

BCl₃-Activated Synthesis of COO-BODIPY Laser Dyes: General Scope and High Yields under Mild Conditions

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1. Photophysical and computational results. Table S1 and Figures S1-S2

Table S1. Fluorescence signatures of the new *COO*-BODIPYs **11-21** in different solvents.

Dye	λ_{ab} (nm)	$\epsilon_{max} 10^{-4}$ ($M^{-1} cm^{-1}$)	λ_{fl} (nm)	ϕ	τ (ns)	$k_f 10^8$ (s^{-1})	$k_{nr} 10^8$ (s^{-1})
11							
c-hex	514	8.2	521	1.00	5.89	1.70	0.00
EtOAc	512	7.2	520	1.00	6.46	1.55	0.00
MeOH	512	6.8	521	1.00	6.91	1.45	0.00
12							
c-hex	523	8.6	540	0.82	6.09	1.34	0.29
EtOAc	519	7.3	536	0.80	6.31	1.27	0.32
MeOH	519	7.2	535	0.82	6.96	1.18	0.26
13							
c-hex	524	6.5	541	0.87	6.34	1.37	0.20
EtOAc	521	5.9	536	0.80	7.02	1.14	0.28
MeOH	520	6.3	534	0.82	7.55	1.09	0.24
14							
c-hex	524	8.2	540	0.93	6.18	1.50	0.11
EtOAc	520	7.0	536	0.92	6.84	1.35	0.12
MeOH	520	6.1	538	0.86	7.43	1.16	0.19
15							
c-hex	525	7.8	540	0.91	6.49	1.40	0.14
EtOAc	521	6.6	538	0.95	6.84	1.39	0.07
MeOH	520	6.0	538	0.87	7.43	1.17	0.17
16							
c-hex	524	7.9	540	0.91	6.18	1.47	0.14
EtOAc	520	7.0	535	0.90	6.49	1.39	0.15
MeOH	519	6.7	534	0.87	7.01	1.24	0.18
17							
c-hex	524	7.7	541	0.95	6.09	1.56	0.08
EtOAc	520	7.5	538	0.85	6.60	1.29	0.22
MeOH	520	7.1	536	0.71	6.03	1.18	0.48
18							
c-hex	524	7.6	540	0.83	6.11	1.35	0.28
EtOAc	520	7.5	536	0.80	6.45	1.24	0.31
MeOH	520	7.3	535	0.83	6.99	1.19	0.24
19							
c-hex	524	7.0	540	0.89	6.24	1.43	0.17
EtOAc	521	6.2	544	0.01	0.05	2.80	197
MeOH	520	6.1	542	0.00	-	-	-
20							
c-hex	528	5.5	571	0.49	5.45	0.90	0.93
EtOAc	522	5.3	562	0.51	5.73	0.89	0.85
MeOH	521	5.1	559	0.53	5.61	0.94	0.84

21							
c-hex	527	6.4	566	0.54	5.64	0.96	0.81
EtOAc	521	5.5	559	0.59	6.07	0.97	0.67
MeOH	521	5.5	557	0.53	6.07	0.87	0.77

Maximum absorption (λ_{ab}) and fluorescence (λ_{fl}) wavelengths; maximum molar absorption (ϵ_{max}); fluorescence quantum yield (ϕ) and lifetime (τ); radiative (k_{fl}) and non-radiative (k_{nr}) rate constants. c-hex: cyclohexane; EtOAc: ethyl acetate; MeOH: methanol.

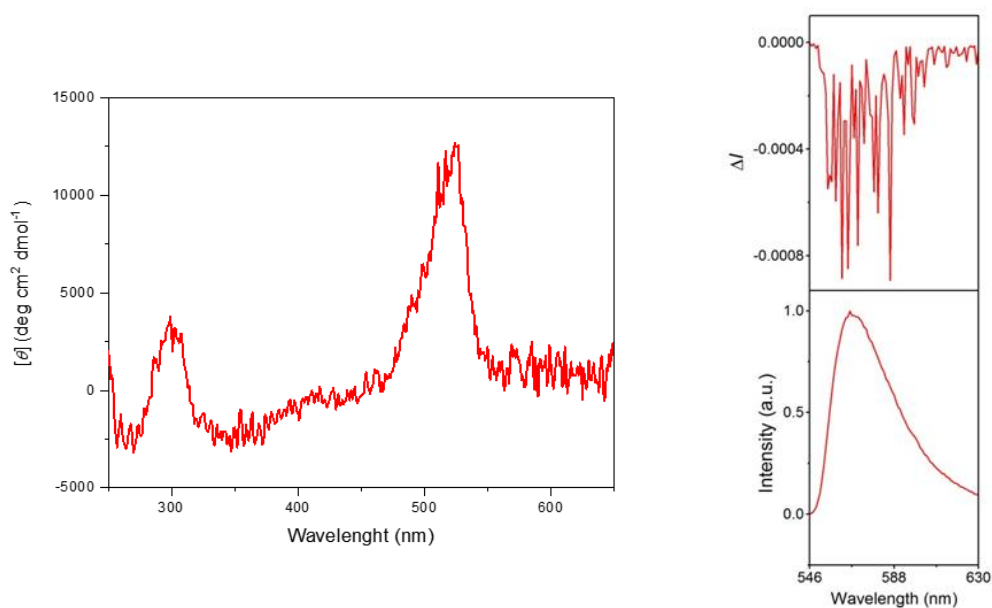


Figure S1. CD (left), CPL (right, up) and total luminescence (right, down) spectra of COO-BODIPY **13** in chloroform.

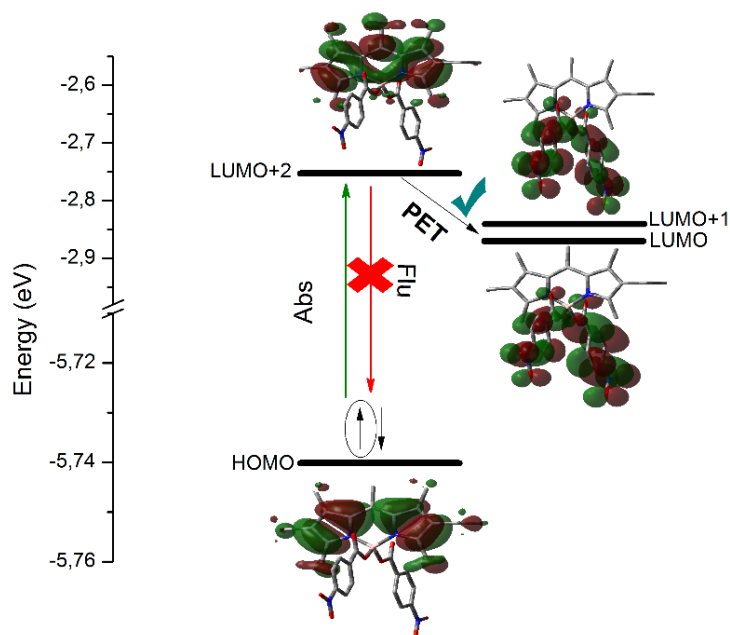


Figure S2. Energetic distribution of key molecular orbitals computed for the optimized ground-state geometry (PCM-B3LYP/6-311g*) of COO-BODIPY **19** (see Table S3), and schematic representation of the fluorescence quenching by oxidative PET.

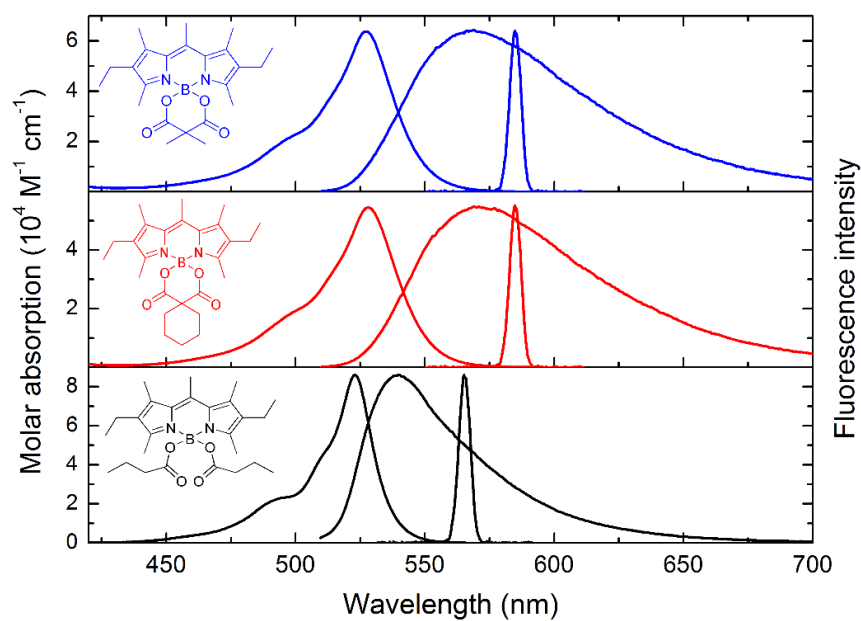


Figure S3. Absorption and corresponding normalized fluorescence and laser spectra of spiranic COO-BODIPYs **20** (in red) and **21** (in blue) in ethyl acetate. The corresponding spectra of **12** (in black) are shown in this figure, as a representative non-spiranic COO-BODIPY, for comparison.

