Electronic supplementary information

for

Structural revision of aristol: a fresh look at the oxidative coupling of thymol under iodination conditions

Niko S. Radulović*, Miljana R. Đorđević and Polina D. Blagojević

Department of Chemistry, Faculty of Science and Mathematics, University of Niš, Višegradska 33, 18000, Niš, Serbia

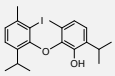
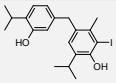
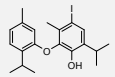
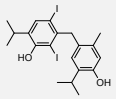
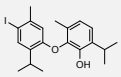
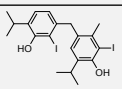
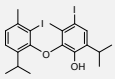
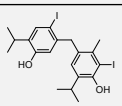
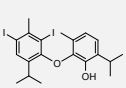
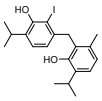
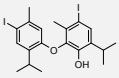
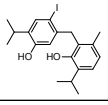
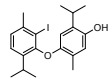
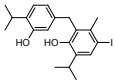
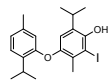
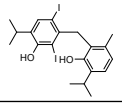
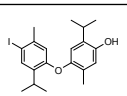
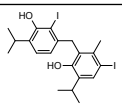
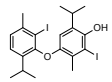
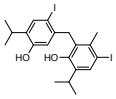
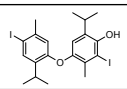
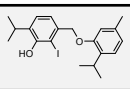
Table of Contents page

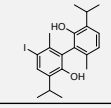
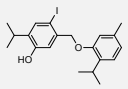
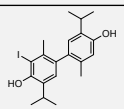
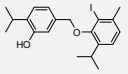
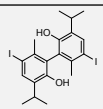
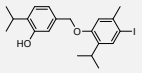
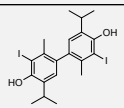
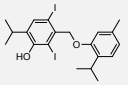
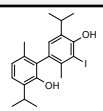
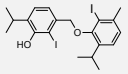
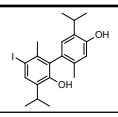
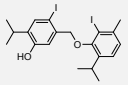
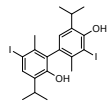
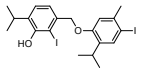
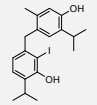
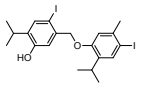
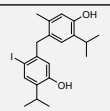
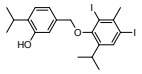
* Correspondence e-mail: nikoradulovic@yahoo.com.

Table S1. Calculated (calc) and experimental (exp) values of chemical shifts of selected protons of compounds **10**-**13** and **16**

Position	**10**	**11**	**12**	**13**	**16**
	δ, ppm (calc/exp)				
H2	6.64/6.57	/	6.49/6.66	/	3.86/6.09
H5	7.32/7.08	7.17/7.05	7.33/7.54	7.19/7.57	7.85/7.59
H6	6.97/6.73	6.87/6.81	/	/	/
H2′	/	/	/	/	6.55/6.61
H5′	/	/	/	/	6.99/6.89

Table S2. List of all possible coupling products used in the QSPR study, the predicted values of the retention indices and the corresponding QSPR variables

Compound structure	M[a] [g mol^{-1}]	Bp[b] [ºC]	MTI[c]	RIpred[d]	Compound structure	M [g mol^{-1}]	Bp [ºC]	MTI	RIpred
	424	445.31	8484	2666		424	468.09	9098	2823
	424	445.31	8524	2670		550	517.04	9570	2923
	424	445.31	8596	2678		550	517.04	9620	2929
	550	494.25	9040	2775		550	517.04	9626	2929
	550	494.25	9106	2782		424	468.09	8914	2804
	550	494.25	9156	2787		424	468.09	8920	2804
	424	445.31	8618	2680		424	468.09	8976	2810
	424	445.31	8646	2683		550	517.04	9430	2909
	424	445.31	8730	2692		550	517.04	9492	2915
	550	494.25	9168	2789		550	517.04	9498	2916
	550	494.25	9284	2801		424	445.31	9506	2773

	424	482.17	7932	2756		424	445.31	9512	2773
	424	482.17	8188	2785		424	445.31	9528	2775
	550	531.12	8454	2864		424	445.31	9640	2787
	550	531.12	8710	2891		550	494.26	10056	2882
	424	482.17	8054	2771		550	494.26	10078	2884
	424	482.17	8066	2772		550	494.26	10084	2885
	550	531.12	8582	2877		550	494.26	10194	2896
	424	468.09	9048	2817		550	517.04	9430	2897
	424	468.09	9054	2818		550	494.26	10206	2897

[a]M- molar mass, [b]Bp- predicted boiling points [ºC], [c]MTI- molecular topological index, [d]RIpred- the predicted values of the retention indices

Figure S1. ^{1}H NMR shifts of polar and "aromatic" protons of compounds **7**, **10**-**17** given in parallel; for clarity and uniformity reasons (signals of polar protons were not sharp singlets), simulated spectra (with experimentally observed values of coupling constants and chemical shifts) are shown. Signals in the gray rectangle correspond to protons that fall within the benzene shielding cone; signals with similar values of chemical shifts are grouped within cyan rectangles.

