Supporting Information to Accompany:

Fluorescent stilbazolium dyes as probes of the norepinephrine transporter: structural insights into substrate binding

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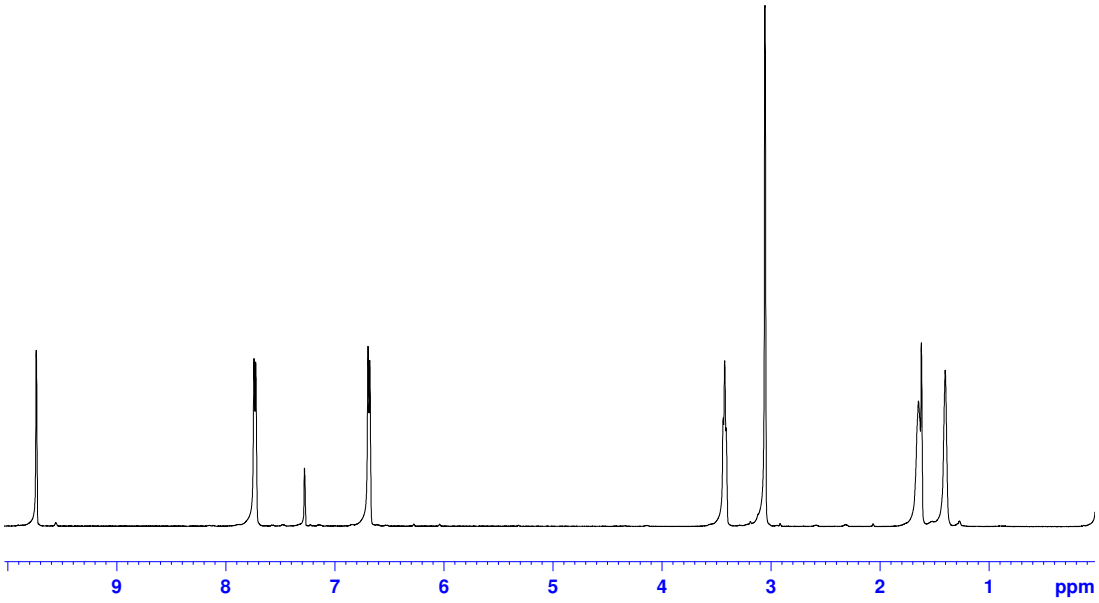
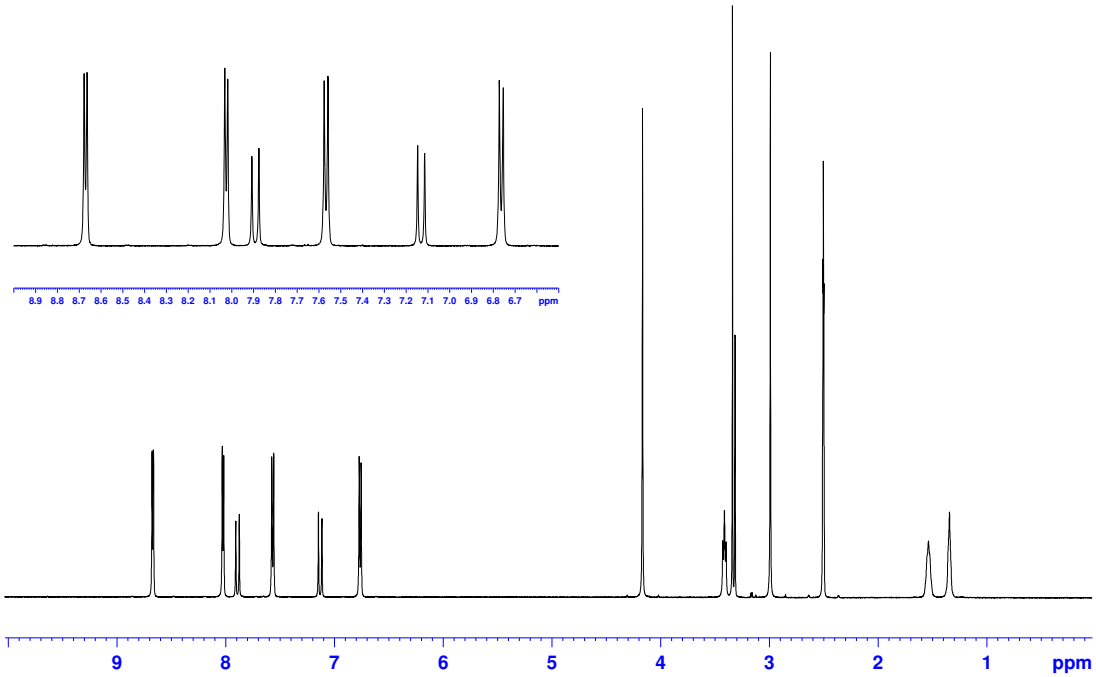
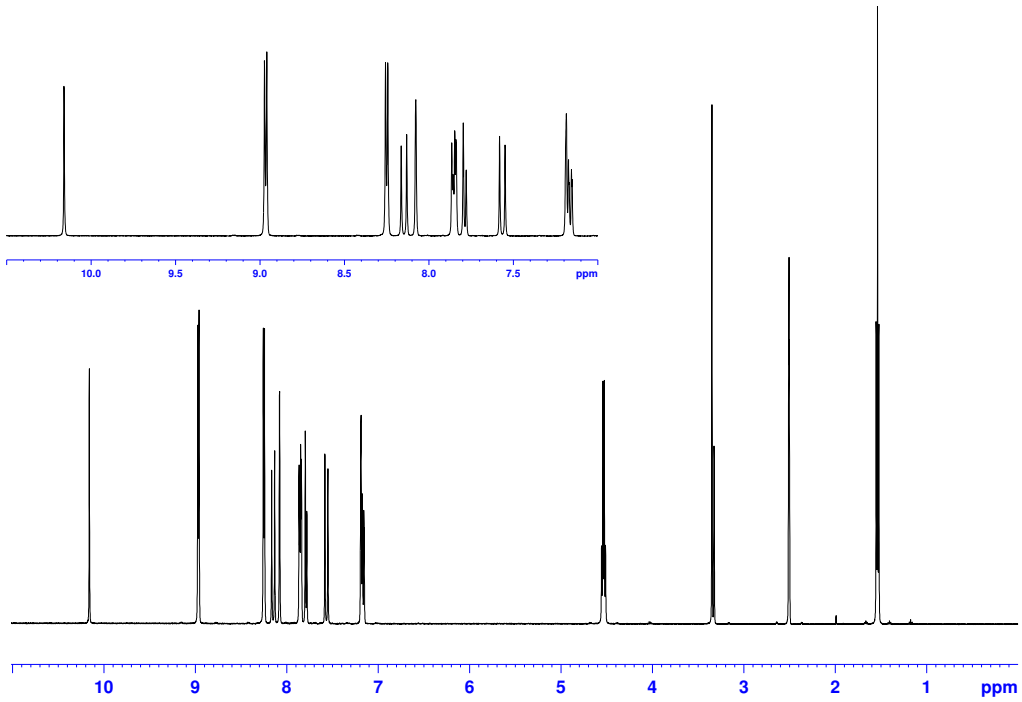
^{1}H NMR of **11**



