

Supporting Information for

Novel Derivatives of 1,6,7,12-Tetrachloroperylene- 3,4,9,10-Tetracarboxylic Acid: Synthesis, Electrochemical and Optical Properties

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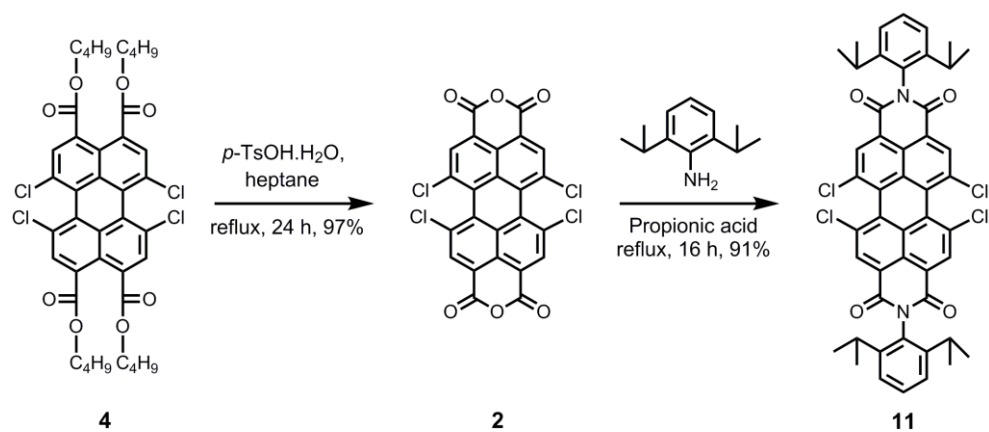
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The supporting information contains following items:

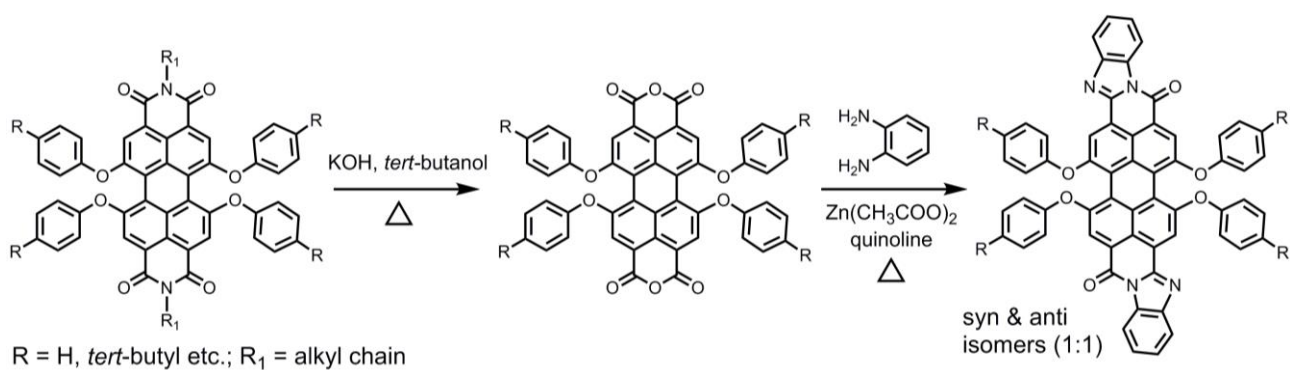
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Table S1. Synthesis of compound **5** from **4** under various reaction conditions.

Entry	<i>T</i> (°C)	<i>t</i> (h)	<i>p</i> -TsOH	Solvent	Amount of solvent per gram of 4	Relative Yield (%)		
						4	5	2
1	90	6	1.3 eq.	heptane	4 mL	90	10	–
2	99	18	3.5 eq.	heptane	16 mL	–	10	90
3	99	3	1.2 eq.	heptane	8 mL	75	20	5
4	99	22	1.2 eq.	heptane	14 mL	20	65	15
5	99	40	1.2 eq.	heptane	18 mL	5	60	35
6	99	48	1.1 eq.	heptane	8 mL	13	77	10
7	100	8	2.0 eq.	toluene	16 mL	40	40	20
8	110	3	16 eq.	toluene	24 mL	20	25	55
9	110	24	10 eq.	chlorobenzene	16 mL	–	4	96



Scheme S1. Synthesis of 1,6,7,12-tetrachloroperylene bisanhydride 2 and bisimide 11.



Scheme S2. Previously followed approach to synthesize 1,6,7,12-tetraphenoxyperylene bisbenzimidazoles.

Figure S1. Cyclic voltammogram of perylene derivatives 4, 6, 7, and 10.

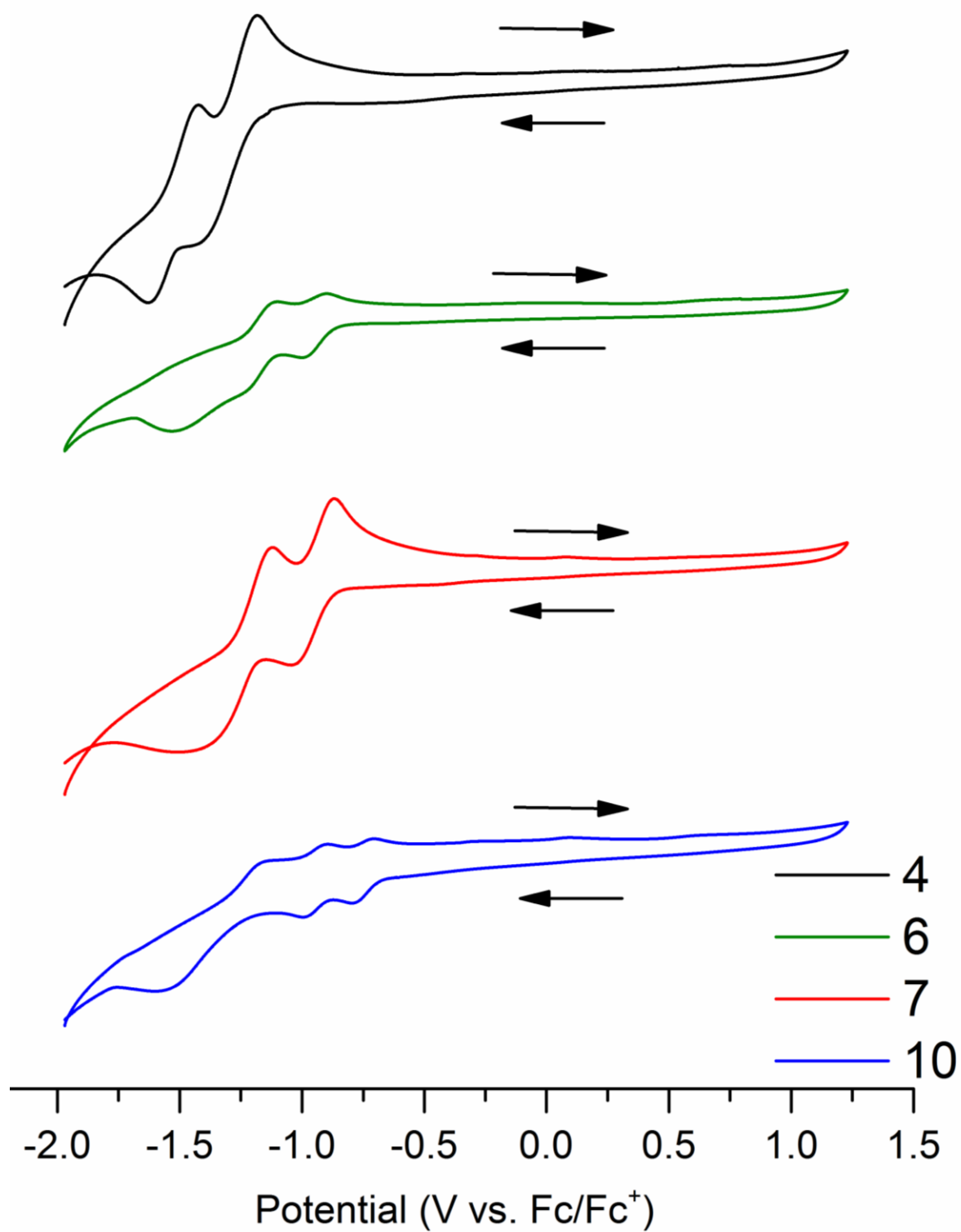


Figure S2. Cyclic voltammogram of perylene derivatives 11, 12, and 14.

