Supplementary Materials

Exploring mannosylpurines as copper chelators and cholinesterase inhibitors with potential to Alzheimer's disease

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^{1}H NMR and ^{13}C NMR spectra of the new compounds 5-8, 9,10, 12, 13, 15 and 16

Compound **5** (in CD_3OD)

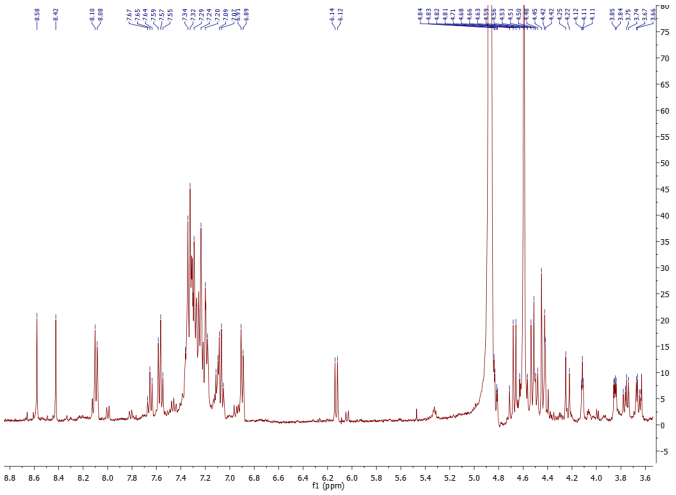


Figure S1. ^{1}H NMR spectrum for compound **5**.

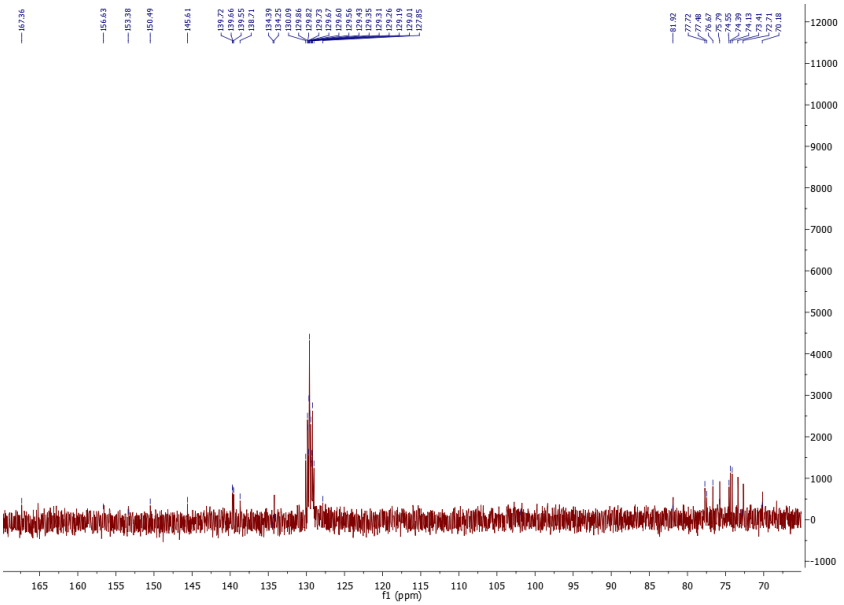


Figure S2. ^{13}C NMR spectrum for compound **5**.

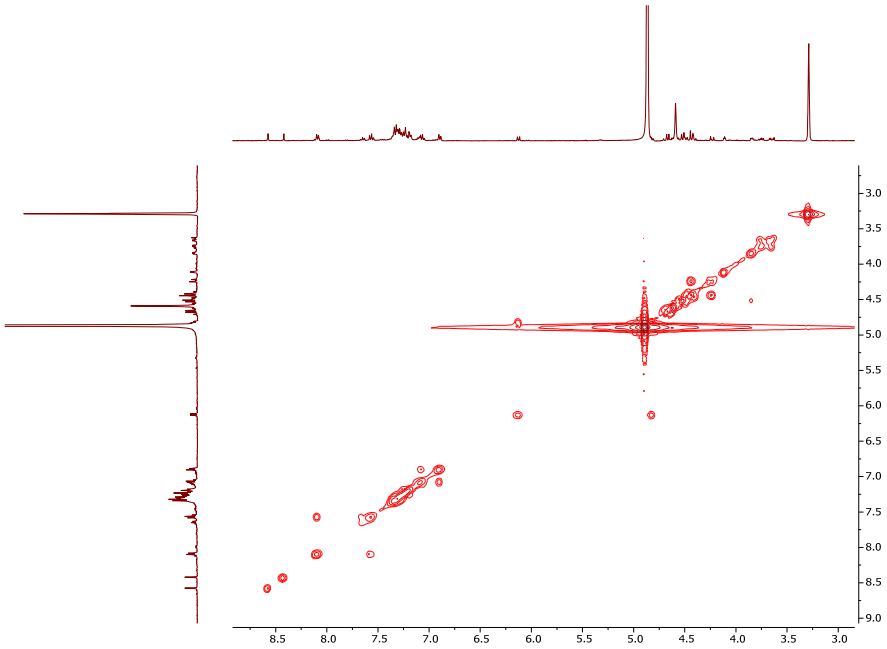


Figure S3. COSY spectrum for compound **5**.

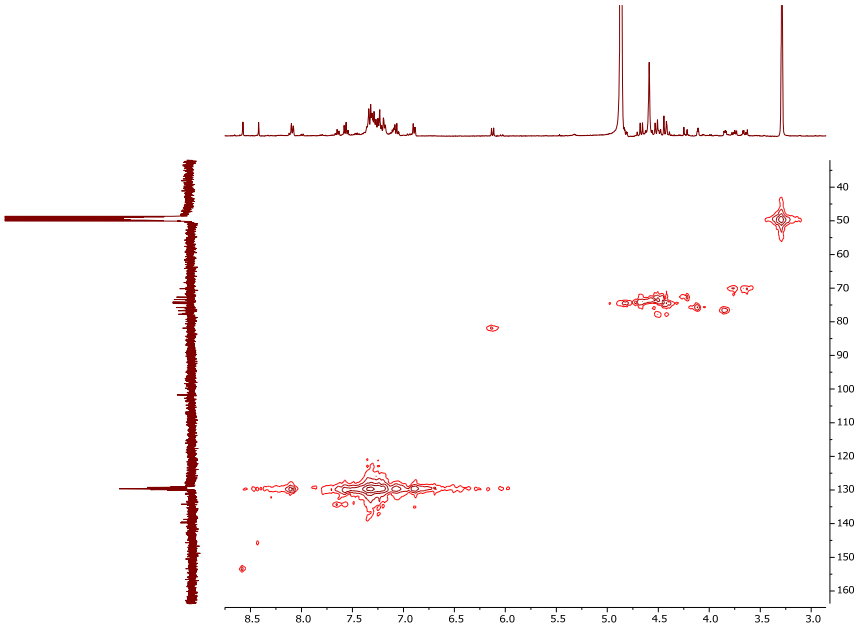


Figure S4. HSQC spectrum for compound **5**.

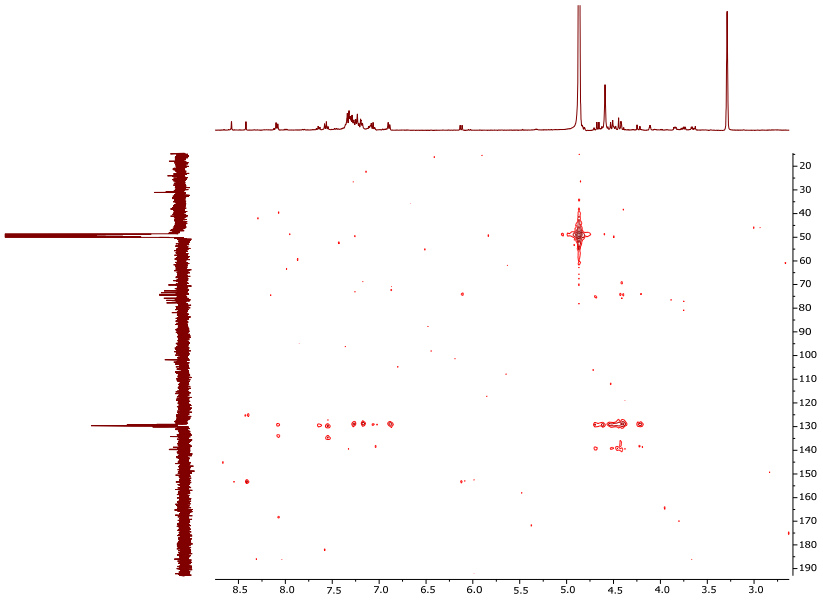


Figure S5. HMBC spectrum for compound **5**.

Compound **6** (in $CDCl_3$)

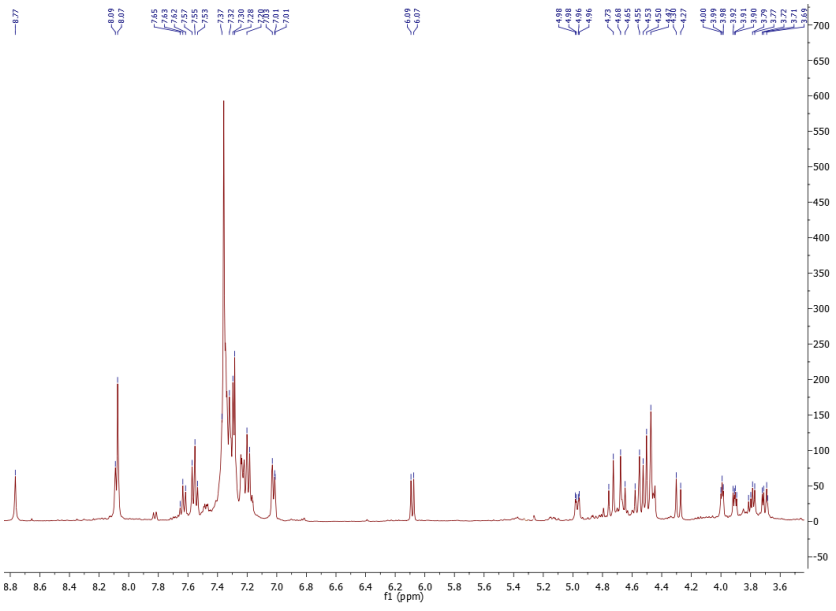


Figure S6. ^{1}H NMR spectrum for compound **6**.

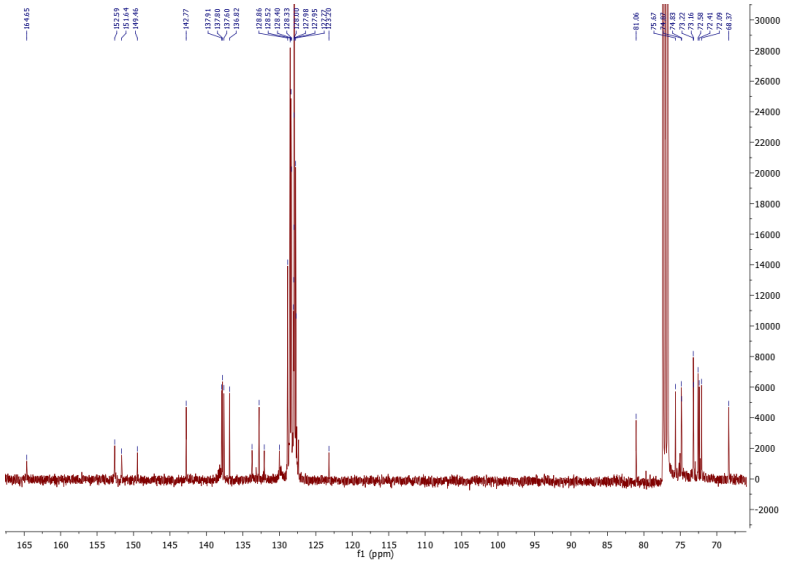


Figure S7. ^{13}C NMR spectrum for compound **6**.

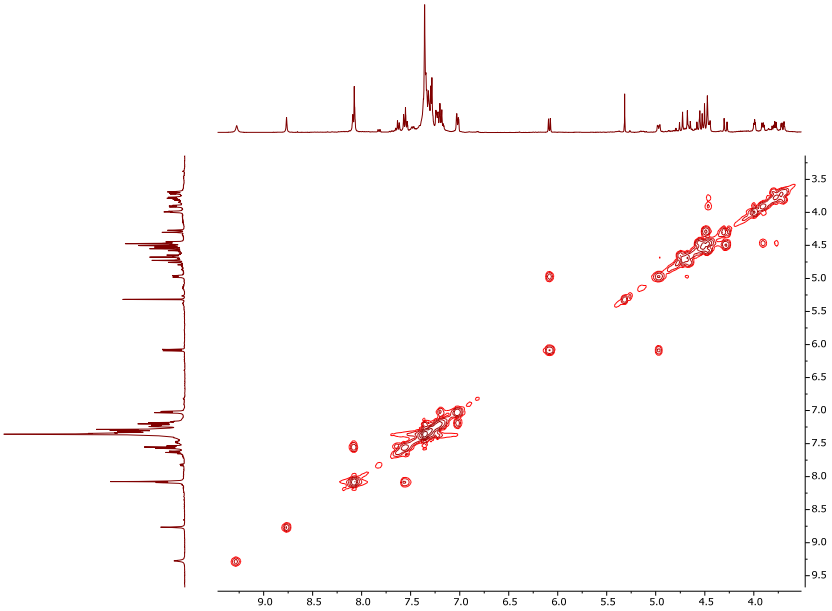


Figure S8. COSY spectrum for compound **6**.

