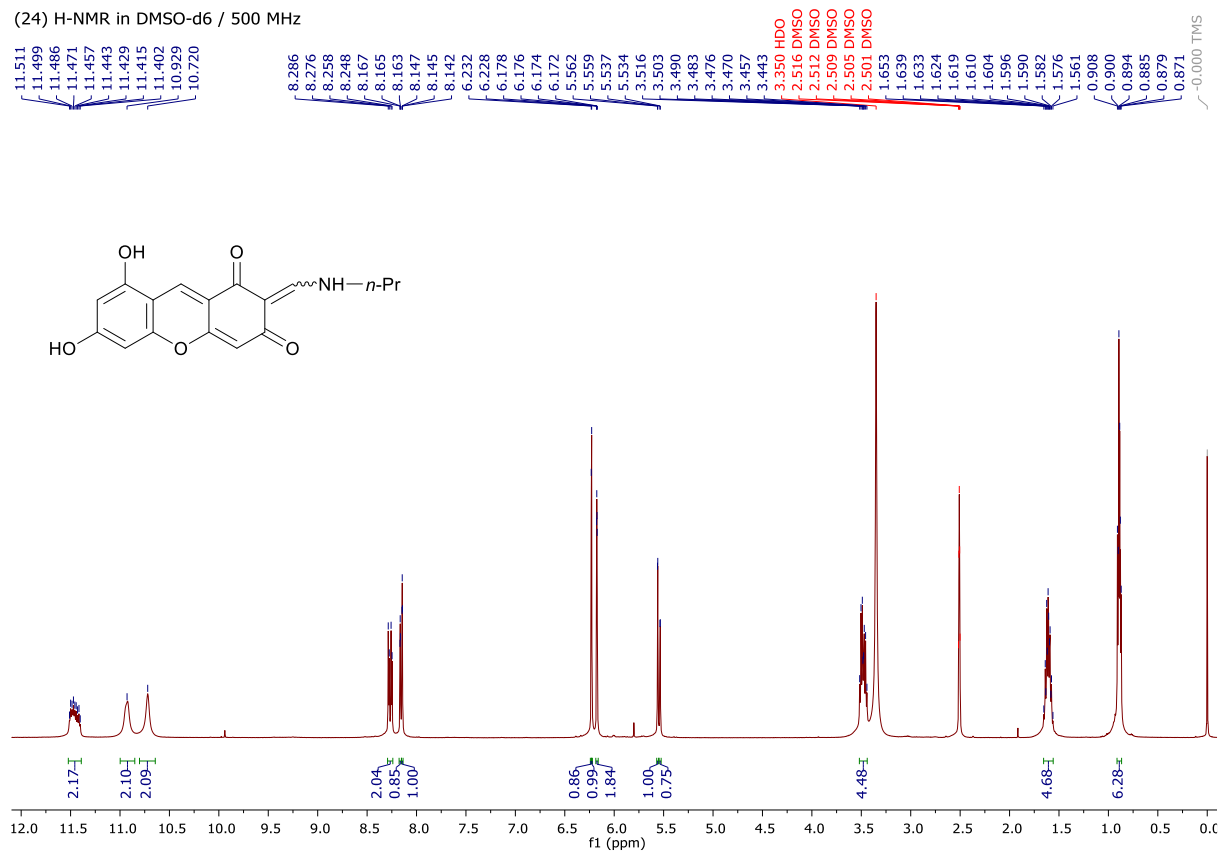


Figure S36. ¹H NMR spectrum of 24 in DMSO-d₆ / 500 MHz.

(24) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

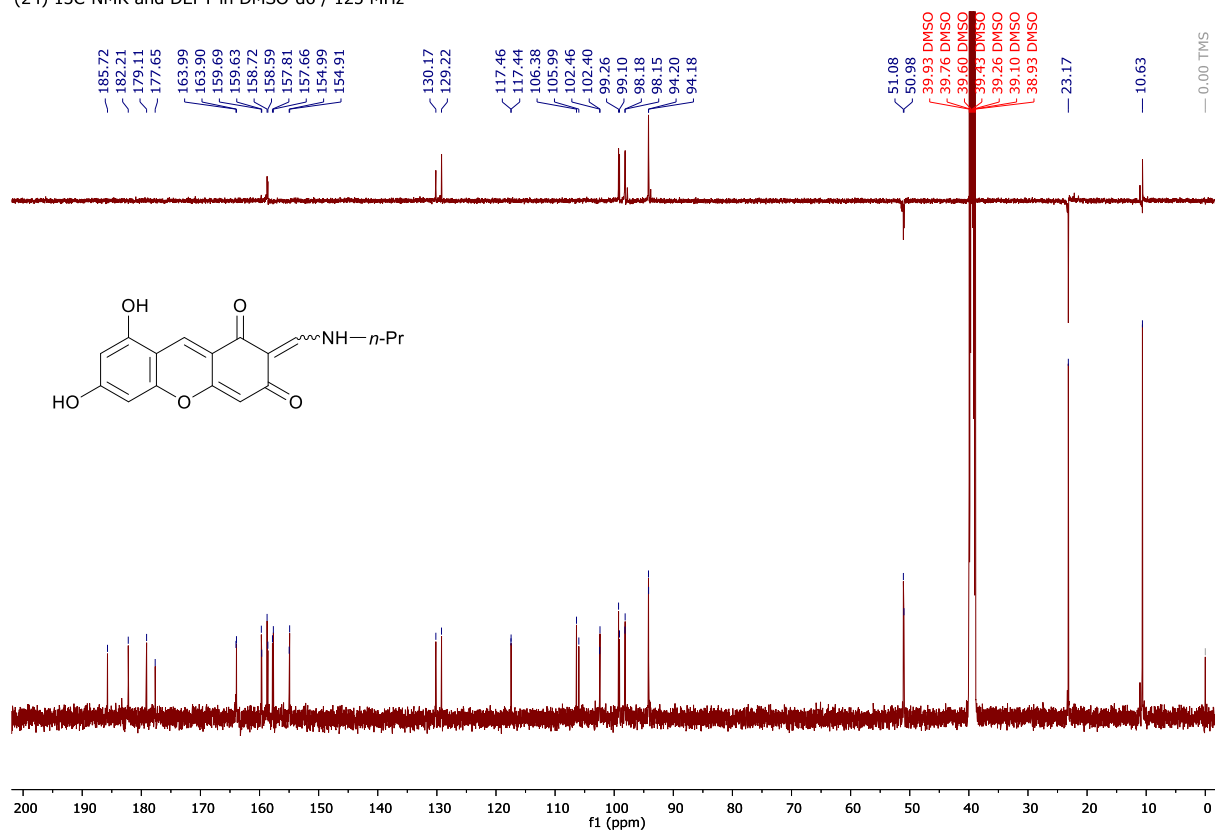


Figure S37. ¹³C NMR and DEPT spectra of 24 in DMSO-d₆ / 125 MHz.

(25) ¹H-NMR in DMSO-d₆ / 500 MHz

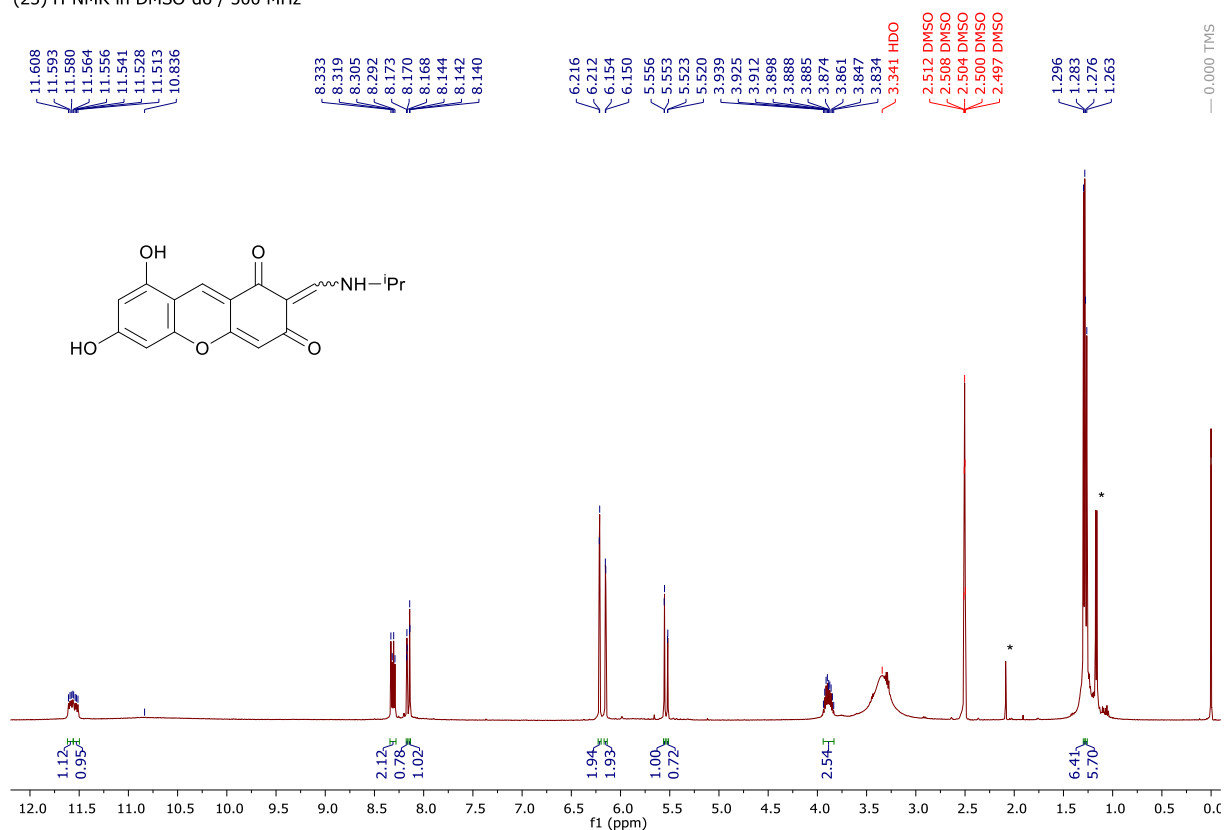


Figure S38. ¹H NMR spectrum of **25** in DMSO-d₆ / 500 MHz.

(25) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

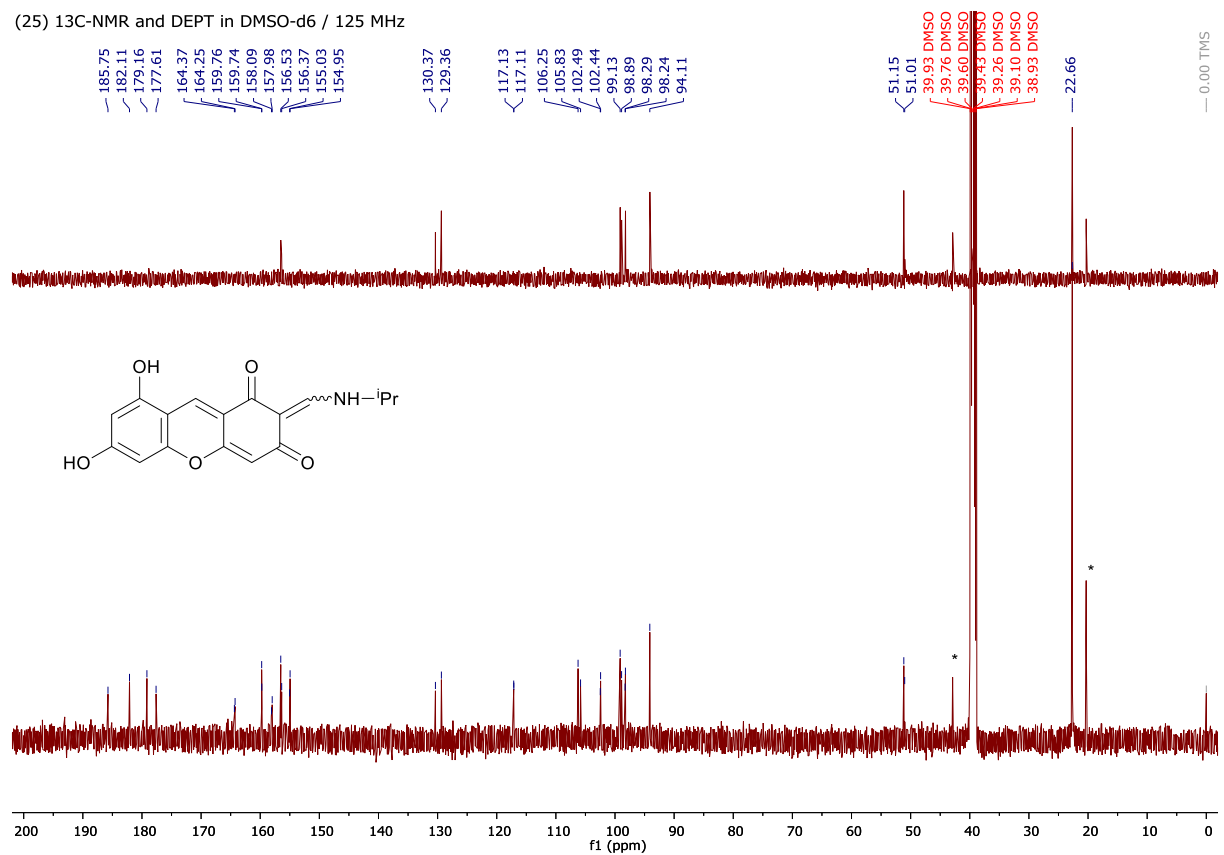


Figure S39. ¹³C NMR and DEPT spectra of **25** in DMSO-d₆ / 125 MHz.

(26) ¹H-NMR in DMSO-d₆ / 500 MHz

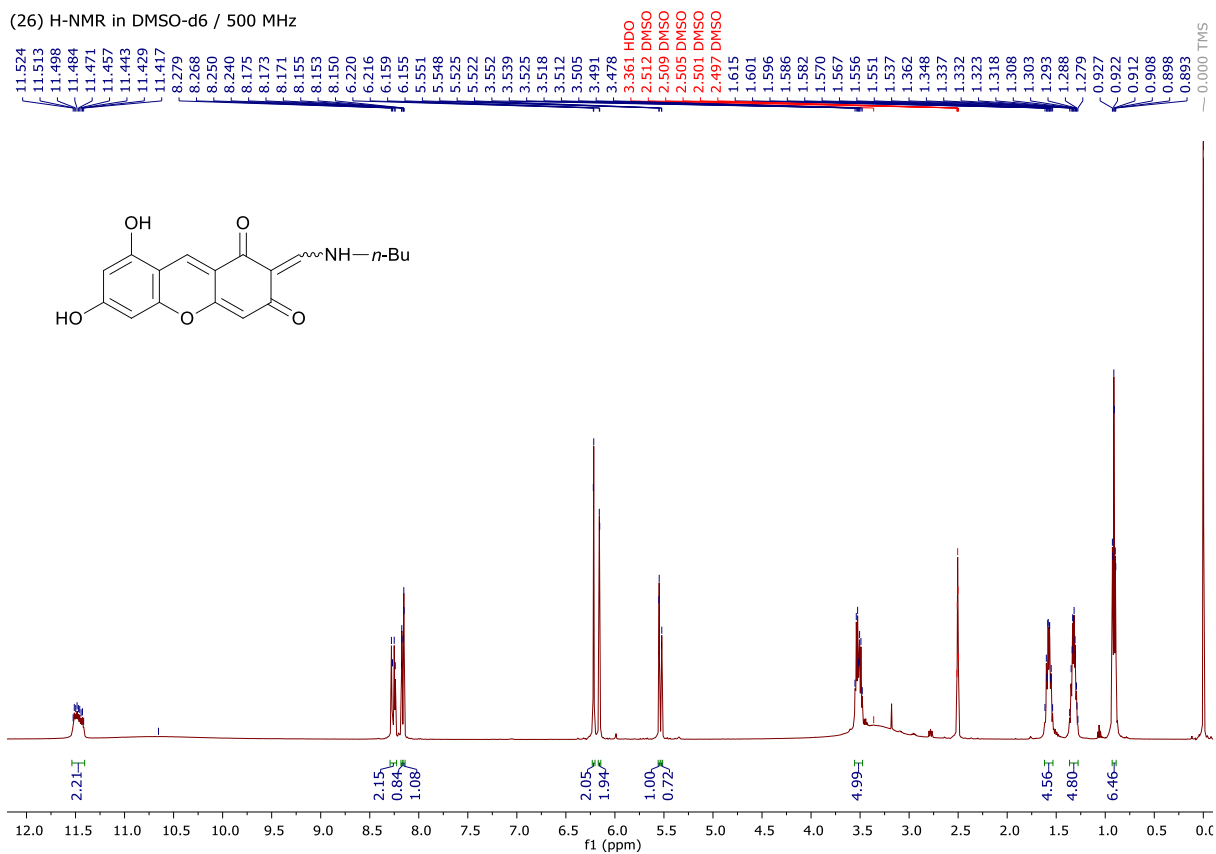


Figure S40. ¹H NMR spectra of 26 in DMSO-d₆ / 500 MHz.

