molecules

MDPI

Supplementary information for,

Synthesis and Evaluation of the *N*-(3-trifluoroacetylindol-7-yl)acetamides for potential *in vitro* antiplasmodial properties

M.J. Mphahlele, M.M. Mmonwa and Y.S. Choong

Supplementary 1: **Copies of ^{1}H- and ^{13}C NMR spectra of compounds 2–4 and ^{19}F NMR spectra of compounds 4**

Supplementary 2: **% cell viability and LC_{50} values of chloroquine and compounds 3 and 4**

Supplementary 3: **% cell viability of Vero cells exposed Doxorubicin chloride, 3a, 3f, 4a and 4g**

Supplementary 4: **Crystal data and structure refinement, bond lengths and torsion angles of 4g**

Supplementary 1: ^{1}H- and ^{13}C-NMR Spectra of Compounds 2–4 and ^{19}F NMR spectra of compounds 4

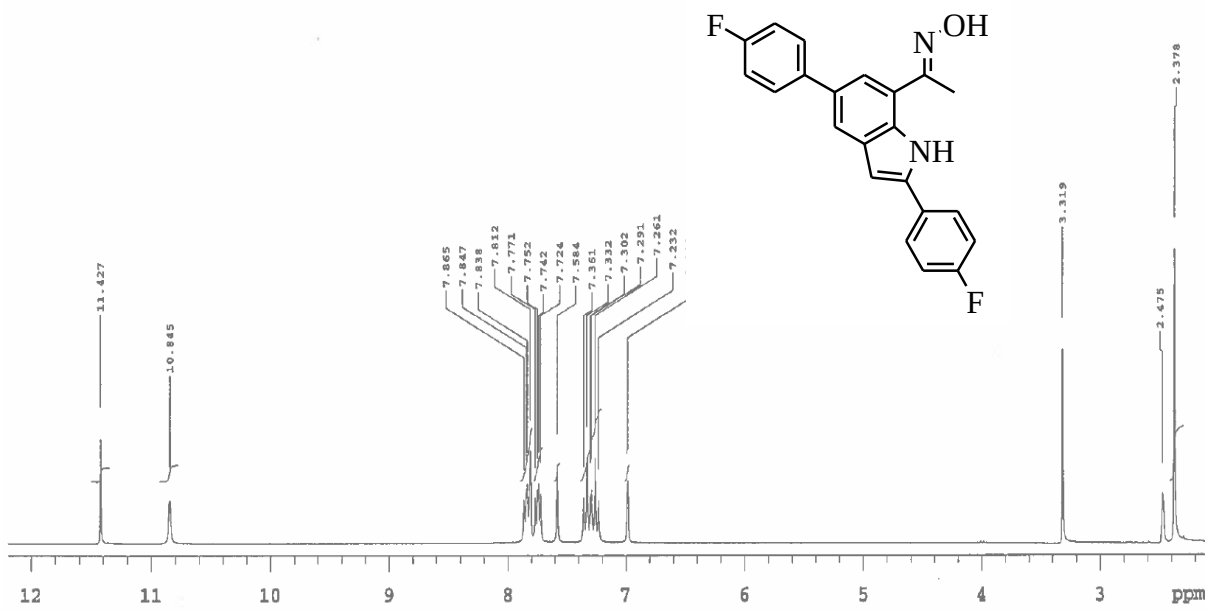


Figure S1. ^{1}H NMR Spectrum of Compound 2a DMSO-d_6 at 300 MHz

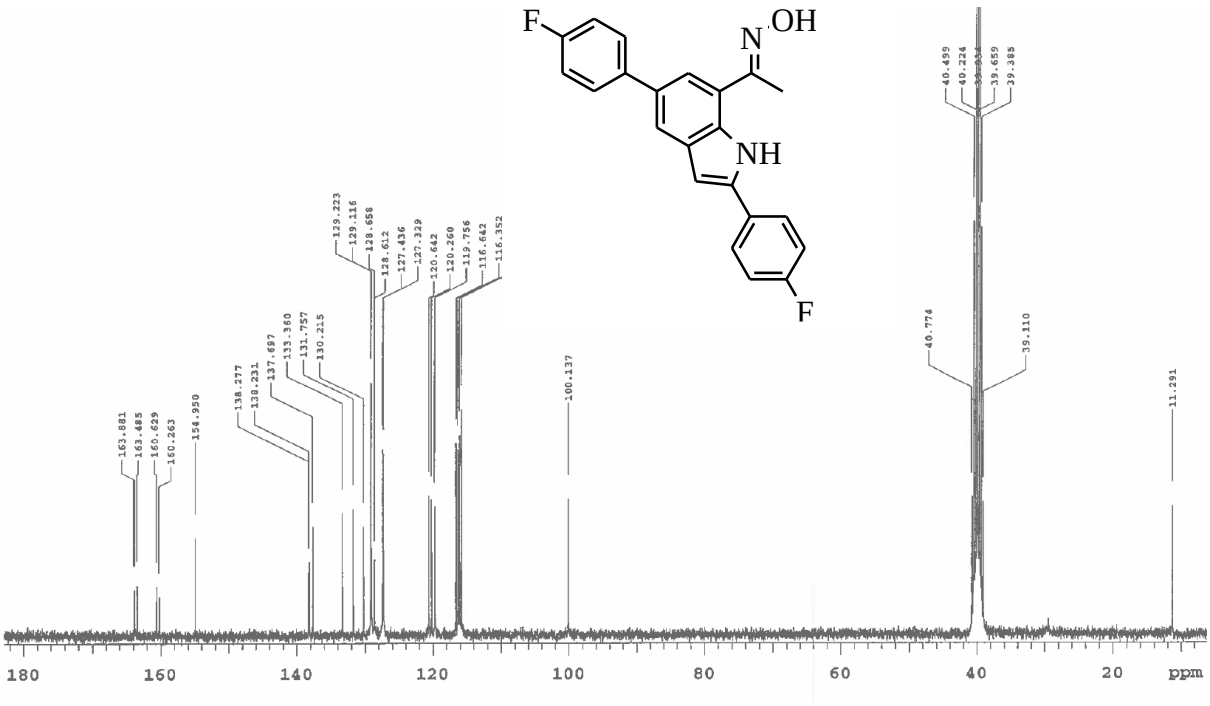


Figure S2. ^{13}C NMR Spectrum of Compound 2a in DMSO-d_6 at 75 MHz

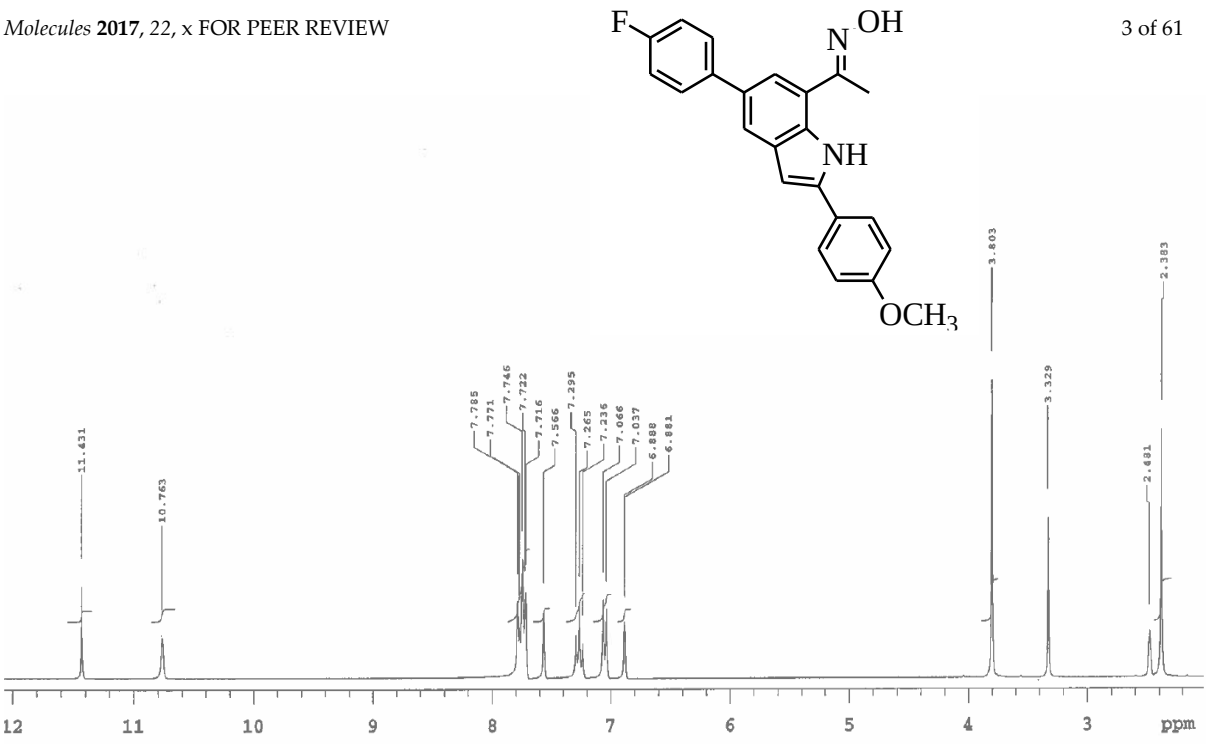


Figure S3. [1]H NMR Spectrum of Compound 2b in DMSO-*d*$_6$ at 300 MHz

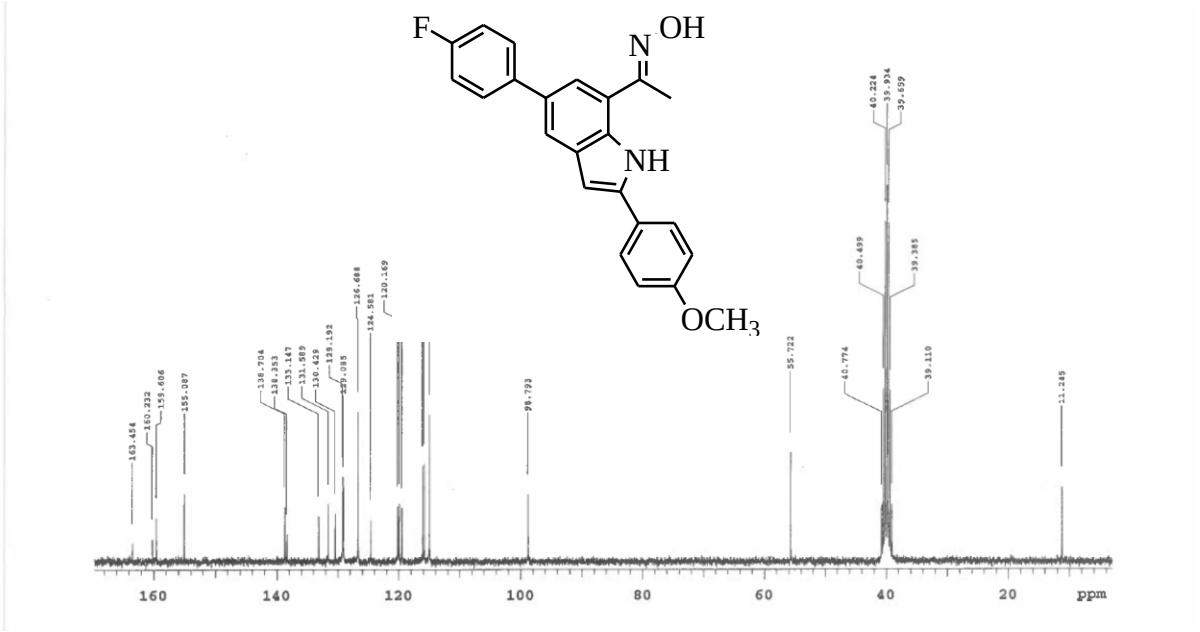


Figure S4. [13]C NMR Spectrum of Compound 2b in DMSO-*d*$_6$ at 75 MHz

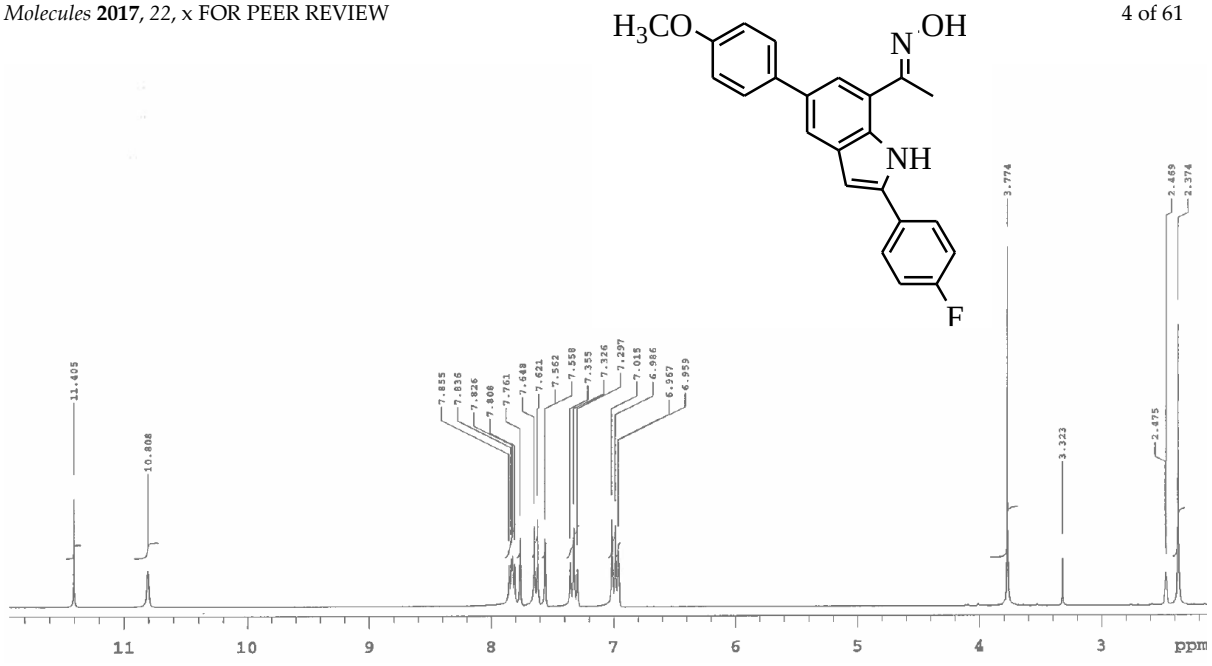