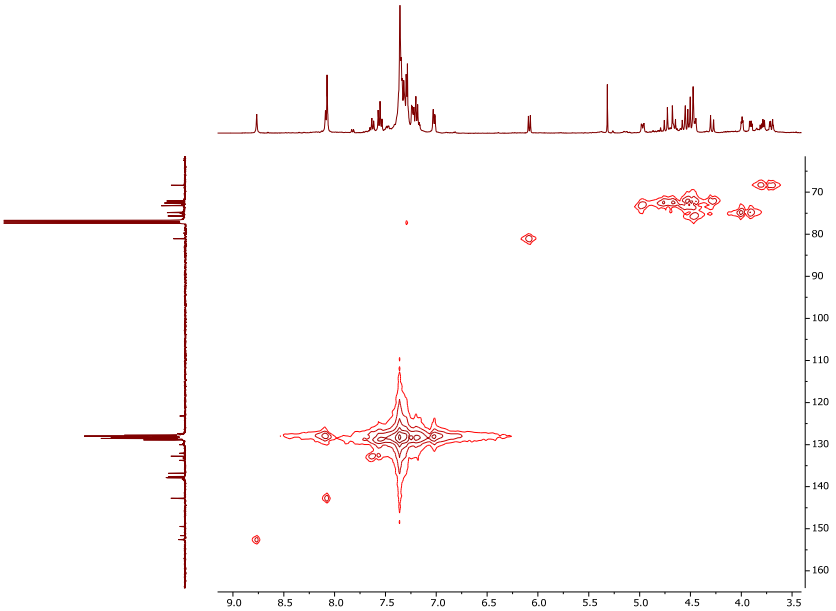


Figure S9. HSQC spectrum for compound **6**.

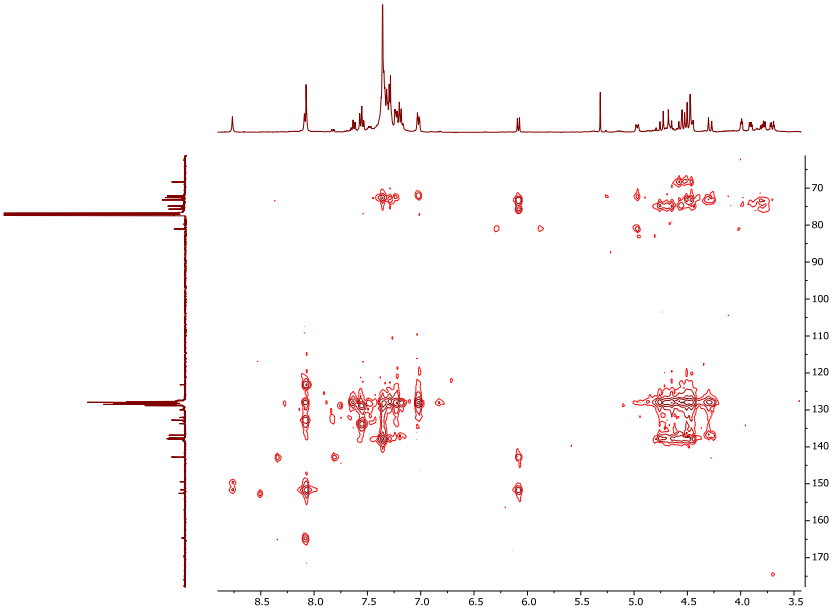


Figure S10. HMBC spectrum for compound **6**.

Compound **7** (in CD_3OD)

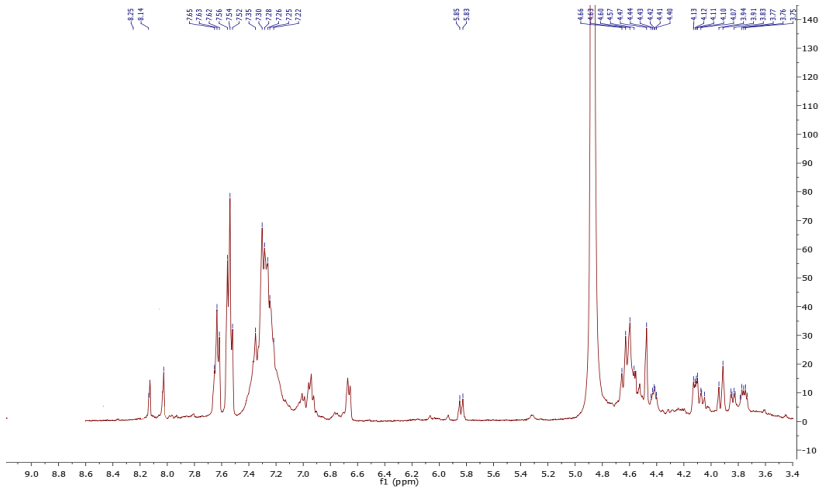


Figure S11. ^{1}H NMR spectrum for compound **7**.

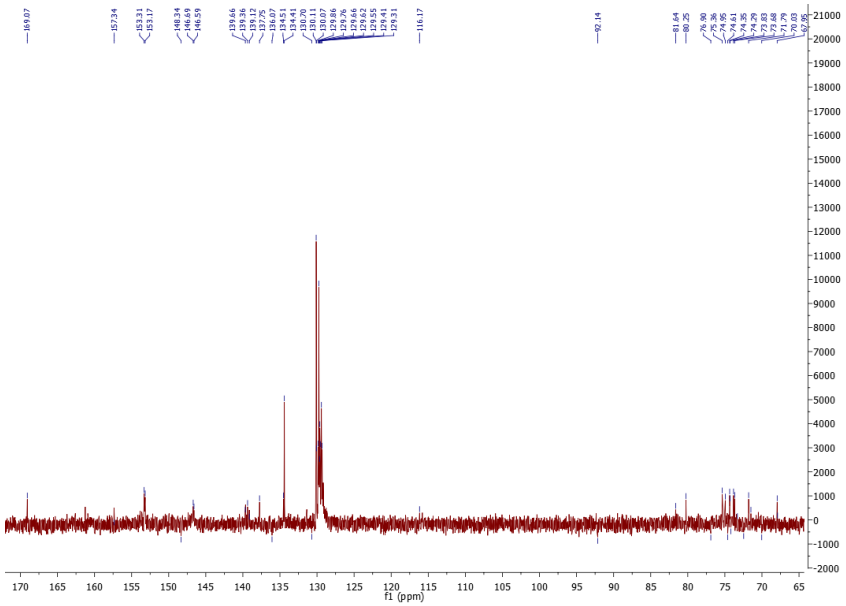


Figure S12. ^{13}C NMR spectrum for compound **7**.

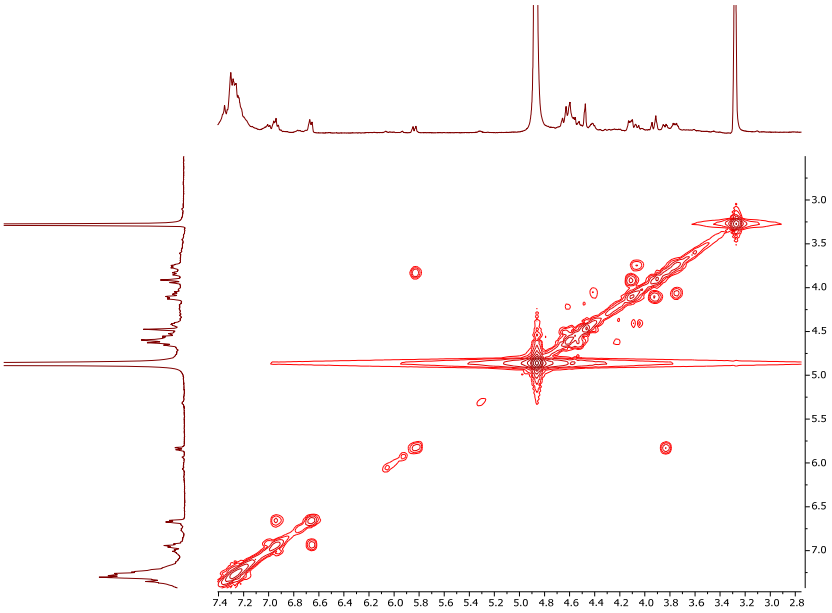


Figure S13. COSY spectrum for compound **7**.

Compound **8** (in CD_3OD)

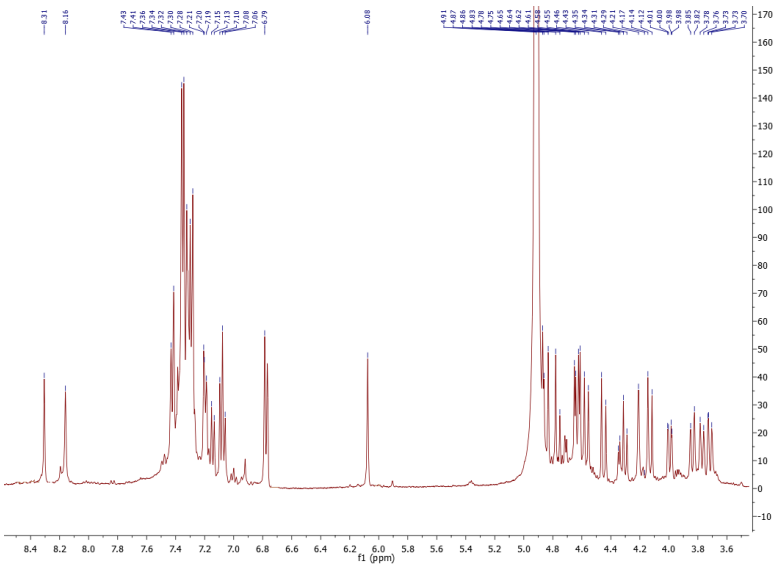


Figure S14. ^1H NMR spectrum for compound **8**.

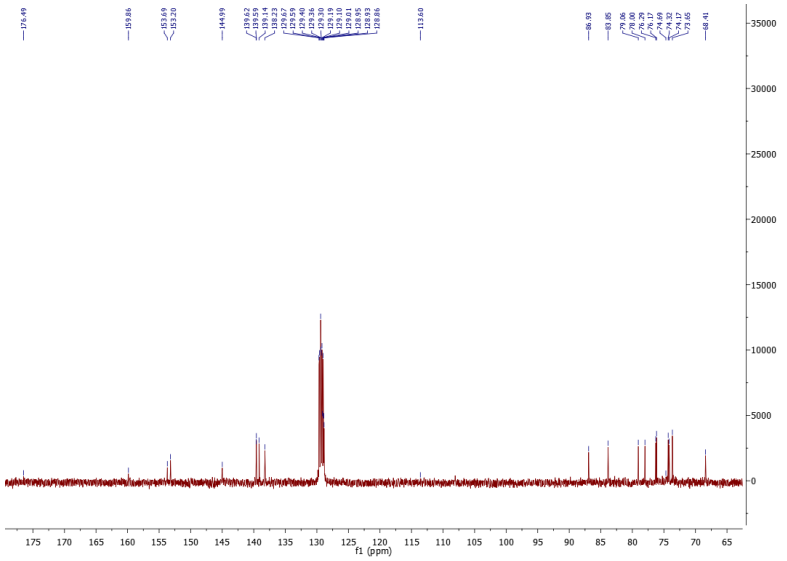


Figure S15. ^{13}C NMR spectrum for compound **8**.

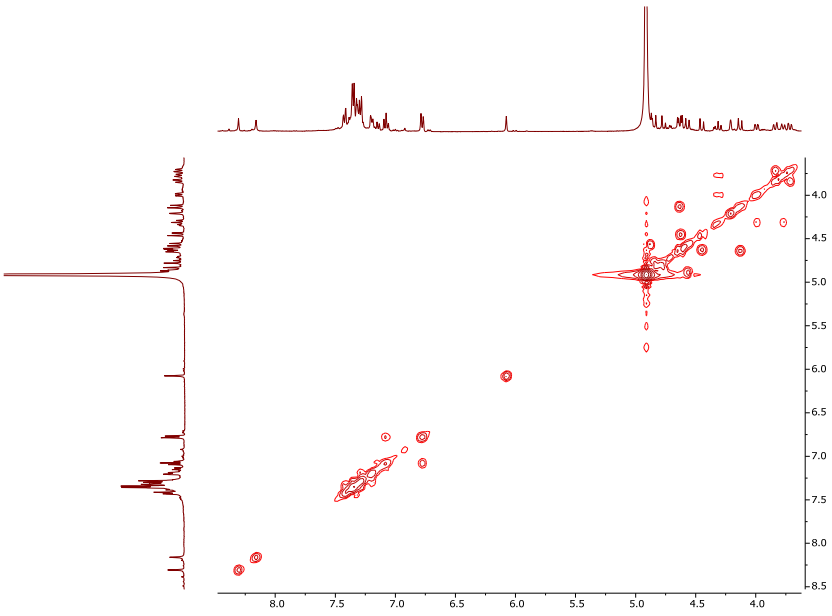


Figure S16. COSY spectrum for compound **8**.

