Supporting Information

Exploiting the *p*-Bromodienone Route for the Formation and Trapping of Calixarene Oxenium Cations with Enamine Nucleophiles

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TABLE OF CONTENTS

CHART S1

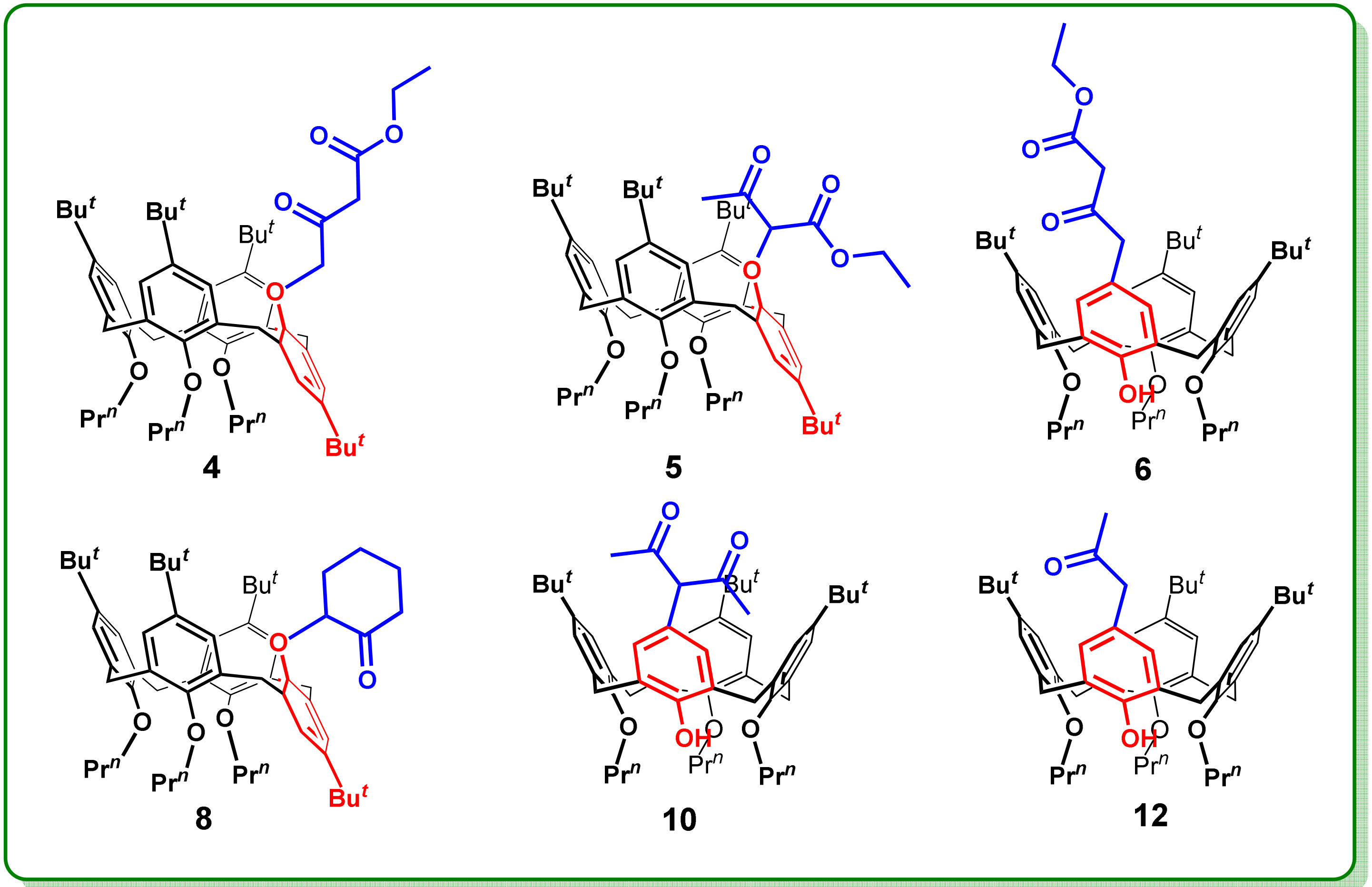


Chart S1. Derivative **4, 5, 6, 8, 10** and **12** (600 MHz, $CDCl_3$, 298 K).

^{1}H and ^{13}C NMR spectra of derivative 4, 5, 6, 8, 10 and 12.

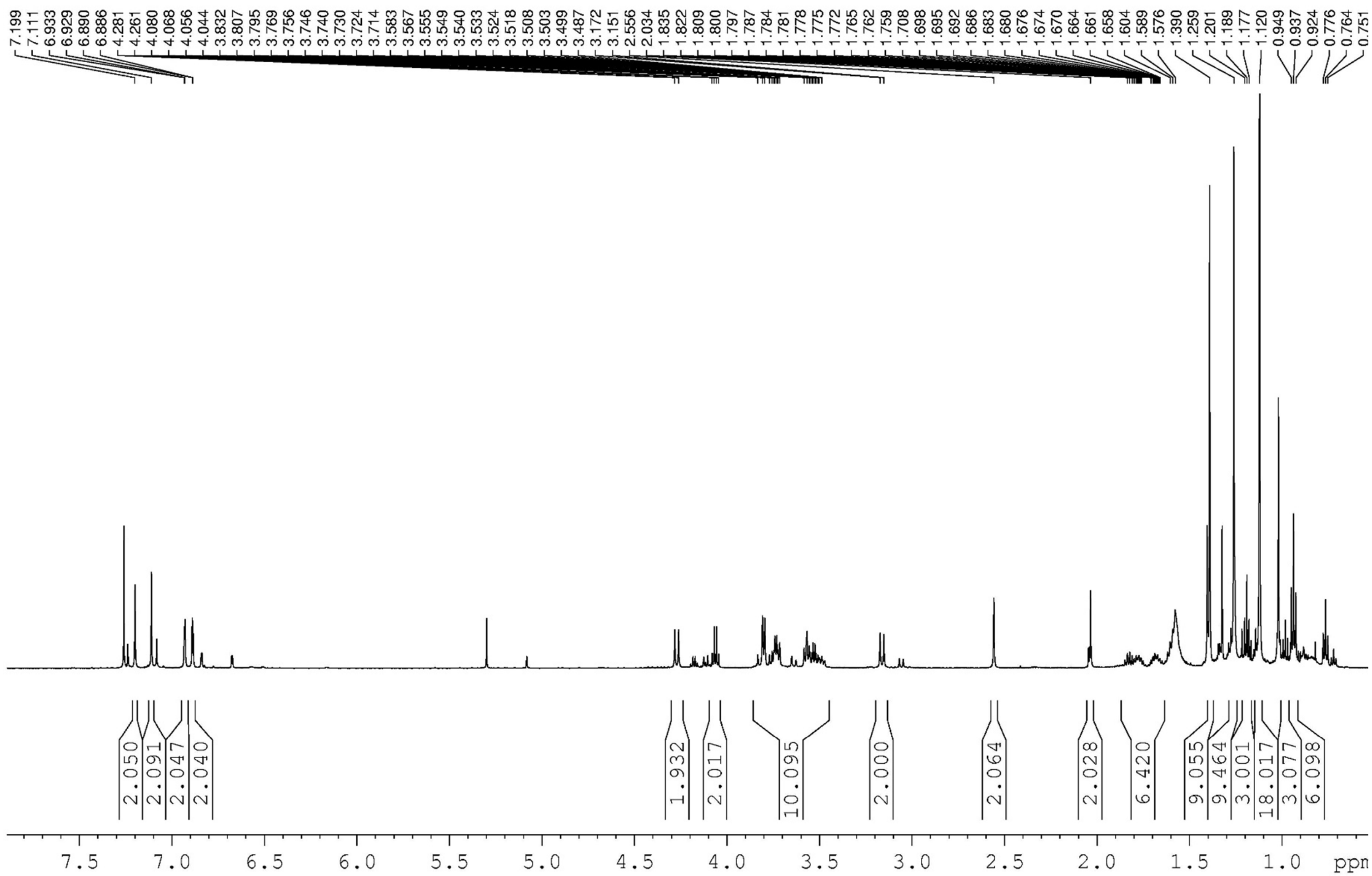


Figure S1. ^{1}H NMR of derivative **4** (600 MHz, $CDCl_3$, 298 K).

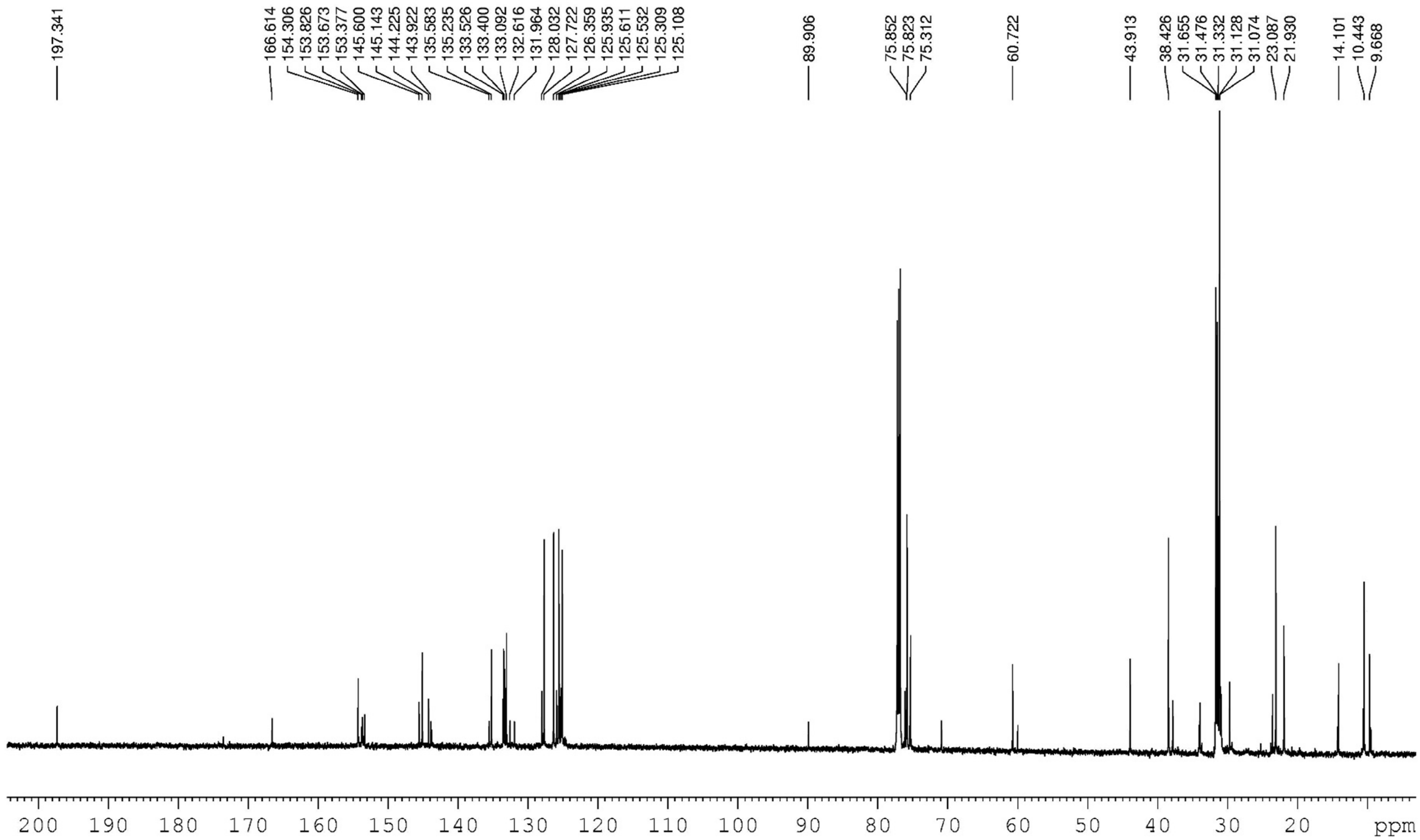


Figure S2. ^{13}C NMR of derivative **4** (150 MHz, $CDCl_3$, 298 K).