Figure S5. ^{1}**H NMR Spectrum of Compound 2c in DMSO-***d*$_6$ **at 300 MHz**

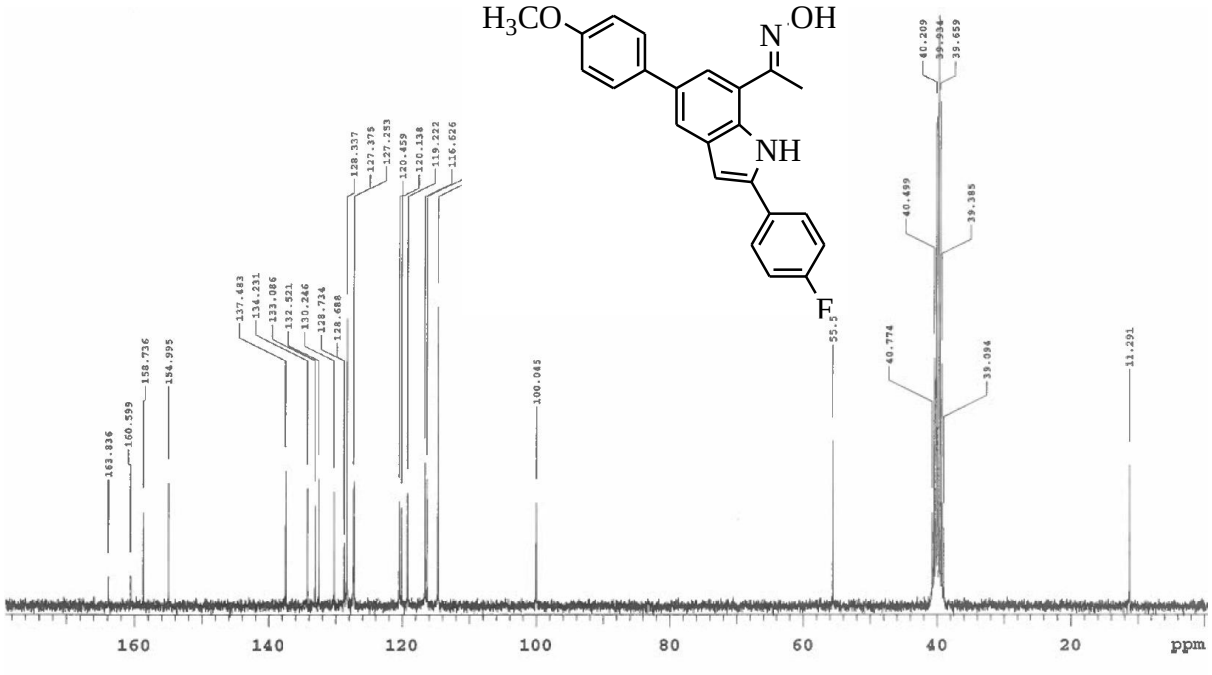


Figure S6. ^{13}**C NMR Spectrum of Compound 2c in DMSO-***d*$_6$ **at 75 MHz**

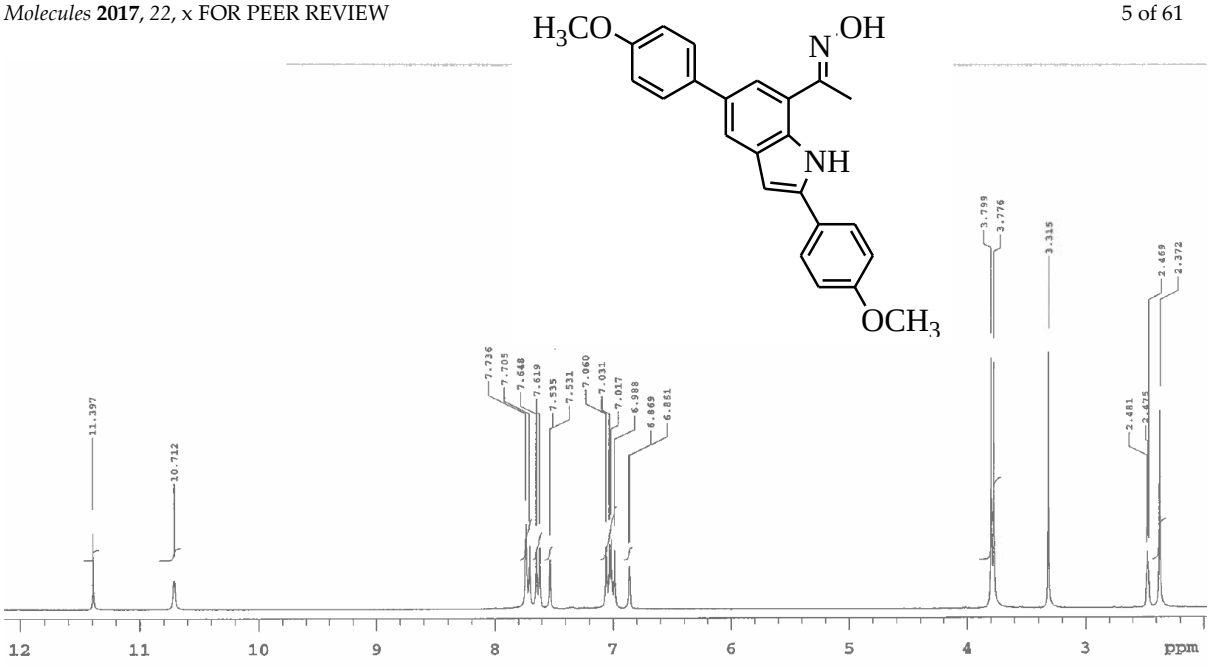


Figure S7. ^{1}H NMR Spectrum of Compound 2d in DMSO-*d*$_6$ at 300 MHz

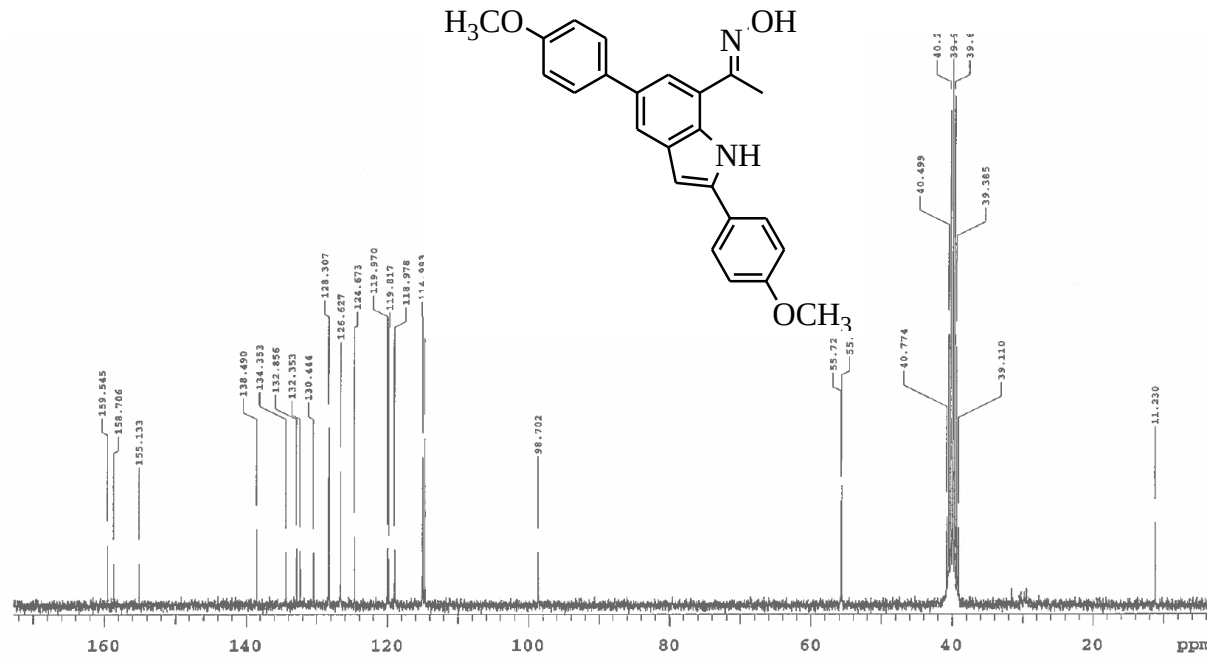


Figure S8. ^{13}C NMR Spectrum of Compound 2d in DMSO-*d*$_6$ at 75 MHz

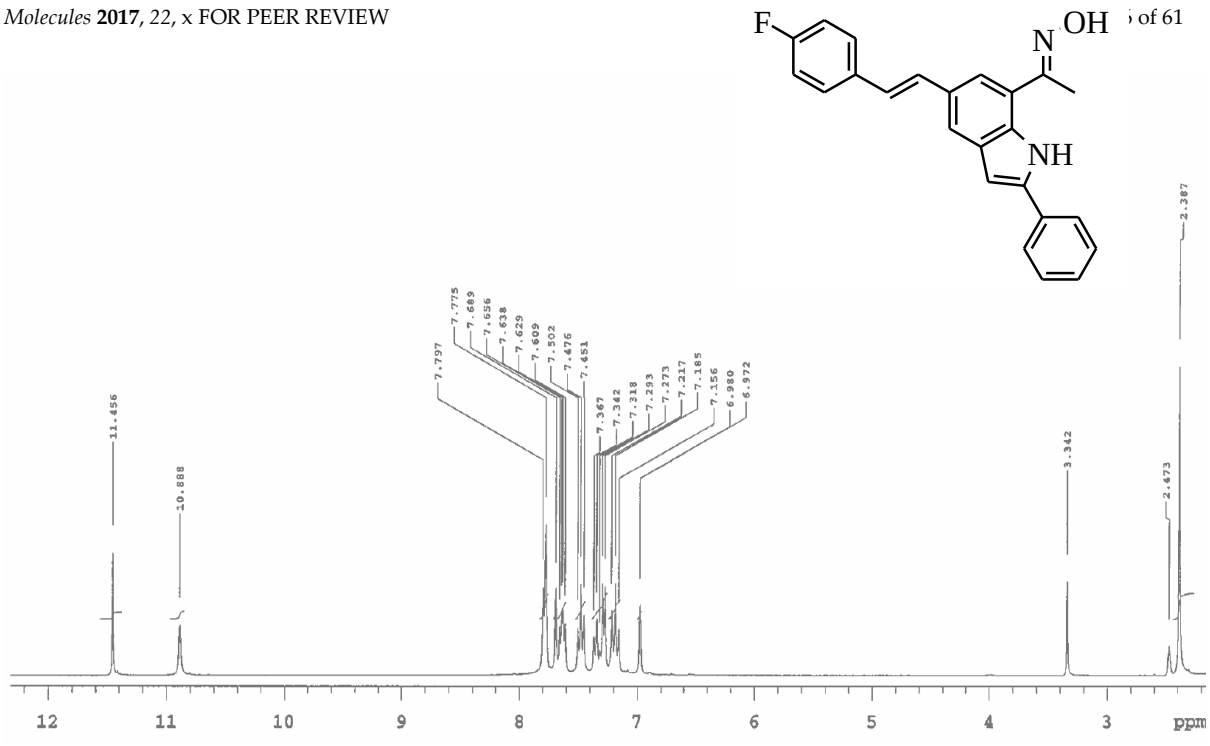


Figure S9. ^{1}H NMR Spectrum of Compound 2e in DMSO-*d*$_6$ at 300 MHz

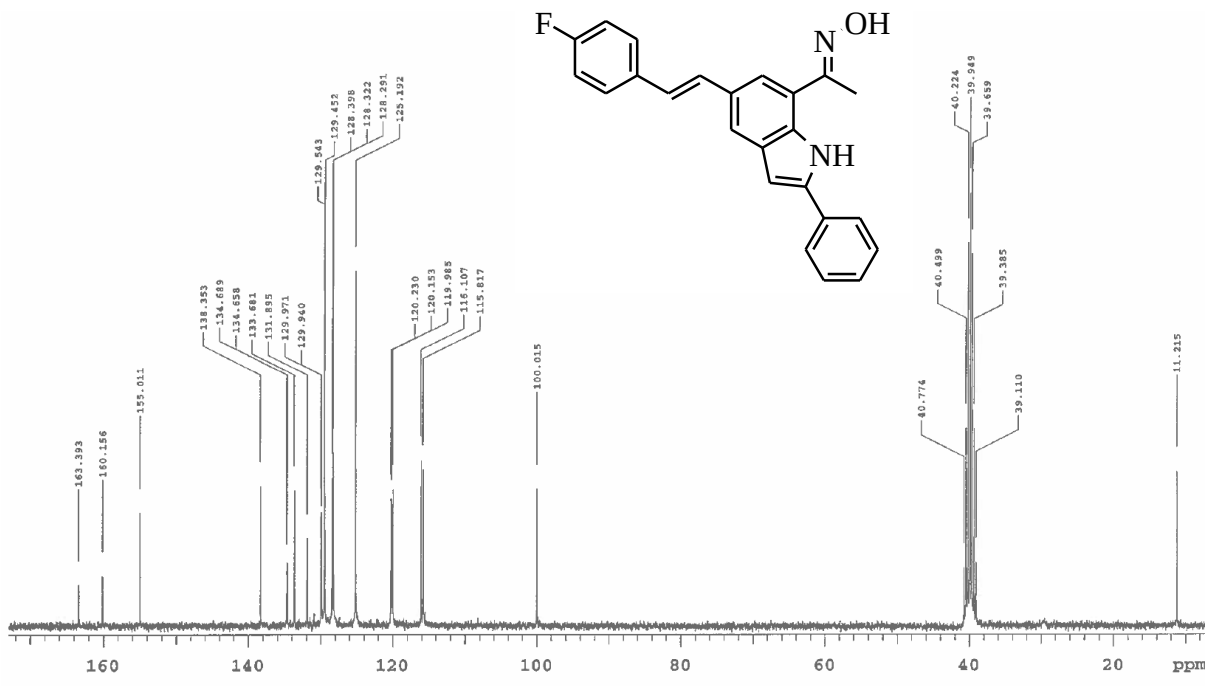


Figure S10. ^{13}C NMR Spectrum of Compound 2e in DMSO-*d*$_6$ at 75 MHz

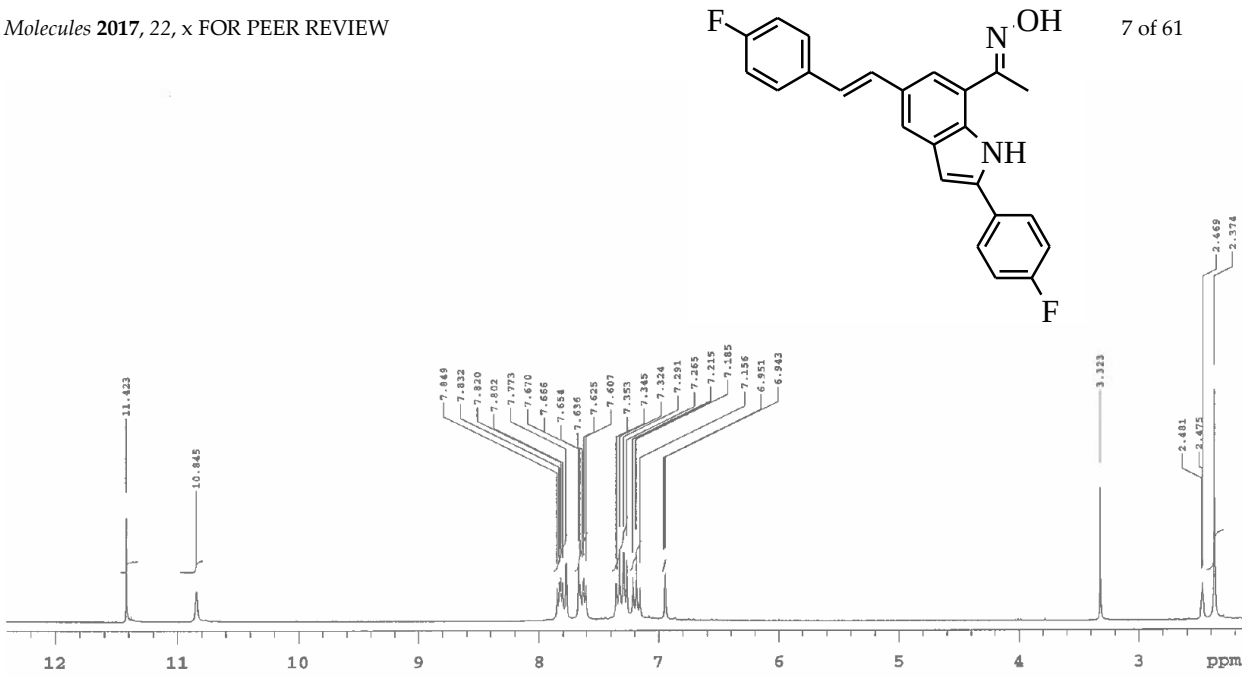


Figure S11. ^{1}H NMR Spectrum of Compound 2f in DMSO-*d*$_6$ at 300 MHz

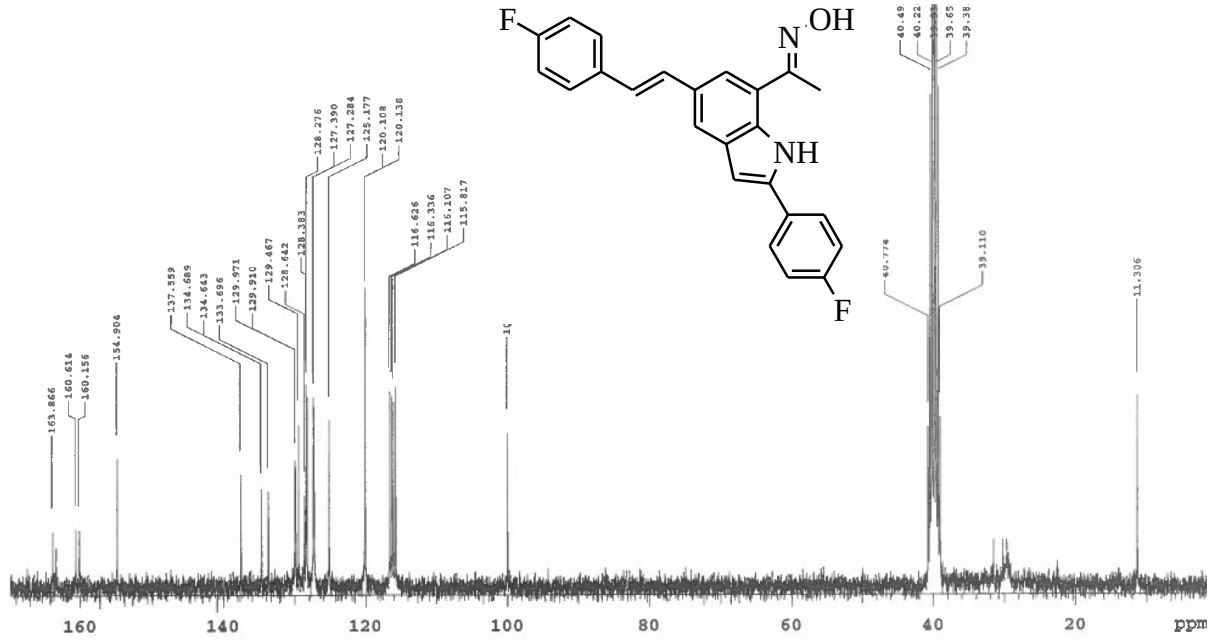


Figure S12. ^{13}C NMR Spectrum of Compound 2f in DMSO-*d*$_6$ at 75 MHz

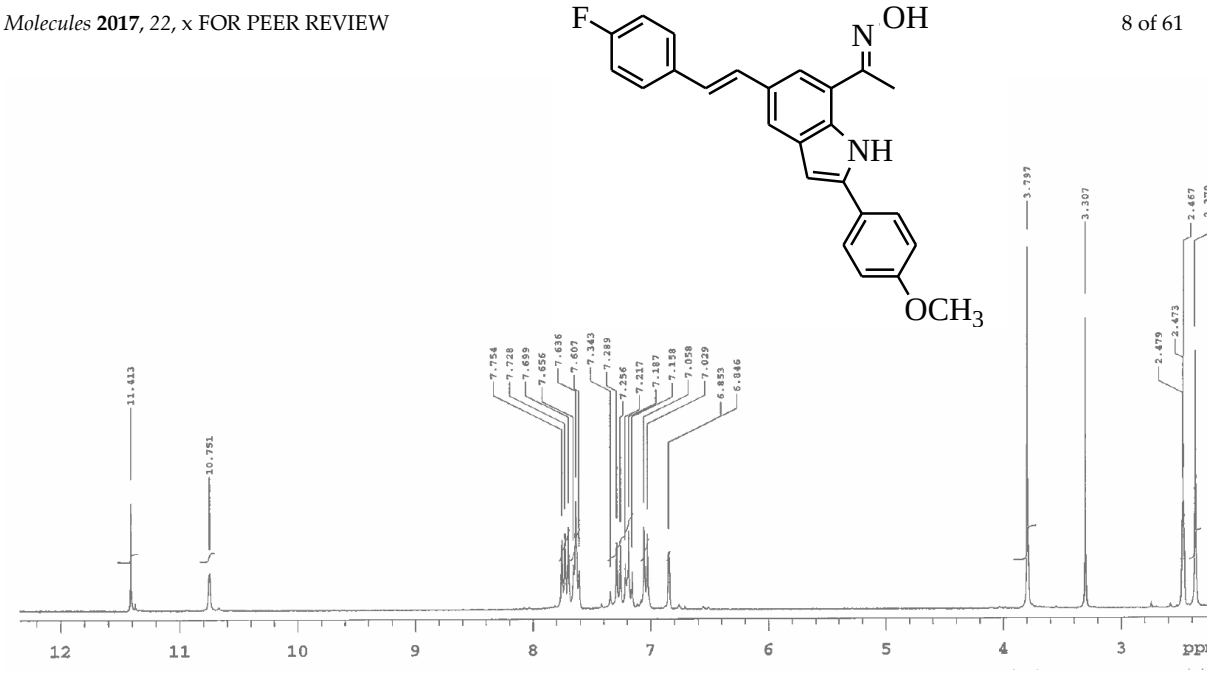


Figure S13. ^{1}**H NMR Spectrum of Compound 2g in DMSO-*d*$_6$ at 300 MHz**

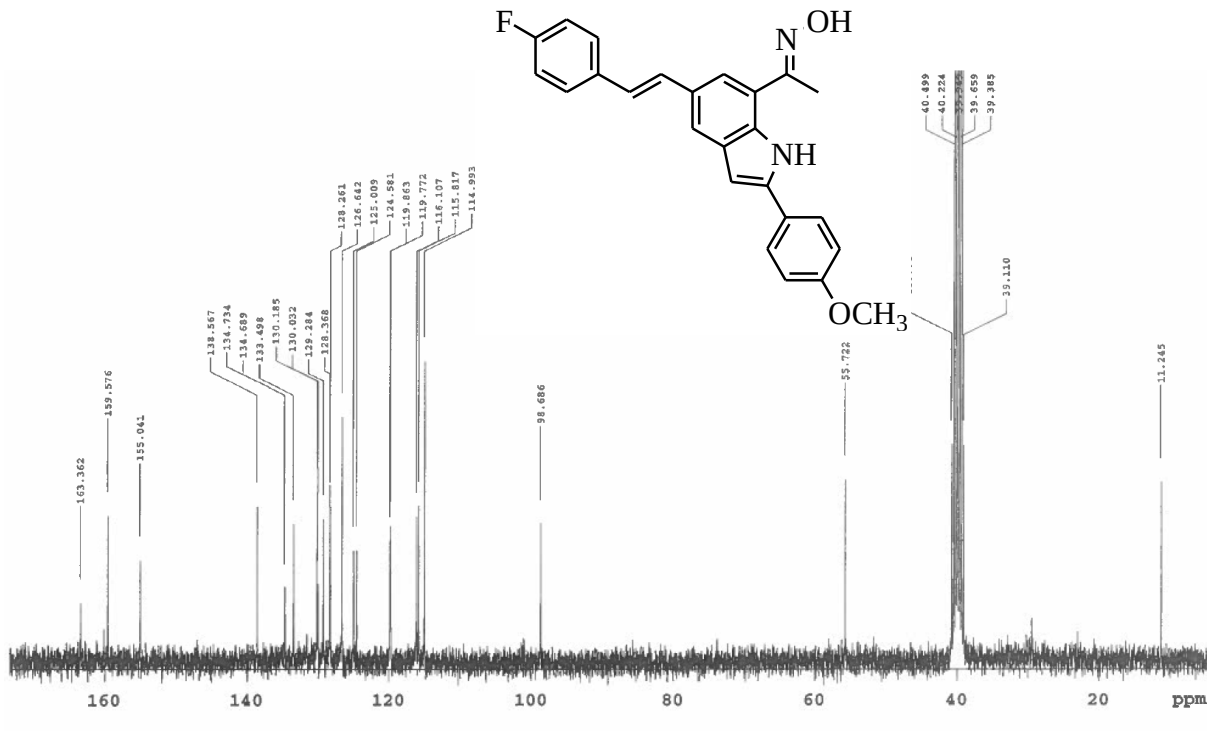


Figure S14. ^{13}**C NMR Spectrum of Compound 2g in DMSO-*d*$_6$ at 75 MHz**

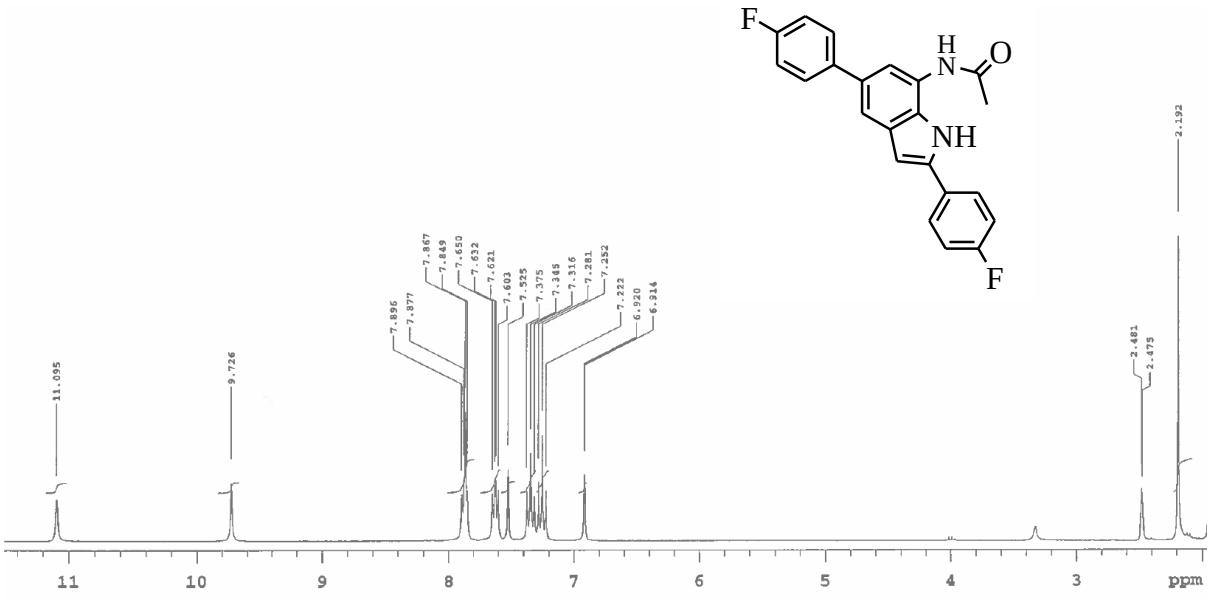