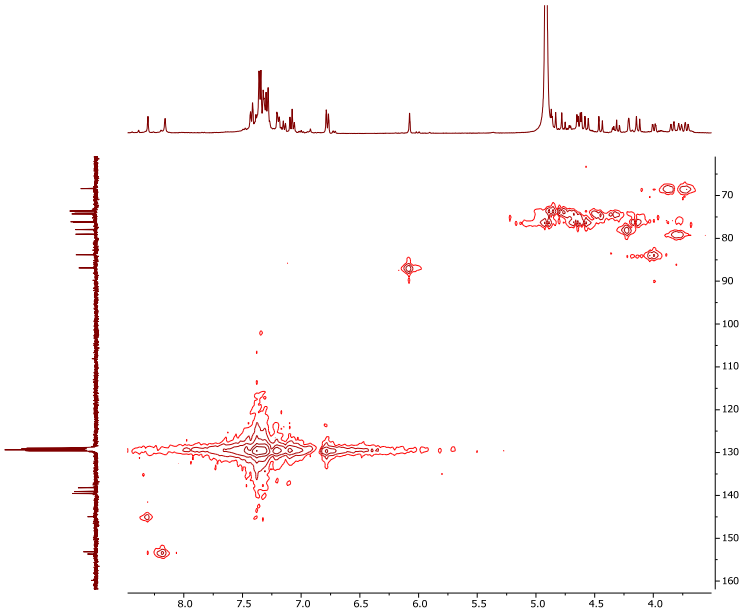


Figure S17. HSQC spectrum for compound **8**.

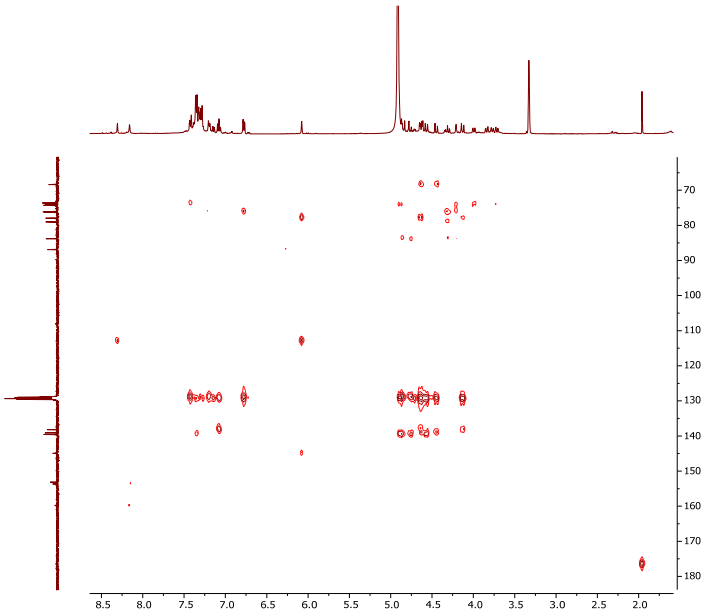


Figure S18. HMBC spectrum for compound **8**.

Compound **9** (in CD_3OD)

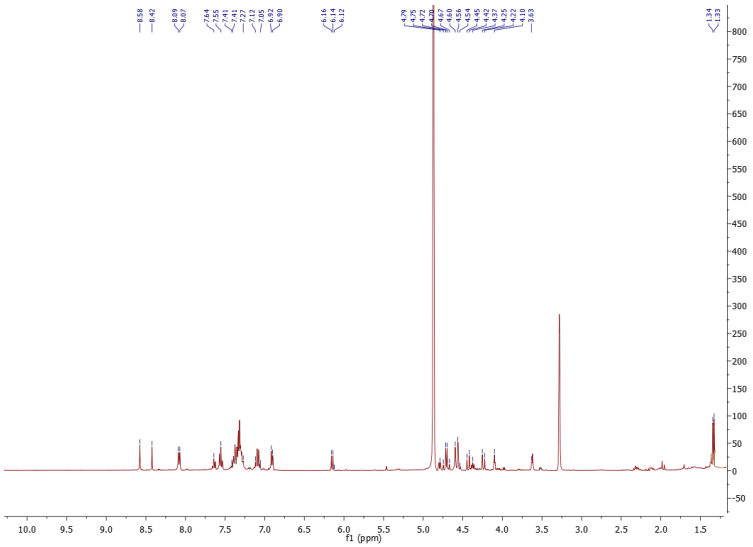


Figure S19. ^{1}H NMR spectrum for compound **9**.

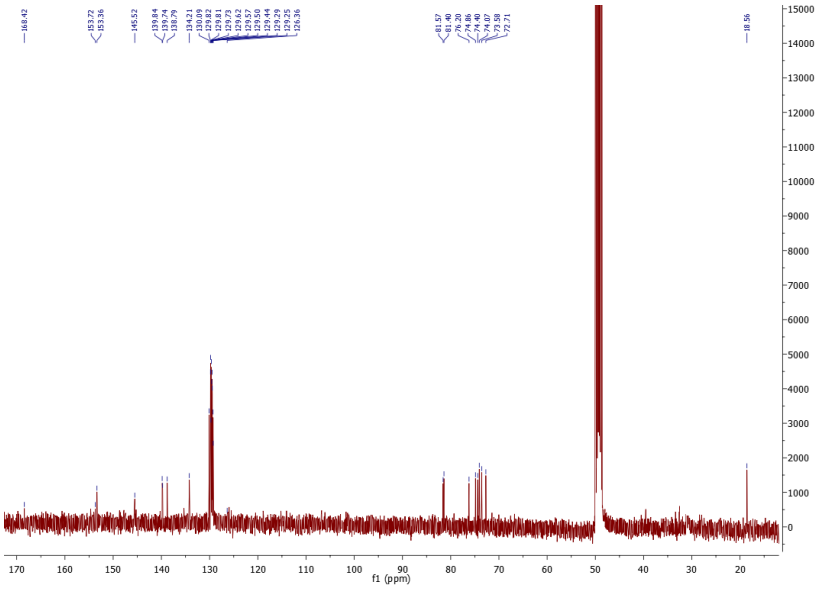


Figure S20. ^{13}C NMR spectrum for compound **9**.

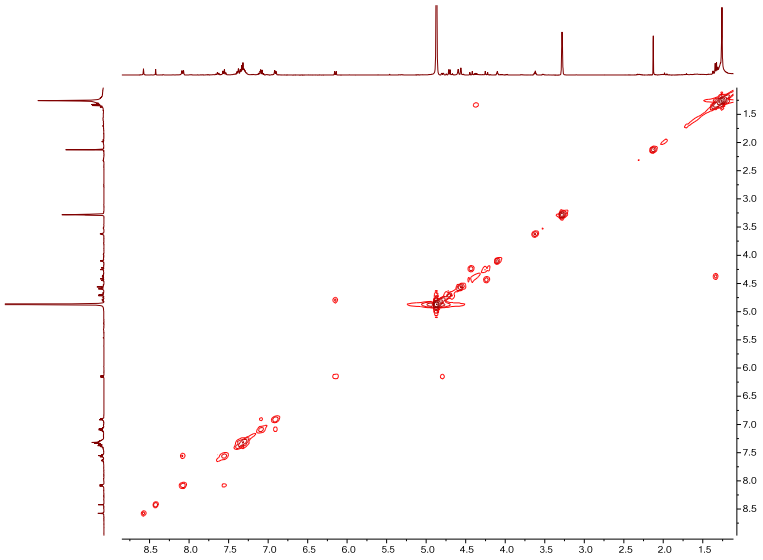


Figure S21. COSY spectrum for compound **9**.

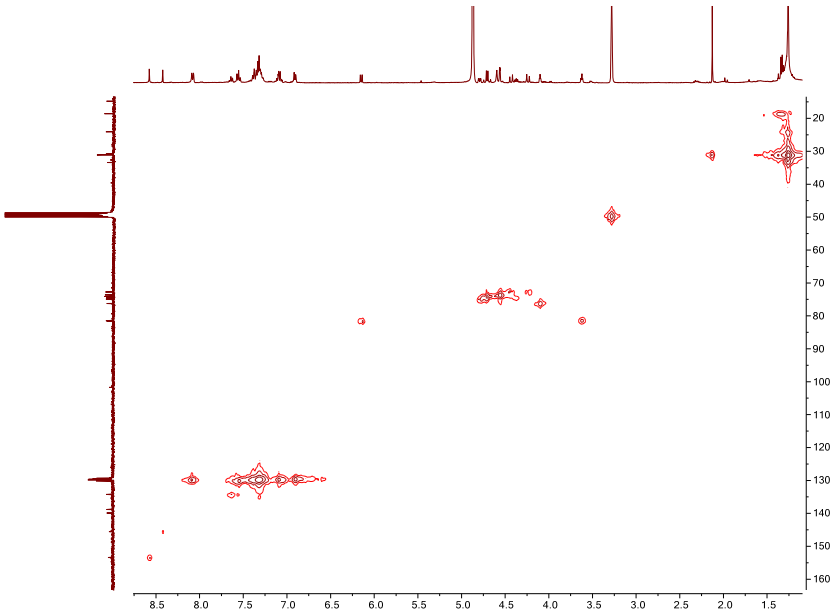


Figure S22. HSQC spectrum for compound **9**.

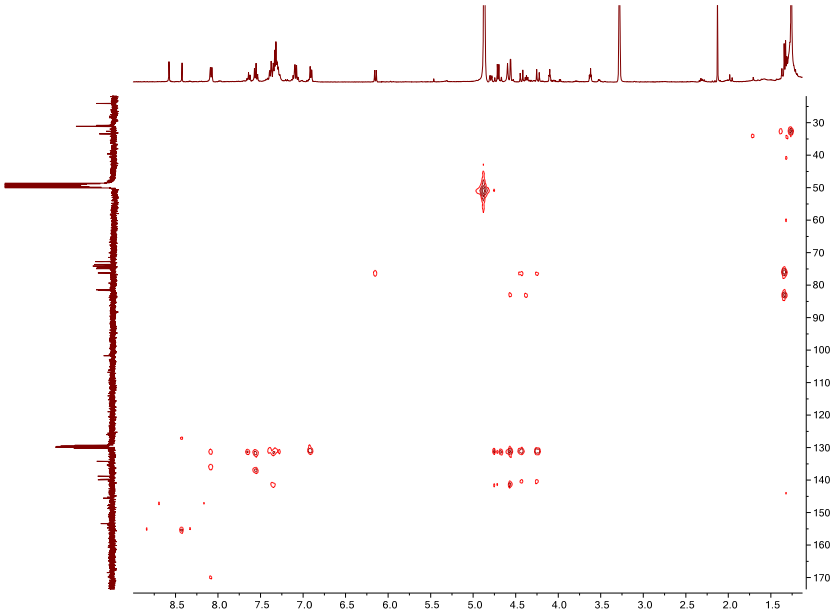


Figure S23. HMBC spectrum for compound **9**.

Compound **10** (in CD_3OD)

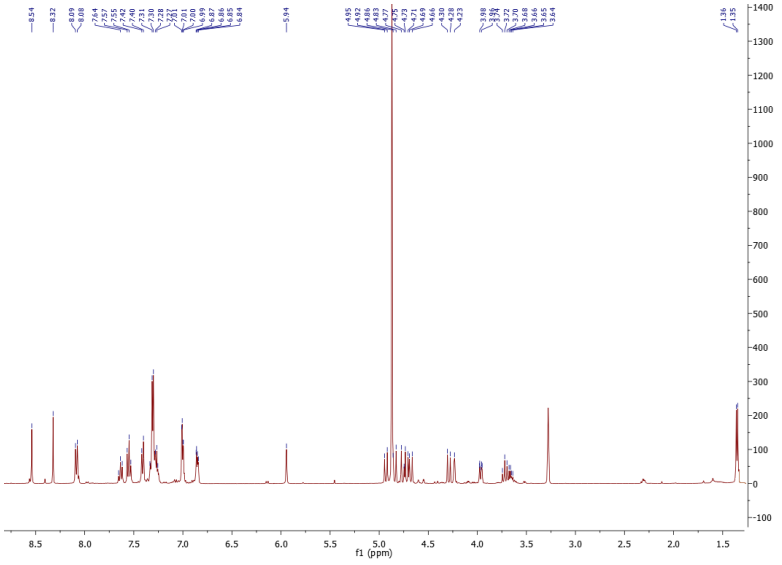


Figure S24. ^1H NMR spectrum for compound **10**.

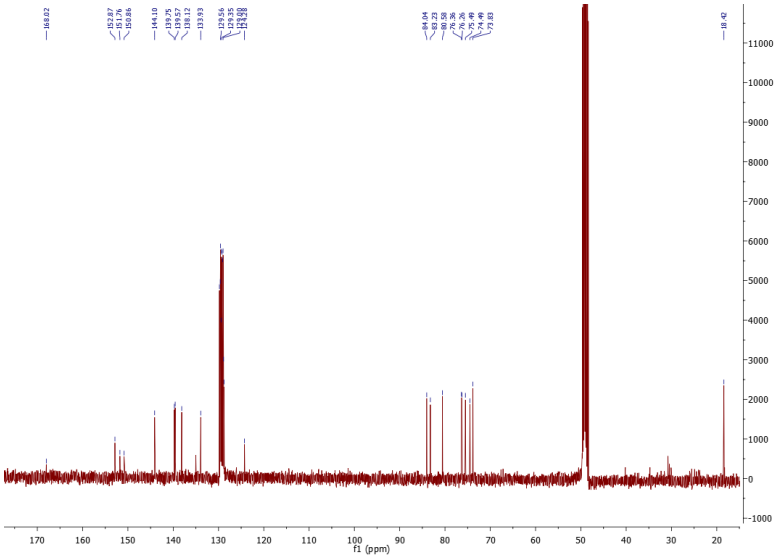


Figure S25. ^{13}C NMR spectrum for compound **10**.