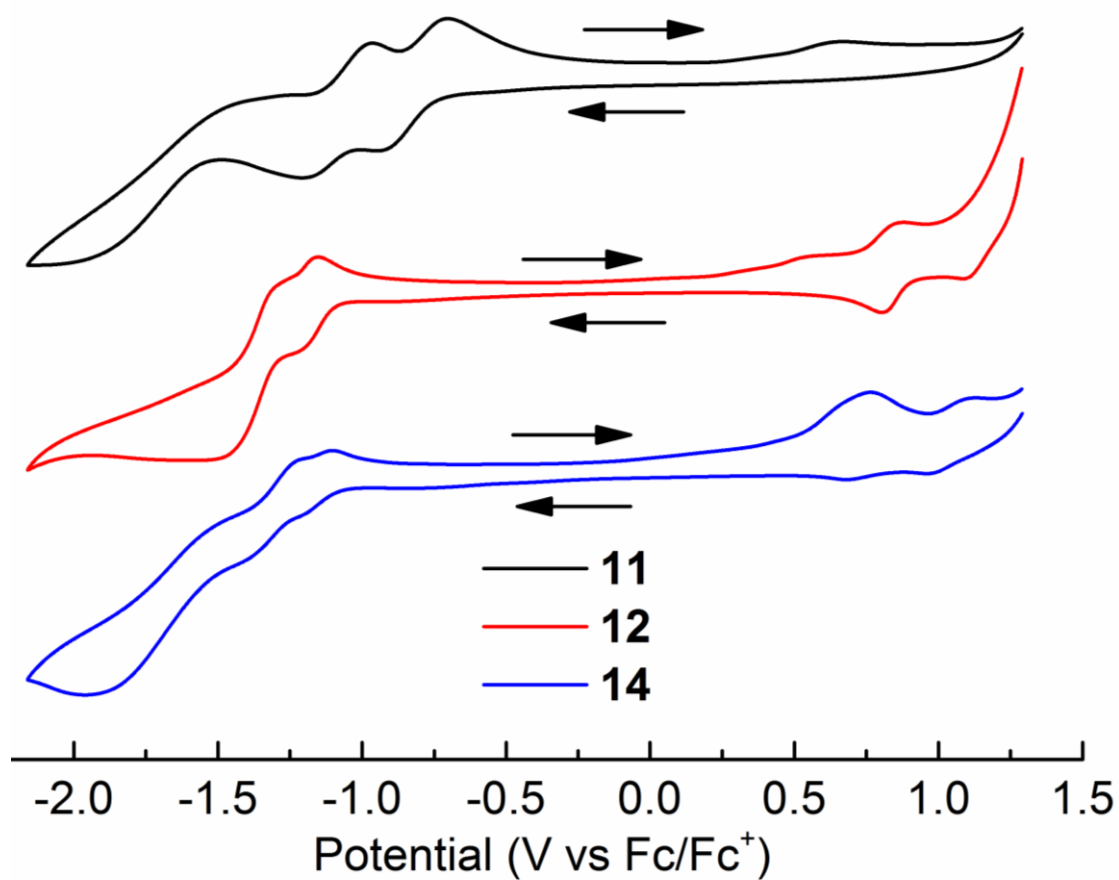


Figure S3. UV/Vis absorption spectra (Vs molar extinction coefficient) of synthesized compounds in chloroform.

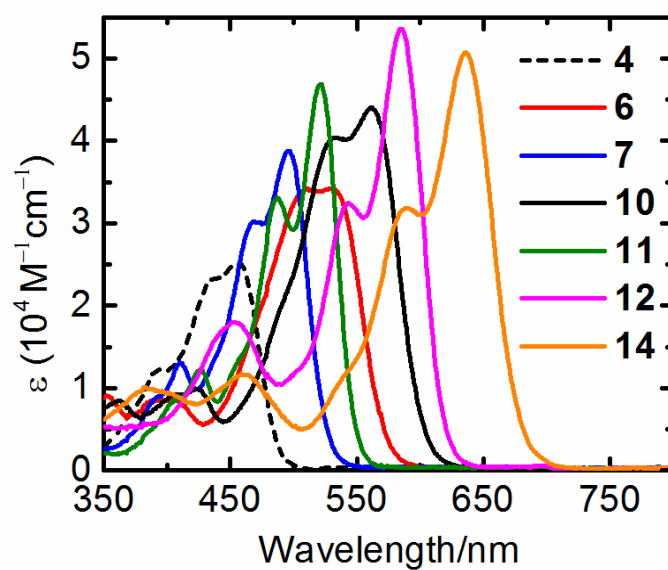


Figure S4. ^1H NMR spectrum of mixture of 1,6,7,12-tetrachloro- and 1,2,6,7,12-pentachloro-perylene-3,4,9,10-tetracarboxy bisanhydride (**2+3**) in D_2SO_4 .

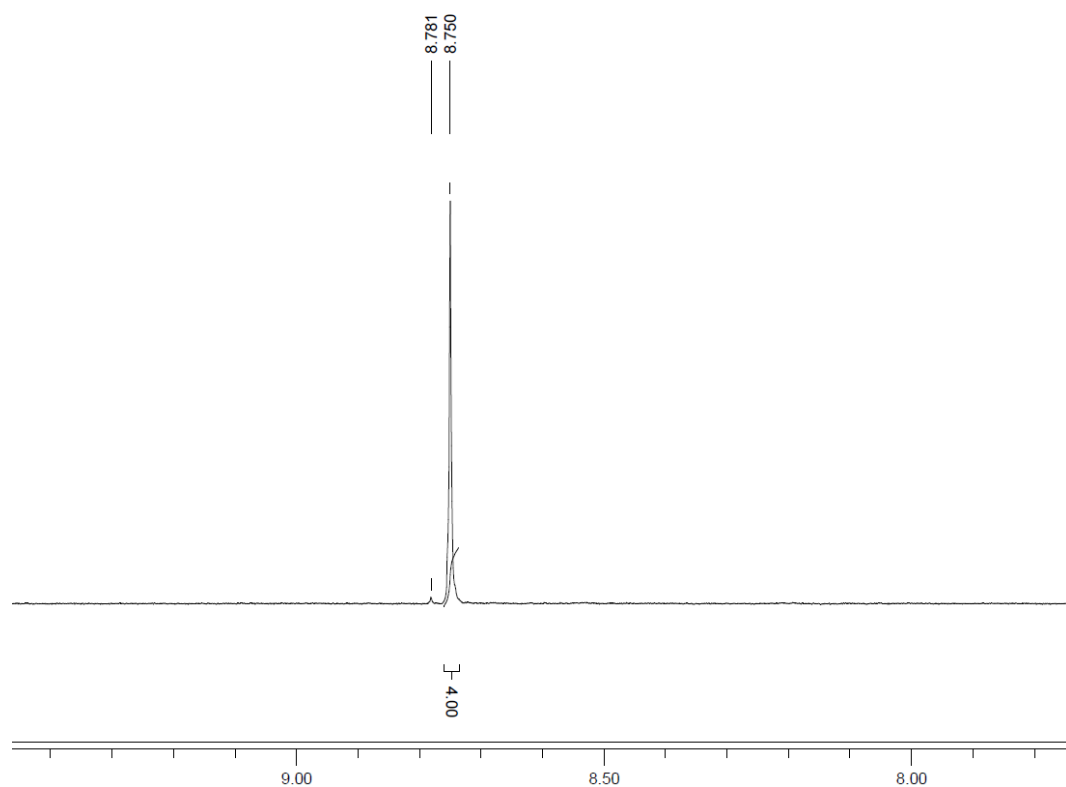


Figure S5. ^1H NMR spectrum of 1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy bisanhydride (**2**) in D_2SO_4 .