(26) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

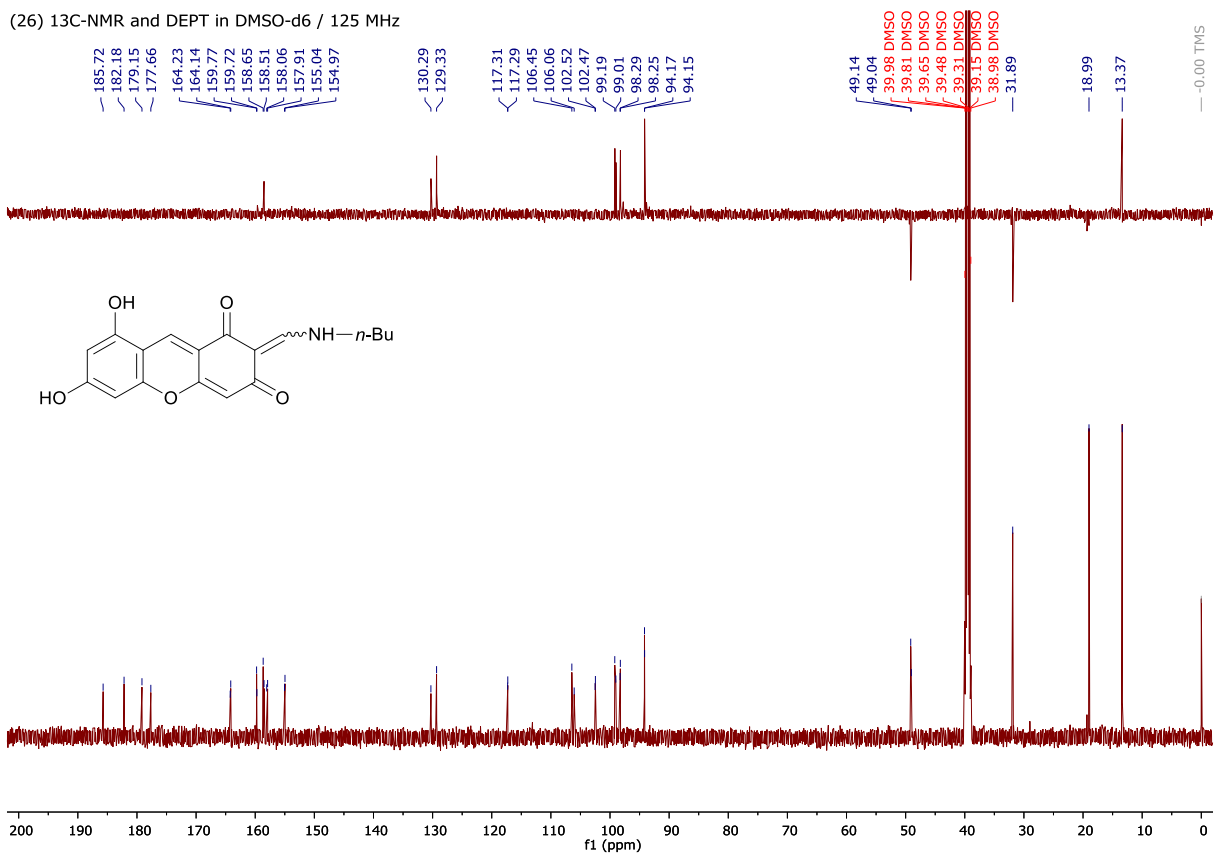


Figure S41. ¹³C NMR and DEPT spectra of 26 in DMSO-d₆ / 125 MHz.

(27) ¹H-NMR in DMSO-d₆ / 500 MHz

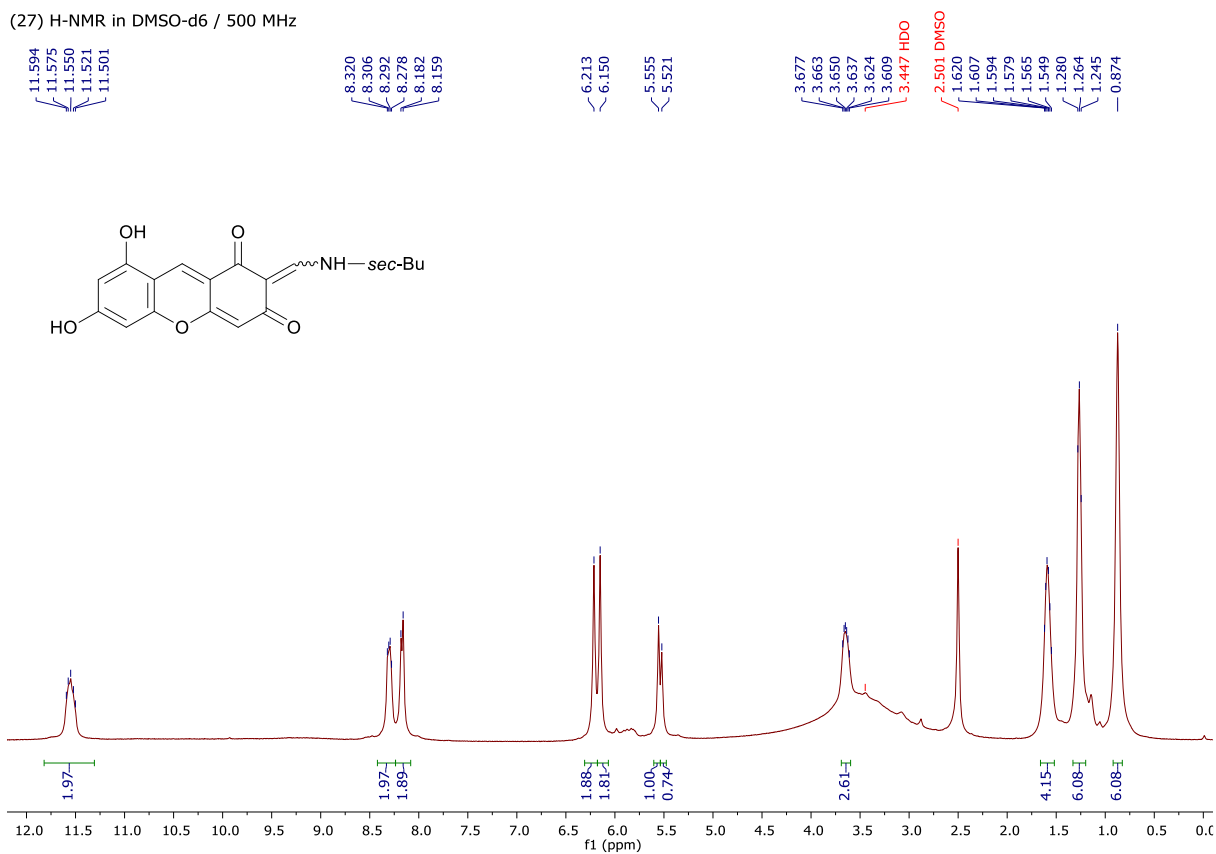


Figure S42. ¹H NMR spectrum of **27** in DMSO-d₆ / 500 MHz.

(27) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

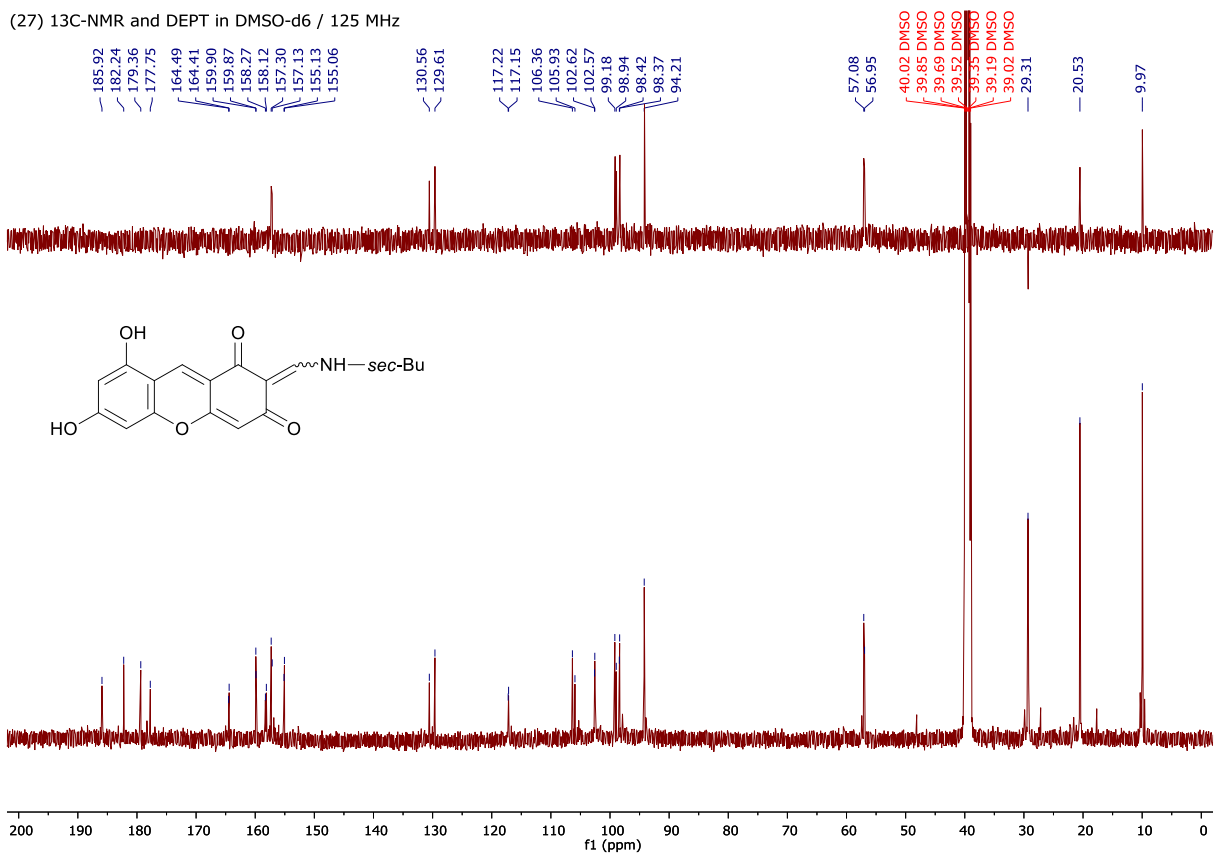


Figure S43. ¹³C NMR and DEPT spectra of **27** in DMSO-d₆ / 125 MHz.

(28) ¹H-NMR in DMSO-d₆ / 500 MHz

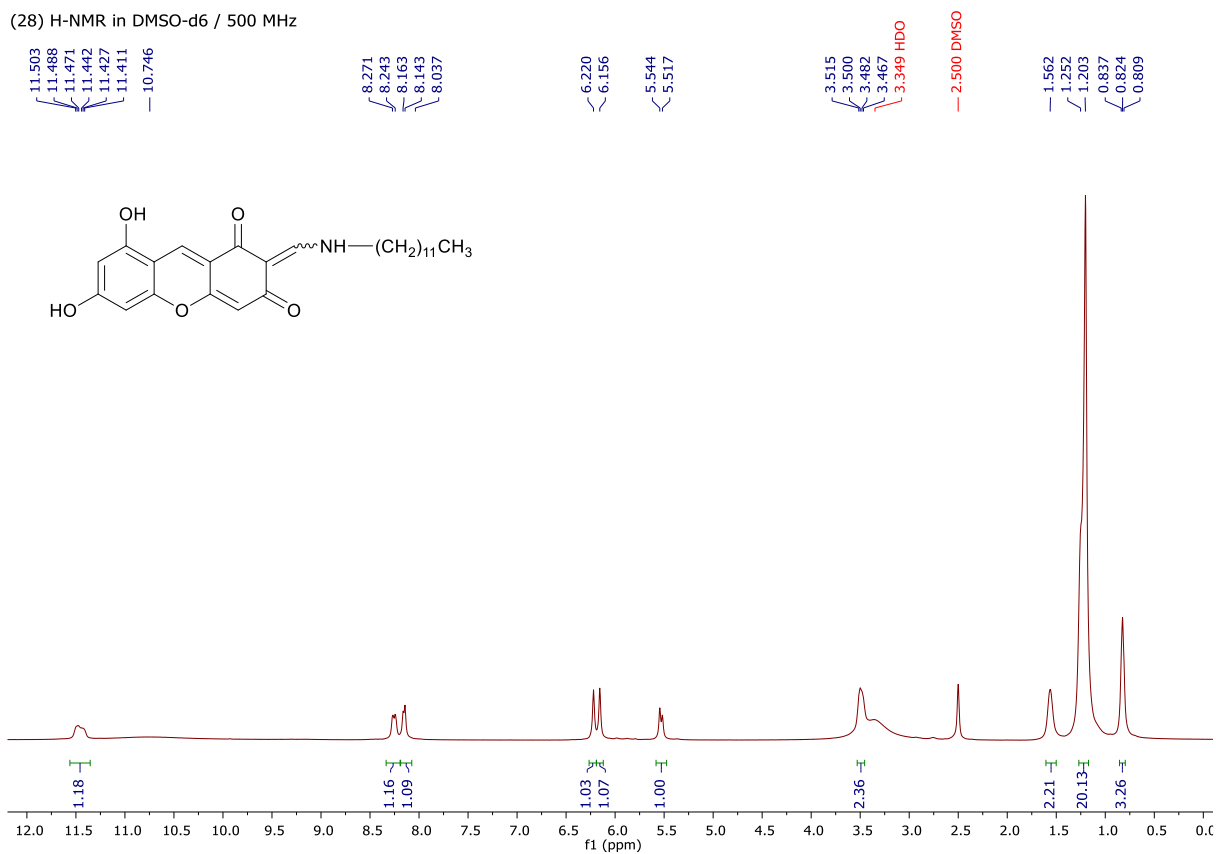


Figure S44. ¹H NMR spectrum of **28** in DMSO-d₆ / 500 MHz.