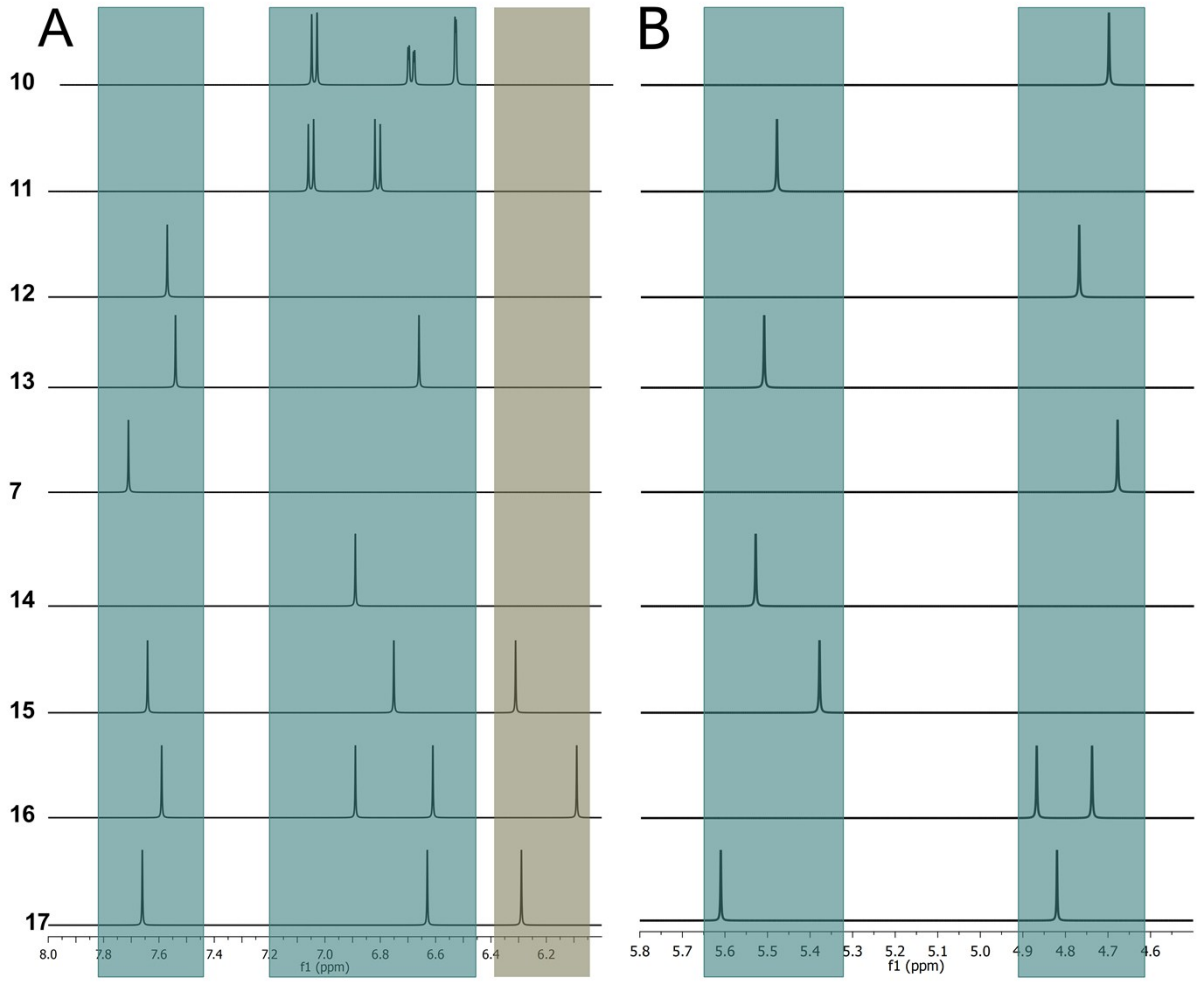


Figure S2. EI Mass spectrum of **14**

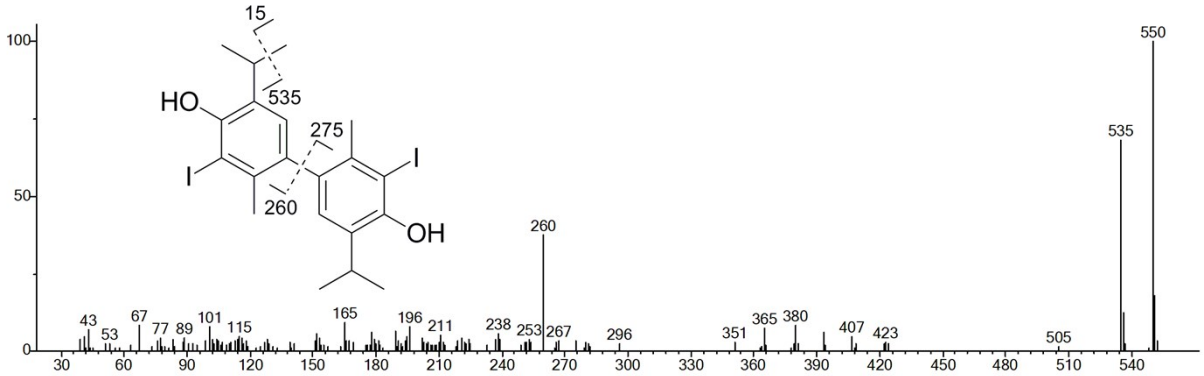
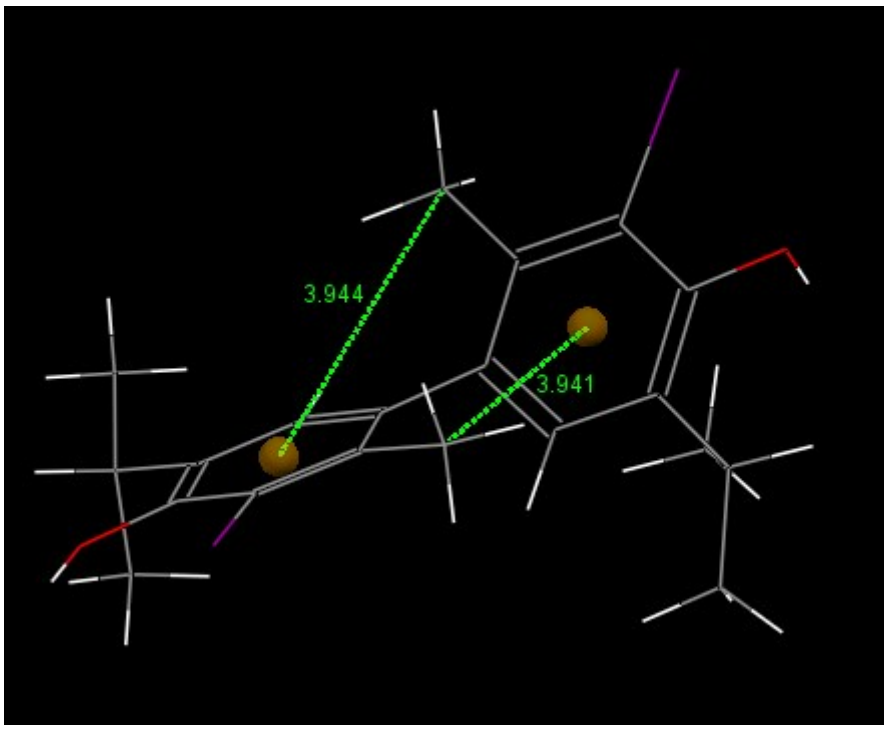


Figure S3. Spatial relationship between benzene ring shielding cones and protons placed above the plane of the ring (compound **14**)



Optimized geometry (for optimization details see Experimental section) of compound **16**.

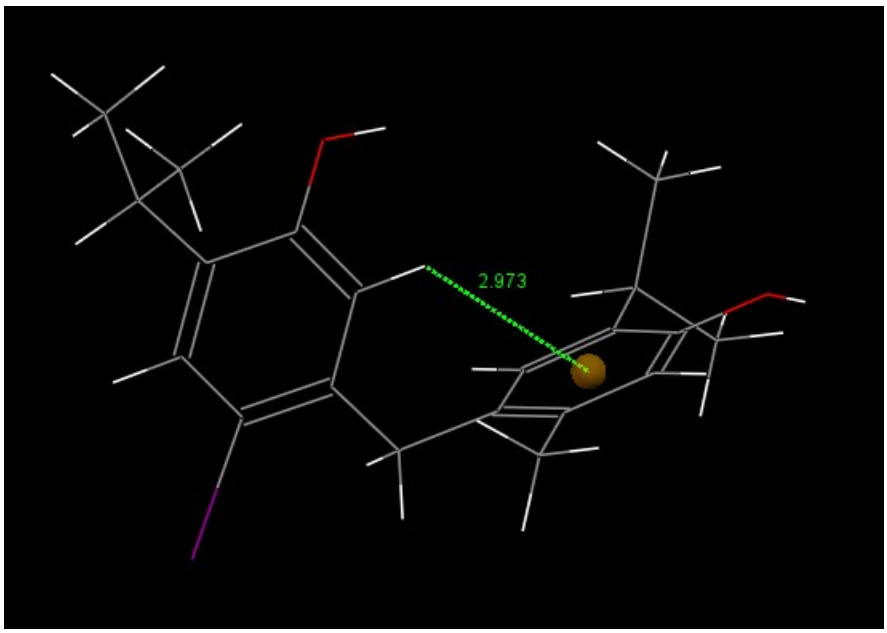


Figure S4. The order of elution of aristol constituents from an SiO_2 column eluted by diethyl ether-hexane mixtures

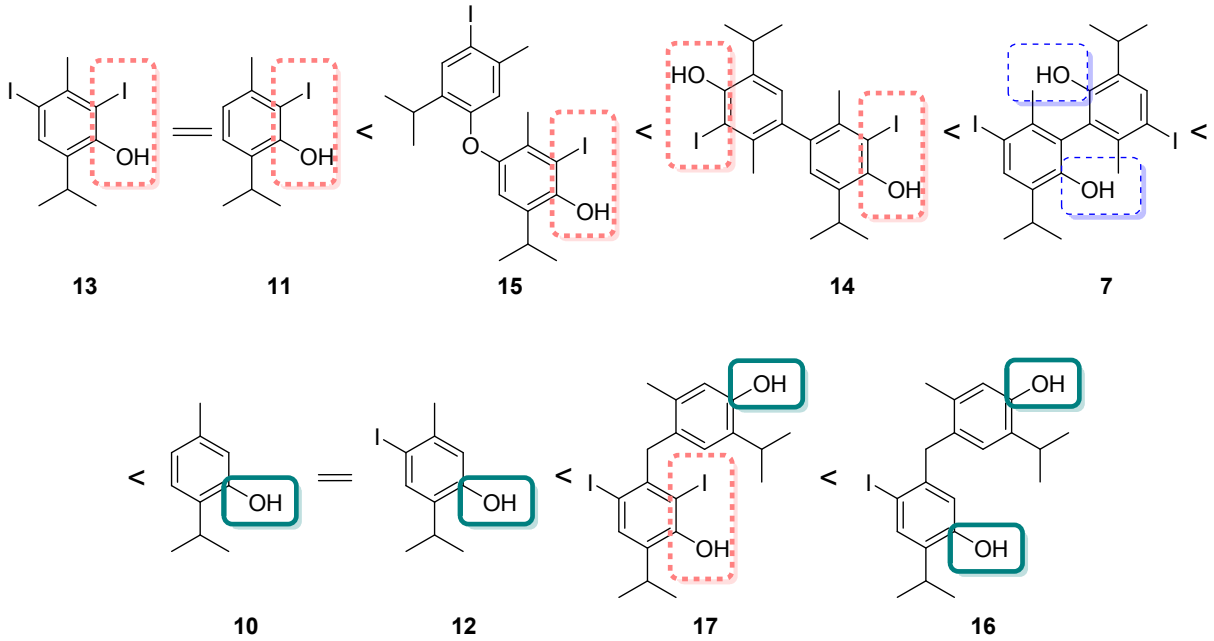


Figure S5. Correlation between experimentally determined and calculated RI values according to equation RIpred = 116.09 + 4.07Bp+ 0.10MTI – 147.55N_I