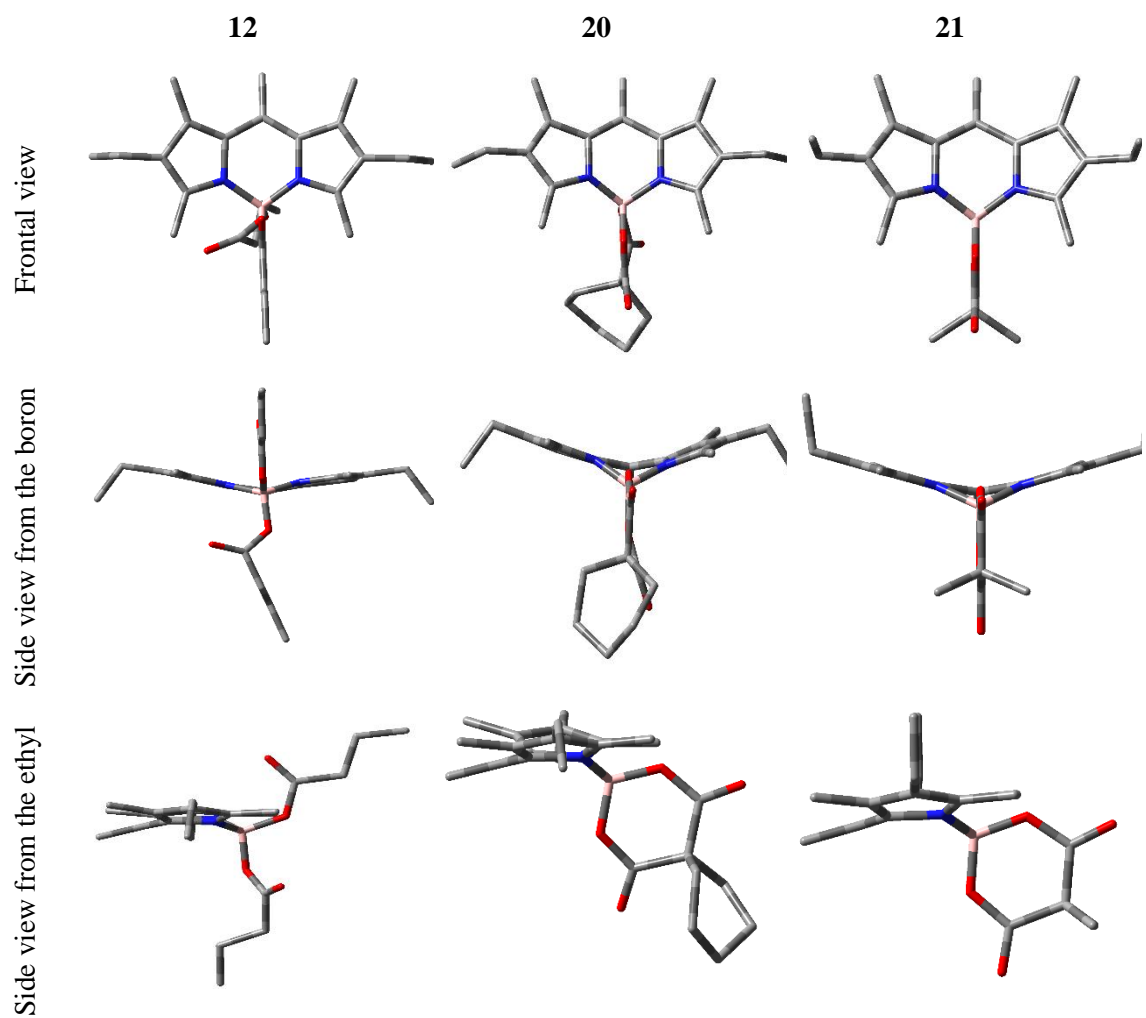
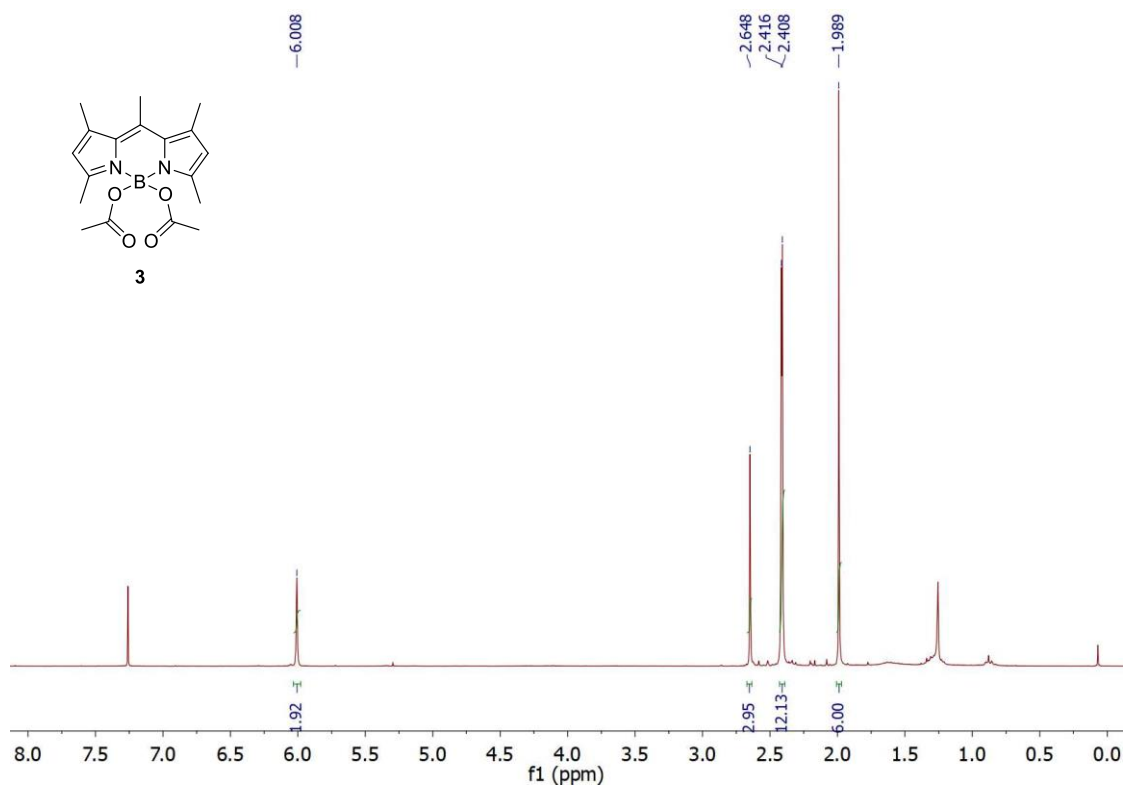


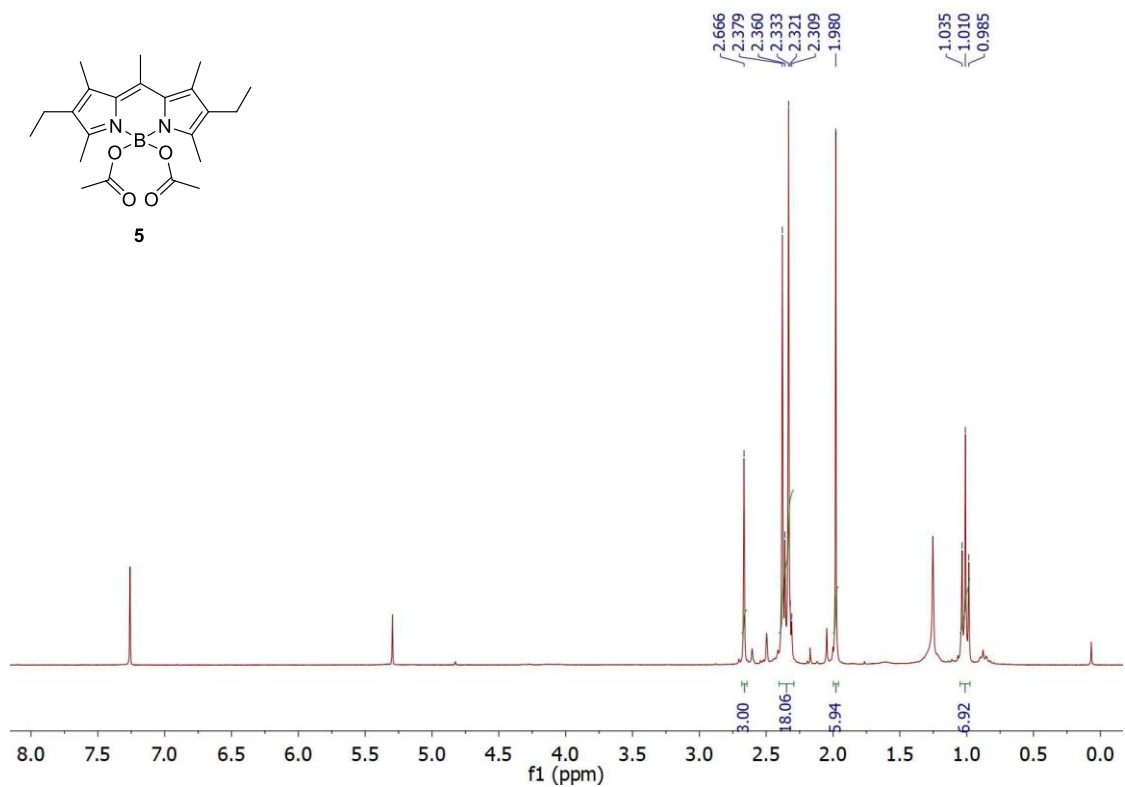
Figure S4. Optimized geometries at the first singlet excited state (TD-PCM-B3LYP/6-311g*) in different views for spiranic COO-BODIPYs **20** and **21** with respect to non-spiranic analog **12** (see Table S2), highlighting the geometrical distortion in the former dyes.