(28) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

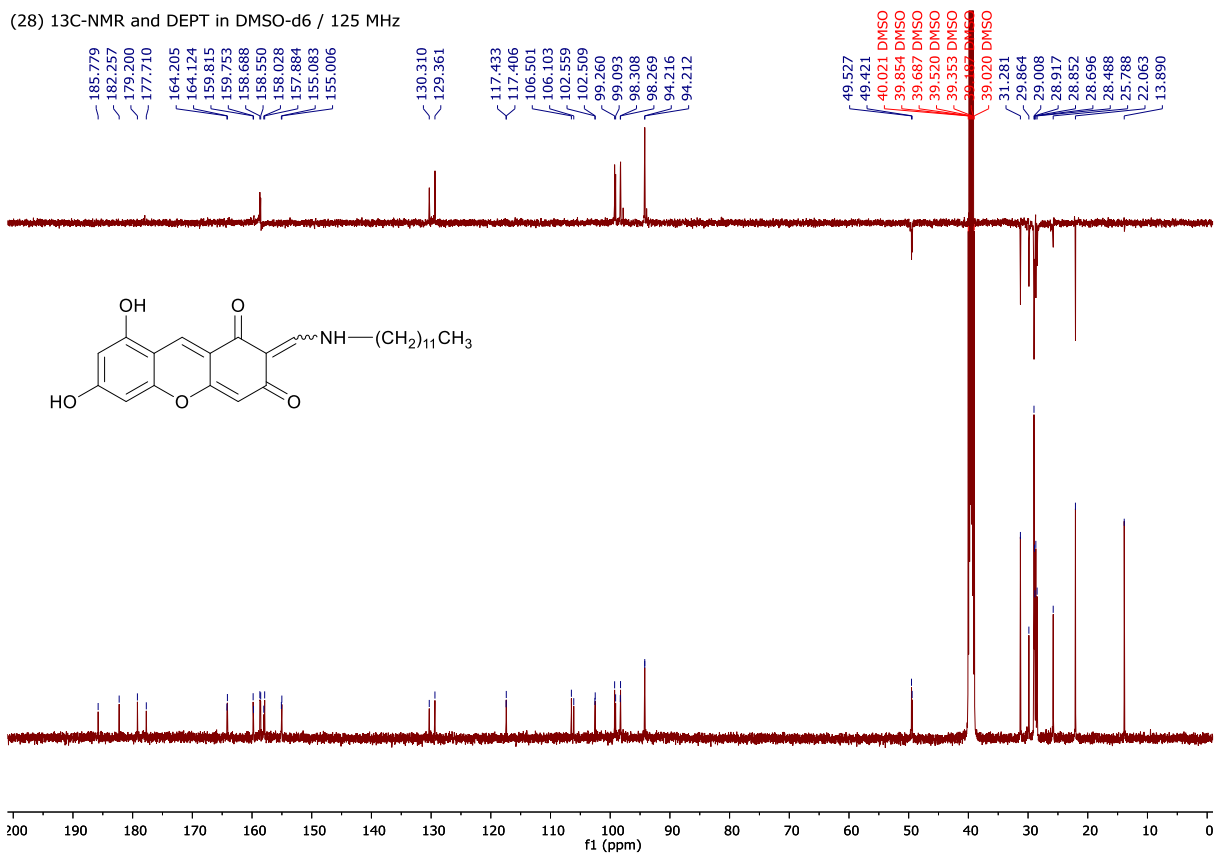


Figure S45. ¹³C NMR and DEPT spectra of **28** in DMSO-d₆ / 125 MHz.

(29) ¹H-NMR in DMSO-d₆ / 500 MHz

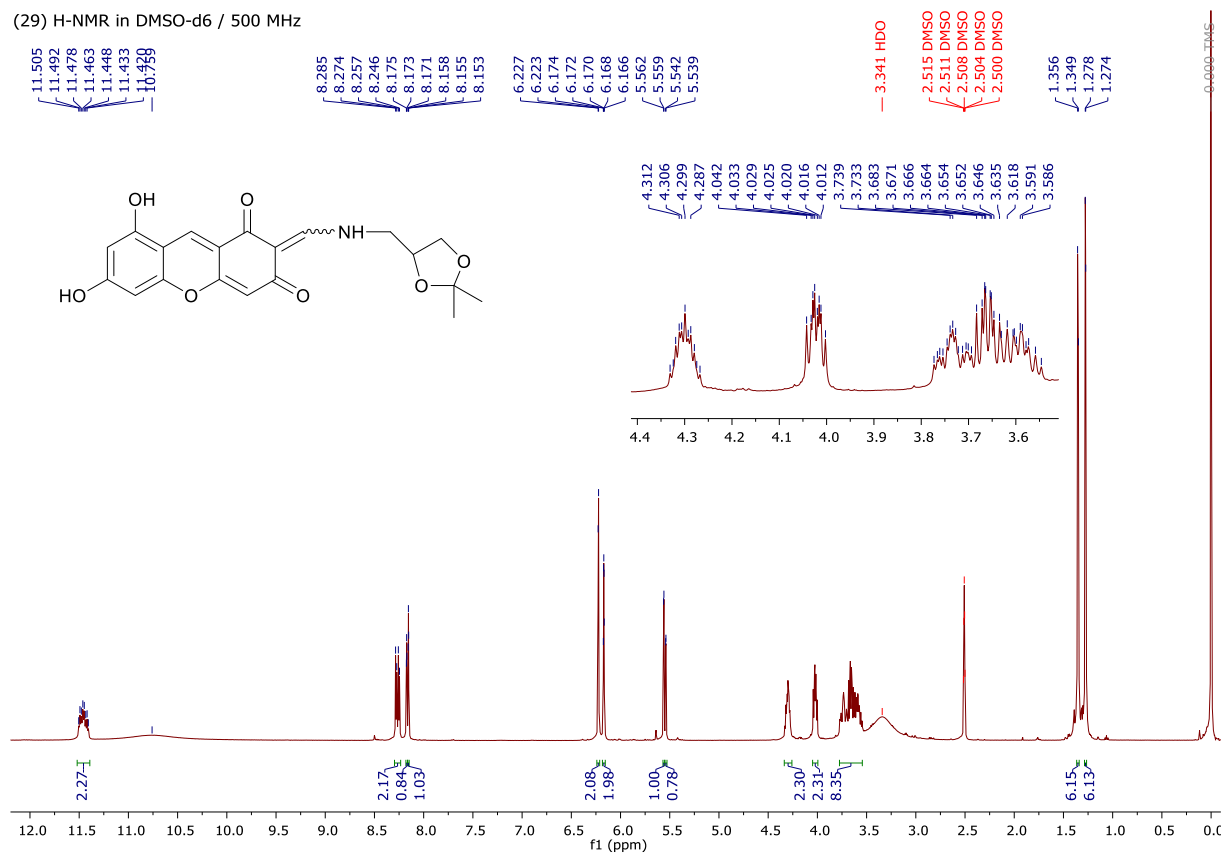


Figure S46. ¹H NMR spectrum of 29 in DMSO-d₆ / 500 MHz.

(29) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

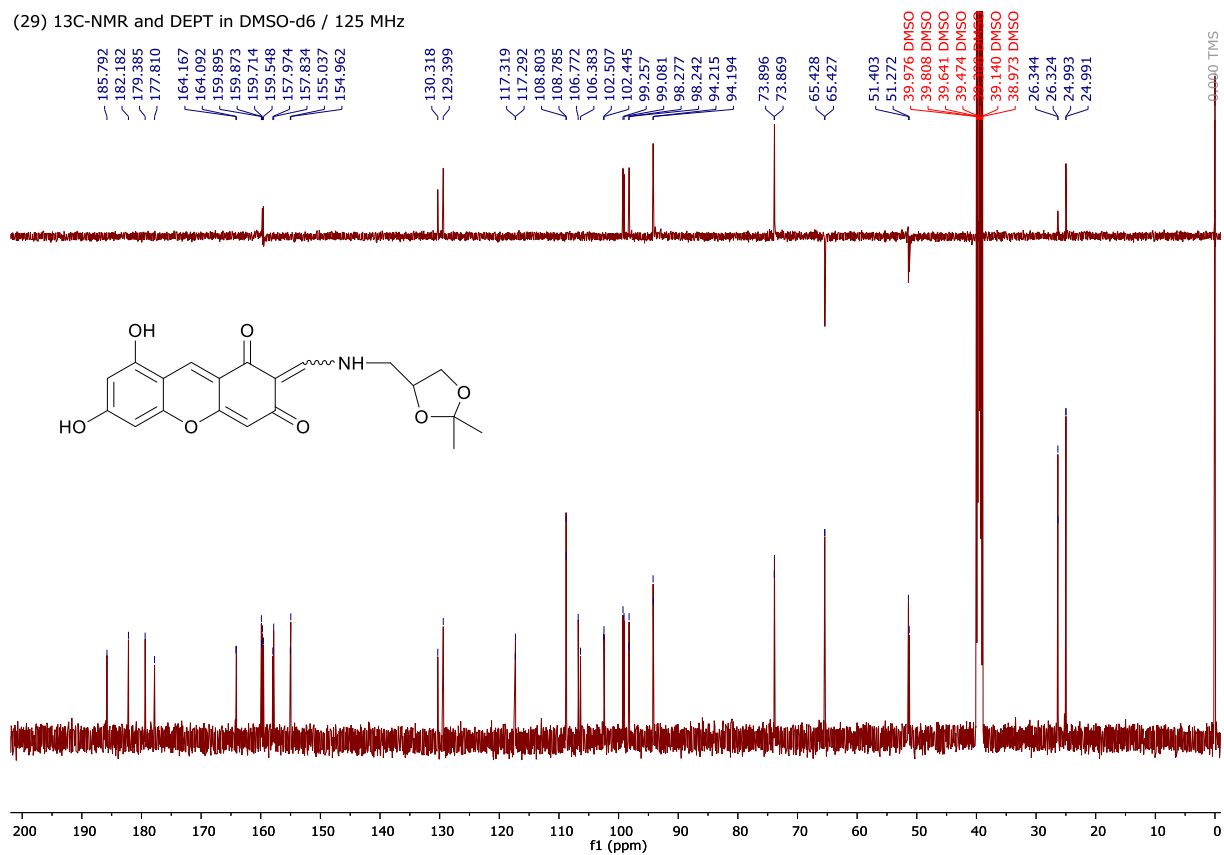


Figure S47. ¹³C NMR and DEPT spectra of 29 in DMSO-d₆ / 125 MHz.

(30) ¹H-NMR in DMSO-d₆ / 500 MHz

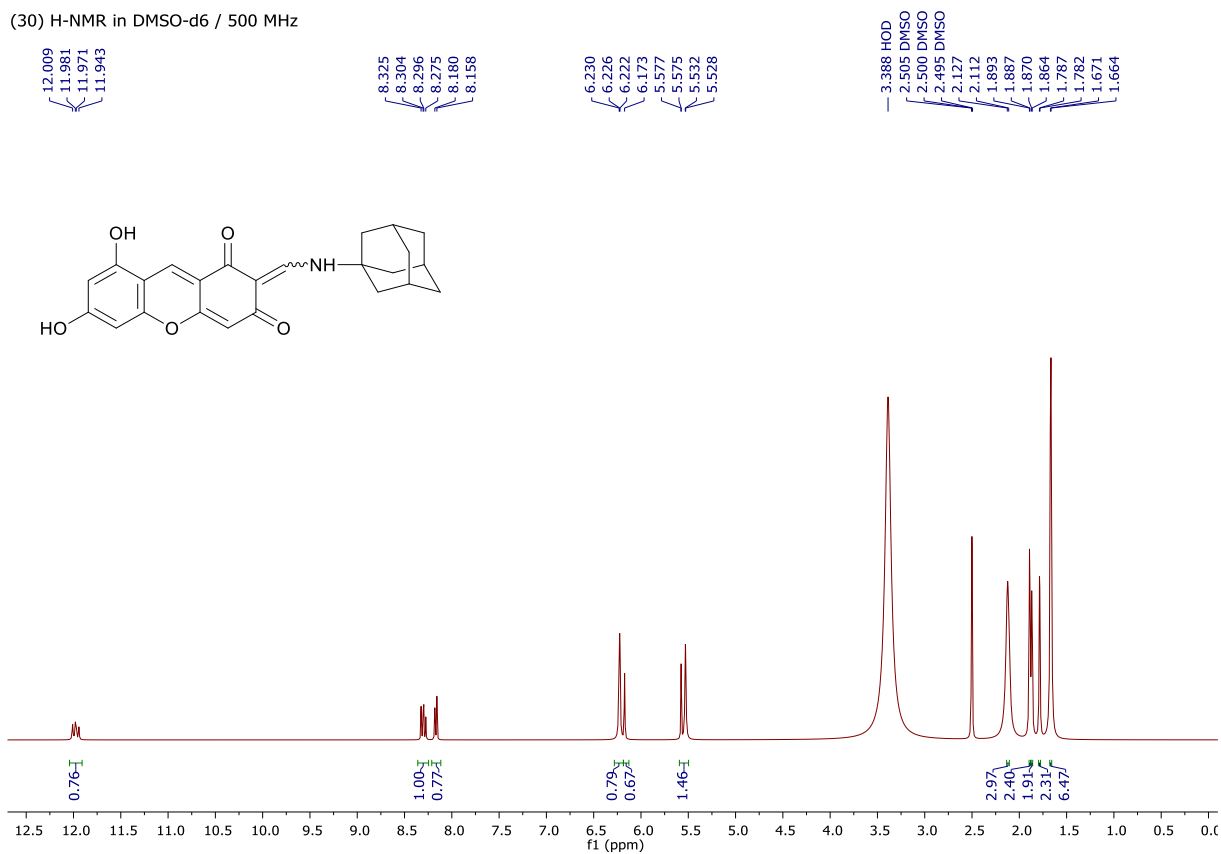


Figure S48. ¹H NMR spectrum of 30 in DMSO-d₆ / 500 MHz.

(30) ¹³C-NMR in DMSO-d₆ / 125 MHz

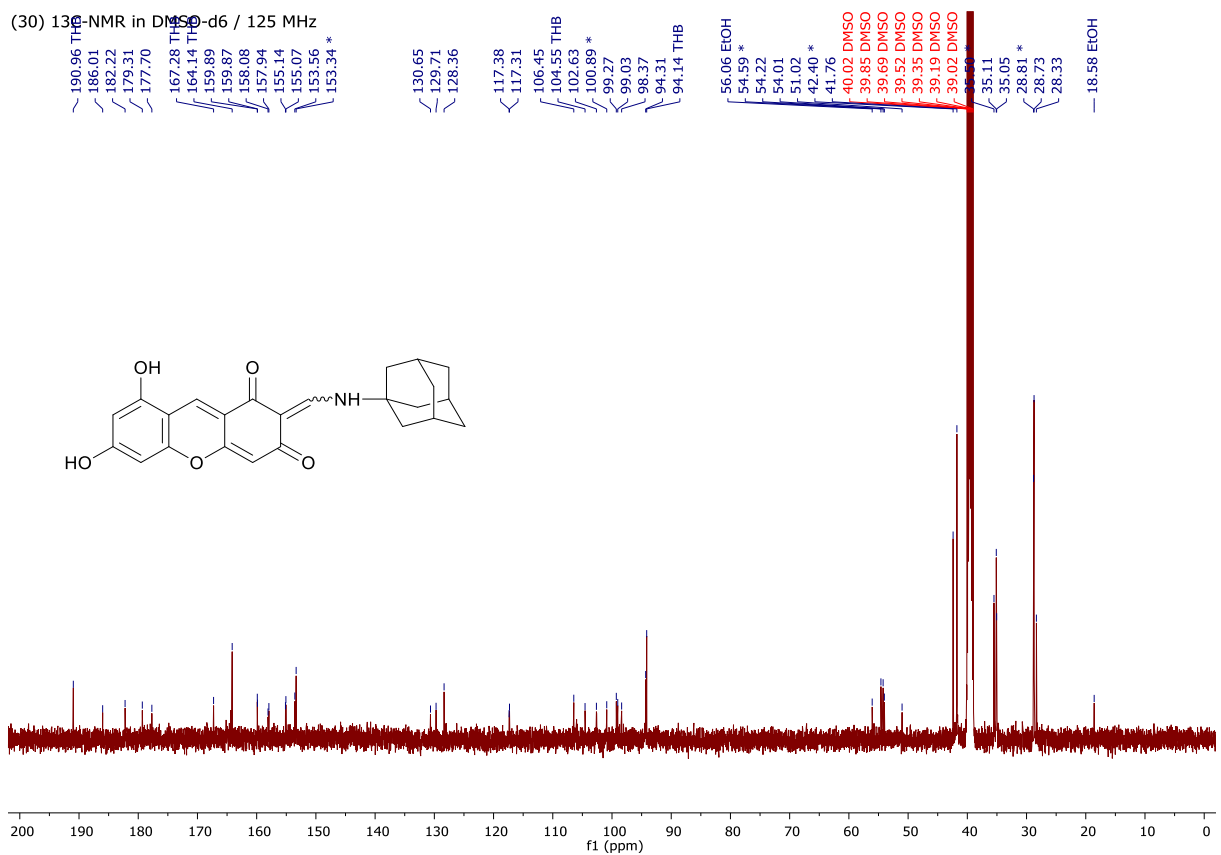


Figure S49. ¹³C NMR and DEPT spectra of 30 in DMSO-d₆ / 125 MHz.