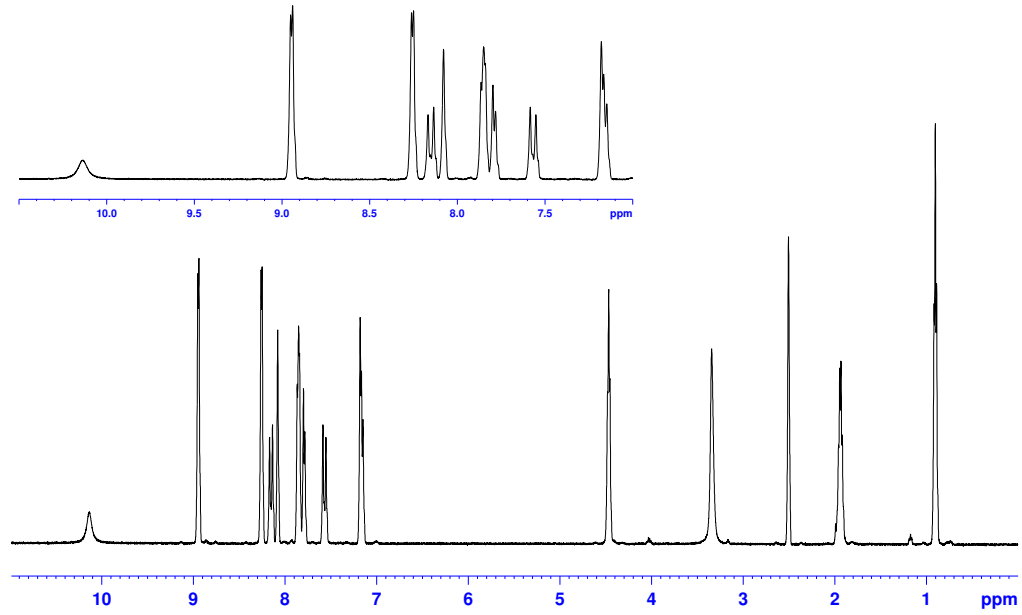
^{1}H NMR of **D2**



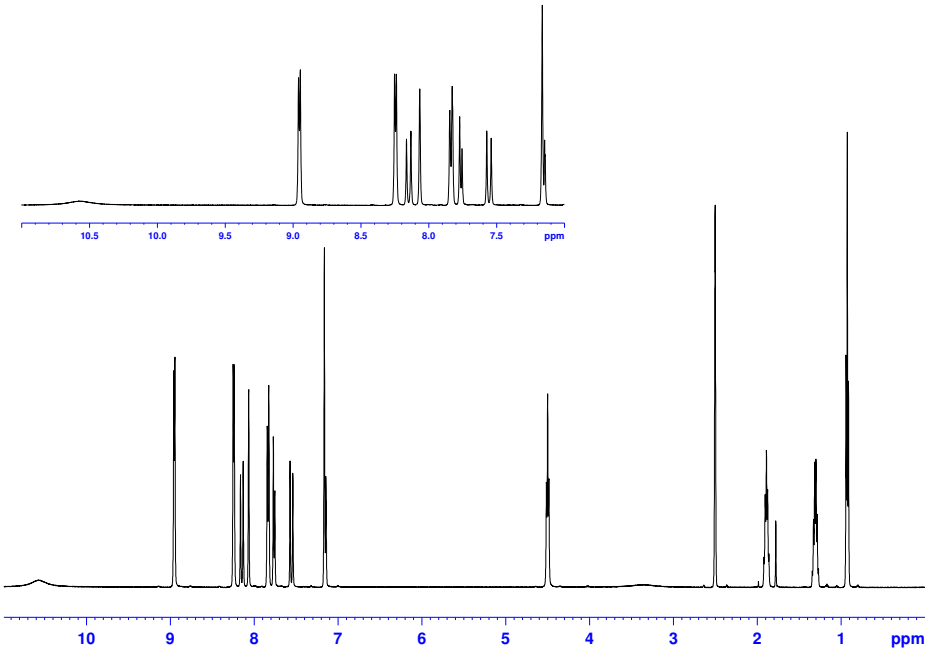
^{1}H NMR of **H2**



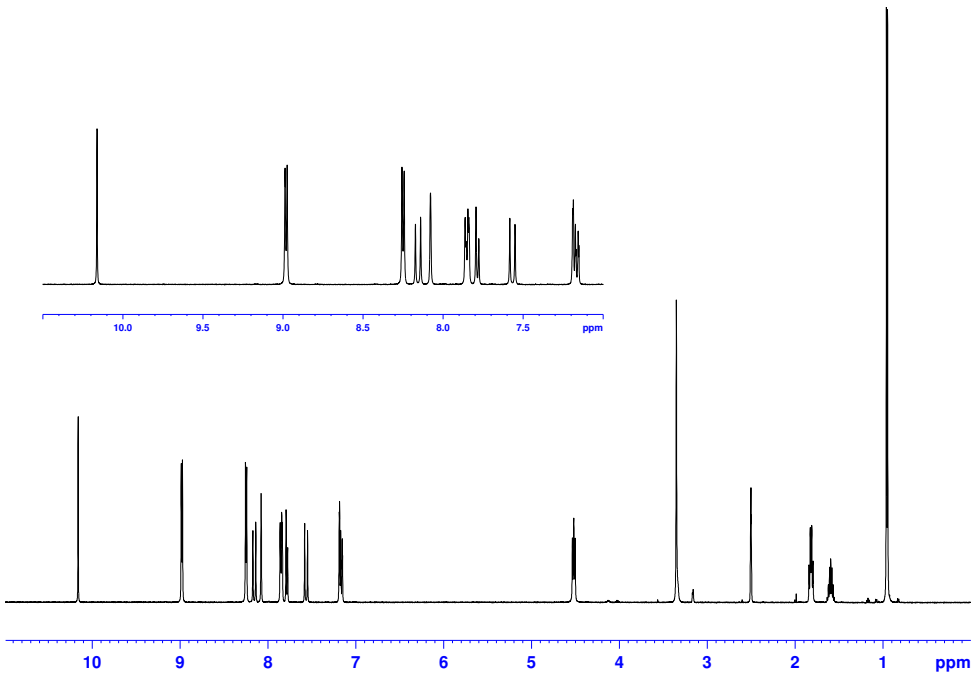
^{1}H NMR of **H3**



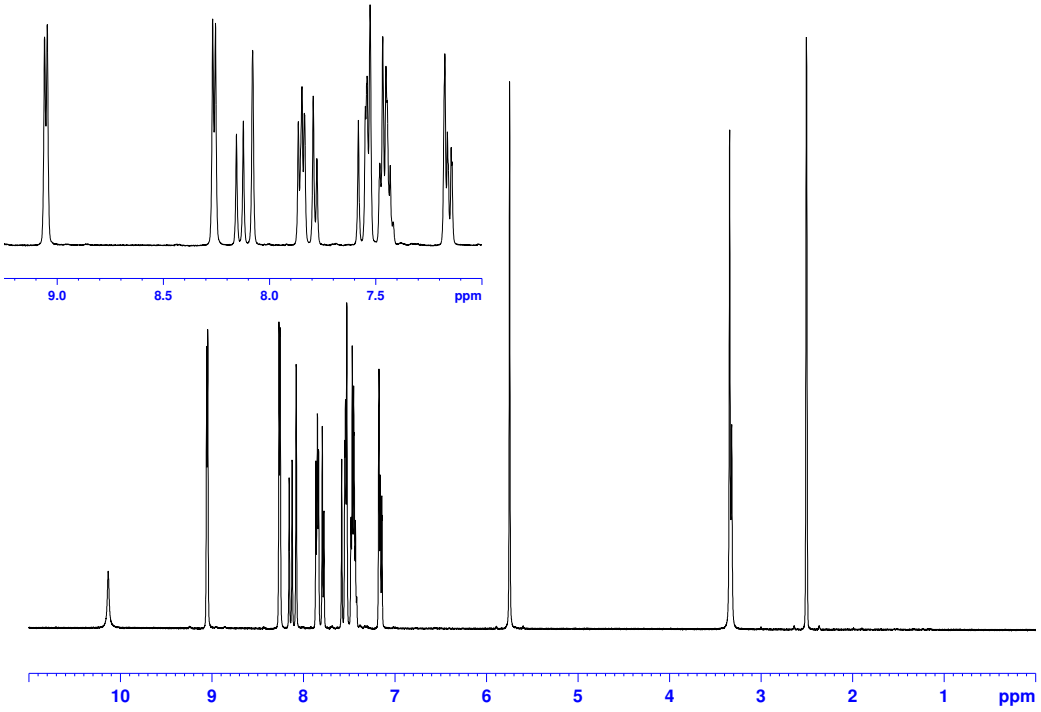
^{1}H NMR of **H4**



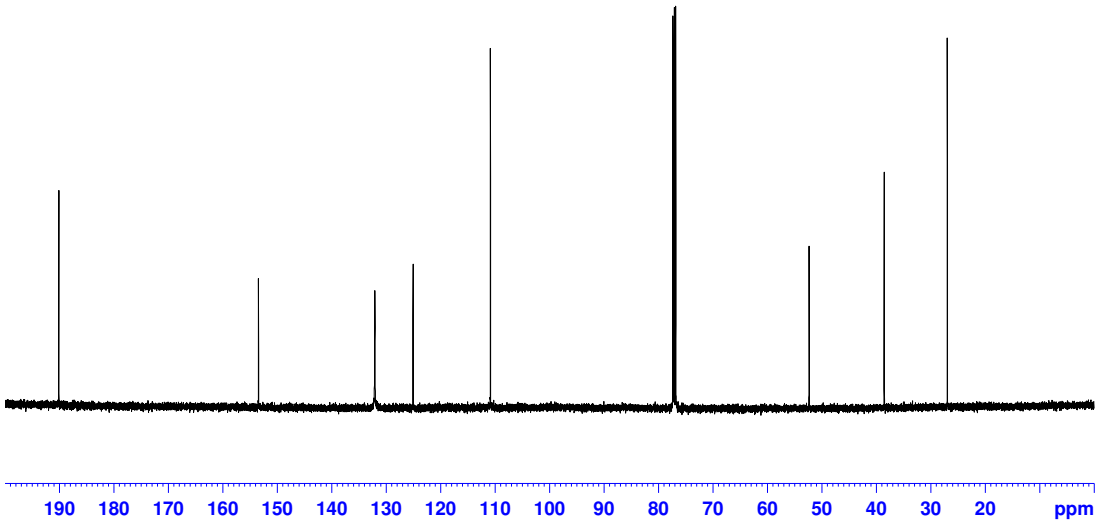