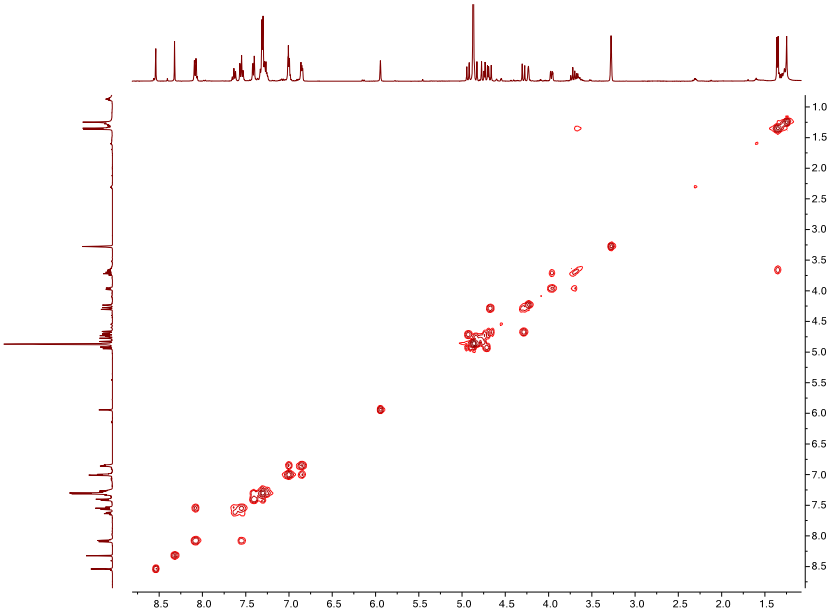


Figure S26. COSY spectrum for compound **10**.

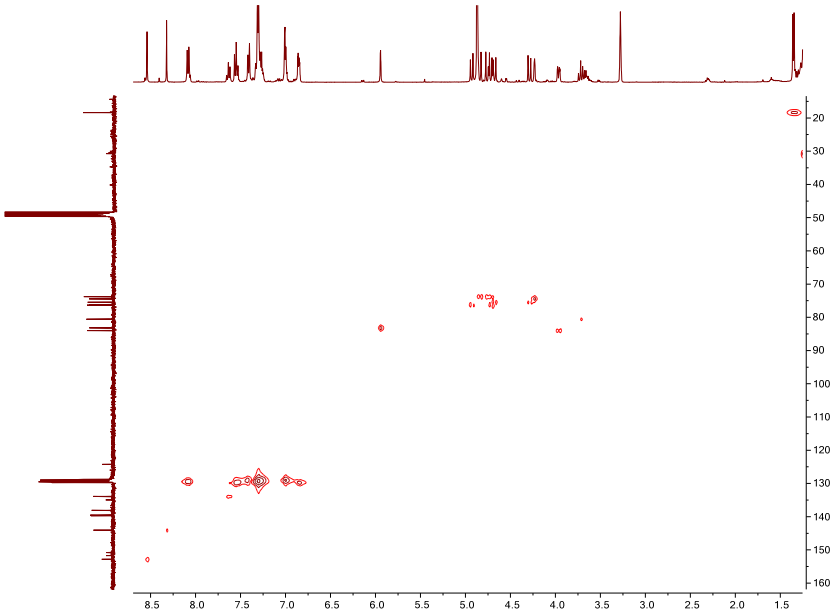


Figure S27. HSQC spectrum for compound **10**.

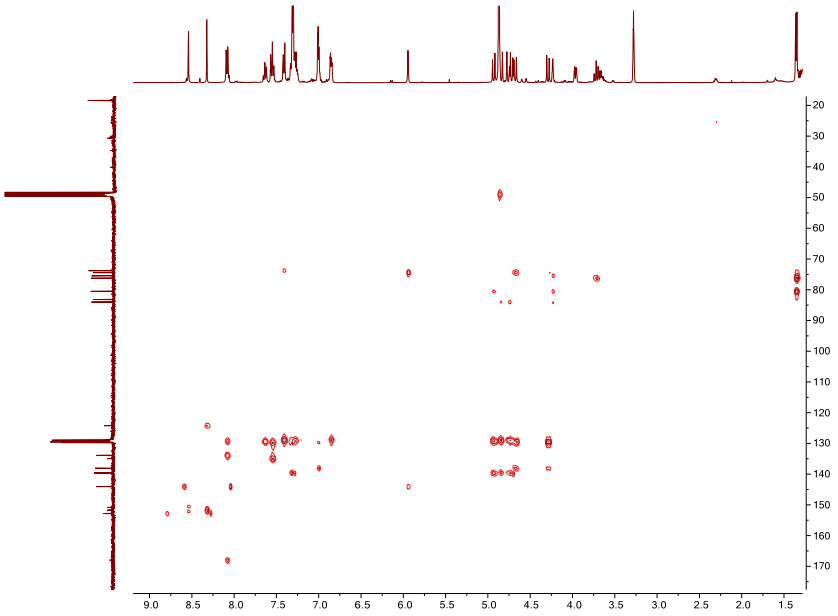


Figure S28. HMBC spectrum for compound **10**.

Compound **12** (in CD_3OD)

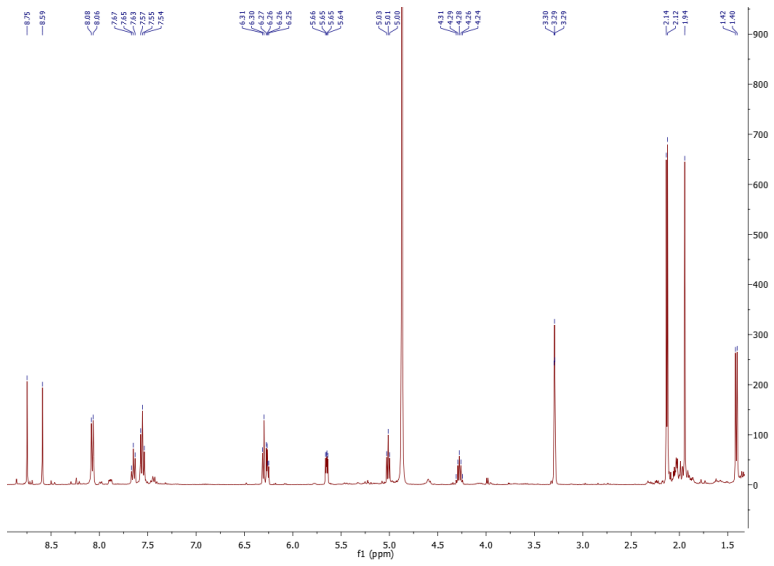


Figure S29. ^{1}H NMR spectrum for compound **12**.

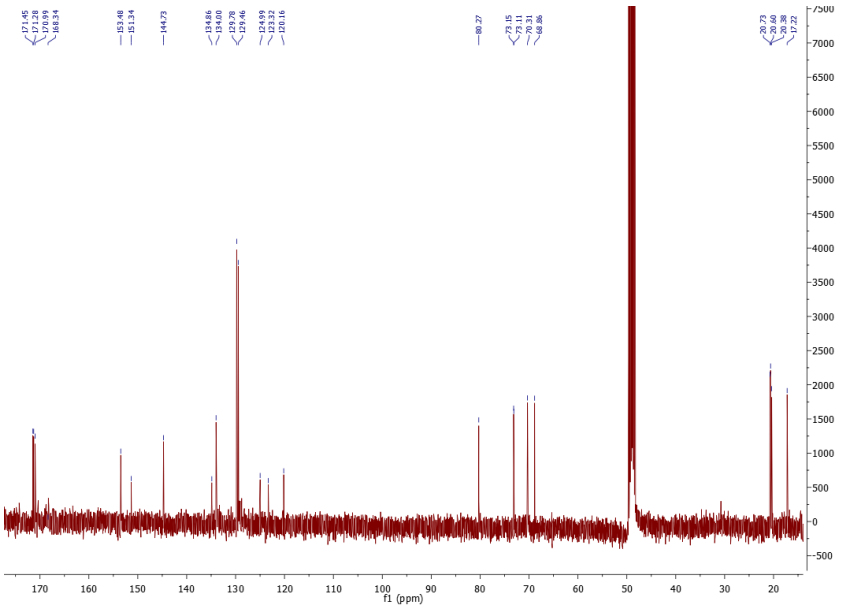


Figure S30. ^{13}C NMR spectrum for compound **12**.

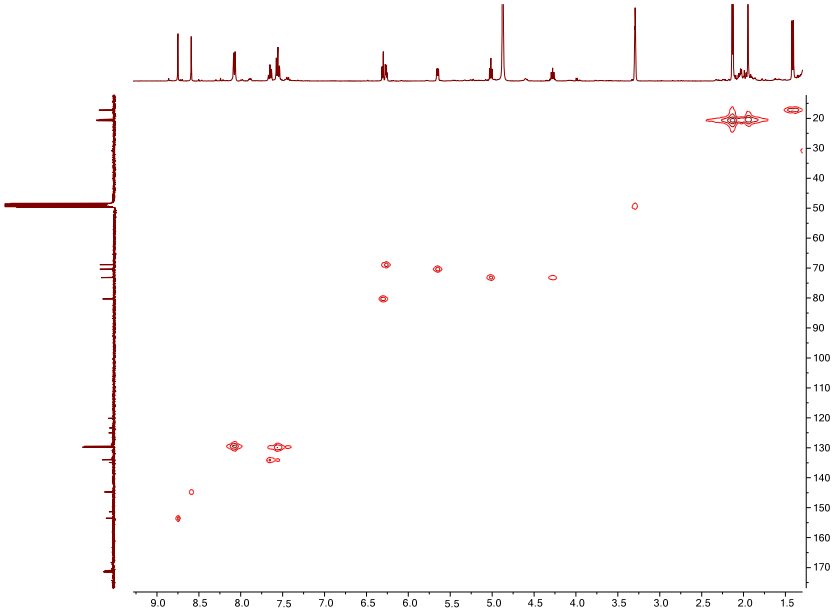


Figure S31. HSQC spectrum for compound **12**.

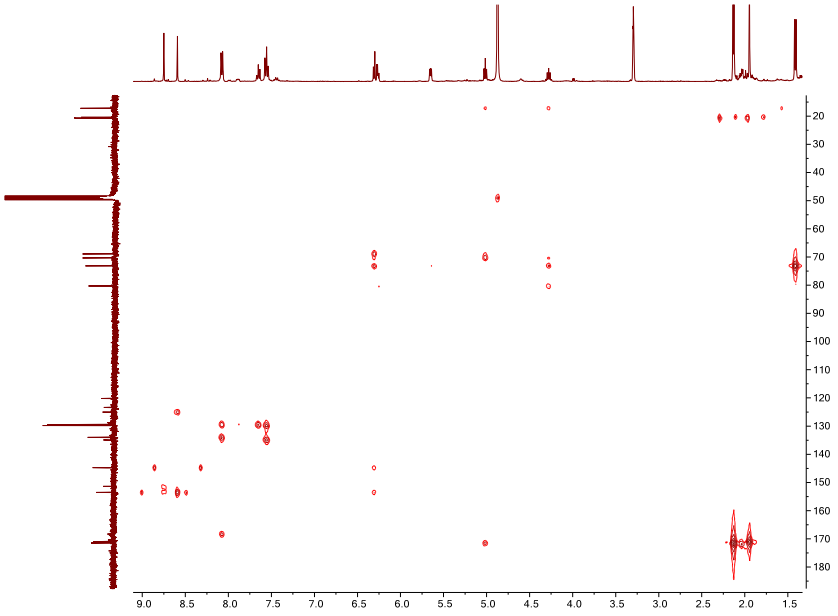


Figure S32. HMBC spectrum for compound **12**.

Compound **13 (**in CD_3OD)

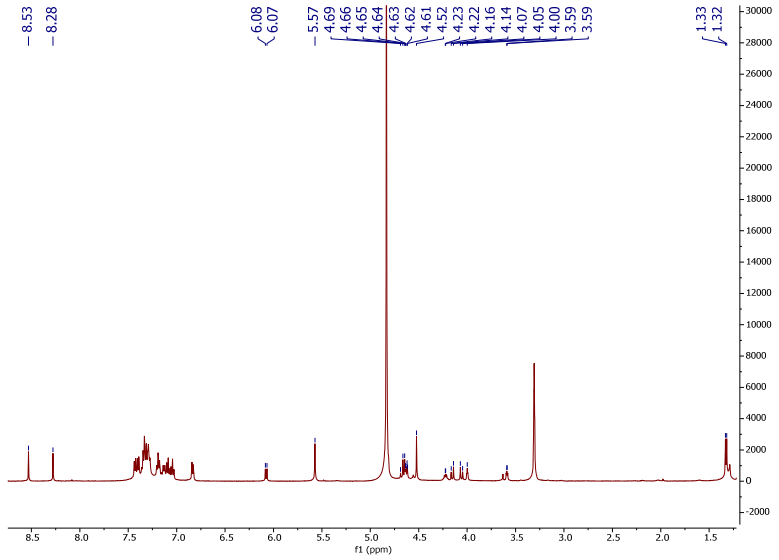


Figure S33. ^{1}H NMR spectrum for compound **13**.