2. ^1H NMR spectra of known compounds

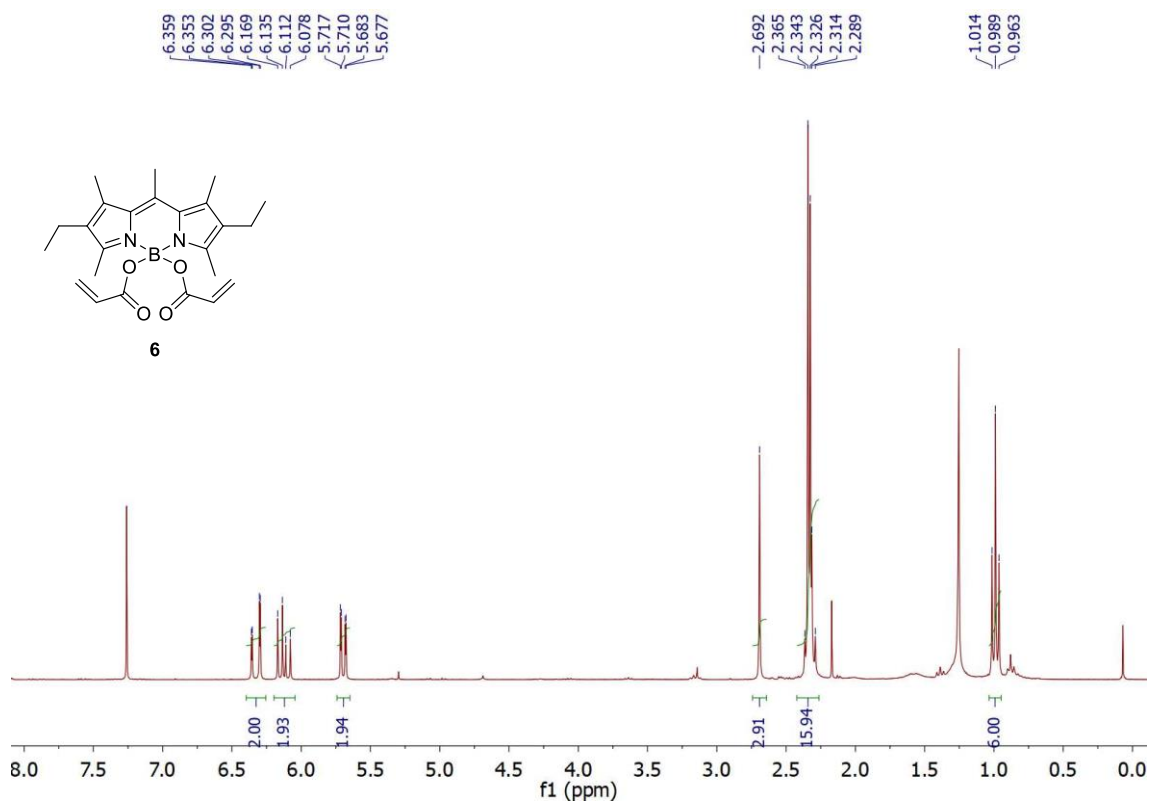
^1H NMR (300 MHz, CDCl_3)



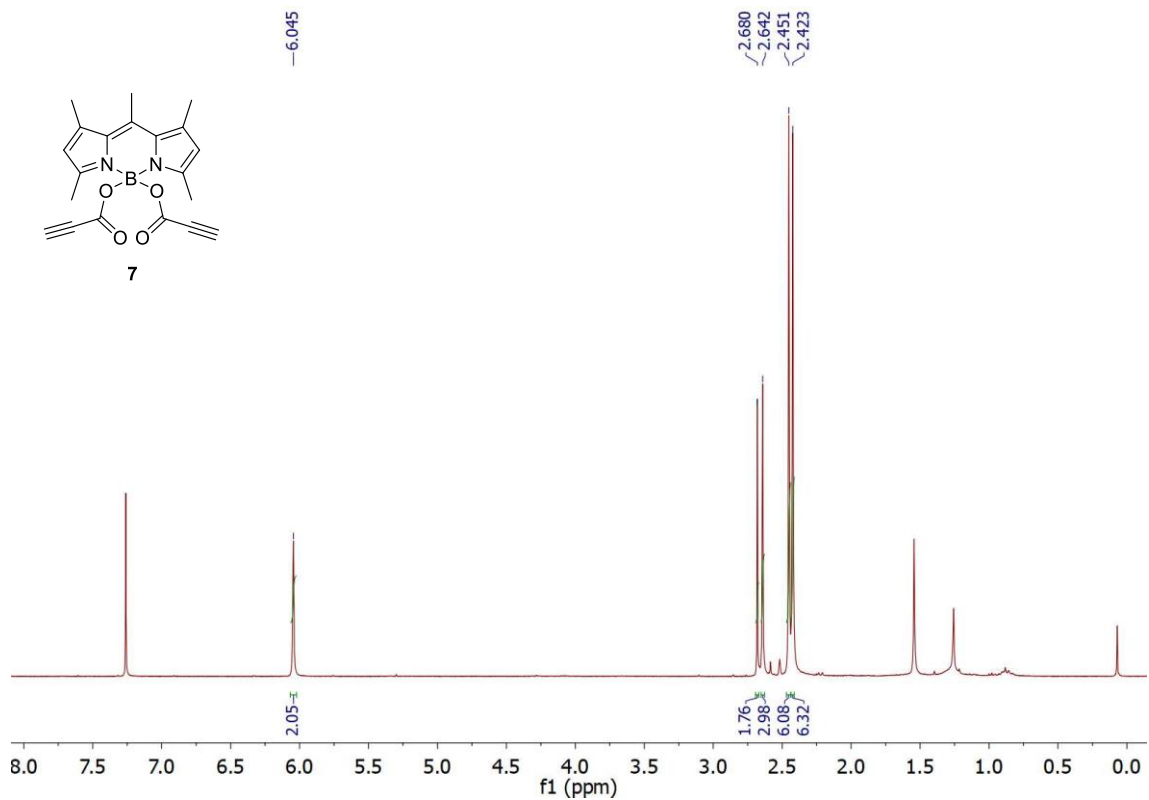
^1H NMR (300 MHz, CDCl_3)



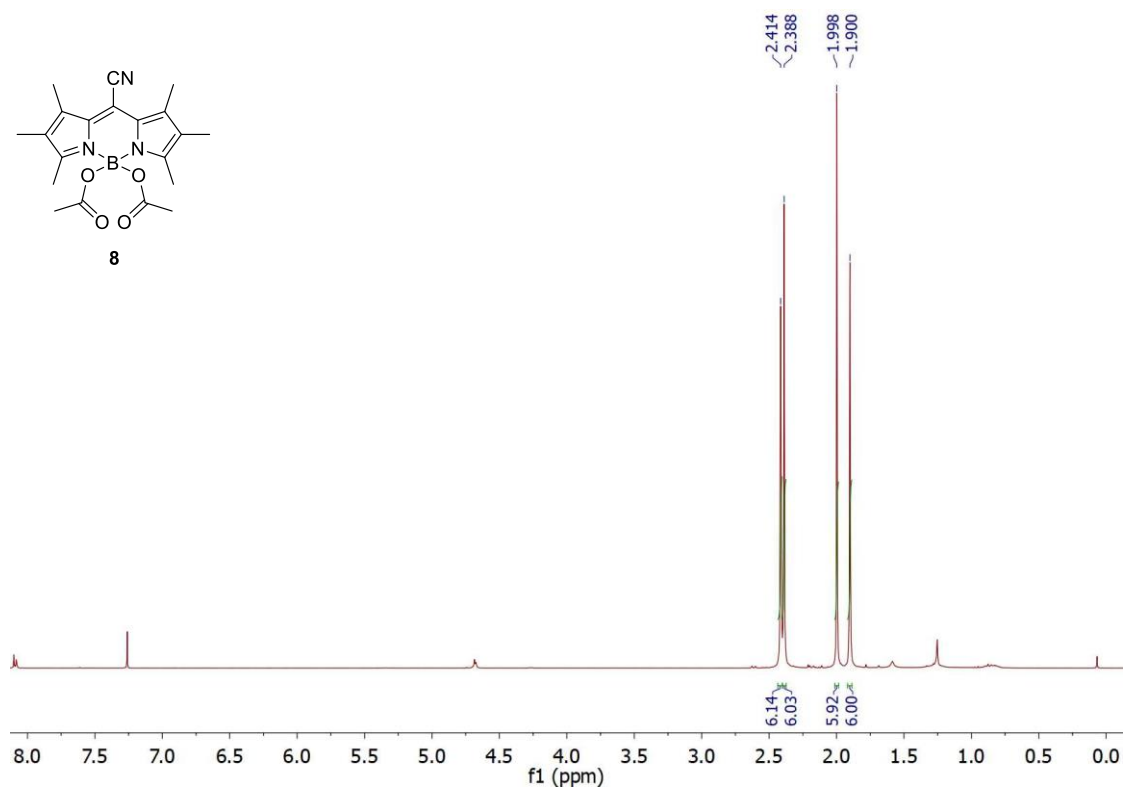
¹H NMR (300 MHz, CDCl₃)