Figure S15. ^{1}H NMR Spectrum of Compound 3a in DMSO-*d*$_6$ at 300 MHz

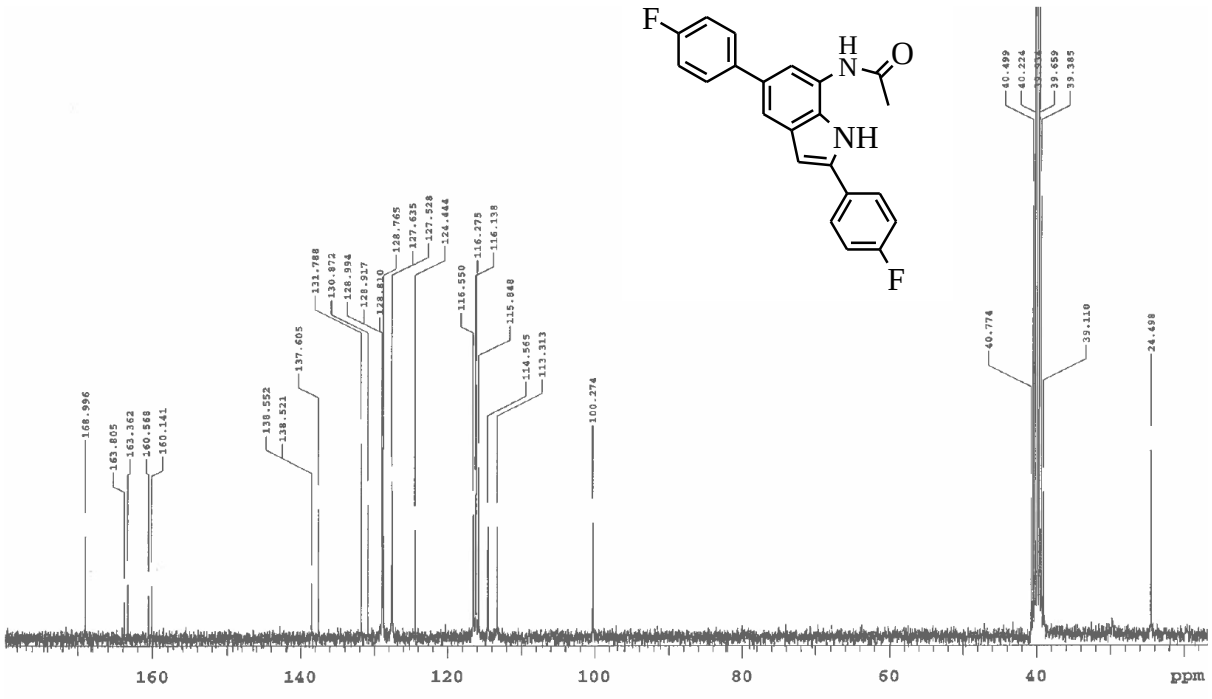


Figure S16. ^{13}C NMR Spectrum of Compound 3a in DMSO-*d*$_6$ at 75 MHz

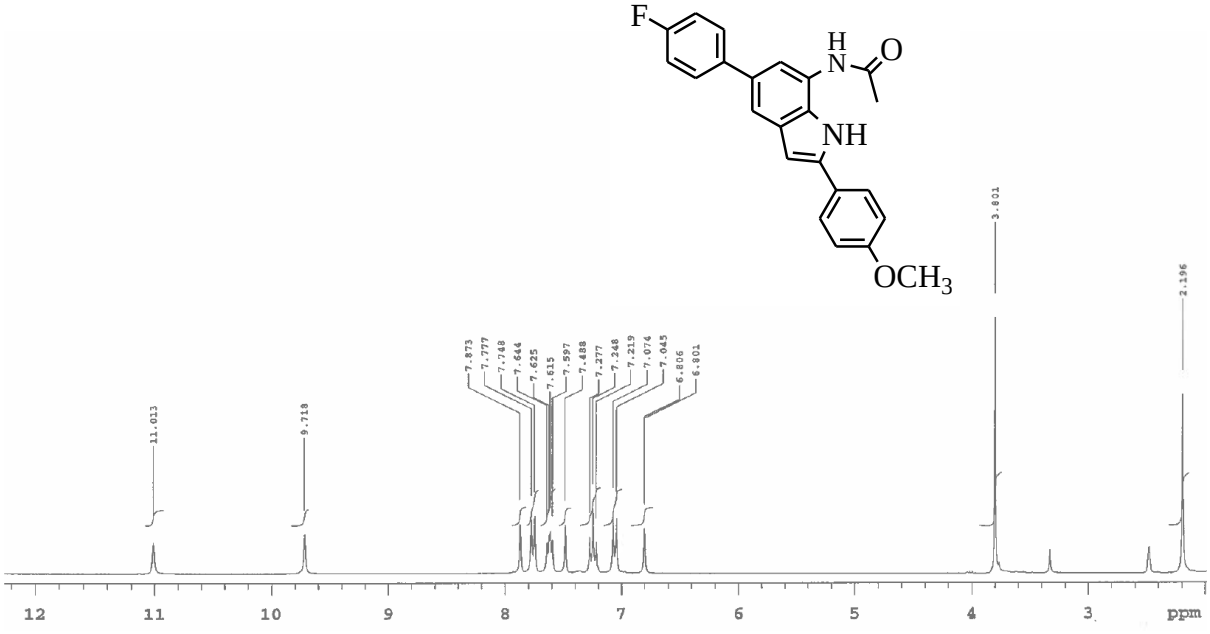


Figure S17. ^{1}**H NMR Spectrum of Compound 3b in DMSO-***d*$_6$ **at 300 MHz**

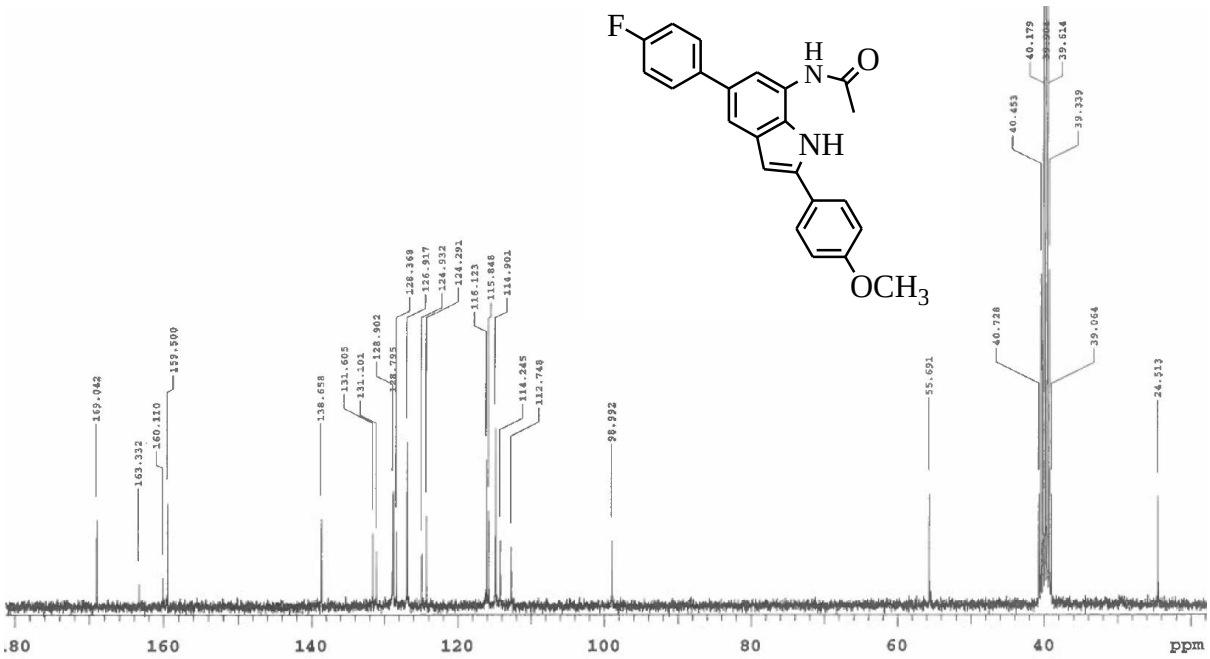


Figure S18. ^{13}**C NMR Spectrum of Compound 3b in DMSO-***d*$_6$ **at 75 MHz**

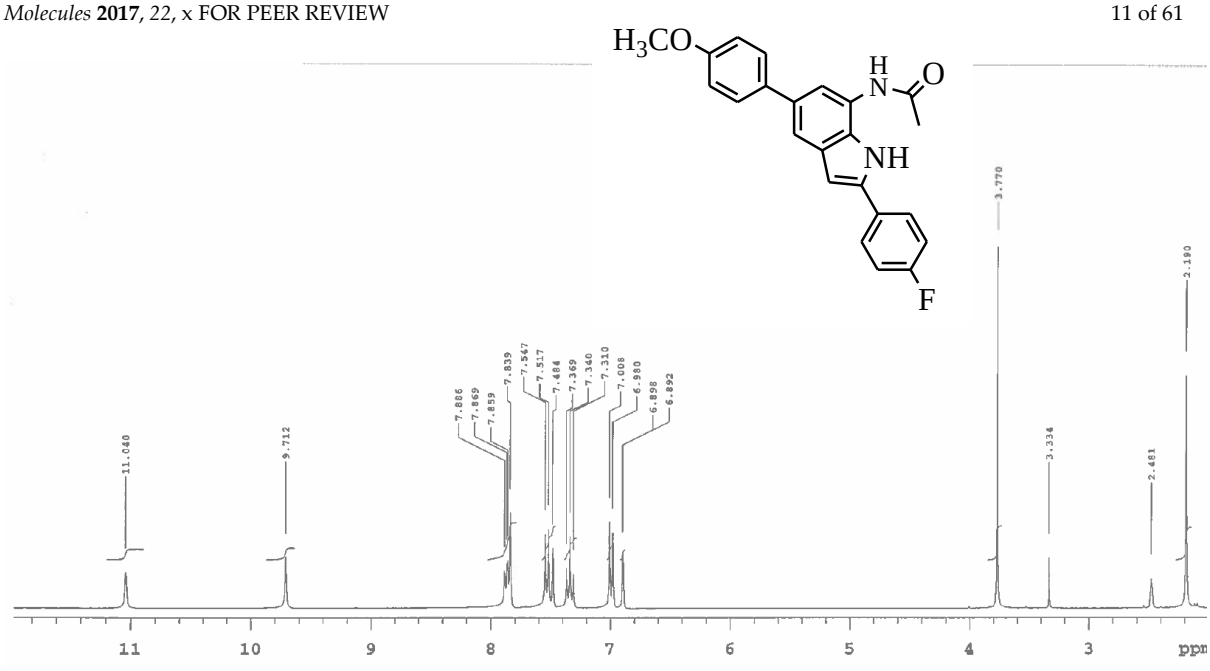


Figure S19. ^{1}H NMR Spectrum of Compound 3c in DMSO-*d*$_6$ at 300 MHz

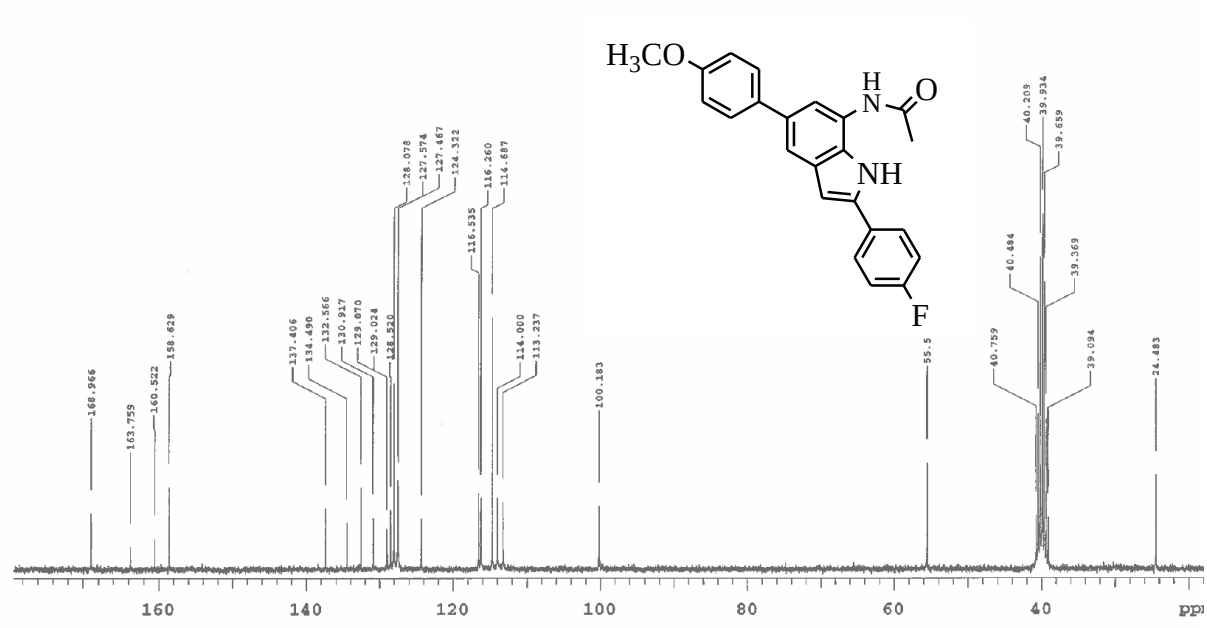


Figure S20. ^{13}C NMR Spectrum of Compound 3c in DMSO-*d*$_6$ at 75 MHz

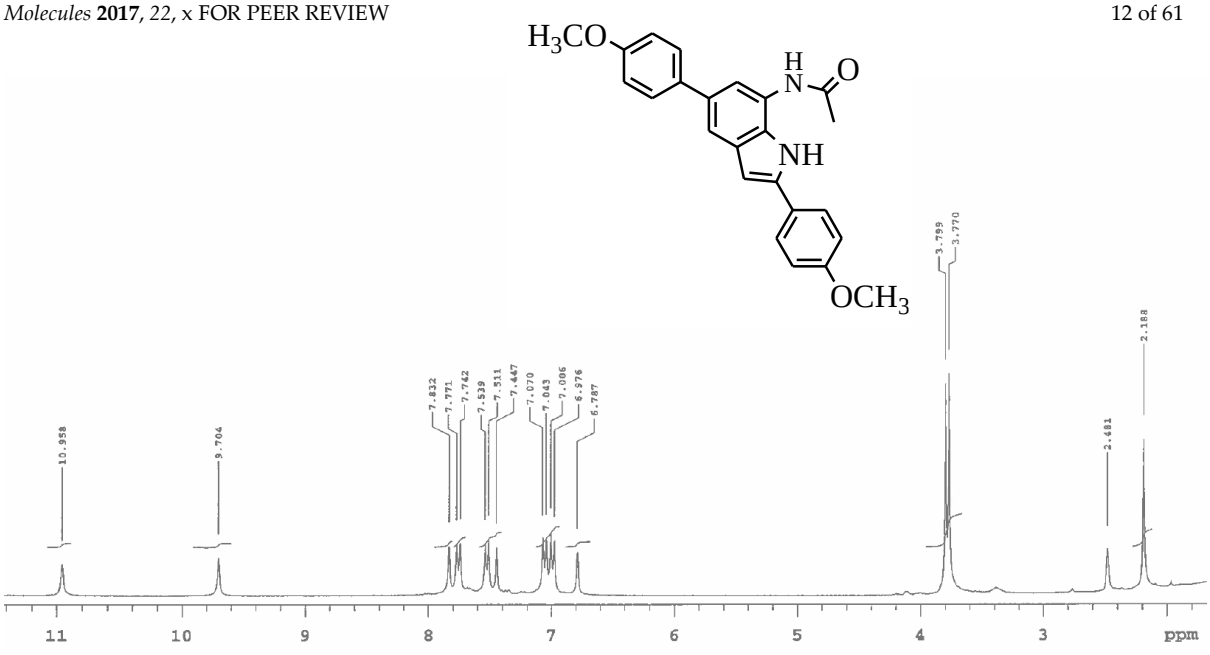


Figure S21. ^{1}H NMR Spectrum of Compound 3d in DMSO-*d*$_6$ at 300 MHz

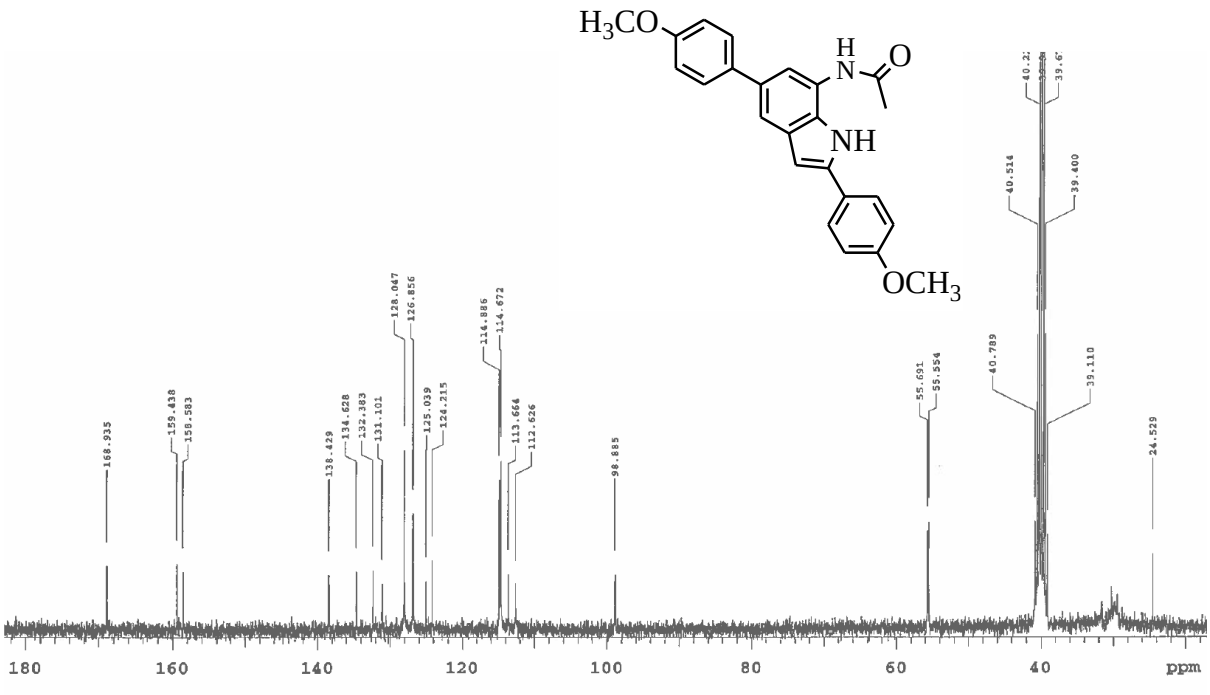


Figure S22. ^{13}C NMR Spectrum of Compound 3d in DMSO-*d*$_6$ at 75 MHz

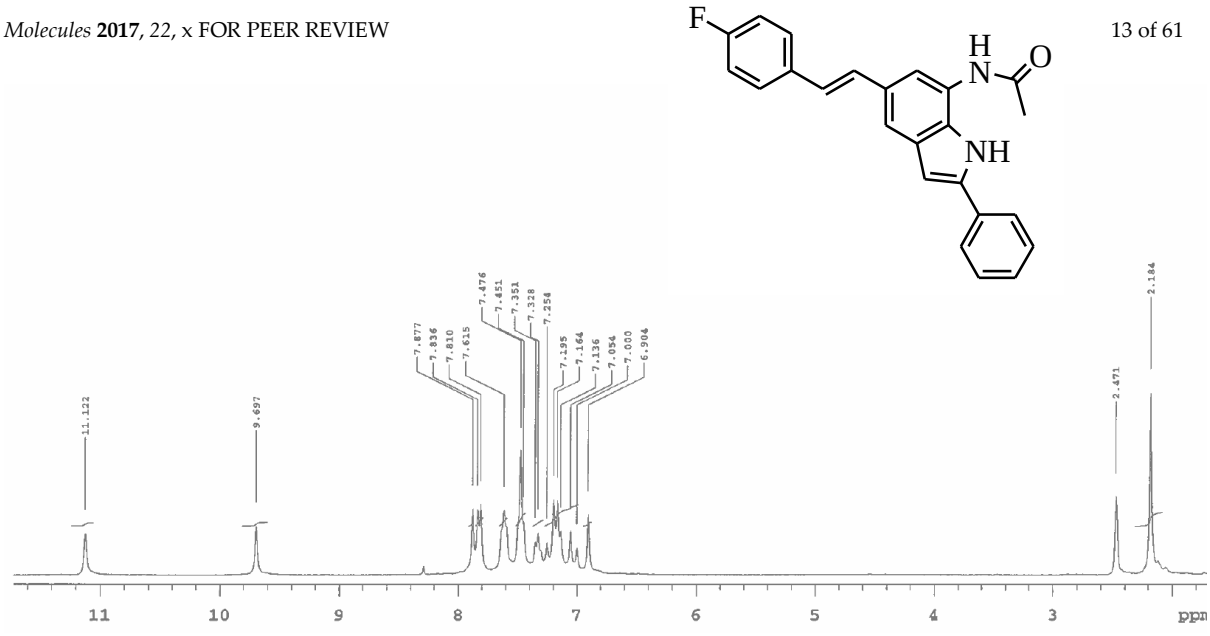


Figure S23. ^{1}**H NMR Spectrum of Compound 3e in DMSO-*d*$_6$ at 300 MHz**

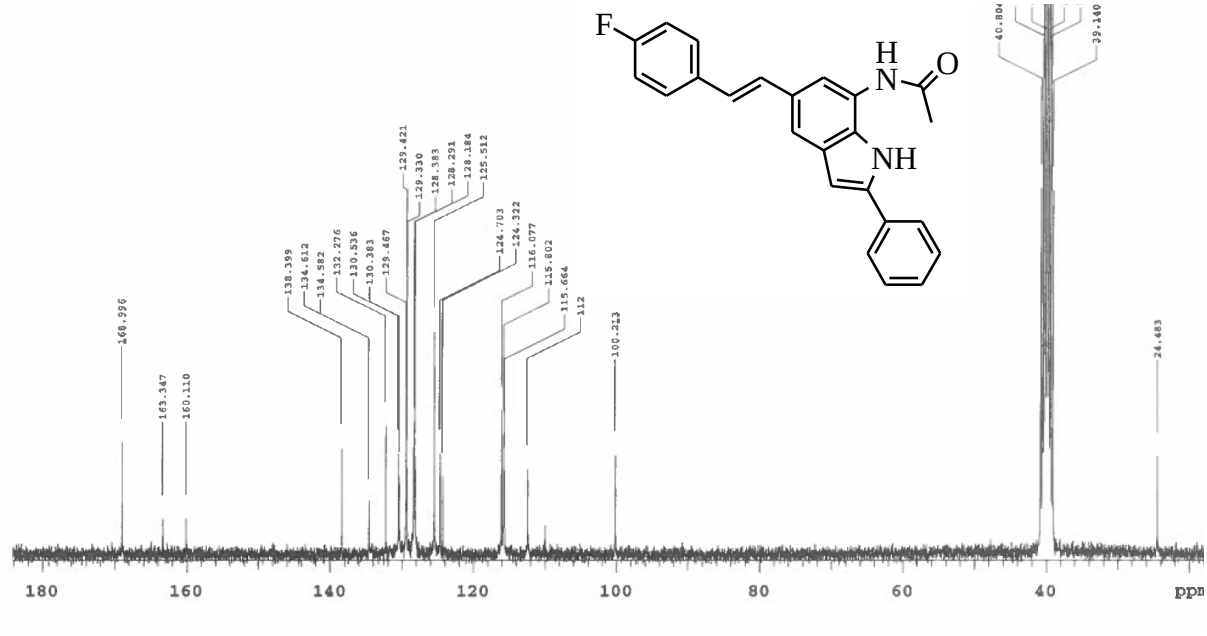


Figure S24. ^{13}**C NMR Spectrum of Compound 3e in DMSO-*d*$_6$ at 75 MHz**

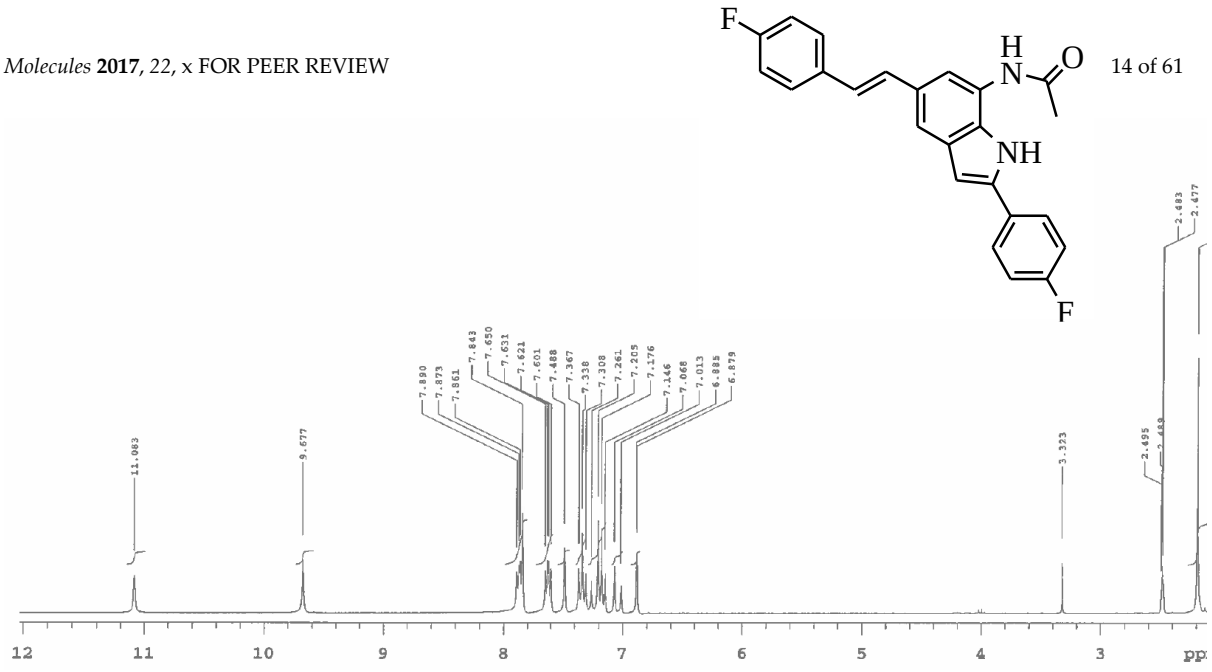


Figure S25. ^{1}H NMR Spectrum of Compound 3f in DMSO-*d*$_6$ at 300 MHz