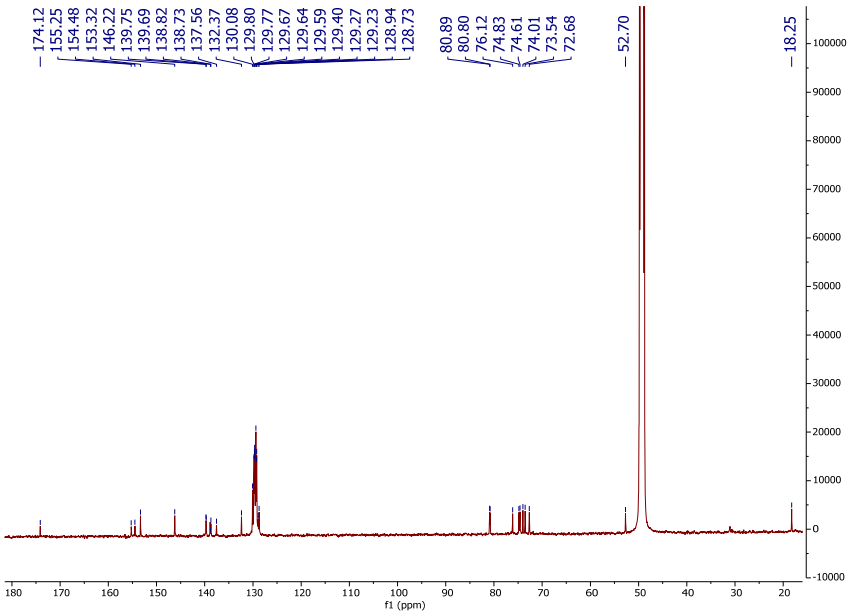


Figure S34. ^{13}C NMR spectrum for compound **13**.

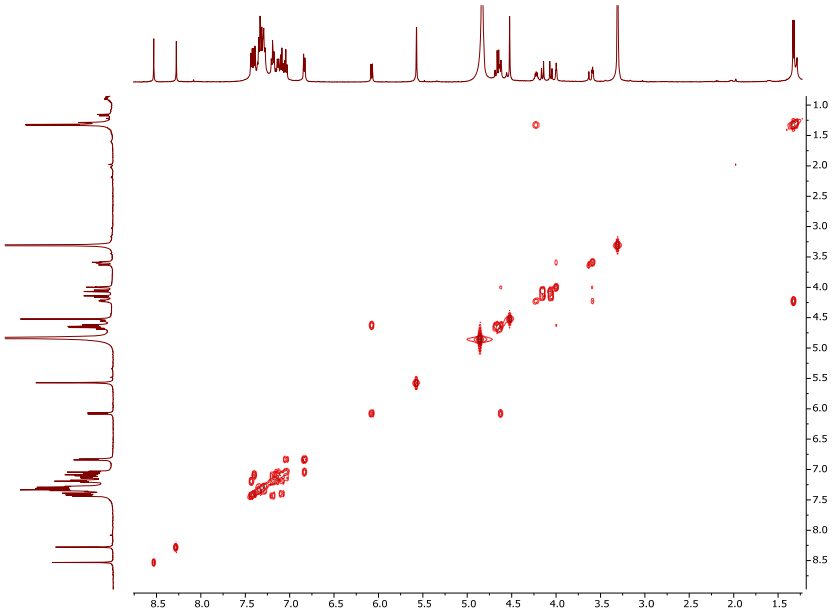


Figure S35. COSY spectrum for compound **13**.

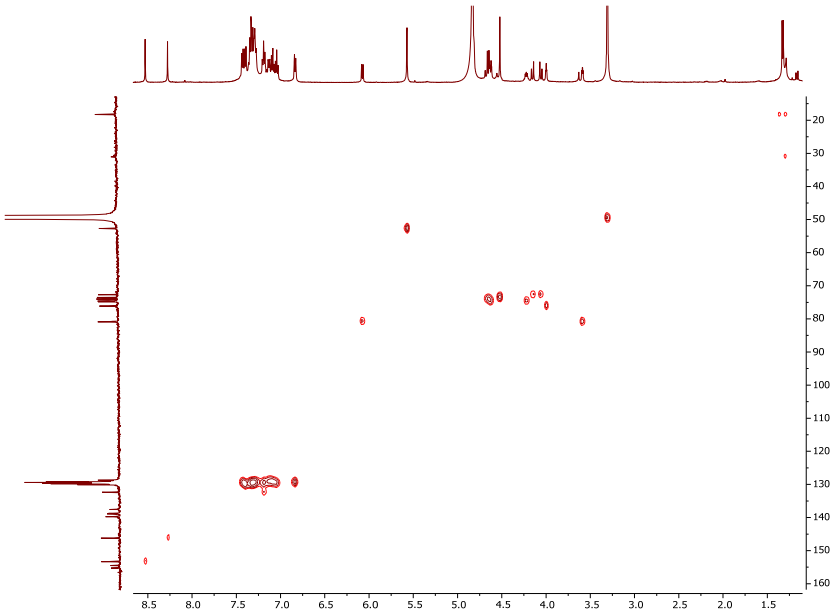


Figure S36. HSQC spectrum for compound **13**.

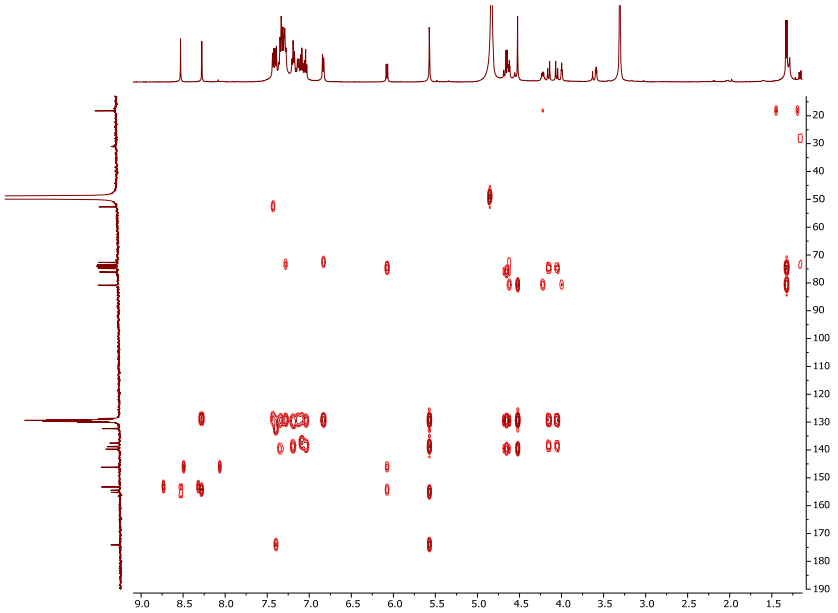


Figure S37. HMBC spectrum for compound **13**.

Compound **15** (in CD_3OD)

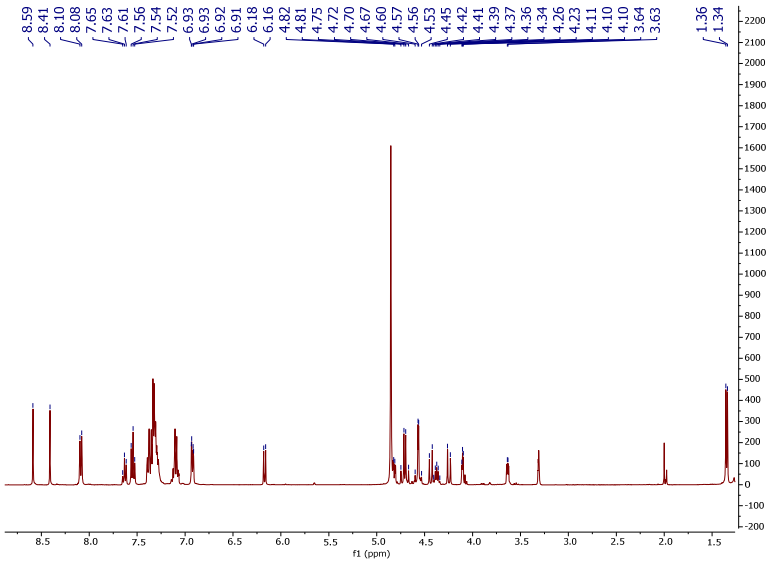


Figure S38. ^{1}H NMR spectrum for compound **15**.

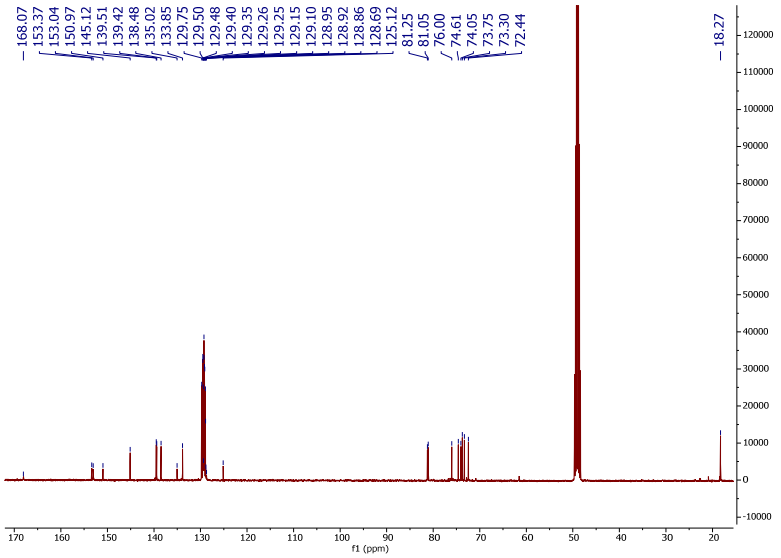


Figure S39. ^{13}C NMR spectrum for compound **15**.

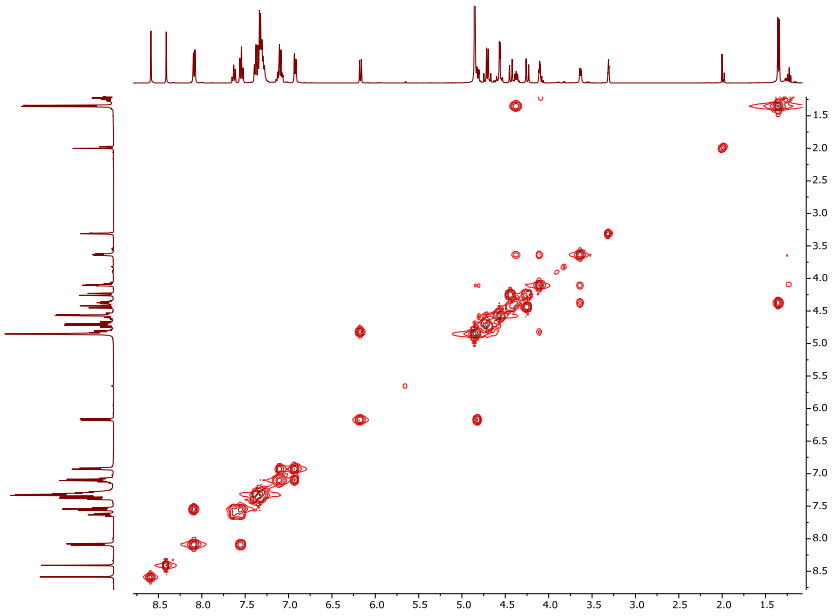


Figure S40. COSY spectrum for compound **15**.

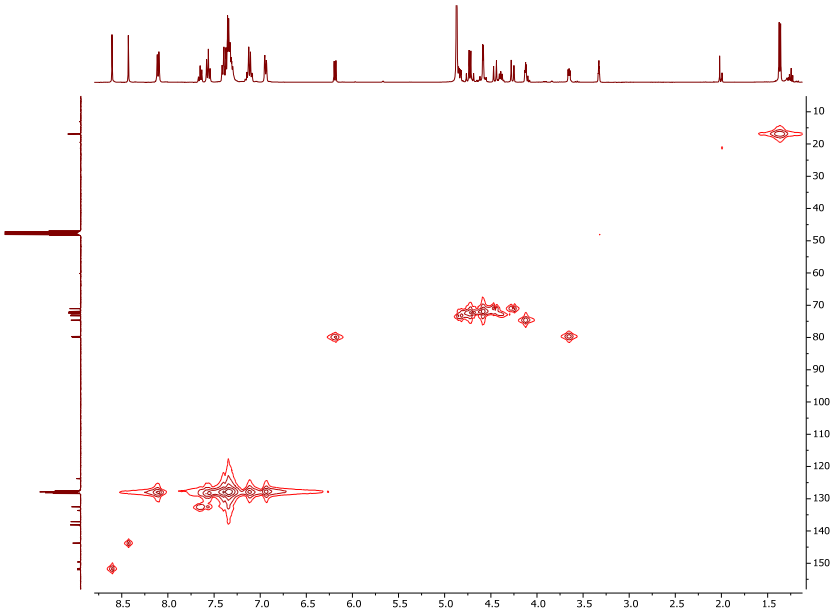


Figure S41. HSQC spectrum for compound **15**.

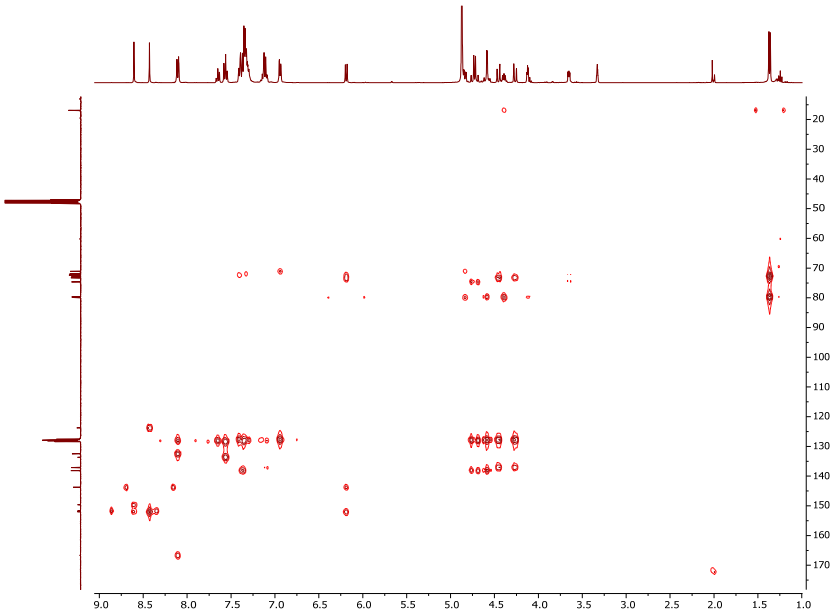


Figure S42. HMBC spectrum for compound **15**.