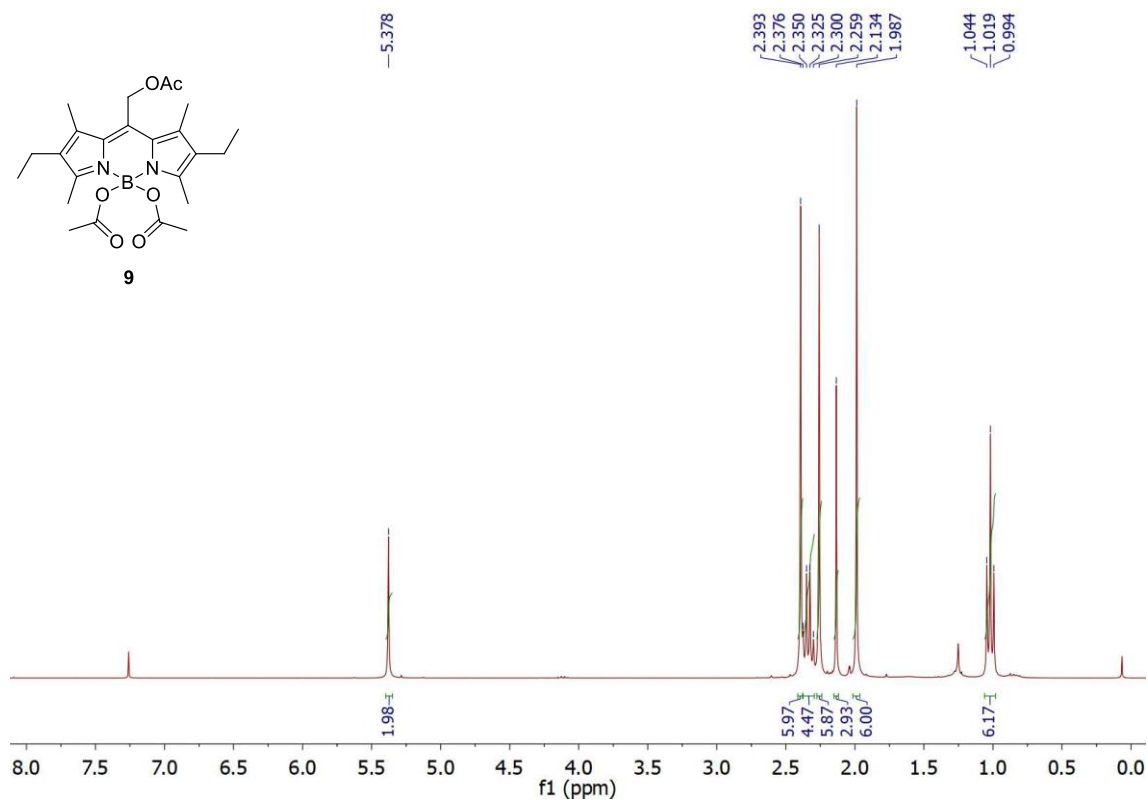
¹H NMR (300 MHz, CDCl₃)



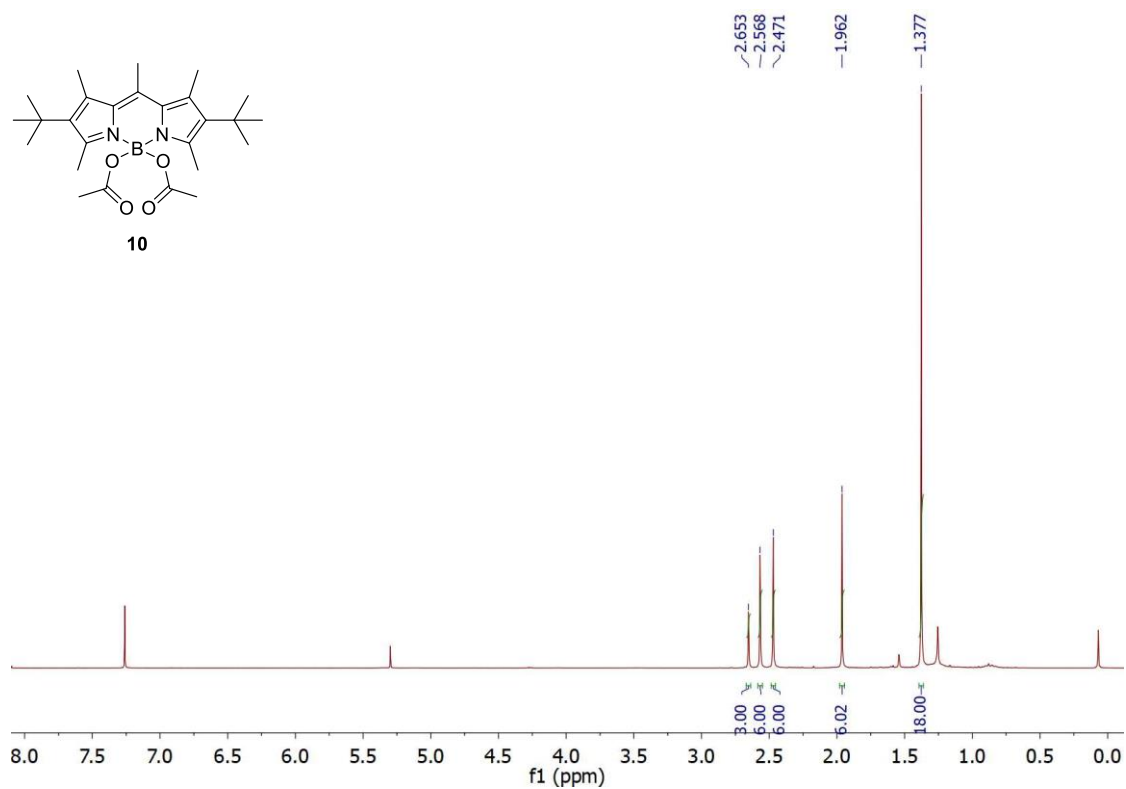
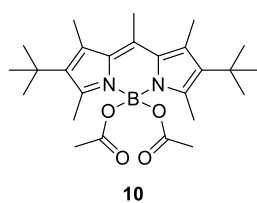
¹H NMR (300 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)

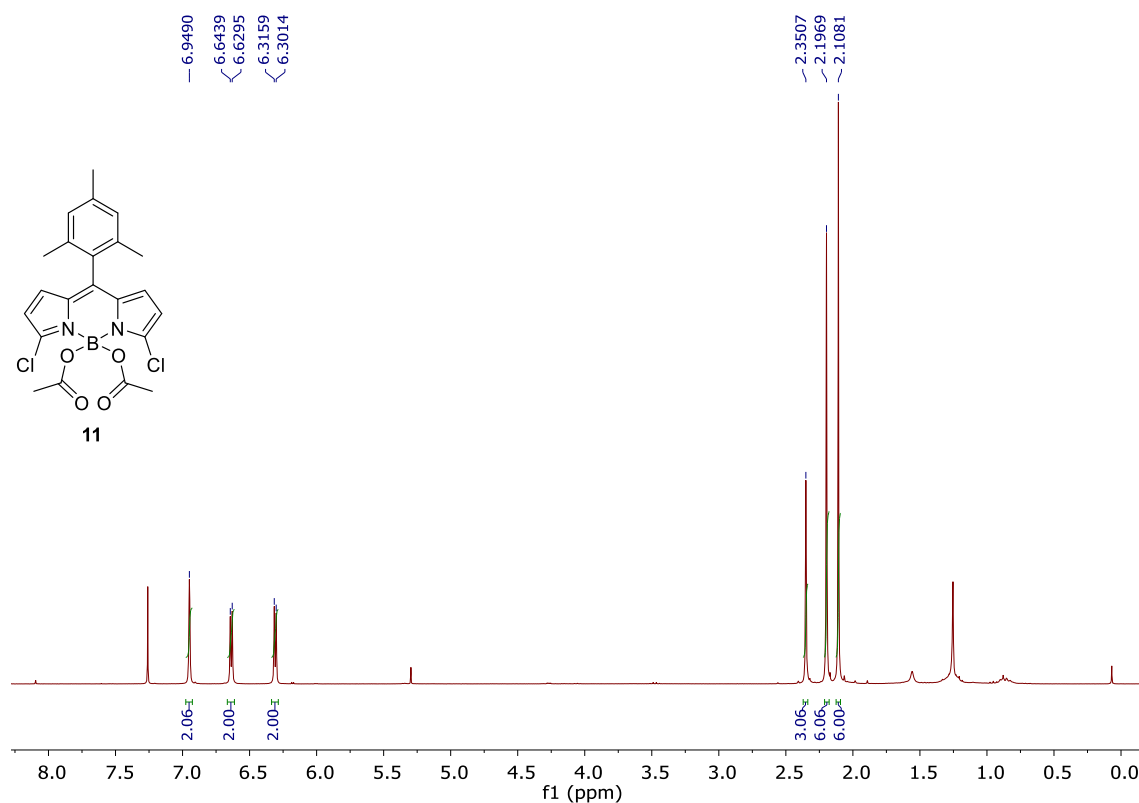


¹H NMR (300 MHz, CDCl₃)