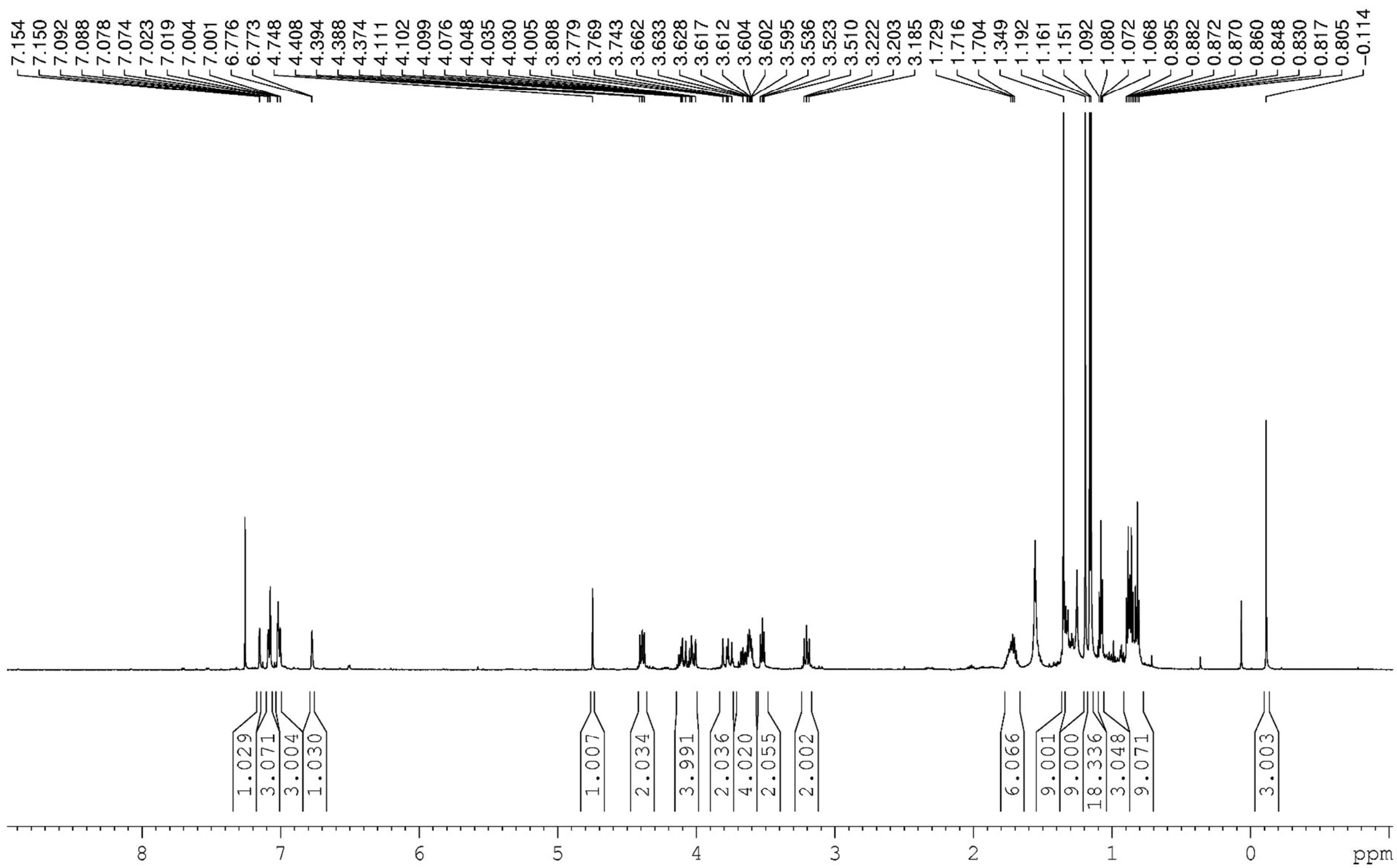


Figure S3. [1]H NMR of derivative **5** (600 MHz, $CDCl_3$, 298 K).

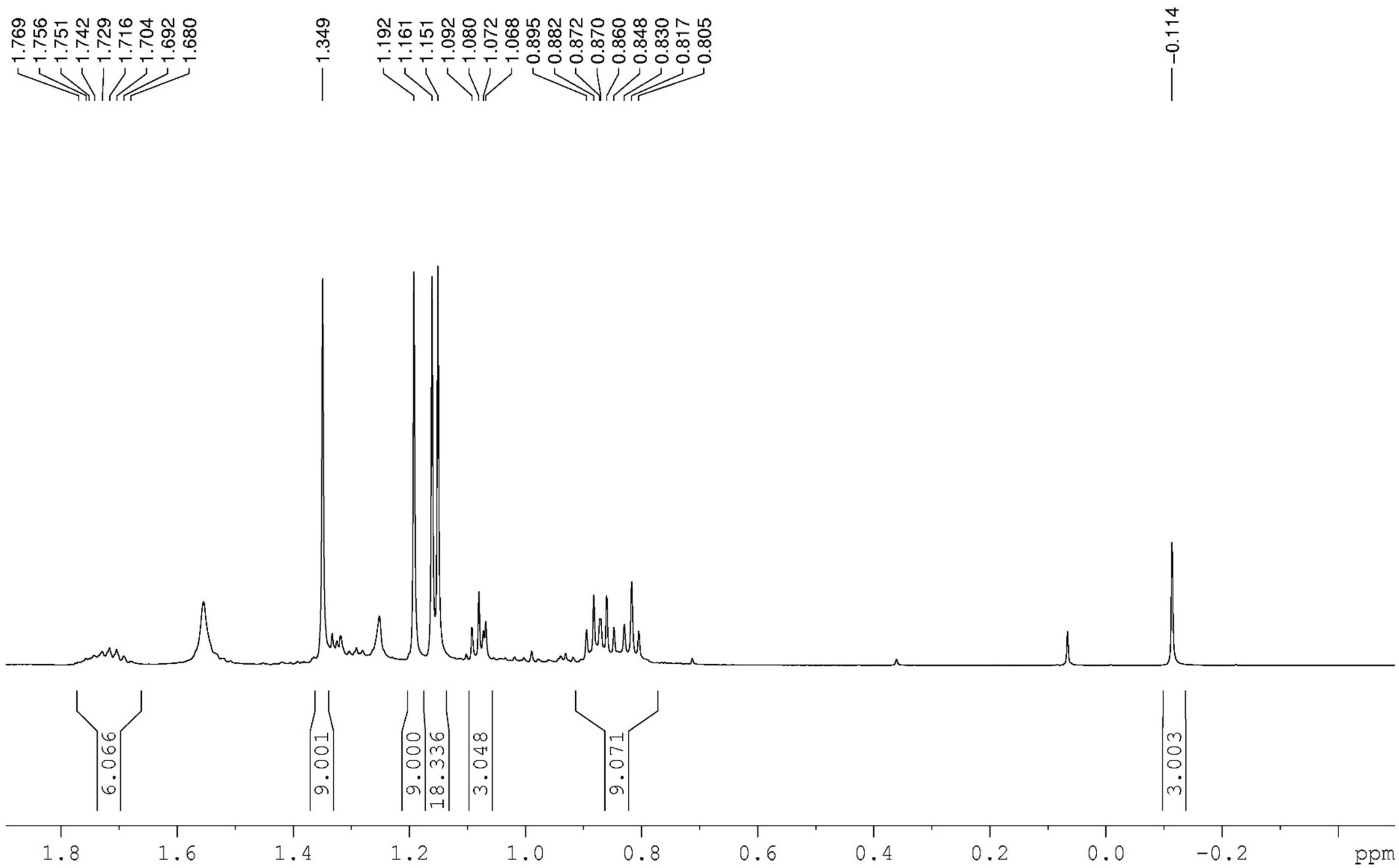


Figure S4. Portion of [1]H NMR of derivative **5** (600 MHz, $CDCl_3$, 298 K).

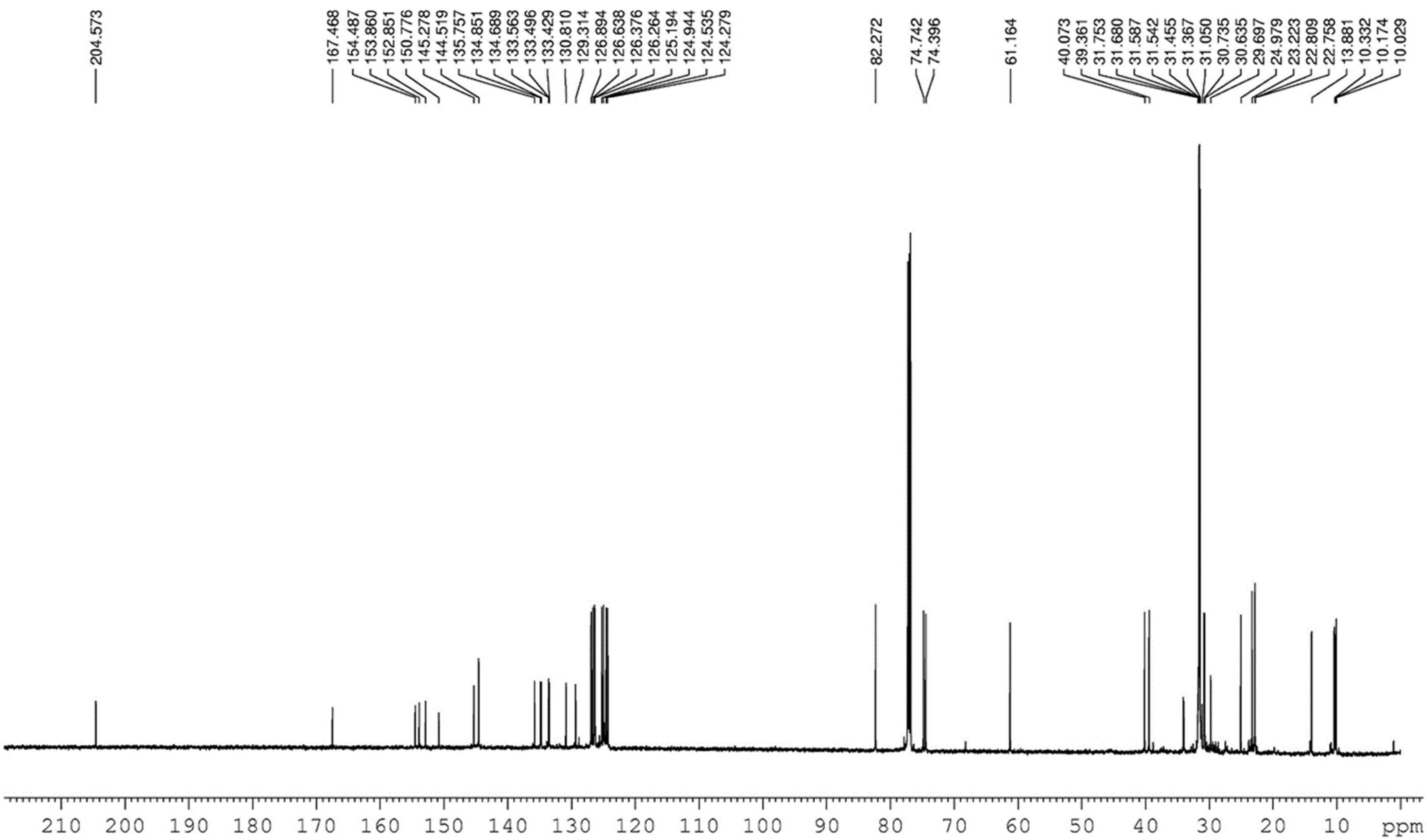


Figure S5. ^{13}C NMR of derivative **5** (150 MHz, $CDCl_3$, 298 K).