Compound **16** (in CD_3OD)

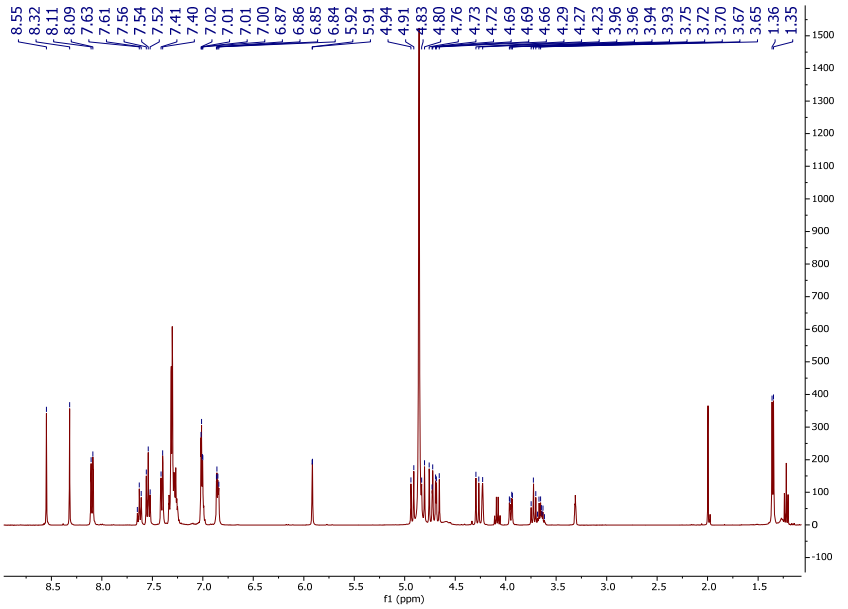


Figure S43. ^{1}H NMR spectrum for compound **16**.

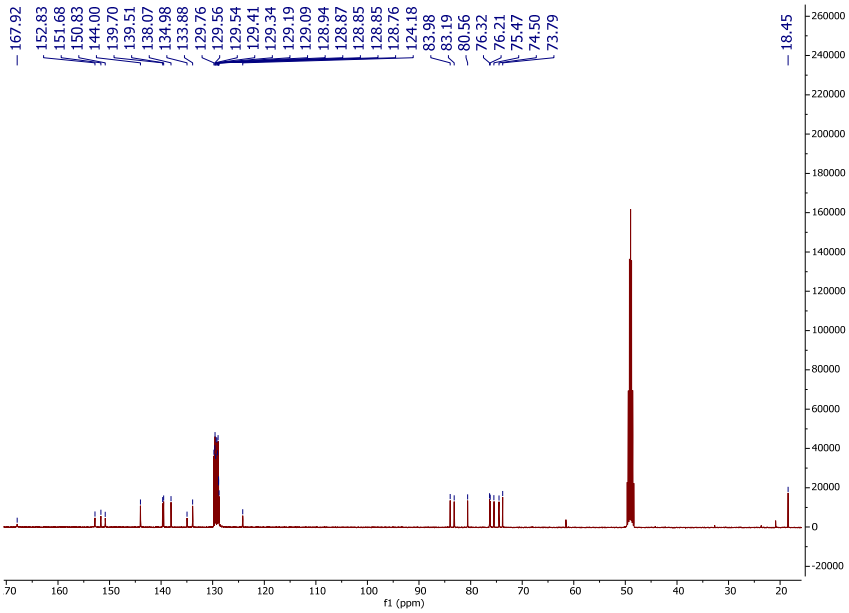


Figure S44. ^{13}C NMR spectrum for compound **16**.

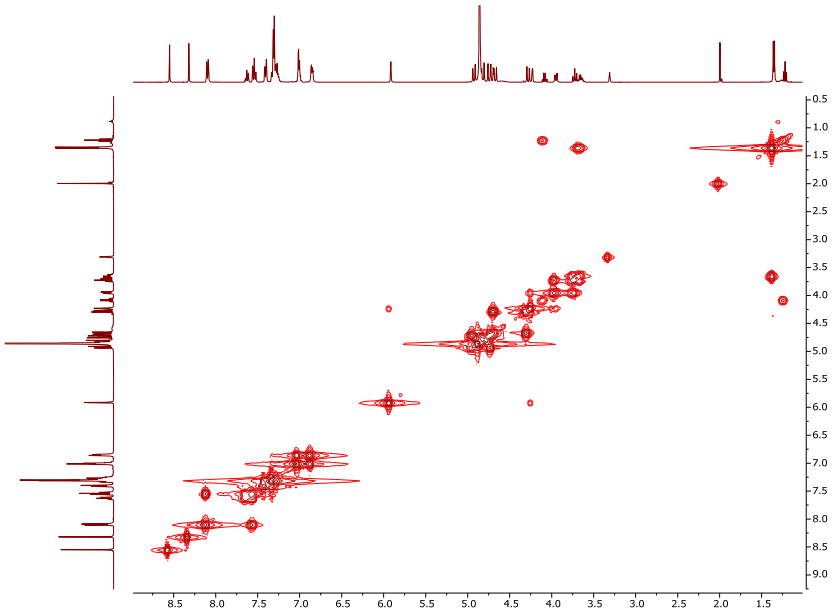


Figure S45. COSY spectrum for compound **16**.

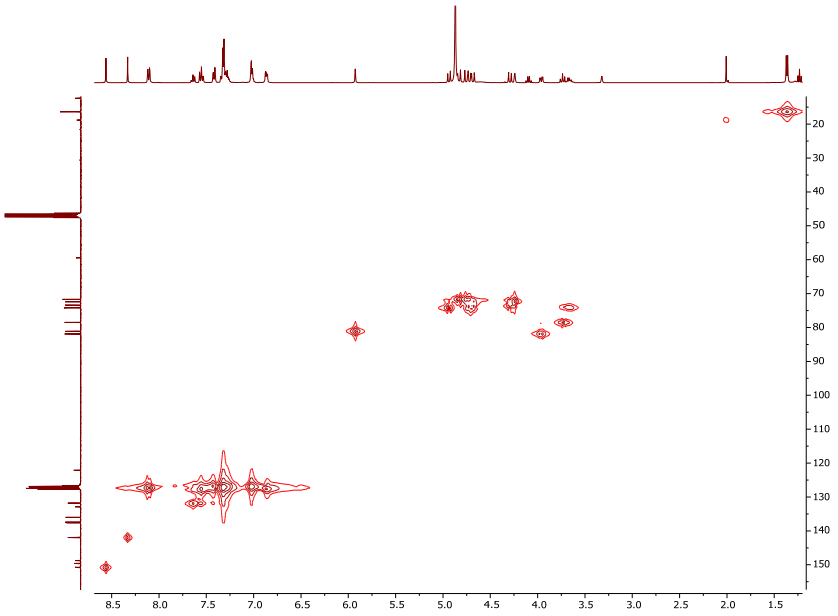


Figure S46. HSQC spectrum for compound **16**.

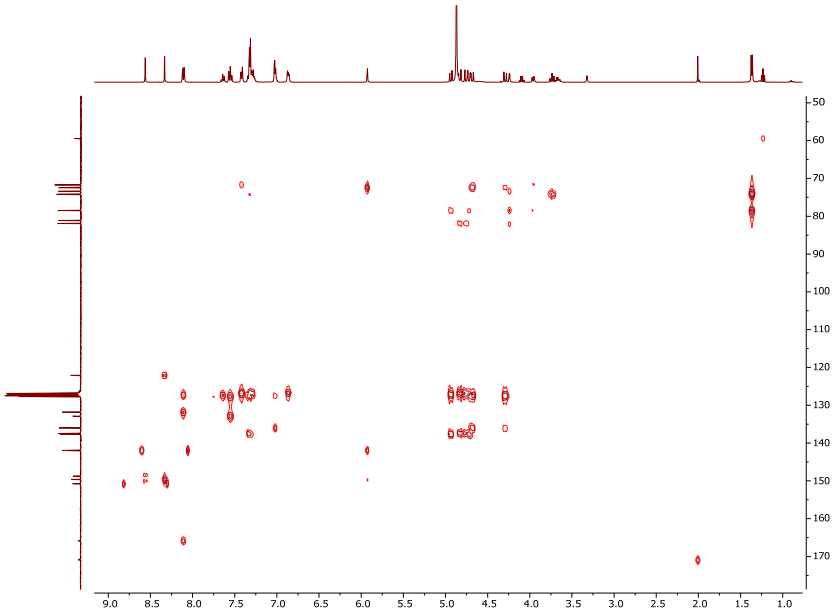


Figure S47. HMBC spectrum for compound **16**.

^{1}H NMR and ^{13}C NMR spectra by computational calculation

Table S1. NMR chemical shifts calculated for compound **5**.

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.36	8.58	Ph	126.8	130.1-129.0
H-8	7.89	8.42	Ph	126.8	130.1-129.0
NH	8.70	7.36-6.89	Ph	129.1	130.1-129.0
ortho PhCO	7.90	8.09	Ph-Cq	137.6	139.7
ortho PhCO	8.03	8.09	Ph	129.2	130.1-129.0
meta PhCO	7.54	7.57	Ph	126.8	130.1-129.0
meta PhCO	7.56	7.57	CH_2Ph	72.6	74.6
para PhCO	7.65	7.65	C-6'	67.4	70.2
H-4'	3.93	3.85	C-5'	73.2	74.1
H-3'	4.39	4.11	C-1'	73.8	81.9
H-5'	4.26	4.60-4.43	C-2'	76.8	74.4
H-2'	3.98	4.78	C-3'	74.4	75.8
H-1'	5.99	6.13	C-4'	74.5	76.7
H-6'b	4.06	3.76	CH_2Ph	70.8	73.4
H-6'a	3.46	3.65	Ph-Cq	137.2	139.6
CH_2Ph-2'	3.97	4.25, 4.22	Ph	129.4	130.1-129.0
CH_2Ph-2'	4.56	4.60 -4.43	Ph	126.9	130.1-129.0
CH_2Ph-4'	4.09	4.60-4.43	Ph	126.9	130.1-129.0
CH_2Ph-4'	4.30	4.60-4.43	Ph	126.8	130.1-129.0
CH_2Ph-3'	4.57	4.71, 4.68, 4.66, 4.63	Ph	129.1	130.1-129.0
CH_2Ph-3'	4.83	4.71, 4.68, 4.66, 4.63	CH_2Ph	74.9	77.7
CH_2Ph-6'	3.80	4.60-4.43	Ph-Cq	137.8	139.7
CH_2Ph-6'	4.10	4.60-4.43	Ph	129.9	130.1-129.0
Ph-2'	6.50	7.36-6.89	Ph	127.3	130.1-129.0
Ph-2'	7.26	7.36-6.89	Ph	127.0	130.1-129.0
Ph-2'	7.02	7.36-6.89	Ph	126.7	130.1-129.0

Ph-2'	7.23	7.36-6.89	Ph	128.8	130.1-129.0
Ph-2'	7.19	7.36-6.89	CH_2Ph	70.4	72.7
Ph-3'	7.76	7.36-6.89	Ph-Cq	136.7	138.7
Ph-3'	7.17	7.36-6.89	Ph	128.8	130.1-129.0
Ph-3'	7.64	7.36-6.89	Ph	126.7	130.1-129.0
Ph-3'	7.34	7.36-6.89	Ph	126.7	130.1-129.0
Ph-3'	7.42	7.36-6.89	Ph	126.5	130.1-129.0
Ph-4'	7.48	7.36-6.89	Ph	128.0	130.1-129.0
Ph-4'	7.40	7.36-6.89	C-4	148.9	156.6
Ph-4'	7.41	7.36-6.89	C-5	119.3	127.9
Ph-4'	7.40	7.36-6.89	C-8	139.1	145.6
Ph-4'	7.38	7.36-6.89	C-6	147.6	150.5
Ph-6'	7.54	7.36-6.89	C-2	149.8	153.4
Ph-6'	7.37	7.36-6.89	CONH	162.9	167.4
Ph-6'	7.49	7.36-6.89	Ph-Cq	133.8	134.4
Ph-6'	7.37	7.36-6.89	Ph	124.9	130.1-129.0
Ph-6'	7.38	7.36-6.89	Ph	126.9	130.1-129.0
			Ph	131.9	134.3
			Ph	127.5	130.1-129.0
			Ph	128.2	130.1-129.0

Table S2. NMR chemical shifts calculated for compound **6**.