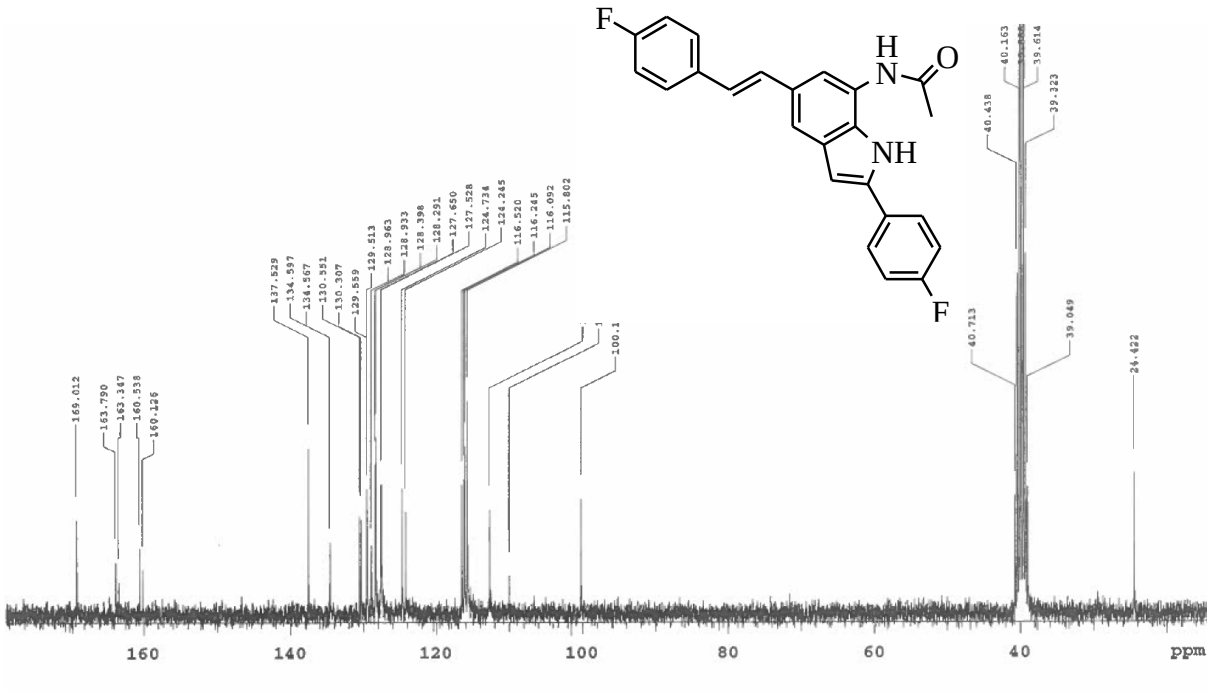


Figure S26. ^{13}C NMR Spectrum of Compound 3f in DMSO-*d*$_6$ at 75 MHz

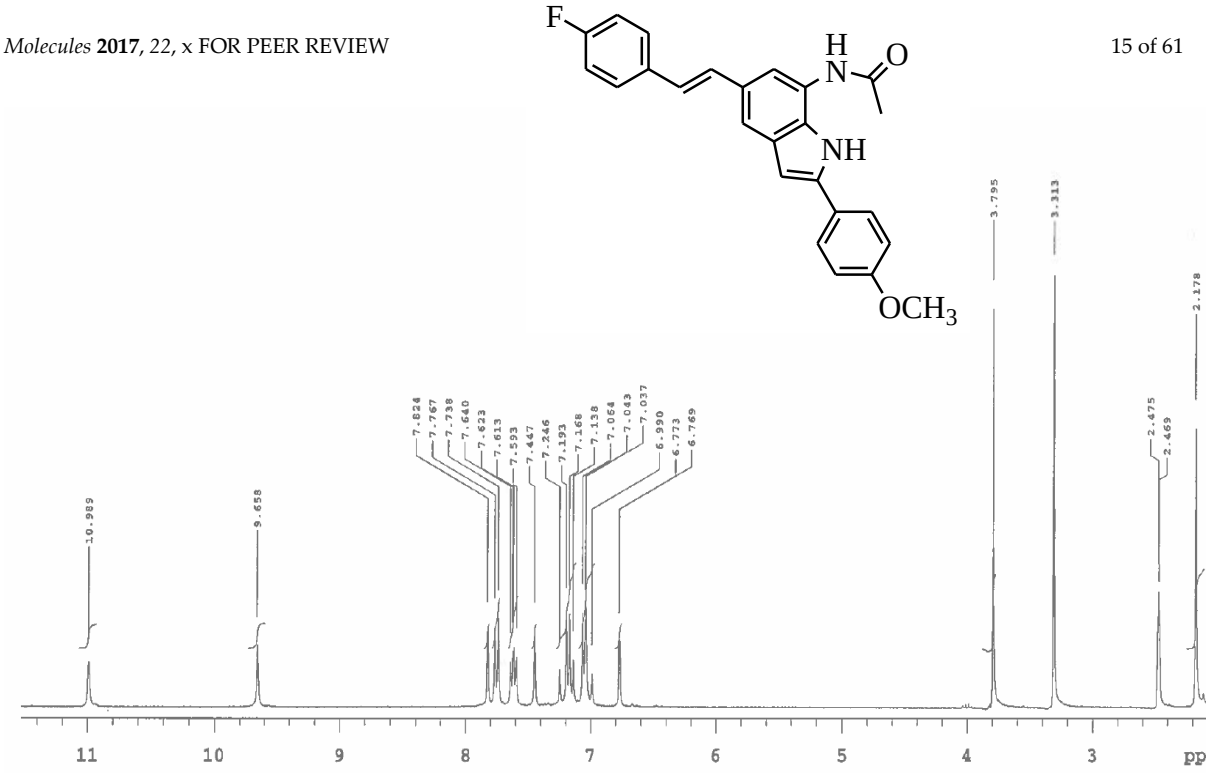


Figure S27. ^{1}H NMR Spectrum of Compound 3g in DMSO-*d*$_6$ at 300 MHz

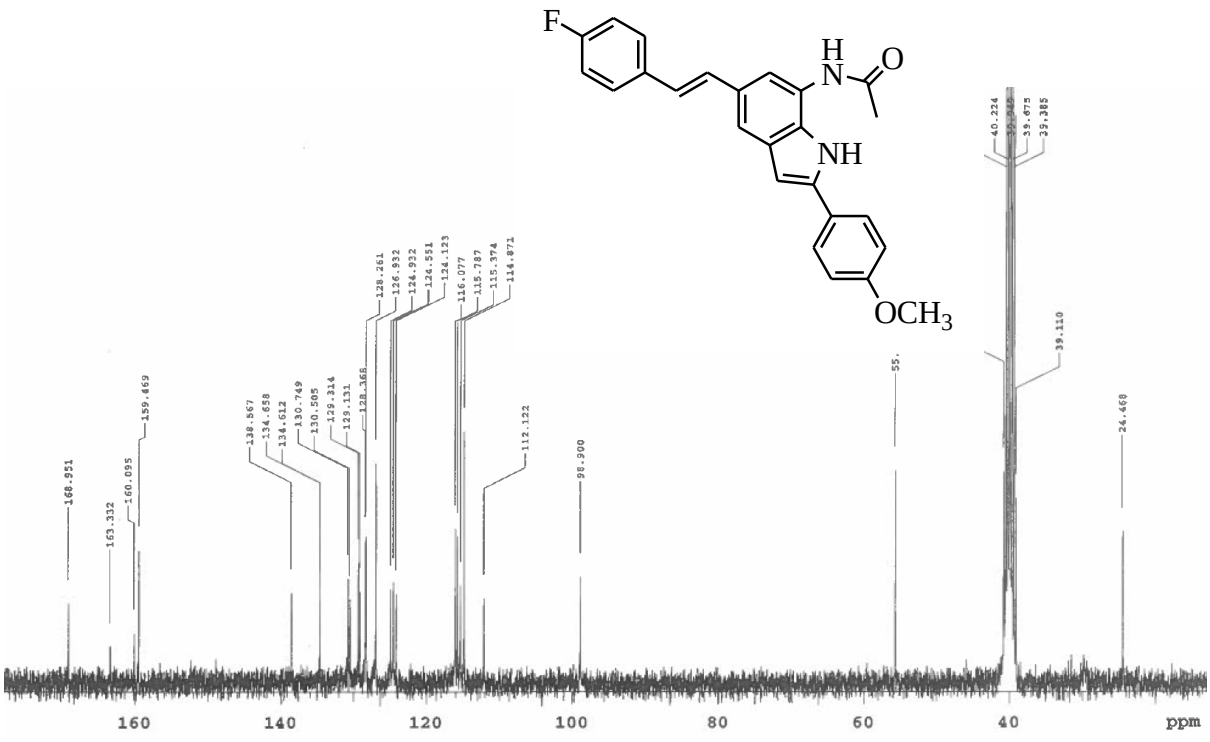


Figure S28. ^{13}C NMR Spectrum of Compound 3g in DMSO-*d*$_6$ at 75 MHz

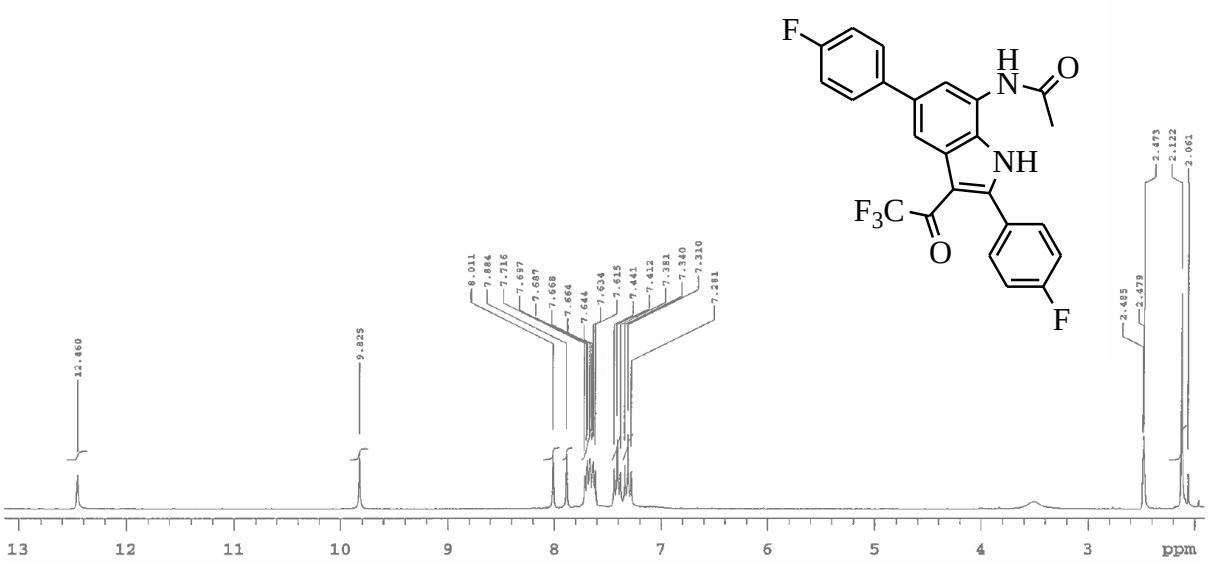


Figure S29. ^{1}H NMR Spectrum of Compound 4a in DMSO-*d*$_6$ at 300 MHz

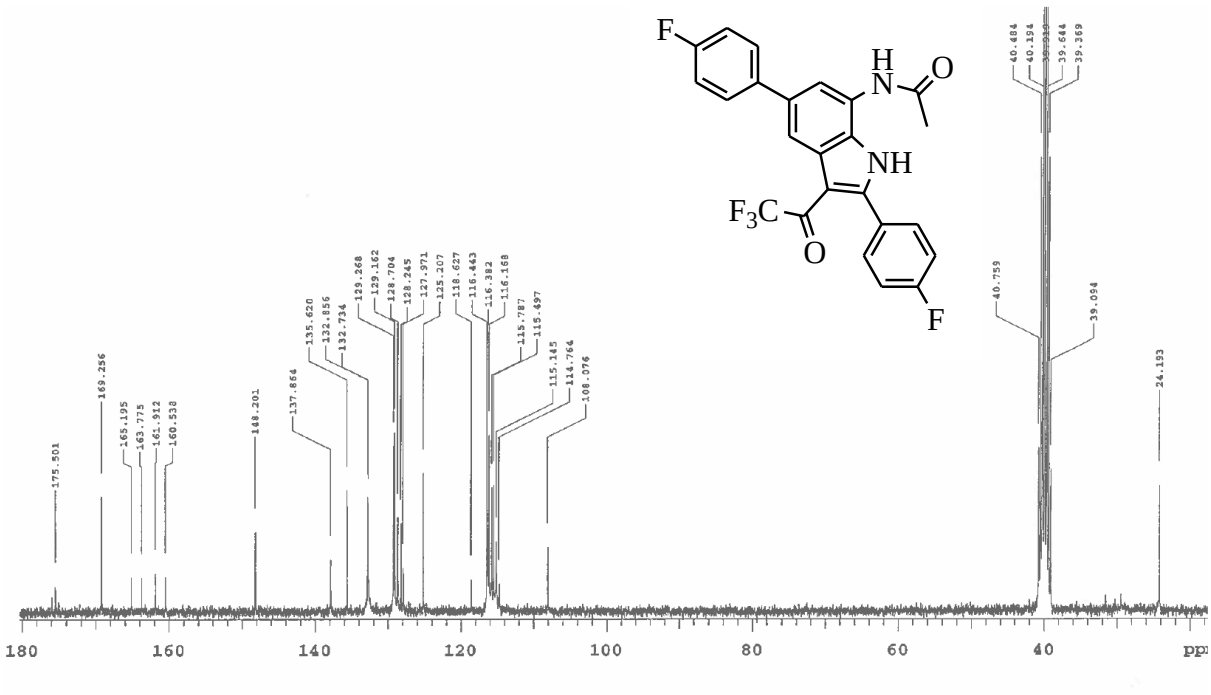


Figure S30. ^{13}C NMR Spectrum of Compound 4a in DMSO-*d*$_6$ at 75 MHz

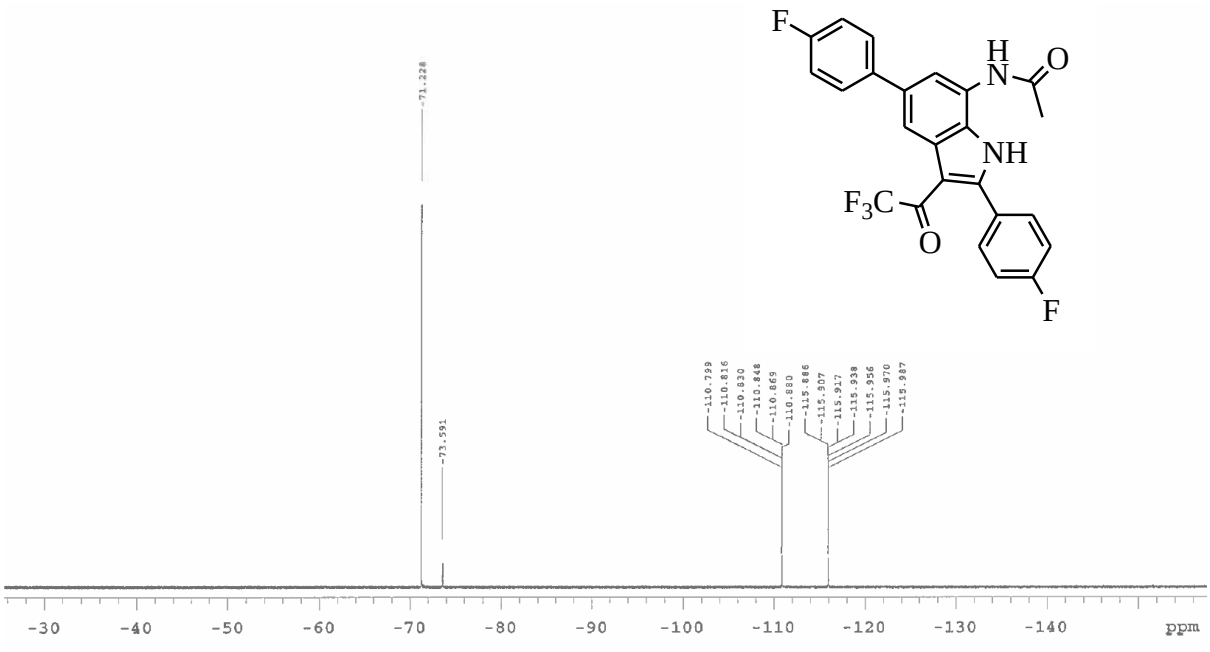


Figure S31. ^{19}F NMR Spectrum of Compound 4a in DMSO-*d*$_6$ at 282 MHz

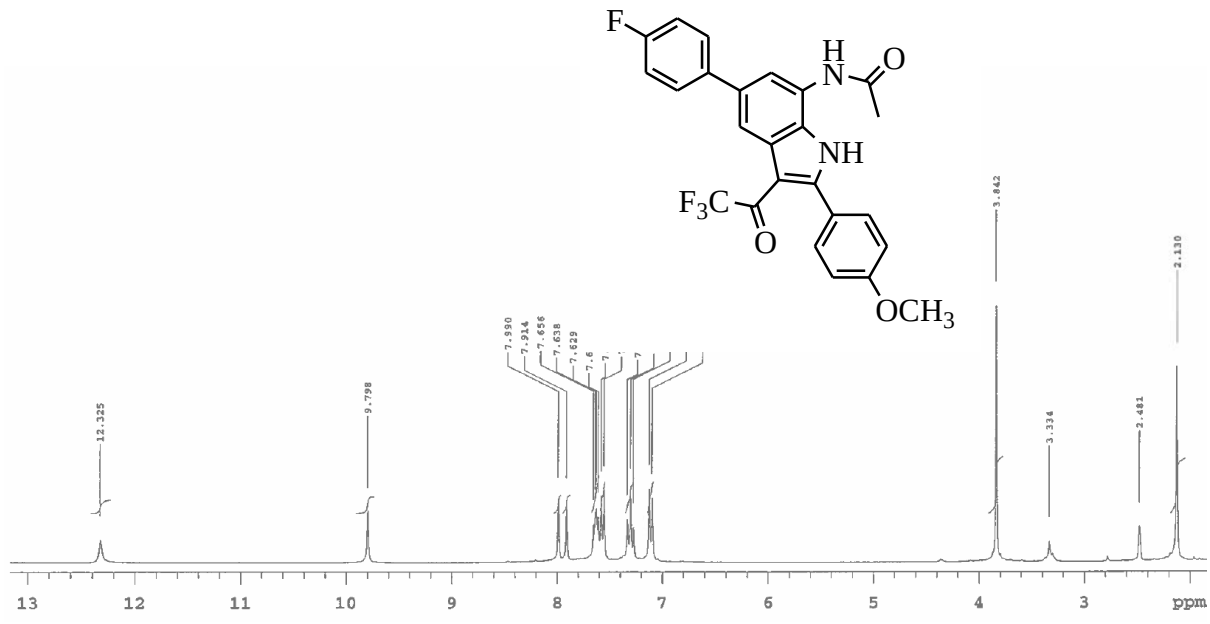
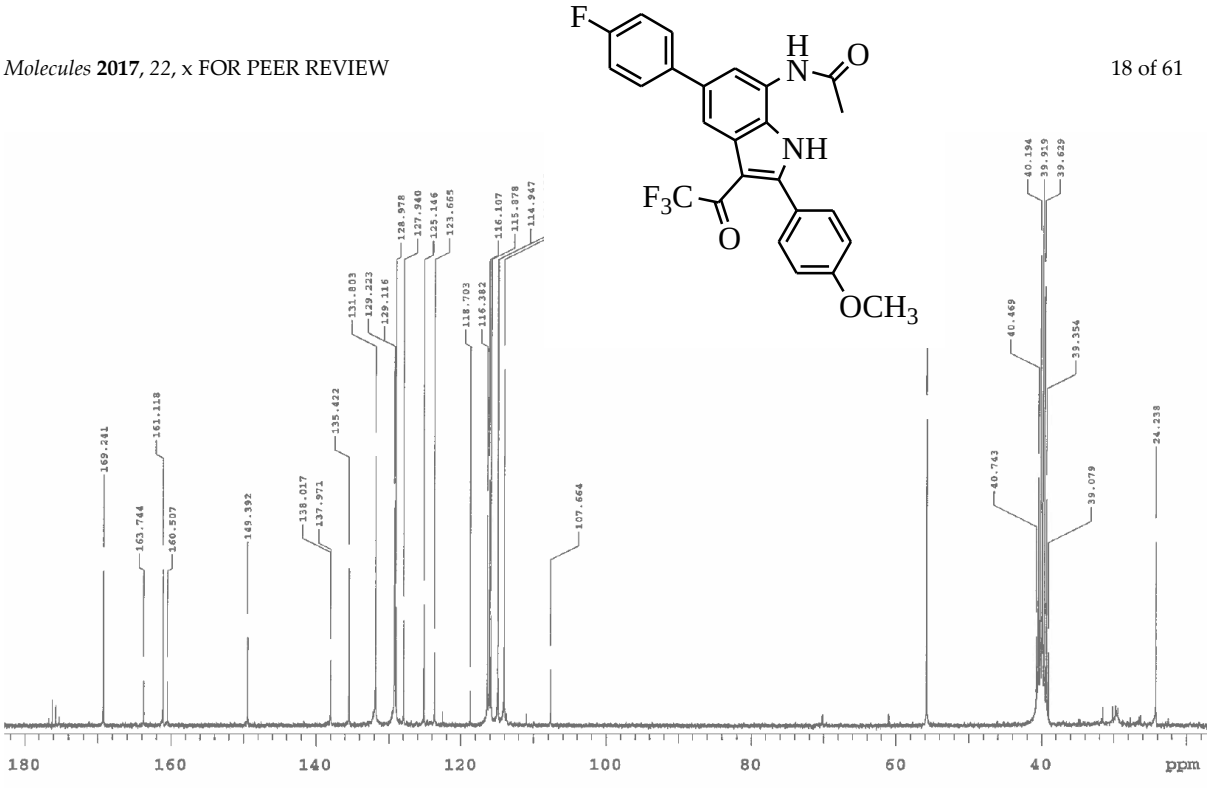


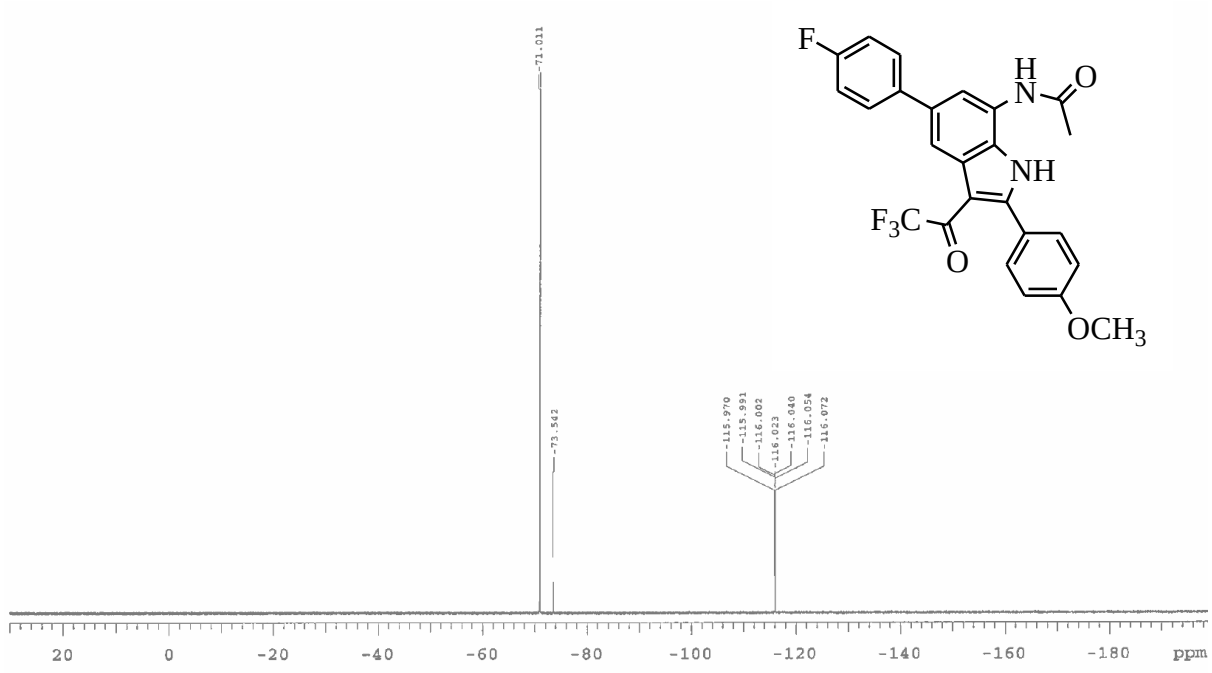
Figure S32. ^{1}H NMR Spectrum of Compound 4b in DMSO-*d*$_6$ at 300 MHz



135

136 **Figure S33. ^{13}C NMR Spectrum of Compound 4b in DMSO-*d*$_6$ at 75 MHz**

137



138

139 **Figure S34. ^{19}F NMR Spectrum of Compound 4b in DMSO-*d*$_6$ at 282 MHz**

140

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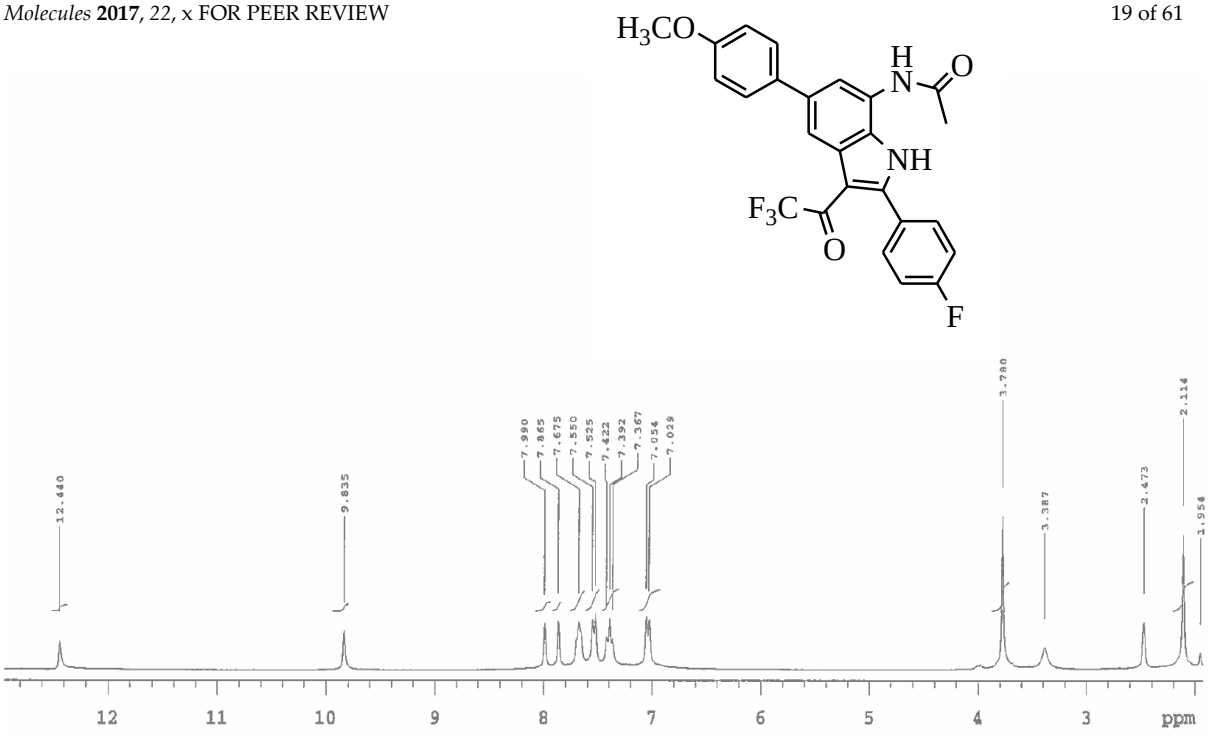