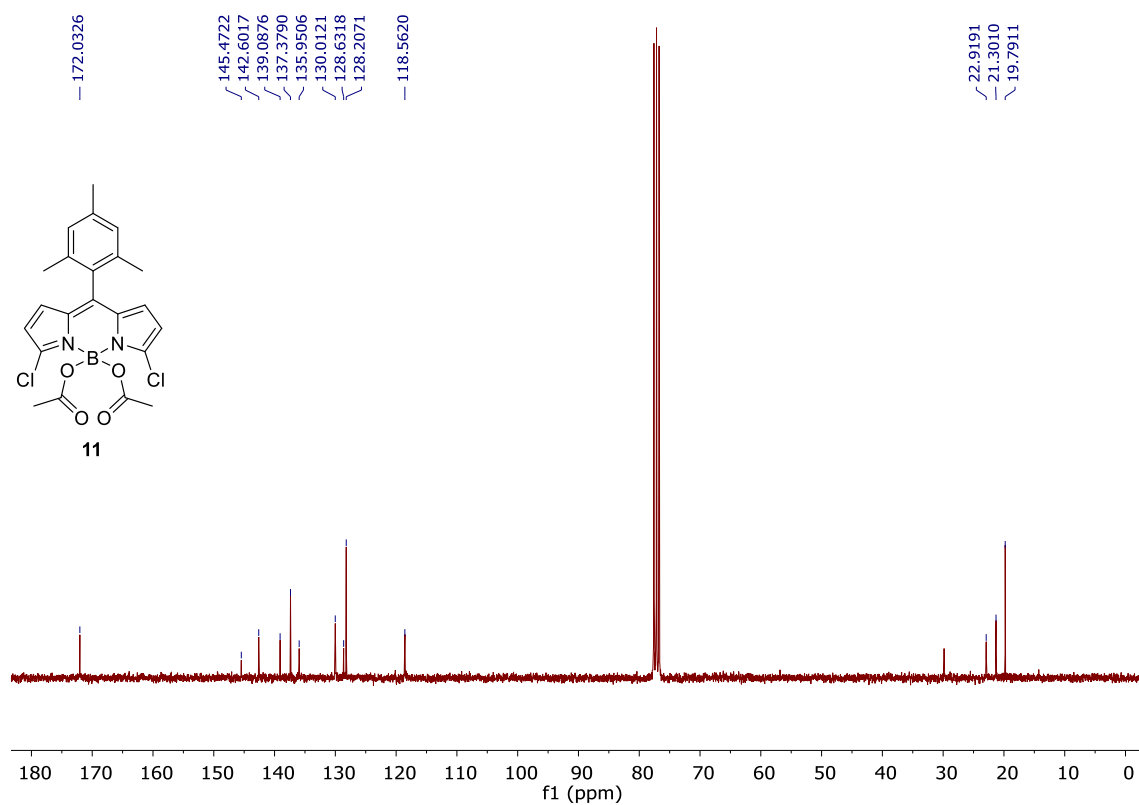


3. ^1H , $^{13}\text{C}\{^1\text{H}\}$ and ^{11}B NMR spectra of new compounds

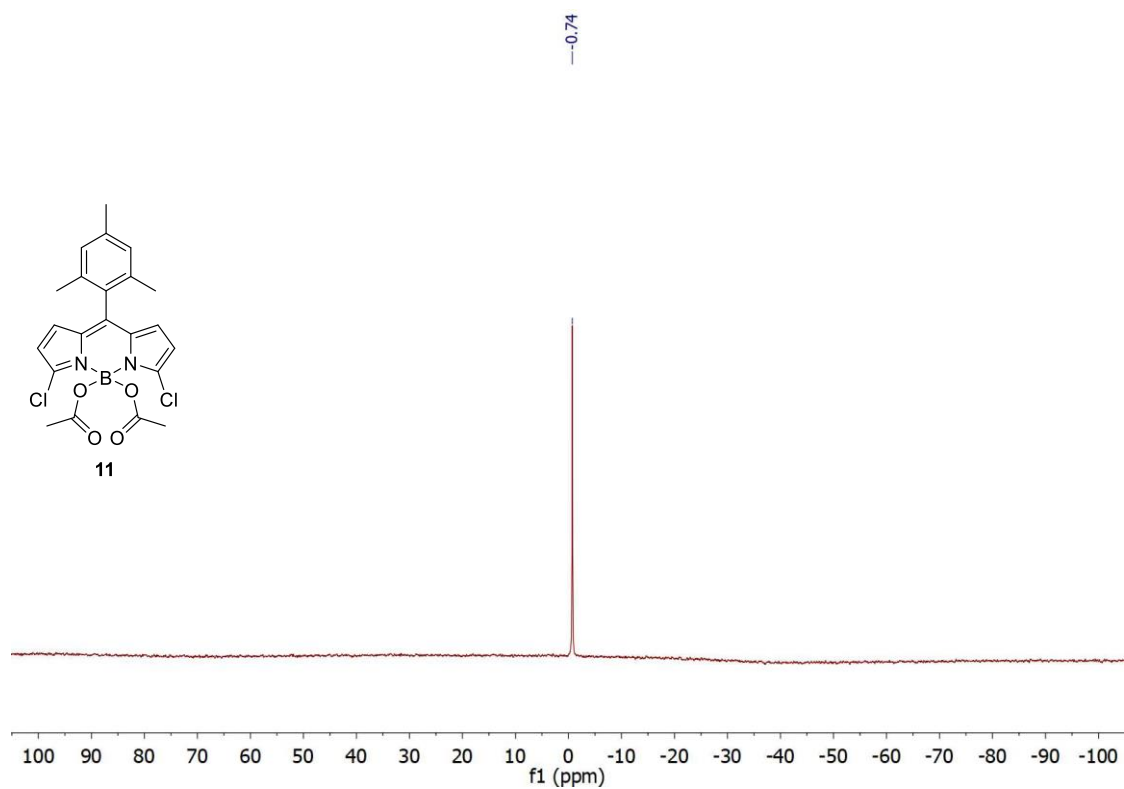
^1H NMR (300 MHz, CDCl_3)



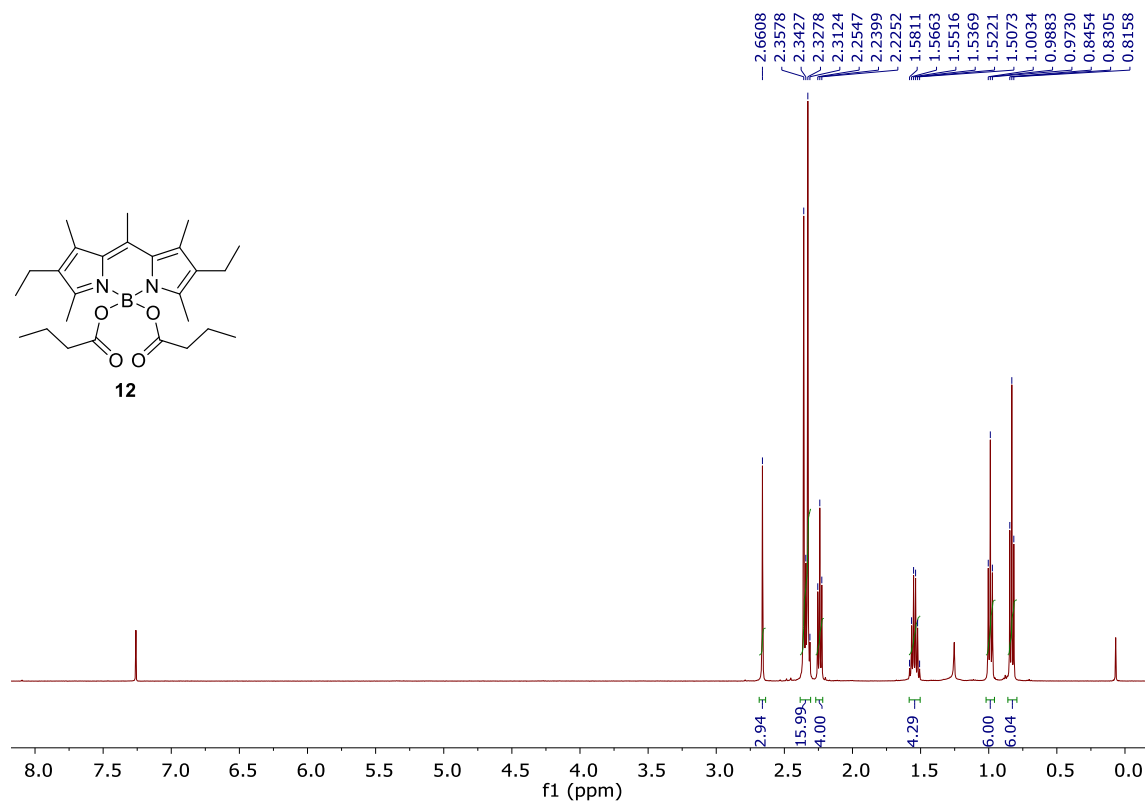
$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3)



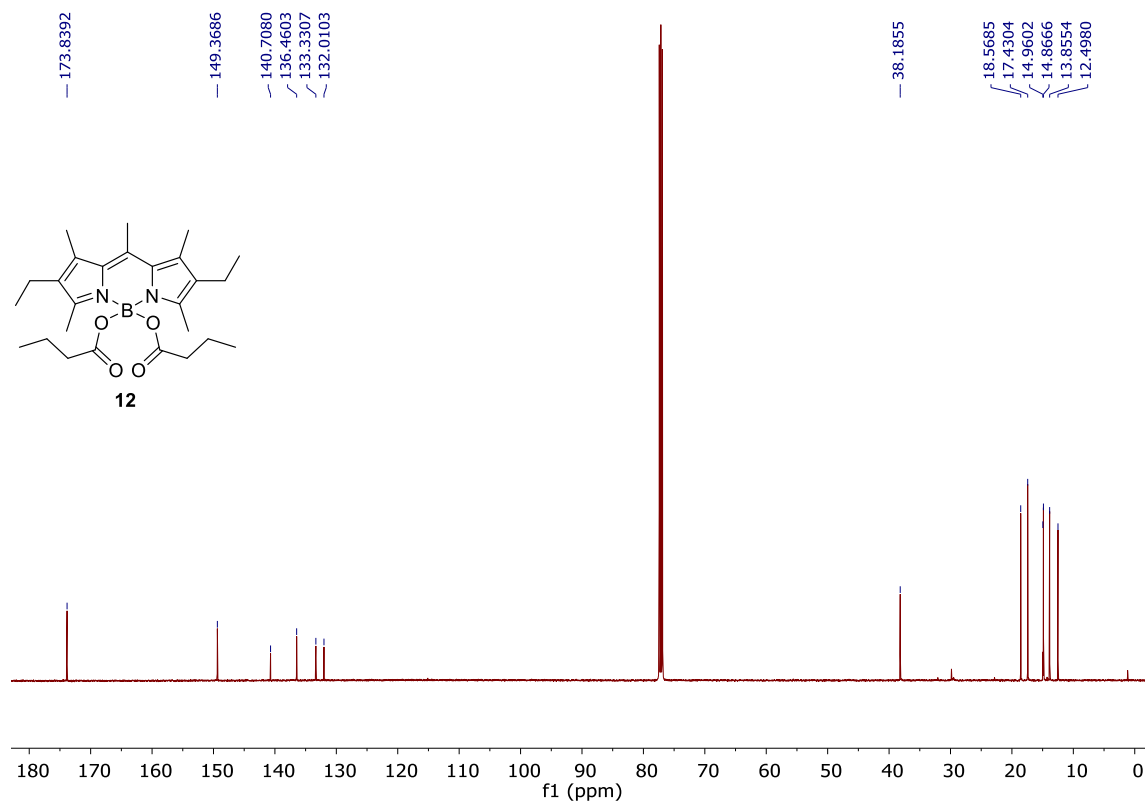
^{11}B NMR (160 MHz, CDCl_3)



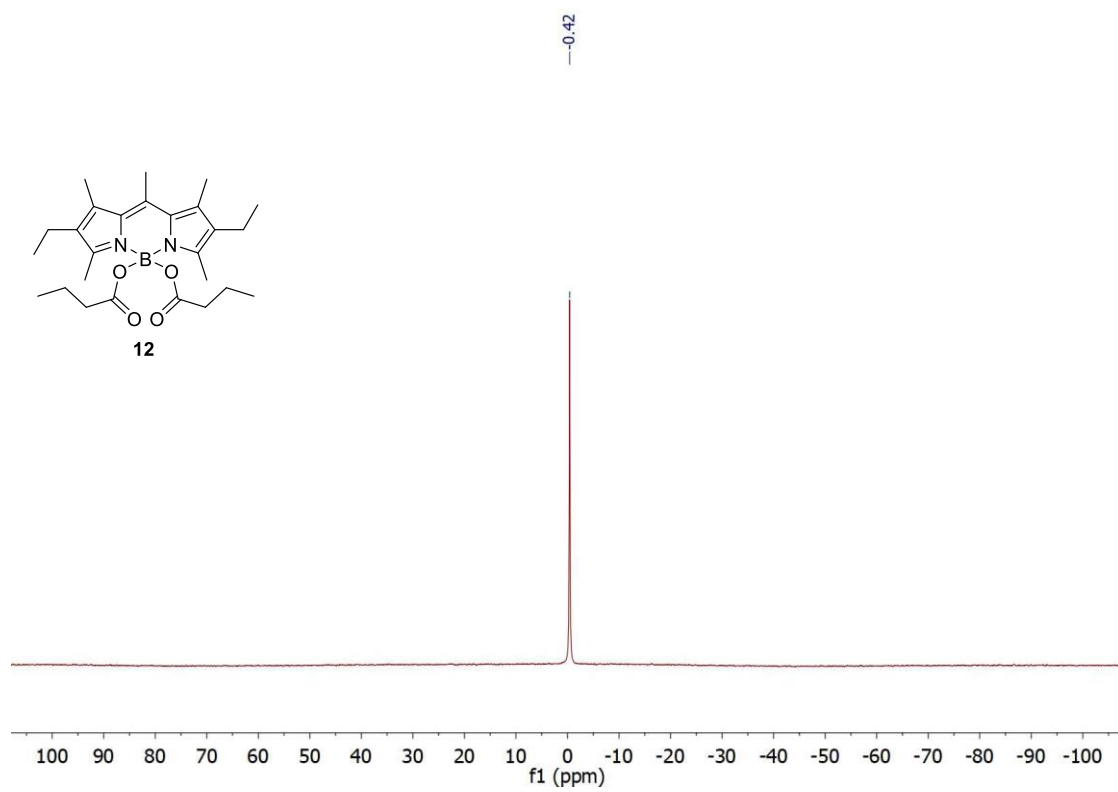
¹H NMR (500 MHz, CDCl₃)



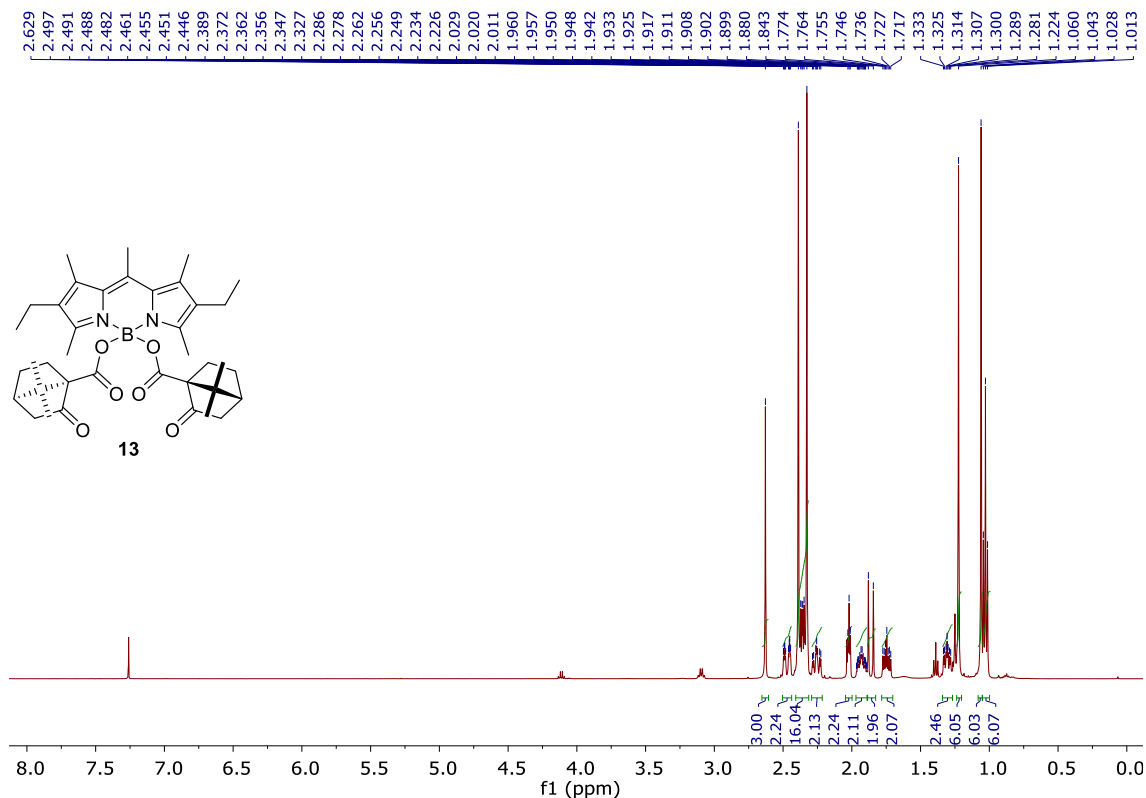
¹³C{¹H} NMR (75 MHz, CDCl₃)



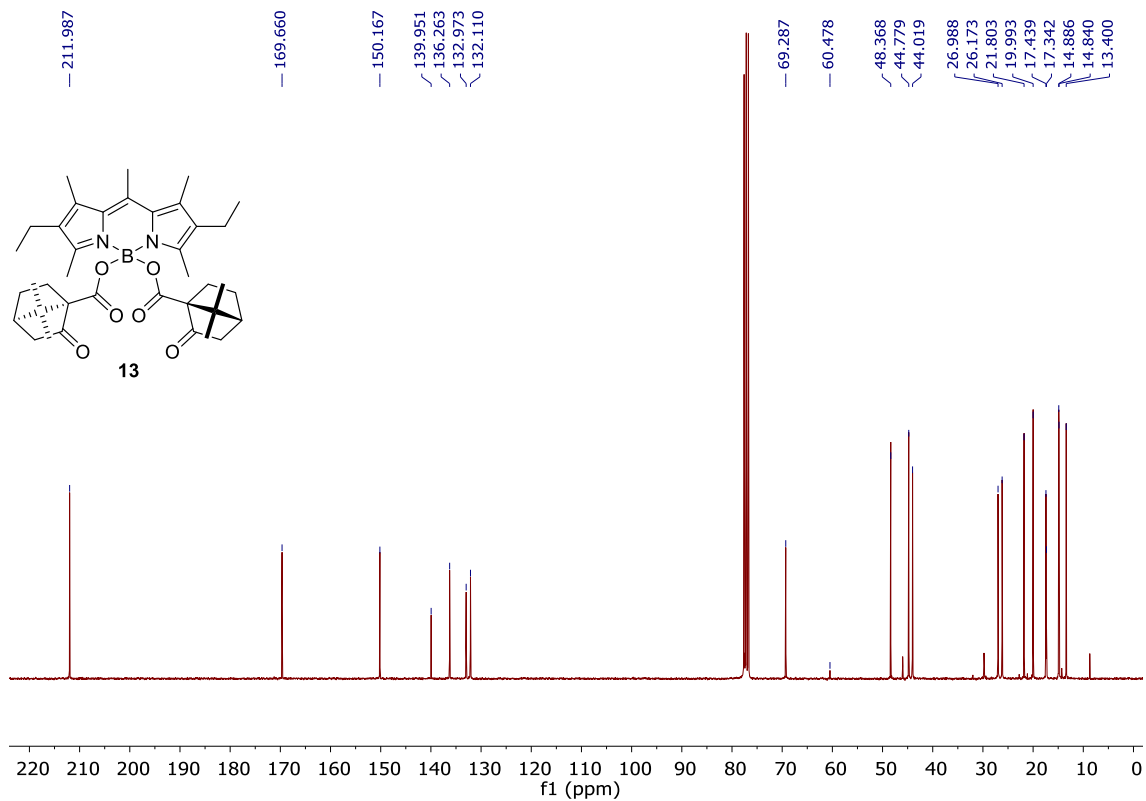
^{11}B NMR (160 MHz, CDCl_3)