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.49	8.77	C-4	147.6	151.6
H-8	8.14	8.09	C-5	118.8	123.2
NH	8.72	7.37-7.01	C-6	147.4	149.6
ortho PhCO	7.85	8.08	C-2	149.6	152.6
ortho PhCO	8.05	8.08	C-8	141.5	142.8
meta PhCO	7.52	7.55	CONH	162.7	164.6
meta PhCO	7.56	7.55	Ph-Cq	133.6	136.8
para PhCO	7.64	7.63	Ph	124.8	127.8-128.9

H-4'	4.35	3.91	Ph	128.2	127.8-128.9
H-3'	3.86	3.99	Ph	126.9	127.8-128.9
H-5'	3.43	4.55-4.43	Ph	127.5	127.8-128.9
H-2'	4.10	4.97	Ph	131.9	127.8-128.9
H-1'	5.87	6.08	C-4'	70.7	74.9, 74.8
H-6'b	3.67	3.71	C-3'	82.9	74.9, 74.8
H-6'a	4.22	3.78	C-5'	80.2	75.7
CH_2Ph-2'	4.84	4.55-4.43	C-2'	72.7	73.2
CH_2Ph-2'	3.96	4.55-4.43	C-1'	78.1	81.1
CH_2Ph-3'	4.78	4.68, 4.65	C-6'	68.0	68.4
CH_2Ph-3'	5.16	4.76, 4.73	CH_2Ph	74.2	73.2
CH_2Ph-4'	4.87	4.55-4.43	CH_2Ph	67.9	72.1
CH_2Ph-4'	4.37	4.55-4.43	CH_2Ph	73.8	72.4
CH_2Ph-6'	4.67	4.55-4.43	CH_2Ph	74.1	72.4
CH_2Ph-6'	4.08	4.30, 4.27	Ph-Cq	137.3	137.5
Ph-2'	7.84	7.37-7.01	Ph	129.9	127.8-128.9
Ph-2'	7.31	7.37-7.01	Ph	129.4	127.8-128.9
Ph-2'	7.69	7.37-7.01	Ph	127.4	127.8-128.9
Ph-2'	7.42	7.37-7.01	Ph	127.0	127.8-128.9
Ph-2'	7.51	7.37-7.01	Ph	127.2	127.8-128.9
Ph-3'	8.00	7.37-7.01	Ph-Cq	139.2	137.9
Ph-3'	7.26	7.37-7.01	Ph	122.5	127.8-128.9
Ph-3'	7.49	7.37-7.01	Ph	123.4	127.8-128.9
Ph-3'	7.38	7.37-7.01	Ph	127.1	127.8-128.9
Ph-3'	7.25	7.37-7.01	Ph	126.5	127.8-128.9
Ph-4'	7.10	7.37-7.01	Ph	124.4	127.8-128.9
Ph-4'	7.29	7.37-7.01	Ph-Cq	137.7	137.5
Ph-4'	7.17	7.37-7.01	Ph	129.0	127.8-128.9
Ph-4'	7.29	7.37-7.01	Ph	129.1	127.8-128.9
Ph-4'	7.25	7.37-7.01	Ph	126.6	127.8-128.9
Ph-6'	6.71	7.37-7.01	Ph	126.7	127.8-128.9
Ph-6'	7.41	7.37-7.01	Ph	126.6	127.8-128.9

Ph-6'	7.26	7.37-7.01	Ph-Cq	138.3	137.7
Ph-6'	7.38	7.37-7.01	Ph	128.6	127.8-128.9
Ph-6'	7.34	7.37-7.01	Ph	129.2	127.8-128.9
			Ph	126.4	127.8-128.9
			Ph	126.8	127.8-128.9
			Ph	126.5	127.8-128.9

Table S3. NMR chemical shifts calculated for compound **7**.

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.61	8.25	C-4	159.7	157.3
H-8	8.09	8.14	C-5	117.2	116.2
NH	7.46	7.35-6.60	C-6	141.7	153.2
ortho PhCO	7.68	7.35-6.60	C-2	149.3	153.3
ortho PhCO	7.66	7.35-6.60	C-8	145.6	146.7
meta PhCO	7.35	7.35-6.60	CONH	164.8	169.1
meta PhCO	7.10	7.35-6.60	Ph-Cq	132.8	136.1
para PhCO	7.38	7.35-6.60	Ph	124.9	129.9-129.3
H-4'	3.94	4.12-4.06	Ph	128.0	129.9-129.3
H-3'	4.18	4.66-4.40	Ph	126.6	129.9-129.3
H-5'	4.39	3.91	Ph	127.4	129.9-129.3
H-2'	3.81	3.85	Ph	131.6	134.5
H-1'	5.94	5.84	C-4'	74.2	73.7
H-6'a	4.18	4.12-4.06	C-3'	75.0	80.3
H-6'b	3.64	3.75	C-5'	73.7	71.8
CH_2Ph-2'	4.01	4.66-4.40	C-2'	77.5	74.4
CH_2Ph-2'	4.80	4.66-4.40	C-1'	76.5	81.6
CH_2Ph-4'	4.07	4.66-4.40	C-6'	67.5	67.9
CH_2Ph-4'	4.32	4.66-4.40	CH_2Ph	67.3	73.8
CH_2Ph-3'	4.39	4.66-4.40	CH_2Ph	70.9	74.3
CH_2Ph-3'	4.61	4.66-4.40	CH_2Ph	75.1	75.4
CH_2Ph-6'	4.15	4.66-4.40	CH_2Ph	72.9	75.0

CH_2Ph-6'	4.30	4.66-4.40	Ph-Cq	138.0	139.1
Ph-2'	7.00	7.35-6.60	Ph	121.8	129.9-129.3
Ph-2'	6.96	7.35-6.60	Ph	123.0	129.9-129.3
Ph-2'	7.21	7.35-6.60	Ph	126.7	129.9-129.3
Ph-2'	7.21	7.35-6.60	Ph	126.2	129.9-129.3
Ph-2'	7.12	7.35-6.60	Ph	124.3	129.9-129.3
Ph-3'	7.48	7.35-6.60	Ph-Cq	138.7	139.7
Ph-3'	6.80	7.35-6.60	Ph	124.8	129.9-129.3
Ph-3'	7.40	7.35-6.60	Ph	124.8	129.9-129.3
Ph-3'	7.29	7.35-6.60	Ph	126.8	129.9-129.3
Ph-3'	7.26	7.35-6.60	Ph	126.7	129.9-129.3
Ph-4'	7.45	7.35-6.60	Ph	125.8	129.9-129.3
Ph-4'	7.42	7.35-6.60	Ph-Cq	137.1	137.8
Ph-4'	7.40	7.35-6.60	Ph	129.5	134.4
Ph-4'	7.41	7.35-6.60	Ph	129.0	130.1
Ph-4'	7.38	7.35-6.60	Ph	126.9	129.9-129.3
Ph-6'	7.55	7.35-6.60	Ph	126.8	129.9-129.3
Ph-6'	7.49	7.35-6.60	Ph	126.9	129.9-129.3
Ph-6'	7.41	7.35-6.60	Ph-Cq	137.8	139.4
Ph-6'	7.41	7.35-6.60	Ph	128.6	130.0
Ph-6'	7.37	7.35-6.60	Ph	129.4	130.7
			Ph	126.7	129.9-129.3
			Ph	126.9	129.9-129.3
			Ph	126.8	129.9-129.3

Table S4. NMR chemical shifts calculated for compound **9**.

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.35	8.58	C-4	148.8	153.7
H-8	7.90	8.42	C-5	119.2	126.4
NH	8.73	7.40-7.27	C-6	147.5	153.4
ortho PhCO	7.91	8.08	C-2	149.7	153.4

ortho PhCO	8.04	8.08	C-8	139.2	145.5
meta PhCO	7.54	7.55	CONH	162.8	168.4
meta PhCO	7.56	7.55	Ph-Cq	133.7	134.2
para PhCO	7.64	7.64	Ph	124.8	129.2-130.1
H-4'	3.69	3.62	Ph	128.2	129.2-130.1
H-3'	4.33	4.10	Ph	126.9	129.2-130.1
H-5'	4.39	4.37	Ph	127.5	129.2-130.1
H-2'	3.94	4.79	Ph	131.9	129.2-130.1
H-1'	6.05	6.15	C-4'	78.6	81.4
CH3	1.96	1.34	C-3'	74.3	76.2
CH3	1.12	1.34	C-5'	71.8	74.4
CH3	1.00	1.34	C-2'	77.4	74.9
OCH_2-2'	3.97	4.25, 4.22	C-1'	72.2	81.6
OCH_2-2'	4.54	4.45, 4.42	C-6'	16.1	18.6
OCH_2-4'	4.29	4.59, 4.56, 4.56, 4.53	OCH_2-2'	70.6	72.7
OCH_2-4'	4.48	4.59, 4.56, 4.56, 4.53	OCH_2-4'	71.0	73.6
OCH_2-3'	4.50	4.75, 4.72, 4.70, 4.67	OCH_2-3'	74.6	74.1
OCH_2-3'	4.75	4.75, 4.72, 4.70, 4.67	Ph-Cq	136.8	139.7
Ph-2'	6.45	6.91	Ph	128.7	129.2-130.1
Ph-2'	7.22	7.40-7.27	Ph	127.8	129.2-130.1
Ph-2'	7.00	6.91	Ph	126.6	129.2-130.1
Ph-2'	7.20	7.12-7.05	Ph	126.4	129.2-130.1
Ph-2'	7.17	7.12-7.05	Ph	126.7	129.2-130.1
Ph-3'	7.53	7.40-7.27	Ph-Cq	137.6	139.8
Ph-3'	7.13	7.12-7.05	Ph	129.4	129.2-130.1
Ph-3'	7.43	7.40-7.27	Ph	129.0	129.2-130.1
Ph-3'	7.29	7.40-7.27	Ph	126.9	129.2-130.1
Ph-3'	7.36	7.40-7.27	Ph	126.7	129.2-130.1
Ph-4'	7.58	7.40-7.27	Ph	126.9	129.2-130.1

Ph-4'	7.45	7.40-7.27	Ph-Cq	137.4	138.8
Ph-4'	7.46	7.40-7.27	Ph	129.5	129.2-130.1
Ph-4'	7.43	7.40-7.27	Ph	129.1	129.2-130.1
Ph-4'	7.41	7.40-7.27	Ph	127.0	129.2-130.1
			Ph	126.8	129.2-130.1
			Ph	126.9	129.2-130.1

Table S5. NMR chemical shifts calculated for compound **12**, "conformer a".

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.47	8.75	C-4	148.5	153.5
H-8	7.87	8.59	C-5	119.0	125.0
NH	8.67	7.57-7.54	C-6	147.6	151.3
ortho PhCO	7.83	8.07	C-2	150.1	153.5
ortho PhCO	8.02	8.07	C-8	138.4	144.7
meta PhCO	7.52	7.57-7.54	COPh	162.7	168.3
meta PhCO	7.54	7.57-7.54	Cq, Ph	133.6	134.0
para PhCO	7.63	7.65	Ph	124.8	120.2
H-1'	6.22	6.30	Ph	128.2	129.8
H-2'	5.27	6.26	Ph	126.9	123.3
H-3'	5.38	5.65	Ph	127.5	129.5
H-4'	4.62	5.01	Ph	131.9	134.0
H-5'	4.13	4.28	C-3'	66.7	70.3
CH_3-6'	1.36	1.41-2.14	C-2'	67.8	68.9
CH_3-6'	1.34	1.41-2.14	C-1'	70.4	80.3
CH_3-6'	2.37	1.41-2.14	C-5'	74.4	73.1
CH_3	1.59	1.41-2.14	C-4'	71.2	73.2
CH_3	1.52	1.41-2.14	C-6'	15.3	17.2
CH_3	1.88	1.41-2.14	CO	169.0	171.2
CH_3	1.91	1.41-2.14	CH_3	20.2	20.4
CH_3	2.36	1.41-2.14	CO	169.5	171.2
CH_3	2.43	1.41-2.14	CH_3	20.8	20.6

CH_3	2.35	1.41-2.14	CO	169.0	171.2
CH_3	2.35	1.41-2.14	CH_3	20.9	20.7
CH_3	1.89	1.41-2.14			

Table S6. NMR chemical shifts calculated for compound **12**, "conformer b".

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.44	8.75	C-4	150.7	153.5
H-8	7.92	8.59	C-5	121.8	125.0
NH	7.72	7.57-7.54	C-6	148.0	151.3
ortho PhCO	7.88	8.07	C-2	149.5	153.5
ortho PhCO	8.03	8.07	C-8	138.5	144.7
meta PhCO	7.51	7.57-7.54	COPh	164.0	168.3
meta PhCO	7.53	7.57-7.54	Cq, Ph	132.4	134.0
para PhCO	7.64	7.65	Ph	126.1	120.2
H-1'	6.29	6.30	Ph	128.1	129.8
H-2'	5.32	6.26	Ph	126.9	123.3
H-3'	5.39	5.65	Ph	127.2	129.5
H-4'	4.63	5.01	Ph	132.2	134.0
H-5'	4.12	4.28	C-3'	66.8	70.3
CH_3-6'	1.36	1.41-2.14	C-2'	67.4	68.9
CH_3-6'	1.36	1.41-2.14	C-1'	70.2	80.3
CH_3-6'	2.38	1.41-2.14	C-5'	74.4	73.1
CH_3	1.59	1.41-2.14	C-4'	71.2	73.2
CH_3	1.54	1.41-2.14	C-6'	15.4	17.2
CH_3	1.89	1.41-2.14	CO	169.0	171.2
CH_3	1.91	1.41-2.14	CH_3	20.3	20.4
CH_3	2.36	1.41-2.14	CO	169.5	171.2
CH_3	2.43	1.41-2.14	CH_3	20.8	20.6
CH_3	2.35	1.41-2.14	CO	169.0	171.2
CH_3	2.35	1.41-2.14	CH_3	20.9	20.7
CH_3	1.88	1.41-2.14			

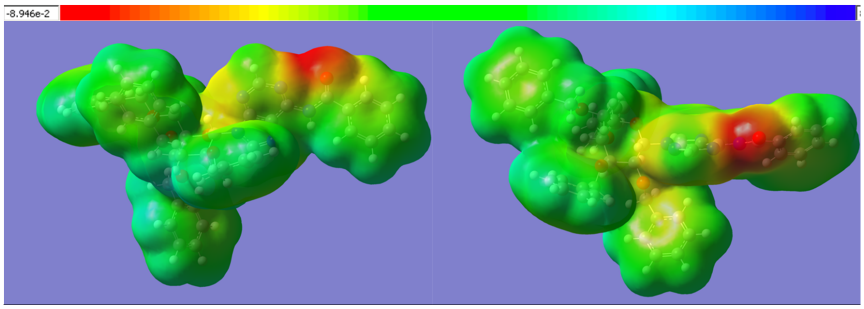
Table S7. NMR chemical shifts calculated for compound **15**.