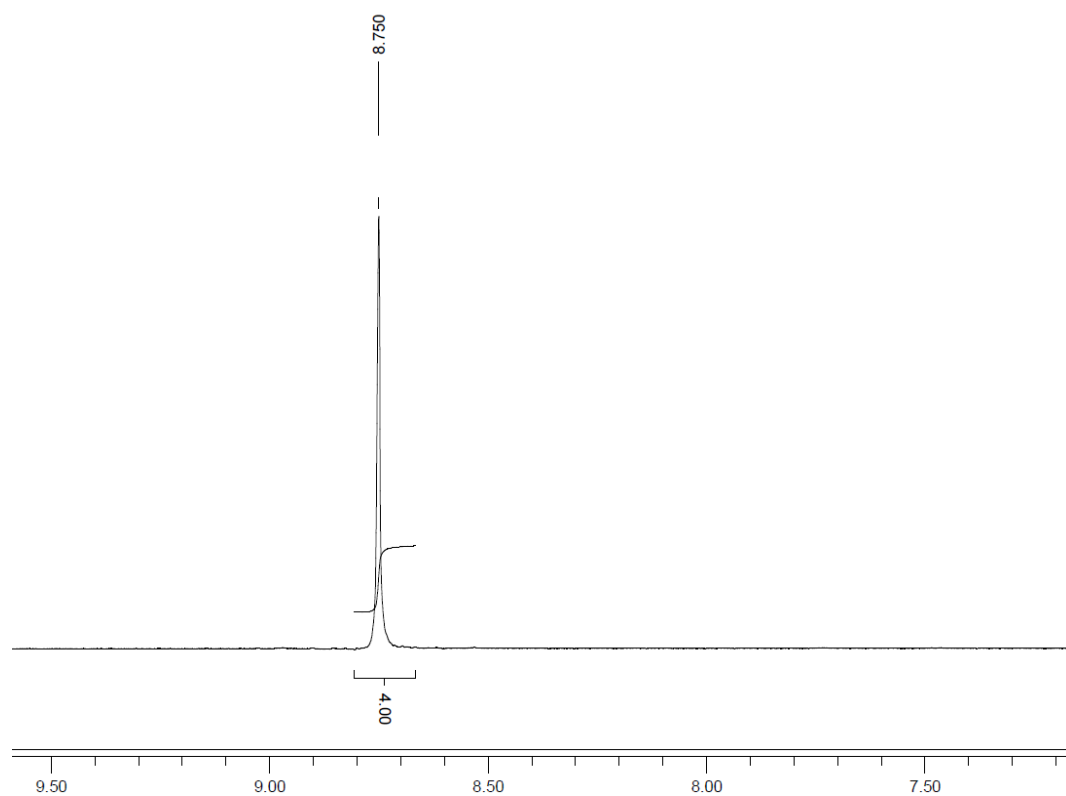


Figure S6. ^1H and ^{13}C NMR (APT) spectra of 1,6,7,12-Tetrachloroperylene-3,4,9,10-tetracarboxy Tetrabutylester (**4**).

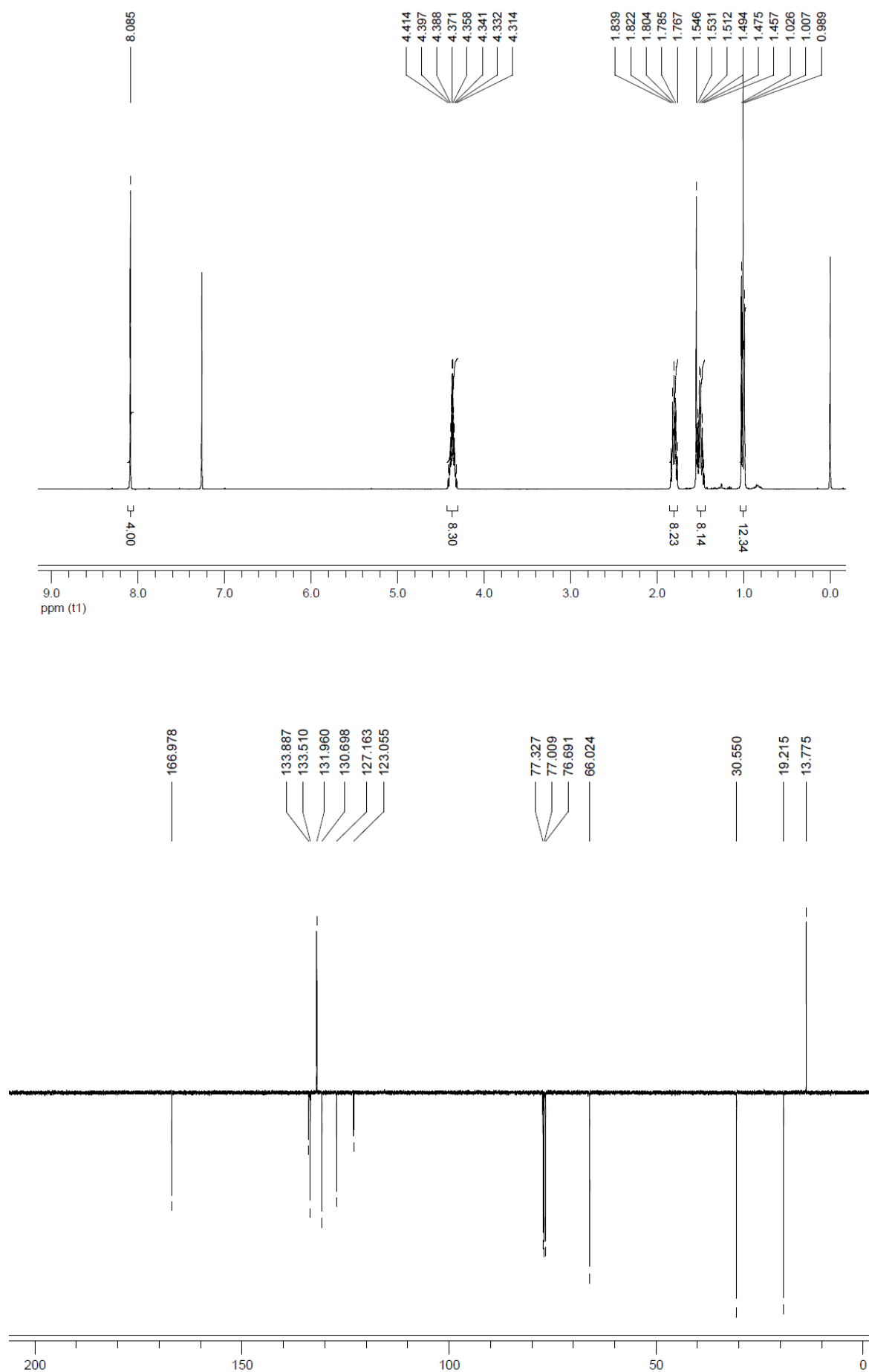


Figure S7. ^1H and ^{13}C NMR (APT) spectra of 1,6,7,12-Tetrachloroperylene-3,4,9,10-tetracarboxy Monoanhydride Dibutylester (**5**).

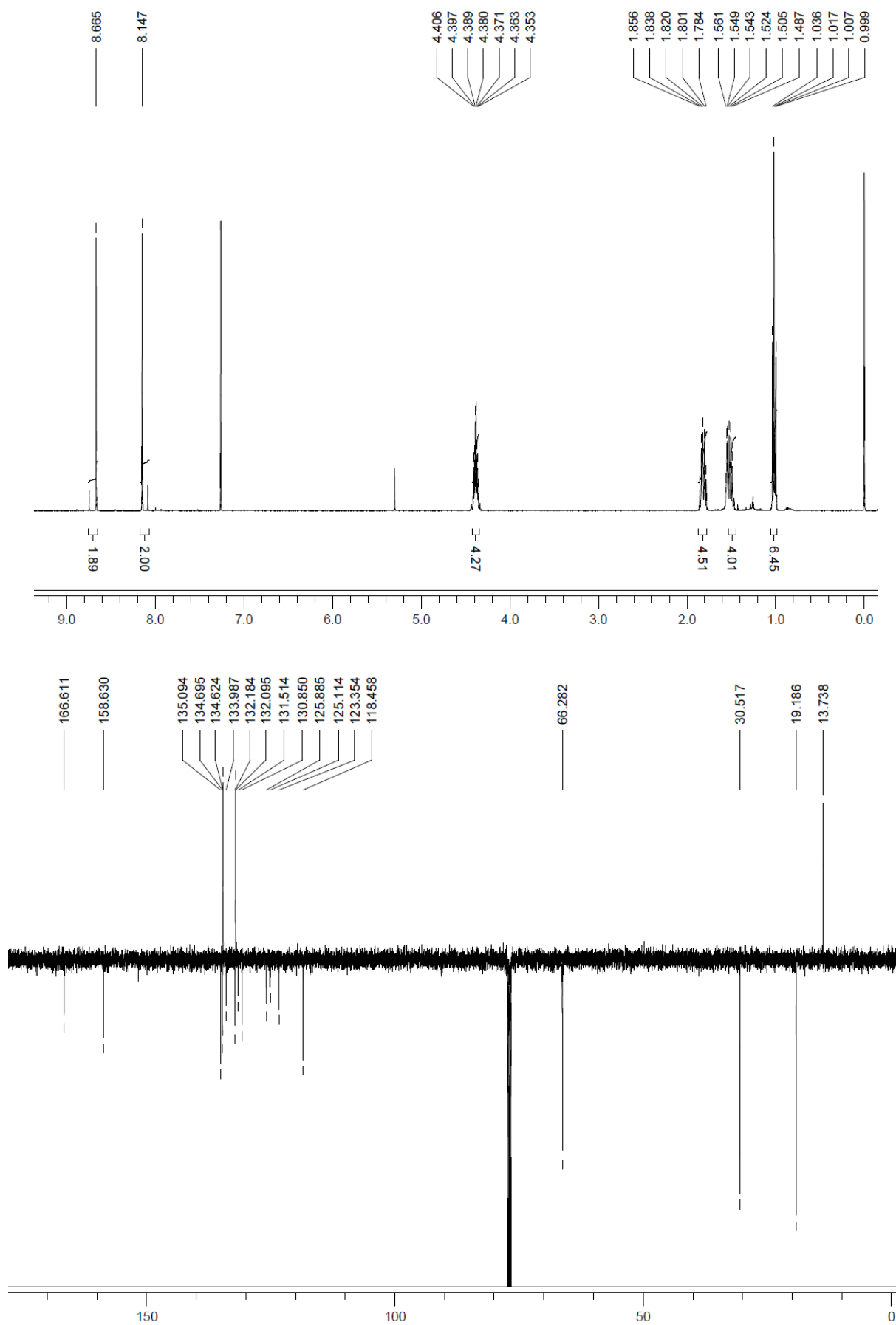


Figure S8. ^1H and ^{13}C NMR (APT) spectra of 1,6,7,12-Tetrachloroperylene-3,4,9,10-tetracarboxy Monobenzimidazole Dibutylester (**6**).

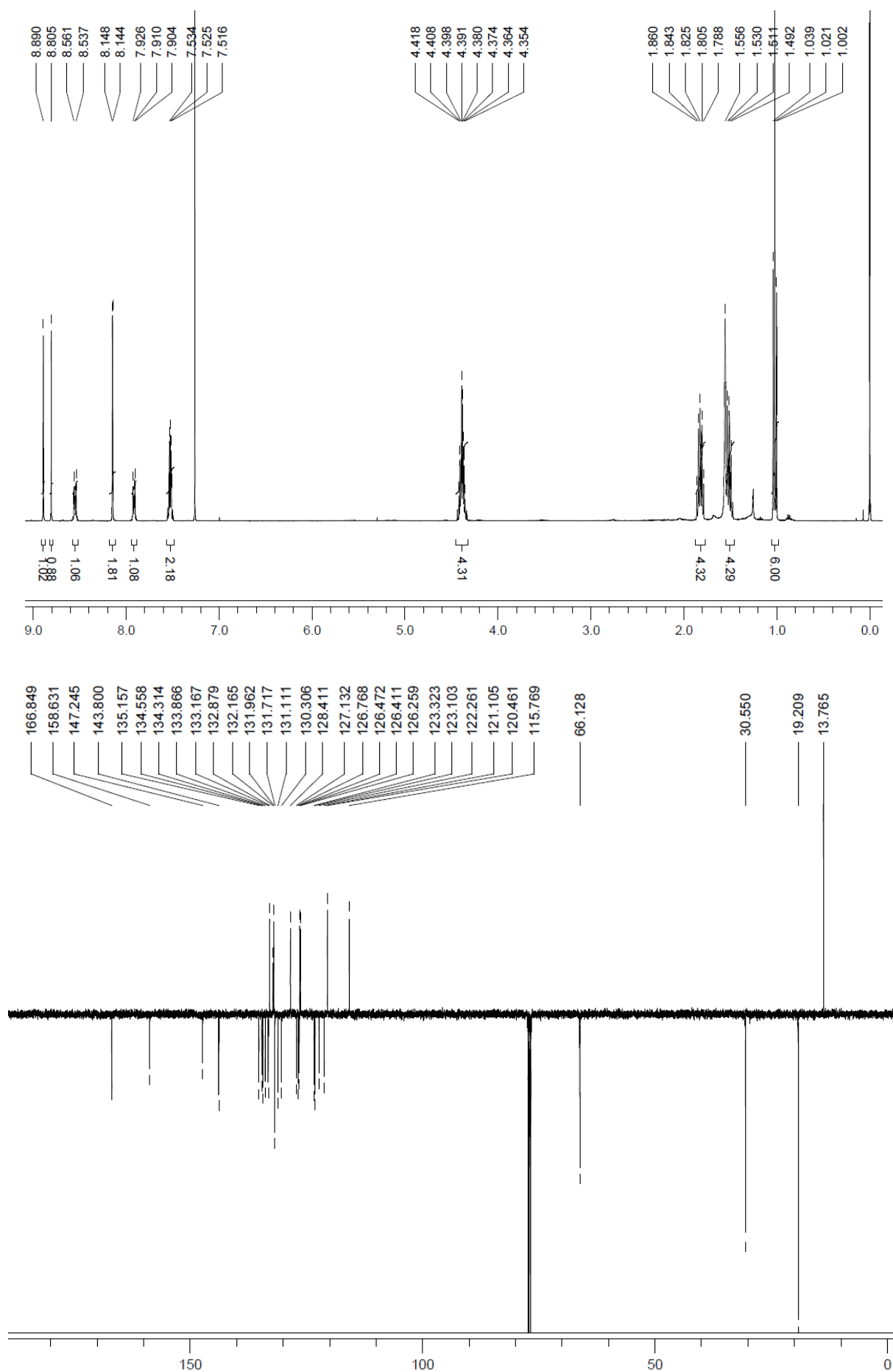


Figure S9. ^1H and ^{13}C NMR (APT) spectra of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Dibutylester (**7**).

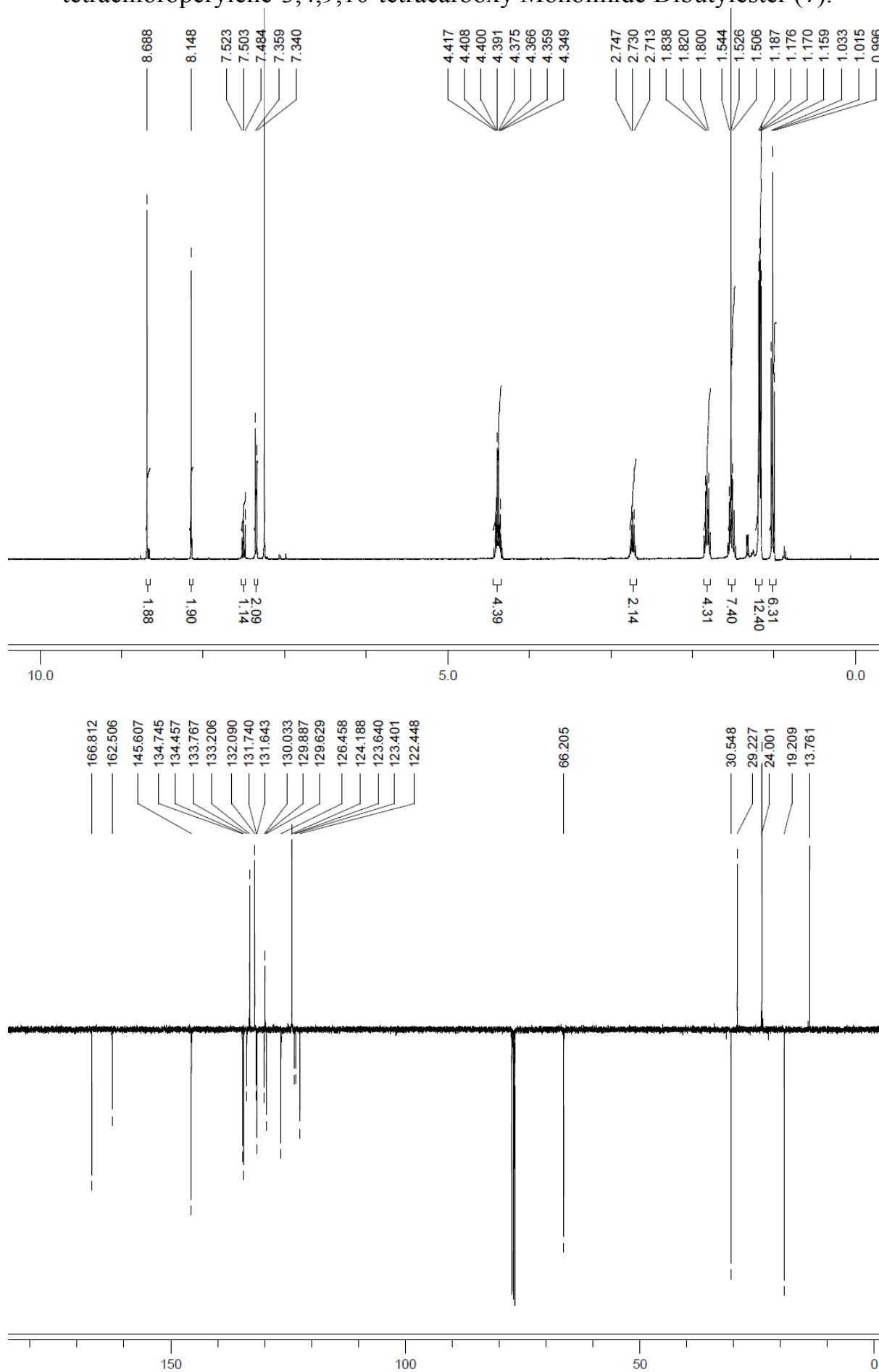


Figure S10. ^1H and ^{13}C NMR (APT) spectra of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Monoanhydride (**8**).

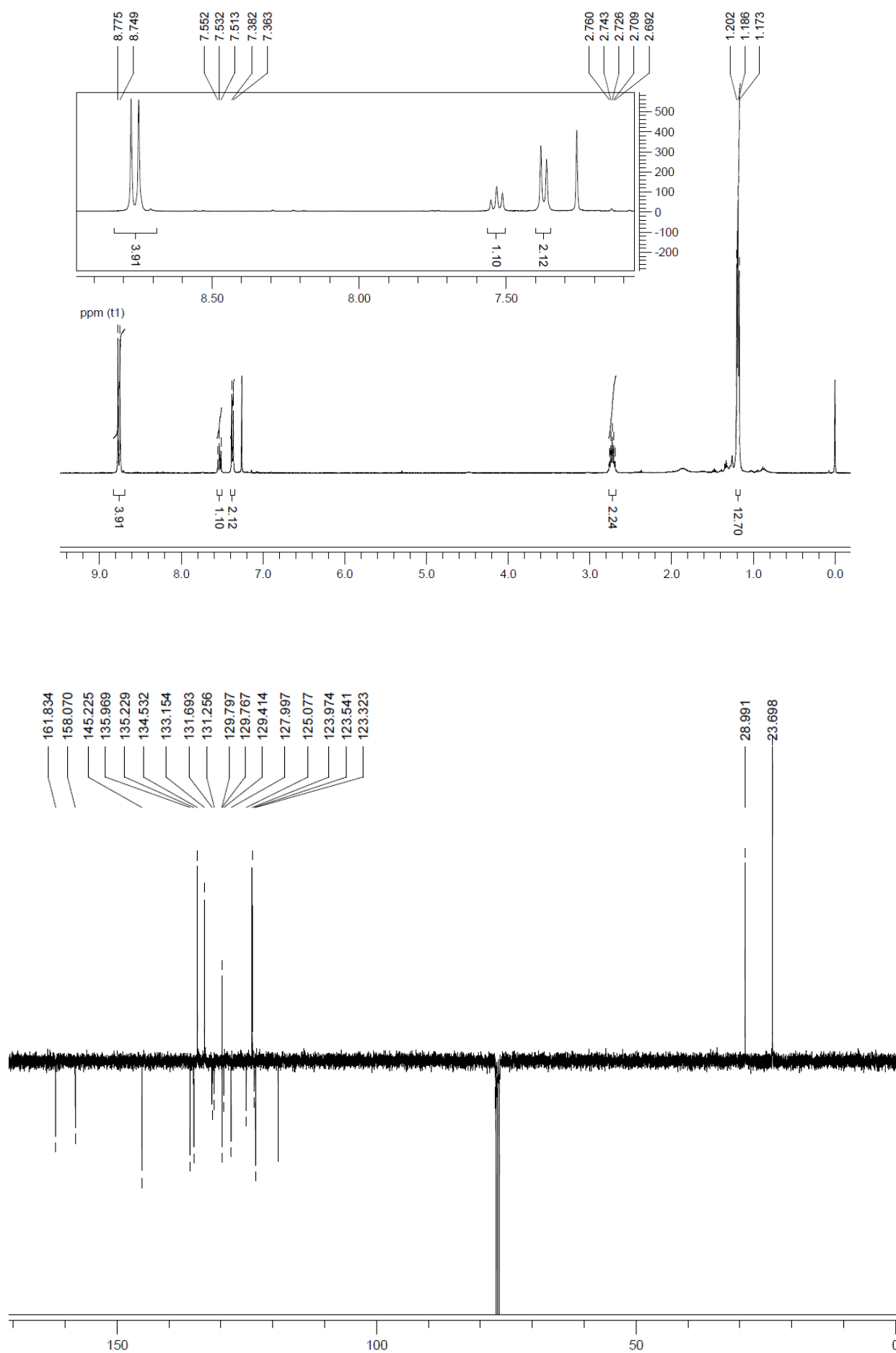


Figure S11. ^1H and ^{13}C NMR (APT) spectra of *N*-(2,6-Diisopropylphenyl)-*N'*-(4-Methoxyphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Bisimide (**9**).

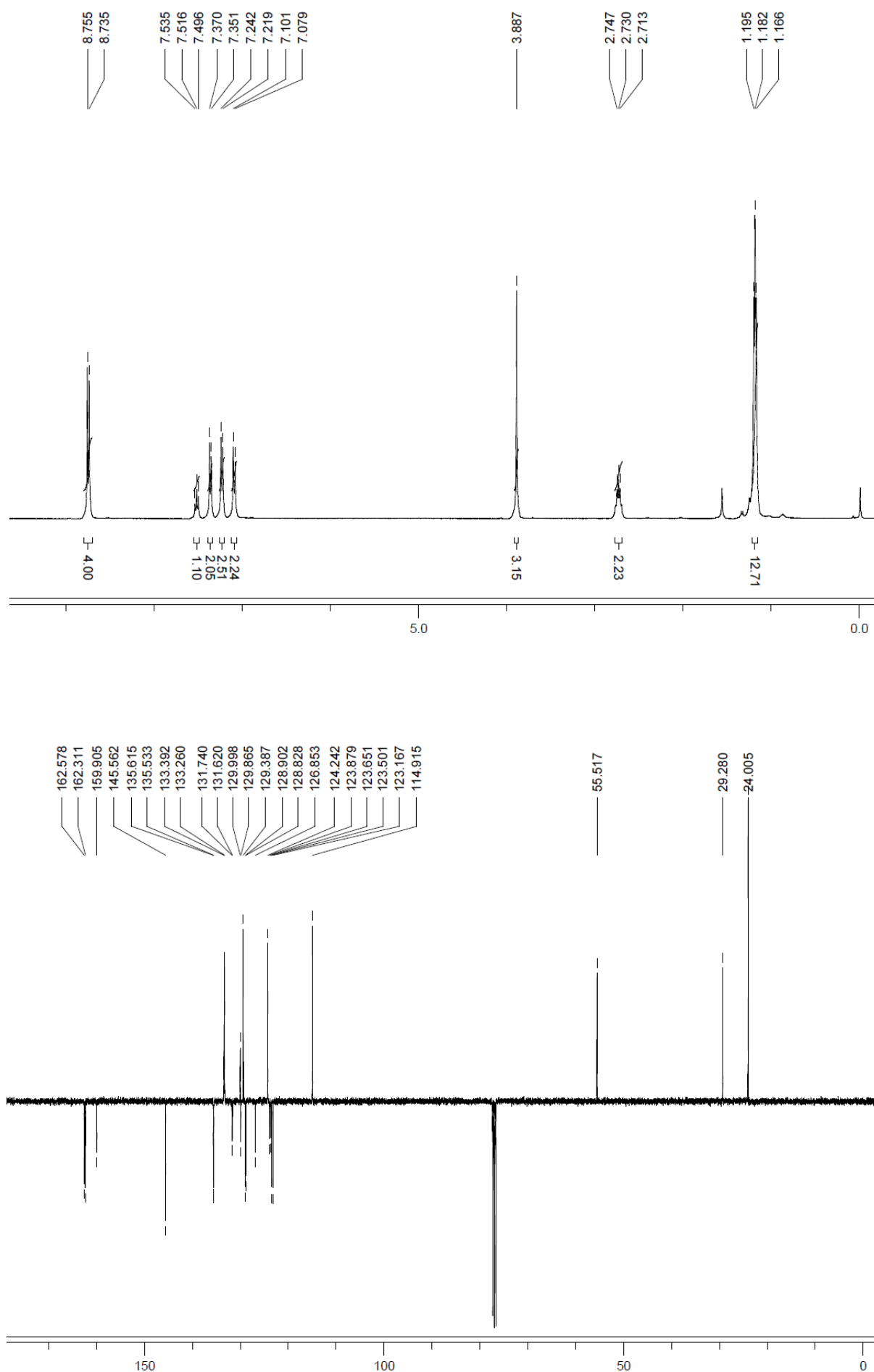


Figure S12. ^1H and ^{13}C NMR (APT) spectra of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Monobenzimidazole (**10**).