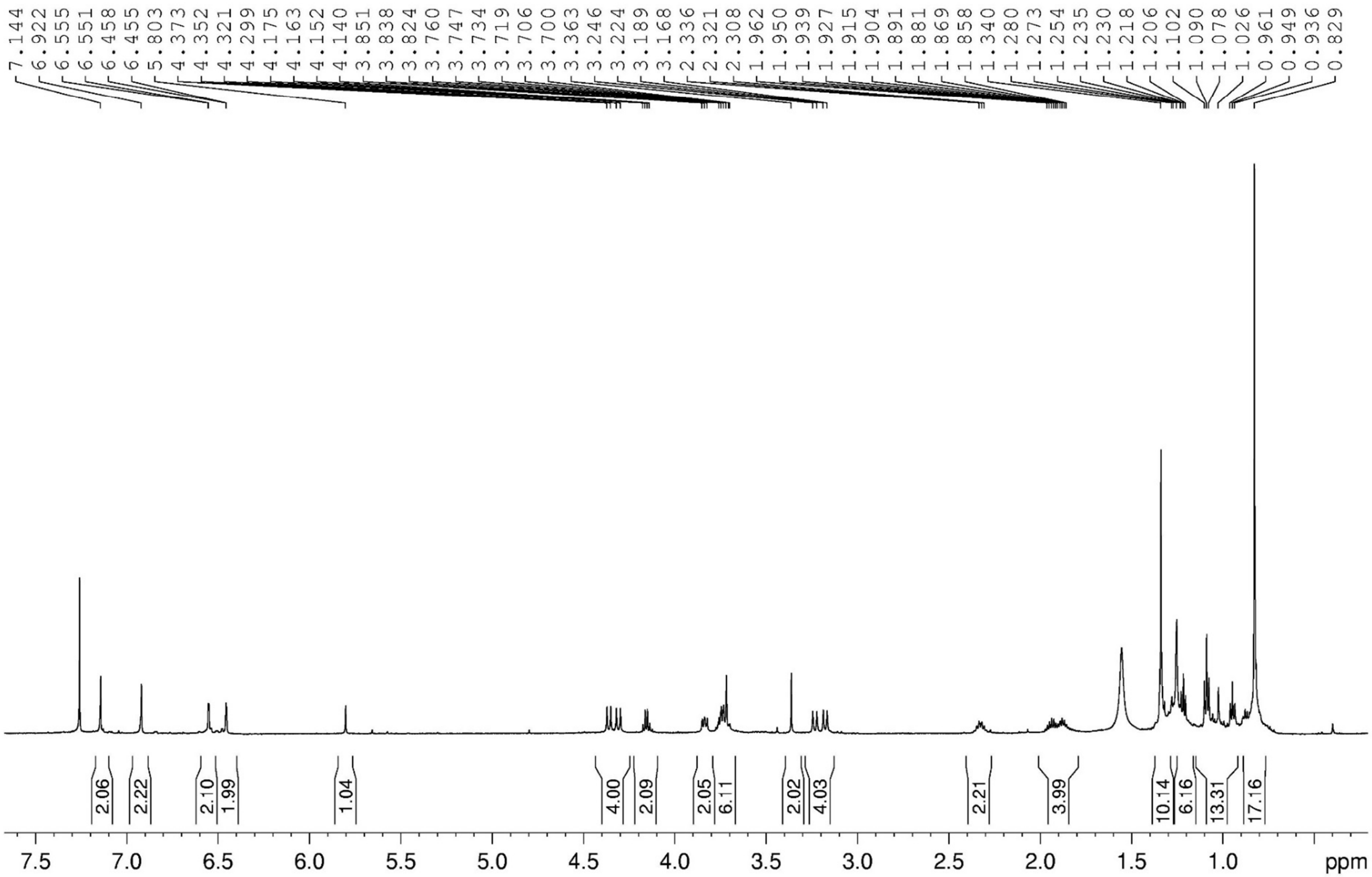


Figure S6. [1]H NMR of derivative **6** (600 MHz, $CDCl_3$, 298 K).

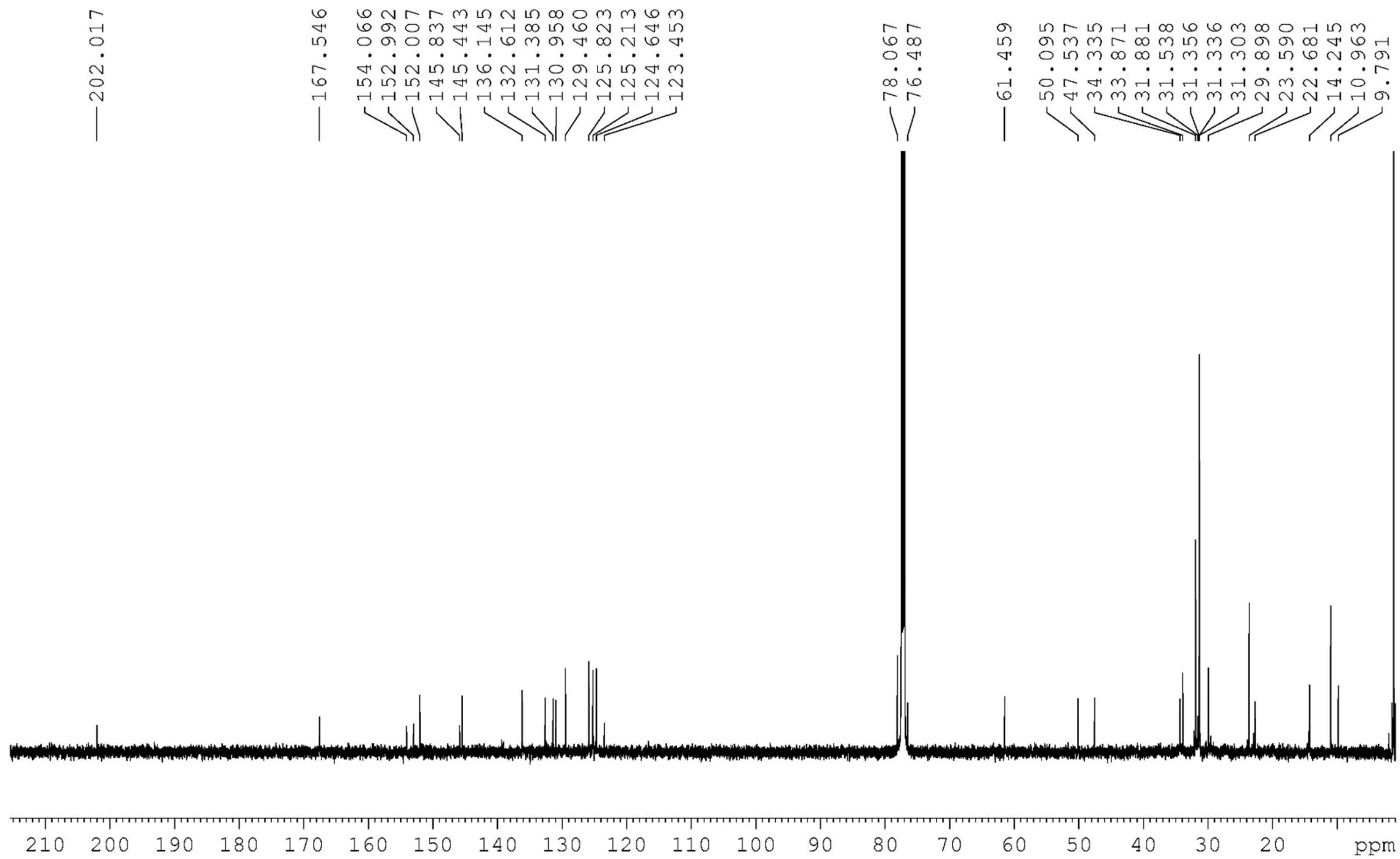


Figure S7. ^{13}C NMR of derivative **6** (150 MHz, $CDCl_3$, 298 K).