Figure S35. ^{1}H NMR Spectrum of Compound 4c in DMSO-*d*$_6$ at 300 MHz

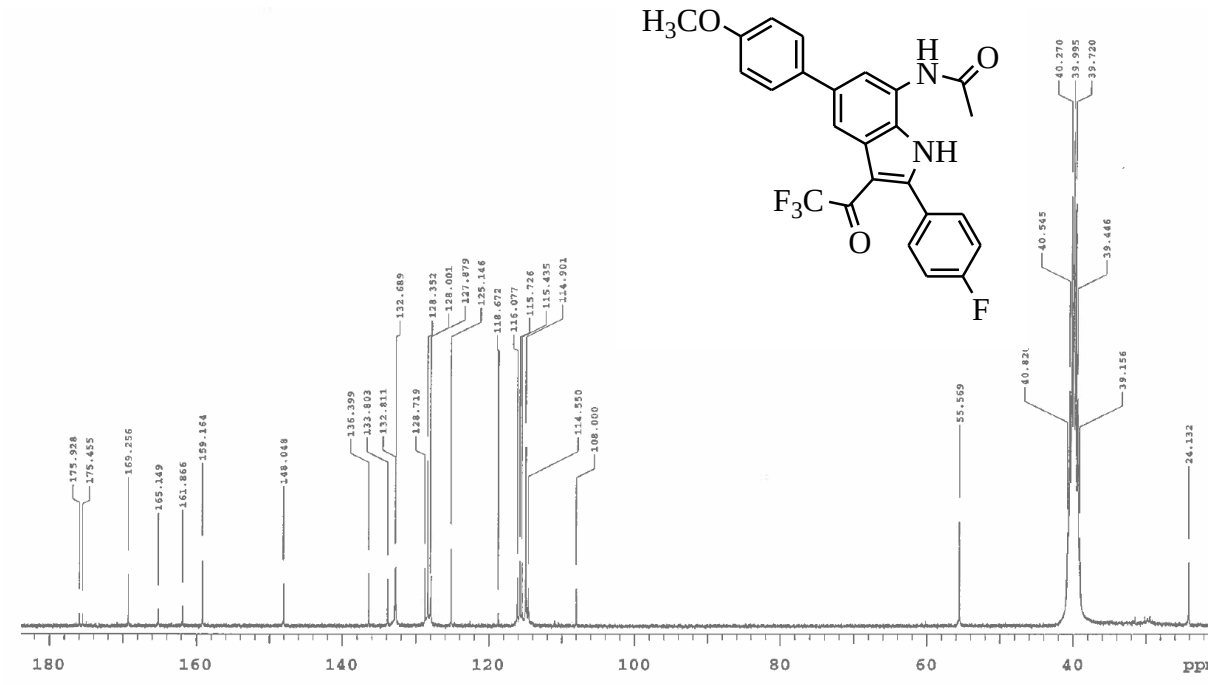


Figure S36. ^{13}C NMR Spectrum of Compound 4c in DMSO-*d*$_6$ at 75 MHz

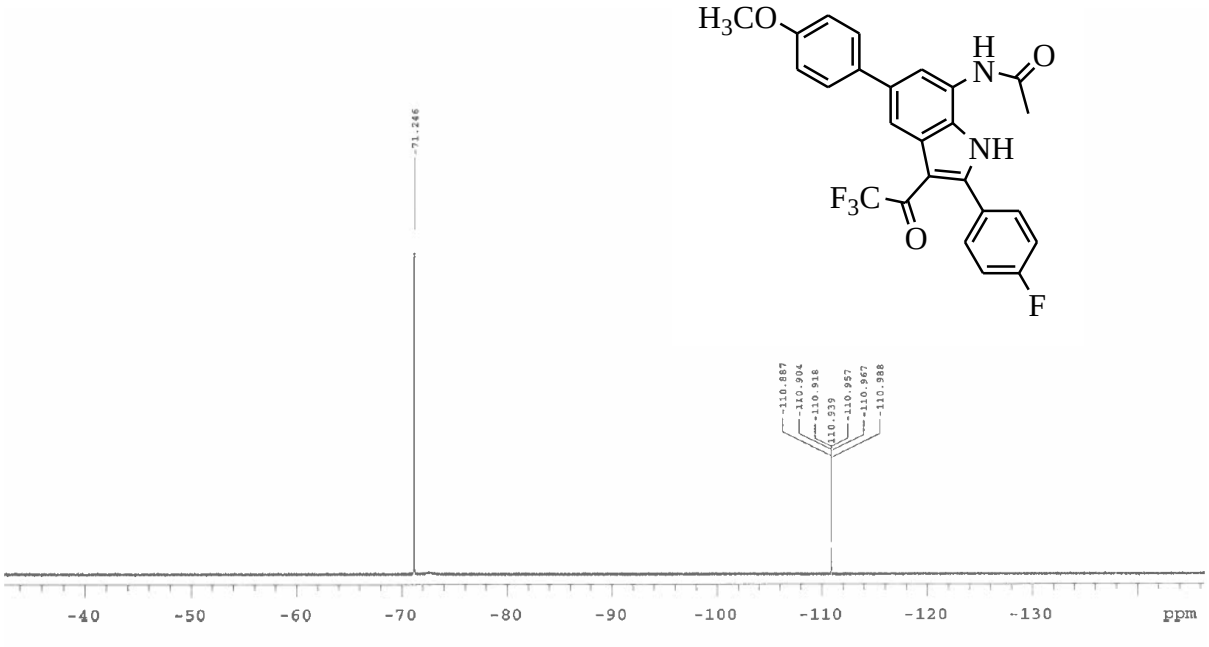


Figure S37. ^{19}F NMR Spectrum of Compound 4c in DMSO-*d*$_6$ at 282 MHz

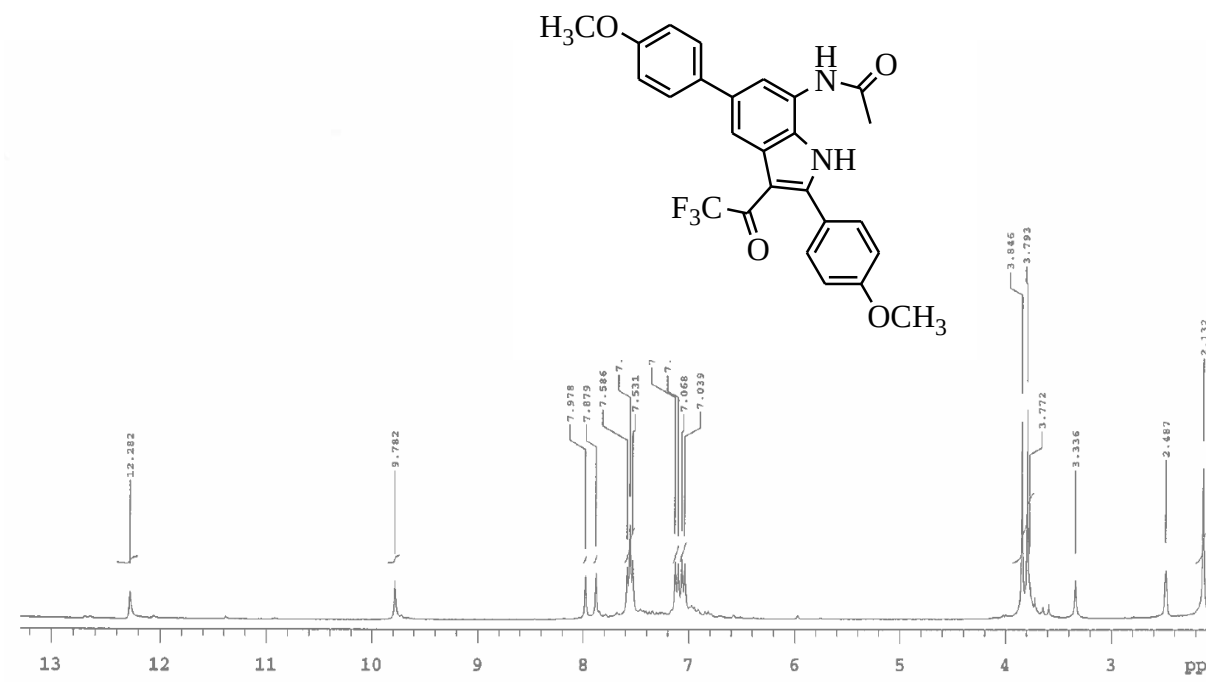


Figure S38. ^{1}H NMR Spectrum of Compound 4d in DMSO-*d*$_6$ at 300 MHz

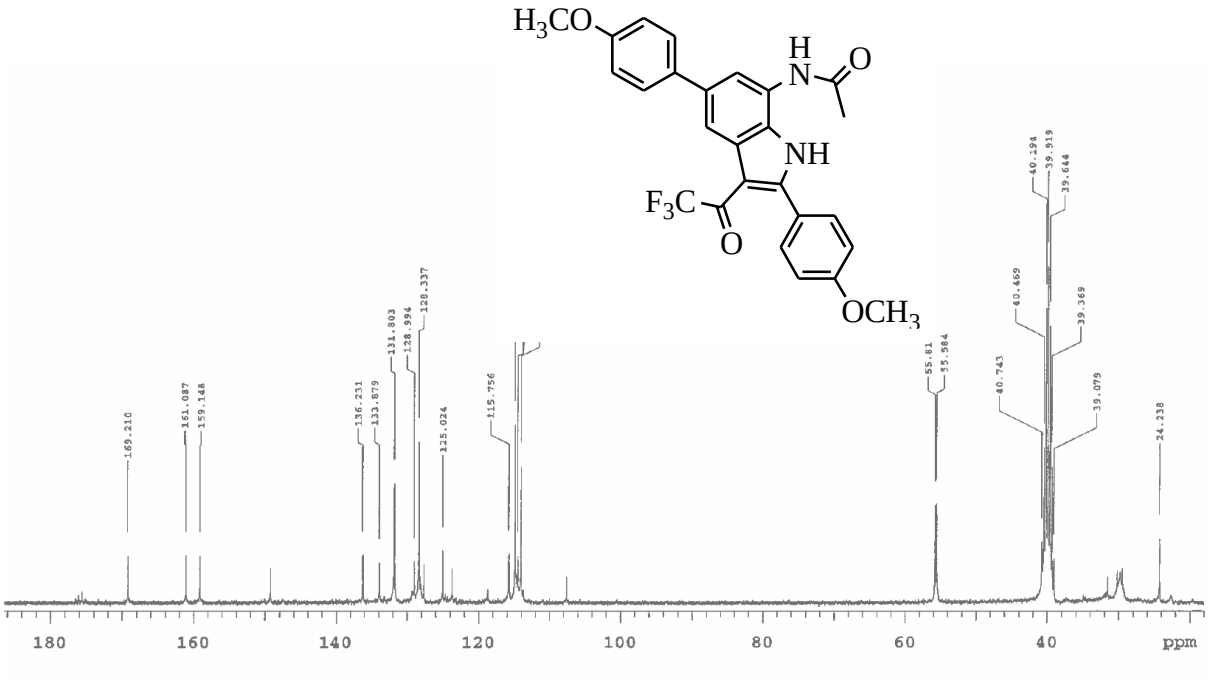


Figure S39. ^{13}C NMR Spectrum of Compound 4d in DMSO-*d*$_6$ at 75 MHz

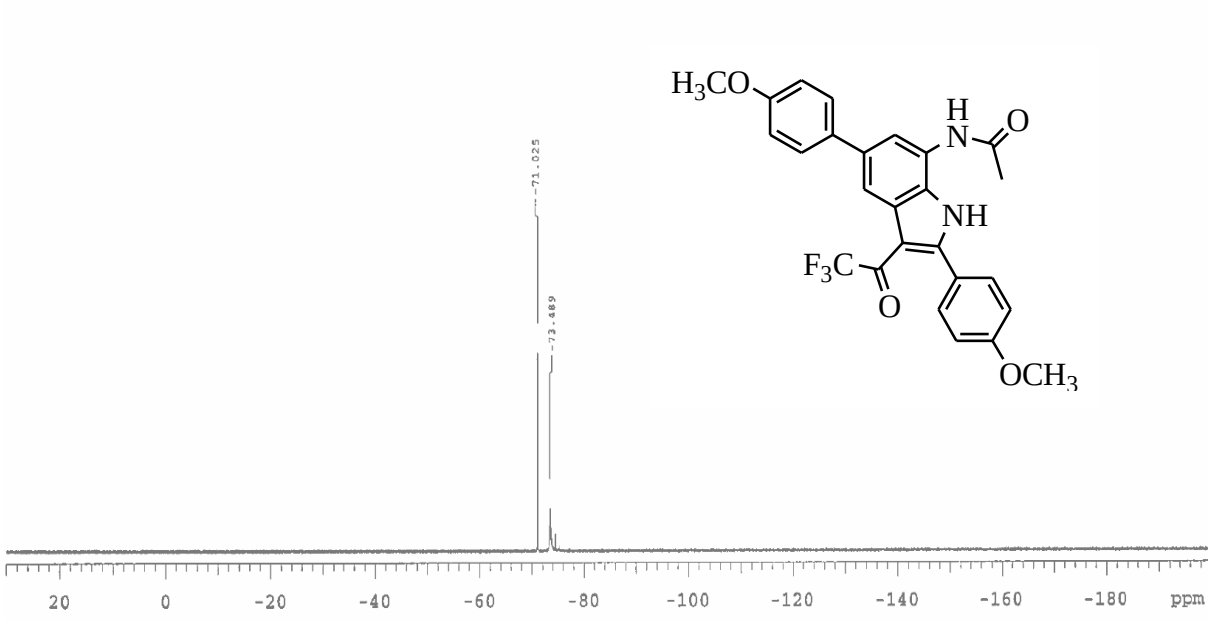


Figure S40. ^{19}F NMR Spectrum of Compound 4d in DMSO-*d*$_6$ at 282 MHz

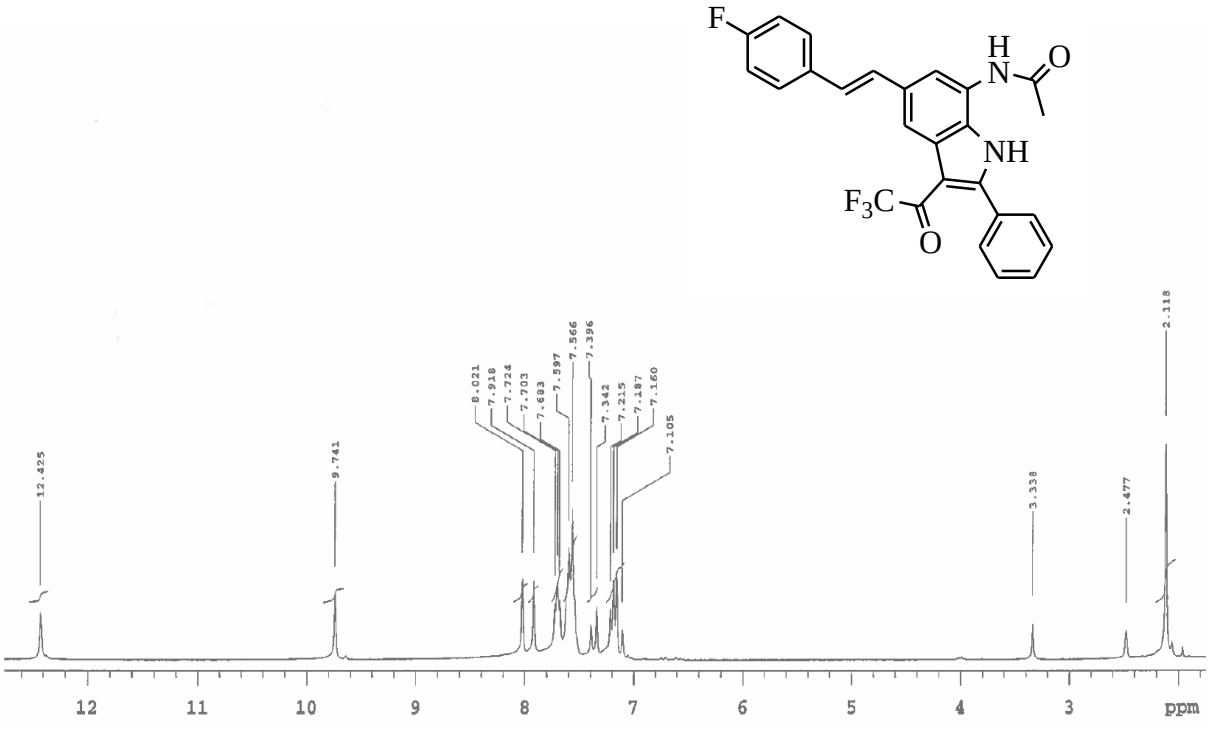


Figure S41. ^{1}H NMR Spectrum of Compound 4e in DMSO-*d*$_6$ at 300 MHz

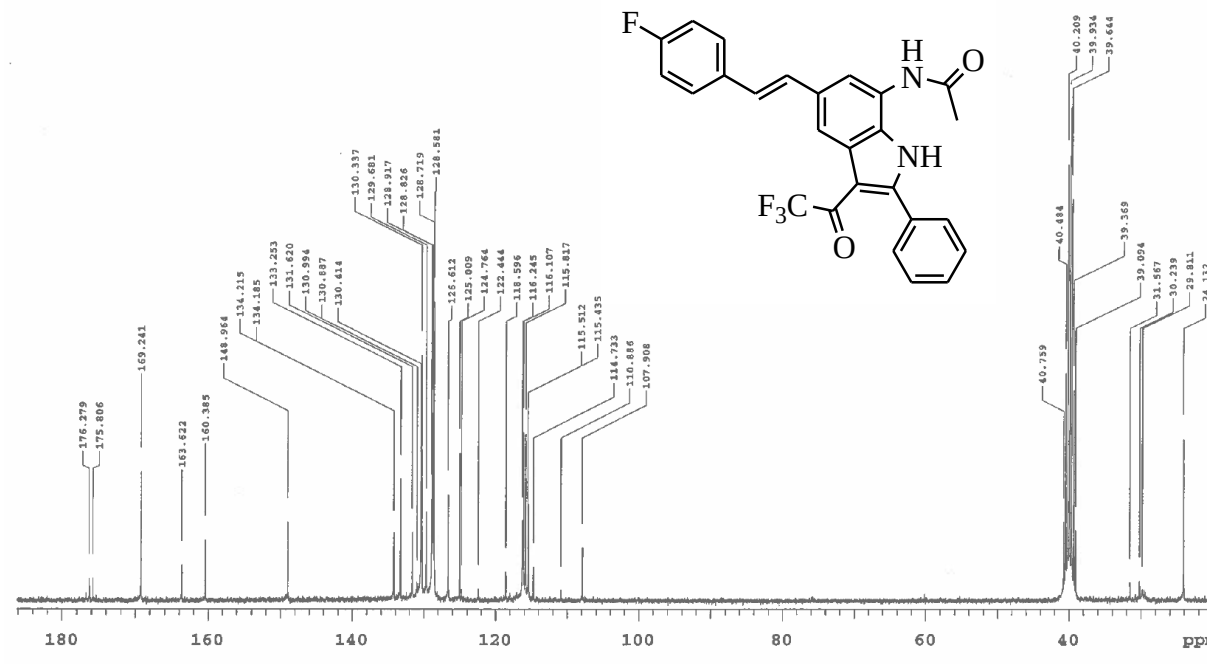


Figure S42. ^{13}C NMR Spectrum of Compound 4e in DMSO-*d*$_6$ at 75 MHz

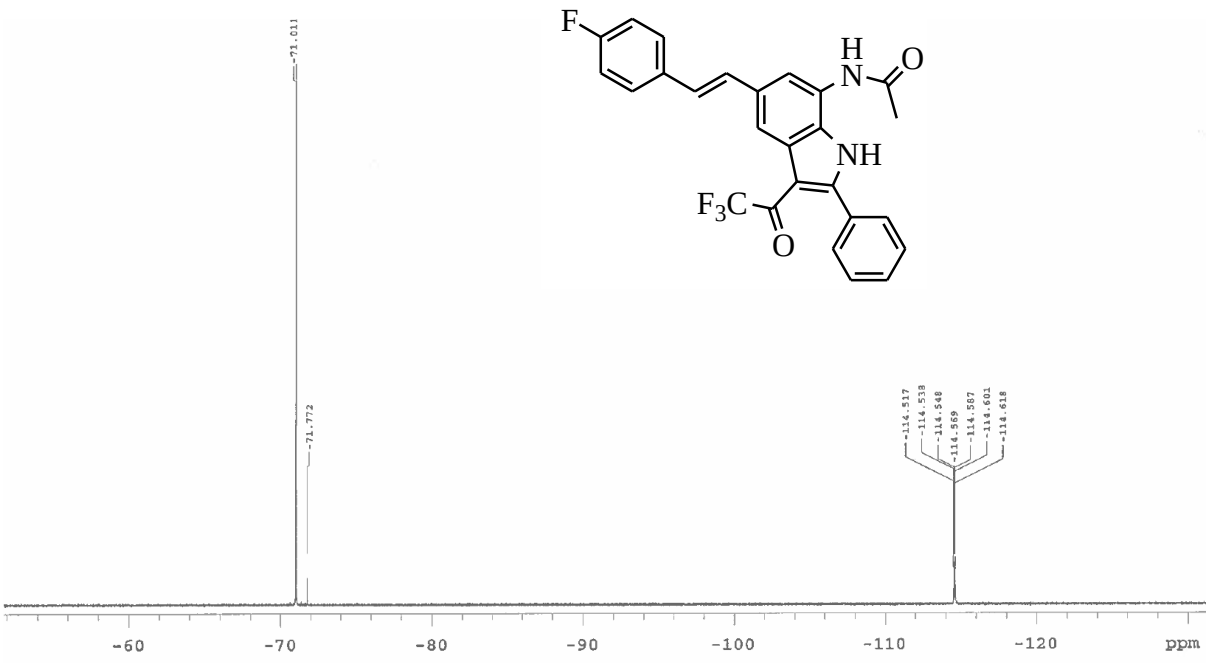


Figure S43. ^{19}F NMR Spectrum of Compound 4e in DMSO-d_6 at 282 MHz

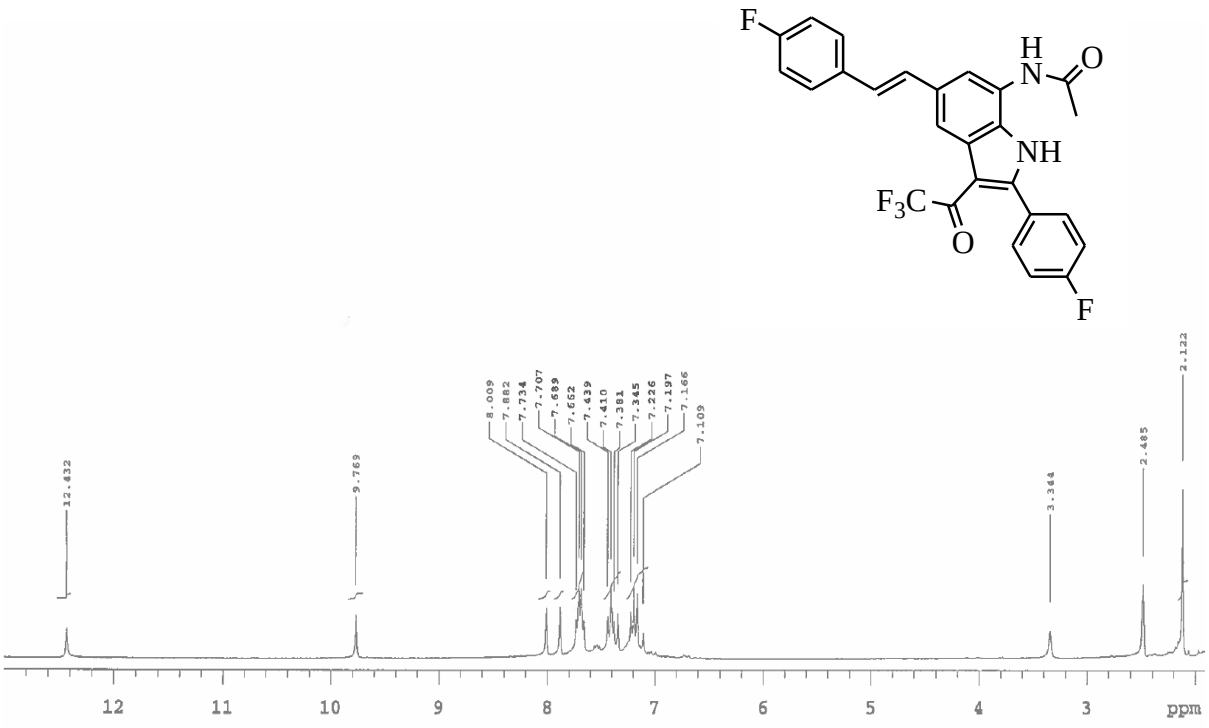


Figure S44. ^{1}H NMR Spectrum of Compound 4f in DMSO-d_6 at 300 MHz

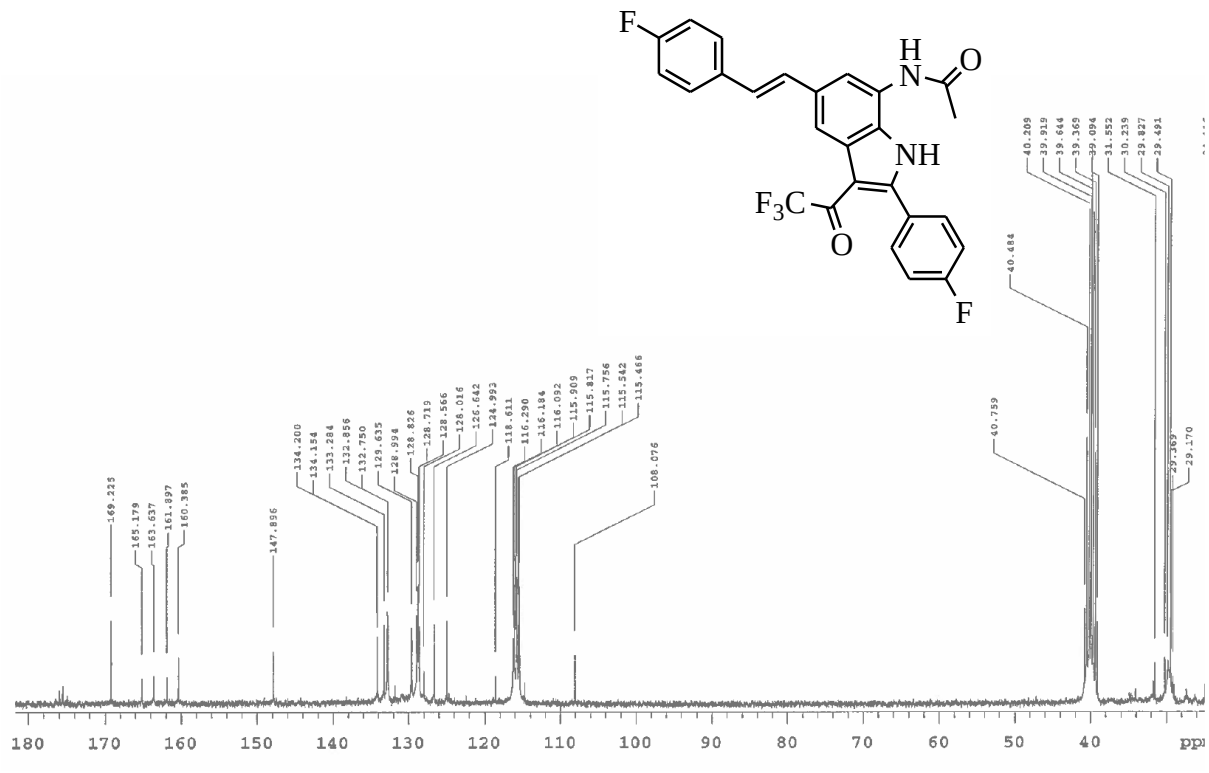


Figure S45. ^{13}C NMR Spectrum of Compound 4f in DMSO-*d*$_6$ at 75 MHz

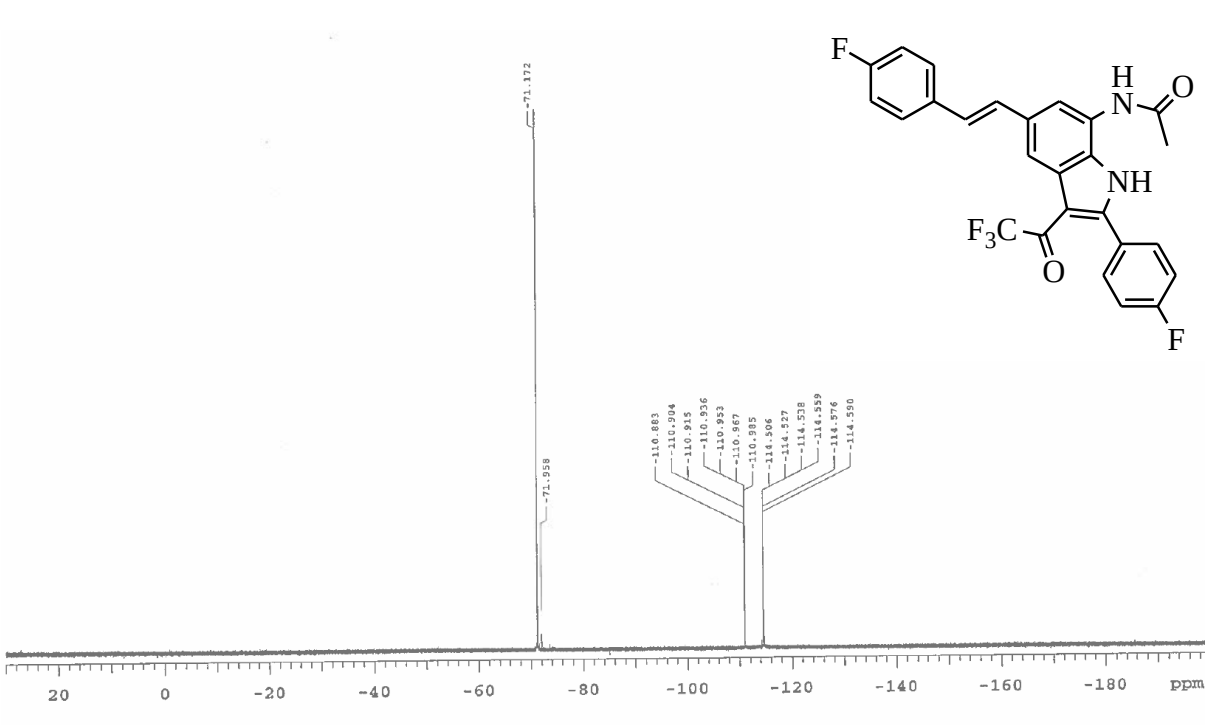


Figure S46. ^{19}F NMR Spectrum of Compound 4f in DMSO-*d*$_6$ at 282 MHz

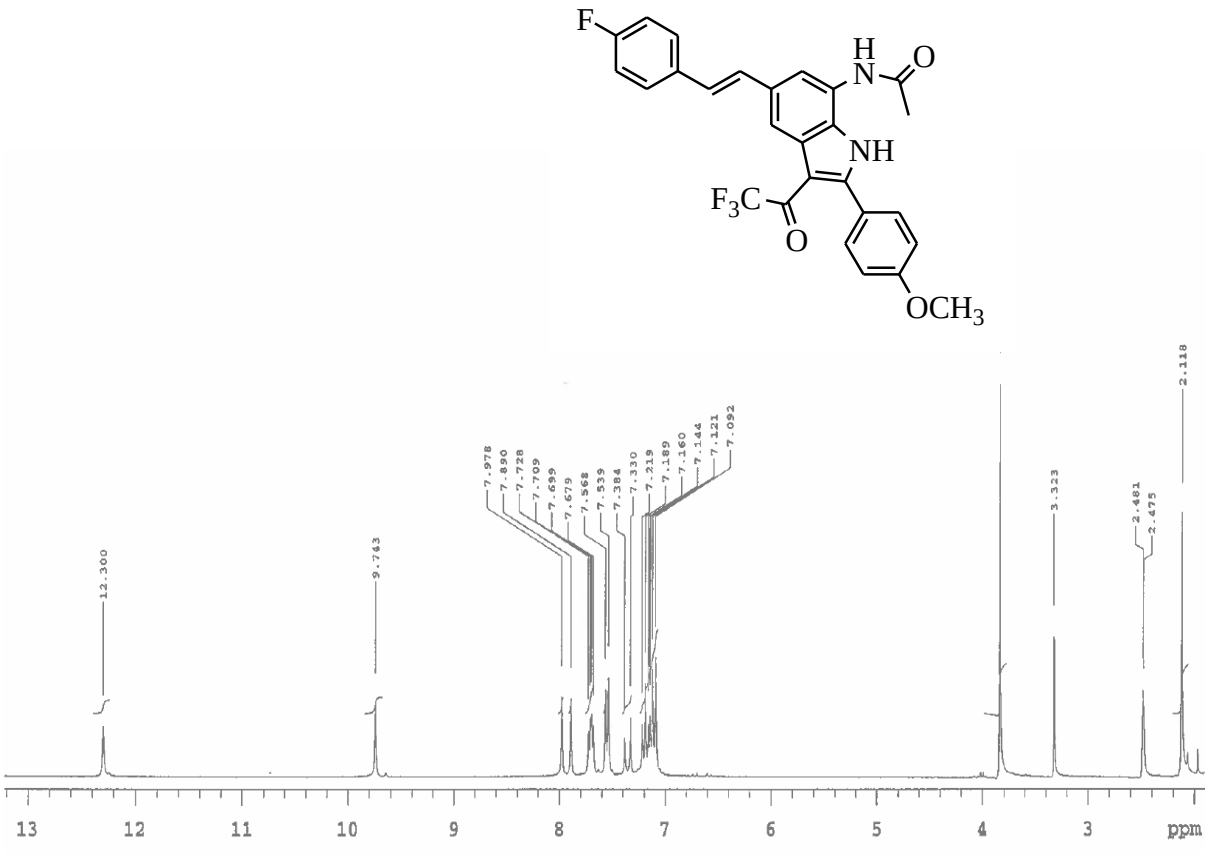


Figure S47. ^{1}H NMR Spectrum of Compound 4g in DMSO-*d*$_6$ at 300 MHz

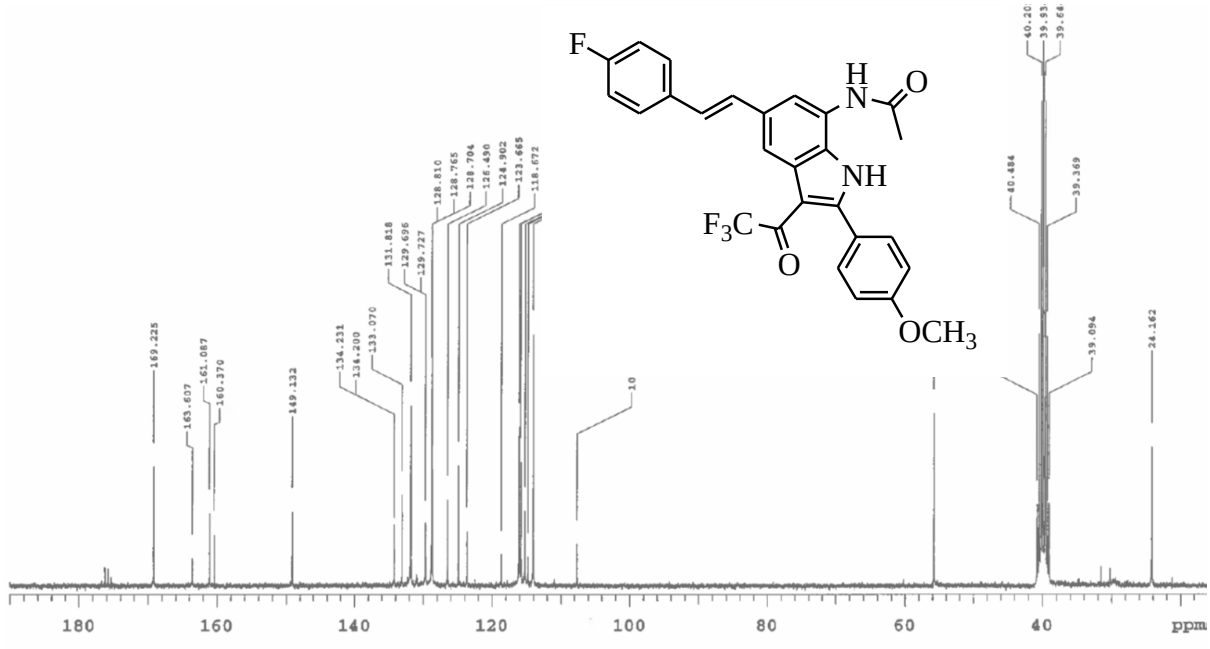


Figure S48. ^{13}C NMR Spectrum of Compound 4g in DMSO-*d*$_6$ at 75 MHz

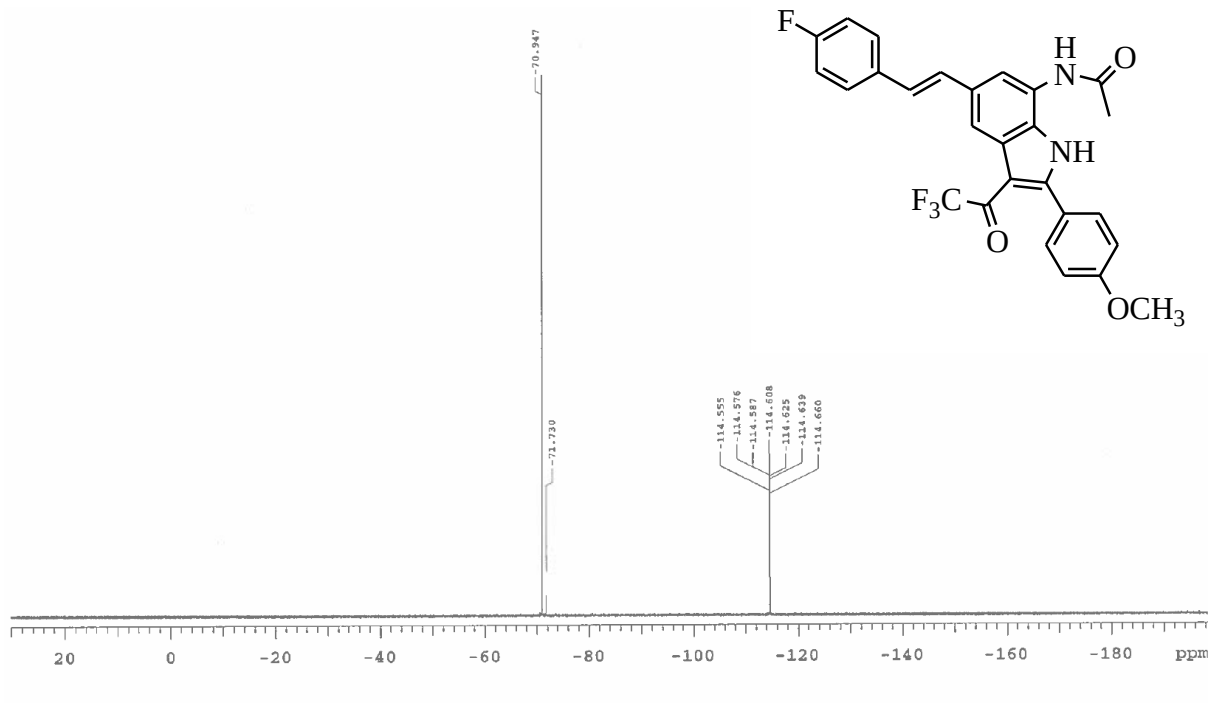
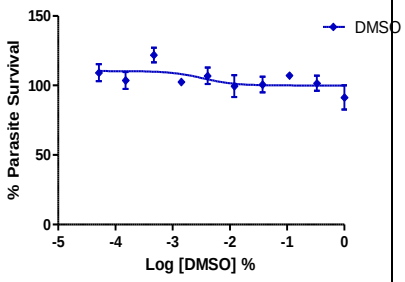


Figure S49. ^{19}F NMR Spectrum of Compound 4g in DMSO-*d*$_6$ at 282 MHz

Supplementary 2: % cell viability and LC_{50} values of chloroquine and compounds 3 and 4

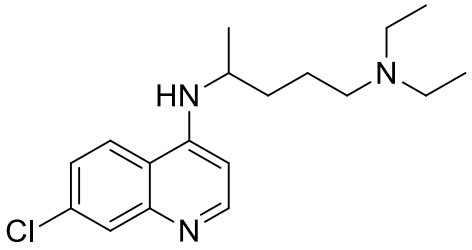
Table 1. Log solvent percentage vs. % Parasite survival data used to plot dose-response curve for DMSO.

Log Solv. Perc (%)[a]	DMSO	
	%PS	SD
0.00	91.41	8.66
-0.48	101.62	5.42
-0.96	107.17	1.17
-1.43	100.72	5.58
-1.92	99.56	7.82
-2.39	106.94	5.85
-2.85	102.51	1.52
-3.33	121.92	5.28
-3.82	103.65	6.05
-4.29	109.18	6.16



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

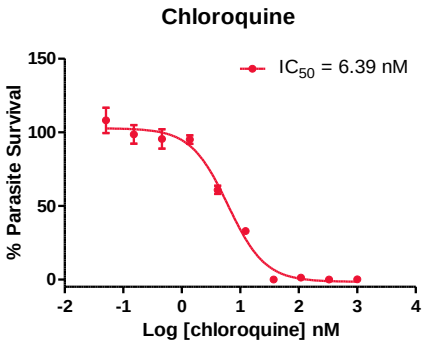
Table 2. Log concentration vs. % Parasite survival data used to plot dose-response curve for chloroquine



Chloroquine

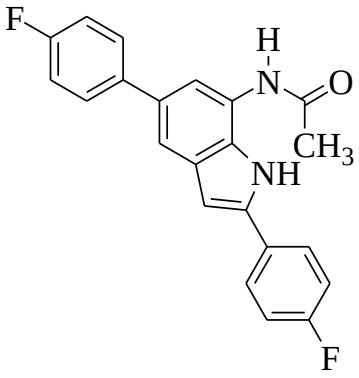
Figure S50. Chemical structure of chloroquine

.Log Conc (nM)[a]	CQ	
	%PS	SD
3.000	0.11	0.20
2.520	0.00	0.00
2.040	1.21	2.10
1.560	0.00	0.00
1.090	32.89	2.13
0.614	60.87	2.79
0.137	94.99	2.90
-0.340	95.42	6.61
-0.818	98.51	6.29
-1.294	108.04	8.58



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

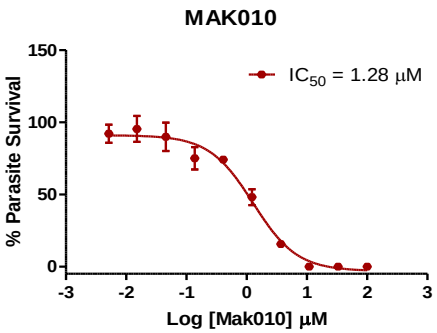