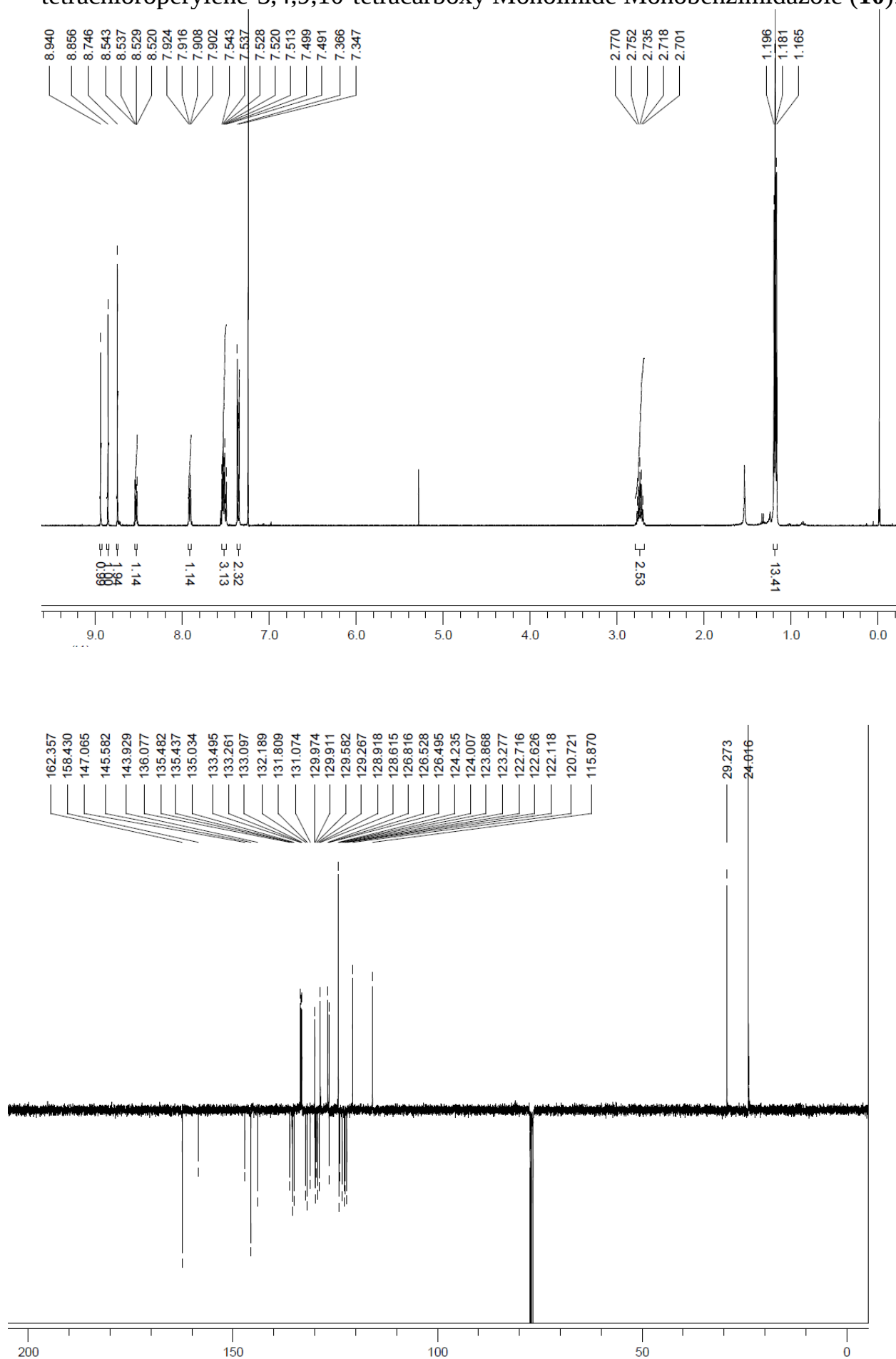


Figure S13. ^1H and ^{13}C NMR (APT) spectra of *N,N'*-Bis(2,6-Diisopropylphenyl)-1,6,7,12-tetra(4-*tert*-butylphenoxy)perylene-3,4,9,10-tetracarboxy Bisimide (**12**).

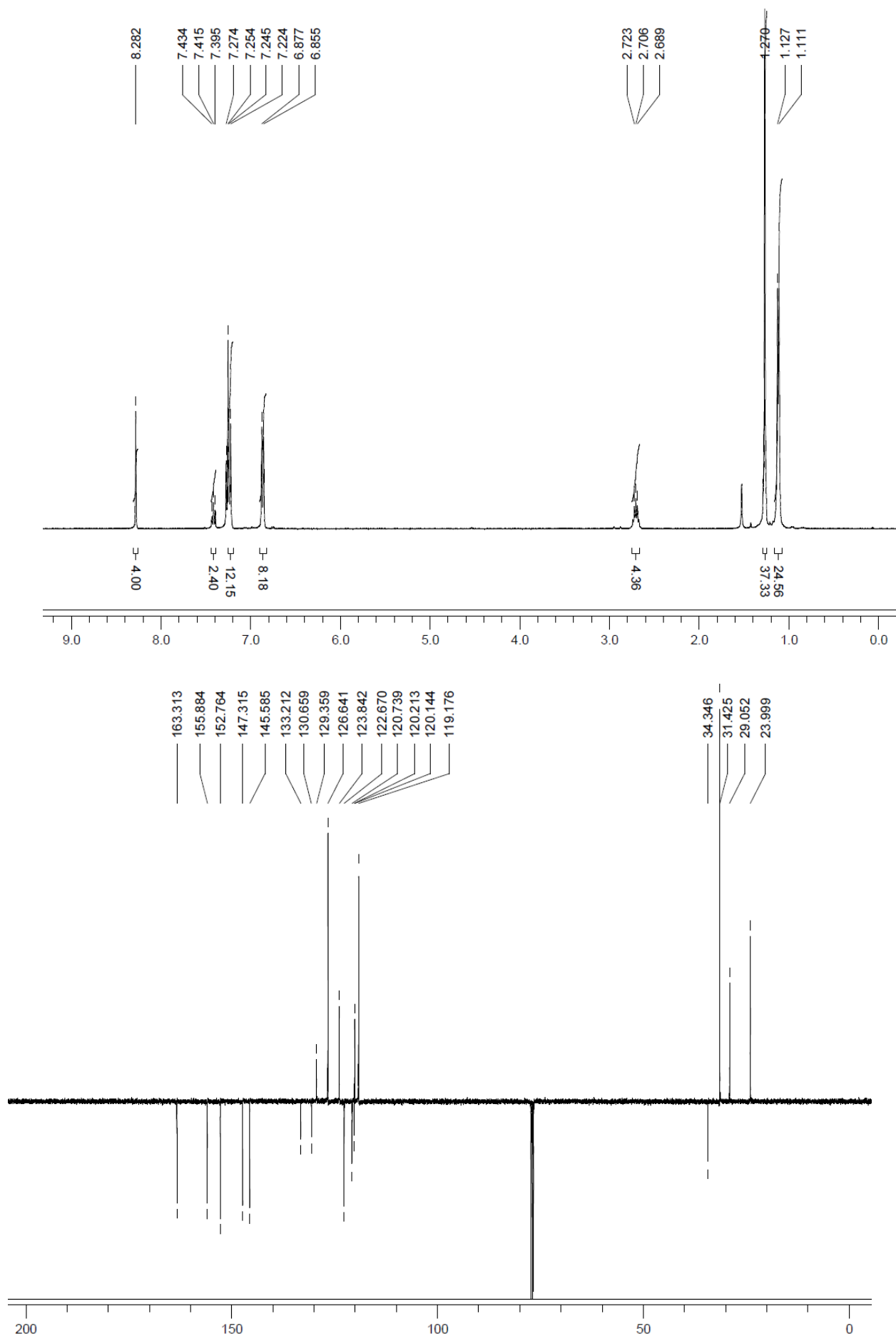


Figure S14. ^1H NMR spectrum of 1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Bisbenzimidazole (**13**) measured in CF_3COOD .