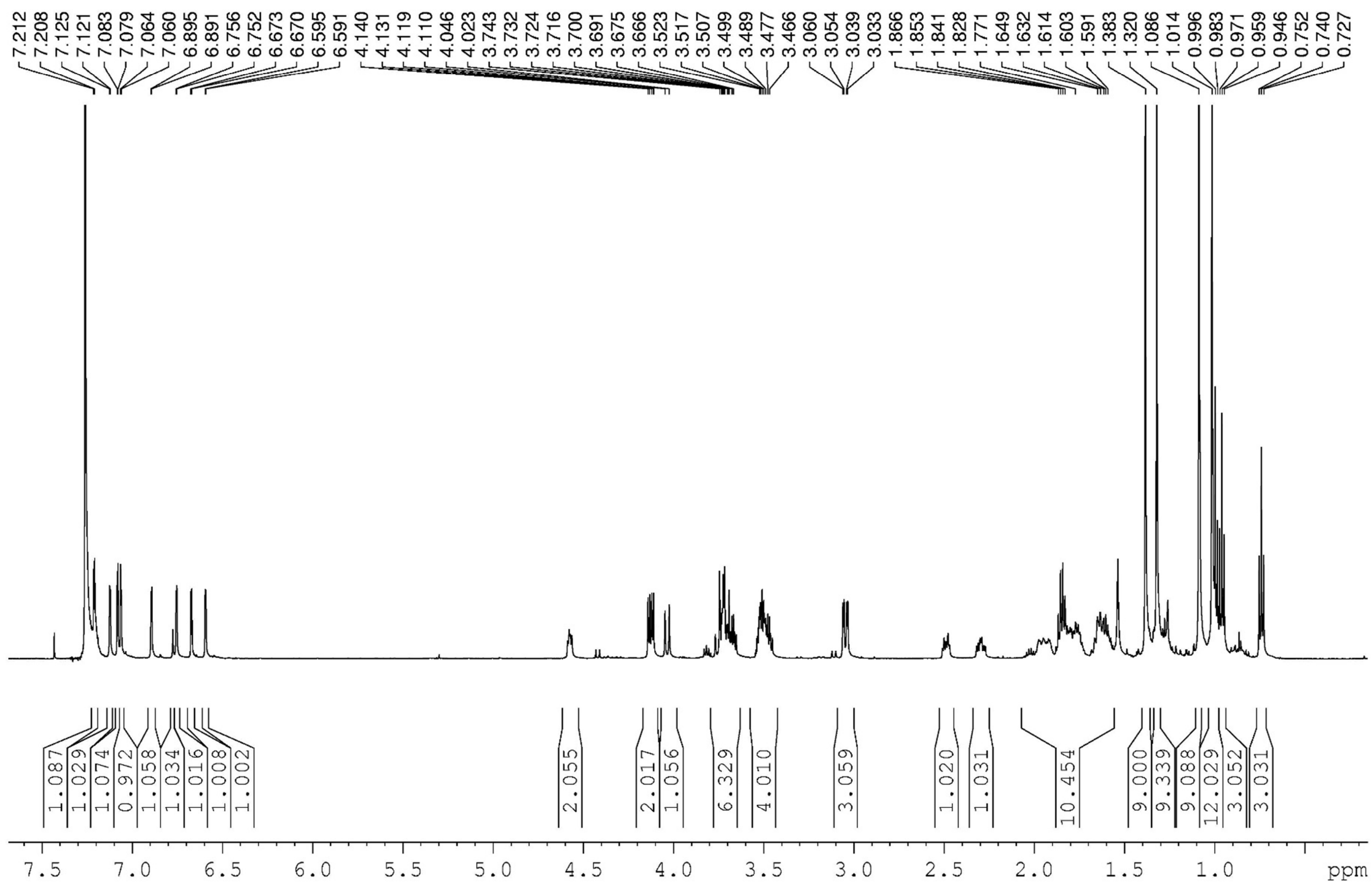


Figure S8. ^{1}H NMR of derivative **8** (600 MHz, $CDCl_3$, 298 K).

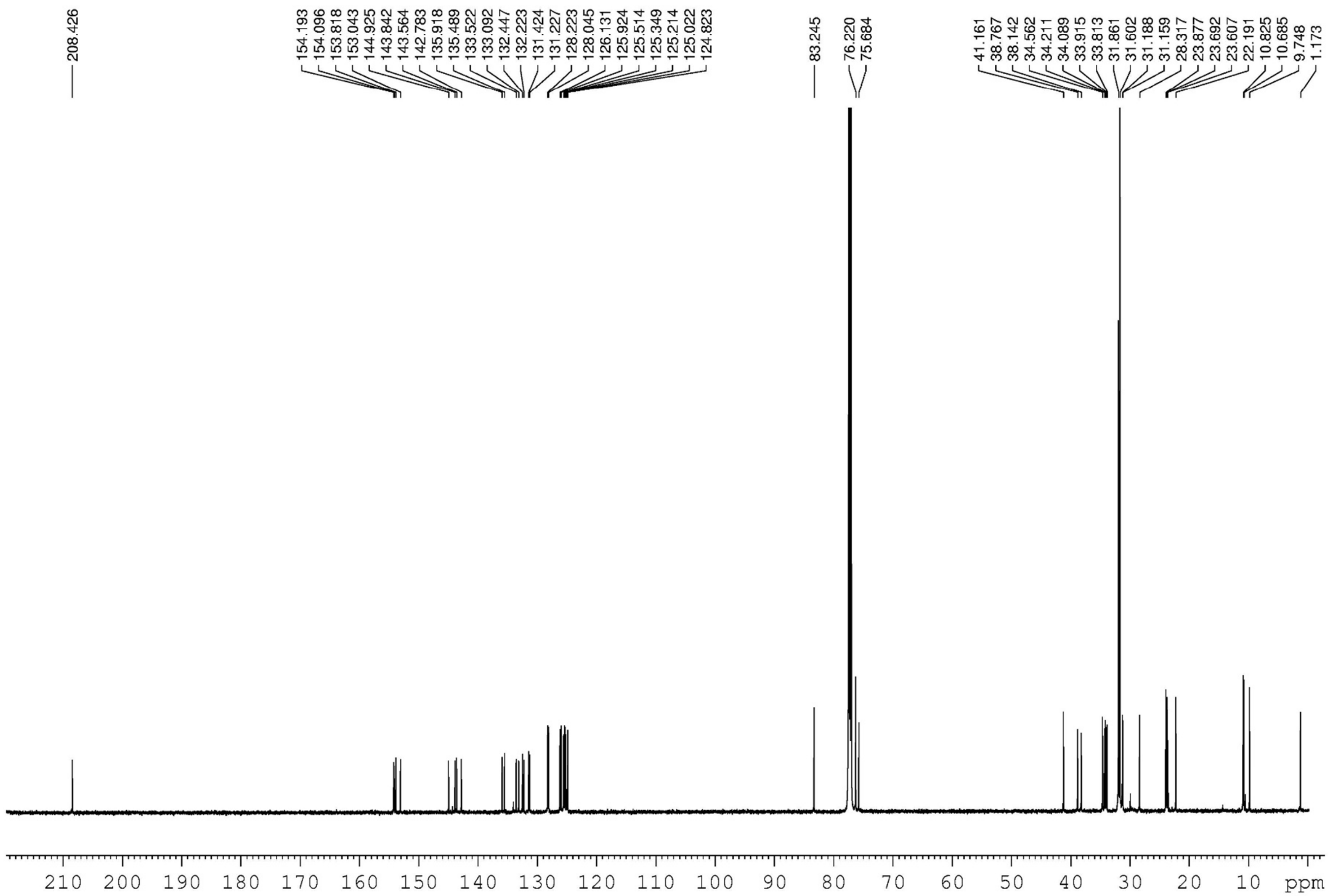


Figure S9. ^{13}C NMR of derivative **8** (150 MHz, $CDCl_3$, 298 K).

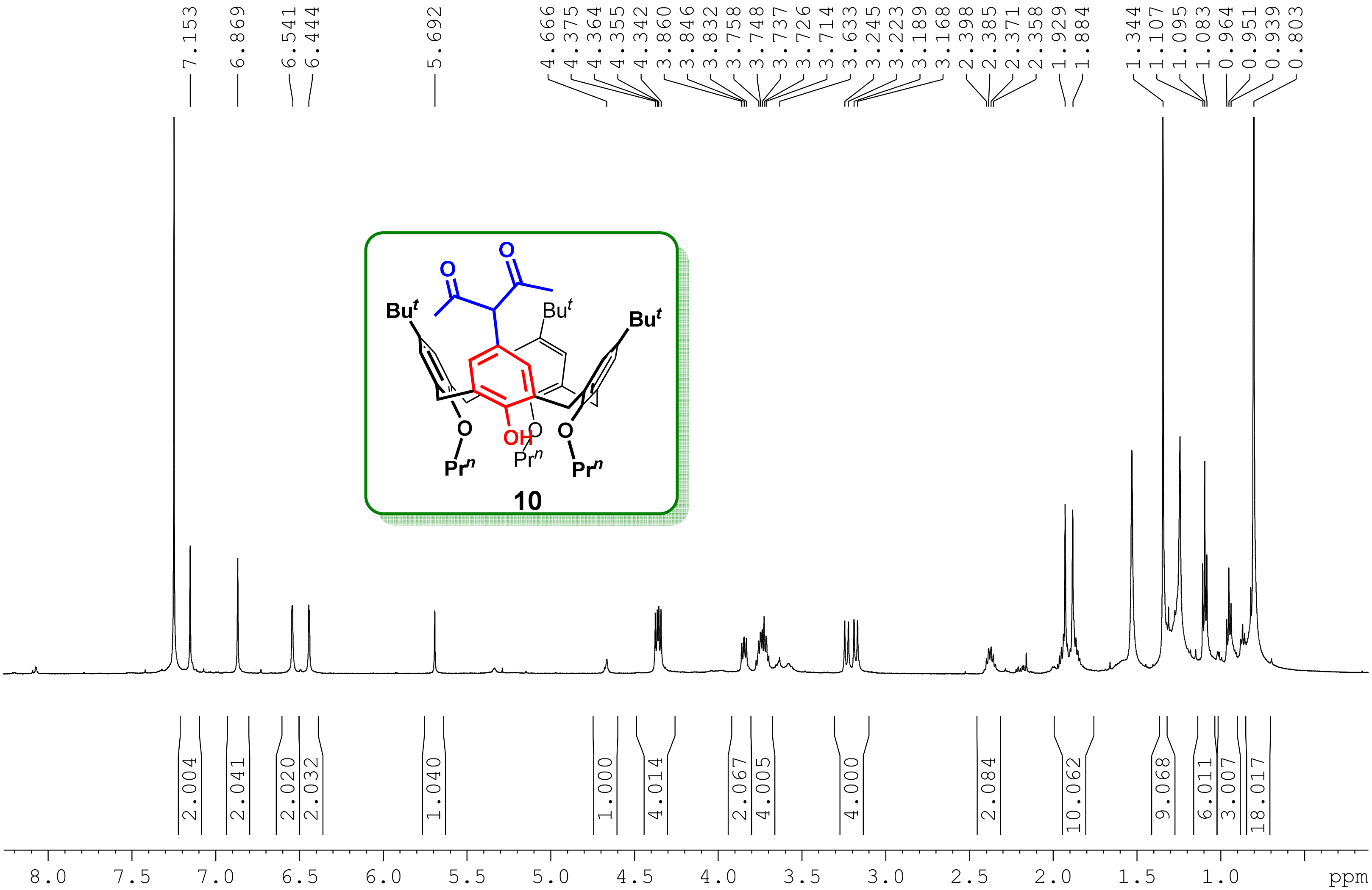


Figure S10. ^{1}H NMR of derivative **10** (600 MHz, $CDCl_3$, 298 K)