^{1}H NMR of **H5**



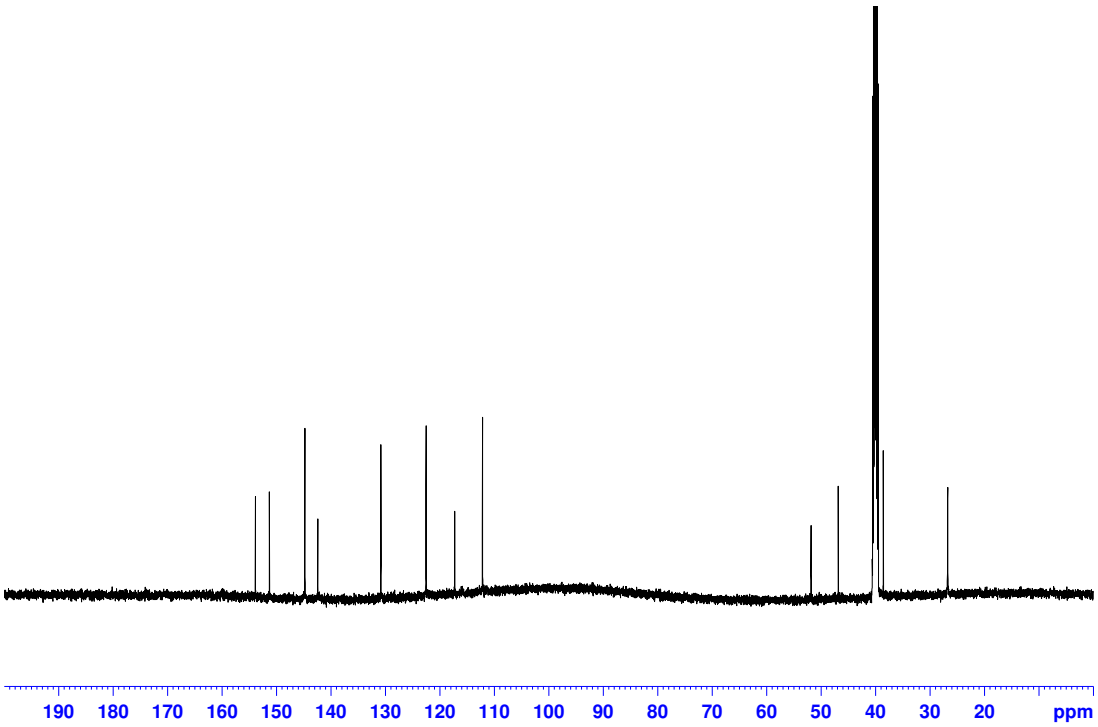
^{1}H NMR of **H6**



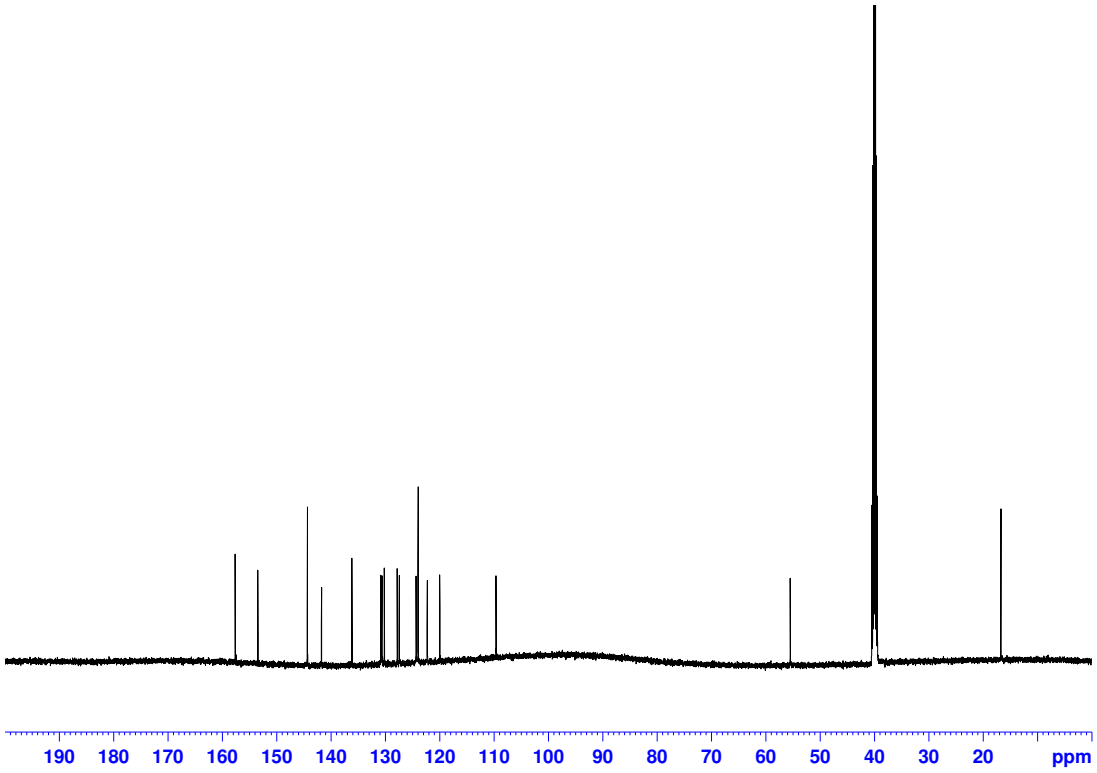
^{13}C NMR of **11**



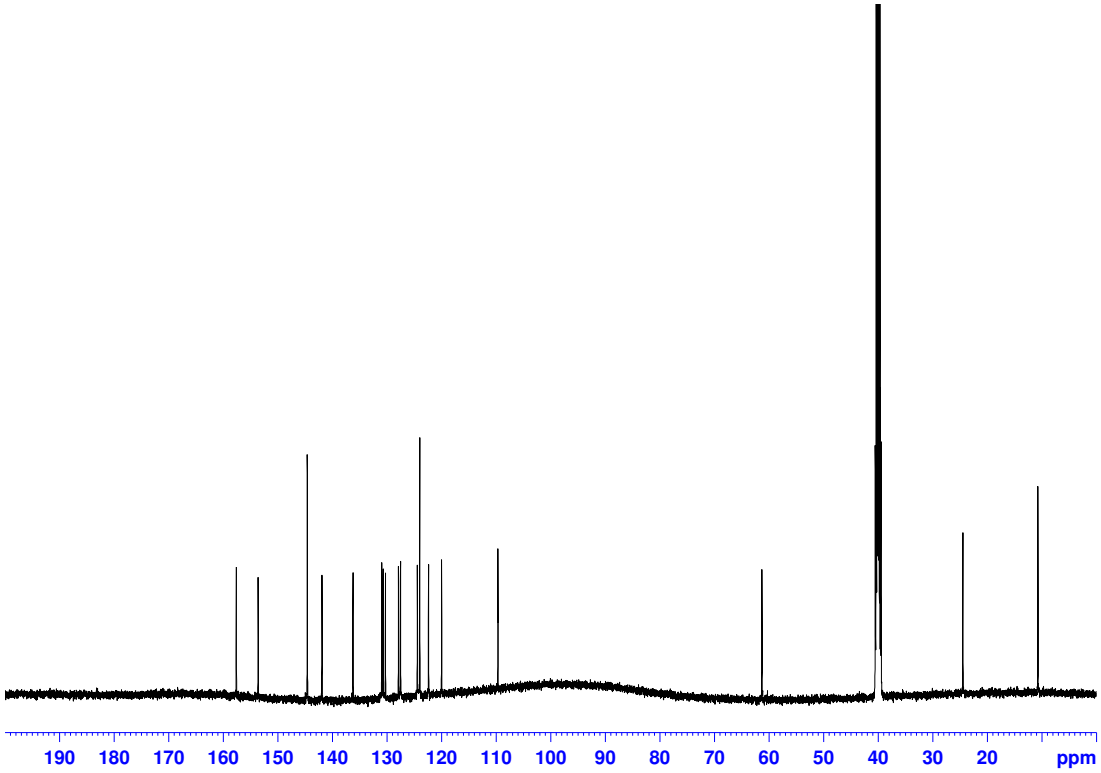
^{13}C NMR of **D2**



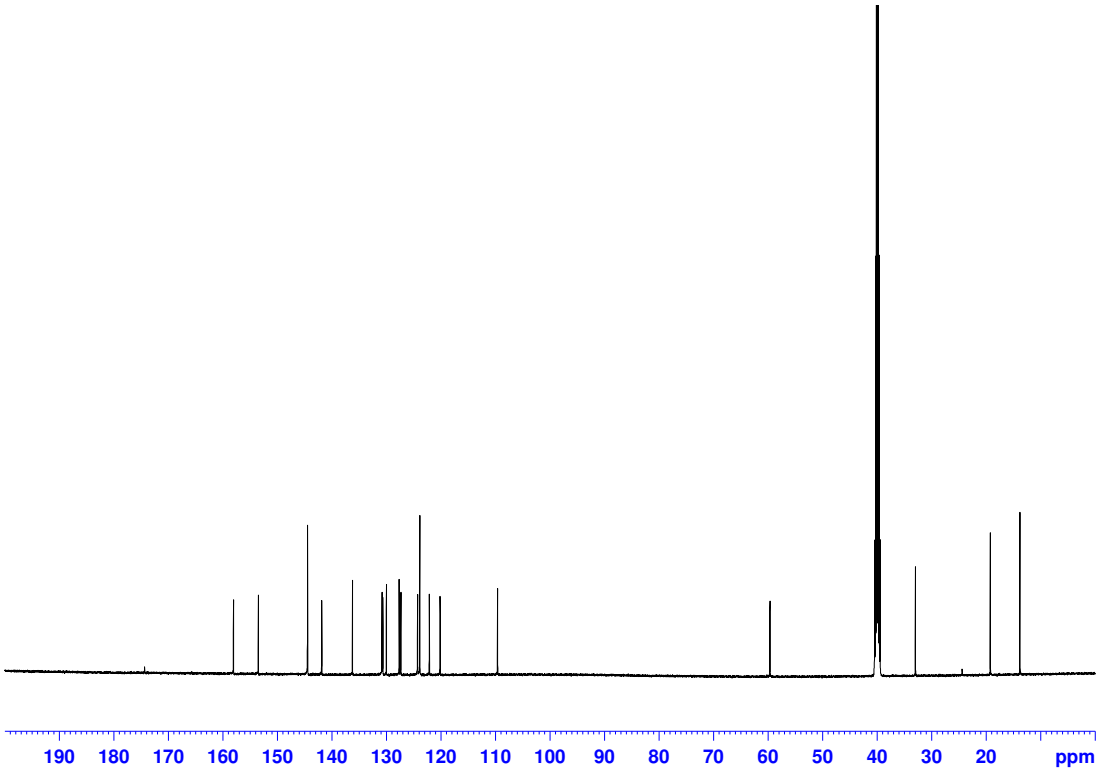
^{13}C NMR of **H2**



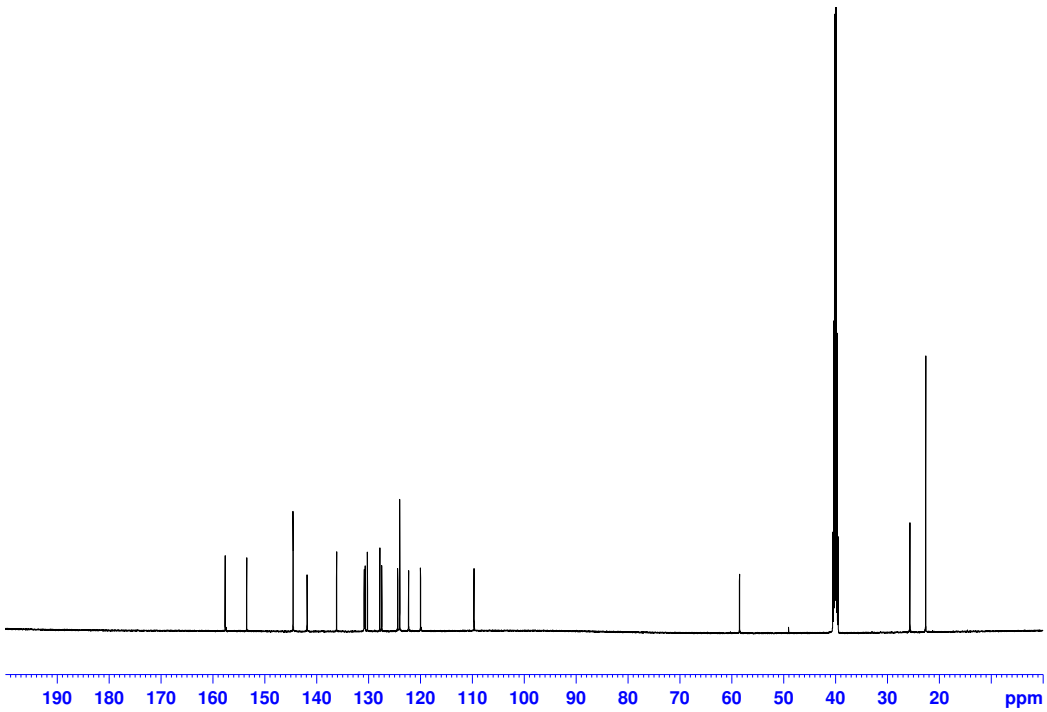