Table 3. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3a**.



3a

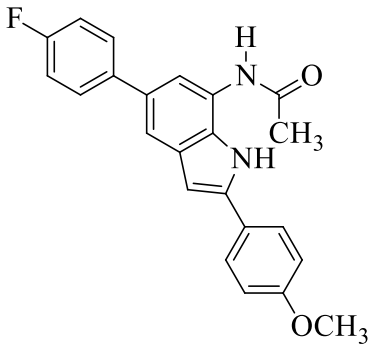
Figure S51. Chemical structure of **3a**

Log Conc (μM)[a]	Mak010	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	15.64	1.59
0.09	48.11	5.47
-0.39	74.07	1.57
-0.86	74.96	7.75
-1.34	89.87	9.82
-1.82	95.34	8.94
-2.29	92.04	6.29



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

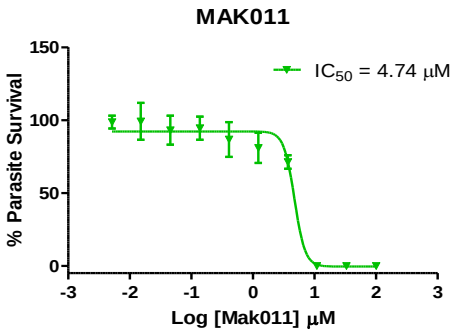
Table 4. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3b**.



3b

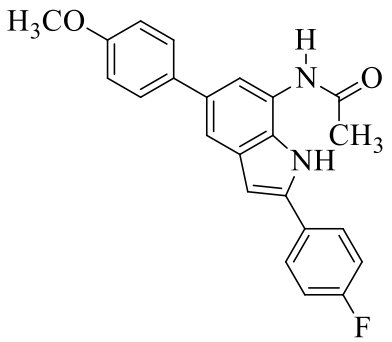
Figure S52. Chemical structure of **3b**

Log Conc (μM)[a]	Mak011	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	71.29	4.66
0.09	80.98	10.32
-0.39	86.71	11.94
-0.86	94.49	7.96
-1.34	93.10	9.89
-1.82	99.18	12.64
-2.29	98.70	4.40



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

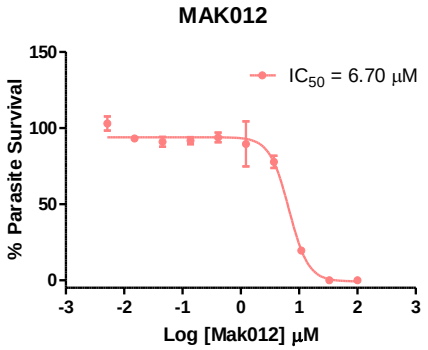
Table 5. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3c**.



3c

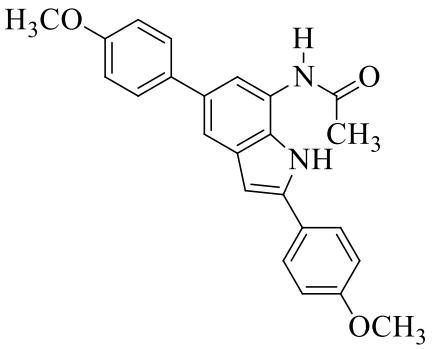
Figure S53. Chemical structure of **3c**

Log Conc (nM)[a]	Mak012	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	19.52	1.14
0.57	77.74	3.97
0.09	89.50	14.79
-0.39	93.80	3.17
-0.86	91.69	2.31
-1.34	90.90	3.20
-1.82	93.13	2.22
-2.29	102.94	4.69



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

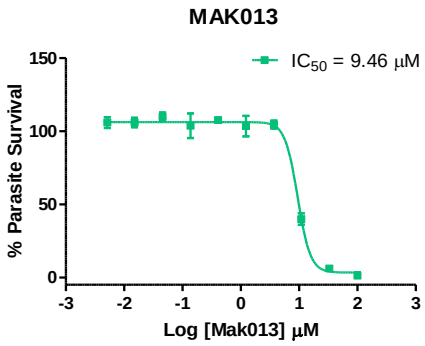
Table 6. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3d**.



3d

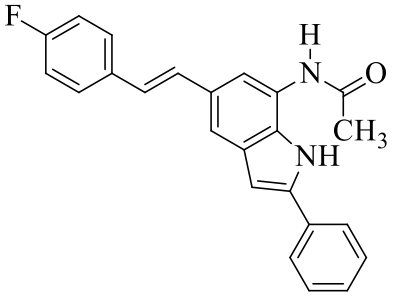
Figure S54. Chemical structure of **3d**

Log Conc (nM)[a]	Mak013	
	%PS	SD
2.00	1.29	2.24
1.52	6.22	0.66
1.04	39.93	3.90
0.57	104.47	2.71
0.09	103.42	6.94
-0.39	107.59	2.04
-0.86	103.72	8.42
-1.34	109.86	2.87
-1.82	105.85	3.24
-2.29	105.83	3.62



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

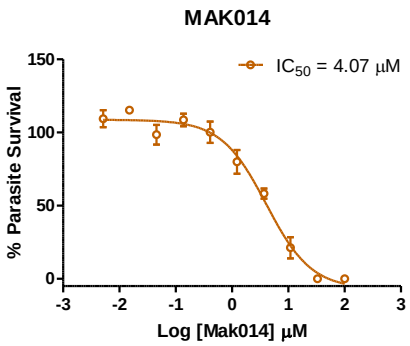
Table 7. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3e**.



3e

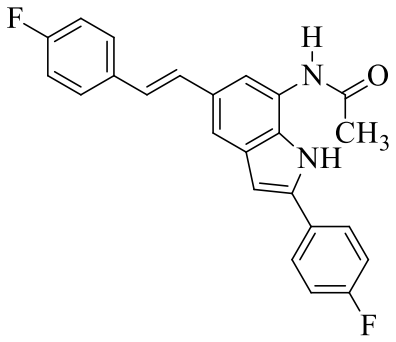
Figure S55. Chemical structure of **3e**

Log Conc (nM)[a]	Mak014	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	21.22	7.20
0.57	58.26	3.47
0.09	79.97	8.12
-0.39	100.22	7.27
-0.86	108.57	4.25
-1.34	98.49	6.72
-1.82	115.28	0.79
-2.29	109.42	5.80



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

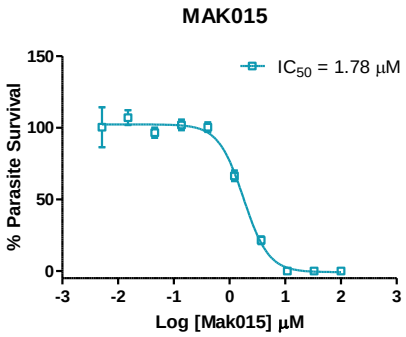
Table 8. Log concentration vs. % Parasite survival data used to plot dose-response curves for **3f**.



3f

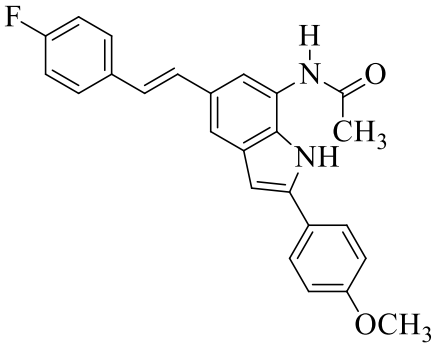
Figure S56. Chemical structure of **3f**

Log Conc (nM)[a]	Mak015	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	21.48	2.58
0.09	66.49	3.66
-0.39	100.45	3.36
-0.86	102.03	3.69
-1.34	96.58	3.50
-1.82	107.12	5.16
-2.29	100.44	13.95



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

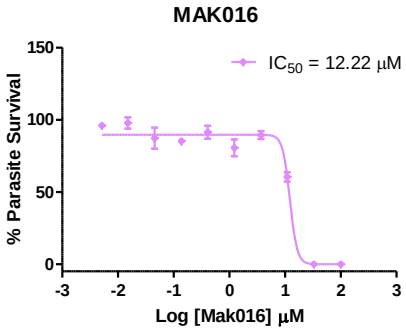
Table 9. Log concentration vs. % Parasite survival data used to plot dose-response curve for **3g**.