H (paper)	^{1}H δ calc	^{1}H δ exp	C (paper)	^{13}C δ calc	^{13}C δ exp
H-2	8.36	8.59	C-4	148.8	153.0
H-8	7.87	8.41	C-5	119.1	125.1
NH	8.77	7.41-7.24	C-6	147.4	151.0
ortho PhCO	7.91	8.09	C-2	149.7	153.0
ortho PhCO	8.05	8.09	C-8	139.1	145.1
meta PhCO	7.54	7.54	CONH	162.5	168.1
meta PhCO	7.55	7.54	Ph-Cq	133.6	138.5
para PhCO	7.64	7.63	Ph	124.7	138.5-128.7
H-1'	6.07	6.17	Ph	128.2	138.5-128.7
H-2'	4.13	4.82	Ph	126.9	138.5-128.7
H-3'	4.66	4.10	Ph	127.5	138.5-128.7
H-4'	3.65	3.64	Ph	131.9	138.5-128.7
H-5'	4.06	4.37	C-3'	70.2	76.0
CH_3	1.03	1.35	C-2'	77.8	74.6
CH_3	1.02	1.35	C-1'	72.4	81.3
CH_3	1.98	1.35	C-5'	77.0	74.1
CH_2Ph-2'	4.18	4.26, 4.23	C-4'	78.7	81.1
CH_2Ph-2'	4.75	4.45, 4.42	C-6'	16.6	18.3
Ph-2'	7.30	7.27-7.24, 7.15-7.04, 6.93	CH_2Ph	70.9	72.4
Ph-2'	6.46	7.27-7.24, 7.15-7.04, 6.93	Ph-Cq	137.0	139.4
Ph-2'	7.24	7.27-7.24, 7.15-7.04, 6.93	Ph	127.8	138.5-128.7
Ph-2'	7.02	7.27-7.24, 7.15-7.04, 6.93	Ph	128.6	138.5-128.7
Ph-2'	7.20	7.27-7.24, 7.15-7.04, 6.93	Ph	126.4	138.5-128.7

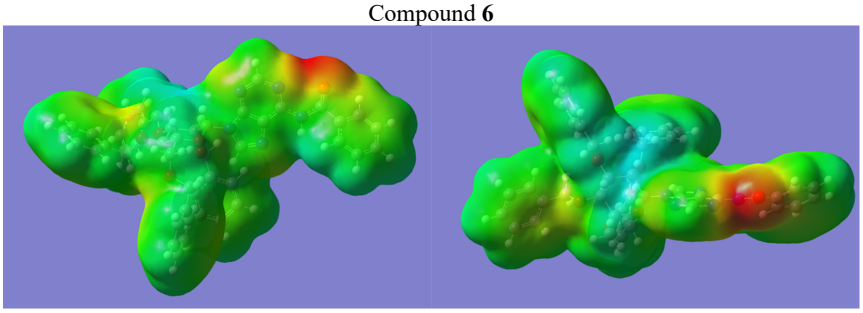
CH_2Ph-3'	4.83	4.75, 4.72	Ph	126.7	138.5-128.7
CH_2Ph-3'	4.54	4.70, 4.67	Ph	126.7	138.5-128.7
Ph-3'	7.16	7.27-7.24, 7.15-7.04, 6.93	CH_2Ph	74.3	73.8
Ph-3'	7.53	7.27-7.24, 7.15-7.04, 6.93	Ph-Cq	137.6	153.4
Ph-3'	7.30	7.27-7.24, 7.15-7.04, 6.93	Ph	129.0	138.5-128.7
Ph-3'	7.43	7.27-7.24, 7.15-7.04, 6.93	Ph	129.4	138.5-128.7
Ph-3'	7.36	7.27-7.24, 7.15-7.04, 6.93	Ph	126.7	138.5-128.7
CH_2Ph-4'	4.42	4.56, 4.53	Ph	126.9	138.5-128.7
CH_2Ph-4'	4.73	4.69, 4.57	Ph	126.9	138.5-128.7
Ph-4'	7.53	7.27-7.24, 7.15-7.04, 6.93	CH_2Ph	71.7	73.3
Ph-4'	7.53	7.27-7.24, 7.15-7.04, 6.93	Ph-Cq	137.4	139.5
Ph-4'	7.45	7.27-7.24, 7.15-7.04, 6.93	Ph	129.6	138.5-128.7
Ph-4'	7.44	7.27-7.24, 7.15-7.04, 6.93	Ph	128.9	138.5-128.7
Ph-4'	7.41	7.27-7.24, 7.15-7.04, 6.93	Ph	127.0	138.5-128.7
			Ph	126.8	138.5-128.7
			Ph	126.9	138.5-128.7

Molecular Electrostatic Potential Maps

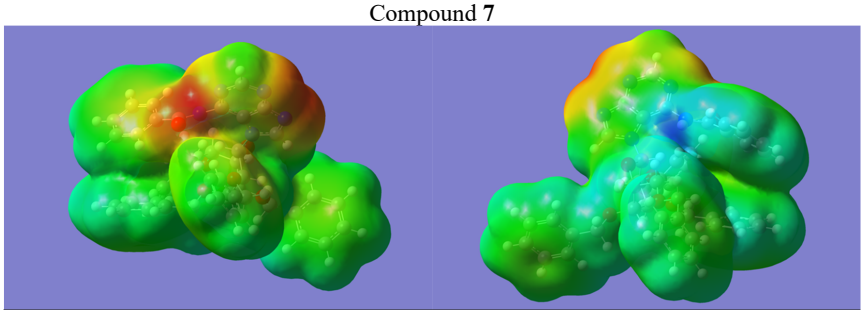
Compound **5**



Compound **6**



Compound **7**



Compound **9**

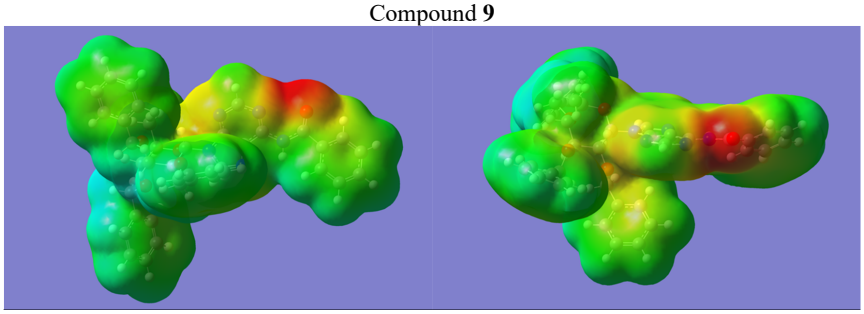
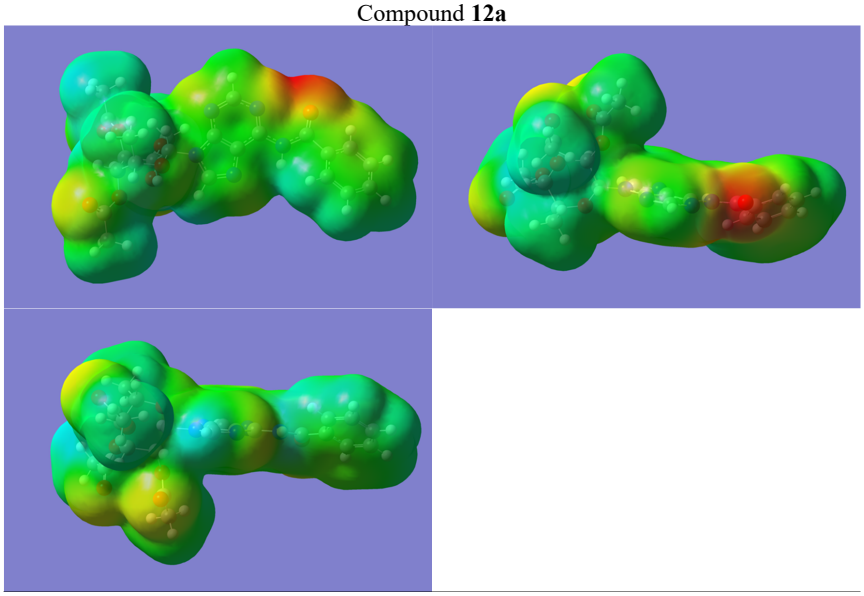


Figure S48. Different views of the electrostatic potential maps for compounds **5**, **6**, **7** and **9.**

Compound **12a**



Compound **12b**

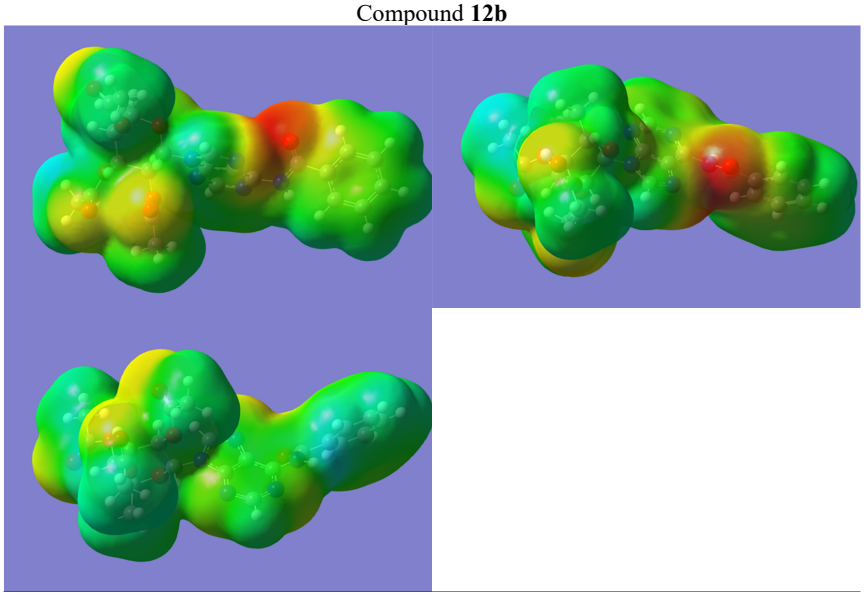


Figure S49. Different views of the electrostatic potential maps for conformers **12**a and **12**b.

Compound **15**

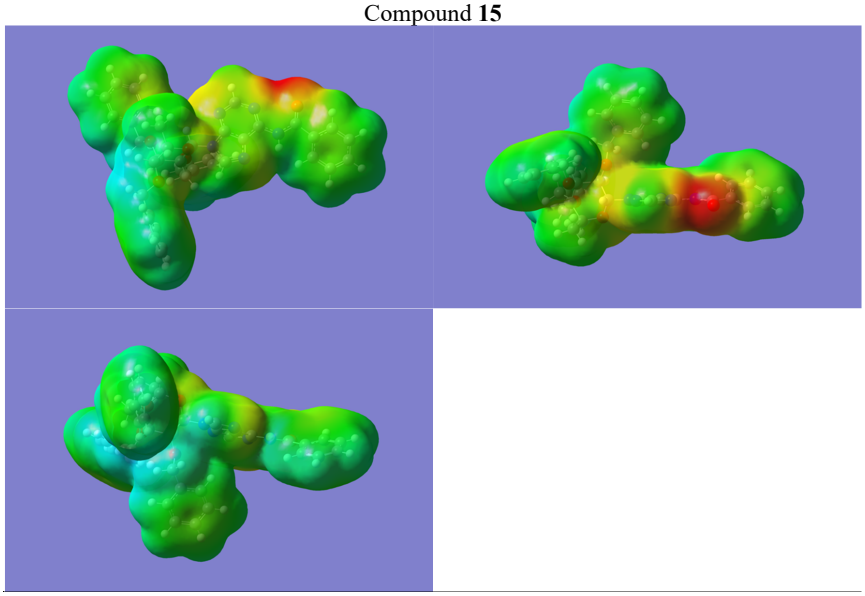


Figure S50. Different views of the electrostatic potential maps for compound **15**.

Energy differences between the most stable conformers found for compound 12 (α and β anomers)

Table S8. Energy differences between conformers "a" and "b" for compound 12 (α and β) and between compound 12a (α anomer) and 12b (β anomer).

Compound 12: α anomer			
conformer	E / kcal.mol^{-1}	ΔE(a-b) / kcal.mol^{-1}	Boltzmann population
a	-1132494.89	-0.55	0.72
b	-1132494.34		0.28
Compound 12: β anomer			
conformer	E / kcal.mol^{-1}	ΔE(a-b) / kcal.mol^{-1}	Boltzmann population
a	-1132488.59	-1.51	0.93
b	-1132487.08		0.07
Compound 12: α and β anomer			
Anomer	E / kcal.mol^{-1}	ΔE(α-β) / kcal.mol^{-1}	Boltzmann population
α	-1132494.89	-6.30	1.00
β	-1132488.59		0.00