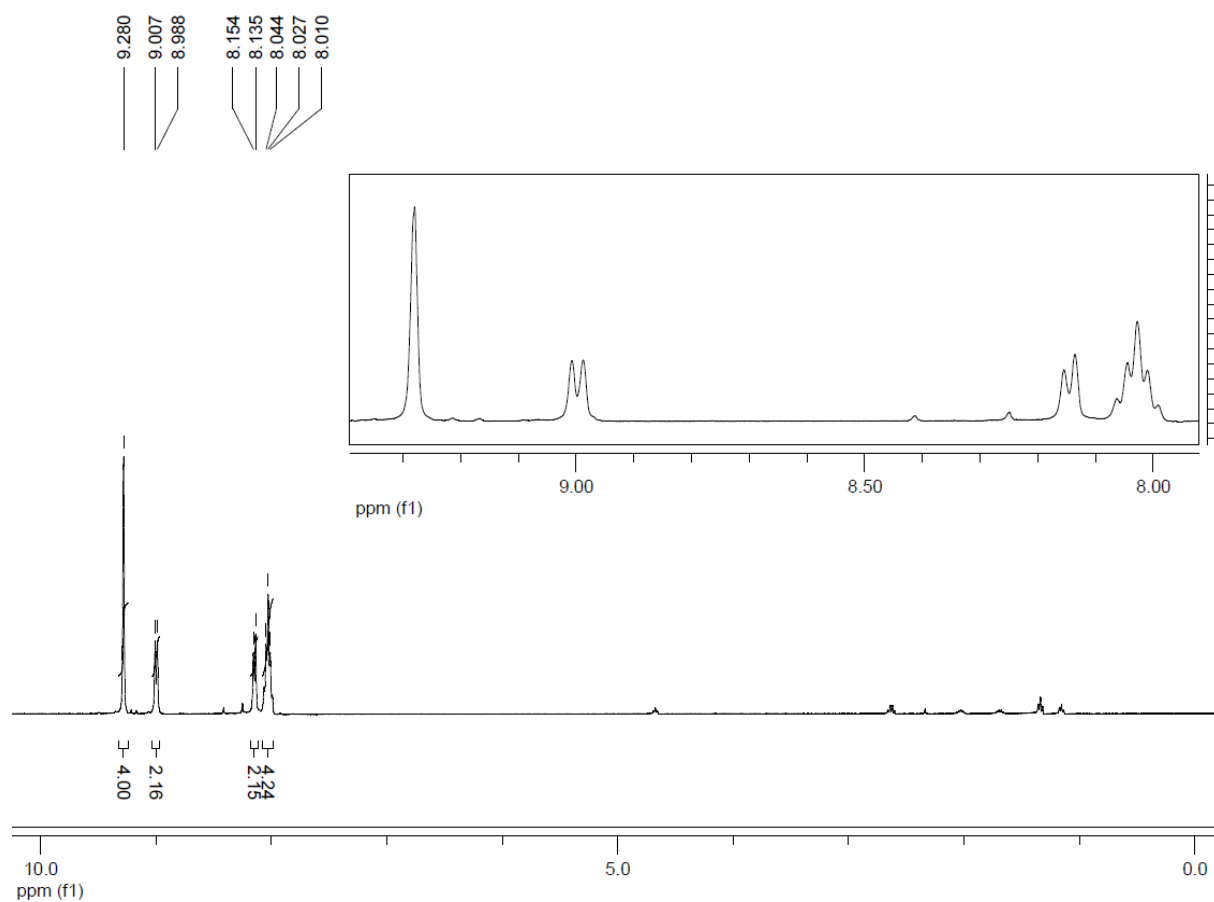


Figure S15. ^1H and ^{13}C NMR (APT) spectra of 1,6,7,12-tetra(4-*tert*-butylphenoxy)perylene-3,4,9,10-tetracarboxy Bisbenzimidazole (**14**).

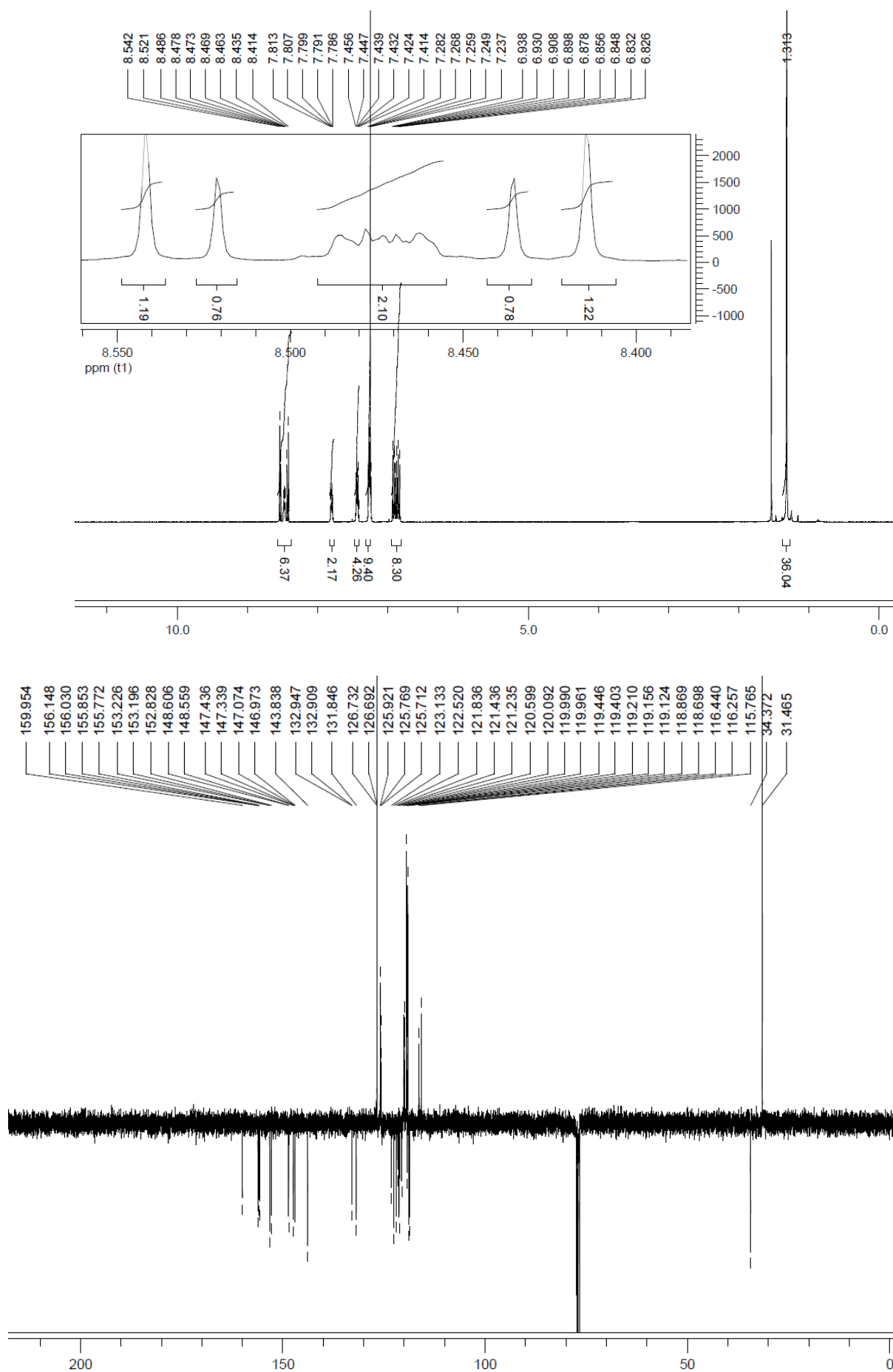
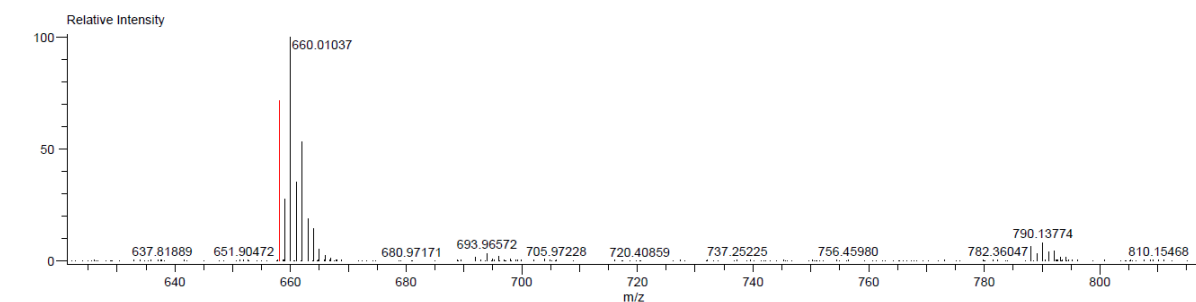
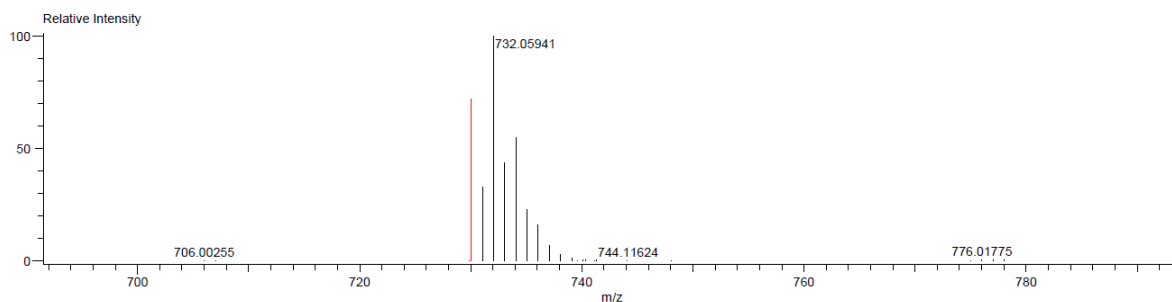


Figure S16. Mass spectrum of 1,6,7,12-Tetrachloroperylene-3,4,9,10-tetracarboxy Monoanhydride Dibutylester (**5**).



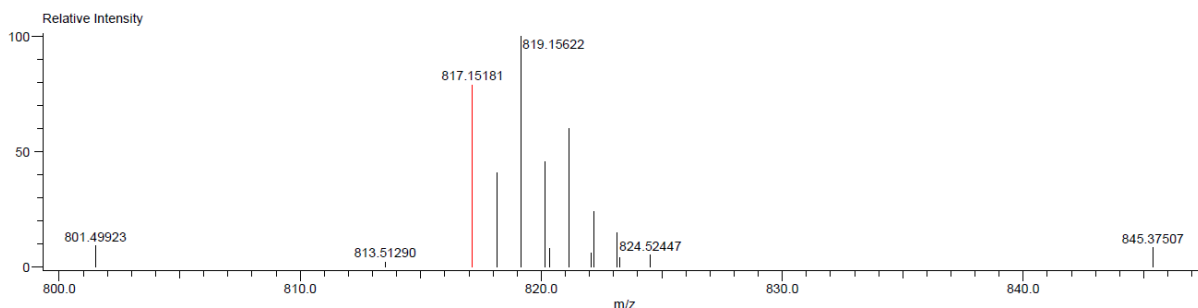
Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference [ppm]	Possible Formula	¹² C	¹ H	³⁵ Cl	³⁷ Cl	¹⁶ O	Unsaturation Number
658.01054	259279.50	71.49	658.01196	-2.16	¹² C ₃₂ ¹ H ₂₂ ³⁵ Cl ₄ ¹⁶ O ₇	32	22	4		7	20.0

Figure S17. Mass spectrum of 1,6,7,12-Tetrachloroperylene-3,4,9,10-tetracarboxy Monobenzimidazole Dibutylester (**6**).



Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference [ppm]	Possible Formula	¹² C	¹ H	³⁵ Cl	³⁷ Cl	¹⁴ N	¹⁶ O	Unsaturation Number
730.06121	455219.25	71.99	730.05958	2.23	¹² C ₃₈ ¹ H ₂₆ ³⁵ Cl ₄ ¹⁴ N ₂ ¹⁶ O ₅	38	26	4		2	5	25.0

Figure S18. Mass spectrum of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Dibutylester (**7**).



Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference [ppm]	Possible Formula	¹² C	¹ H	³⁵ Cl	³⁷ Cl	¹⁴ N	¹⁶ O	Unsaturation Number
817.15181	5578.16	79.00	817.15315	-1.64	¹² C ₄₄ ¹ H ₃₉ ³⁵ Cl ₄ ¹⁴ N ₁ ¹⁶ O ₆	44	39	4		1	6	24.0

Figure S19. Mass spectrum of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Monoanhydride (**8**).

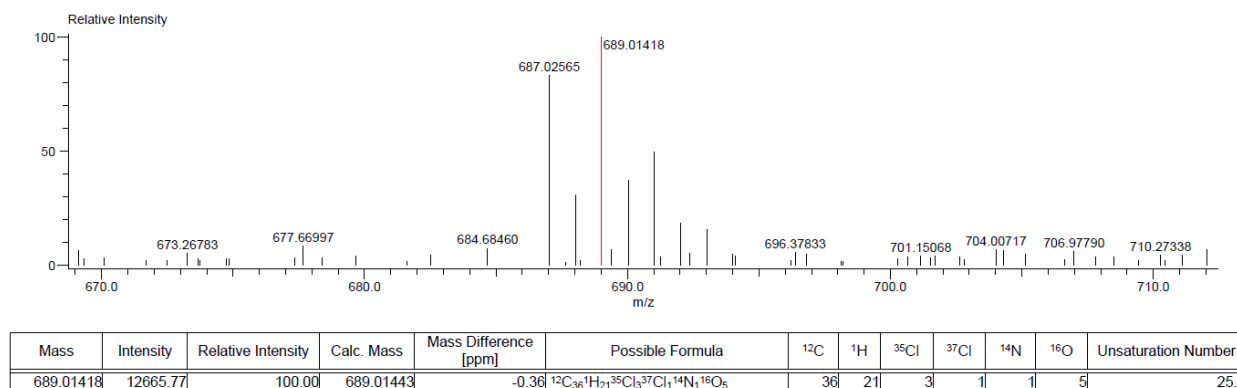


Figure S20. Mass spectrum of *N*-(2,6-Diisopropylphenyl)-*N'*-(4-Methoxyphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Bisimide (**9**).

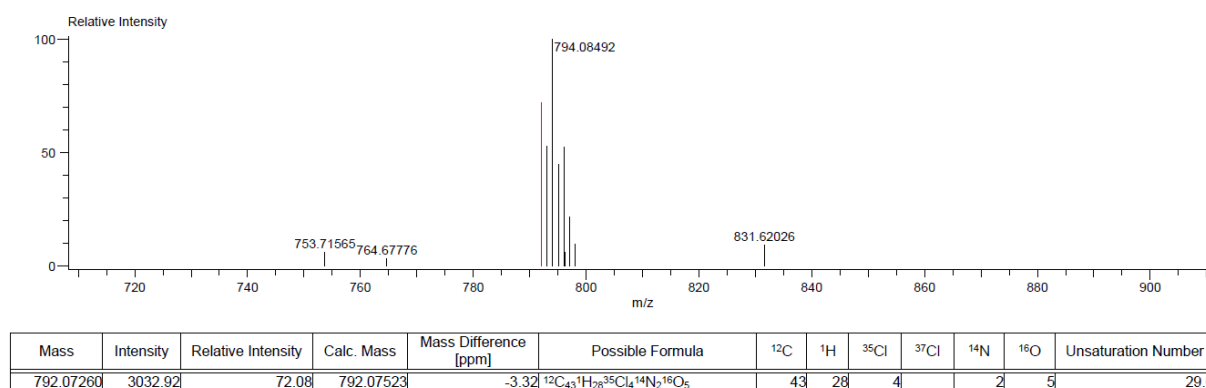


Figure S21. Mass spectrum of *N*-(2,6-Diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxy Monoimide Monobenzimidazole (**10**).