3g

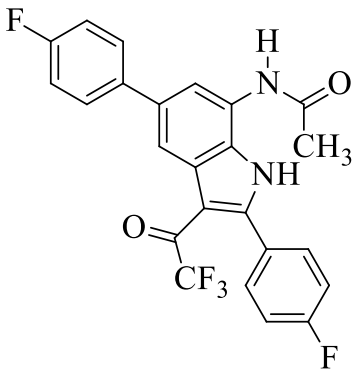
Figure S57. Chemical structure of **3g**

Log Conc (nM)[a]	Mak016	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	60.43	3.21
0.57	89.42	2.84
0.09	80.58	5.76
-0.39	91.40	4.44
-0.86	85.19	2.22
-1.34	87.26	7.30
-1.82	97.74	3.83
-2.29	95.92	0.24



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

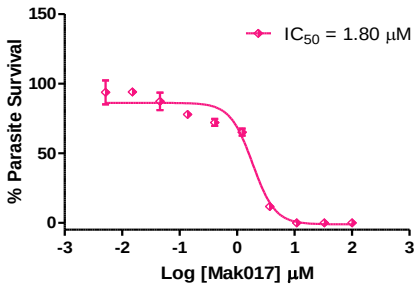
Table 10. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4a**.



4a

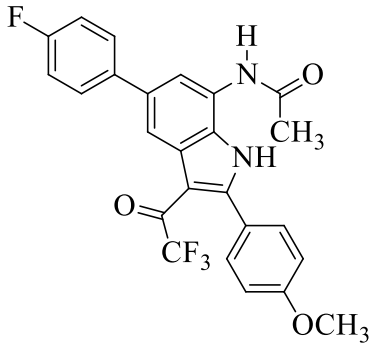
Figure S58. Chemical structure of **4a**

Log Conc (nM)[a]	Mak017	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	11.72	2.10
0.09	65.14	2.55
-0.39	72.07	2.54
-0.86	77.87	1.99
-1.34	87.25	6.26
-1.82	93.96	1.95
-2.29	93.73	8.60



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

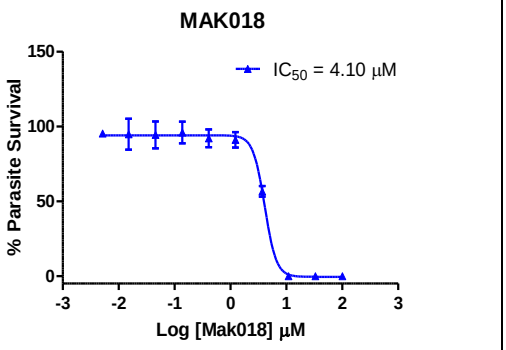
Table 11. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4b**.



4b

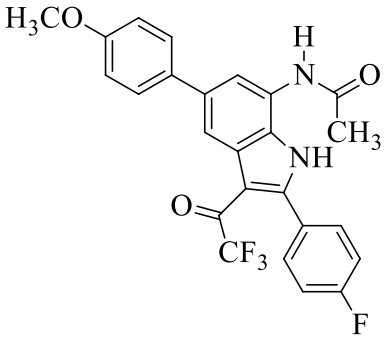
Figure S59. Chemical structure of **4b**

Log Conc (nM)[a]	Mak018	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	56.59	6.18
0.09	91.05	8.86
-0.39	92.10	10.32
-0.86	95.97	12.54
-1.34	94.36	15.51
-1.82	94.82	17.88
-2.29	95.33	0.31



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

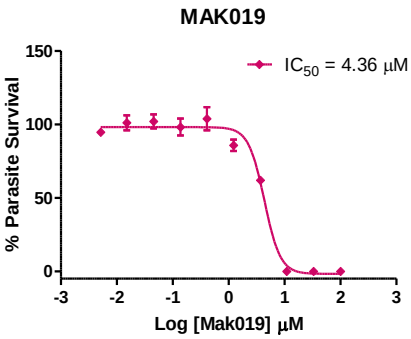
Table 12. Log concentration vs. % Parasite survival data used to plot dose-response curves for **4c**.



4c

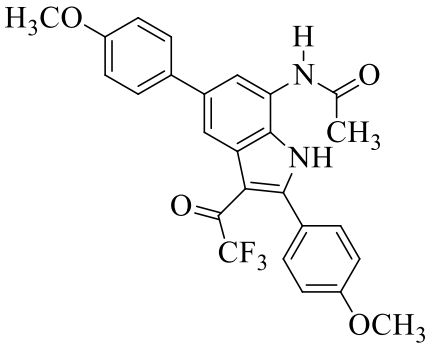
Figure S60. Chemical structure of **4c**

Log Conc (nM)[a]	Mak019	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	61.91	1.75
0.09	85.74	6.81
-0.39	103.78	13.62
-0.86	98.19	10.00
-1.34	102.00	8.27
-1.82	101.10	8.85
-2.29	94.61	3.19



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

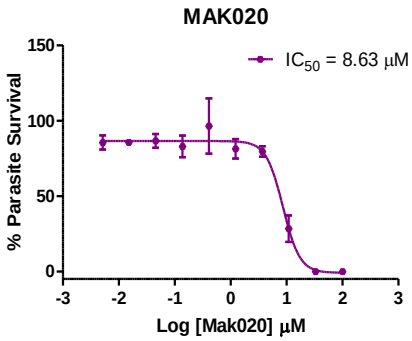
Table 13. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4d**.



4d

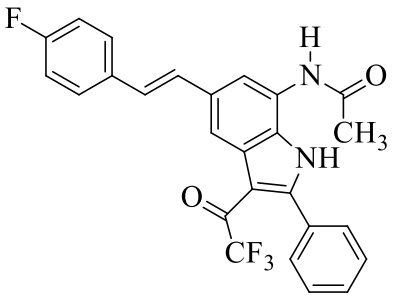
Figure S61. Chemical structure of **4d**

Log Conc (nM)[a]	Mak020	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	28.38	8.73
0.57	79.58	3.47
0.09	81.36	6.46
-0.39	96.45	18.29
-0.86	82.93	7.17
-1.34	86.61	4.56
-1.82	85.55	1.87
-2.29	85.53	4.67



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

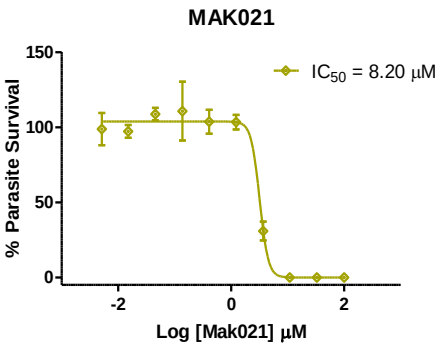
Table 14. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4e**.



4e

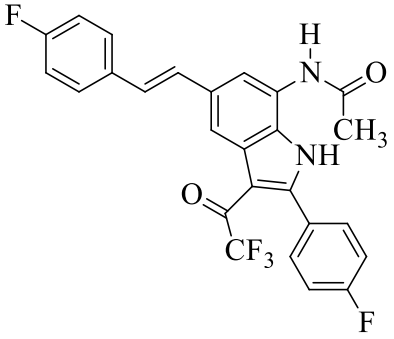
Figure S62. Chemical structure of **4e**

Log Conc (nM)[a]	Mak021	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	30.89	6.27
0.09	103.39	4.80
-0.39	103.65	7.91
-0.86	110.72	19.57
-1.34	108.71	4.13
-1.82	97.23	4.24
-2.29	98.80	10.71



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

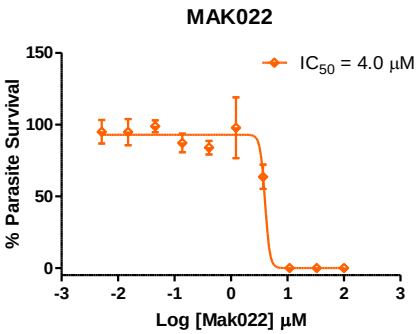
Table 15. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4f**.



4f

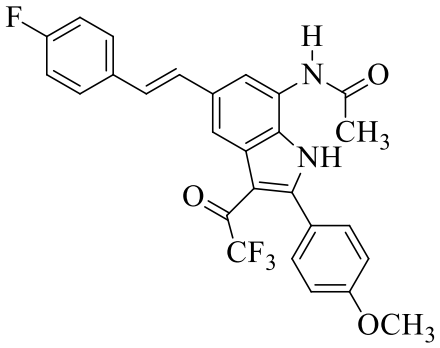
Figure S63. Chemical structure of **4f**

Log Conc (nM)[a]	Mak022	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	63.56	8.43
0.09	97.76	21.21
-0.39	83.88	4.74
-0.86	87.18	6.48
-1.34	98.80	4.11
-1.82	94.74	9.07
-2.29	94.97	8.18



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

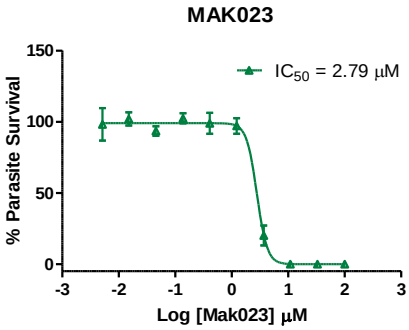
Table 16. Log concentration vs. % Parasite survival data used to plot dose-response curve for **4g**.



4g

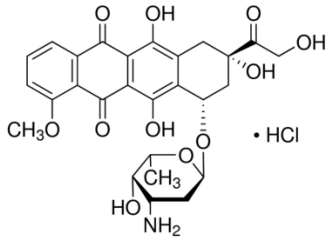
Figure S64. Chemical structure of **4g**

Log Conc (nM)[a]	Mak023	
	%PS	SD
2.00	0.00	0.00
1.52	0.00	0.00
1.04	0.00	0.00
0.57	20.17	6.97
0.09	97.06	5.47
-0.39	98.95	7.36
-0.86	102.44	3.56
-1.34	93.46	3.39
-1.82	101.99	4.62
-2.29	98.20	11.43



[a]Data are expressed as means of triplicate values. SD = standard deviation; %PS = Percentage Parasite Survival.

Supplementary 3: % cell viability of Vero cells exposed Doxorubicin chloride, 3a, 3f, 4a and 4g



Doxorubicin hydrochloride

Table 17: Percentage cell viability of Vero cells exposed to different concentrations of Doxorubicin hydrochloride

Conc. (µM)	%Viability	SD
100	44.05	3.44
10	63.48	0.93
1	75.68	4.77
0.1	87.74	3.35
0.01	95.00	4.86
0.001	100.00	4.01

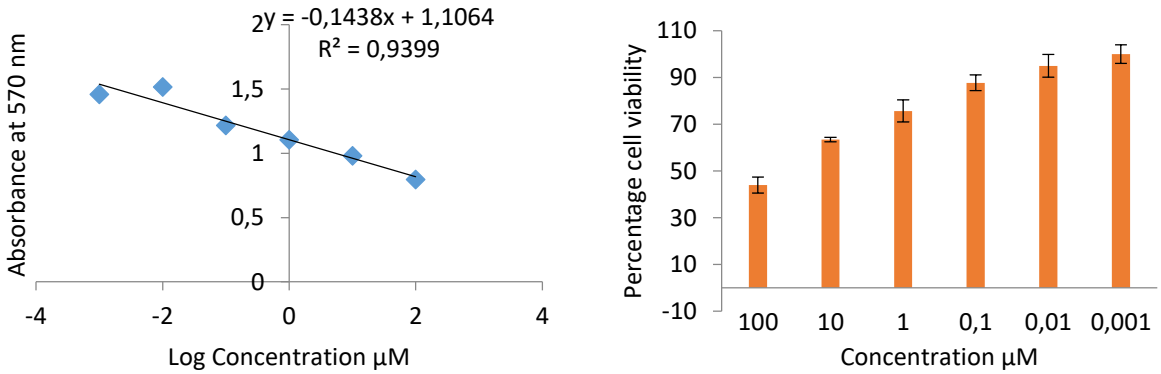
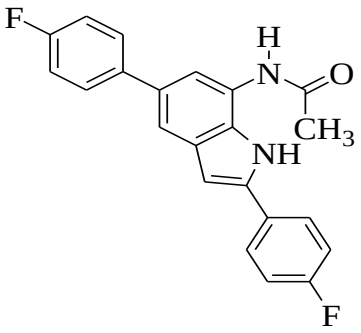


Figure S65. Linear regression plots and percentage cell viability graphs Vero cells exposed to different concentrations of doxorubicin hydrochloride

Table 18: Percentage cell viability of Vero cells exposed to different concentrations of **3a**



3a

Conc. (µg/ml)	%Viability	SD
100	26.13	0.48
10	51.69	2.71
1	86.54	2.98
0.1	100.00	1.44

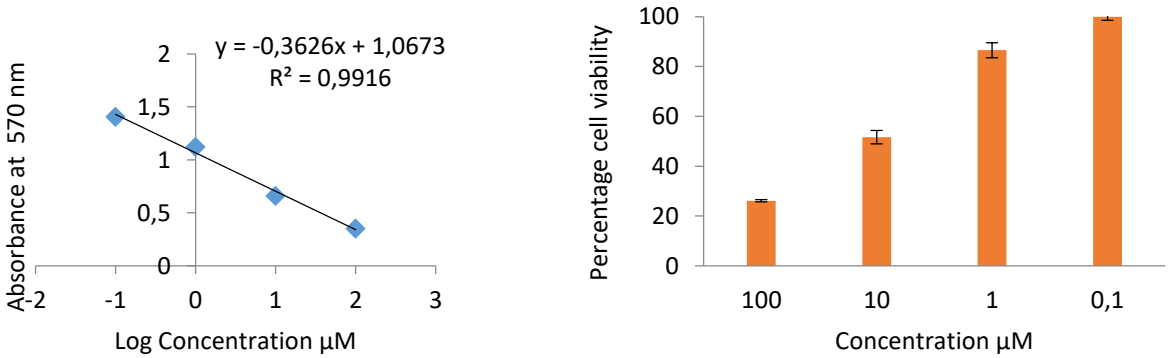
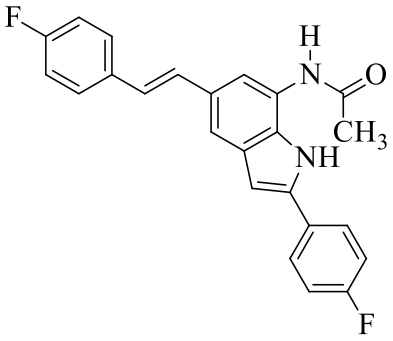


Figure S66. Linear regression plots and percentage cell viability graphs of Vero cells exposed to different concentrations of **3a**

Table 19: Percentage cell viability of Vero cells exposed to different concentrations of **3f**



3f

Conc. (µg/ml)	%Viability	SD
100	13.76	7.23
10	94.81	1.81
1	98.5	0.71
0.1	99.00	1.41

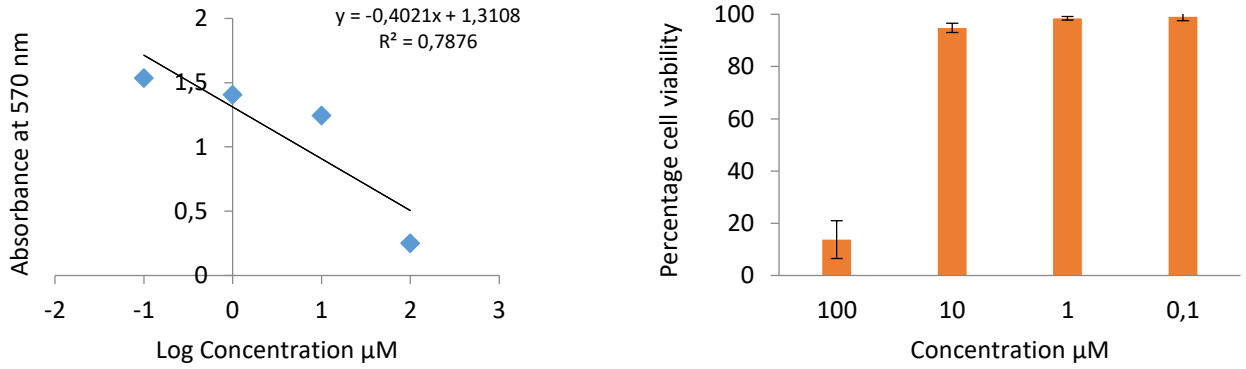
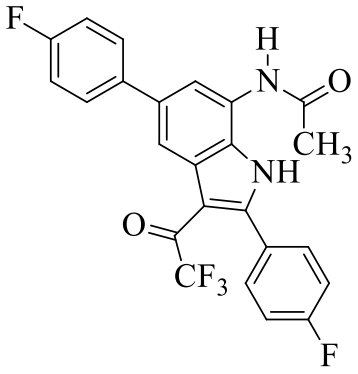


Figure S67. Linear regression plots and percentage cell viability graphs of Vero cells exposed to different concentrations of **3f**

Table 20: Percentage cell viability of Vero cells exposed to different concentrations of **4a**



4a

Conc. (µg/ml)	%Viability	SD
100	5.45	0.16
10	96.5	2.12
1	98.50	0.71
0.1	99.5	0.71

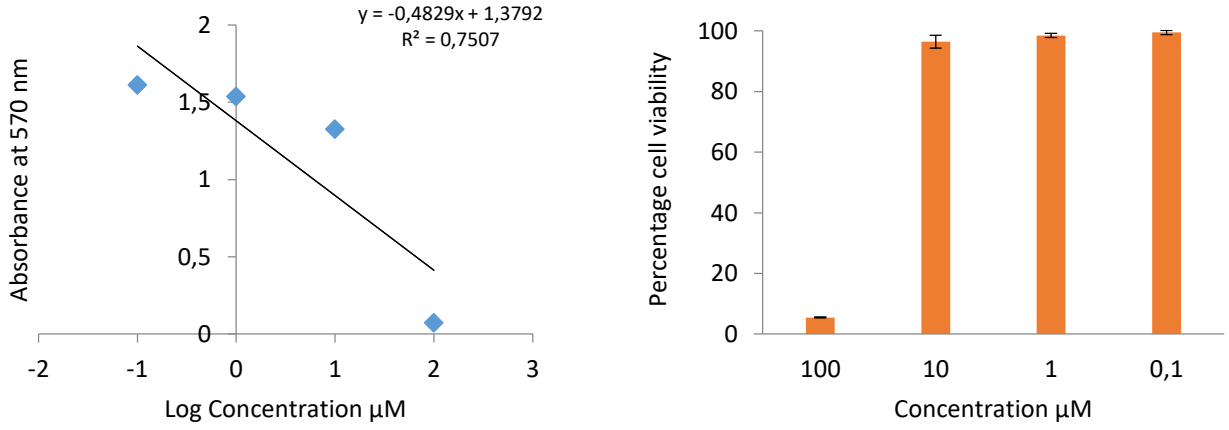
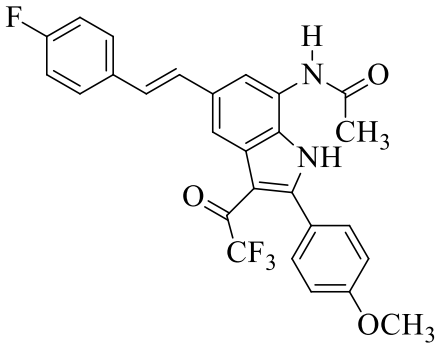


Figure S68. Linear regression plots and percentage cell viability graphs of Vero cells exposed to different concentrations of **4a**

Table 21: Percentage cell viability of Vero cells exposed to different concentrations of **4g**



4g

Conc. (µg/ml)	%Viability	SD
100	35.56	0.37
10	98.5	0.71
1	99.00	0.71
0.1	99.50	1.41

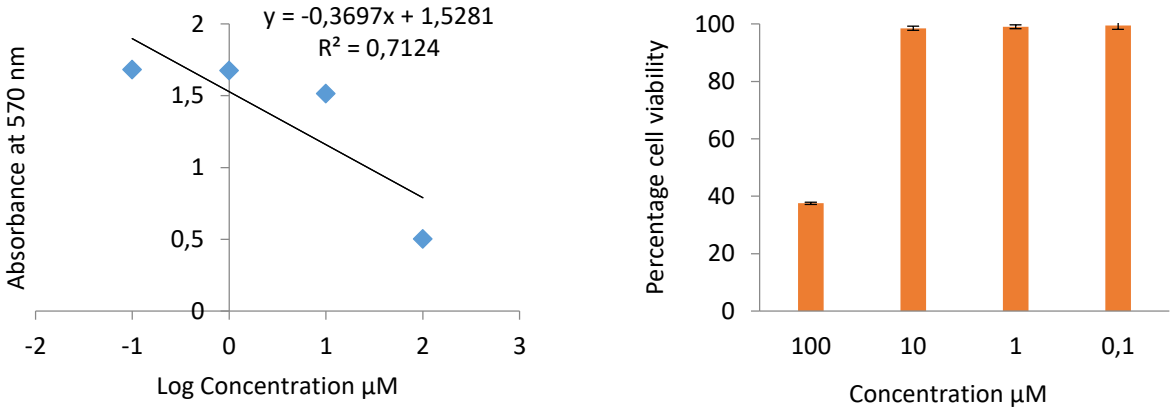


Figure S69. Linear regression plots and percentage cell viability graphs of Vero cells exposed to different concentrations of **4g**

678 **Supplementary 4: Crystal data and structure refinement, bond lengths and torsion angles of 4g**
679
680 **Table 22. Crystal data and structure refinement for 4g**

681	Identification code	16a_mak001_p	
682	Empirical formula	C27 H20 F4 N2 O3	
683	Formula weight	496.45	
684	Temperature	173(2) K	
685	Wavelength	0.71073 Å	
686	Crystal system	Triclinic	
687	Space group	P-1	
688	Unit cell dimensions	a = 11.1351(10) Å	α= 68.965(3)°.
689		b = 14.9334(13) Å	β= 72.856(3)°.
690		c = 18.7080(16) Å	γ = 68.716(3)°.
691	Volume	2656.7(4) Å^3	
692	Z	4	
693	Density (calculated)	1.241 Mg/m^3	
694	Absorption coefficient	0.100 mm^{-1}	
695	F(000)	1024	
696	Crystal size	0.40 x 0.13 x 0.04 mm^3	
697	Theta range for data collection	3.06 to 25.50°.	
698	Index ranges	-11<=h<=13, -17<=k<=18, -22<=l<=22	
699	Reflections collected	26244	
700	Independent reflections	9846 [R(int) = 0.0581]	
701	Completeness to theta = 25.50°	99.5 %	
702	Absorption correction	Semi-empirical from equivalents	
703	Max. and min. transmission	0.9960 and 0.9610	
704	Refinement method	Full-matrix least-squares on F^2	
705	Data / restraints / parameters	9846 / 0 / 649	
706	Goodness-of-fit on F^2	1.077	
707	Final R indices [I>2sigma(I)]	R1 = 0.0788, wR2 = 0.2115	
708	R indices (all data)	R1 = 0.1203, wR2 = 0.2286	
709	Largest diff. peak and hole	0.432 and -0.390 e.Å^{-3}	

710

Table 23. Bond lengths [Å] and angles [°] for 4g

C(1)-C(2)	1.355(6)
C(1)-C(6)	1.356(6)
C(1)-F(1)	1.359(4)
C(2)-C(3)	1.406(6)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.359(6)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.404(6)
C(4)-C(7)	1.468(5)
C(5)-C(6)	1.369(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.286(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.482(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.390(5)
C(9)-C(14)	1.411(5)
C(10)-C(11)	1.402(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.397(5)
C(11)-C(15)	1.445(5)
C(12)-N(1)	1.387(4)
C(12)-C(13)	1.394(5)
C(13)-C(14)	1.367(5)
C(13)-N(2)	1.409(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.407(5)
C(15)-C(17)	1.457(5)
C(16)-N(1)	1.373(4)
C(16)-C(19)	1.464(5)
C(17)-O(1)	1.208(4)
C(17)-C(18)	1.534(5)
C(18)-F(4)	1.317(4)
C(18)-F(2)	1.336(4)
C(18)-F(3)	1.355(4)