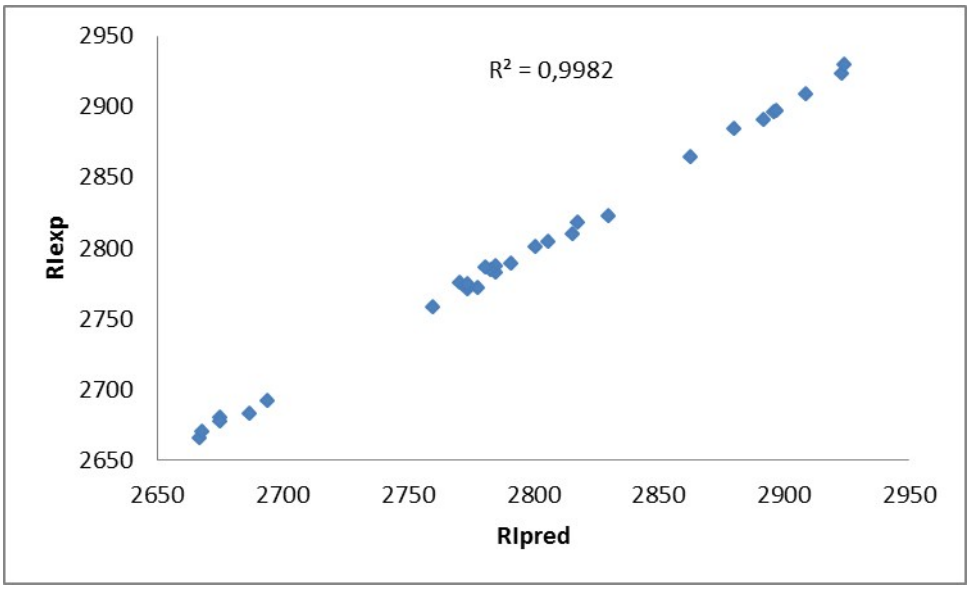


Figure S6. Partial ion current chromatograms [35-52 min] of a sample of aristol

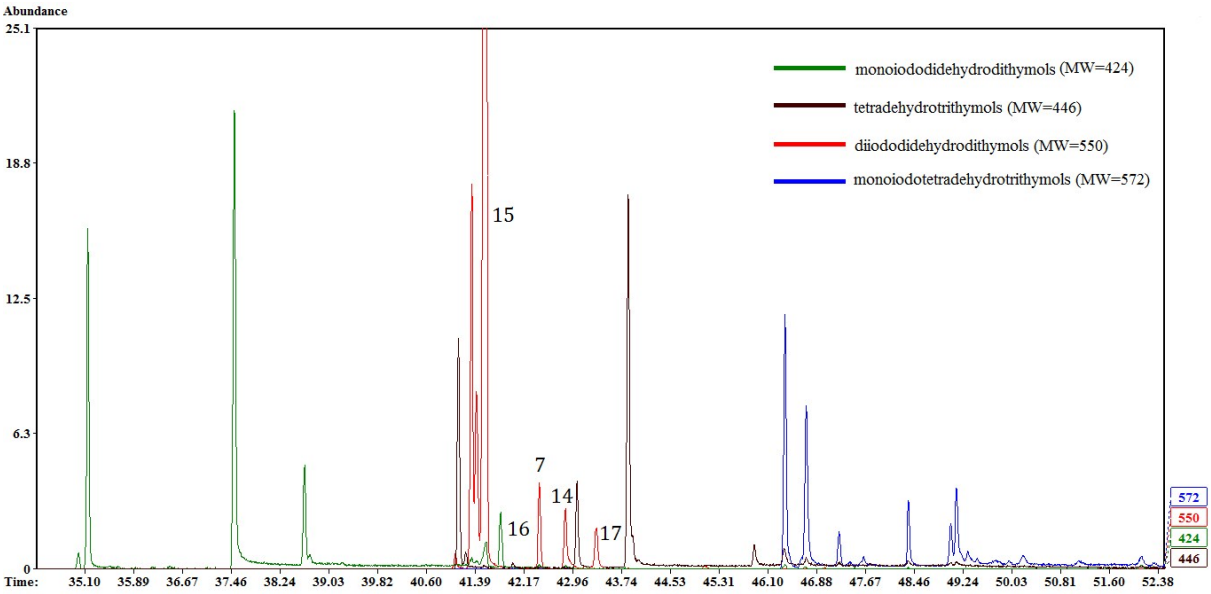
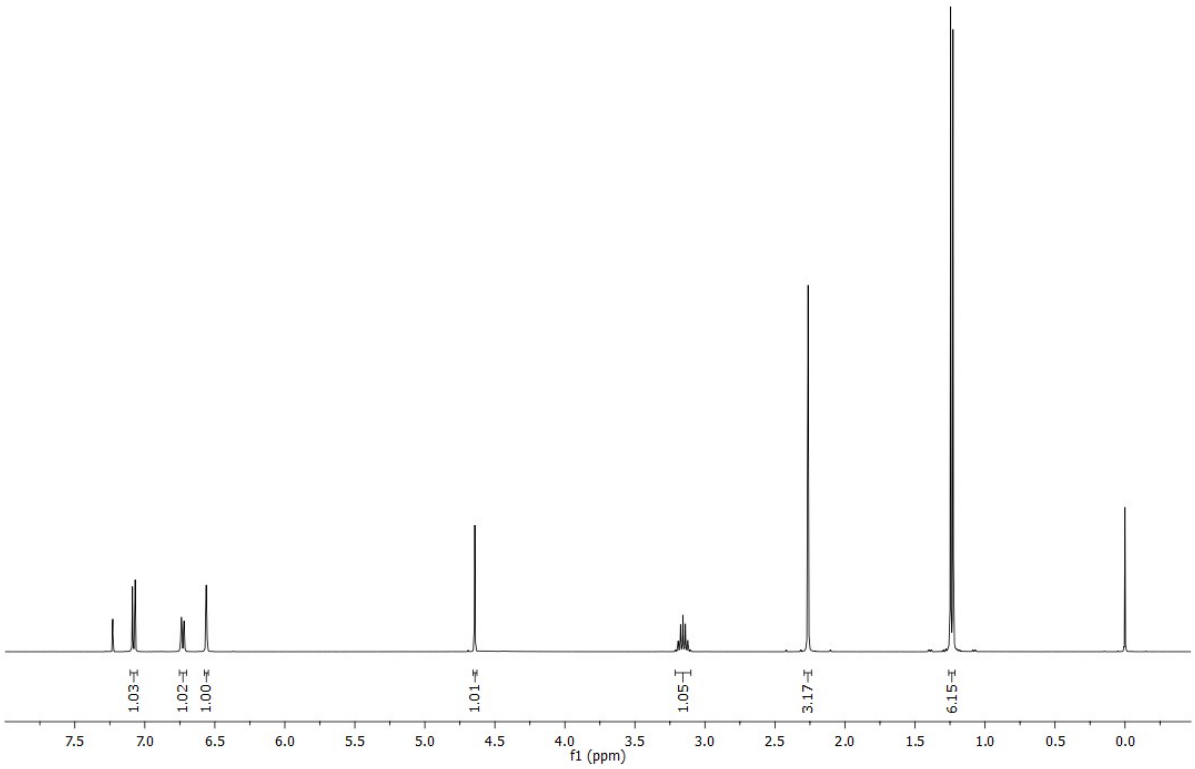
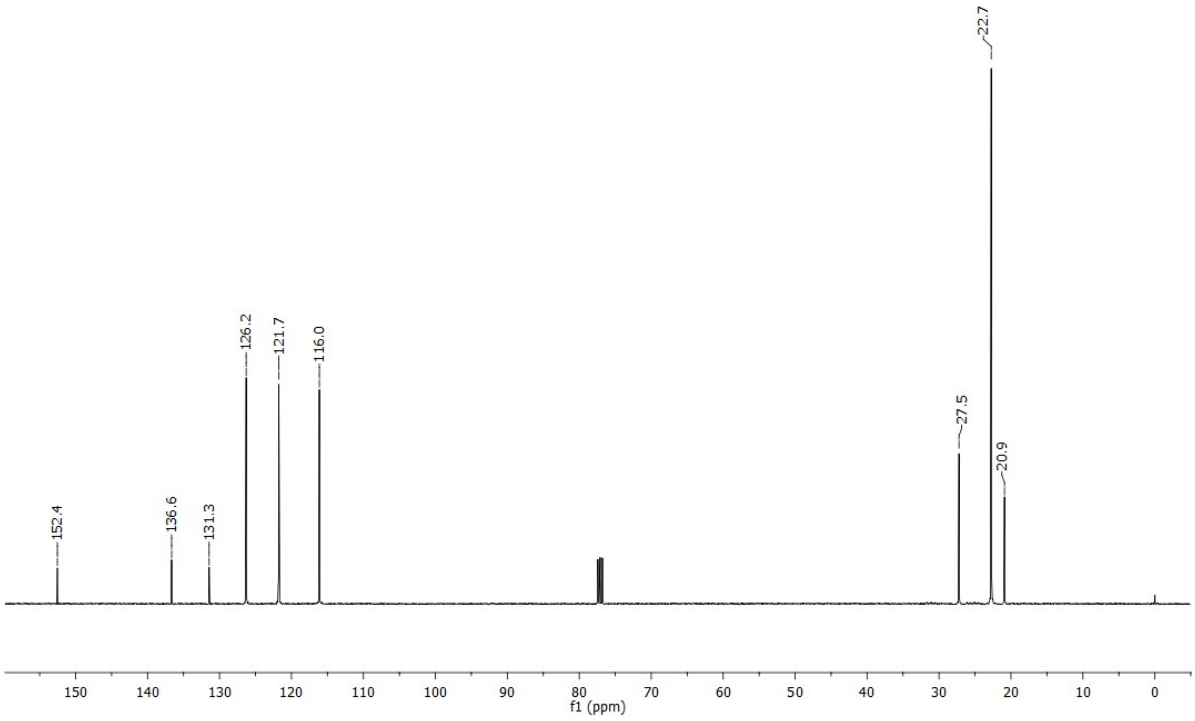


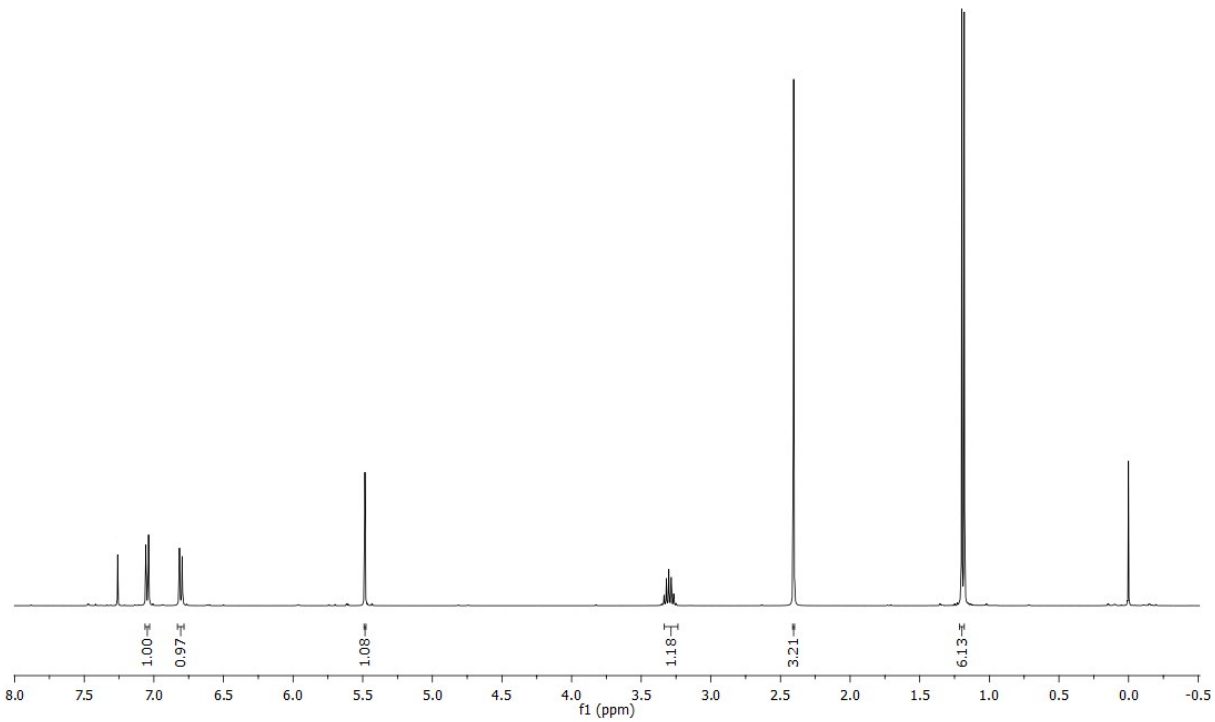
Figure S7. ^{1}H and ^{13}C NMR spectra of compounds **7**, **10-17**



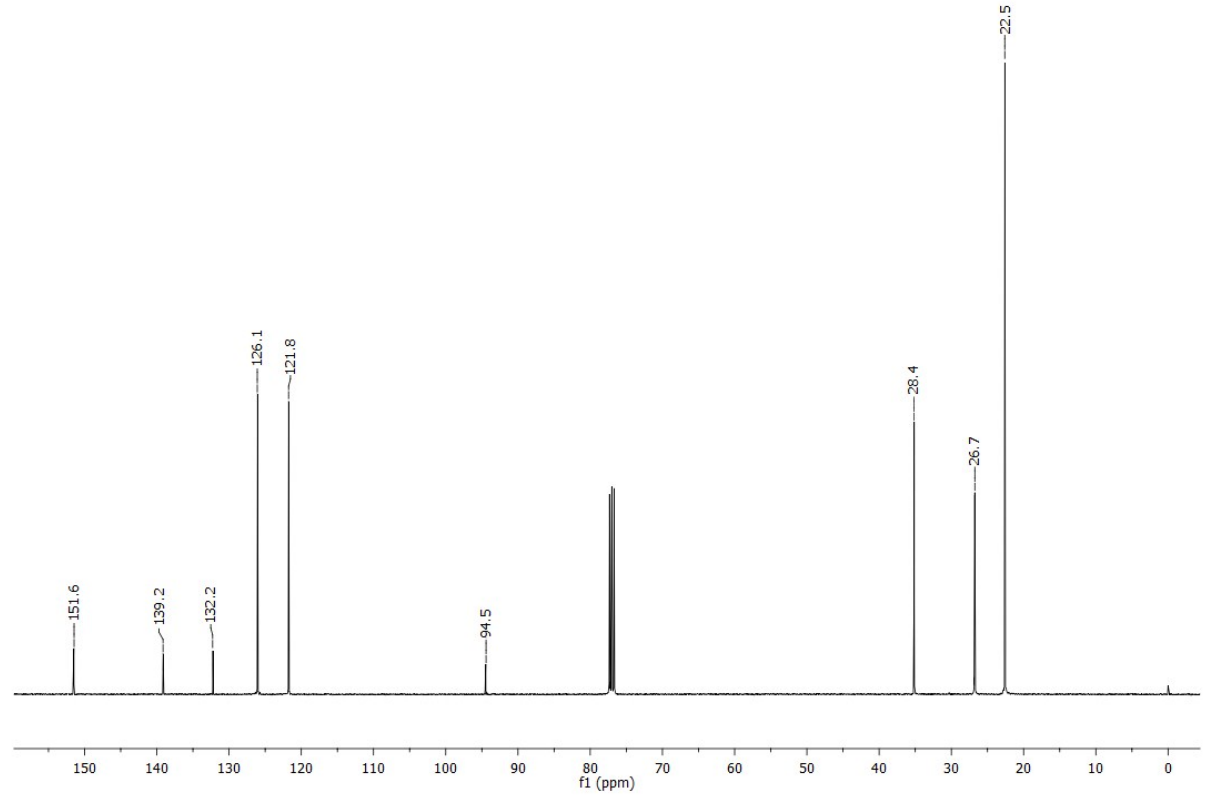
^{1}H NMR (400 MHz) spectrum of compound **10** in $CDCl_3$



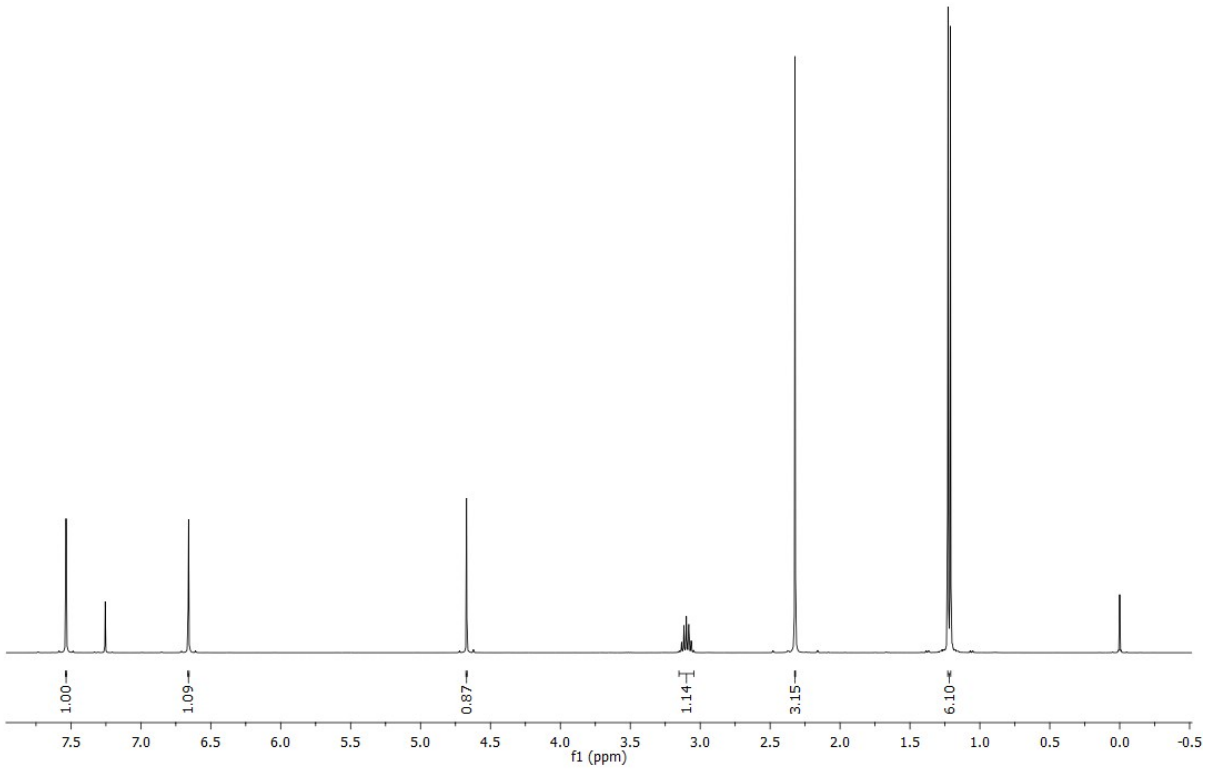
^{13}C NMR (100 MHz) spectrum of compound **10** in $CDCl_3$



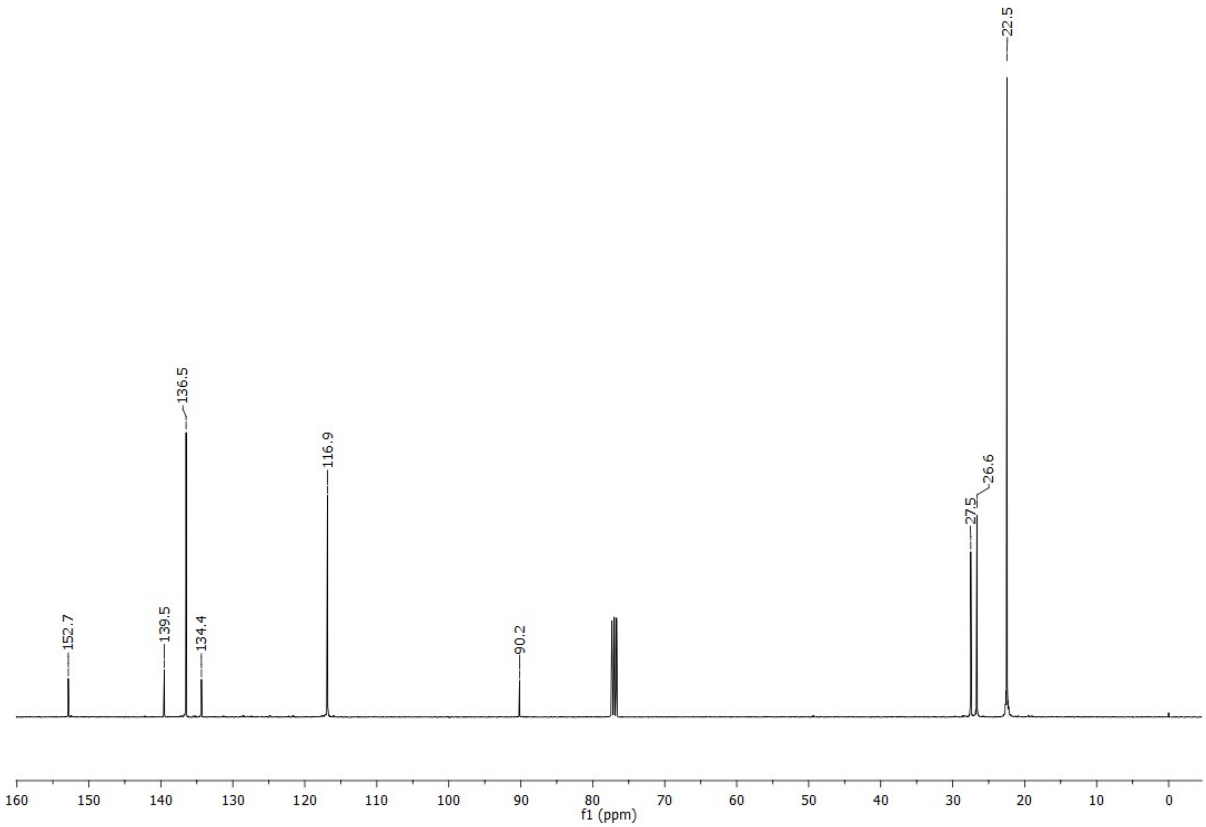
^{1}H NMR (400 MHz) spectrum of compound **11** in $CDCl_3$



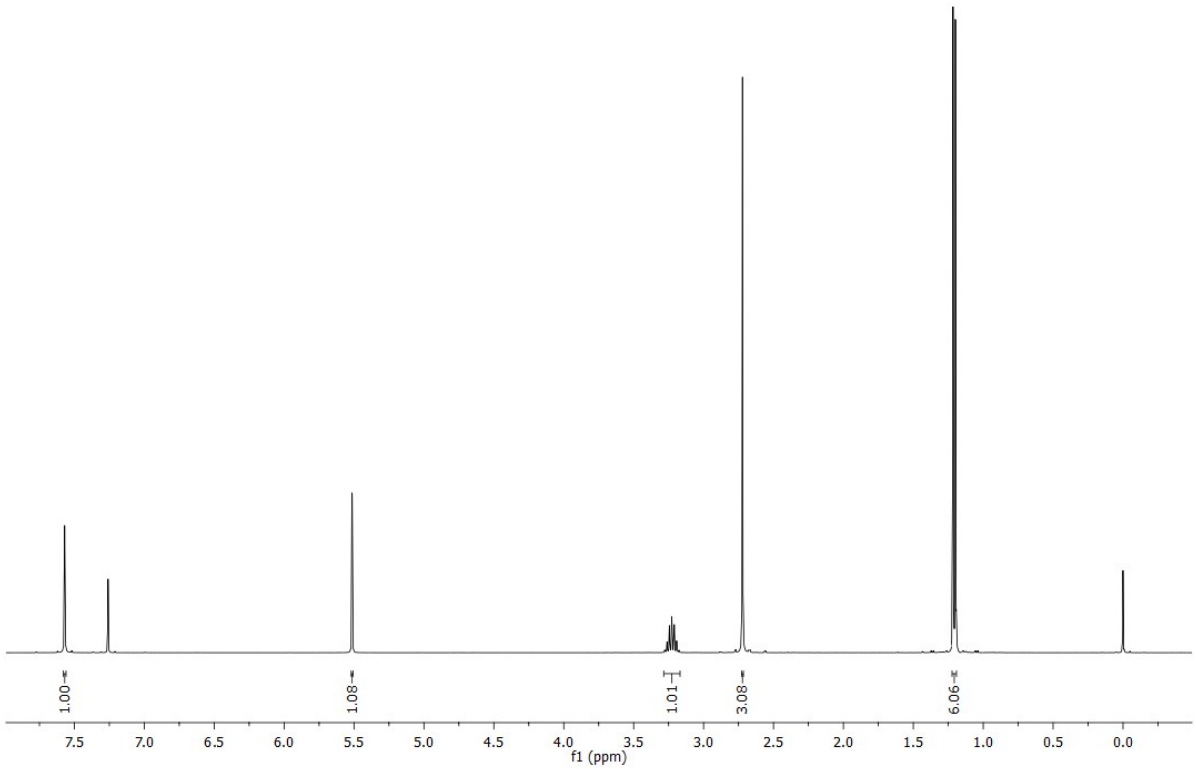
^{13}C NMR (100 MHz) spectrum of compound **11** in $CDCl_3$



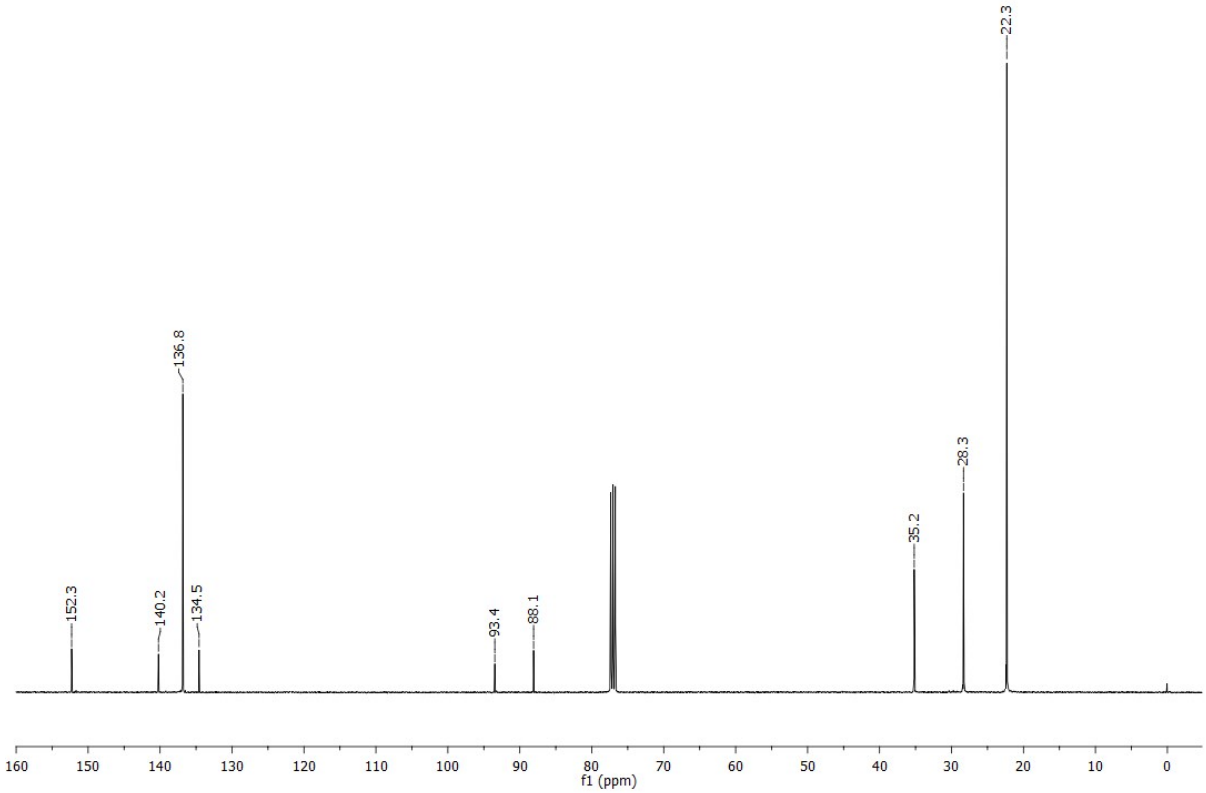
^{1}H NMR (400 MHz) spectrum of compound **12** in $CDCl_3$



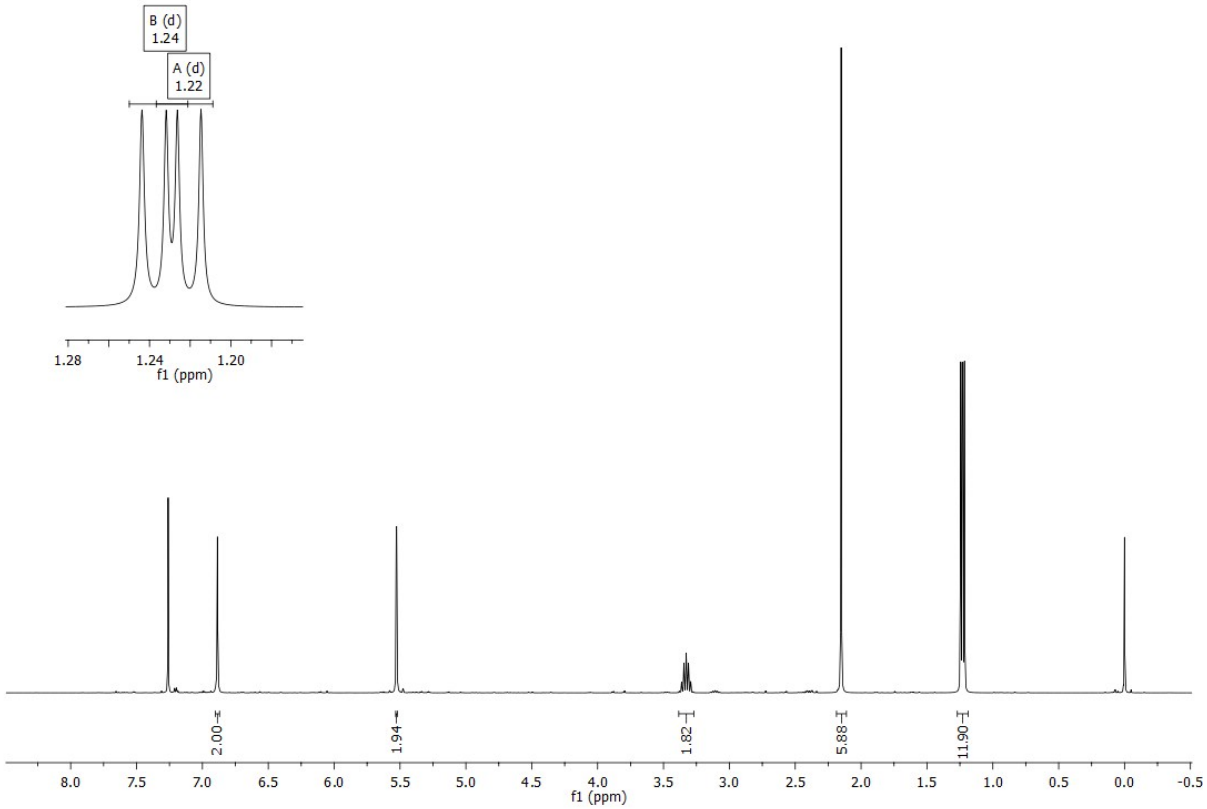
^{13}C NMR (100 MHz) spectrum of compound **12** in $CDCl_3$



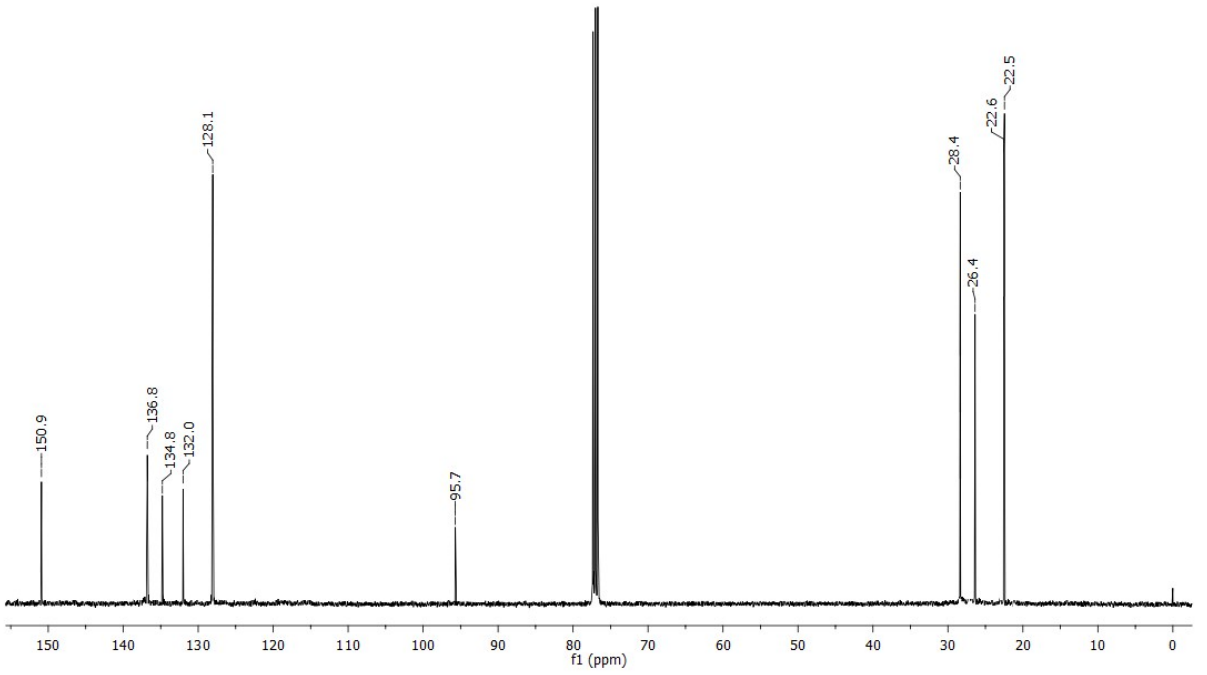
^{1}H NMR (400 MHz) spectrum of compound **13** in $CDCl_3$



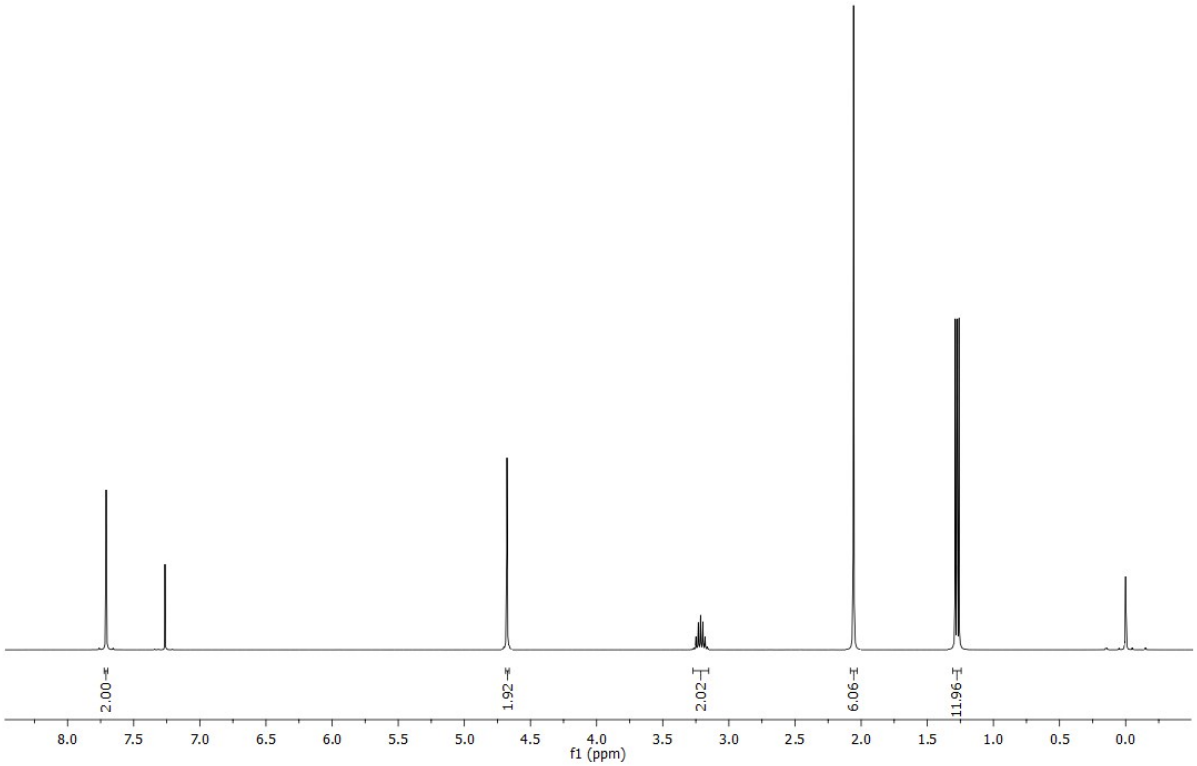
^{13}C NMR (100 MHz) spectrum of compound **13** in $CDCl_3$