(31) ¹H-NMR in DMSO-d₆ / 500 MHz

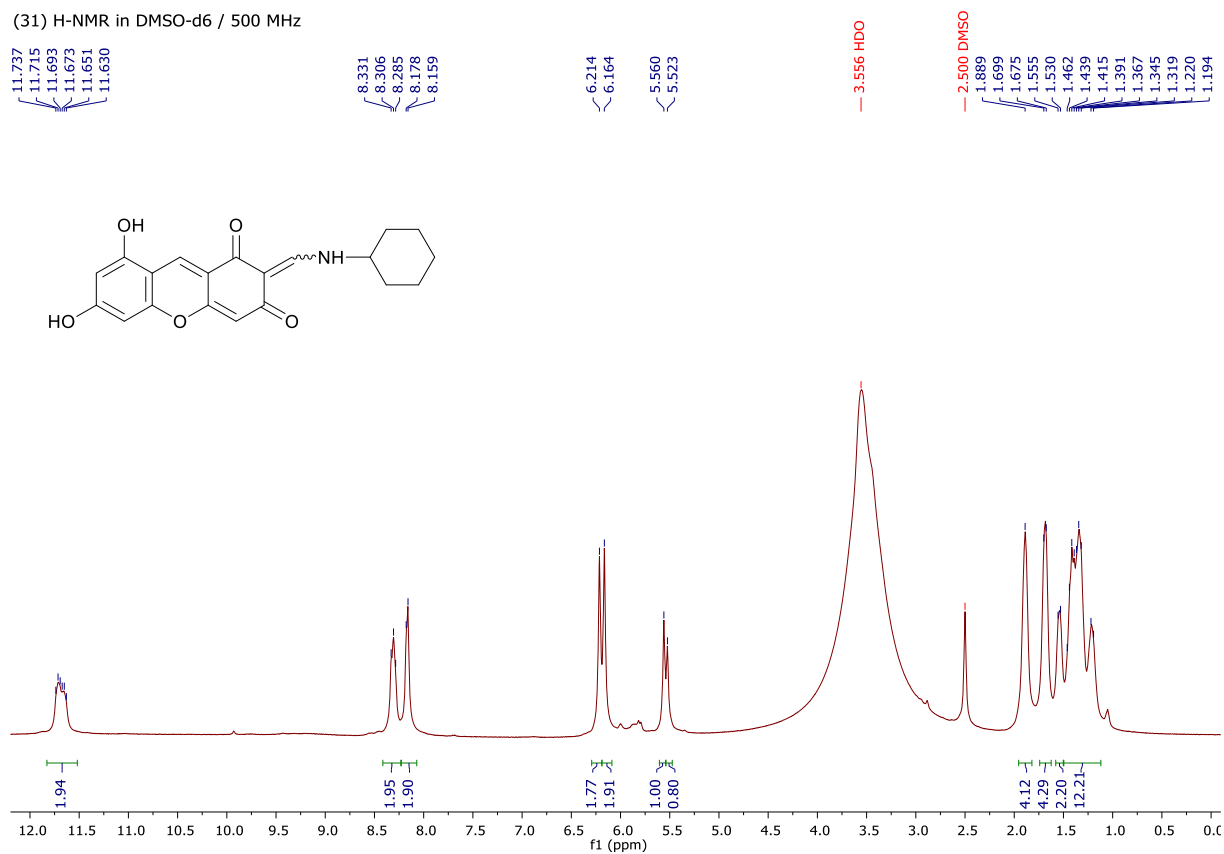


Figure S50. ¹H NMR spectrum of **31** in DMSO-d₆ / 500 MHz.

(31) ¹³C-NMR and DEPT in DMSO-d₆ / 125 MHz

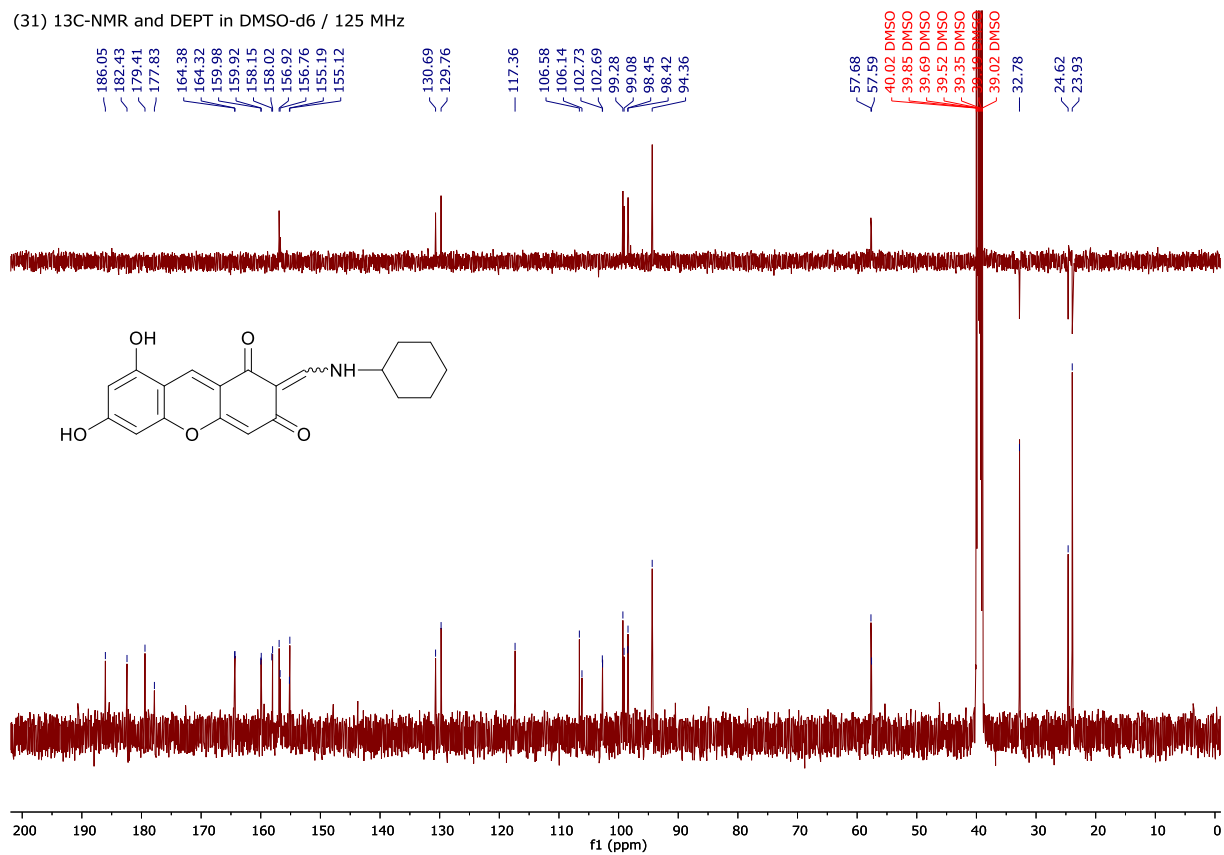


Figure S51. ¹³C NMR and DEPT spectra of **31** in DMSO-d₆ / 125 MHz.

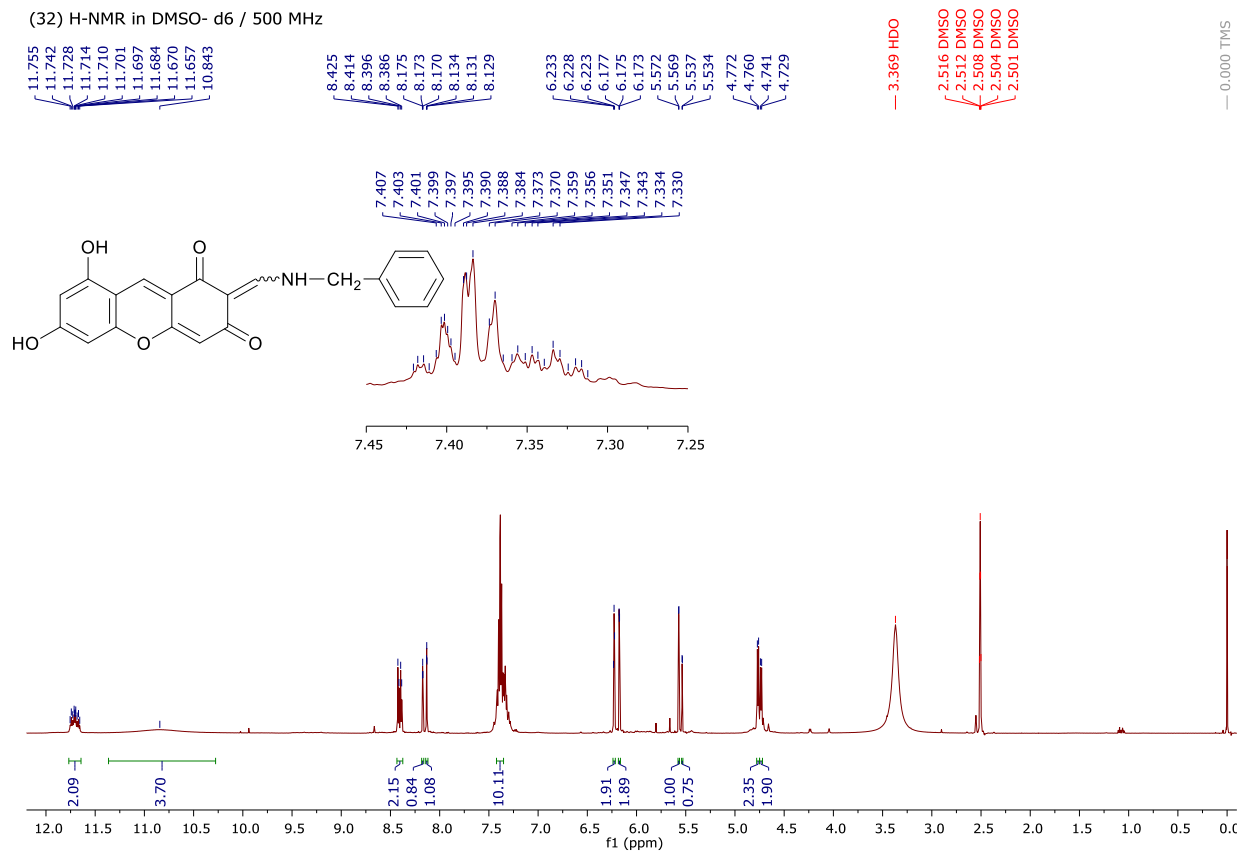


Figure S52. ¹H NMR spectrum of **32** in DMSO-*d*₆ / 500 MHz.

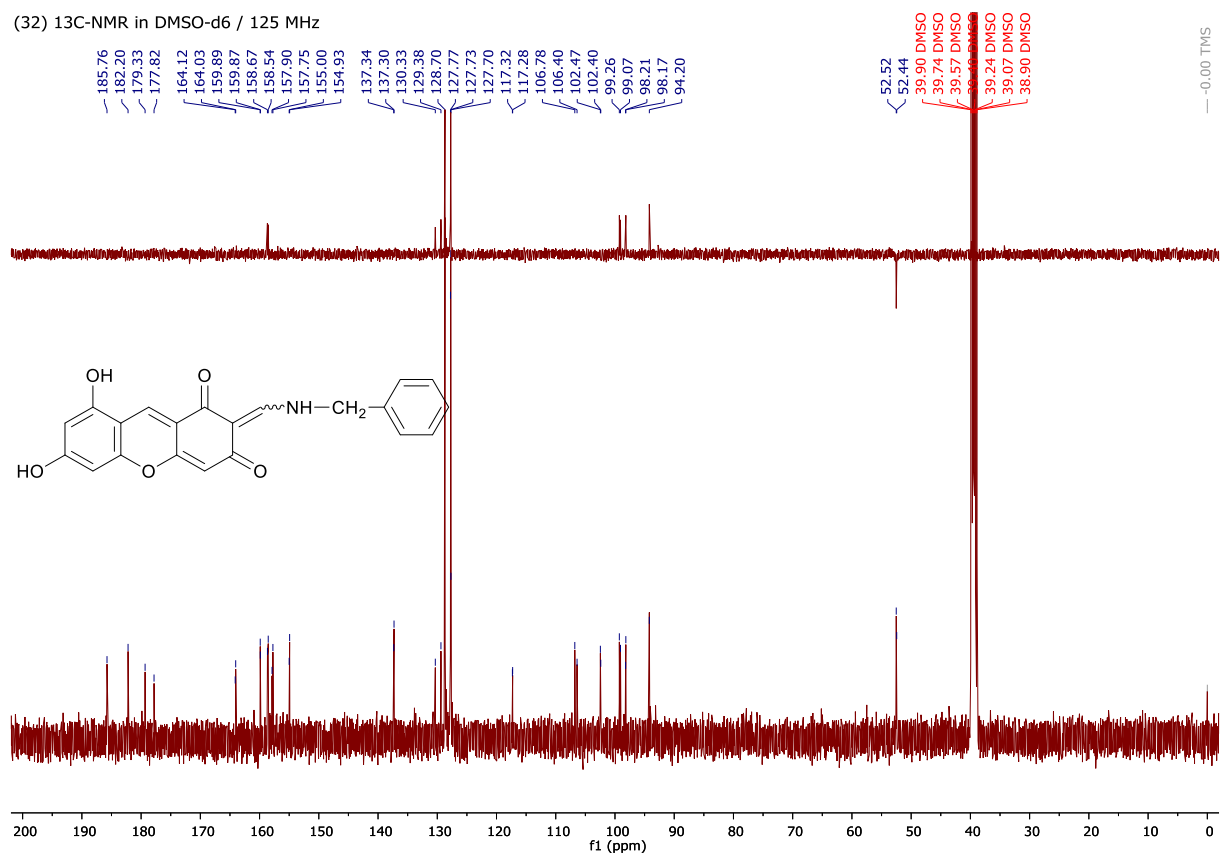


Figure S53. ¹³C NMR and DEPT spectra of **32** in DMSO-*d*₆ / 125 MHz.

(33) H-RMN in DMSO-d6 / 500 MHz

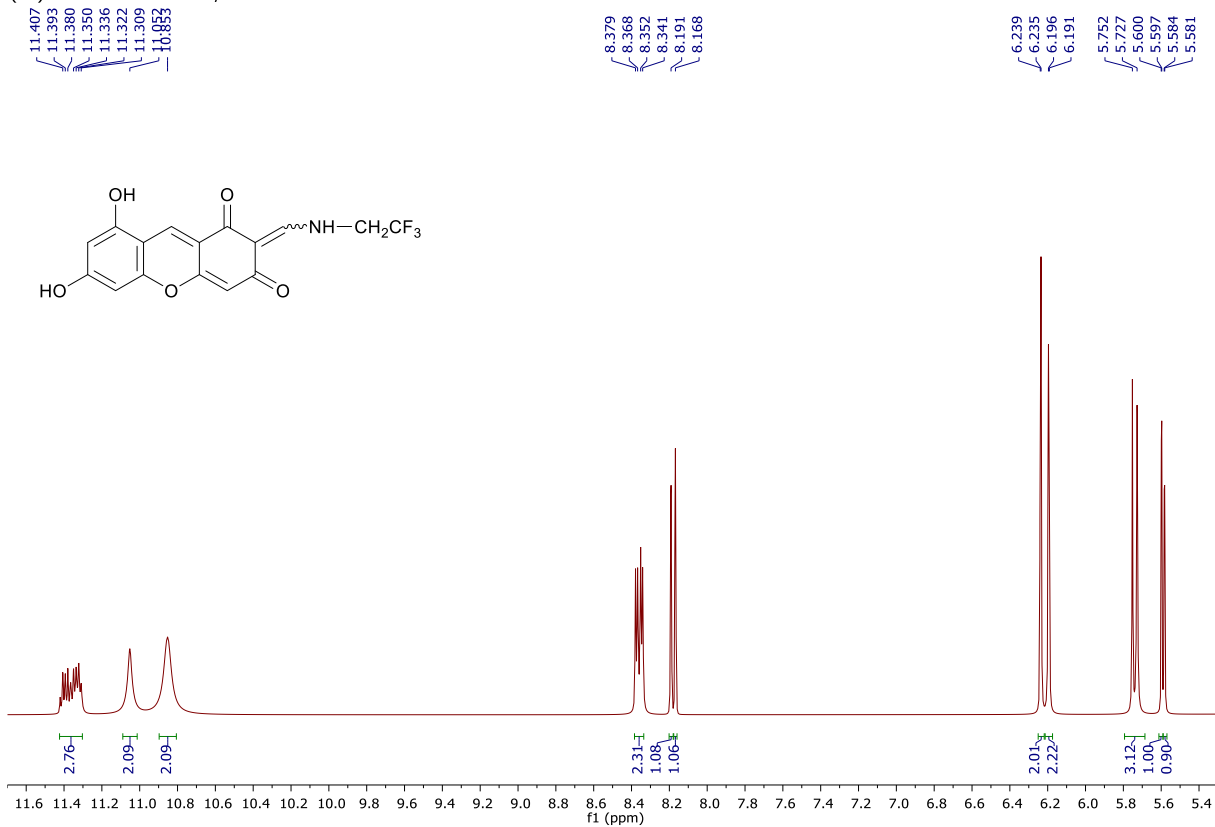


Figure S54. ¹H NMR spectrum of 33 in DMSO-d₆ / 500 MHz.