750	C(19)-C(20)	1.402(5)
751	C(19)-C(24)	1.403(5)
752	C(20)-C(21)	1.375(5)
753	C(20)-H(20)	0.9500
754	C(21)-C(22)	1.397(5)
755	C(21)-H(21)	0.9500
756	C(22)-O(3)	1.358(4)
757	C(22)-C(23)	1.380(5)
758	C(23)-C(24)	1.392(5)
759	C(23)-H(23)	0.9500
760	C(24)-H(24)	0.9500
761	C(25)-O(3)	1.431(4)
762	C(25)-H(25A)	0.9800
763	C(25)-H(25B)	0.9800
764	C(25)-H(25C)	0.9800
765	C(26)-O(2)	1.208(5)
766	C(26)-N(2)	1.366(5)
767	C(26)-C(27)	1.531(6)
768	N(1)-H(1)	0.8800
769	N(2)-H(2)	0.8800
770	C(27)-H(27A)	0.9800
771	C(27)-H(27B)	0.9800
772	C(27)-H(27C)	0.9800
773	C(28)-C(33)	1.360(6)
774	C(28)-C(29)	1.361(5)
775	C(28)-F(5)	1.365(4)
776	C(29)-C(30)	1.374(5)
777	C(29)-H(29)	0.9500
778	C(30)-C(31)	1.395(5)
779	C(30)-H(30)	0.9500
780	C(31)-C(32)	1.403(5)
781	C(31)-C(34)	1.470(5)
782	C(32)-C(33)	1.388(5)
783	C(32)-H(32)	0.9500
784	C(33)-H(33)	0.9500
785	C(34)-C(35)	1.338(5)
786	C(34)-H(34)	0.9500
787	C(35)-C(36)	1.468(5)
788	C(35)-H(35)	0.9500

789	C(36)-C(37)	1.394(5)
790	C(36)-C(41)	1.419(5)
791	C(37)-C(38)	1.390(5)
792	C(37)-H(37)	0.9500
793	C(38)-C(39)	1.403(5)
794	C(38)-C(42)	1.455(5)
795	C(39)-N(3)	1.384(4)
796	C(39)-C(40)	1.394(5)
797	C(40)-C(41)	1.381(5)
798	C(40)-N(4)	1.416(4)
799	C(41)-H(41)	0.9500
800	C(42)-C(43)	1.396(5)
801	C(42)-C(44)	1.445(5)
802	C(43)-N(3)	1.358(5)
803	C(43)-C(48)	1.466(5)
804	C(44)-O(4)	1.230(4)
805	C(44)-C(45)	1.517(6)
806	C(45)-F(6)	1.337(5)
807	C(45)-F(7)	1.345(5)
808	C(45)-F(8)	1.347(5)
809	C(48)-C(53)	1.377(5)
810	C(48)-C(49)	1.402(5)
811	C(49)-C(50)	1.363(5)
812	C(49)-H(49)	0.9500
813	C(50)-C(51)	1.394(5)
814	C(50)-H(50)	0.9500
815	C(51)-O(6)	1.364(4)
816	C(51)-C(52)	1.379(5)
817	C(52)-C(53)	1.381(5)
818	C(52)-H(52)	0.9500
819	C(53)-H(53)	0.9500
820	C(54)-O(6)	1.410(5)
821	C(54)-H(54A)	0.9800
822	C(54)-H(54B)	0.9800
823	C(54)-H(54C)	0.9800
824	C(55)-O(5)	1.205(4)
825	C(55)-N(4)	1.366(5)
826	C(55)-C(56)	1.509(5)
827	C(56)-H(56A)	0.9800

C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
N(3)-H(3)	0.8800
N(4)-H(4)	0.8800
C(2)-C(1)-C(6)	122.3(4)
C(2)-C(1)-F(1)	117.9(4)
C(6)-C(1)-F(1)	119.8(4)
C(1)-C(2)-C(3)	118.0(4)
C(1)-C(2)-H(2A)	121.0
C(3)-C(2)-H(2A)	121.0
C(4)-C(3)-C(2)	122.2(4)
C(4)-C(3)-H(3A)	118.9
C(2)-C(3)-H(3A)	118.9
C(3)-C(4)-C(5)	116.7(4)
C(3)-C(4)-C(7)	120.7(4)
C(5)-C(4)-C(7)	122.7(4)
C(6)-C(5)-C(4)	122.0(4)
C(6)-C(5)-H(5)	119.0
C(4)-C(5)-H(5)	119.0
C(1)-C(6)-C(5)	118.8(4)
C(1)-C(6)-H(6)	120.6
C(5)-C(6)-H(6)	120.6
C(8)-C(7)-C(4)	128.6(4)
C(8)-C(7)-H(7)	115.7
C(4)-C(7)-H(7)	115.7
C(7)-C(8)-C(9)	127.9(4)
C(7)-C(8)-H(8)	116.0
C(9)-C(8)-H(8)	116.0
C(10)-C(9)-C(14)	120.8(3)
C(10)-C(9)-C(8)	121.3(3)
C(14)-C(9)-C(8)	117.8(3)
C(9)-C(10)-C(11)	117.6(3)
C(9)-C(10)-H(10)	121.2
C(11)-C(10)-H(10)	121.2
C(12)-C(11)-C(10)	120.1(3)
C(12)-C(11)-C(15)	107.0(3)
C(10)-C(11)-C(15)	132.9(3)
N(1)-C(12)-C(13)	128.9(3)
N(1)-C(12)-C(11)	108.4(3)

867	C(13)-C(12)-C(11)	122.6(3)
868	C(14)-C(13)-C(12)	116.7(3)
869	C(14)-C(13)-N(2)	125.0(3)
870	C(12)-C(13)-N(2)	118.2(3)
871	C(13)-C(14)-C(9)	122.2(3)
872	C(13)-C(14)-H(14)	118.9
873	C(9)-C(14)-H(14)	118.9
874	C(16)-C(15)-C(11)	106.4(3)
875	C(16)-C(15)-C(17)	132.8(3)
876	C(11)-C(15)-C(17)	120.5(3)
877	N(1)-C(16)-C(15)	108.8(3)
878	N(1)-C(16)-C(19)	117.4(3)
879	C(15)-C(16)-C(19)	133.7(3)
880	O(1)-C(17)-C(15)	122.7(3)
881	O(1)-C(17)-C(18)	114.1(3)
882	C(15)-C(17)-C(18)	123.1(3)
883	F(4)-C(18)-F(2)	108.0(3)
884	F(4)-C(18)-F(3)	106.3(3)
885	F(2)-C(18)-F(3)	106.9(3)
886	F(4)-C(18)-C(17)	110.6(3)
887	F(2)-C(18)-C(17)	115.0(3)
888	F(3)-C(18)-C(17)	109.7(3)
889	C(20)-C(19)-C(24)	117.0(3)
890	C(20)-C(19)-C(16)	121.4(3)
891	C(24)-C(19)-C(16)	121.5(3)
892	C(21)-C(20)-C(19)	121.2(3)
893	C(21)-C(20)-H(20)	119.4
894	C(19)-C(20)-H(20)	119.4
895	C(20)-C(21)-C(22)	120.6(3)
896	C(20)-C(21)-H(21)	119.7
897	C(22)-C(21)-H(21)	119.7
898	O(3)-C(22)-C(23)	125.2(3)
899	O(3)-C(22)-C(21)	115.1(3)
900	C(23)-C(22)-C(21)	119.7(3)
901	C(22)-C(23)-C(24)	119.2(3)
902	C(22)-C(23)-H(23)	120.4
903	C(24)-C(23)-H(23)	120.4
904	C(23)-C(24)-C(19)	122.2(4)
905	C(23)-C(24)-H(24)	118.9

906	C(19)-C(24)-H(24)	118.9
907	O(3)-C(25)-H(25A)	109.5
908	O(3)-C(25)-H(25B)	109.5
909	H(25A)-C(25)-H(25B)	109.5
910	O(3)-C(25)-H(25C)	109.5
911	H(25A)-C(25)-H(25C)	109.5
912	H(25B)-C(25)-H(25C)	109.5
913	O(2)-C(26)-N(2)	124.1(4)
914	O(2)-C(26)-C(27)	123.2(4)
915	N(2)-C(26)-C(27)	112.7(4)
916	C(16)-N(1)-C(12)	109.3(3)
917	C(16)-N(1)-H(1)	125.3
918	C(12)-N(1)-H(1)	125.3
919	C(26)-N(2)-C(13)	127.6(3)
920	C(26)-N(2)-H(2)	116.2
921	C(13)-N(2)-H(2)	116.2
922	C(22)-O(3)-C(25)	117.5(3)
923	C(26)-C(27)-H(27A)	109.5
924	C(26)-C(27)-H(27B)	109.5
925	H(27A)-C(27)-H(27B)	109.5
926	C(26)-C(27)-H(27C)	109.5
927	H(27A)-C(27)-H(27C)	109.5
928	H(27B)-C(27)-H(27C)	109.5
929	C(33)-C(28)-C(29)	123.0(4)
930	C(33)-C(28)-F(5)	118.5(4)
931	C(29)-C(28)-F(5)	118.5(3)
932	C(28)-C(29)-C(30)	118.6(4)
933	C(28)-C(29)-H(29)	120.7
934	C(30)-C(29)-H(29)	120.7
935	C(29)-C(30)-C(31)	121.6(4)
936	C(29)-C(30)-H(30)	119.2
937	C(31)-C(30)-H(30)	119.2
938	C(30)-C(31)-C(32)	117.4(3)
939	C(30)-C(31)-C(34)	123.3(3)
940	C(32)-C(31)-C(34)	119.3(3)
941	C(33)-C(32)-C(31)	121.0(4)
942	C(33)-C(32)-H(32)	119.5
943	C(31)-C(32)-H(32)	119.5
944	C(28)-C(33)-C(32)	118.4(4)

945	C(28)-C(33)-H(33)	120.8
946	C(32)-C(33)-H(33)	120.8
947	C(35)-C(34)-C(31)	125.7(3)
948	C(35)-C(34)-H(34)	117.2
949	C(31)-C(34)-H(34)	117.2
950	C(34)-C(35)-C(36)	126.7(4)
951	C(34)-C(35)-H(35)	116.7
952	C(36)-C(35)-H(35)	116.7
953	C(37)-C(36)-C(41)	120.2(3)
954	C(37)-C(36)-C(35)	117.9(3)
955	C(41)-C(36)-C(35)	121.9(3)
956	C(38)-C(37)-C(36)	119.5(3)
957	C(38)-C(37)-H(37)	120.3
958	C(36)-C(37)-H(37)	120.3
959	C(37)-C(38)-C(39)	119.1(3)
960	C(37)-C(38)-C(42)	133.8(3)
961	C(39)-C(38)-C(42)	106.8(3)
962	N(3)-C(39)-C(40)	130.0(3)
963	N(3)-C(39)-C(38)	107.3(3)
964	C(40)-C(39)-C(38)	122.6(3)
965	C(41)-C(40)-C(39)	117.7(3)
966	C(41)-C(40)-N(4)	124.0(3)
967	C(39)-C(40)-N(4)	118.3(3)
968	C(40)-C(41)-C(36)	121.0(3)
969	C(40)-C(41)-H(41)	119.5
970	C(36)-C(41)-H(41)	119.5
971	C(43)-C(42)-C(44)	133.3(3)
972	C(43)-C(42)-C(38)	106.4(3)
973	C(44)-C(42)-C(38)	120.2(3)
974	N(3)-C(43)-C(42)	108.6(3)
975	N(3)-C(43)-C(48)	119.1(3)
976	C(42)-C(43)-C(48)	132.2(3)
977	O(4)-C(44)-C(42)	124.1(4)
978	O(4)-C(44)-C(45)	112.9(3)
979	C(42)-C(44)-C(45)	123.0(3)
980	F(6)-C(45)-F(7)	106.4(3)
981	F(6)-C(45)-F(8)	106.0(4)
982	F(7)-C(45)-F(8)	107.2(3)
983	F(6)-C(45)-C(44)	109.8(3)

984	F(7)-C(45)-C(44)	111.1(4)
985	F(8)-C(45)-C(44)	115.8(3)
986	C(53)-C(48)-C(49)	117.6(3)
987	C(53)-C(48)-C(43)	121.8(3)
988	C(49)-C(48)-C(43)	120.6(3)
989	C(50)-C(49)-C(48)	120.7(3)
990	C(50)-C(49)-H(49)	119.6
991	C(48)-C(49)-H(49)	119.6
992	C(49)-C(50)-C(51)	121.0(4)
993	C(49)-C(50)-H(50)	119.5
994	C(51)-C(50)-H(50)	119.5
995	O(6)-C(51)-C(52)	125.6(3)
996	O(6)-C(51)-C(50)	115.5(3)
997	C(52)-C(51)-C(50)	118.8(3)
998	C(51)-C(52)-C(53)	119.7(4)
999	C(51)-C(52)-H(52)	120.1
1000	C(53)-C(52)-H(52)	120.1
1001	C(48)-C(53)-C(52)	122.1(3)
1002	C(48)-C(53)-H(53)	118.9
1003	C(52)-C(53)-H(53)	118.9
1004	O(6)-C(54)-H(54A)	109.5
1005	O(6)-C(54)-H(54B)	109.5
1006	H(54A)-C(54)-H(54B)	109.5
1007	O(6)-C(54)-H(54C)	109.5
1008	H(54A)-C(54)-H(54C)	109.5
1009	H(54B)-C(54)-H(54C)	109.5
1010	O(5)-C(55)-N(4)	124.2(3)
1011	O(5)-C(55)-C(56)	122.2(3)
1012	N(4)-C(55)-C(56)	113.5(3)
1013	C(55)-C(56)-H(56A)	109.5
1014	C(55)-C(56)-H(56B)	109.5
1015	H(56A)-C(56)-H(56B)	109.5
1016	C(55)-C(56)-H(56C)	109.5
1017	H(56A)-C(56)-H(56C)	109.5
1018	H(56B)-C(56)-H(56C)	109.5
1019	C(43)-N(3)-C(39)	110.7(3)
1020	C(43)-N(3)-H(3)	124.6
1021	C(39)-N(3)-H(3)	124.6
1022	C(55)-N(4)-C(40)	127.8(3)

C(55)-N(4)-H(4)	116.1
C(40)-N(4)-H(4)	116.1
C(51)-O(6)-C(54)	117.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 24. Torsion angles [°] for 4g

C(6)-C(1)-C(2)-C(3)	-2.7(9)
F(1)-C(1)-C(2)-C(3)	-179.9(5)
C(1)-C(2)-C(3)-C(4)	-0.7(10)
C(2)-C(3)-C(4)-C(5)	3.4(9)
C(2)-C(3)-C(4)-C(7)	-176.7(6)
C(3)-C(4)-C(5)-C(6)	-3.0(7)
C(7)-C(4)-C(5)-C(6)	177.1(4)
C(2)-C(1)-C(6)-C(5)	3.1(8)
F(1)-C(1)-C(6)-C(5)	-179.8(4)
C(4)-C(5)-C(6)-C(1)	-0.1(7)
C(3)-C(4)-C(7)-C(8)	171.2(6)
C(5)-C(4)-C(7)-C(8)	-9.0(8)
C(4)-C(7)-C(8)-C(9)	-177.6(4)
C(7)-C(8)-C(9)-C(10)	3.4(7)
C(7)-C(8)-C(9)-C(14)	-177.6(4)
C(14)-C(9)-C(10)-C(11)	0.3(6)
C(8)-C(9)-C(10)-C(11)	179.3(4)
C(9)-C(10)-C(11)-C(12)	0.2(6)
C(9)-C(10)-C(11)-C(15)	-177.6(4)
C(10)-C(11)-C(12)-N(1)	178.6(3)
C(15)-C(11)-C(12)-N(1)	-3.2(4)
C(10)-C(11)-C(12)-C(13)	-0.2(6)
C(15)-C(11)-C(12)-C(13)	178.1(3)
N(1)-C(12)-C(13)-C(14)	-178.7(4)
C(11)-C(12)-C(13)-C(14)	-0.3(6)
N(1)-C(12)-C(13)-N(2)	0.6(6)
C(11)-C(12)-C(13)-N(2)	179.0(3)
C(12)-C(13)-C(14)-C(9)	0.7(6)
N(2)-C(13)-C(14)-C(9)	-178.5(4)
C(10)-C(9)-C(14)-C(13)	-0.7(6)
C(8)-C(9)-C(14)-C(13)	-179.8(4)
C(12)-C(11)-C(15)-C(16)	3.5(4)
C(10)-C(11)-C(15)-C(16)	-178.5(4)
C(12)-C(11)-C(15)-C(17)	-171.6(3)
C(10)-C(11)-C(15)-C(17)	6.3(7)
C(11)-C(15)-C(16)-N(1)	-2.6(4)
C(17)-C(15)-C(16)-N(1)	171.7(4)

1069	C(11)-C(15)-C(16)-C(19)	173.8(4)
1070	C(17)-C(15)-C(16)-C(19)	-11.9(7)
1071	C(16)-C(15)-C(17)-O(1)	170.5(4)
1072	C(11)-C(15)-C(17)-O(1)	-15.9(6)
1073	C(16)-C(15)-C(17)-C(18)	-12.3(7)
1074	C(11)-C(15)-C(17)-C(18)	161.3(3)
1075	O(1)-C(17)-C(18)-F(4)	27.9(5)
1076	C(15)-C(17)-C(18)-F(4)	-149.5(3)
1077	O(1)-C(17)-C(18)-F(2)	150.4(4)
1078	C(15)-C(17)-C(18)-F(2)	-27.0(5)
1079	O(1)-C(17)-C(18)-F(3)	-89.1(4)
1080	C(15)-C(17)-C(18)-F(3)	93.5(4)
1081	N(1)-C(16)-C(19)-C(20)	133.3(4)
1082	C(15)-C(16)-C(19)-C(20)	-42.9(6)
1083	N(1)-C(16)-C(19)-C(24)	-42.5(5)
1084	C(15)-C(16)-C(19)-C(24)	141.4(4)
1085	C(24)-C(19)-C(20)-C(21)	-3.0(5)
1086	C(16)-C(19)-C(20)-C(21)	-178.9(3)
1087	C(19)-C(20)-C(21)-C(22)	1.4(6)
1088	C(20)-C(21)-C(22)-O(3)	179.5(3)
1089	C(20)-C(21)-C(22)-C(23)	0.7(6)
1090	O(3)-C(22)-C(23)-C(24)	-179.7(3)
1091	C(21)-C(22)-C(23)-C(24)	-1.0(6)
1092	C(22)-C(23)-C(24)-C(19)	-0.7(6)
1093	C(20)-C(19)-C(24)-C(23)	2.6(5)
1094	C(16)-C(19)-C(24)-C(23)	178.5(3)
1095	C(15)-C(16)-N(1)-C(12)	0.7(4)
1096	C(19)-C(16)-N(1)-C(12)	-176.4(3)
1097	C(13)-C(12)-N(1)-C(16)	-179.8(4)
1098	C(11)-C(12)-N(1)-C(16)	1.6(4)
1099	O(2)-C(26)-N(2)-C(13)	-1.5(7)
1100	C(27)-C(26)-N(2)-C(13)	179.4(4)
1101	C(14)-C(13)-N(2)-C(26)	2.6(7)
1102	C(12)-C(13)-N(2)-C(26)	-176.6(4)
1103	C(23)-C(22)-O(3)-C(25)	-2.9(5)
1104	C(21)-C(22)-O(3)-C(25)	178.4(3)
1105	C(33)-C(28)-C(29)-C(30)	1.2(6)
1106	F(5)-C(28)-C(29)-C(30)	-179.8(4)
1107	C(28)-C(29)-C(30)-C(31)	0.9(6)

1108	C(29)-C(30)-C(31)-C(32)	-2.2(6)
1109	C(29)-C(30)-C(31)-C(34)	176.0(4)
1110	C(30)-C(31)-C(32)-C(33)	1.5(6)
1111	C(34)-C(31)-C(32)-C(33)	-176.7(4)
1112	C(29)-C(28)-C(33)-C(32)	-1.8(7)
1113	F(5)-C(28)-C(33)-C(32)	179.1(4)
1114	C(31)-C(32)-C(33)-C(28)	0.4(7)
1115	C(30)-C(31)-C(34)-C(35)	-8.0(6)
1116	C(32)-C(31)-C(34)-C(35)	170.2(4)
1117	C(31)-C(34)-C(35)-C(36)	-176.5(4)
1118	C(34)-C(35)-C(36)-C(37)	164.9(4)
1119	C(34)-C(35)-C(36)-C(41)	-14.5(6)
1120	C(41)-C(36)-C(37)-C(38)	0.0(6)
1121	C(35)-C(36)-C(37)-C(38)	-179.4(3)
1122	C(36)-C(37)-C(38)-C(39)	-1.2(6)
1123	C(36)-C(37)-C(38)-C(42)	-174.3(4)
1124	C(37)-C(38)-C(39)-N(3)	-176.5(3)
1125	C(42)-C(38)-C(39)-N(3)	-1.6(4)
1126	C(37)-C(38)-C(39)-C(40)	1.2(6)
1127	C(42)-C(38)-C(39)-C(40)	176.1(3)
1128	N(3)-C(39)-C(40)-C(41)	177.1(4)
1129	C(38)-C(39)-C(40)-C(41)	0.0(6)
1130	N(3)-C(39)-C(40)-N(4)	-3.4(6)
1131	C(38)-C(39)-C(40)-N(4)	179.5(4)
1132	C(39)-C(40)-C(41)-C(36)	-1.2(6)
1133	N(4)-C(40)-C(41)-C(36)	179.3(4)
1134	C(37)-C(36)-C(41)-C(40)	1.3(6)
1135	C(35)-C(36)-C(41)-C(40)	-179.4(4)
1136	C(37)-C(38)-C(42)-C(43)	175.8(4)
1137	C(39)-C(38)-C(42)-C(43)	2.0(4)
1138	C(37)-C(38)-C(42)-C(44)	-1.0(7)
1139	C(39)-C(38)-C(42)-C(44)	-174.7(4)
1140	C(44)-C(42)-C(43)-N(3)	174.4(4)
1141	C(38)-C(42)-C(43)-N(3)	-1.7(4)
1142	C(44)-C(42)-C(43)-C(48)	-7.8(8)
1143	C(38)-C(42)-C(43)-C(48)	176.0(4)
1144	C(43)-C(42)-C(44)-O(4)	161.5(4)
1145	C(38)-C(42)-C(44)-O(4)	-22.8(6)
1146	C(43)-C(42)-C(44)-C(45)	-21.3(7)

C(38)-C(42)-C(44)-C(45)	154.4(4)
O(4)-C(44)-C(45)-F(6)	39.4(5)
C(42)-C(44)-C(45)-F(6)	-138.0(4)
O(4)-C(44)-C(45)-F(7)	-77.9(5)
C(42)-C(44)-C(45)-F(7)	104.6(4)
O(4)-C(44)-C(45)-F(8)	159.4(4)
C(42)-C(44)-C(45)-F(8)	-18.1(6)
N(3)-C(43)-C(48)-C(53)	-45.7(5)
C(42)-C(43)-C(48)-C(53)	136.7(4)
N(3)-C(43)-C(48)-C(49)	134.4(4)
C(42)-C(43)-C(48)-C(49)	-43.1(6)
C(53)-C(48)-C(49)-C(50)	-0.8(5)
C(43)-C(48)-C(49)-C(50)	179.1(4)
C(48)-C(49)-C(50)-C(51)	-0.1(6)
C(49)-C(50)-C(51)-O(6)	-178.1(4)
C(49)-C(50)-C(51)-C(52)	1.4(6)
O(6)-C(51)-C(52)-C(53)	177.8(4)
C(50)-C(51)-C(52)-C(53)	-1.7(6)
C(49)-C(48)-C(53)-C(52)	0.5(6)
C(43)-C(48)-C(53)-C(52)	-179.4(4)
C(51)-C(52)-C(53)-C(48)	0.7(6)
C(42)-C(43)-N(3)-C(39)	0.7(4)
C(48)-C(43)-N(3)-C(39)	-177.3(3)
C(40)-C(39)-N(3)-C(43)	-176.9(4)
C(38)-C(39)-N(3)-C(43)	0.6(4)
O(5)-C(55)-N(4)-C(40)	-2.6(6)
C(56)-C(55)-N(4)-C(40)	178.0(4)
C(41)-C(40)-N(4)-C(55)	-4.7(6)
C(39)-C(40)-N(4)-C(55)	175.8(4)
C(52)-C(51)-O(6)-C(54)	6.4(7)
C(50)-C(51)-O(6)-C(54)	-174.1(4)

Symmetry transformations used to generate equivalent atoms: