

# Synthesis of 1,8-diazaanthracenes as building blocks for internally functionalized aromatic oligoamide foldamers.

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## 1)X-ray crystallographic data

Table S1: Crystallographic Parameters for complexes 1-Br, 1-OAc, 1-N3, 1-ONO<sub>2</sub>, 2, 2-H<sub>2</sub>

Compound	1-Br	1-Oac	1-N3	1-ONO <sub>2</sub>	2	2-H <sub>2</sub>
Solvent/precipitant	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CHCl <sub>3</sub> /Hexane	CH <sub>2</sub> Cl <sub>2</sub> /MeOH
Formula	C <sub>25</sub> H <sub>29</sub> BrN <sub>2</sub> O <sub>6</sub>	C <sub>27</sub> H <sub>32</sub> N <sub>2</sub> O <sub>8</sub>	C <sub>25</sub> H <sub>29</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>25</sub> H <sub>29</sub> N <sub>3</sub> O <sub>9</sub>	C <sub>25</sub> H <sub>29</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>6</sub>	C <sub>48</sub> H <sub>61</sub> N <sub>4</sub> O <sub>12.5</sub>
Aspect	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow
Crystal System	Triclinic	Monoclinic	Triclinic	monoclinic	Triclinic	Triclinic
Space Group	P-1	P21/c	P-1	P21/n	P-1	P-1
Z	2	4	2	4	2	2
Unit Cell Parameters						
a, Å	9.505(5)	12.781(5)	10.0459(9)	7.790(1)	9.393(2)	8.005
b, Å	10.865(5)	14.374(5)	10.3718(9)	14.768(1)	11.183(3)	14.308
c, Å	12.959(6)	14.946(7)	12.8237(11)	21.795(2)	14.185(2)	20.389
α, °	112.60(3)	90	96.672(6)	90	75.57(3)	84.31
β, °	99.94(4)	107.14(13)	91.767(7)	91.934(6)	71.46(4)	85.91
γ, °	95.09(4)	90	101.295(6)	90	80.53(4)	83.79
Temperature, K	113	100	113	113	100	113
Volume, Å <sup>3</sup>	1199.2(11)	2624.1(19)	1299.4(2)	2505.9(4)	1362.2(5)	2305.8
FW, g.mol <sup>-1</sup>	533.41	512.55	495.53	515.51	559.85	894.01
ρ, g.cm <sup>-3</sup>	1.477	1.297	1.266	1.366	1.365	1.288
λ, E	1.5419	1.5419	1.5419	1.5419	1.5419	1.5419
θ min	6.54	6.9	6.77	6.68	6.73	3.12
θ max	71.75	68.49	71.98	71.92	68.49	68.46
Radiation	CuKα	CuKα	CuKα	CuKα	CuKα	CuKα
Reflections Measured	14708	4817	5114	4938	5016	8495
GOF	1.055	1.041	1.055	1.014	1.054	1.068
R1 (I>2σ(I))	0.1141	0.0353	0.0673	0.0593	0.0497	0.0381
wR2 (all data)	0.2423	0.096	0.1569	0.1379	0.1485	0.1085

Table S2: Crystallographic Parameters for complexes 2-Cl, 2-Br, 2-NH<sub>2</sub>, 2-SBn, 2-Cl<sup>red</sup>, and 4-dimer

Compound	2-Cl	2-Br	2-NH <sub>2</sub>	2-SBn	2-Cl <sup>red</sup>	4-dimer
Solvent/precipitant	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CHCl <sub>3</sub> /Hexane	CHCl <sub>3</sub> /Hexane	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CH <sub>2</sub> Cl <sub>2</sub> /MeOH	CH <sub>2</sub> Cl <sub>2</sub> /MeOH
Formula	C <sub>25</sub> H <sub>29</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>6</sub>	C <sub>25</sub> H <sub>28</sub> BrCl <sub>3</sub> N <sub>2</sub>	C <sub>25</sub> H <sub>32</sub> Cl <sub>3</sub> N <sub>3</sub> O	C <sub>31</sub> H <sub>34</sub> N <sub>2</sub> O <sub>6</sub> S	C <sub>24</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>6</sub>	C <sub>52</sub> H <sub>64</sub> N <sub>6</sub> O <sub>11</sub> 0.1(CH <sub>2</sub> Cl <sub>2</sub> )
Aspect	Yellow	Yellow	red	red	Yellow	Yellow
Crystal System	Triclinic	monoclinic	Triclinic	Triclinic	monoclinic	monoclinic
Space Group	P-1	P21/n	P-1	P-1	P21/C	P21/n
Z	2	4	2	2	4	4
Unit Cell Parameters						
a, Å	9.426(6)	14.965(3)	5.764(5)	13.490(3)	12.5630(8)	18.056(7)
b, Å	11.630(4)	9.4631(16)	11.669(10)	14.415(3)	21.5829(13)	20.067(9)
c, Å	12.474(5)	19.478(4)	21.430(19)	16.347(3)	9.2102(6)	29.141(9)
α, °	80.31(3)	90	90.02(2)	69.791(15)	90	90
β, °	83.65(6)	92.257(7)	95.25(3)	84.884(16)	106.995(5)	103.002(8)
γ, °	81.13(5)	90	97.50(5)	88.811(14)	90	90
Temperature, K	113	100	100	113	113	100
Volume, Å <sup>3</sup>	1326.7(11)	2756.3(9)	1423(2)	2971.1(11)	2388.3(3)	10288(7)
FW, g.mol <sup>-1</sup>	559.85	638.75	592.89	562.66	478.96	1915.81
ρ, g.cm <sup>-3</sup>	1.401	1.539	1.384	1.258	1.332	1.237
λ, E	1.5419	1.5419	1.5419	1.5419	1.5419	1.5419
θ min	6.57	6.9	7.27	6.54	6.7	6.51
θ max	68.87	68.49	68.45	72.05	71.99	68.37
Radiation	CuKα	CuKα	CuKα	CuKα	CuKα	CuKα
Reflections Measured	4913	14708	5216	11699	4701	18883
GOF	1.017	1.055	1.034	1.093	1.008	1.038
R1 (>2σ(I))	0.05	0.0527	0.064	0.081	0.0587	0.072
wR2 (all data)	0.1346	0.1419	0.18	0.2331	0.1421	0.1934

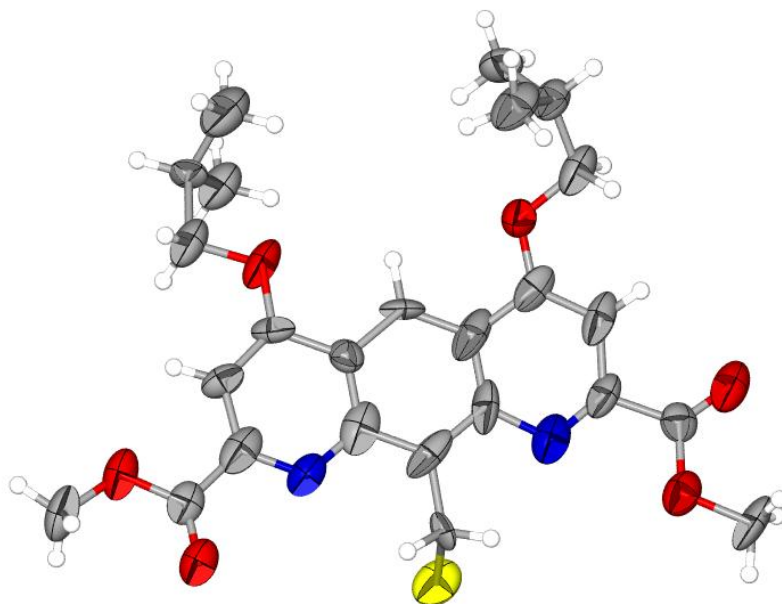


Figure S1: Thermal Ellipsoid Plot at 50% probability for 1-Br

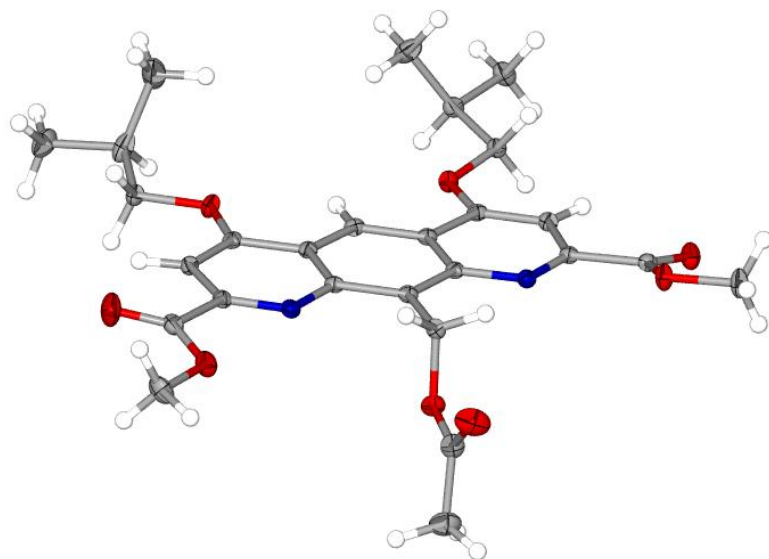


Figure S2: Thermal Ellipsoid Plot at 50% probability for 1-OAc

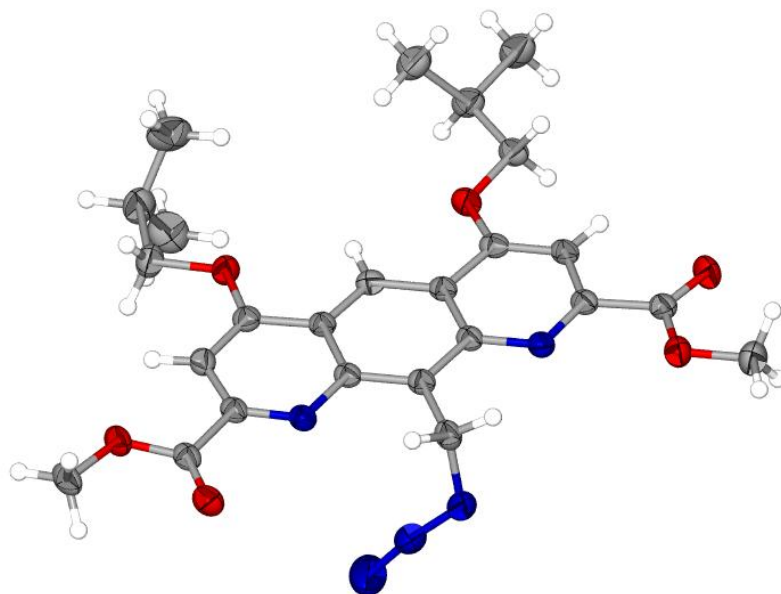


Figure S3: Thermal Ellipsoid Plot at 50% probability for 1-N<sub>3</sub>

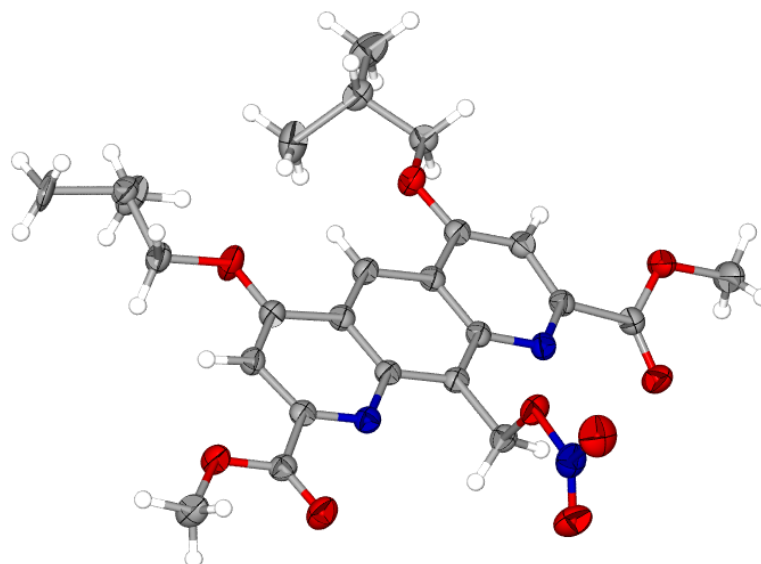


Figure S4: Thermal Ellipsoid Plot at 50% probability for 1-ONO<sub>2</sub>

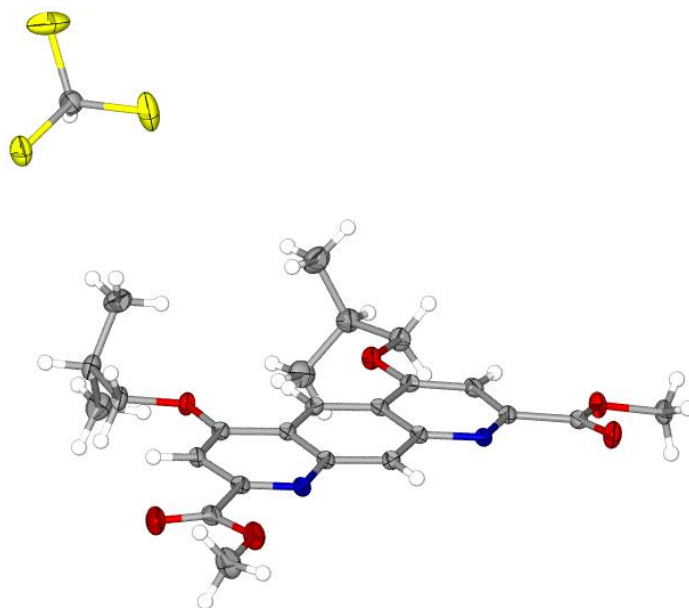


Figure S5: Thermal Ellipsoid Plot at 50% probability for 2

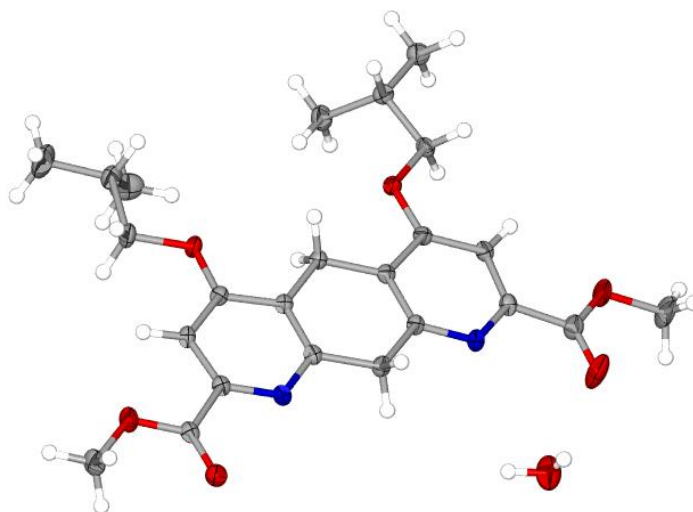


Figure S6: Thermal Ellipsoid Plot at 50% probability for 2-H<sub>2</sub>

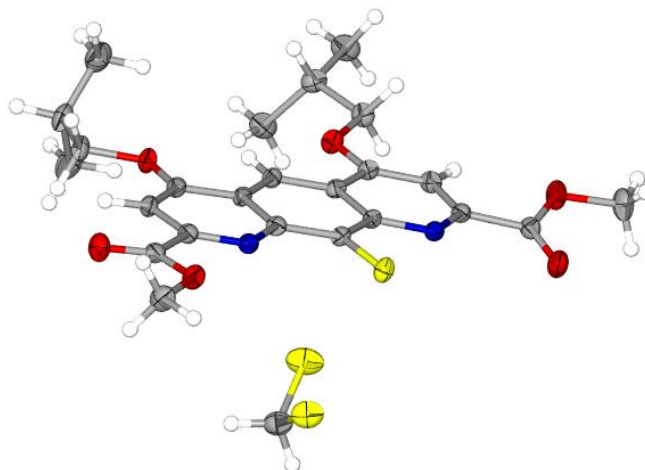


Figure S7: Thermal Ellipsoid Plot at 50% probability for 2-Cl

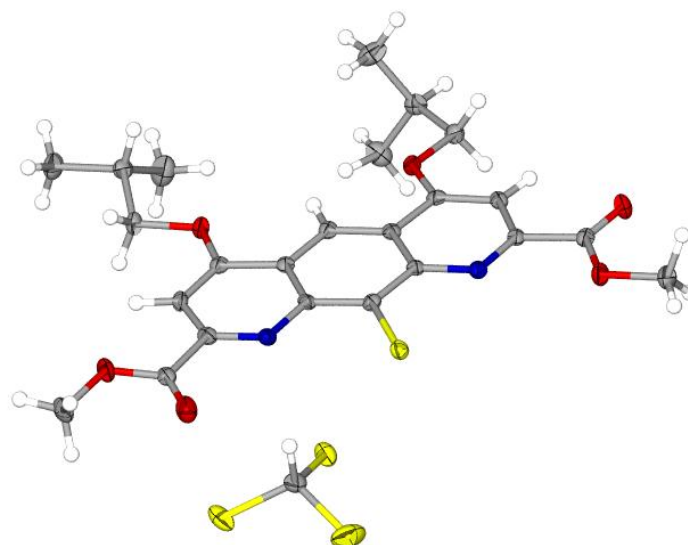


Figure S8: Thermal Ellipsoid Plot at 50% probability for 2-Br

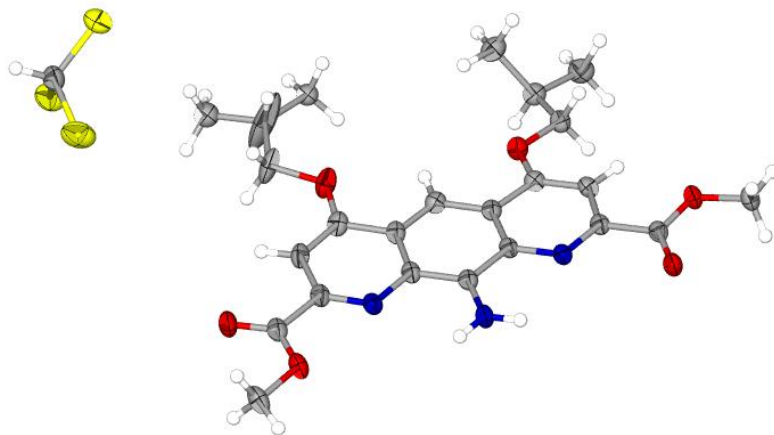


Figure S9: Thermal Ellipsoid Plot at 50% probability for 2-NH2

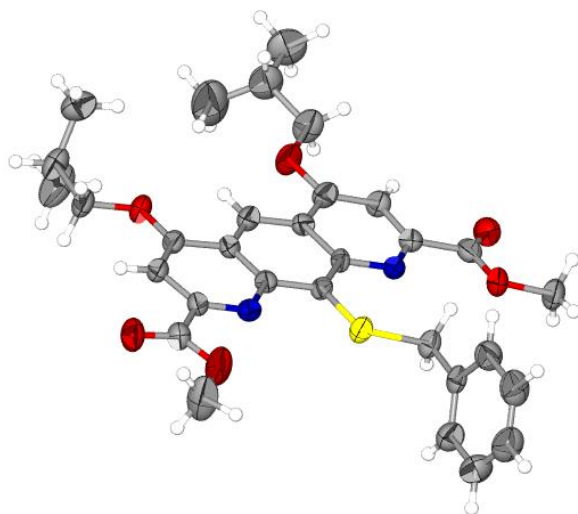


Figure S10: Thermal Ellipsoid Plot at 50% probability for 2-SBn



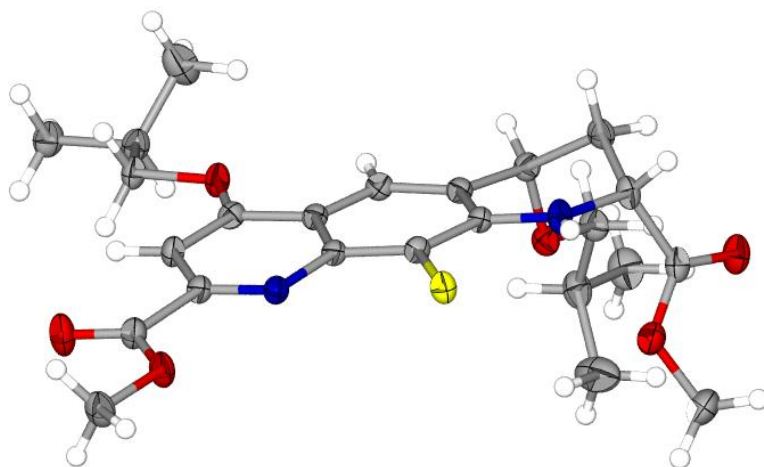


Figure S11: Thermal Ellipsoid Plot at 50% probability for 2-Cl<sup>red</sup>

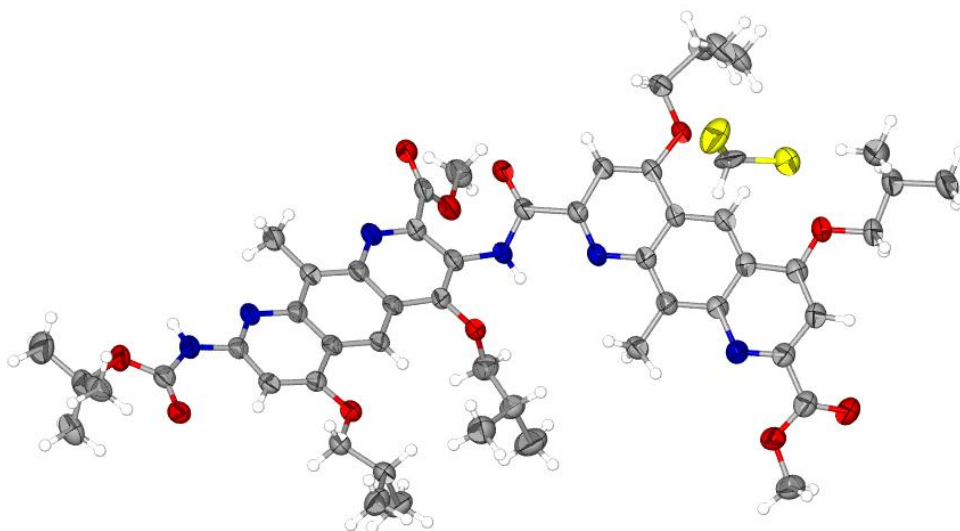
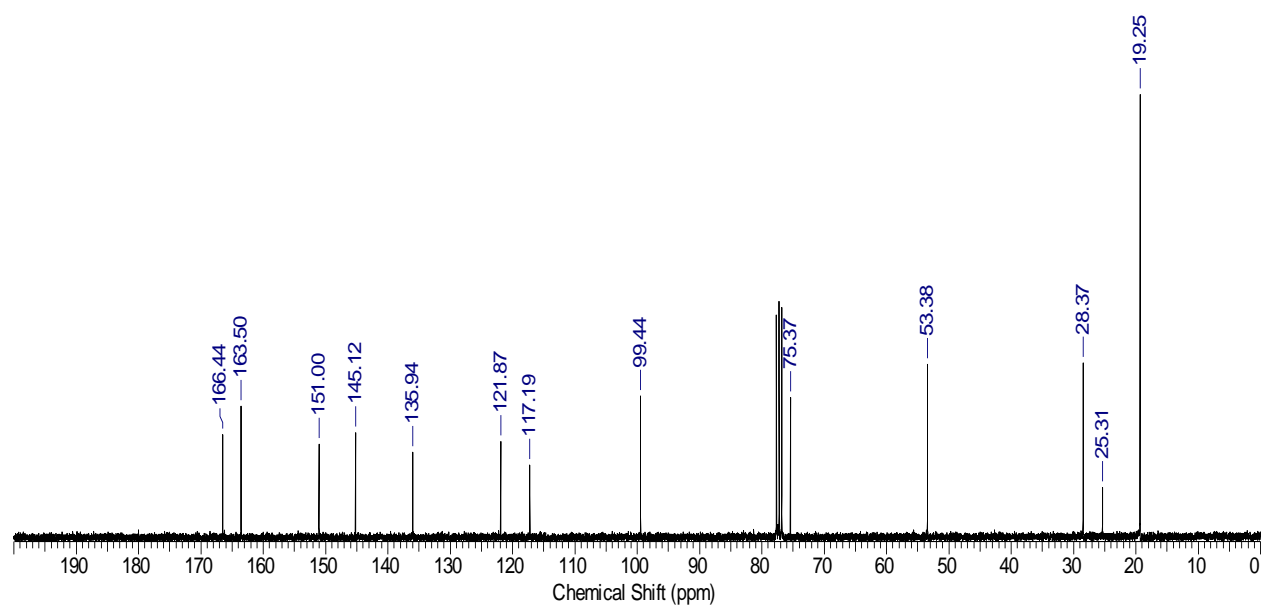
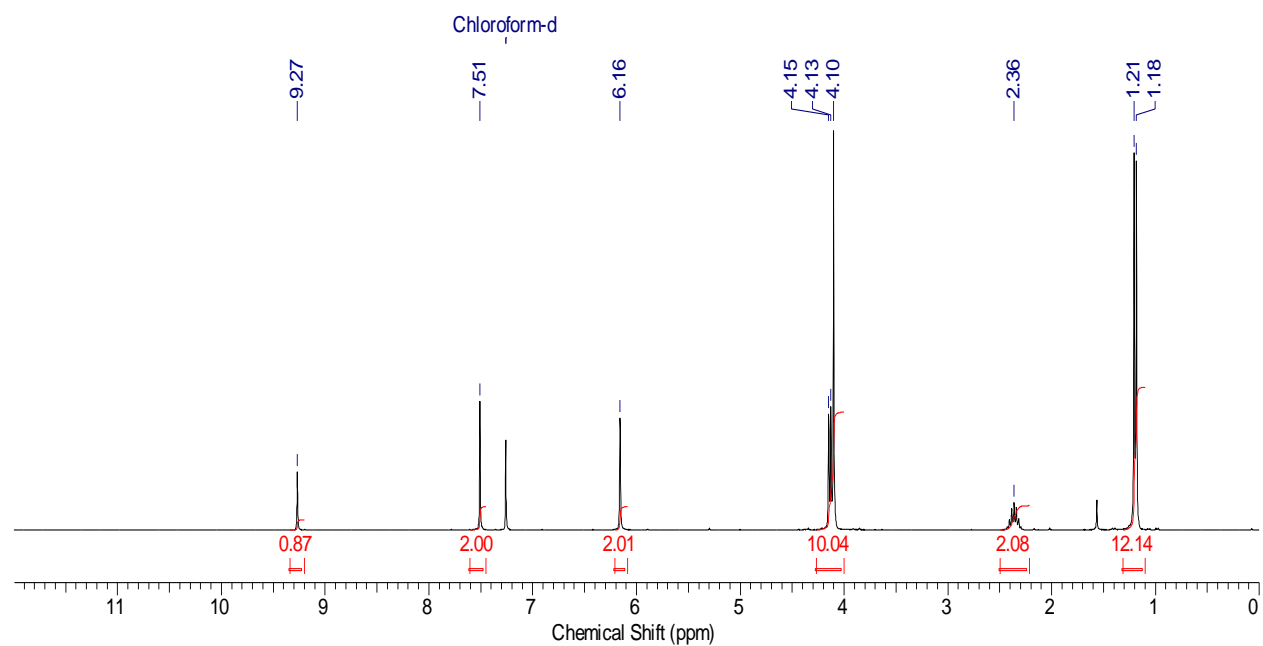
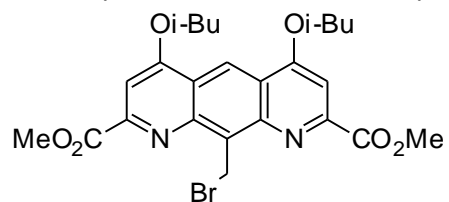


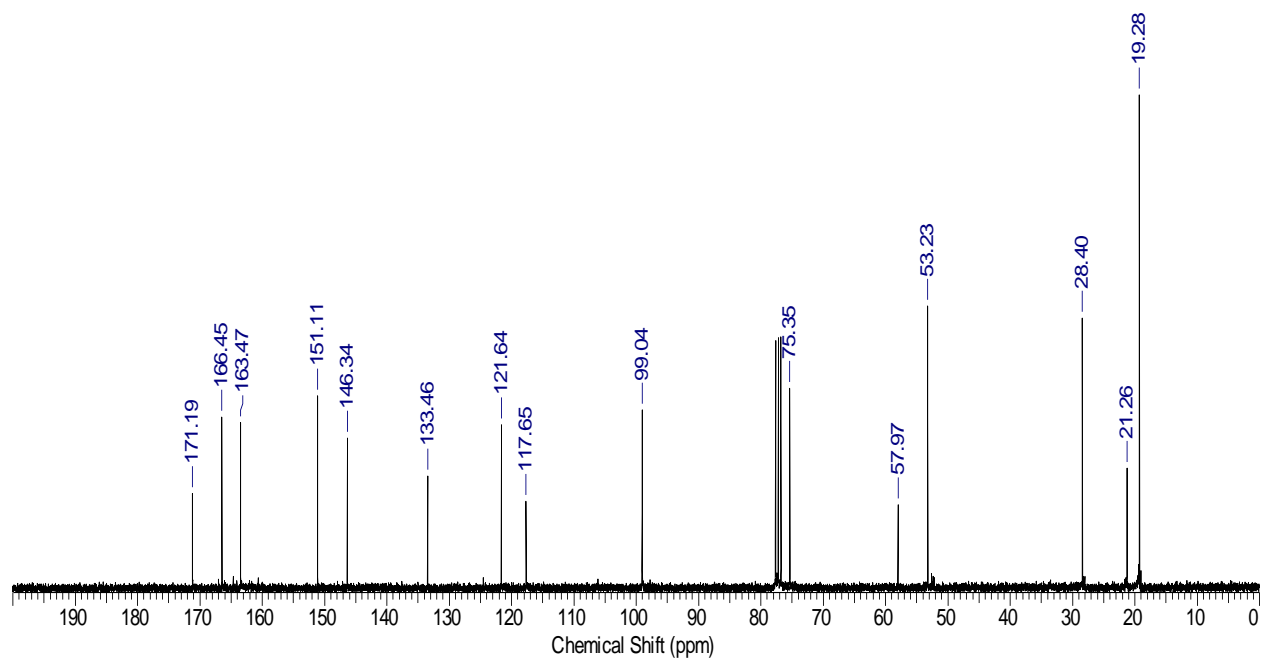
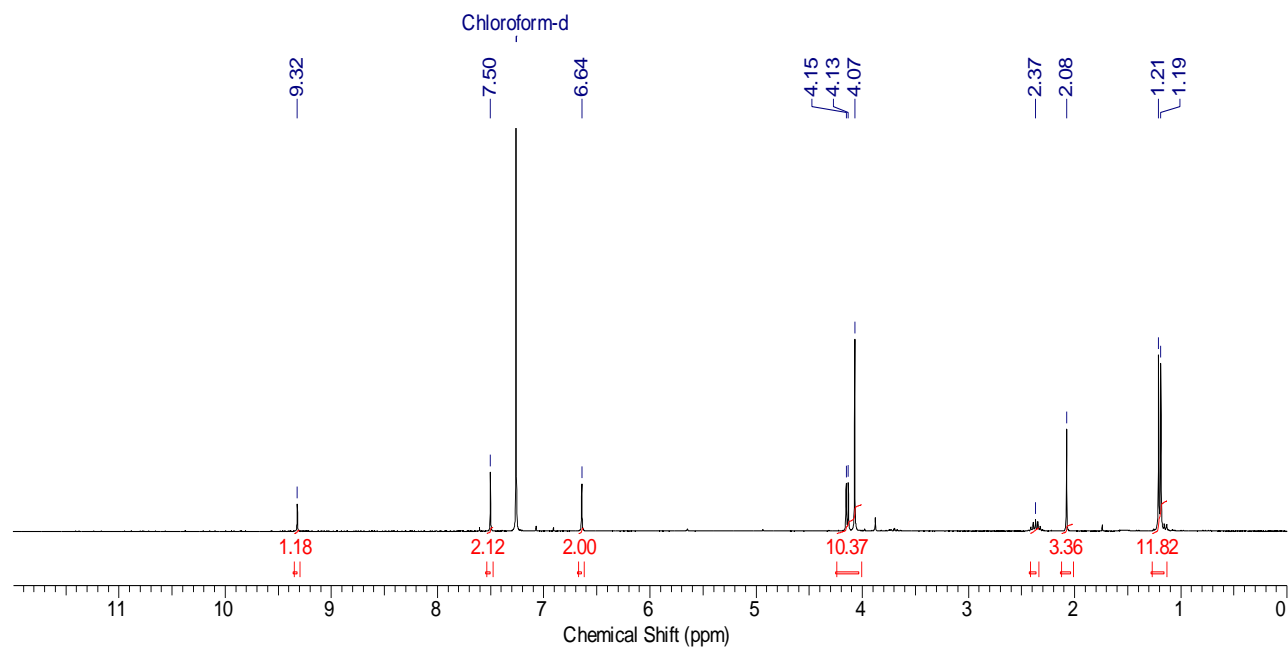
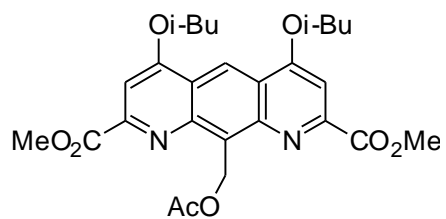
Figure S12: Thermal Ellipsoid Plot at 50% probability for 4-Dimer

## 2)<sup>1</sup>H & <sup>13</sup>C NMR Spectra of compounds 1-4 and their derivatives

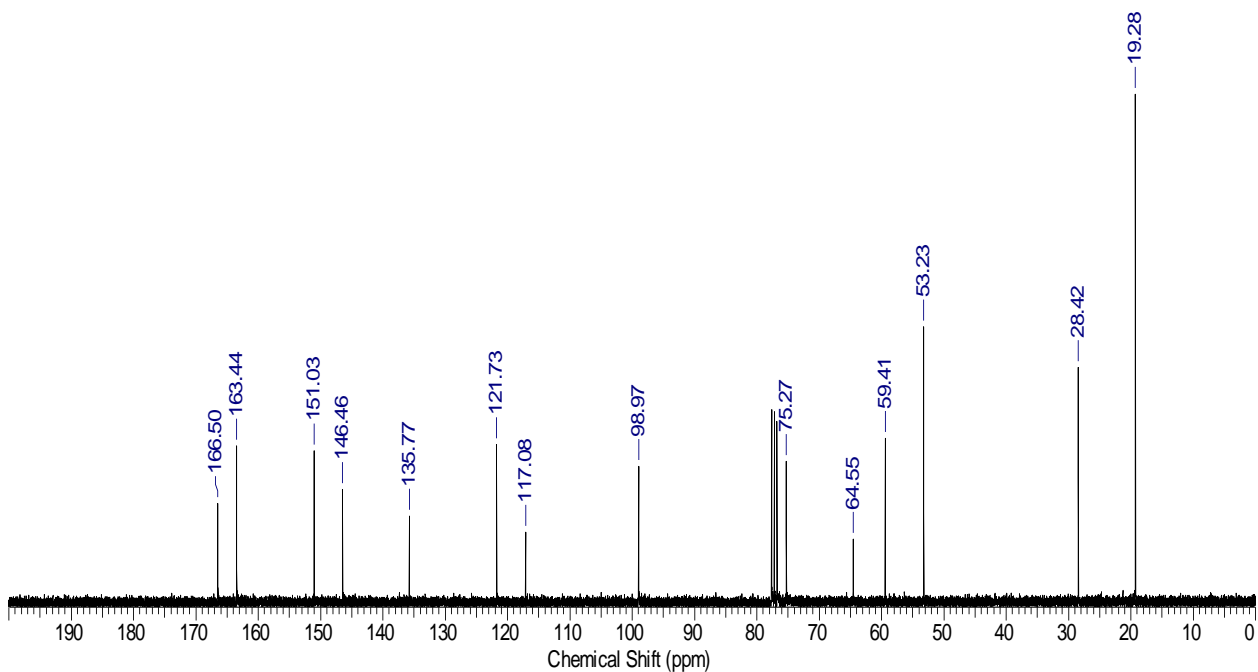
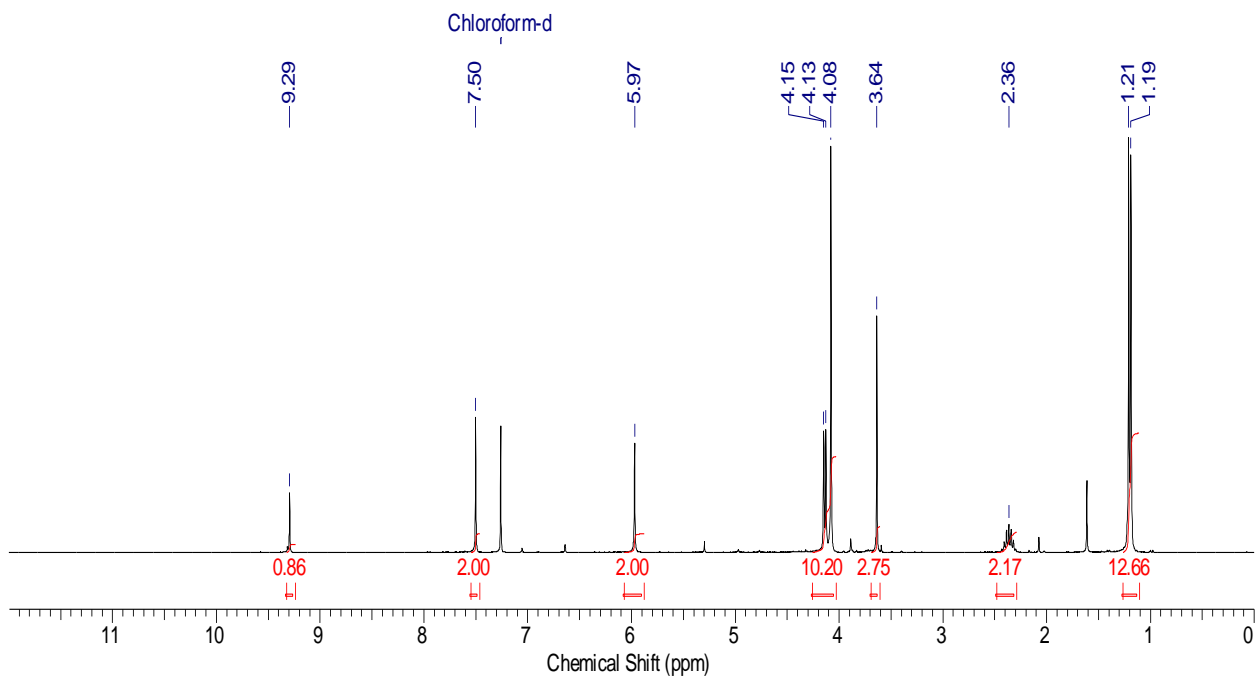
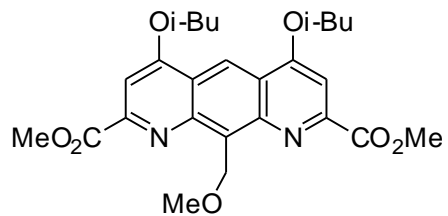
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-(bromomethyl)-2,7-anthracene dicarboxylate; (**1-Br**)



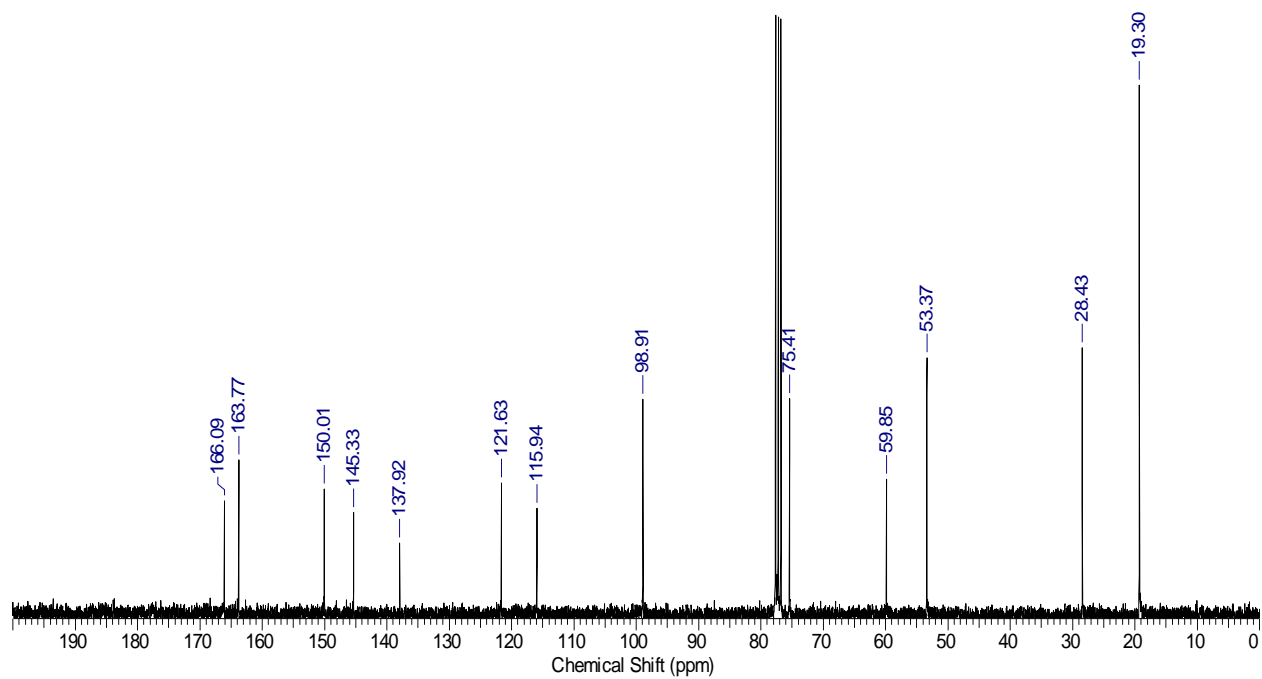
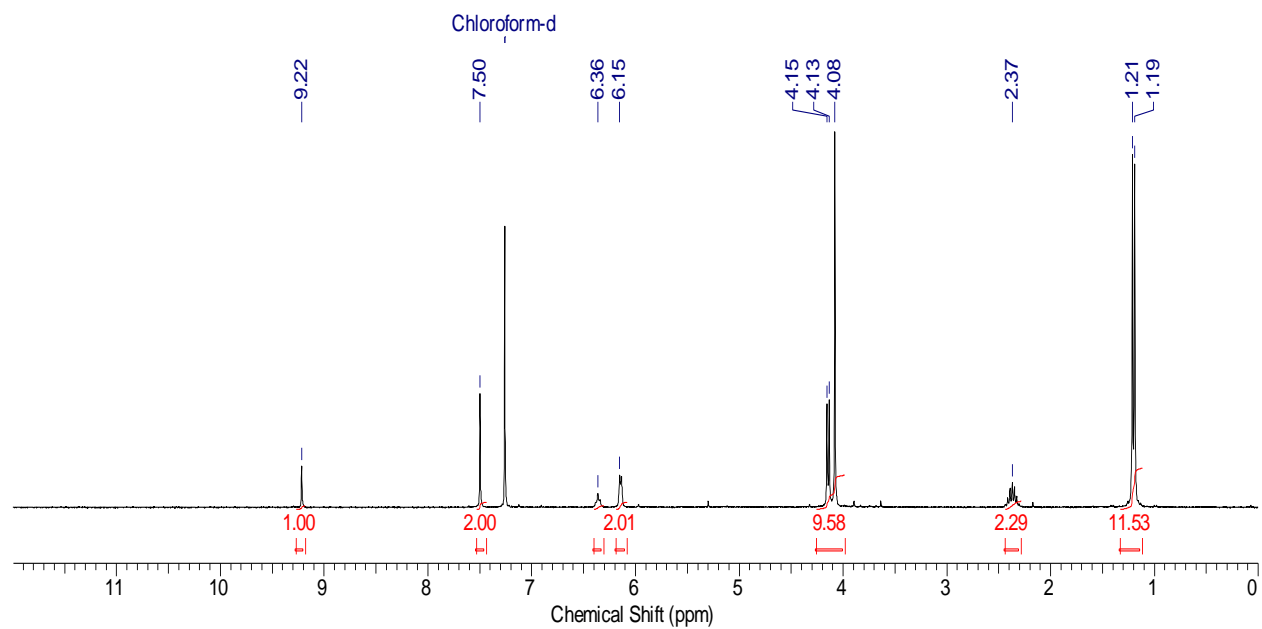
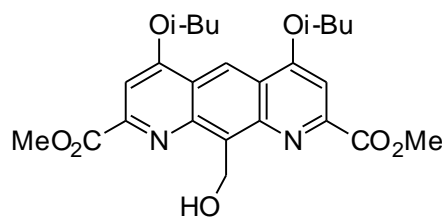
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-[(acetyloxy)methyl]-2,7-anthracene dicarboxylate; (**1-OAc**)



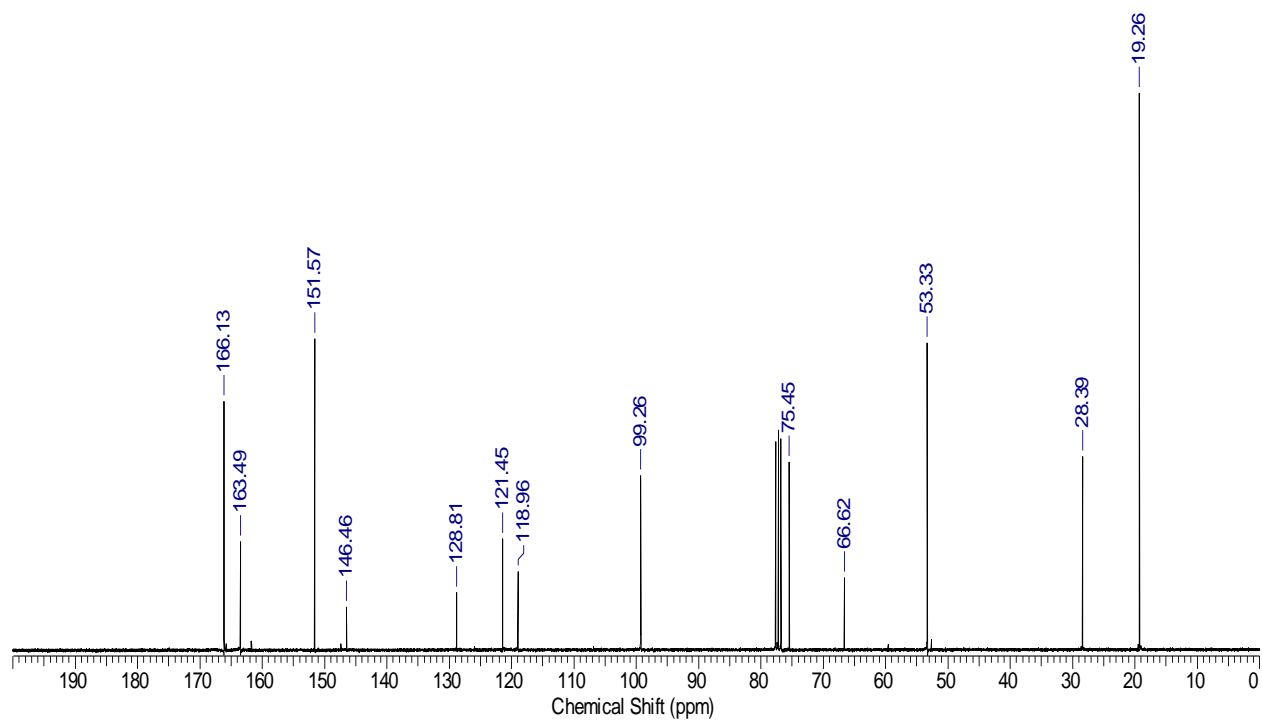
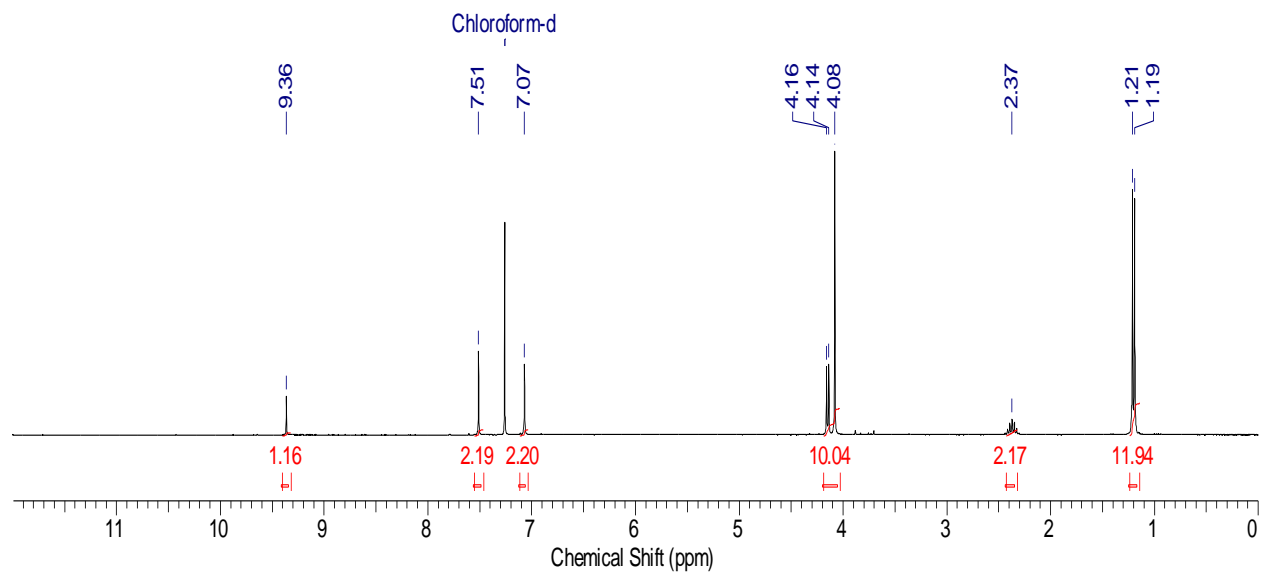
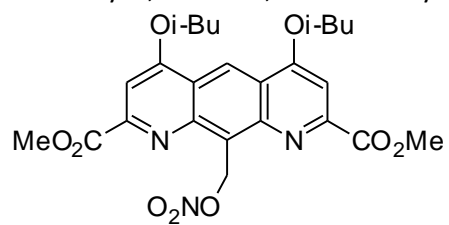
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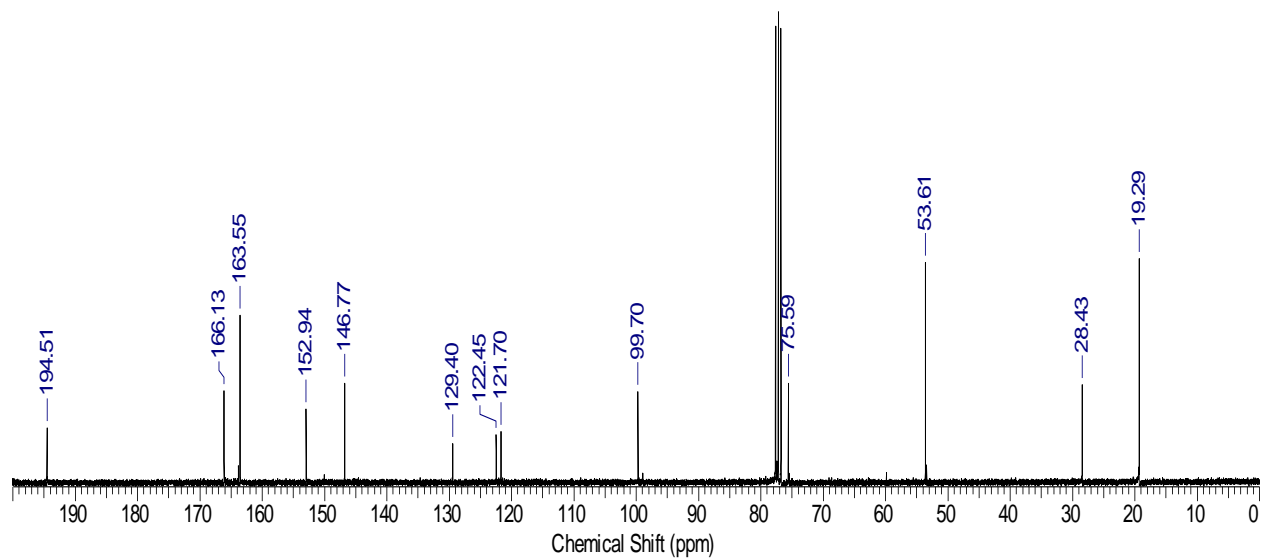
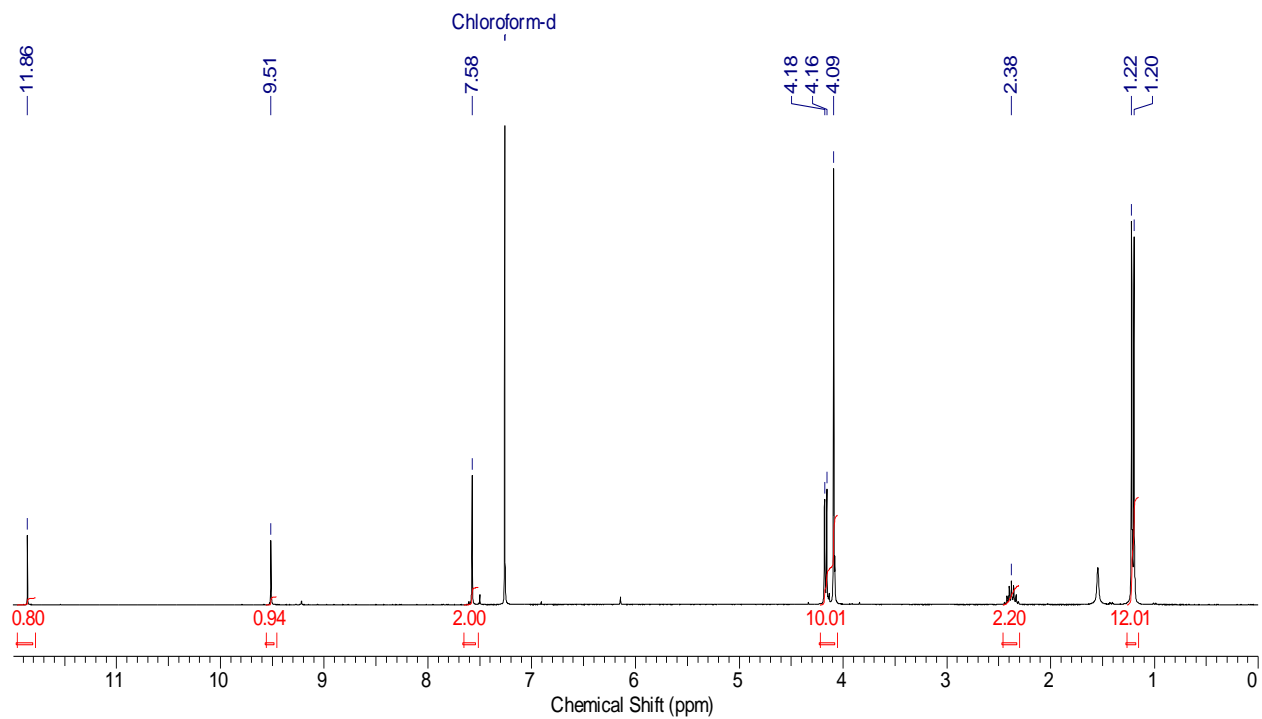
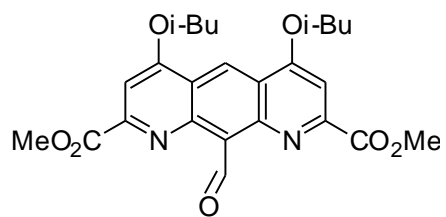
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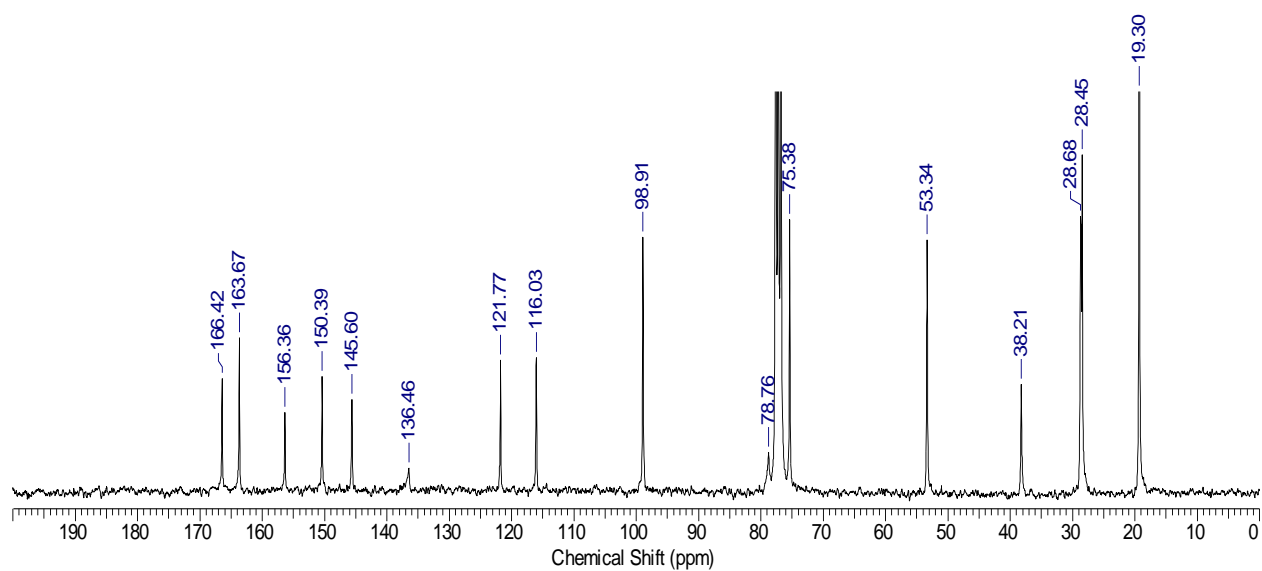
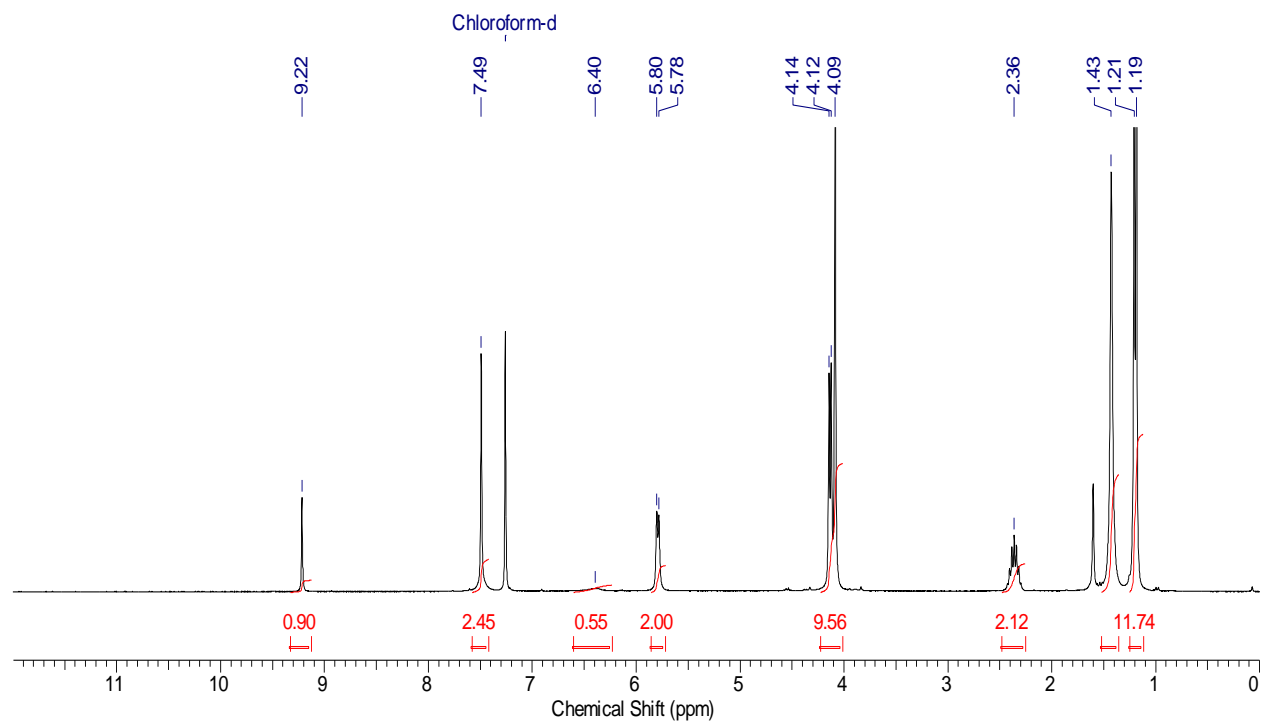
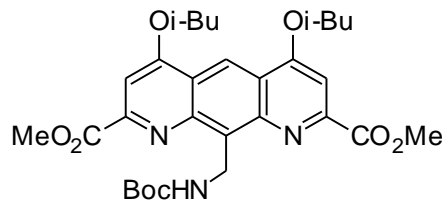
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-(nitrooxymethyl)-2,7-anthracene dicarboxylate; **1-ONO<sub>2</sub>**



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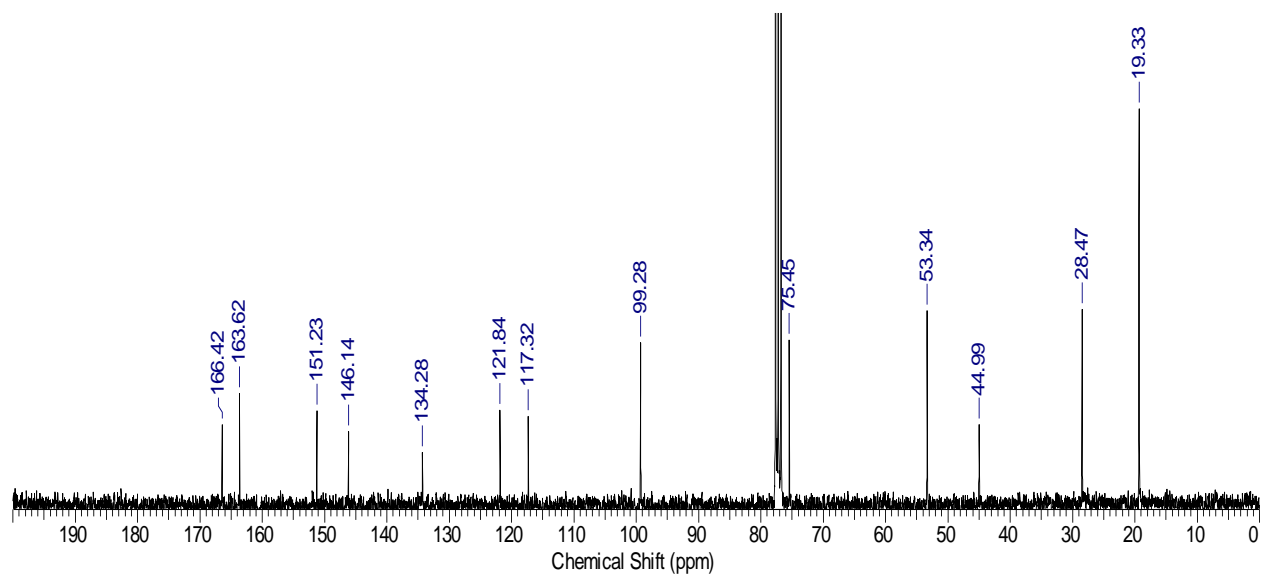
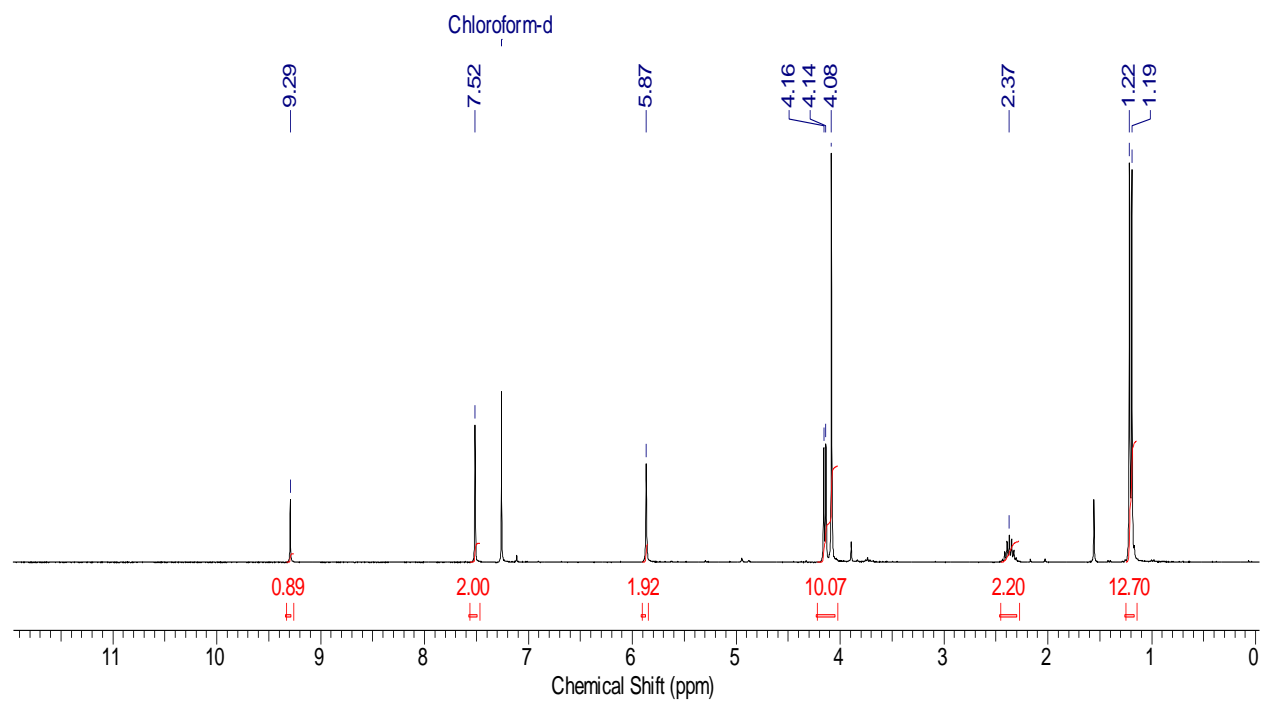
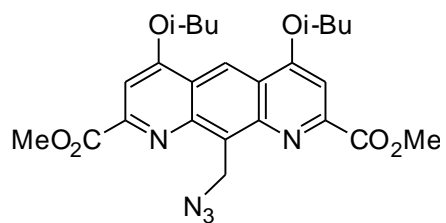


Dimethyl 1,8-diaza-4,5-diisobutoxy-9-[[*(tert*-butoxycarbonyl)amino]methyl]-2,7-anthracene dicarboxylate; (**1-NHBoc**)

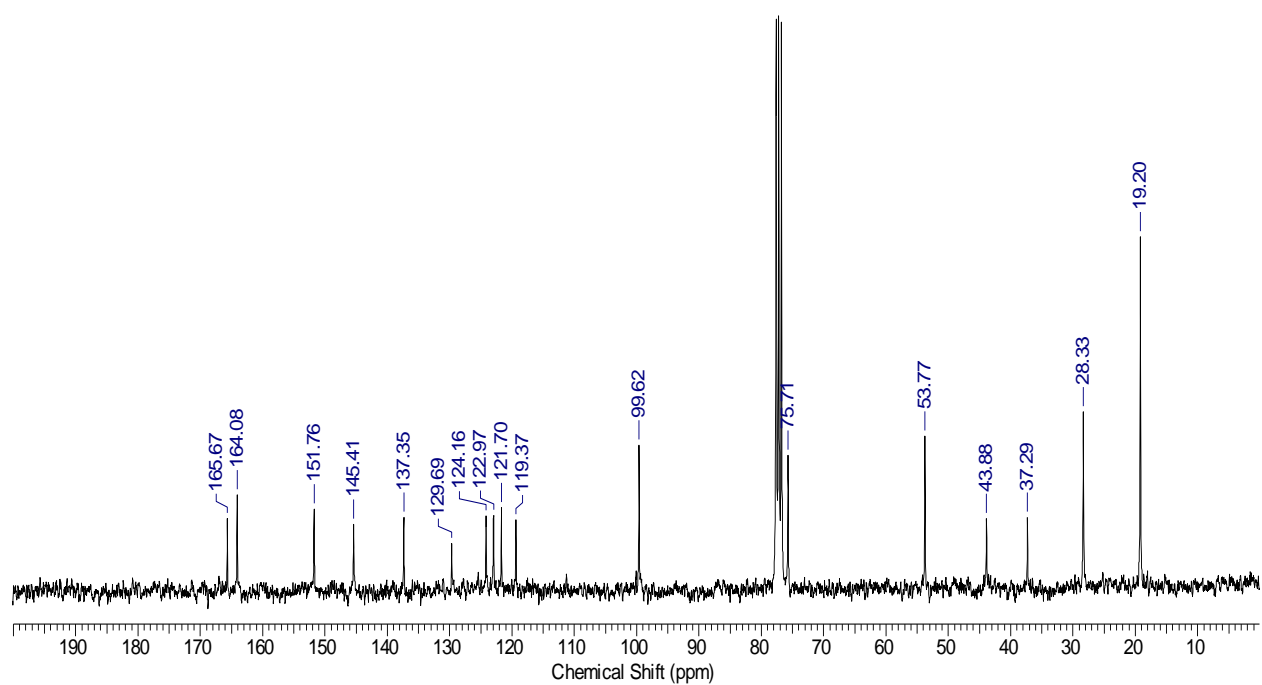
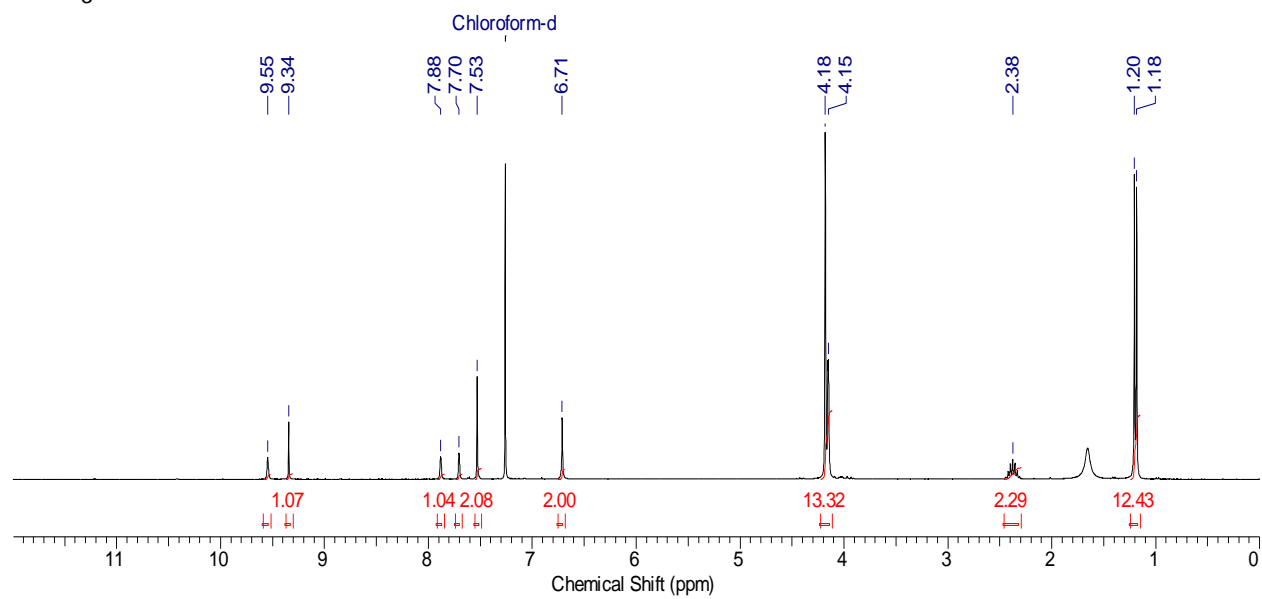
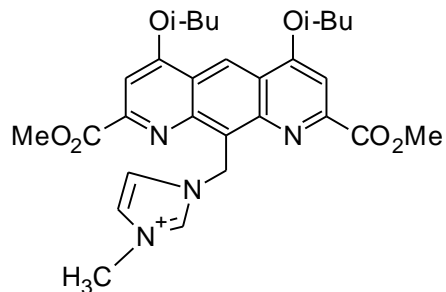




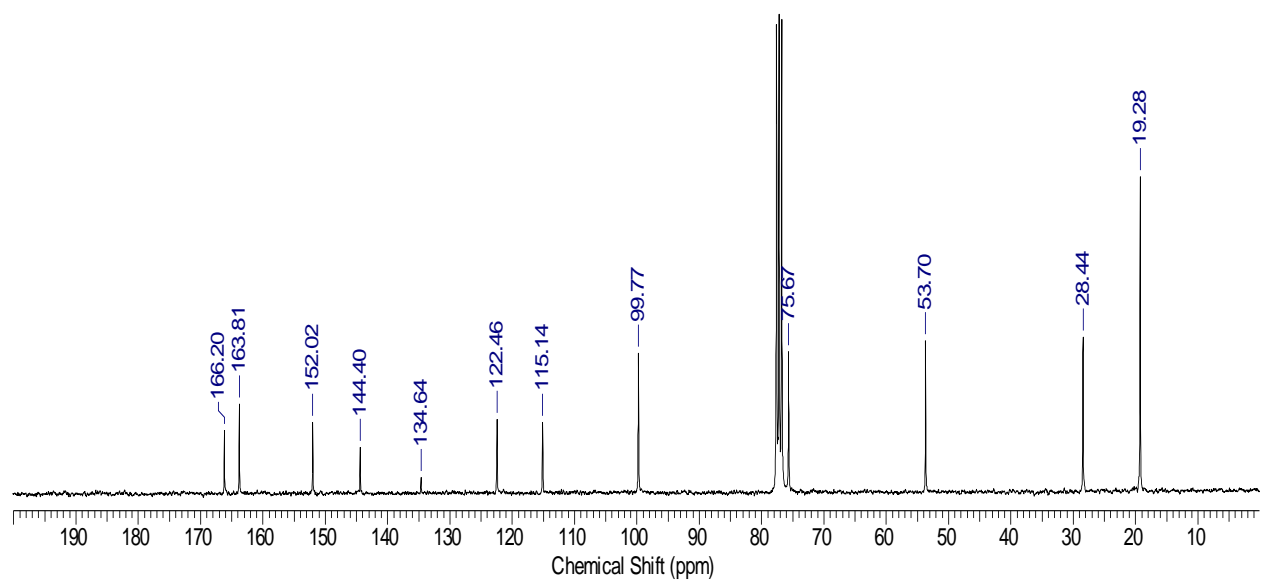
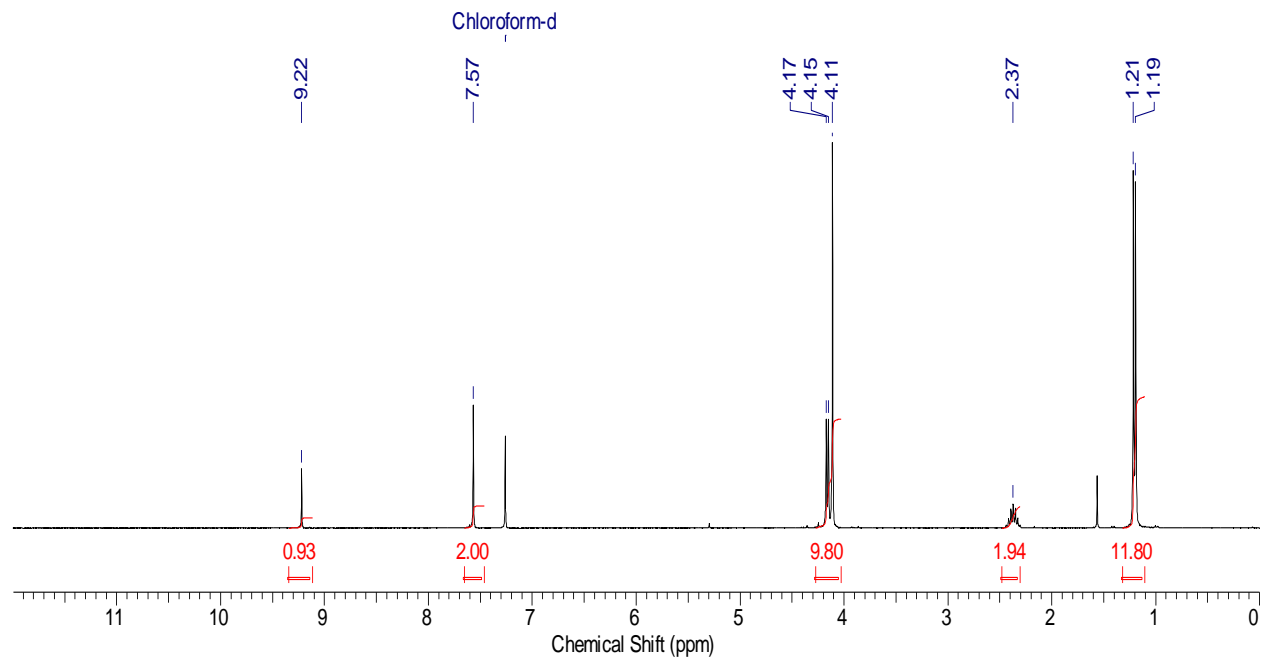
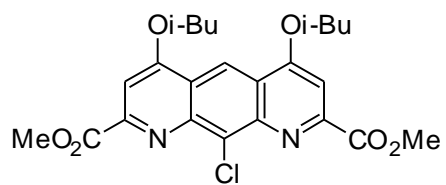
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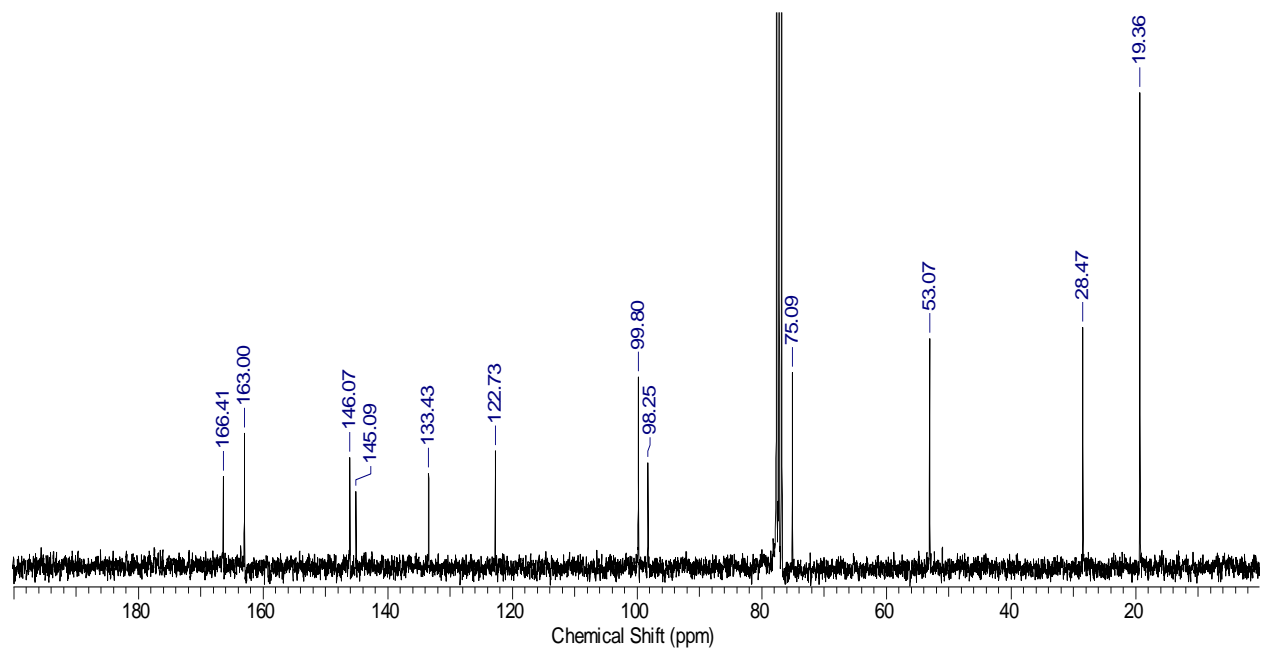
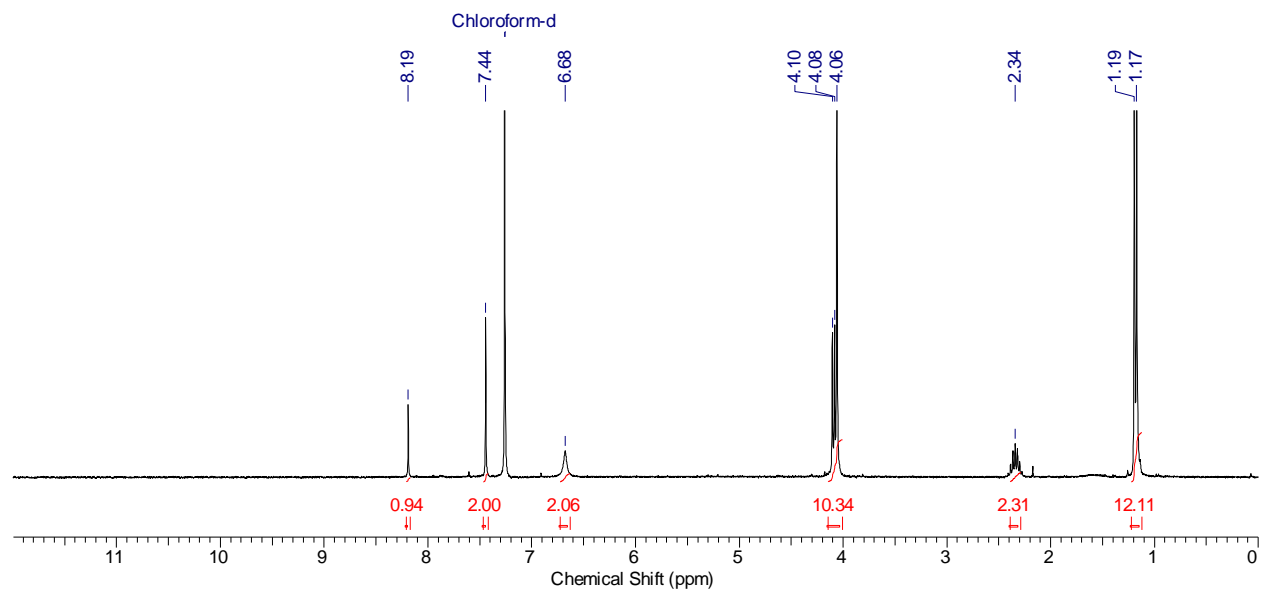
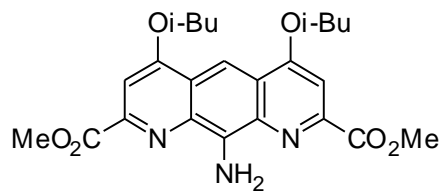
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-[N(N'-Methylimidazolium)methyl]-2,7-anthracene dicarboxylate bromide; (**1-Imid**)



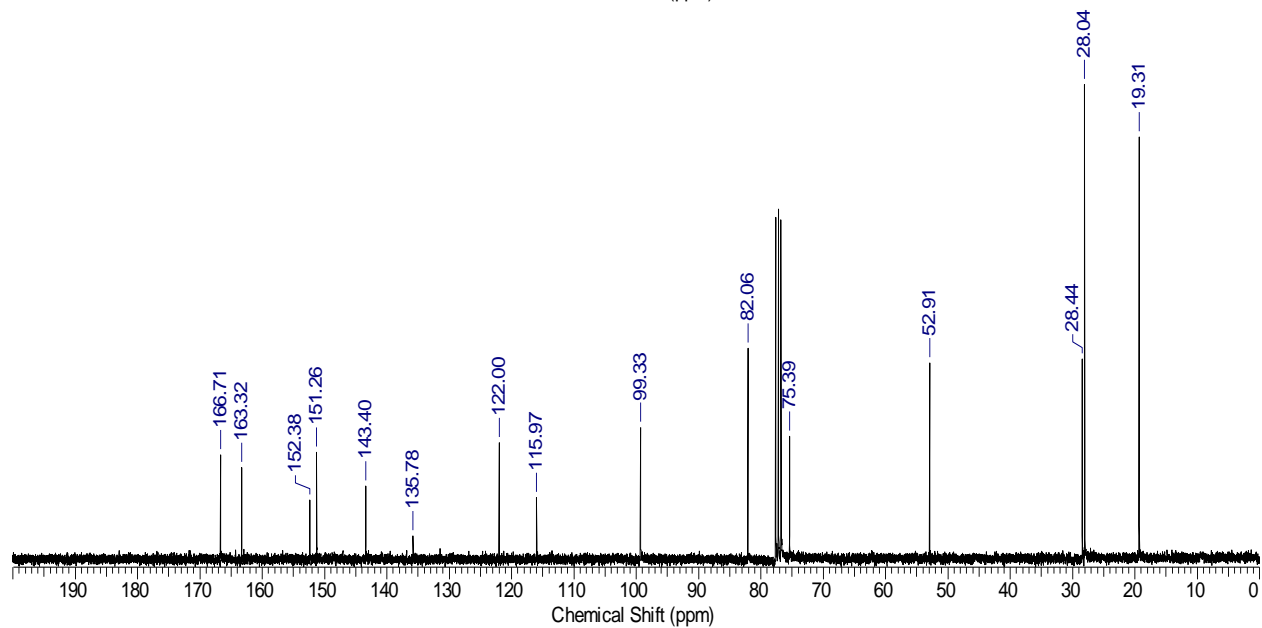
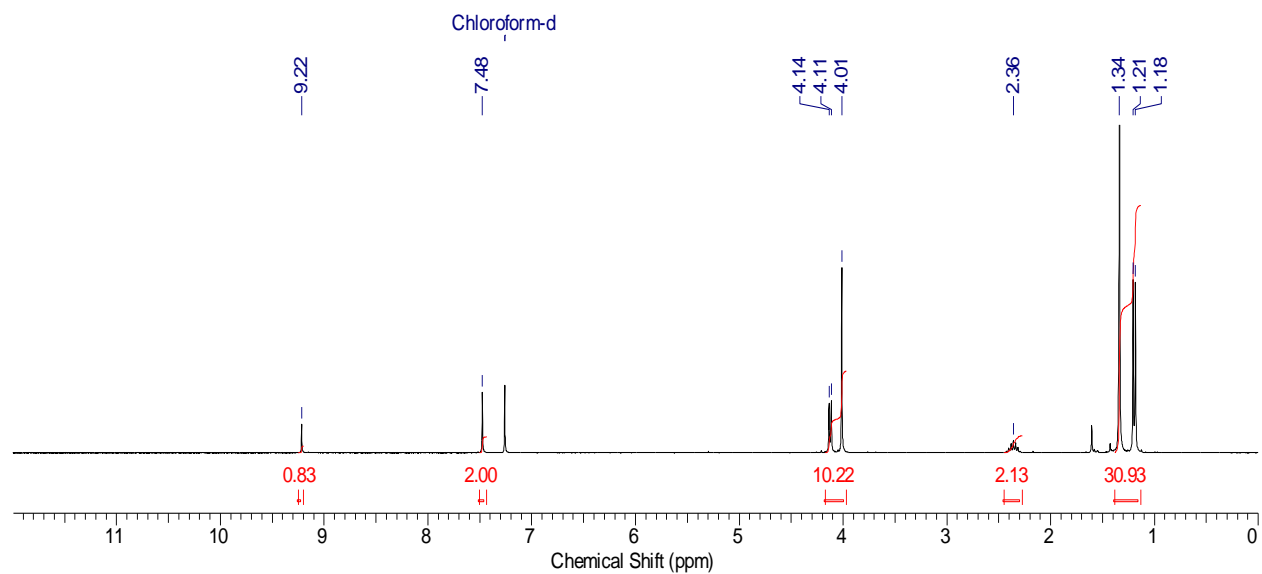
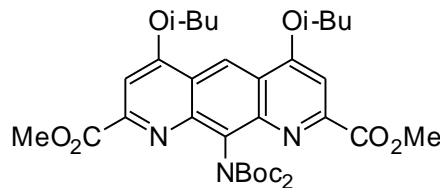
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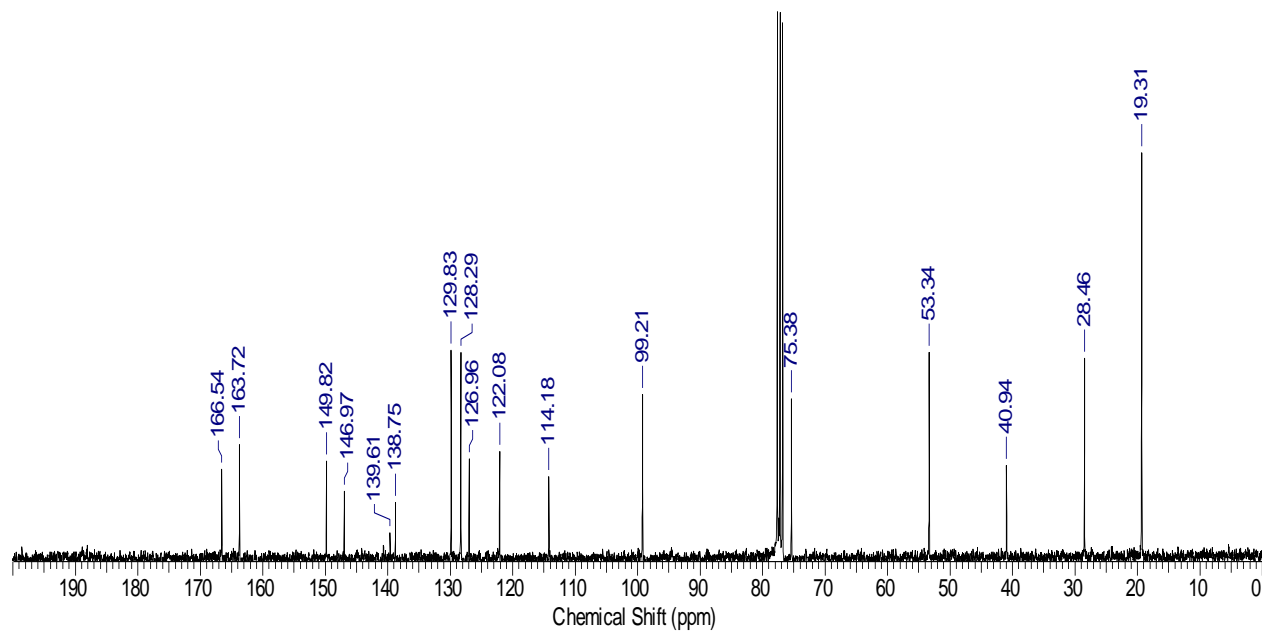
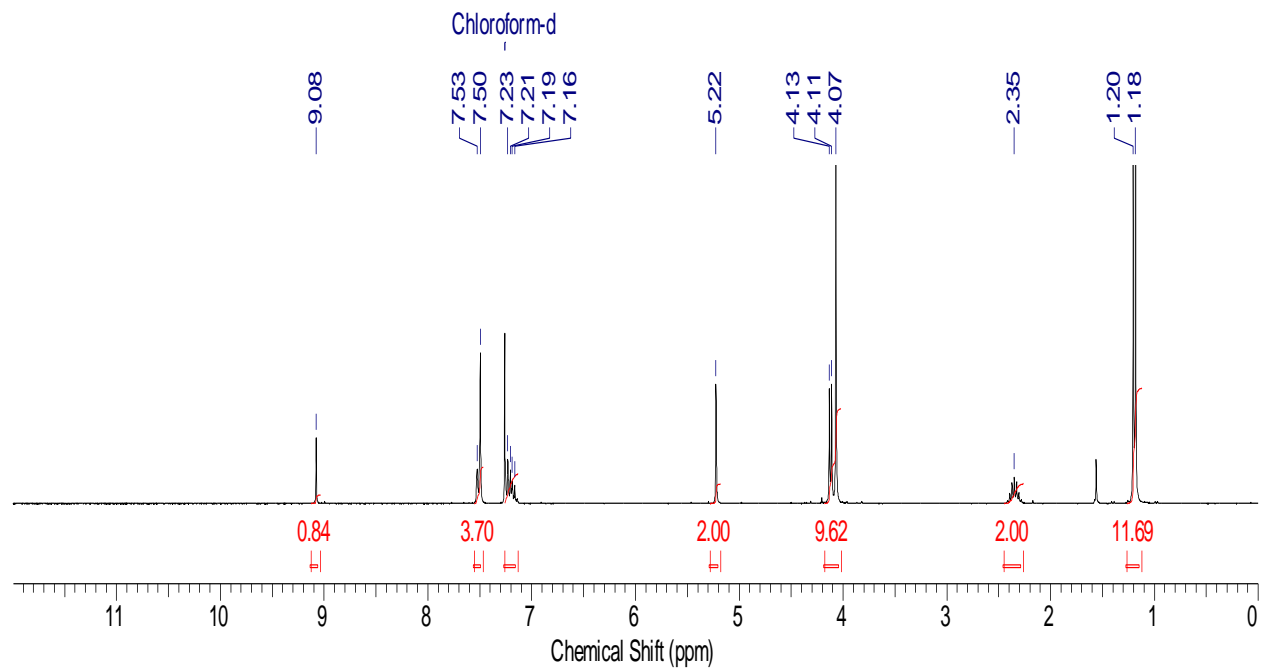
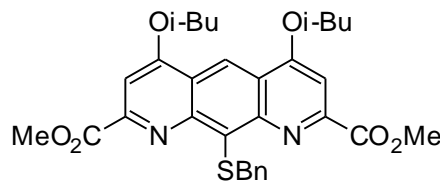
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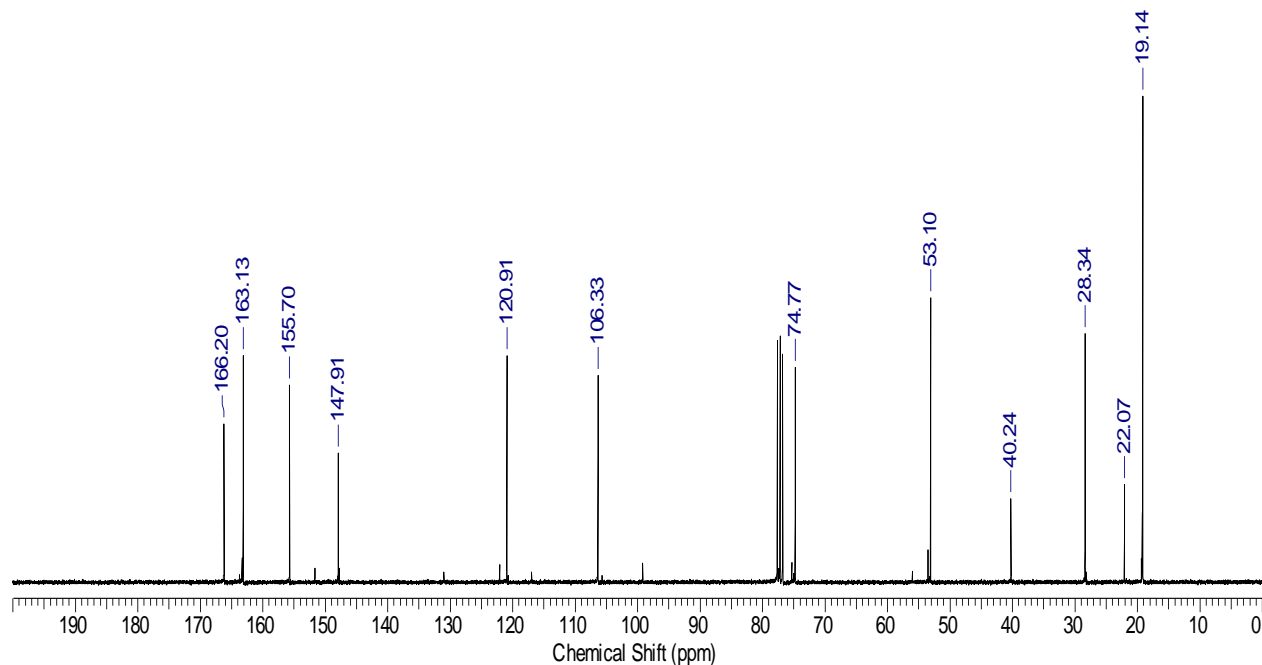
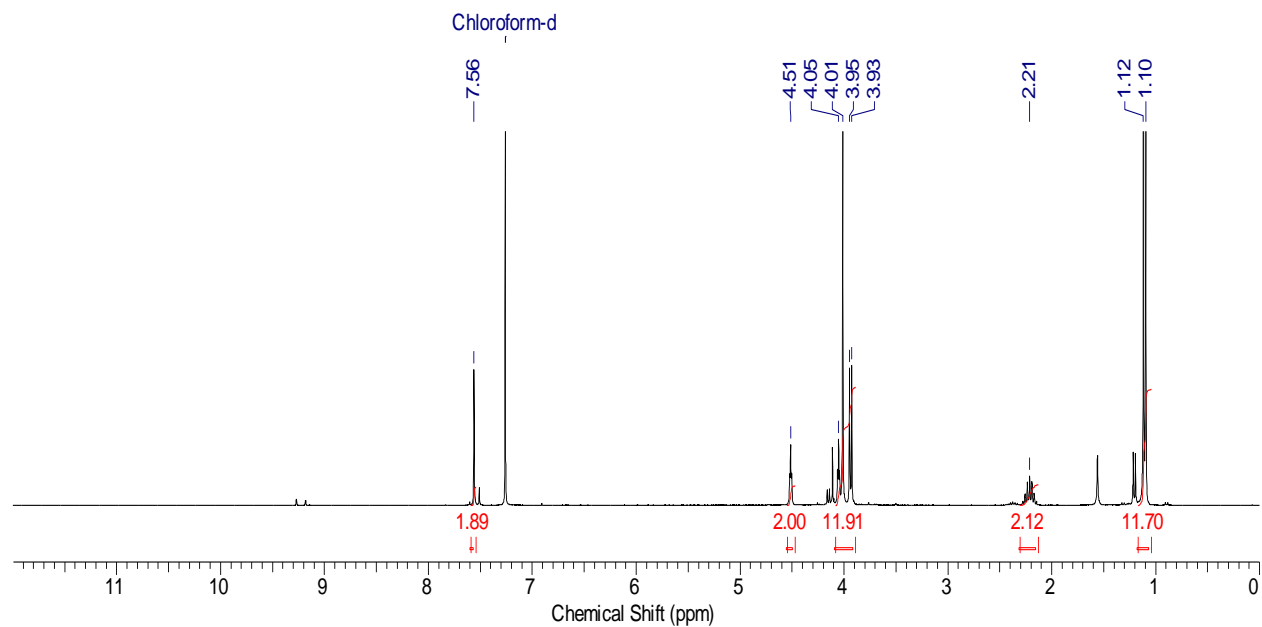
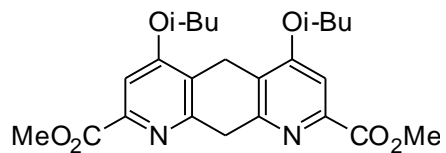
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-[bis(*tert*-butoxycarbonyl)amino]-2,7-anthracene dicarboxylate; (**2-NBoc<sub>2</sub>**)



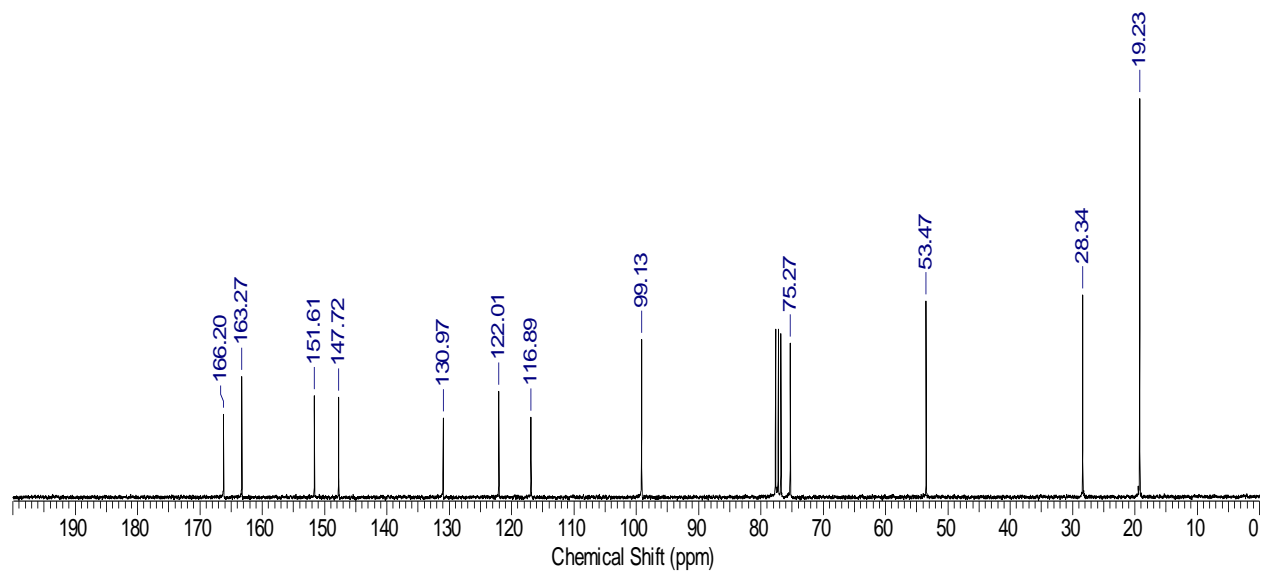
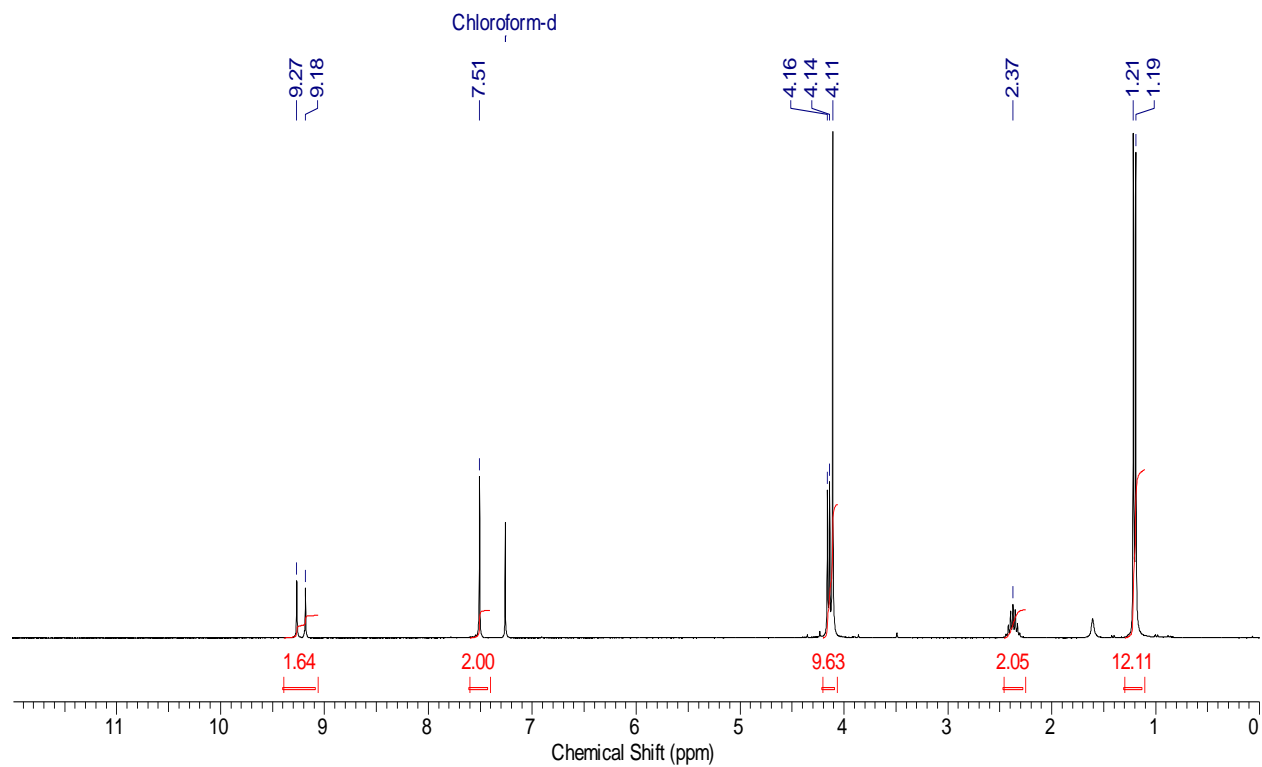
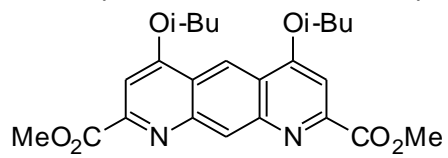
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-[benzylmercato]-2,7-anthracene dicarboxylate; (**2-SBn**)



Dimethyl 1,8-diaza-4,5-diisobutoxy-9,10-dihydro-2,7-anthracene dicarboxylate; (**2-H<sub>2</sub>**)

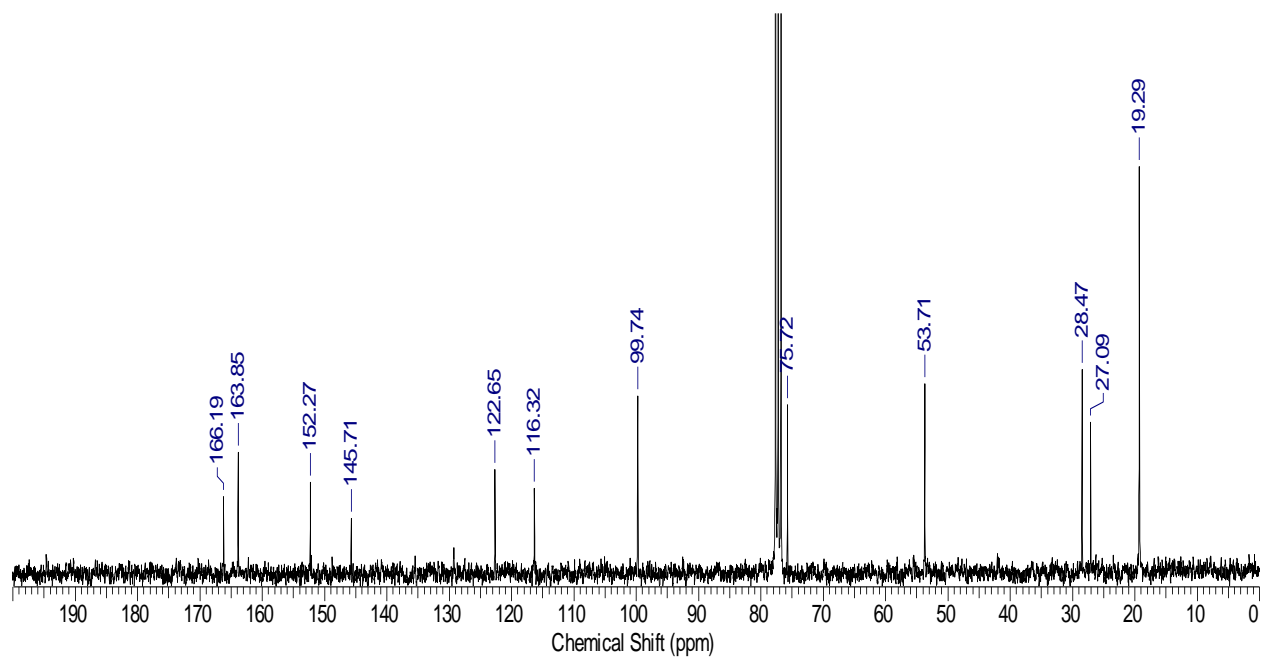
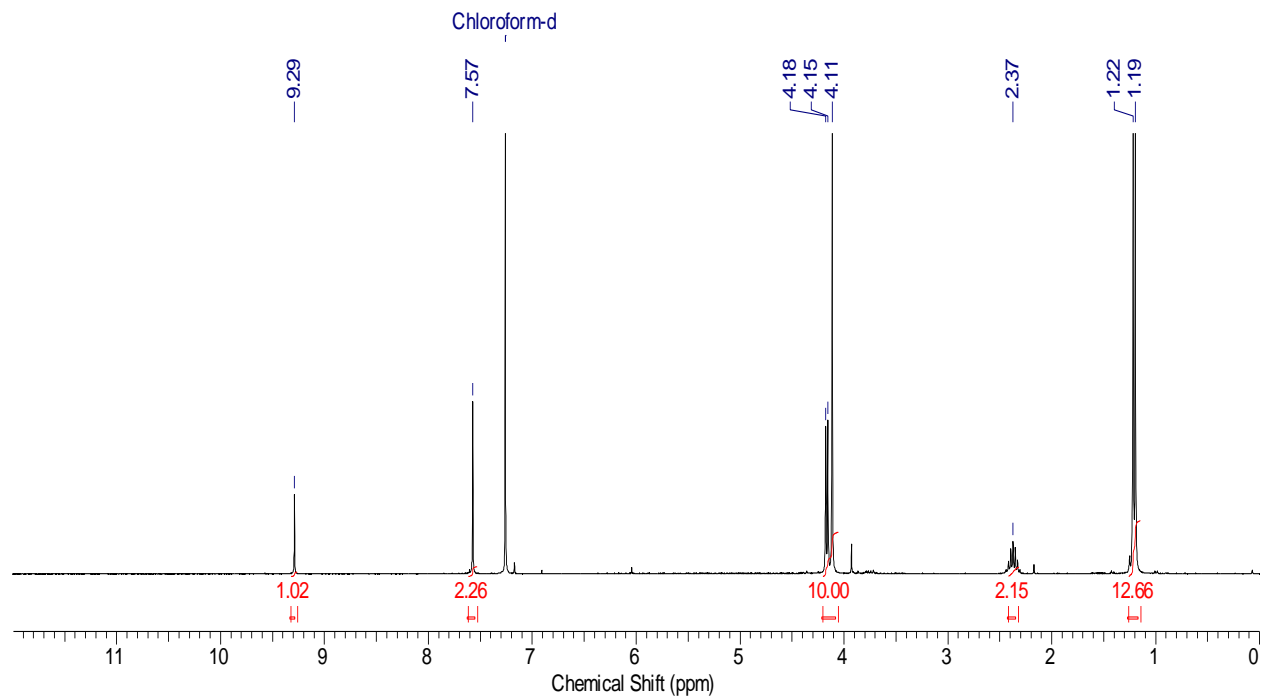
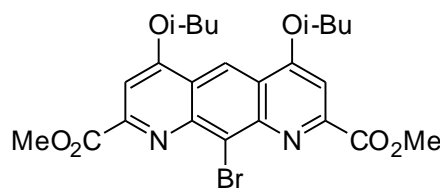


Dimethyl 1,8-diaza-4,5-diisobutoxy-2,7-anthracene dicarboxylate; (2)

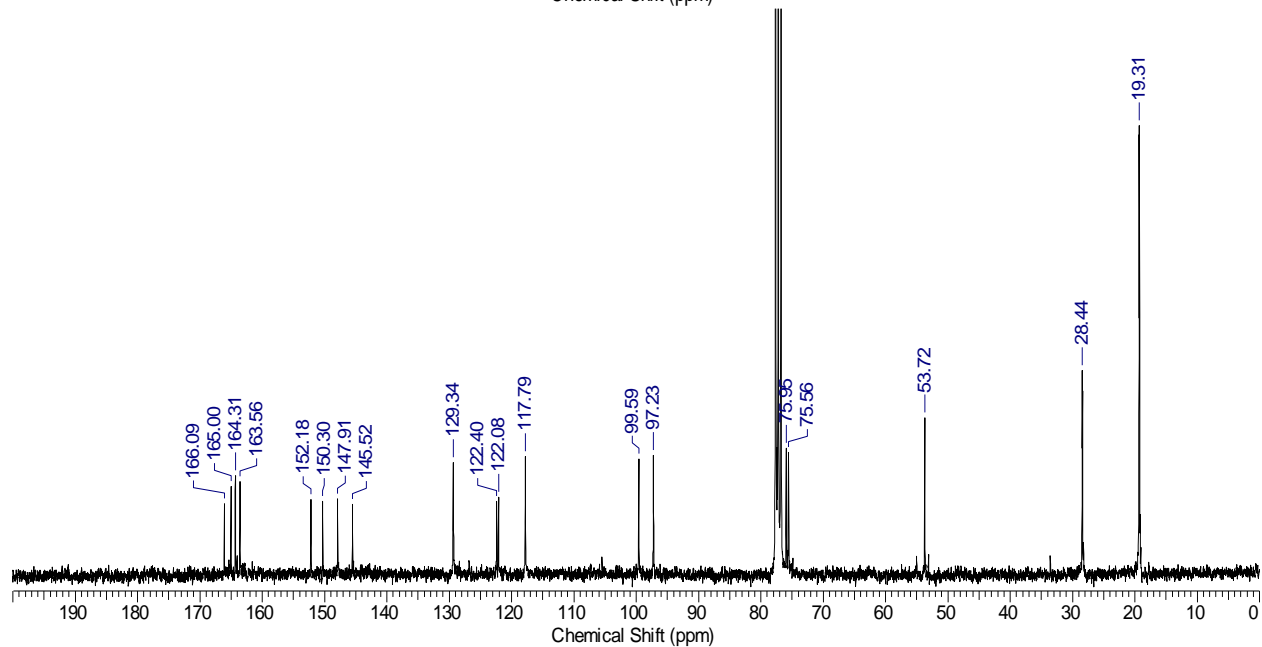
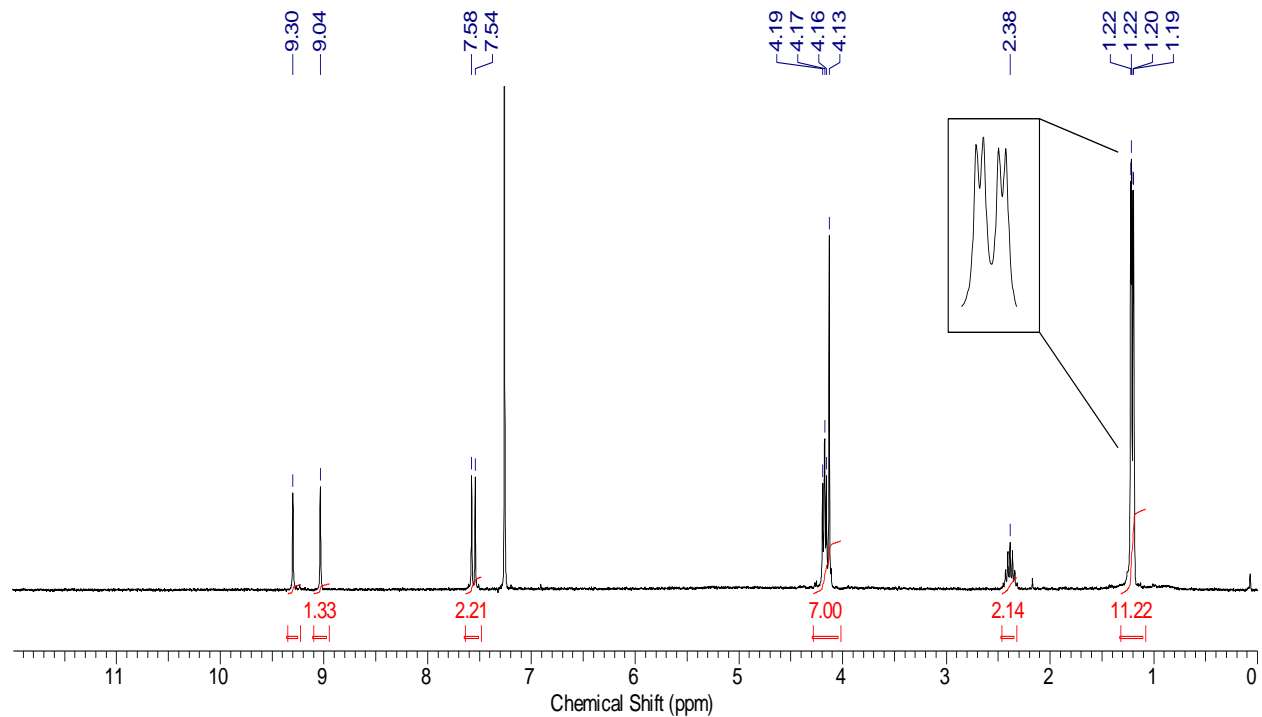
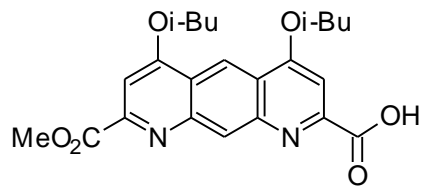




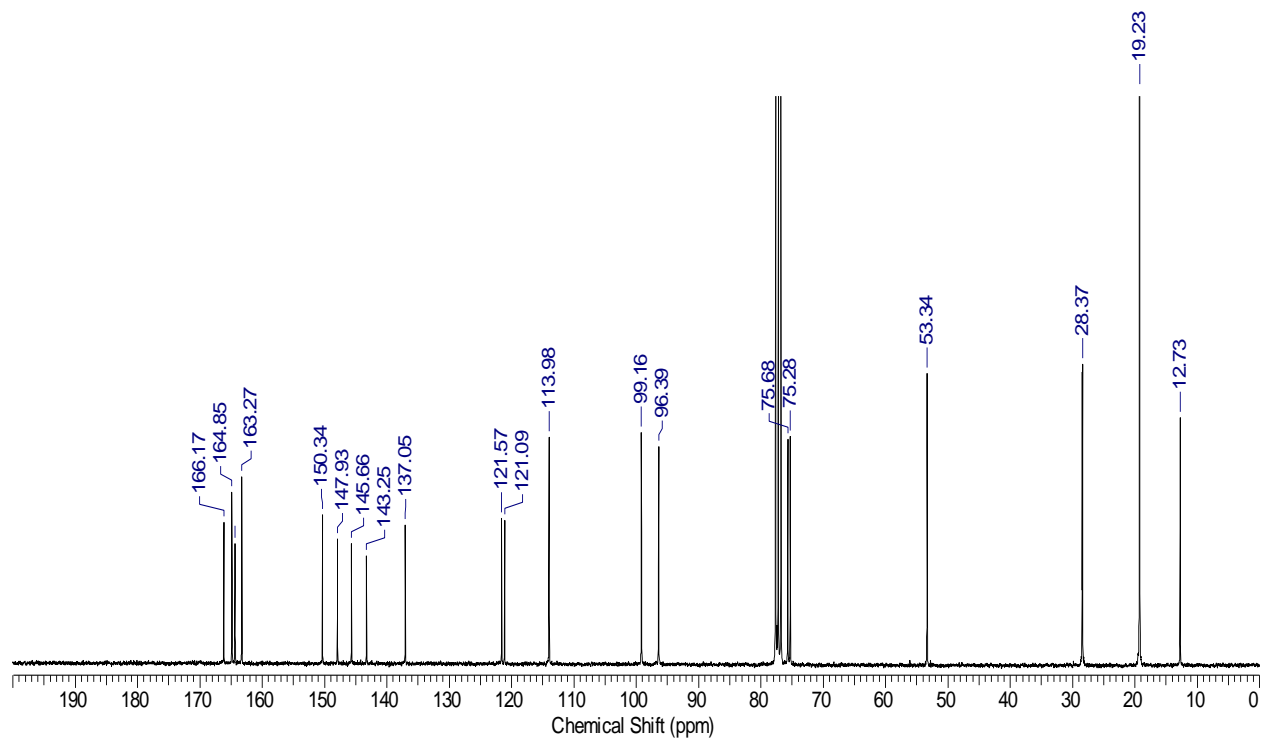
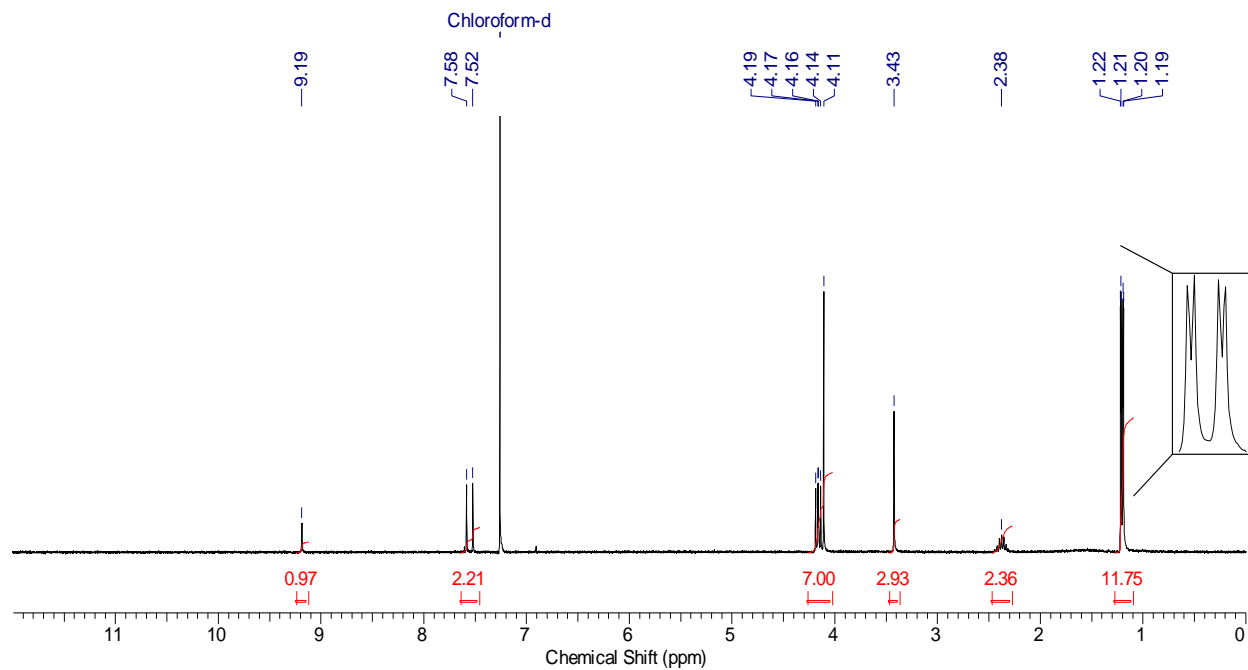
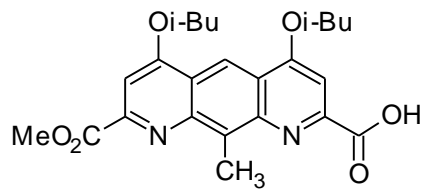
Dimethyl 1,8-diaza-4,5-diisobutoxy-9-bromo-2,7-anthracene dicarboxylate; (**2-Br**)



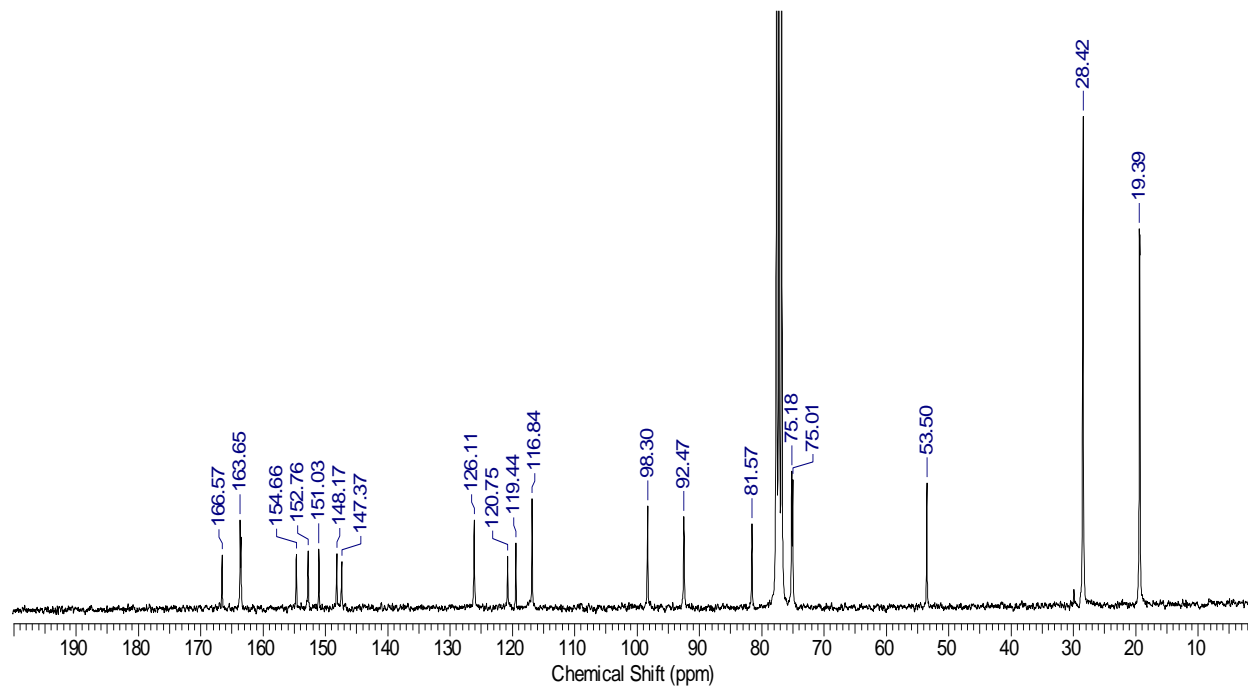
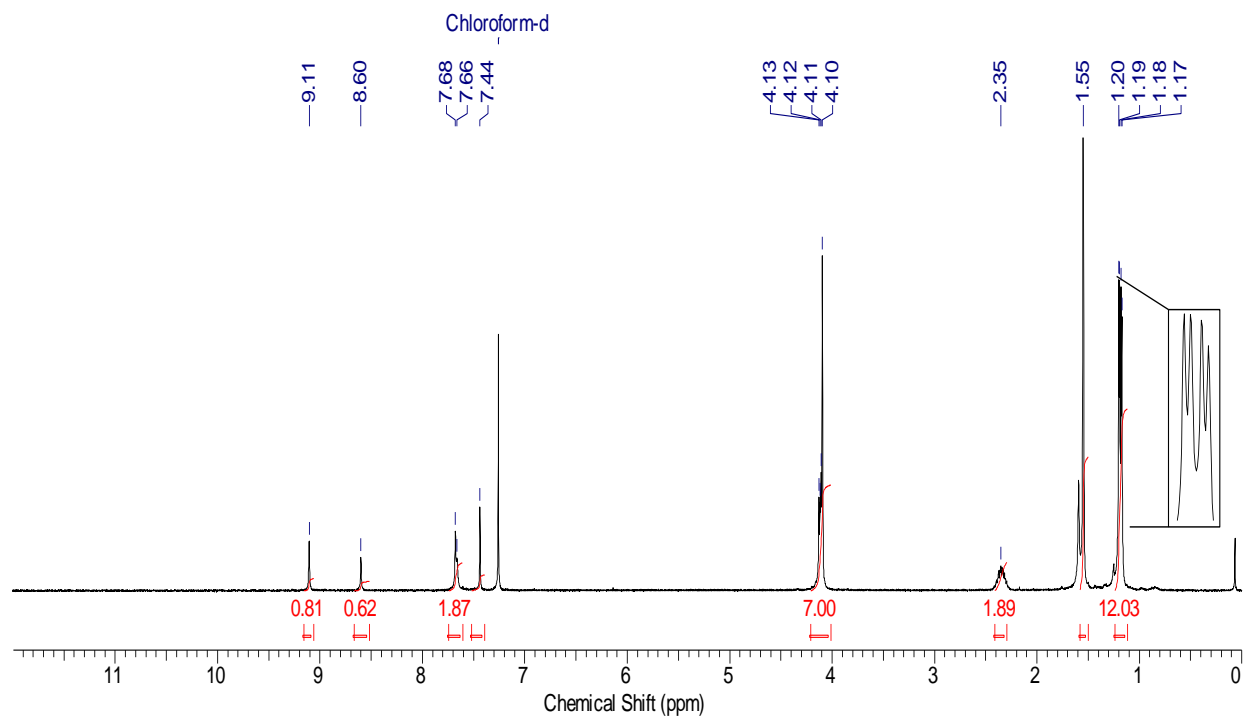
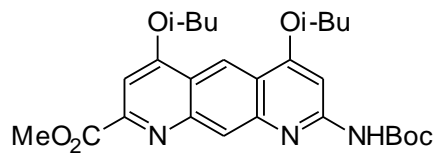
1,8-diaza-4,5-diisobutoxy-7-(methoxycarbonyl)-2-anthracene carboxylic acid (**3**)



1,8-diaza-4,5-diisobutoxy-7-(methoxycarbonyl)-9-methyl-2-anthracene carboxylic acid (**3-Me**)



1,8-diaza-4,5-diisobutoxy-7-[(*tert*-butoxycarbonyl)amino]-2-anthracene carboxylate , **4**



Methyl 1,8-diaza-4,5-diisobutoxy-7-[(*tert*-butoxycarbonyl)amino]-9-methyl-2-anthracene carboxylate, 4-Me