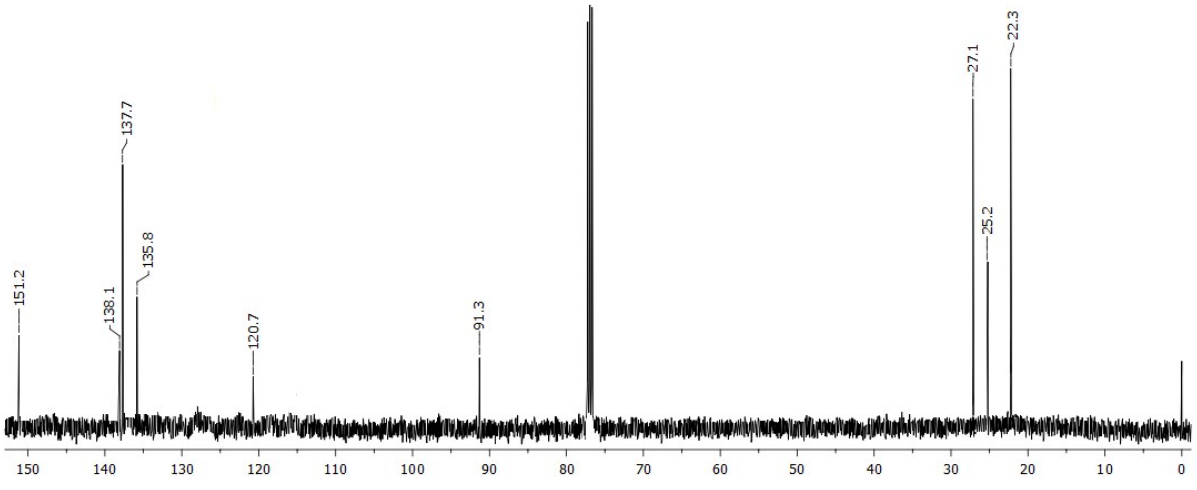
^{1}H NMR (400 MHz) spectrum of compound **14** in $CDCl_3$



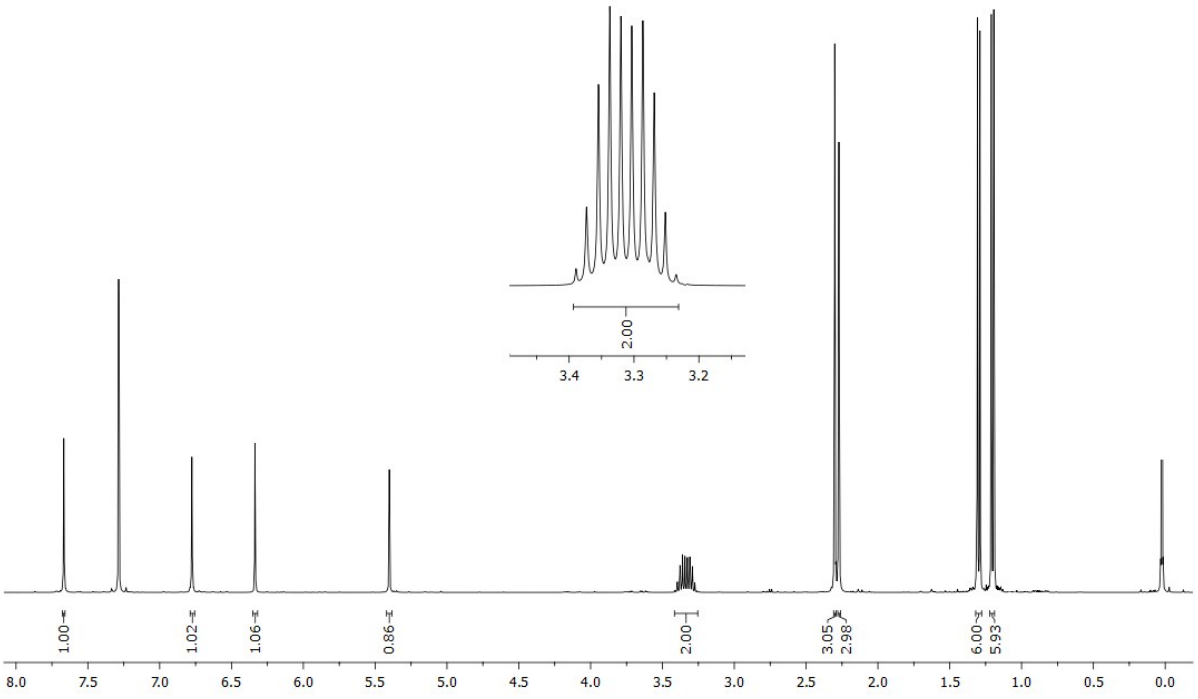
^{13}C NMR (100 MHz) spectrum of compound **14** in $CDCl_3$



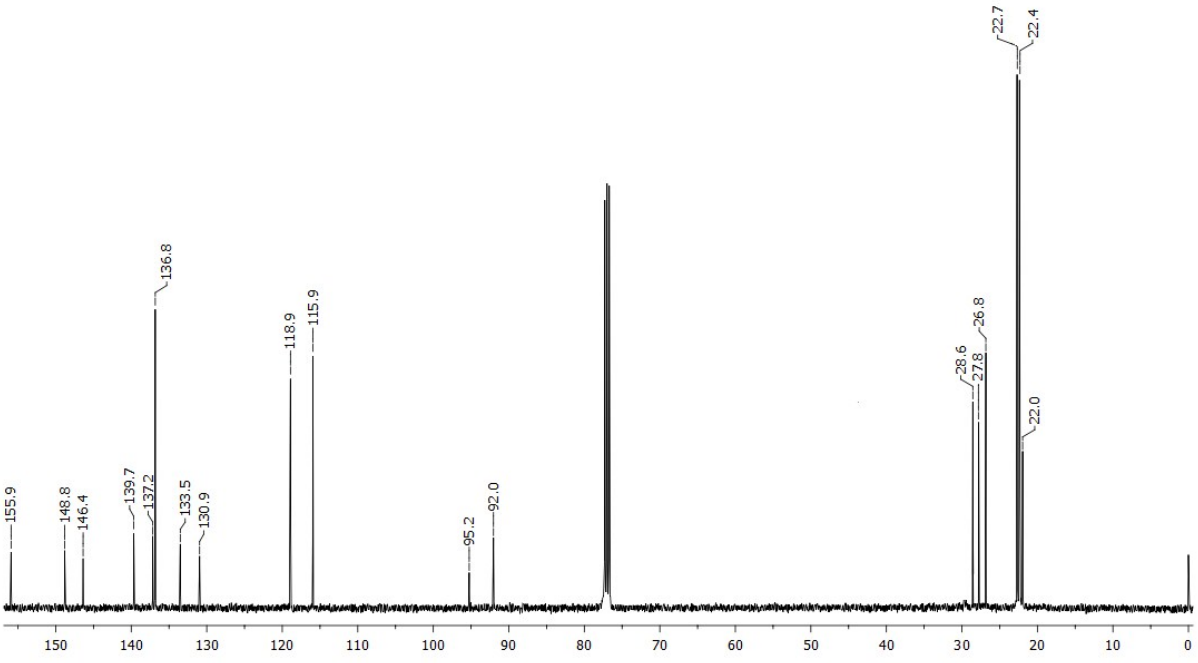
^{1}H NMR (400 MHz) spectrum of compound **7** in $CDCl_3$



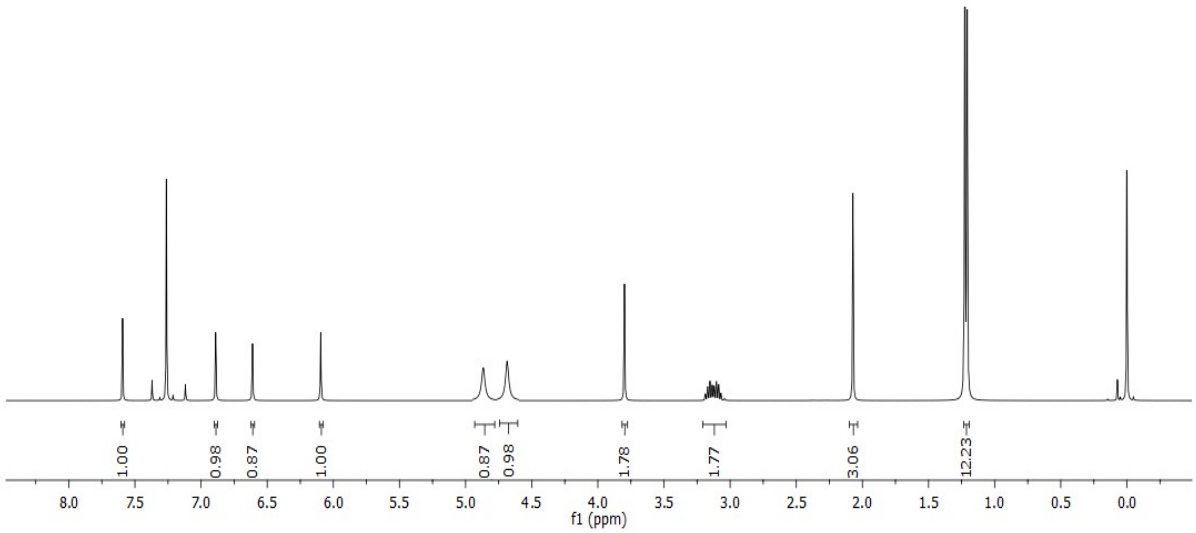
^{13}C NMR (100 MHz) spectrum of compound **7** in $CDCl_3$