^{13}C NMR of **H3**



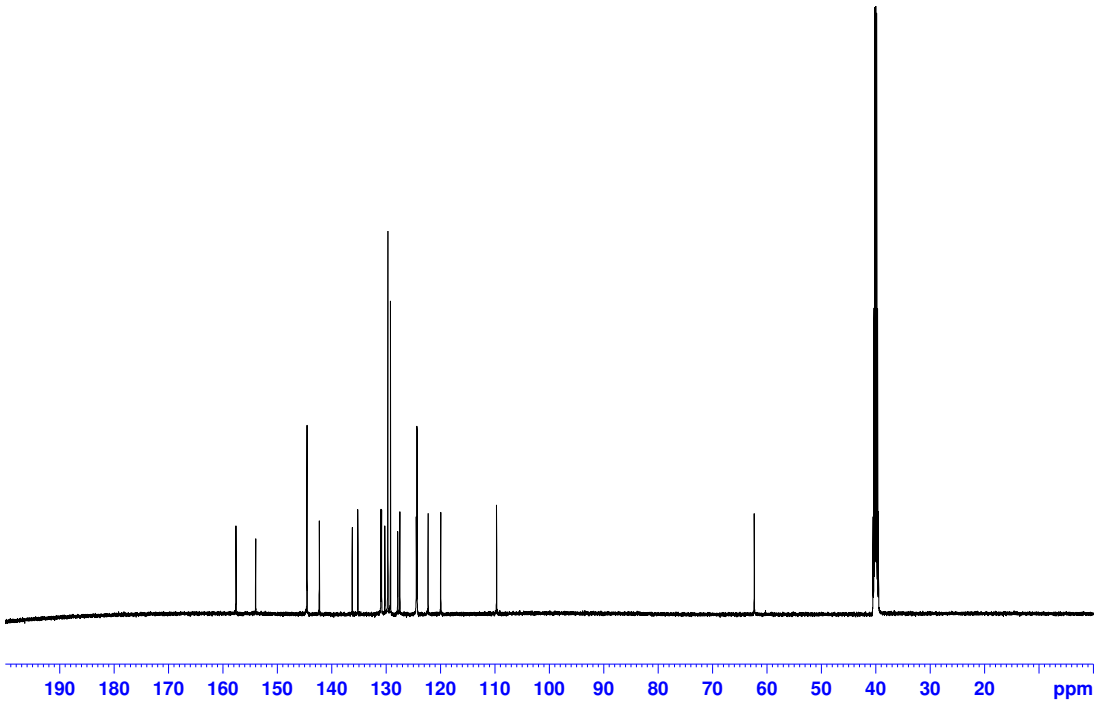
^{13}C NMR of **H4**



^{13}C NMR of **H5**



^{13}C NMR of **H6**



HSQC of **11**

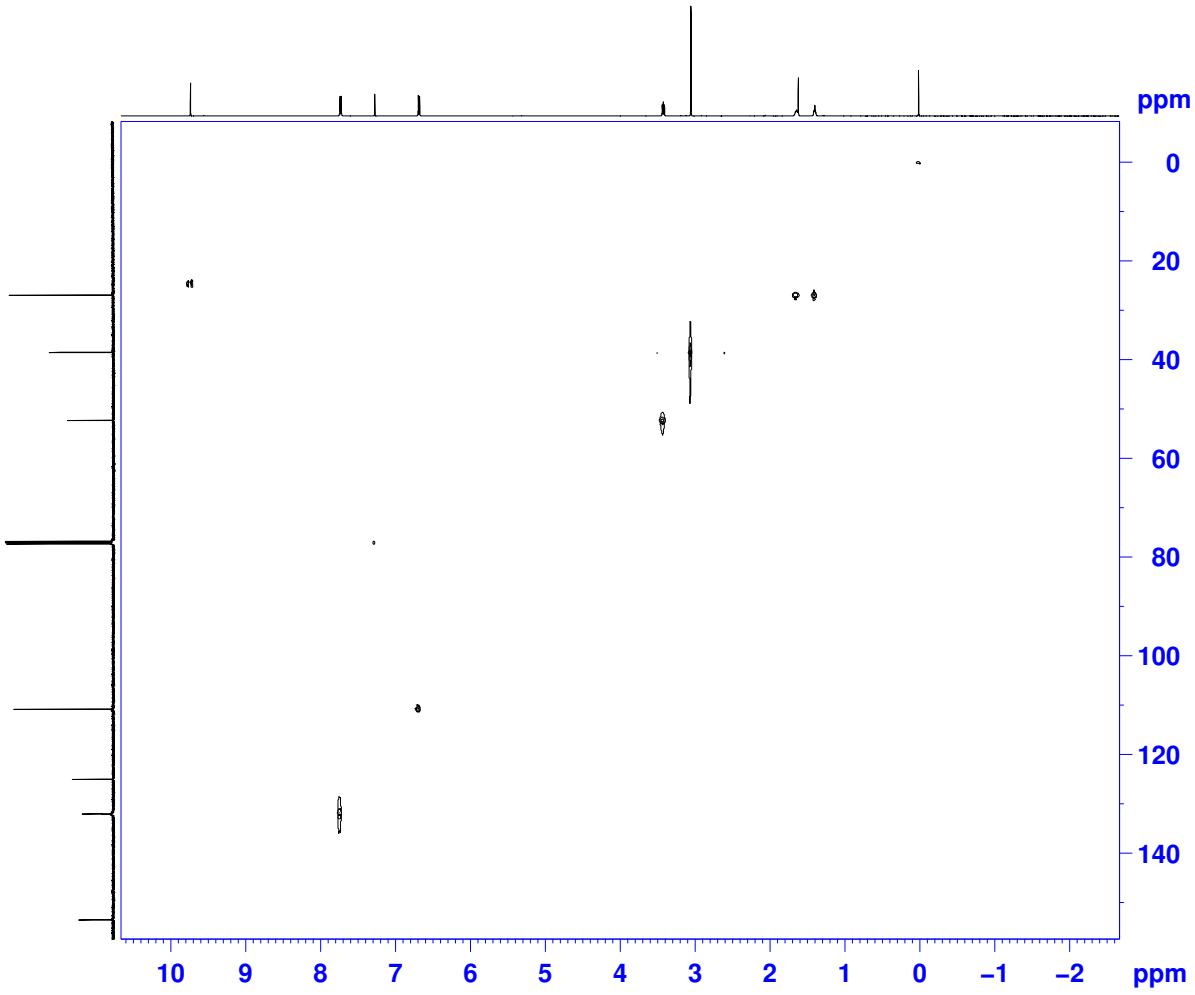


Table S1. Calculated $S_0 \rightarrow S_1$ transition energies and oscillator strength vs. interplanar twist angle.

A1

	toluene		THF		water	
	$S_0 \rightarrow S_1$ E (eV)	*f*	$S_0 \rightarrow S_1$ E (eV)	*f*	$S_0 \rightarrow S_1$ E (eV)	*f*
GS optimized[a]	2.49	1.41	2.56	1.34	2.61	1.29
10	2.48	1.39	2.55	1.31	2.61	1.26
20	2.44	1.31	2.52	1.23	2.57	1.2
30	2.37	1.17	2.45	1.1	2.52	1.05
40	2.25	0.98	2.35	0.91	2.43	0.87
50	2.08	0.74	2.21	0.68	2.30	0.64
60	1.86	0.49	2.03	0.44	2.15	0.41
70	1.59	0.25	1.82	0.22	1.97	0.2
80	1.31	0.07	1.64	0.06	1.83	0.05
90	1.17	0.00	1.57	0.00	1.77	0.00

H1

	toluene		THF		water	
	$S_0 \rightarrow S_1$ E (eV)	*f*	$S_0 \rightarrow S_1$ E (eV)	*f*	$S_0 \rightarrow S_1$ E (eV)	*f*
GS optimized[b]	2.43	0.95	2.61	0.94	2.71	0.93
10	2.41	0.93	2.59	0.92	2.71	0.91
20	2.38	0.87	2.57	0.85	2.69	0.84
30	2.32	0.77	2.53	0.75	2.66	0.74
40	2.23	0.63	2.48	0.62	2.62	0.6
50	2.12	0.48	2.40	0.46	2.56	0.45
60	1.98	0.32	2.31	0.3	2.50	0.28
70	1.83	0.16	2.23	0.15	2.44	0.14
80	1.70	0.04	2.16	0.04	2.40	0.04
90	1.65	0.00	2.00	0.00	2.39	0.00

[a] for **A1** the ground state geometry exhibits interplane twist angles of 0.4°, 0.4° and 0.5° in toluene, THF and water, respectively.
[b] for **H1** the ground state geometry exhibits interplane twist angles of 1.6°, 1.5° and 0.1° in toluene, THF and water, respectively.