(51) H-RMN in DMSO-d6 / 500 MHz

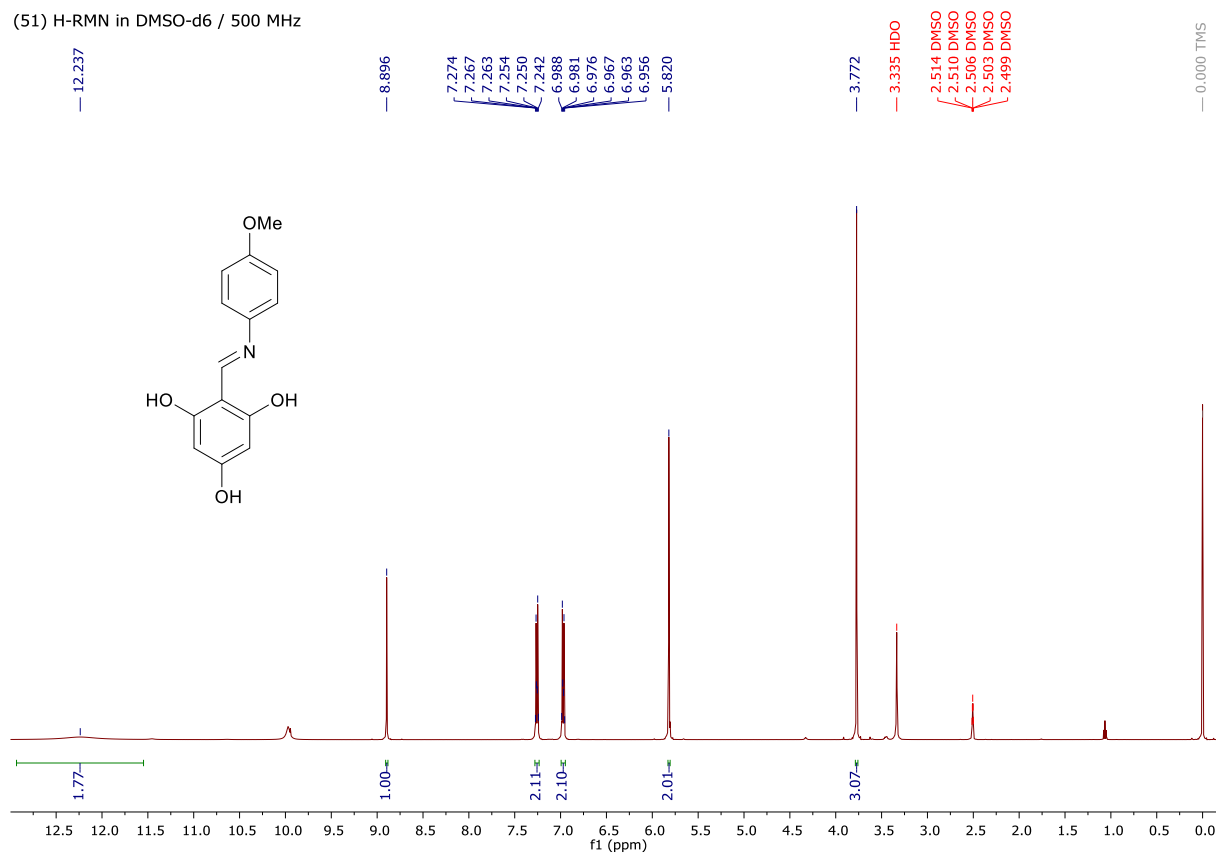


Figure S55. ¹H NMR spectrum of 51 in DMSO-d6 / 500 MHz.

(51) ¹³C-NMR and DEPT in DMSO-d6 / 125 MHz

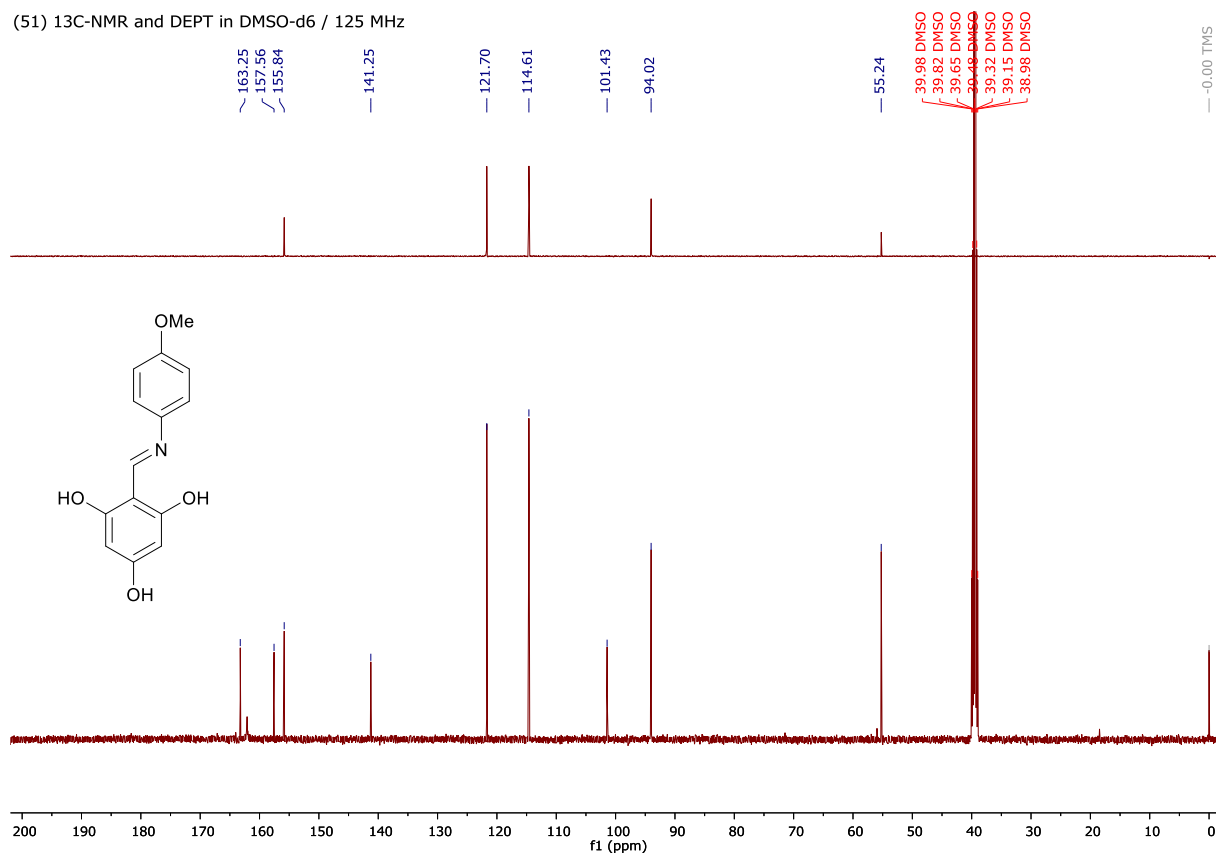


Figure S56. ¹³C NMR and DEPT spectra of 51 in DMSO-d6 / 125 MHz.

COSY, HSQC, HMBC SPECTRA AND VARIABLE-TEMPERATURE EXPERIMENTS

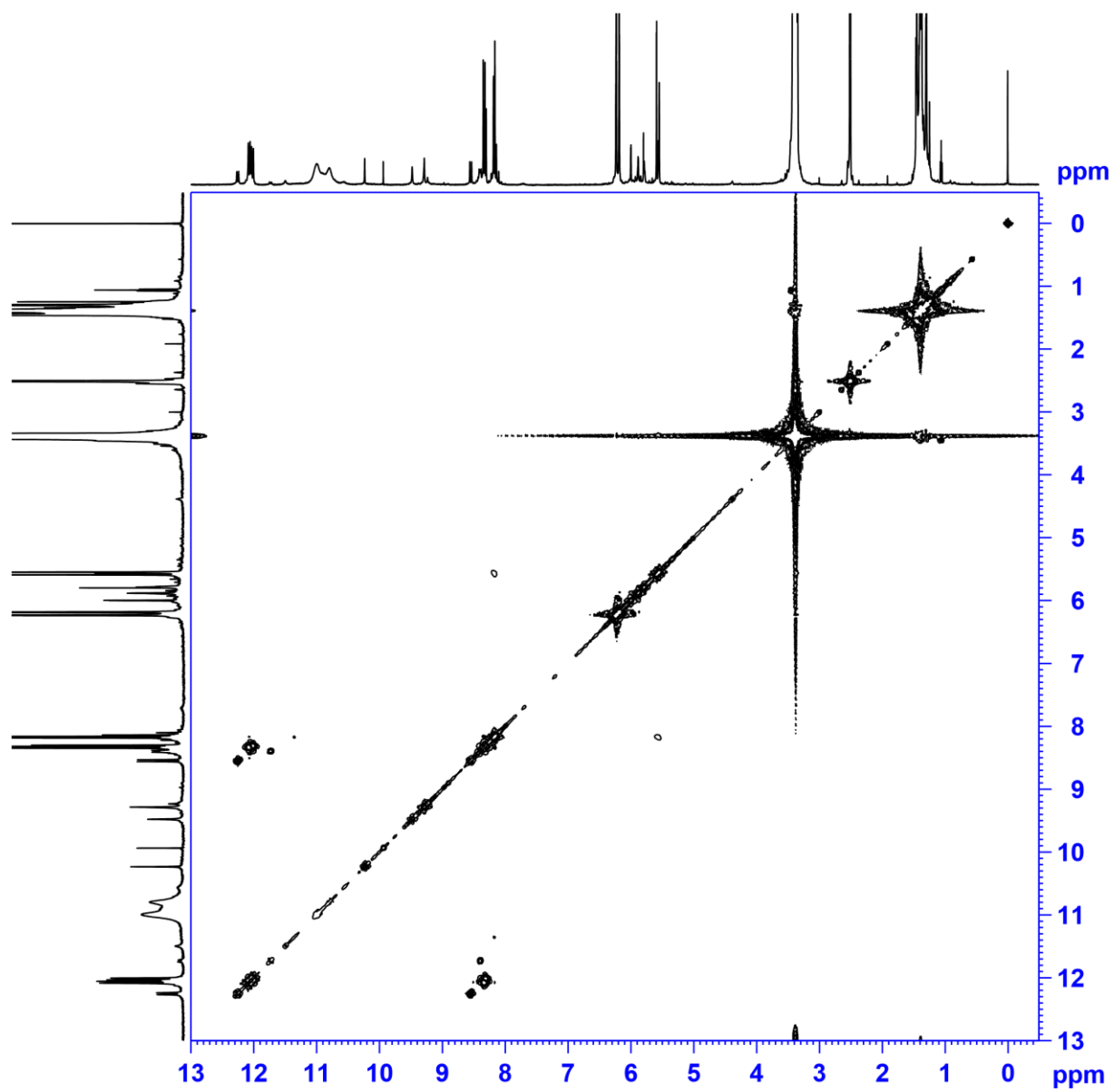


Figure S57. Compound 19 – COSY.

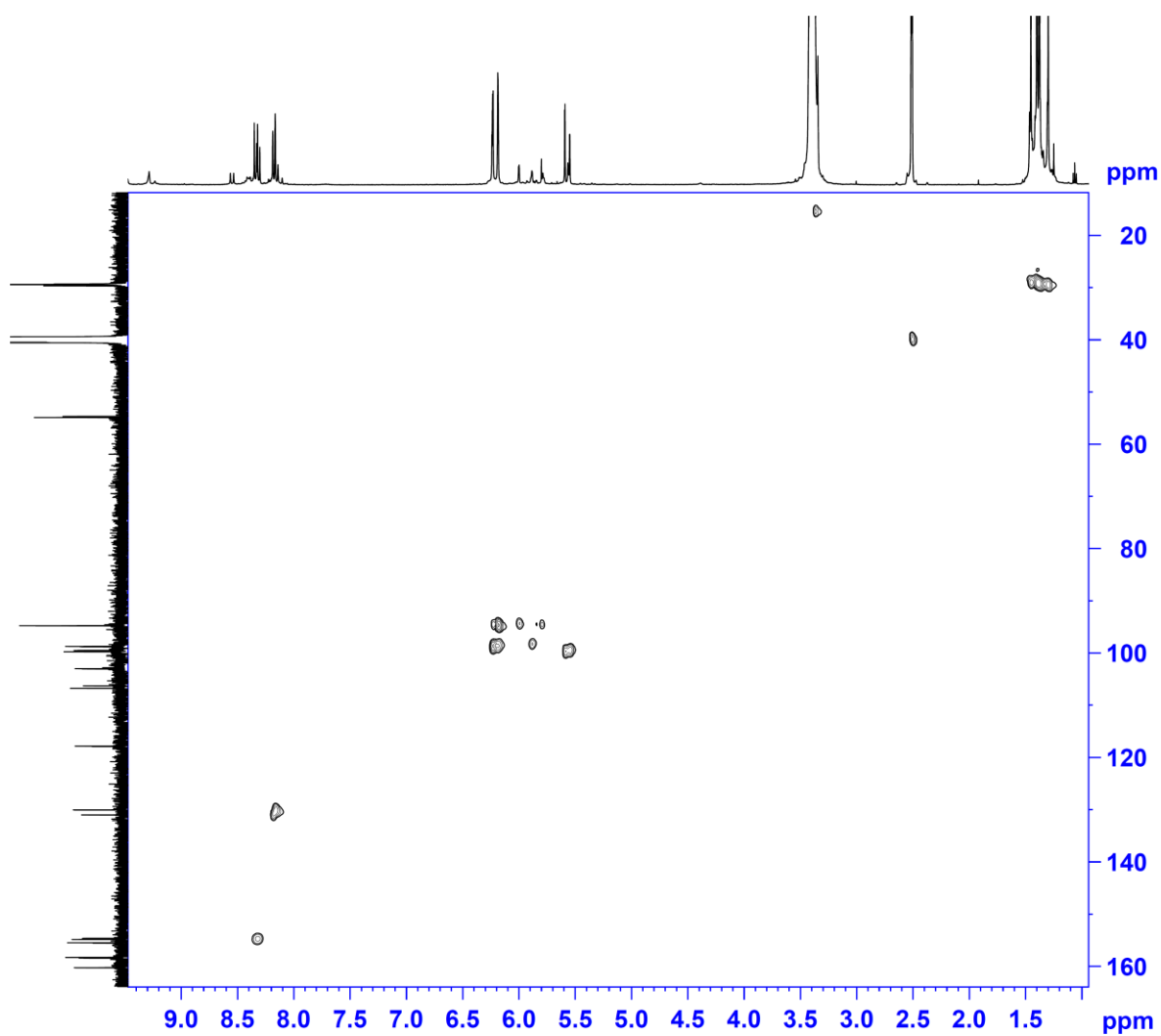


Figure S58. Compound 19 – HSQC.

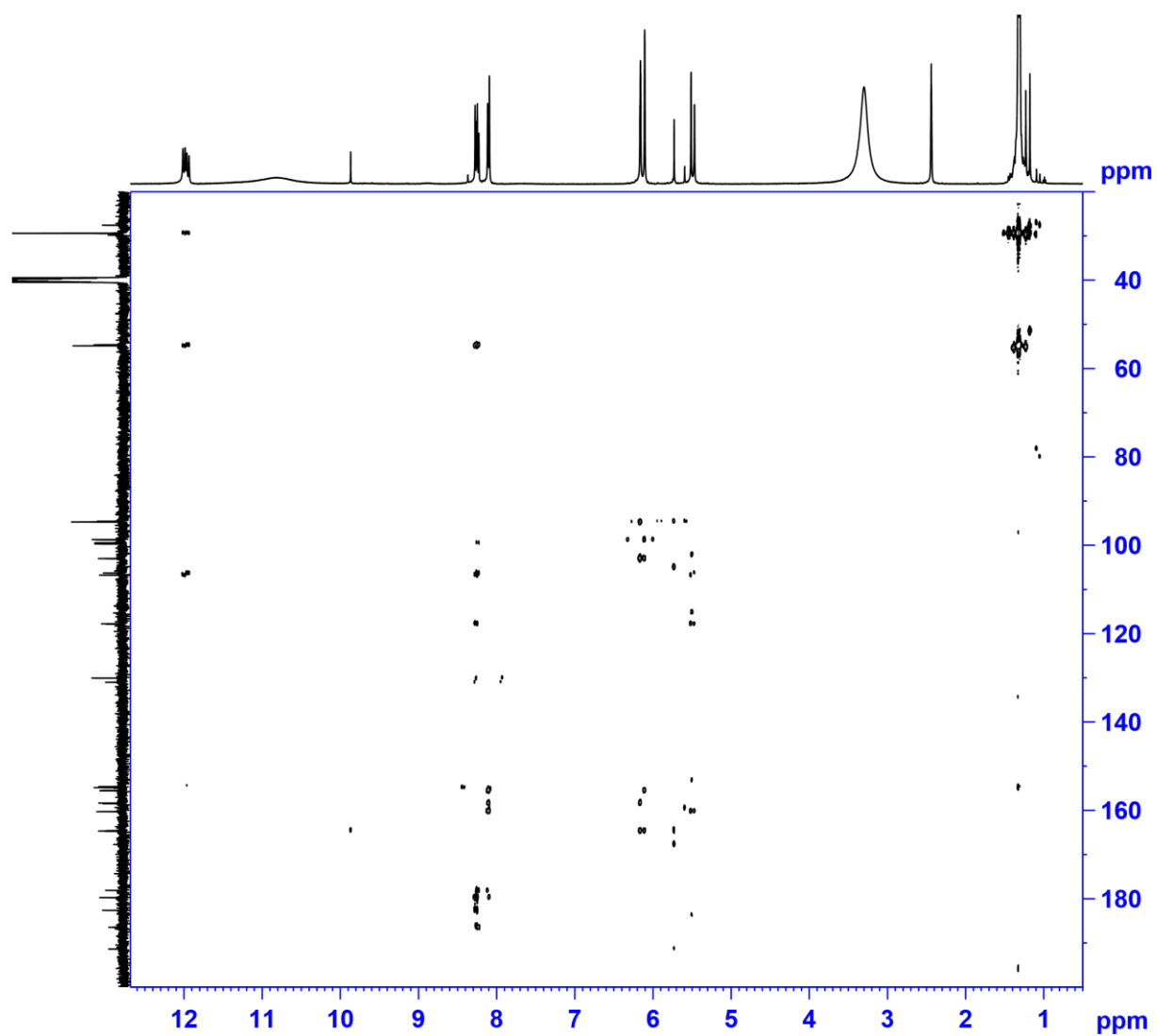


Figure S59. Compound 19 – HMBC.

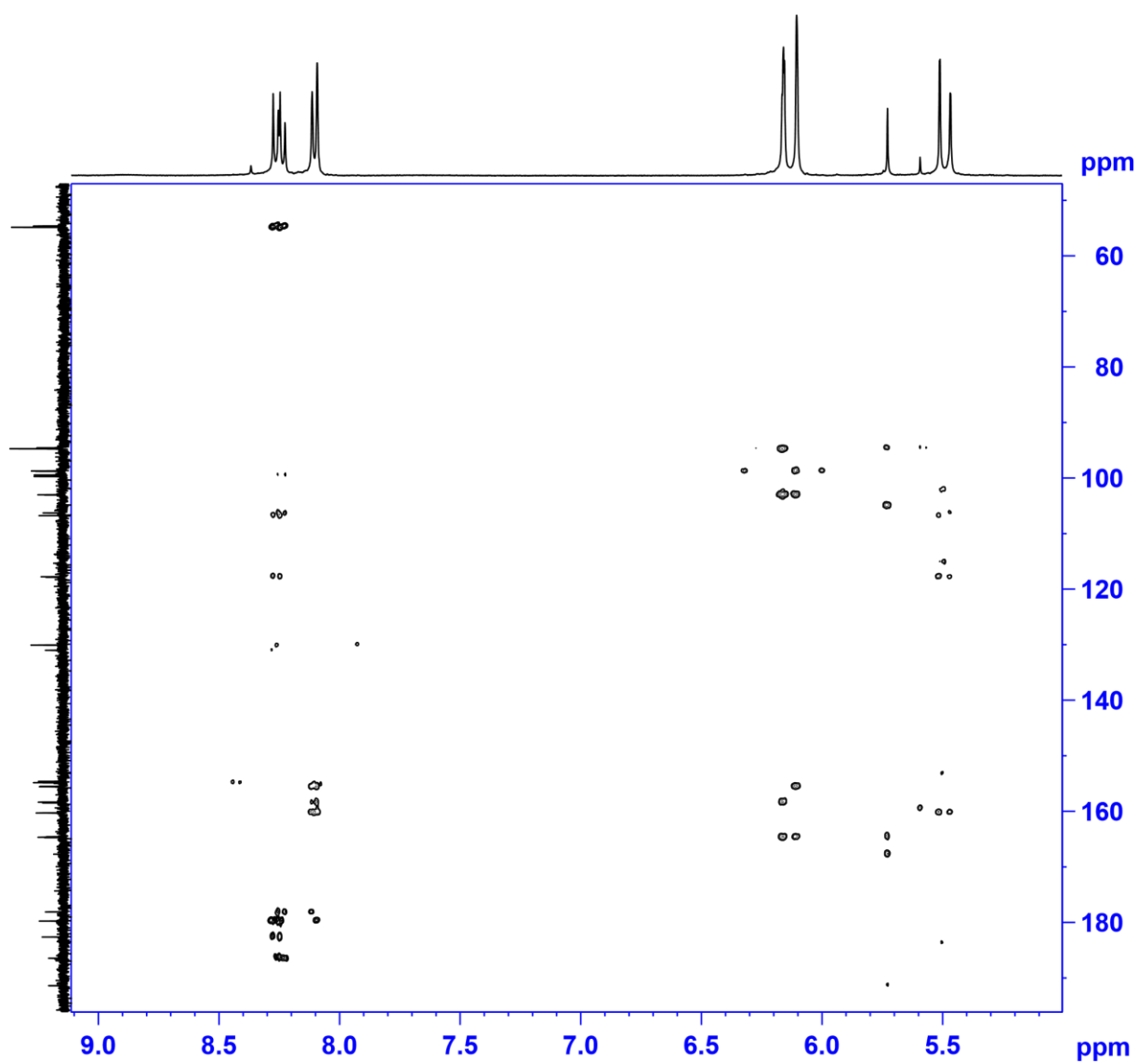


Figure S60. Compound 19 – HMBC (expanded/zoomed areas)

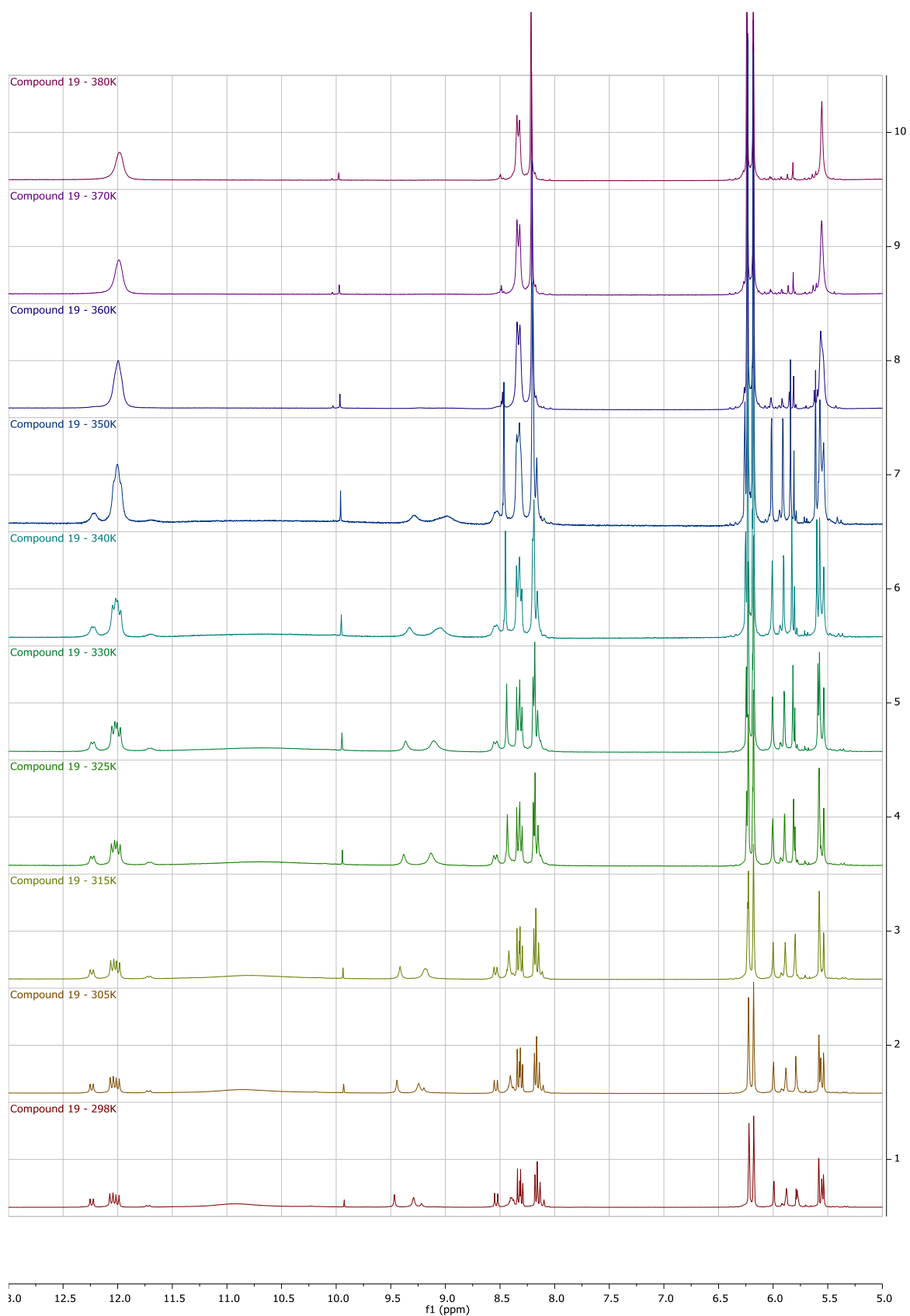


Figure S61. Compound 19. ¹H NMR variable-temperature experiments recorded between 13 and 5 ppm.

(19) ^{13}C -NMR in DMSO- d_6 / 125 MHz / 380K

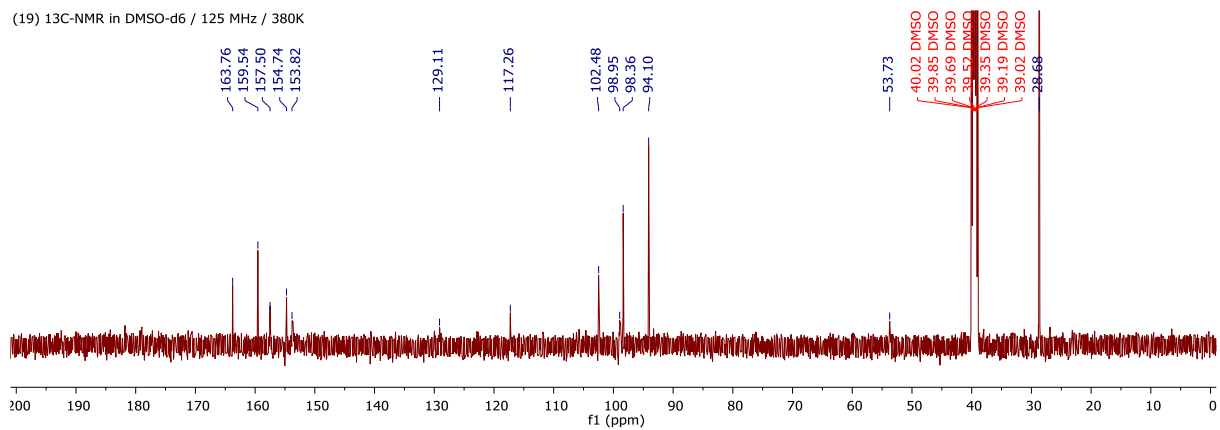


Figure S62. ^{13}C NMR spectrum of **19** at 380 K.

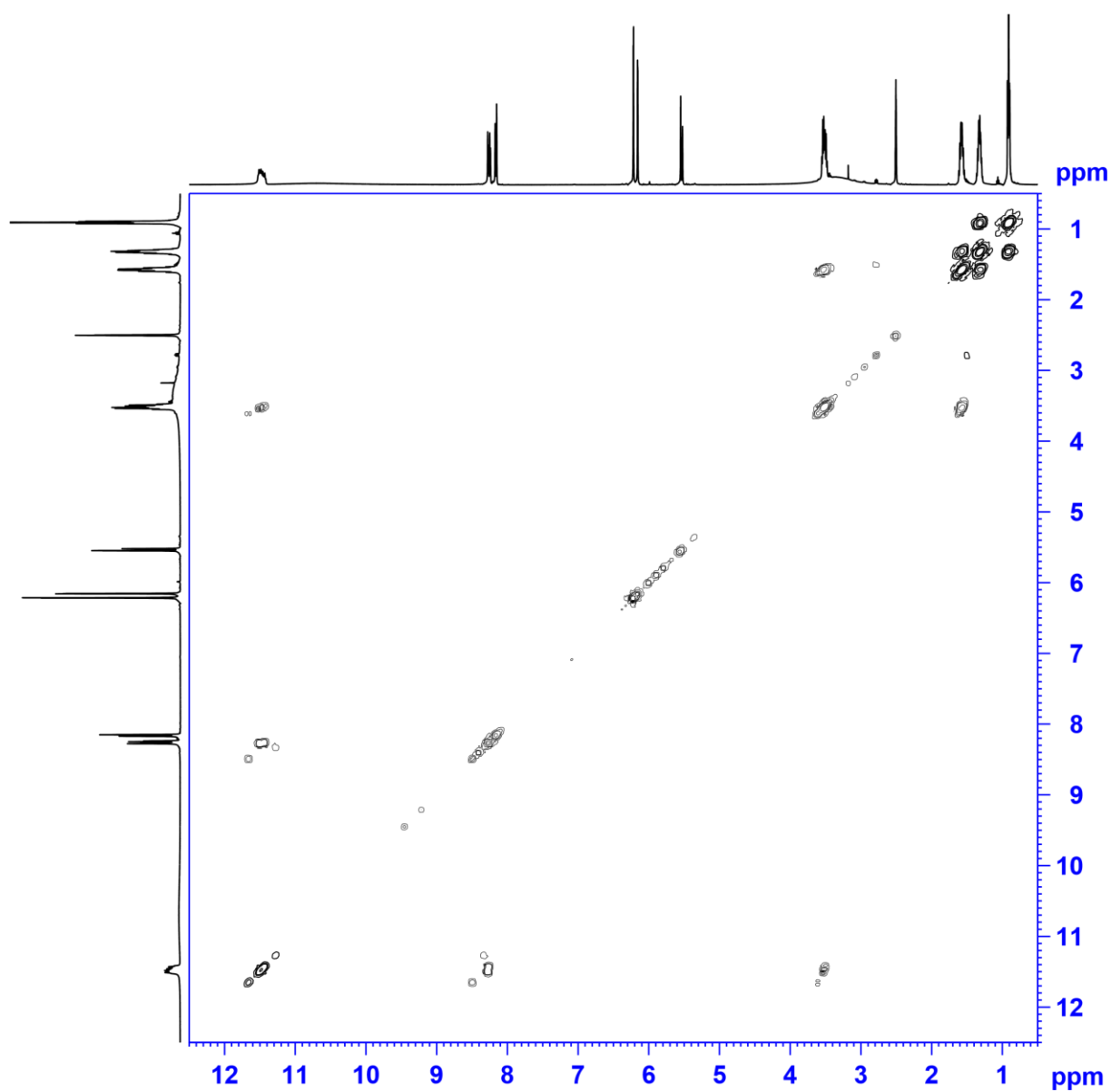


Figure S63. Compound **26** – COSY.

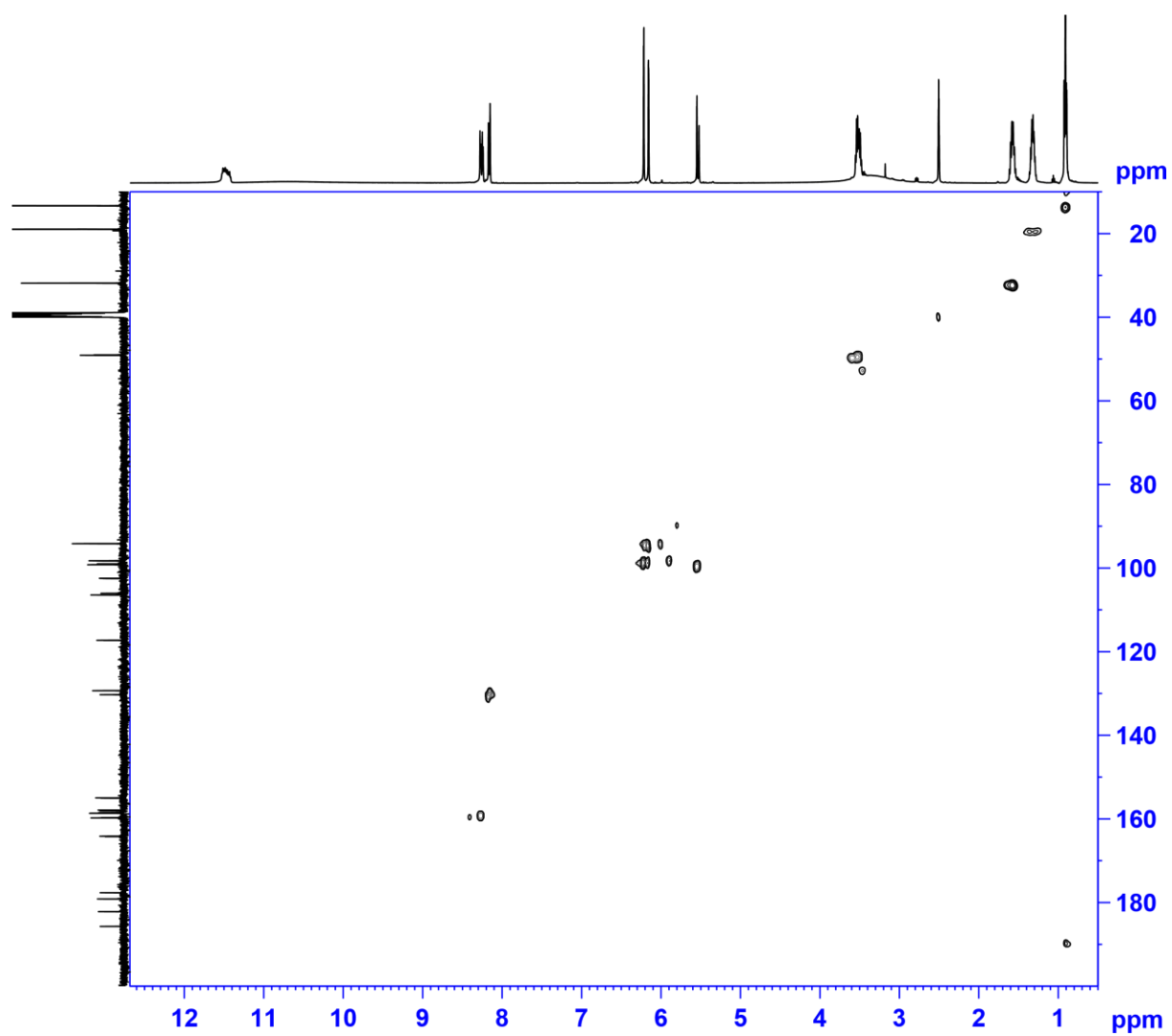


Figure S64. Compound 26 – HSQC.

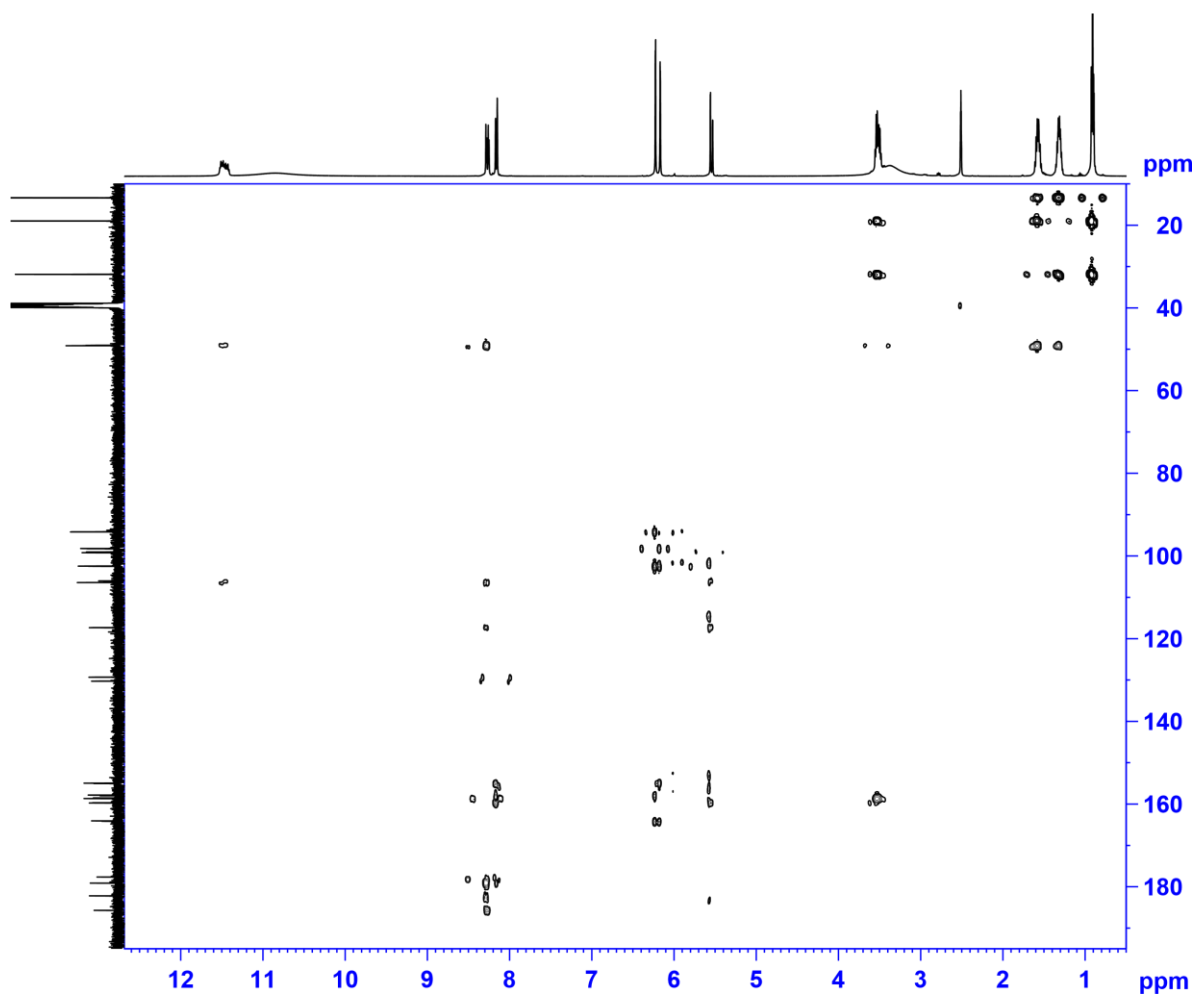


Figure S65. Compound 26 – HMBC.

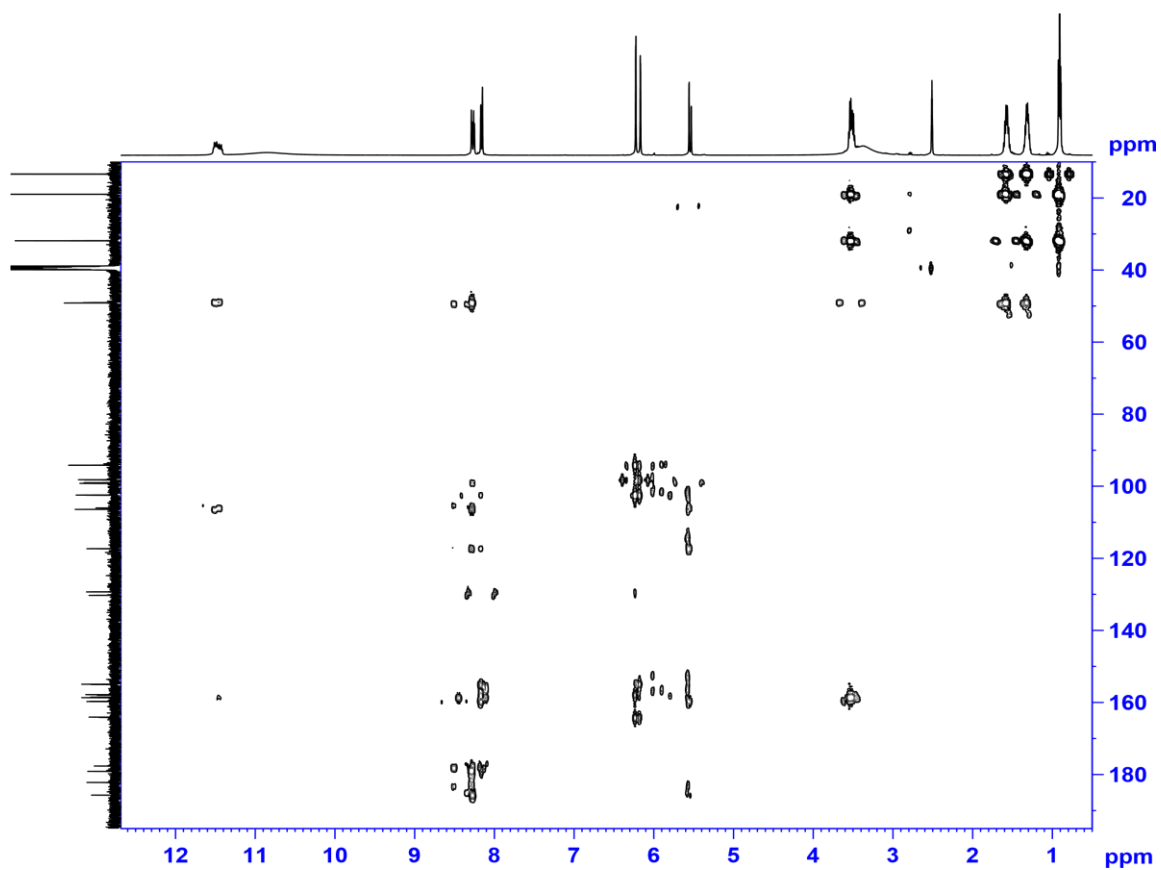


Figure S66. Compound 26 – HMBC (at higher magnification).

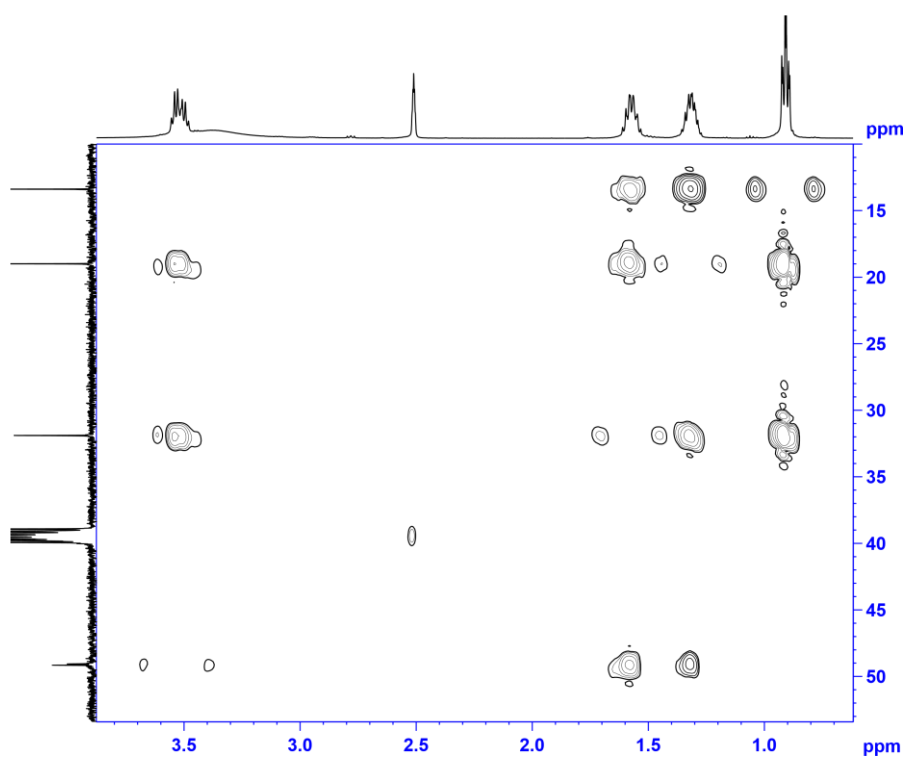


Figure S67. Compound 26 – HMBC (expanded/zoomed areas).