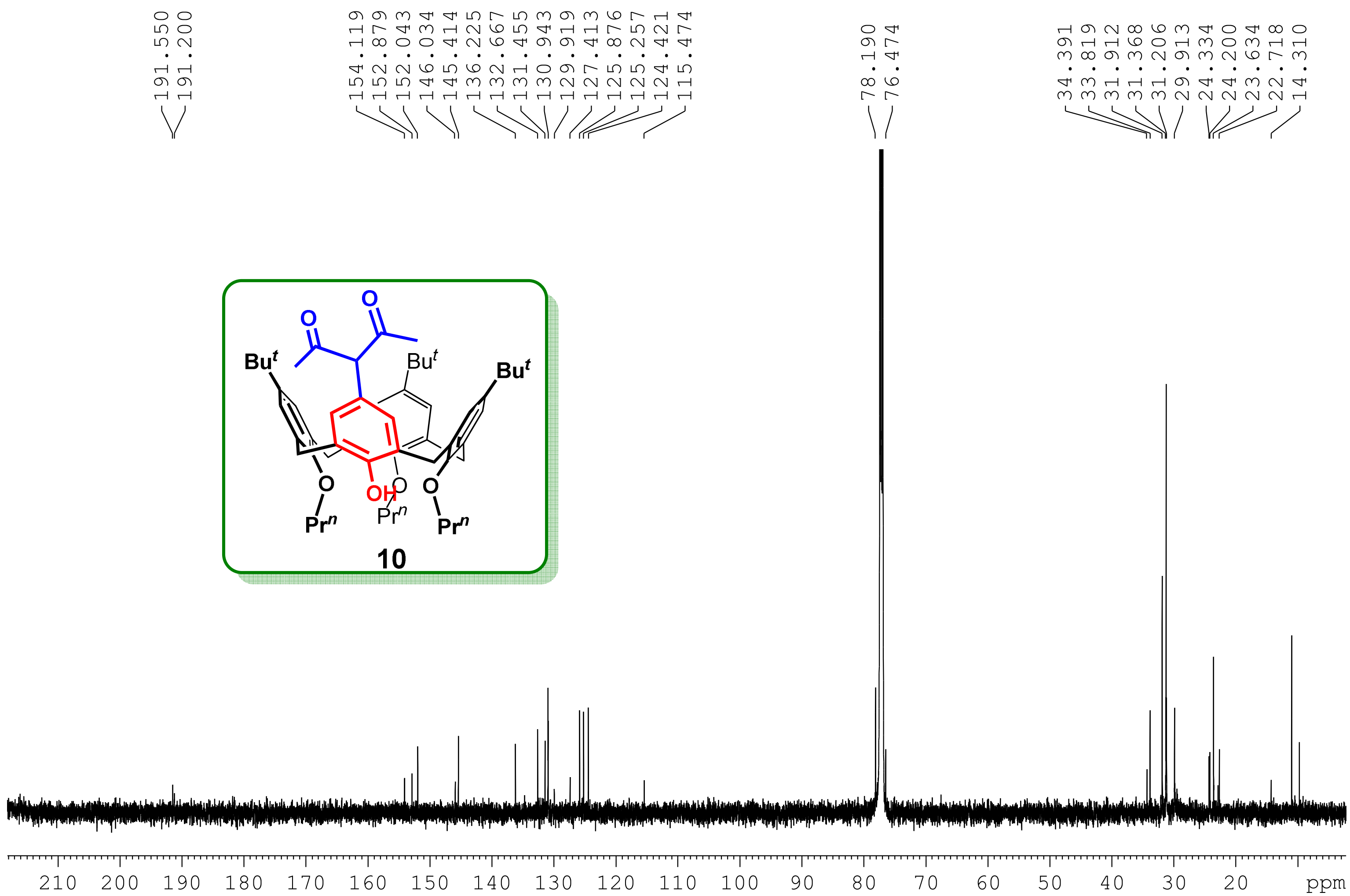


Figure S11. ^{13}C NMR of derivative **10** (150 MHz, $CDCl_3$, 298 K).

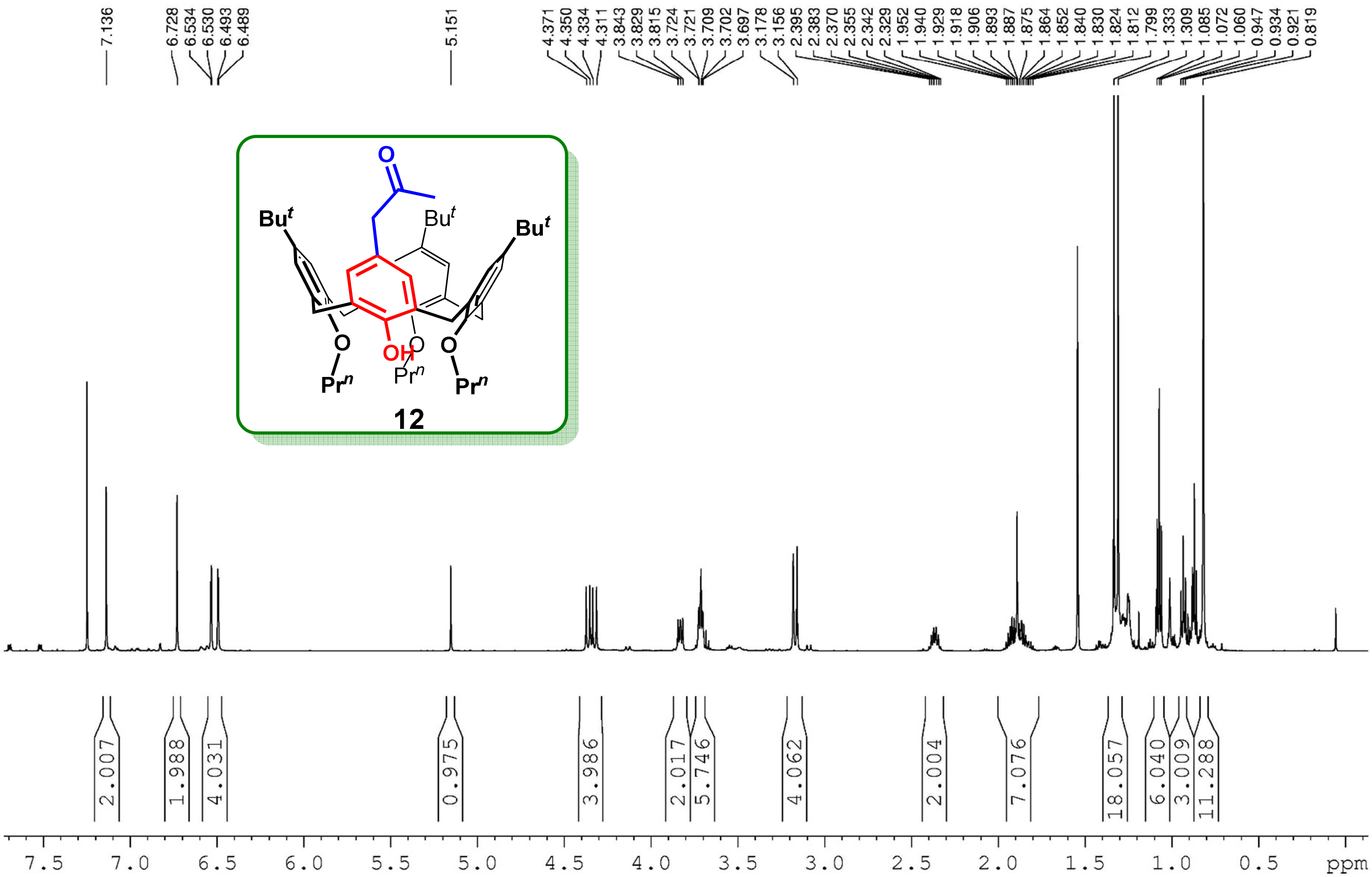


Figure S12. ^{1}H NMR of derivative **12** (600 MHz, $CDCl_3$, 298 K)

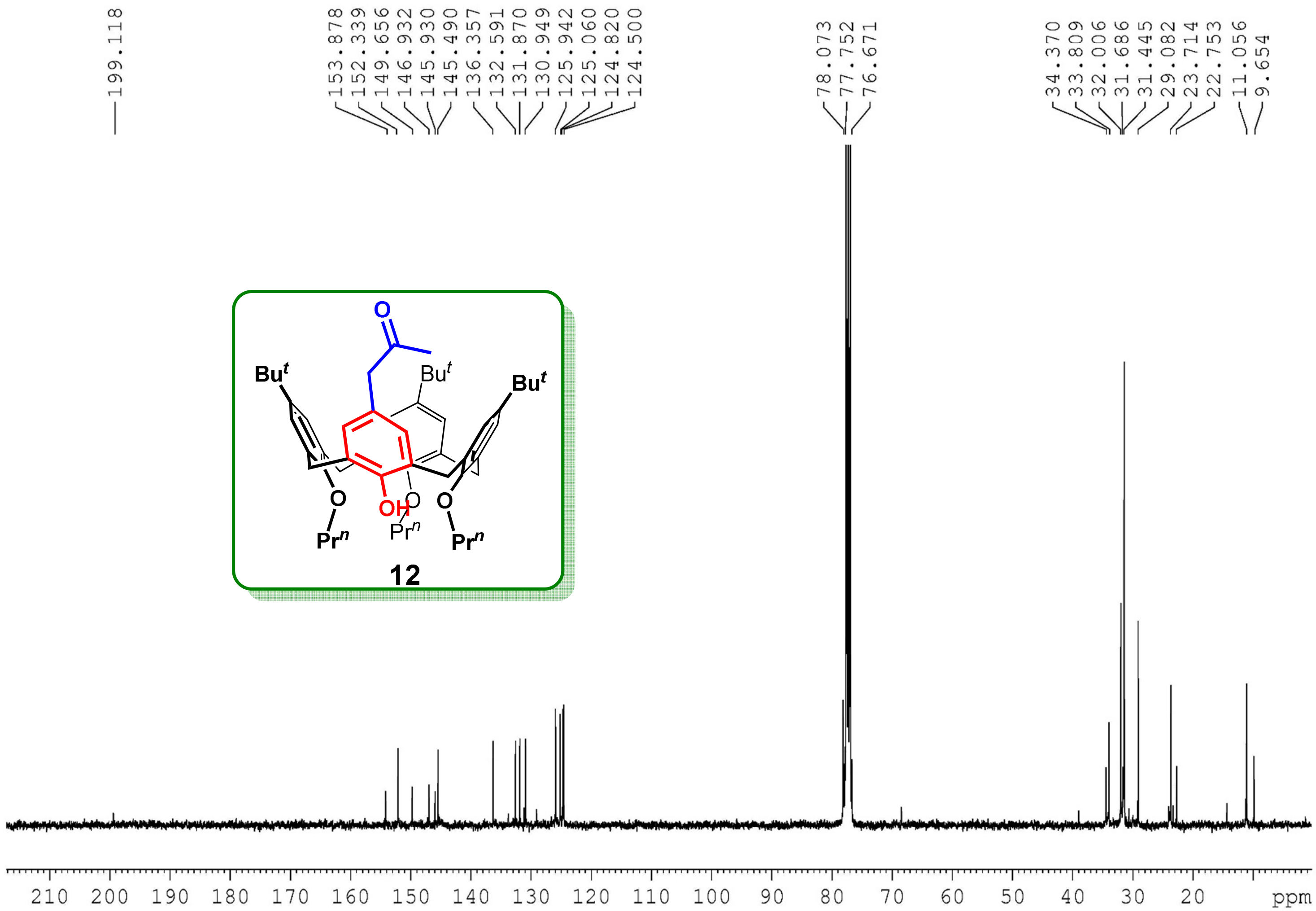


Figure S13. ^{13}C NMR of derivative **12** (100 MHz, $CDCl_3$, 298 K).