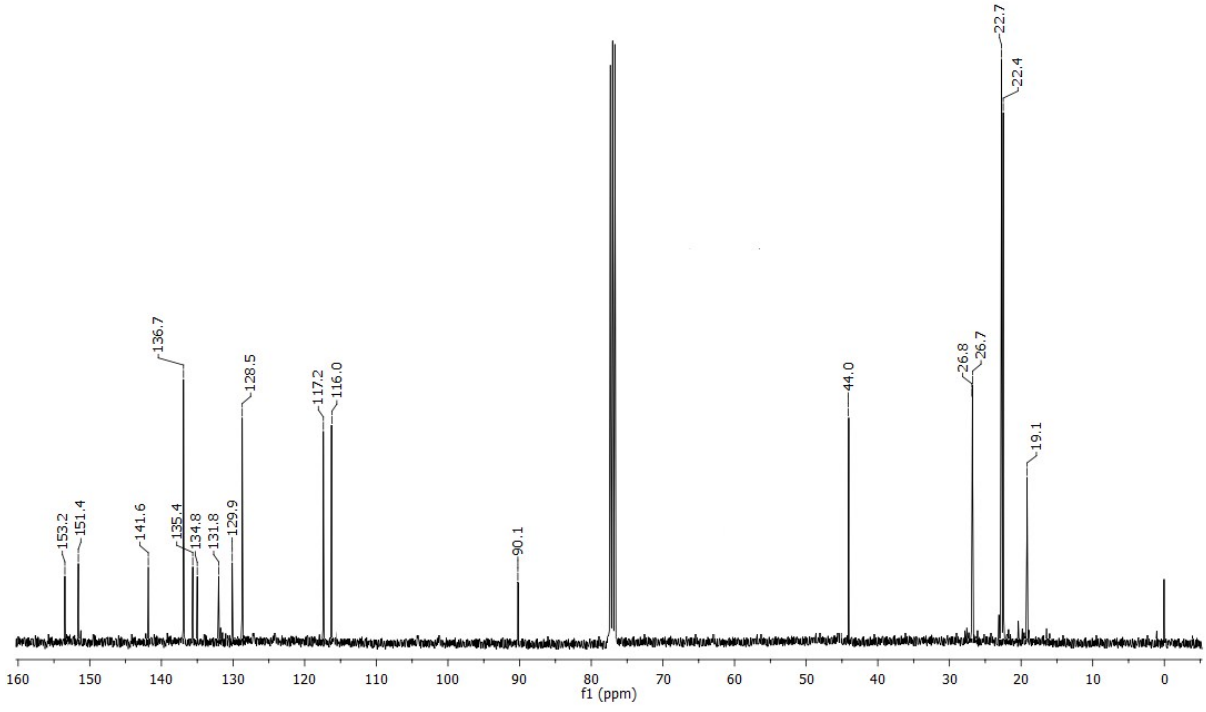
^{1}H NMR (400 MHz) spectrum of compound **15** in $CDCl_3$



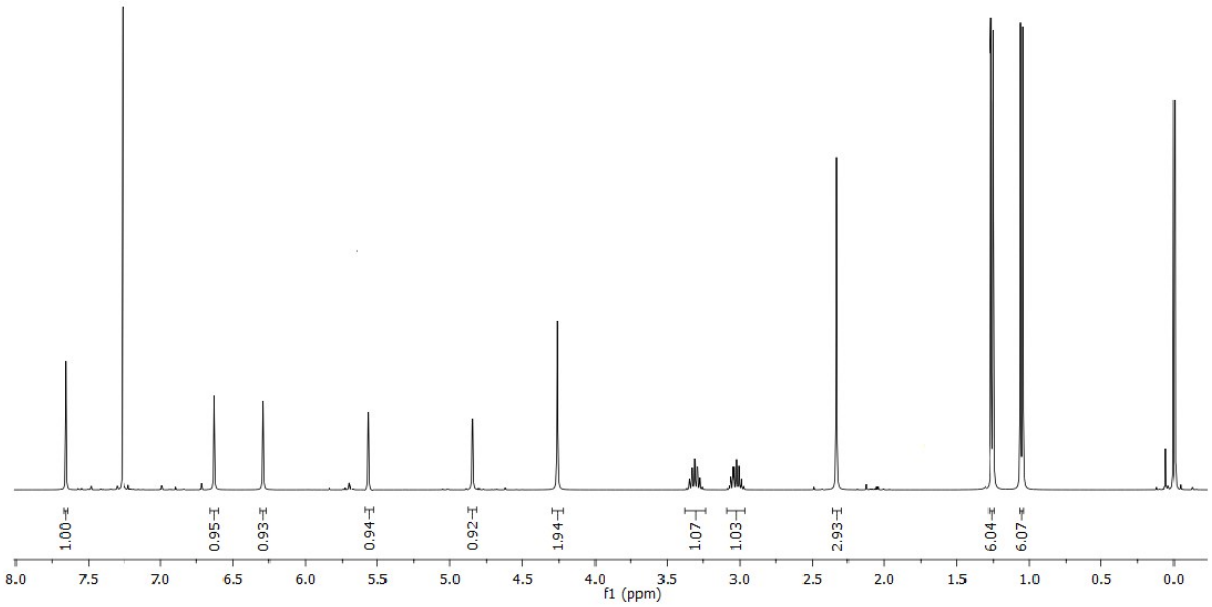
^{13}C NMR (100 MHz) spectrum of compound **15** in $CDCl_3$



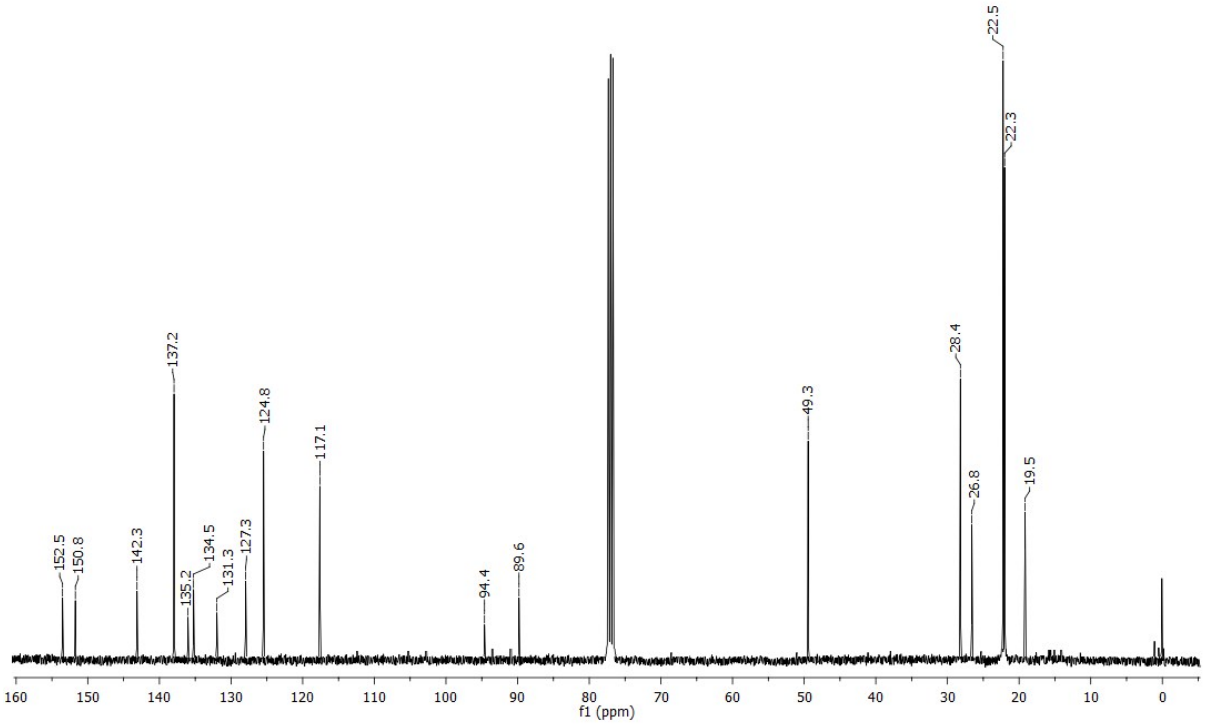
^{1}H NMR (400 MHz) spectrum of compound **16** in $CDCl_3$



^{13}C NMR (100 MHz) spectrum of compound **16** in $CDCl_3$



^{1}H NMR (400 MHz) spectrum of compound **17** in $CDCl_3$



^{13}C NMR (100 MHz) spectrum of compound **17** in $CDCl_3$