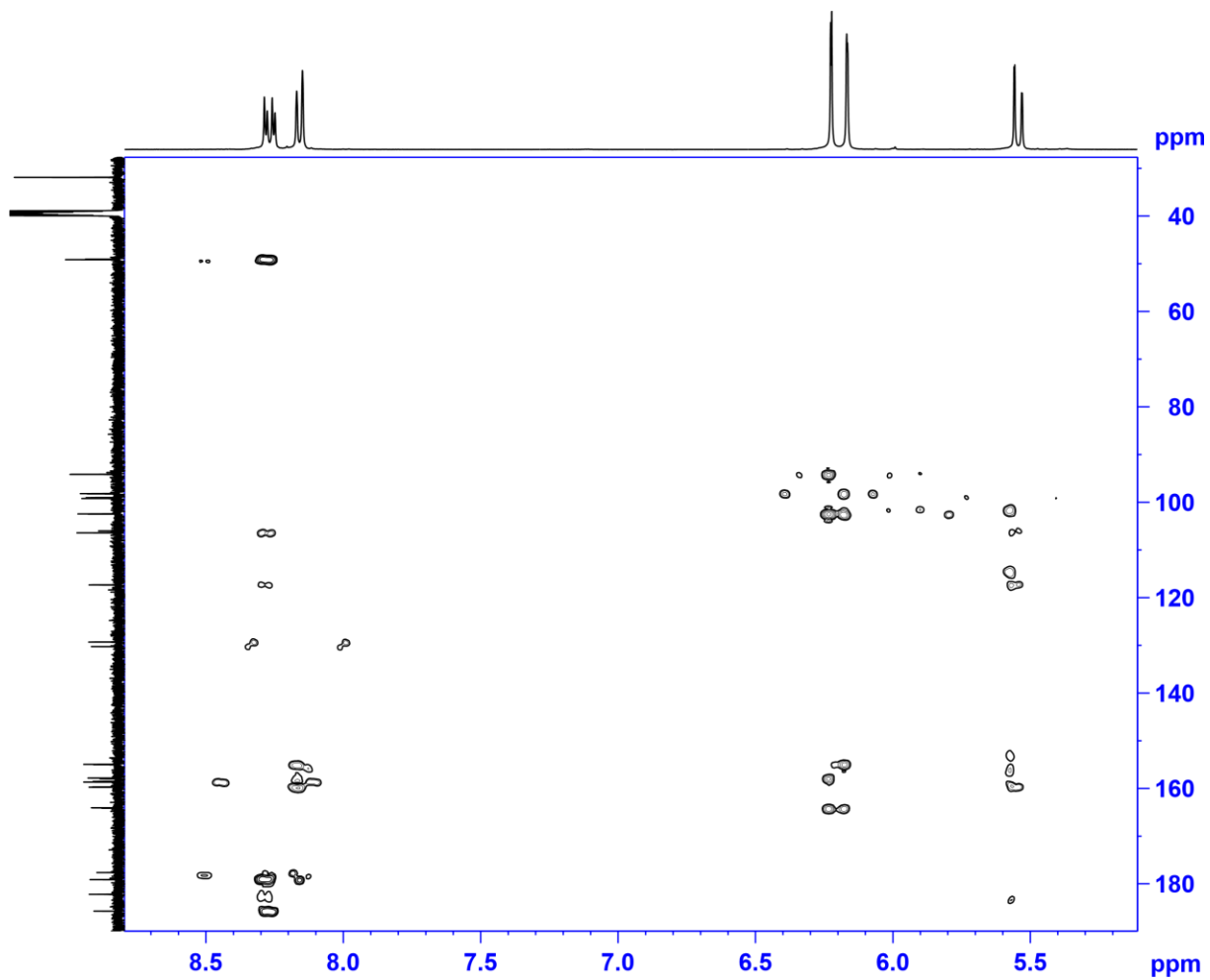


Figure S68. Compound 26 – HMBC (expanded/zoomed spectrum).

CARTESIAN COORDINATES FOR OPTIMIZED STRUCTURES

Compound 21 in DMSO:

<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-0.92484500	-0.32546600	-0.01397900
C	-1.82614900	0.79522700	-0.00783700
C	-1.34948400	2.18676600	-0.00211200
C	0.09122300	2.40649500	-0.00205100
C	0.94966000	1.36381100	-0.00492000
C	0.52913300	-0.01959800	-0.00930900
O	2.28590200	1.64103600	-0.00377300
C	3.22615500	0.66022300	-0.00118700
C	2.84838800	-0.68961600	-0.00221700
C	1.45522800	-1.00716000	-0.00758300
C	4.55006500	1.06582900	0.00259800
C	5.53087600	0.07699800	0.00619800
C	5.20647800	-1.28369400	0.00622000
C	3.87541200	-1.65697200	0.00201900
O	6.84395000	0.38294000	0.01018500
O	3.48344600	-2.94776300	0.00180200
O	-1.30227800	-1.50704900	-0.02131900
C	-3.21038800	0.59801000	-0.00375400
O	-2.12755500	3.14515600	0.00204200
N	-3.82705100	-0.55900900	-0.01192800
C	-5.30055600	-0.72846500	0.00662600
C	-5.55960600	-2.23013300	-0.05352600
C	-5.91196900	-0.03578600	-1.21122200
C	-5.86062000	-0.14105900	1.30246300
H	0.45590600	3.42582900	0.00110200
H	1.13183500	-2.04178900	-0.01015400
H	4.80415700	2.11923500	0.00308100
H	5.99778800	-2.02509000	0.00963400
H	6.96231400	1.34242400	0.00978800
H	4.25625800	-3.52882000	0.00540700
H	-3.83749800	1.48599900	0.00900200
H	-3.23191500	-1.38702300	-0.01821700
H	-5.10191100	-2.73772000	0.79993100
H	-6.63452100	-2.41800200	-0.03019300
H	-5.15521100	-2.65673100	-0.97543500
H	-5.73763800	1.04273300	-1.18769400
H	-6.99143400	-0.20330800	-1.21895800
H	-5.48995300	-0.43979300	-2.13463300
H	-6.94150900	-0.29586400	1.33618000
H	-5.41044400	-0.62917800	2.17038600
H	-5.66858300	0.93314600	1.36420700

Compound 22 in DMSO:

<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	0.72101200	0.89172400	-0.00629600
C	1.79198100	-0.08861100	-0.00917800
C	1.53177100	-1.52291800	-0.01245000
C	0.15019300	-1.97705400	-0.00803500
C	-0.86359900	-1.08433900	-0.00421500
C	-0.66684800	0.34833400	-0.00513500
O	-2.13787200	-1.57161400	0.00067000
C	-3.22297200	-0.75479300	0.00170500
C	-3.06501300	0.63824500	-0.00275000
C	-1.74022600	1.17371600	-0.00538400
C	-4.46446000	-1.36859600	0.00754200
C	-5.59097900	-0.54941700	0.00857900
C	-5.48769300	0.84562400	0.00339600
C	-4.23432700	1.42860800	-0.00241500
O	-6.83914800	-1.05927300	0.01451200
O	-4.05591100	2.76555600	-0.00783100
O	0.90127300	2.10924500	-0.00488500
C	3.09871300	0.40948000	-0.00453300

O	2.45938700	-2.35218700	-0.01785900
N	4.19861400	-0.30360500	-0.00830900
C	5.57263900	0.25241800	0.00771100
C	5.77513900	1.07014500	1.28363300
C	6.51572400	-0.94638100	-0.01119200
C	5.78909800	1.11954700	-1.23279500
H	-0.04202800	-3.04255600	-0.00795100
H	-1.58720900	2.24685000	-0.00703900
H	-4.54501700	-2.44938200	0.01112100
H	-6.38718700	1.45046100	0.00394400
H	-6.80352800	-2.02549000	0.01786700
H	-4.91232200	3.21417100	-0.00676900
H	3.21676300	1.49037400	0.00410000
H	4.07060700	-1.31575400	-0.01441000
H	6.79890400	1.44996300	1.31594400
H	5.09501300	1.92491600	1.31760700
H	5.60420600	0.45006400	2.16692800
H	7.55099000	-0.60109800	0.00087000
H	6.36163000	-1.54539500	-0.91263800
H	6.35273200	-1.58034000	0.86446900
H	5.62819800	0.53523900	-2.14197200
H	5.11142100	1.97679000	-1.24171200
H	6.81376500	1.49820900	-1.23819100

Compound 49 in DMSO:

<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-0.95778000	-0.14790600	0.00019700
C	-1.82710400	0.92259800	0.00015100
C	-1.32943500	2.30530400	0.00007900
C	0.11315800	2.49591200	0.00002100
C	0.94429600	1.43093100	0.00004900
C	0.47808700	0.06151600	0.00013800
O	2.28713700	1.66197400	0.00001000
C	3.19249100	0.65282300	-0.00001600
C	2.76998600	-0.68608400	0.00004000
C	1.37408100	-0.96176000	0.00012600
C	4.52884000	1.01453600	-0.00008800
C	5.47607100	-0.00608800	-0.00010900
C	5.10770400	-1.35721000	-0.00005800
C	3.76773500	-1.68826300	0.00001100
O	6.79694800	0.25426100	-0.00018200
O	3.33304400	-2.96348100	0.00006000
O	-1.38186100	-1.39639100	0.00026300
C	-3.26264700	0.68892600	0.00006200
O	-2.10392800	3.26601100	0.00004800
N	-3.72683600	-0.50461200	0.00023600
C	-5.16850900	-0.80131000	-0.00008600
C	-6.05801800	0.43889600	0.00045700
C	-5.43875900	-1.64087100	1.25194800
C	-5.43848400	-1.63956700	-1.25307200
H	0.50219300	3.50619000	-0.00004300
H	1.02648000	-1.98806400	0.00018700
H	4.81689500	2.05928700	-0.00012300
H	5.87375300	-2.12437200	-0.00007500
H	6.94945900	1.20917400	-0.00021800
H	4.08486800	-3.57170600	0.00004100
H	-2.41513200	-1.33823300	0.00025500
H	-3.89923200	1.57312500	-0.00013400
H	-5.89110900	1.05394000	-0.88789600
H	-7.10351300	0.12309500	0.00046200
H	-5.89085800	1.05327500	0.88922900
H	-4.80697400	-2.53290700	1.25973000
H	-6.48490100	-1.95694200	1.27273200
H	-5.23211100	-1.06095900	2.15545400
H	-5.23166900	-1.05869500	-2.15592000
H	-4.80667900	-2.53158100	-1.26165700
H	-6.48461800	-1.95563200	-1.27435900

Compound 50 in DMSO:

<u>ATOM</u> <u>TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-0.69391100	0.99624100	0.00015400
C	-1.78436300	0.04952500	0.00024700
C	-1.53426500	-1.33172300	0.00031900
C	-0.21784000	-1.88040600	0.00024600
C	0.83414000	-1.02069300	0.00010700
C	0.67331800	0.40883400	0.00010700
O	2.08485000	-1.55026600	0.00005200
C	3.19415100	-0.77160900	0.00000100
C	3.07838000	0.62797200	0.00011300
C	1.77891100	1.20183400	0.00014400
C	4.41551500	-1.42325700	-0.00019000
C	5.56515100	-0.63732700	-0.00026000
C	5.50575400	0.76248300	-0.00010100
C	4.27445300	1.38457400	0.00008800
O	6.79612900	-1.18151500	-0.00047000
O	4.13400300	2.72368200	0.00026100
O	-0.84621500	2.22030900	0.00006100
C	-3.14750400	0.54153100	0.00025500
O	-2.53390800	-2.18774000	0.00057700
N	-4.14219700	-0.26783400	0.00053300
C	-5.54337200	0.17975100	-0.00020900
C	-6.19039300	-0.41821900	-1.25310500
C	-6.19193500	-0.41902400	1.25146600
C	-5.71261100	1.69635600	0.00019000
H	-0.07914500	-2.95324200	0.00031200
H	1.65839200	2.27970700	0.00017900
H	4.46162900	-2.50597000	-0.00029700
H	6.42482200	1.33742600	-0.00014400
H	6.73461900	-2.14672700	-0.00064100
H	5.00224300	3.14940700	0.00001300
H	-3.27004600	1.62481200	-0.00021200
H	-3.40305200	-1.62069200	0.00058200
H	-7.25982300	-0.19300500	-1.26940900
H	-5.73377800	-0.00399100	-2.15601300
H	-6.06333700	-1.50379200	-1.26708300
H	-7.26144300	-0.19411000	1.26645100
H	-5.73668400	-0.00517600	2.15524400
H	-6.06457000	-1.50456600	1.26504100
H	-5.26793600	2.15295100	-0.88828500
H	-6.77917900	1.93263600	0.00036800
H	-5.26769800	2.15234200	0.88887300

Transition state for 21 to 49 tautomerization in DMSO:

<u>ATOM</u> <u>TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-0.98273300	-0.11943500	0.00220200
C	-1.83386600	0.98103500	0.00495900
C	-1.32315400	2.35400000	0.00477700
C	0.12368700	2.52409800	0.00114000
C	0.94058700	1.44809700	-0.00039100
C	0.46043600	0.08250600	0.00111500
O	2.28688700	1.66397900	-0.00390000
C	3.18100700	0.64448200	-0.00264500
C	2.74468600	-0.68954900	0.00122200
C	1.34421500	-0.94924900	0.00222800
C	4.52120600	0.99254400	-0.00539400
C	5.45834700	-0.03735700	-0.00343700
C	5.07569100	-1.38411700	0.00149400
C	3.73181500	-1.70121600	0.00367200
O	6.78231200	0.20964800	-0.00604300
O	3.28493200	-2.97253500	0.00824900
O	-1.44046600	-1.33541500	0.00076800
C	-3.25704100	0.74456000	0.00611400
O	-2.08334600	3.32677400	0.00701100

N	-3.69537200	-0.46517000	0.00254600
C	-5.11769800	-0.84218500	-0.00279500
C	-5.34010900	-1.72903500	1.22504200
C	-5.35129600	-1.65321700	-1.28042000
C	-6.05462200	0.35999700	0.03796900
H	0.52686000	3.52893200	-0.00023400
H	0.98191800	-1.97063500	0.00394500
H	4.81902700	2.03453600	-0.00867200
H	5.83291600	-2.15994600	0.00367000
H	6.94415700	1.16296600	-0.00917800
H	4.03108700	-3.58757300	0.00979000
H	-3.91939100	1.60826300	0.00954200
H	-2.58086400	-1.20101100	0.00047000
H	-5.15845500	-1.16591800	2.14420300
H	-6.36917400	-2.09643500	1.23911600
H	-4.66544100	-2.58890800	1.20485400
H	-5.18259900	-1.03314200	-2.16472600
H	-6.37915100	-2.02359500	-1.30490100
H	-4.67323600	-2.50964200	-1.32123300
H	-7.08648200	0.00275800	0.03748300
H	-5.90275400	0.95500000	0.94252100
H	-5.92031700	1.00516500	-0.83427300

Transition state for 22 to 50 tautomerization in DMSO:

<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	0.68196900	1.04446300	0.00002900
C	1.78014400	0.11153300	0.00000500
C	1.56268000	-1.28767000	0.00002400
C	0.24347800	-1.84501200	-0.00000300
C	-0.81662600	-0.99739300	0.00000400
C	-0.67780000	0.43702200	0.00001300
O	-2.06212300	-1.54261700	0.00001000
C	-3.18209700	-0.77833900	-0.00000200
C	-3.08603300	0.62183200	-0.00000100
C	-1.79260300	1.21384800	0.00000700
C	-4.39442500	-1.44708400	-0.00001100
C	-5.55531600	-0.67776400	-0.00001700
C	-5.51508800	0.72230800	-0.00001400
C	-4.29164300	1.36112100	-0.00000700
O	-6.77905900	-1.23986200	-0.00002800
O	-4.17008700	2.70263400	-0.00000100
O	0.81658100	2.27069800	0.00006800
C	3.13304100	0.59902200	-0.00003400
O	2.57560000	-2.09898400	0.00006400
N	4.11455500	-0.23536300	0.00002300
C	5.53652700	0.13900700	-0.00002200
C	5.75783500	1.64758000	-0.00004200
C	6.15669000	-0.48487700	1.25332200
C	6.15664800	-0.48491000	-1.25336800
H	0.11308200	-2.91903100	0.00000100
H	-1.68679600	2.29319500	0.00001100
H	-4.42431700	-2.53035300	-0.00001000
H	-6.44169700	1.28505800	-0.00001500
H	-6.70300000	-2.20394400	-0.00001300
H	-5.04434400	3.11569500	-0.00000700
H	3.28612100	1.67714800	-0.00010800
H	3.50284600	-1.41694700	0.00007400
H	6.83187200	1.84567700	-0.00002100
H	5.32870500	2.11781100	-0.88893300
H	5.32867500	2.11783800	0.88882000
H	7.23358300	-0.29995100	1.27016700
H	5.98937600	-1.56503200	1.26602600
H	5.71481700	-0.05379100	2.15545500
H	5.98909000	-1.56502600	-1.26618600
H	5.71494400	-0.05365700	-2.15550400
H	7.23358300	-0.30022200	-1.27011600