2D NMR Spectra of derivative 4

2D COSY-45 Spectrum of derivative **4**

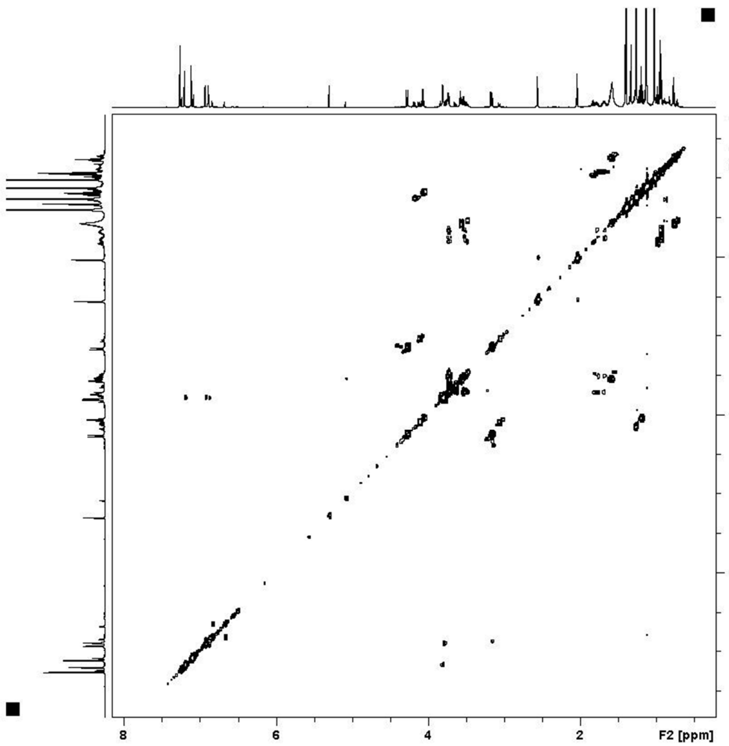


Figure S14. 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **4**.

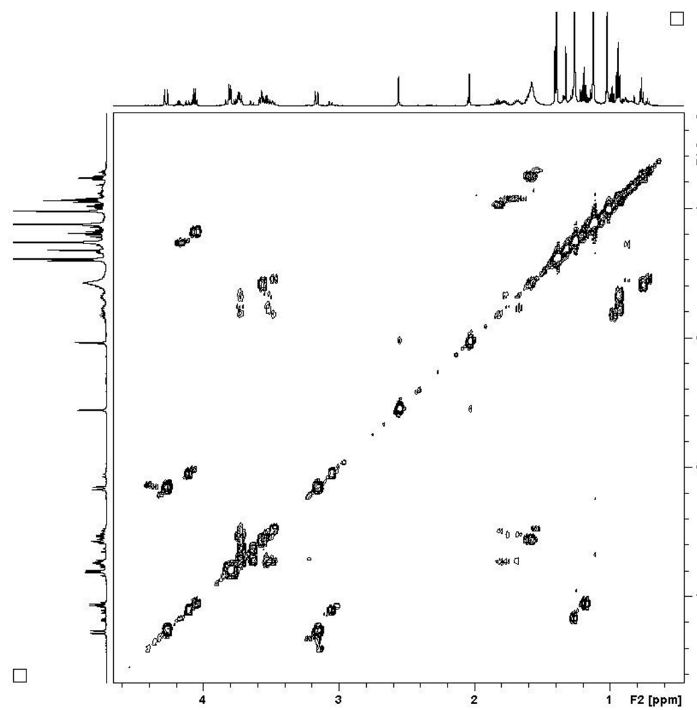


Figure S15. Section of the 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **4**.

2D HSQC Spectrum of derivative **4**

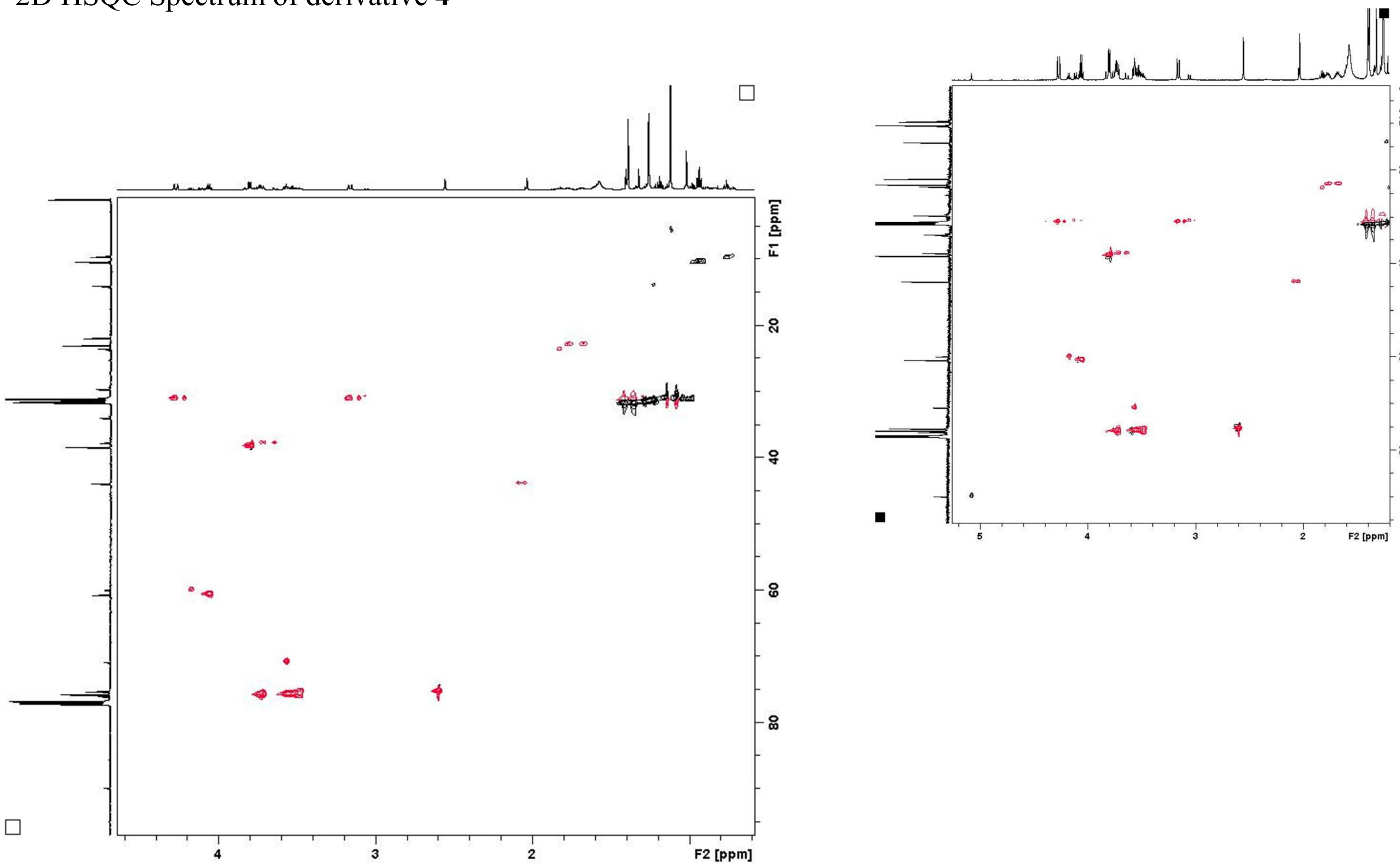


Figure S16. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **4**

2D NMR Spectra of derivative 5

2D COSY-45 Spectrum of derivative **5**

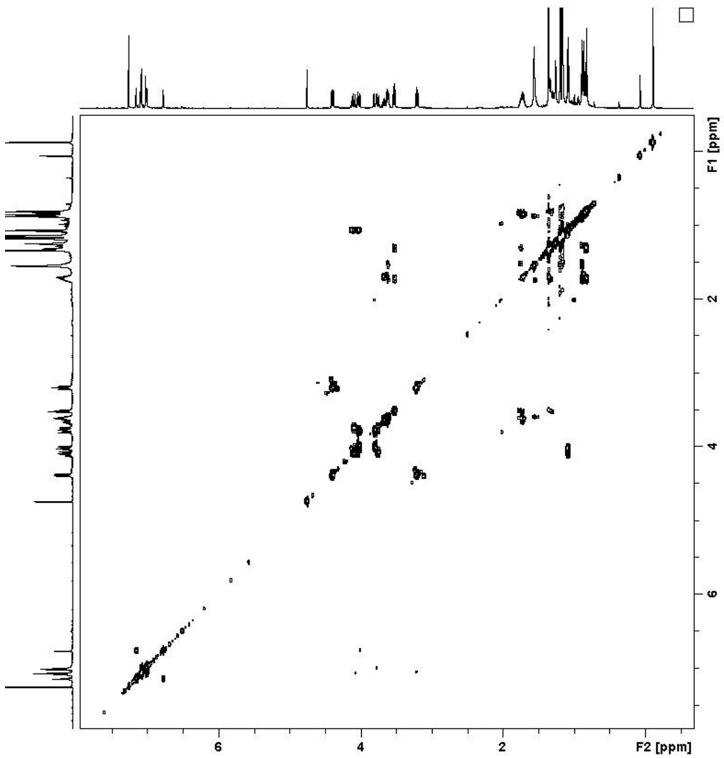


Figure S17. 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

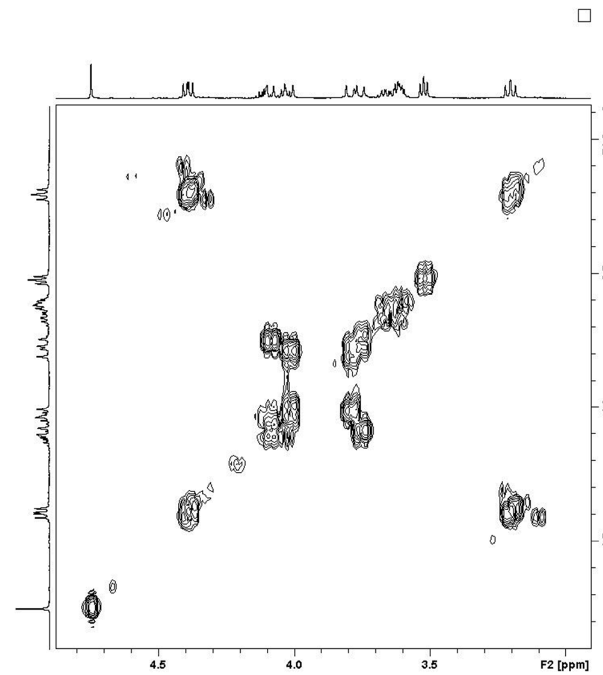


Figure S18. Section of the 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

2D HSQC Spectrum of derivative **5**

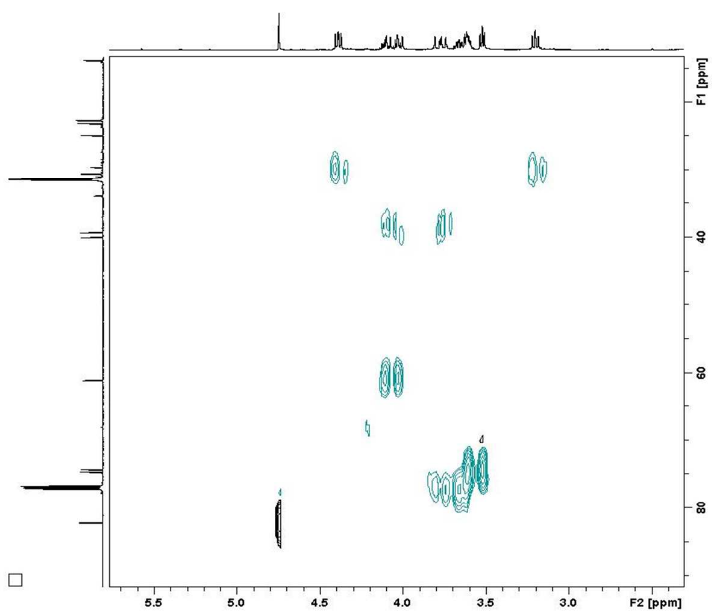


Figure S19. Section of the 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

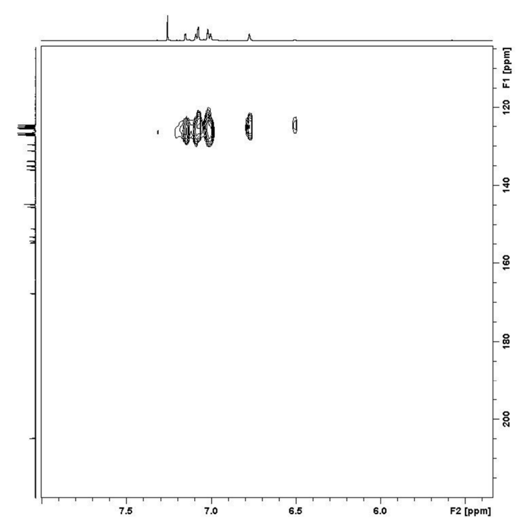


Figure S20. Section of the 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

2D HMBC Spectrum of derivative **5**

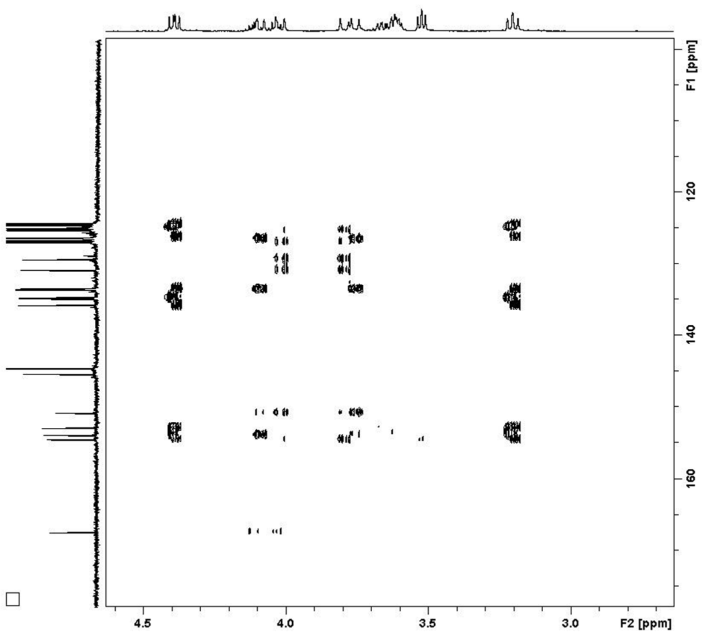


Figure S21. Section of the 2D HMBC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

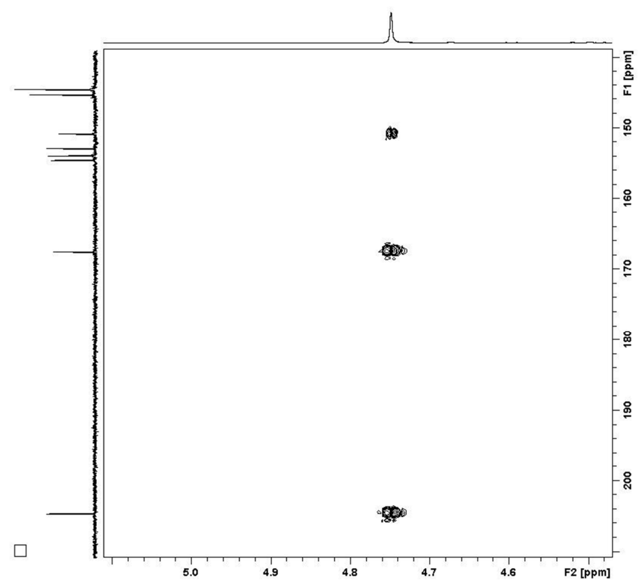


Figure S22. Section of the 2D HMBC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **5**.

2D NMR Spectra of derivative 6

2D COSY-45 Spectrum of derivative **6**

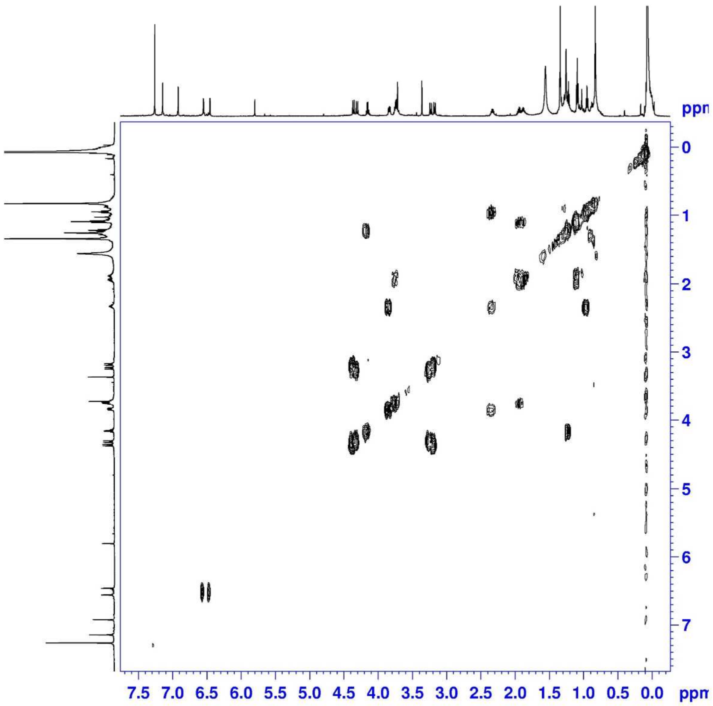


Figure S23. 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **6**.

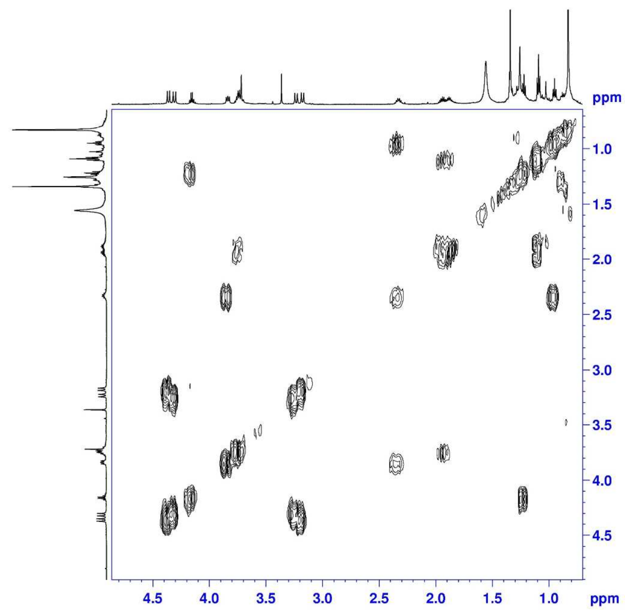


Figure S24. Section of the 2D COSY-45 spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **6**.

2D NMR Spectra of derivative 8

2D COSY-45 Spectrum of derivative **8**

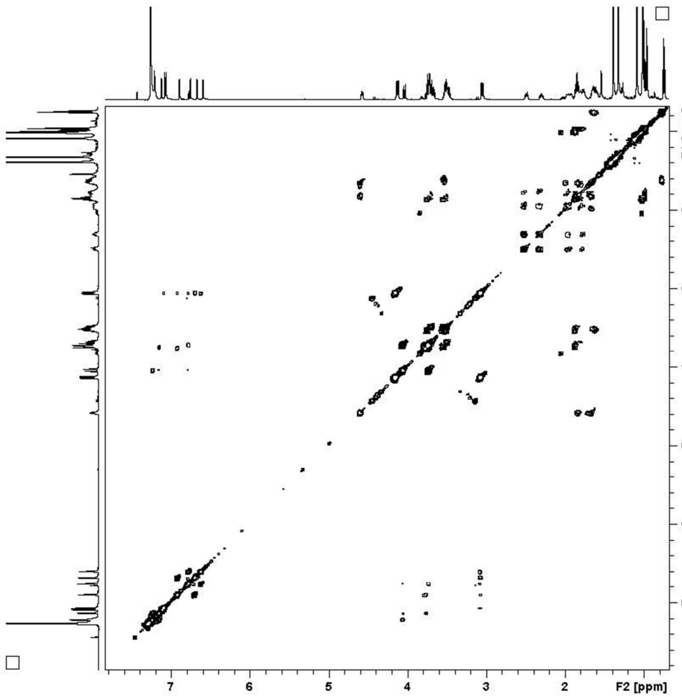


Figure S25 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **8**.

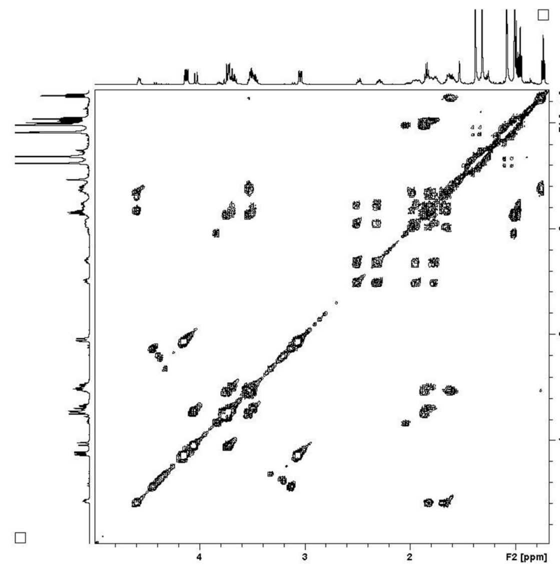


Figure S26. Section of the 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **8**.

2D NMR Spectra of derivative 10

2D COSY-45 Spectrum of derivative **10**

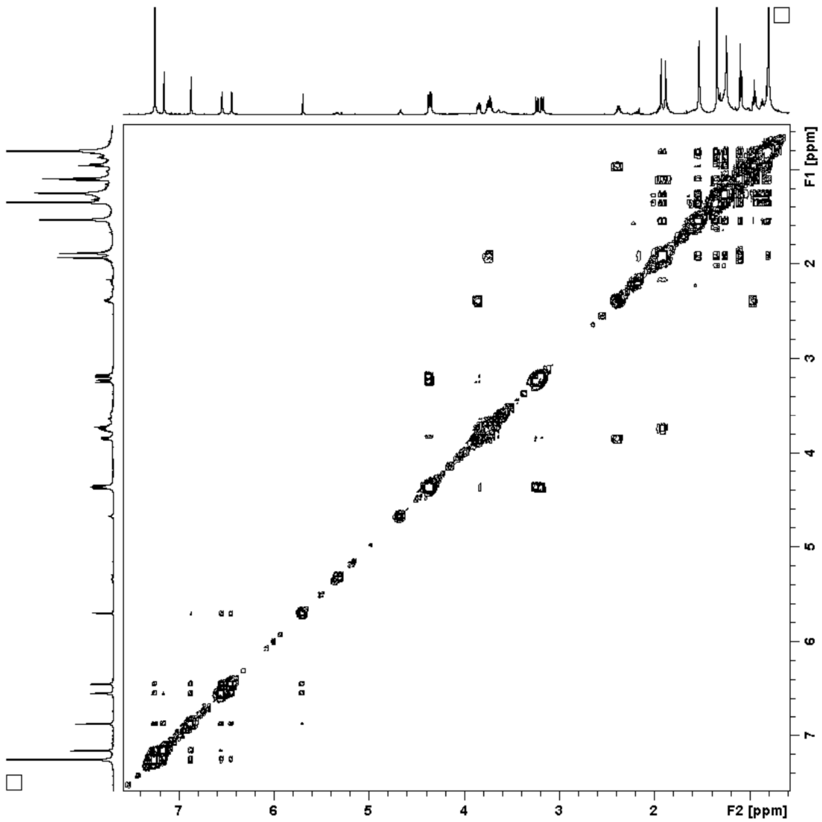


Figure S27 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **10**.

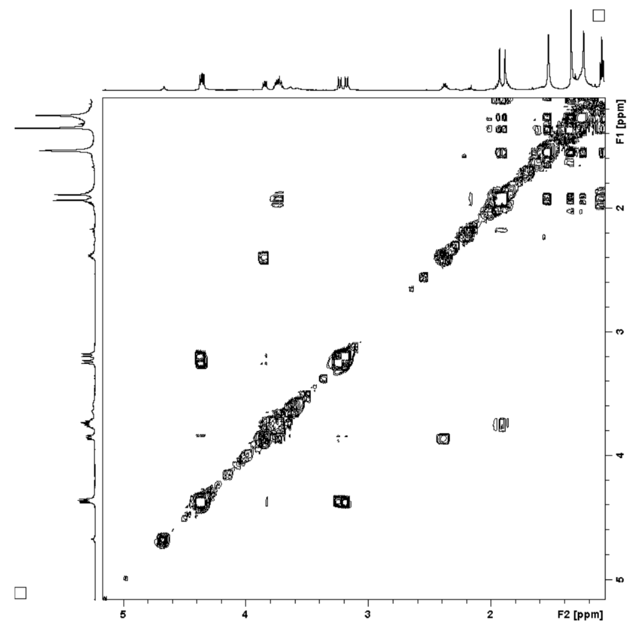
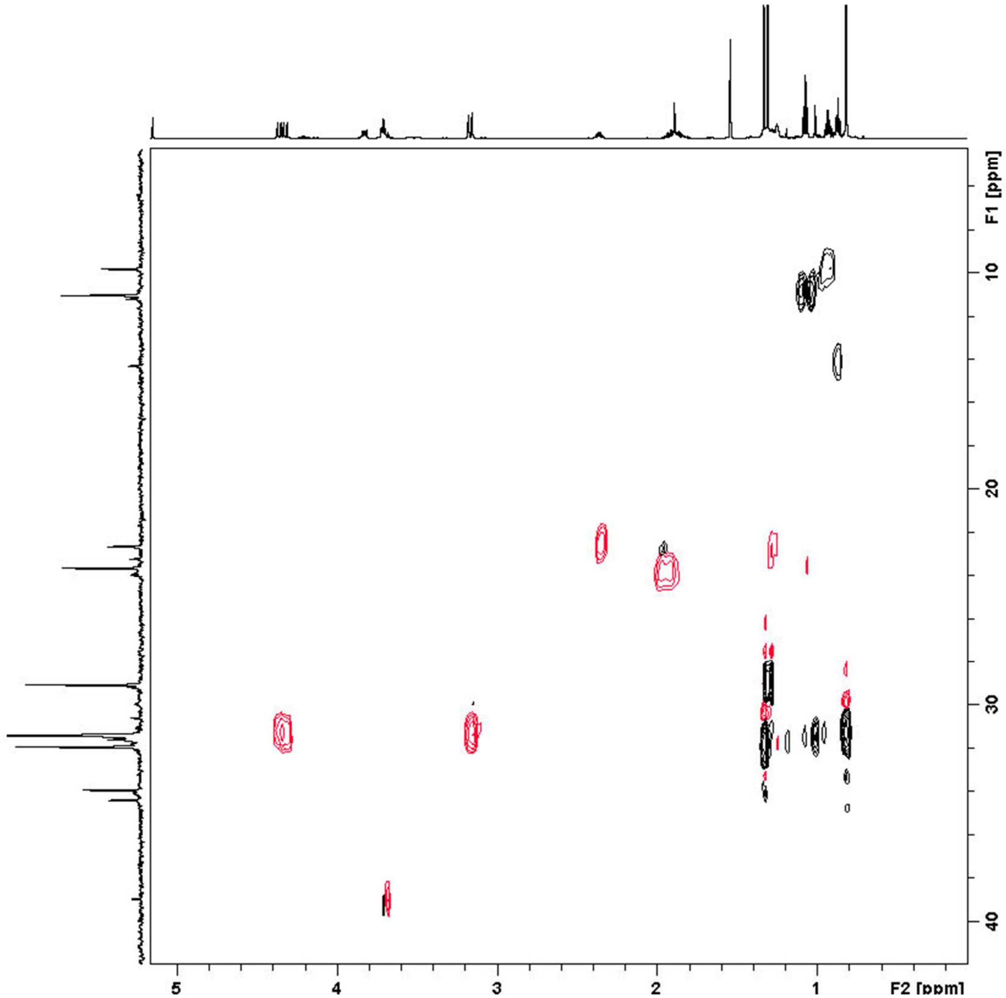


Figure S28. Section of the 2D COSY spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **10**.

2D NMR Spectra of derivative 12

2D HSQC spectrum of derivative **12**.



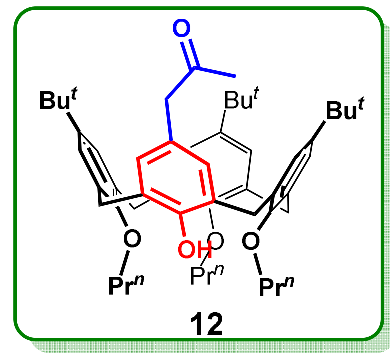


Figure S29. 2D HSQC spectrum (600 MHz, $CDCl_3$, 298 K) of derivative **12**.

DFT Calculations

DFT-optimized structure of **5** at the B3LYP/6-31G(d,p) level of theory

Cartesian coordinates of the optimzed structure of **5**

O	-0.890600	-3.064300	0.965300
O	-0.813400	1.341700	1.280100
O	0.335900	-1.857400	-1.691000
C	-2.007000	0.685100	1.002200
C	-2.719500	1.167700	-0.115500
C	-1.734400	-1.098900	2.899700
C	1.708300	-1.736700	-1.759900
C	1.449700	-2.641600	1.409000
C	0.093700	-2.399400	1.681900
C	-3.925700	0.551900	-0.448400
C	-0.282900	-1.517700	2.708000
C	1.408200	0.057100	-3.549400
C	2.062400	-1.393400	3.434500
C	1.888500	-3.405000	0.164700
C	0.708800	-1.061900	3.586700
C	3.898700	-2.358000	-0.979600
C	3.676400	-0.730200	-2.718400
C	-2.454200	-0.443100	1.716800
C	2.279400	-0.832200	-2.667800
C	4.514100	-1.488200	-1.892900
C	2.511600	-2.493800	-0.887800
C	2.405200	-2.138300	2.298400
C	-4.453200	-0.524200	0.276500
C	-3.683800	-1.004100	1.336500
C	-2.271500	2.389800	-0.915700
C	0.024000	3.402400	-1.217600

C	1.332700	3.436300	-1.727300
C	1.752200	2.322000	-2.461000
C	0.881900	1.276100	-2.801300
C	-0.460500	1.373100	-2.411200
C	-0.875800	2.378900	-1.521900
O	-1.403900	0.492000	-2.924100
C	-0.215700	-2.863600	-2.552700
H	-2.327600	-1.979800	3.168900
H	-1.788600	-0.445500	3.779300
H	0.398800	-0.444900	4.423400
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H	3.448900	-2.362800	2.098300
H	-4.032500	-1.856900	1.907500
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H	-3.015200	2.540600	-1.707200
H	0.561100	-0.510600	-3.935700
H	2.006400	0.384100	-4.407500
H	1.025200	-3.924300	-0.251700
H	2.628000	-4.163100	0.445900
H	2.778300	2.252900	-2.805300
H	4.105500	-0.038900	-3.435400
H	-4.475200	0.946500	-1.298300
H	-0.320100	4.196100	-0.561600
H	0.209100	-3.847100	-2.298900
H	0.064600	-2.655400	-3.596700
H	2.832800	2.211700	1.866900
H	1.822700	0.740000	1.682700
C	-2.349800	-4.982200	0.775400
H	-3.192600	-4.287400	0.685100
H	-1.983800	-5.165200	-0.241000
C	-2.809300	-6.297300	1.412900
H	-3.596700	-6.767200	0.816400
H	-1.983700	-7.013100	1.493600
H	-3.208000	-6.136500	2.420800
C	-1.726100	-2.866100	-2.387200
H	-1.951400	-3.039300	-1.332400
H	-2.092900	-1.864400	-2.620500
C	-2.399700	-3.918500	-3.272500

H	-3.486800	-3.902900	-3.145300
H	-2.192300	-3.747100	-4.335700
H	-2.055600	-4.932100	-3.033200
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H	-2.502900	-0.966500	-4.853300
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C	-3.708500	0.480300	-5.927000
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H	5.112300	-0.085400	4.527100
H	4.816200	-0.980100	3.035300
H	4.052900	0.595600	3.283300
C	2.602500	-0.037200	5.541200
H	3.404400	0.211800	6.243600
H	2.243700	0.901000	5.106200
H	1.788500	-0.481200	6.123300
C	3.618700	-2.297500	5.175600
H	4.384100	-2.063300	5.924300
H	2.787900	-2.798000	5.683800
H	4.049800	-3.007100	4.462500
C	6.051400	-1.403500	-1.954100
C	6.542200	-0.381100	-2.996600
H	7.636800	-0.356400	-3.001600
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C	6.627700	-2.788900	-2.331300
H	7.722300	-2.751000	-2.372300
H	6.347800	-3.556400	-1.603700
H	6.262000	-3.110600	-3.311900
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H	7.698000	-0.915700	-0.601800
H	6.213400	-0.000800	-0.278400
H	6.335500	-1.695100	0.210400
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C	3.651900	4.474900	-2.036500
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H	2.188100	6.761200	-2.215700
H	1.512100	5.609000	-3.383500
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C	2.296900	5.085100	-0.031600
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H	1.310800	5.247000	0.412200
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H	-6.953700	0.330600	1.101200
H	-6.709500	0.846800	-0.571900
C	0.860900	2.408900	2.630300
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C	-1.566100	3.041600	2.948700
O	-2.184200	3.043400	3.989200
O	-1.610600	4.025100	2.029300
C	-2.419400	5.182900	2.373800
H	-2.263200	5.407800	3.431200
H	-2.000700	5.988100	1.766400
C	-3.892600	4.960400	2.071100
H	-4.451800	5.877200	2.286300
H	-4.046300	4.706900	1.018300
H	-4.296800	4.158400	2.692100
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H	-1.205100	1.162300	-4.886000
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