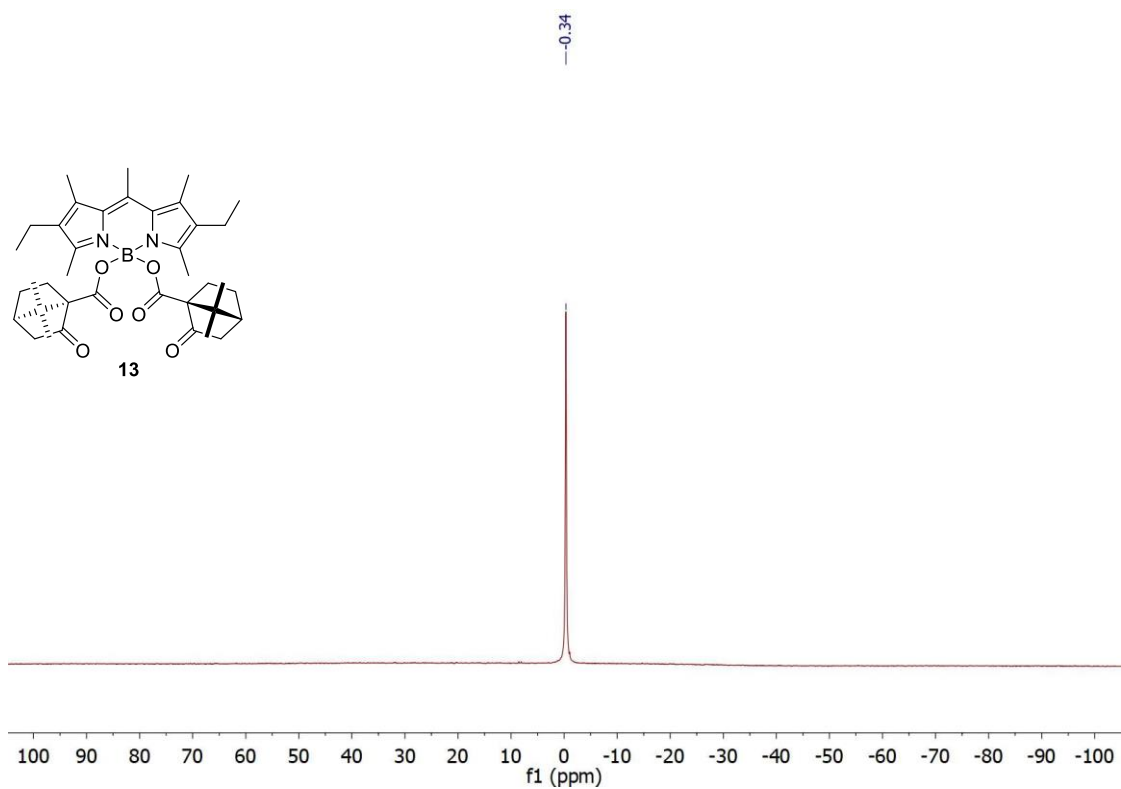
^1H NMR (500 MHz, CDCl_3)



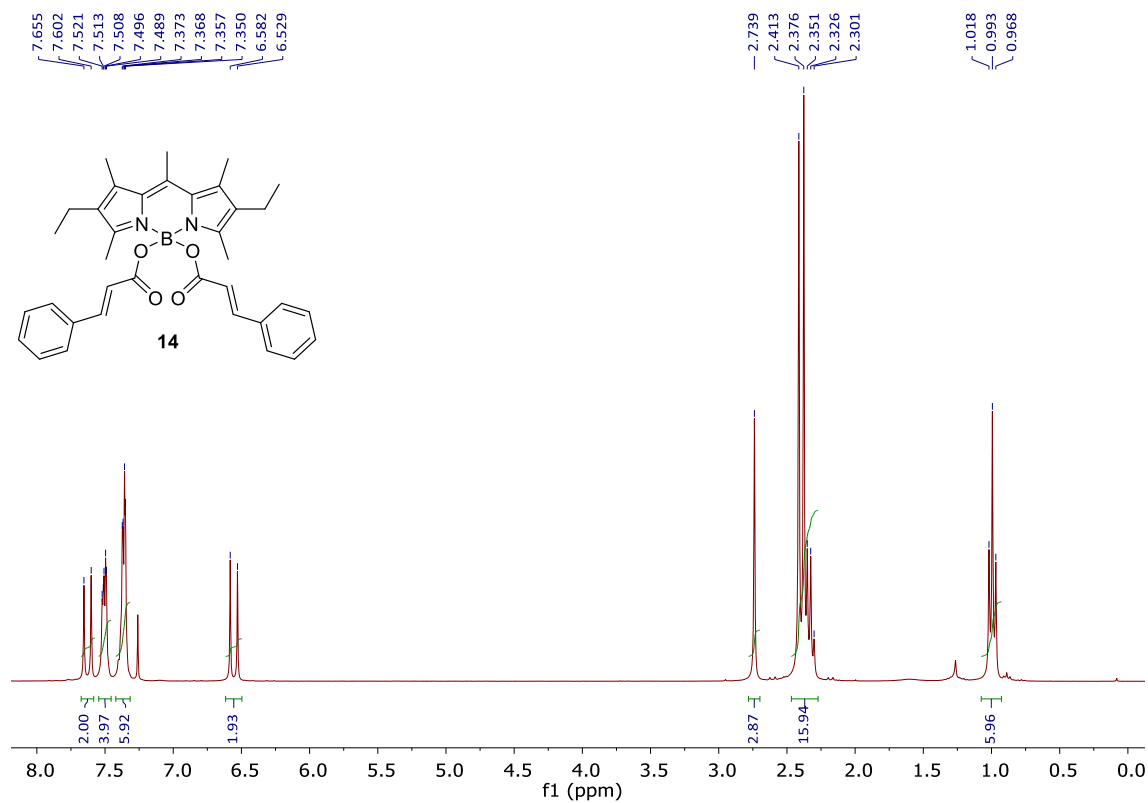
$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3)



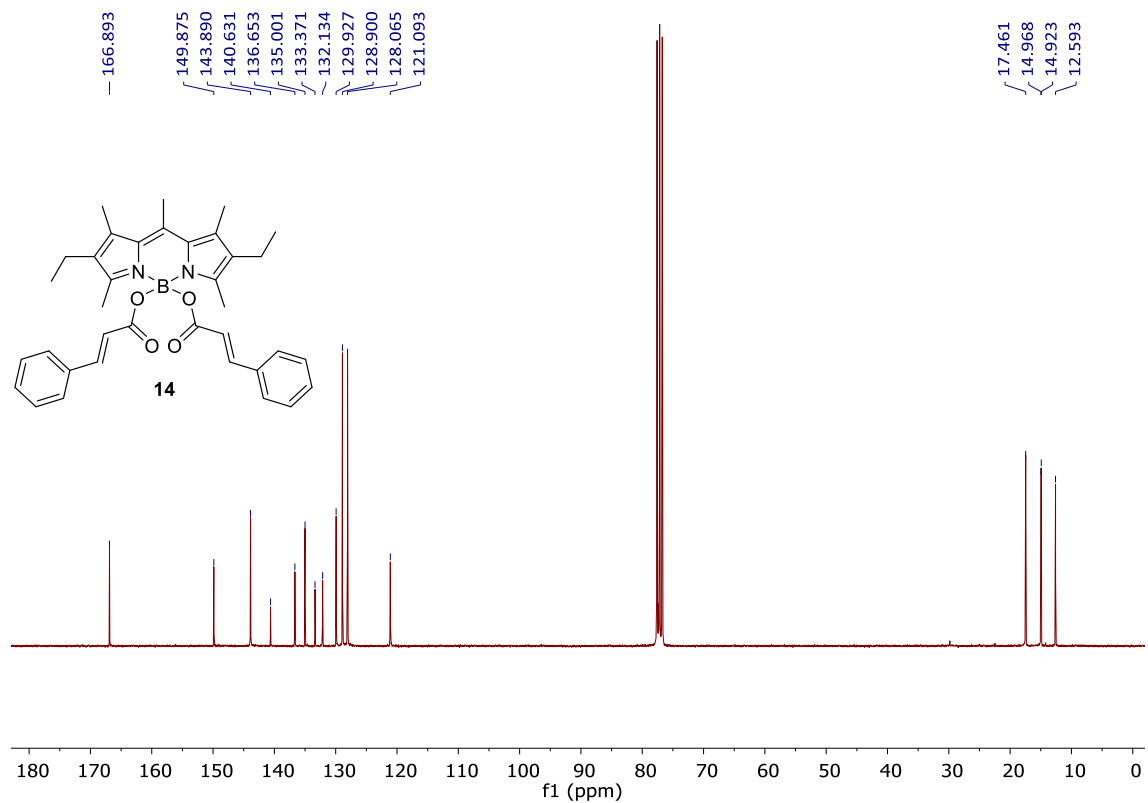
^{11}B NMR (160 MHz, CDCl_3)



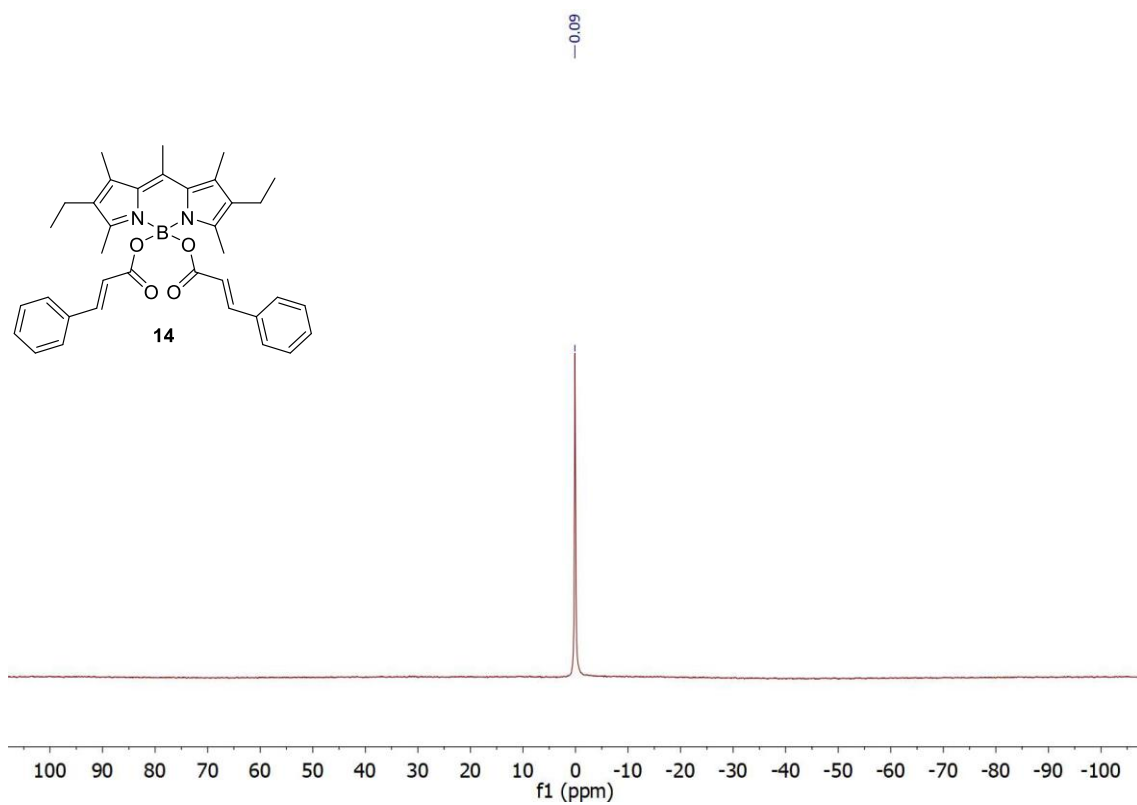
^1H NMR (300 MHz, CDCl_3)



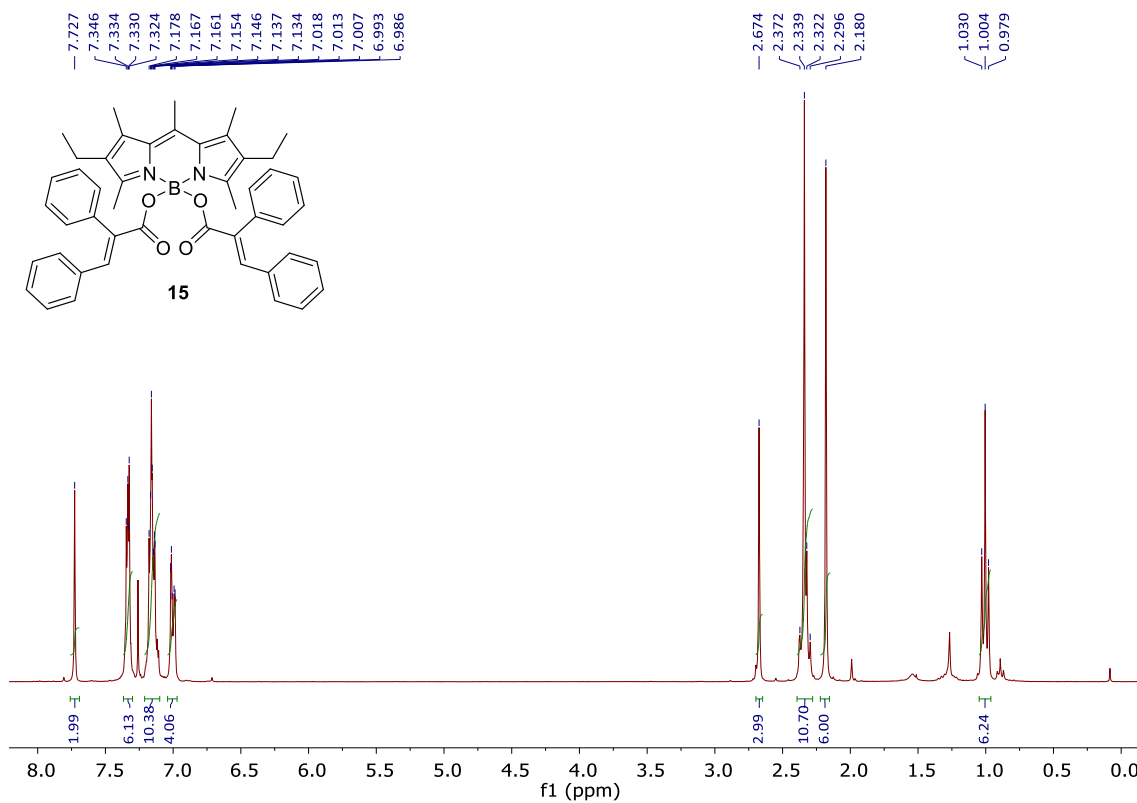
$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3)



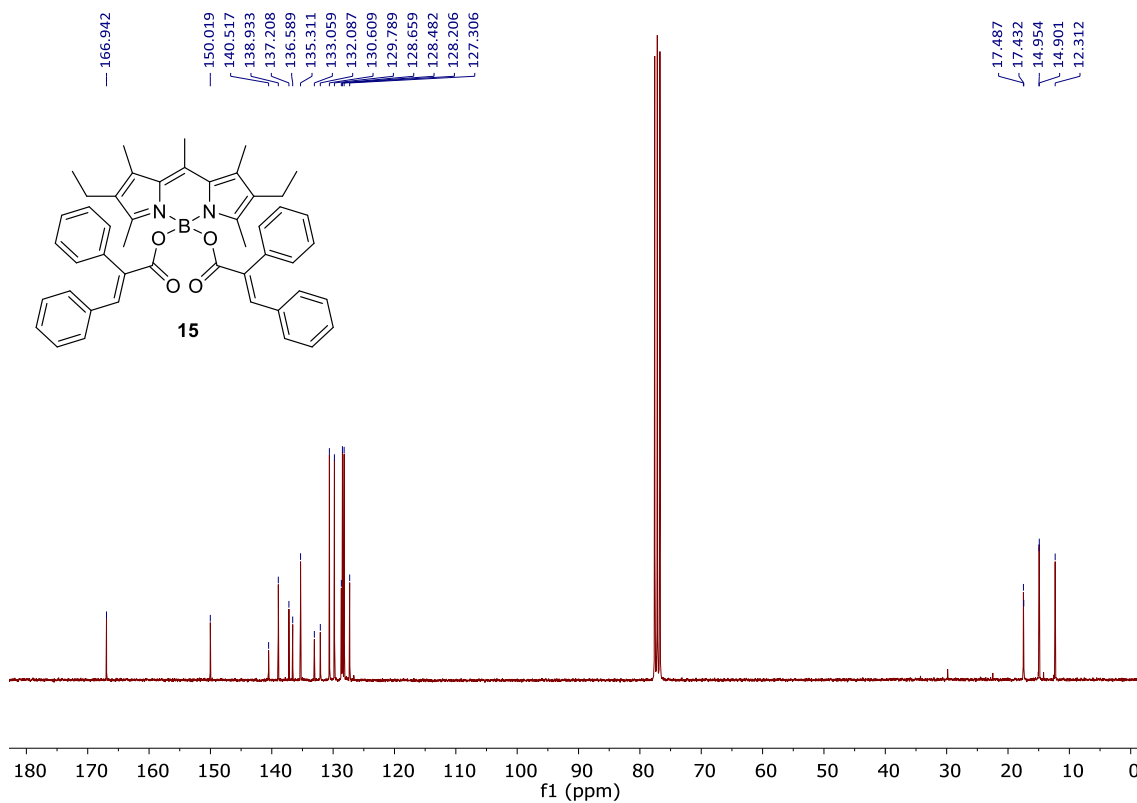
^{11}B NMR (160 MHz, CDCl_3)



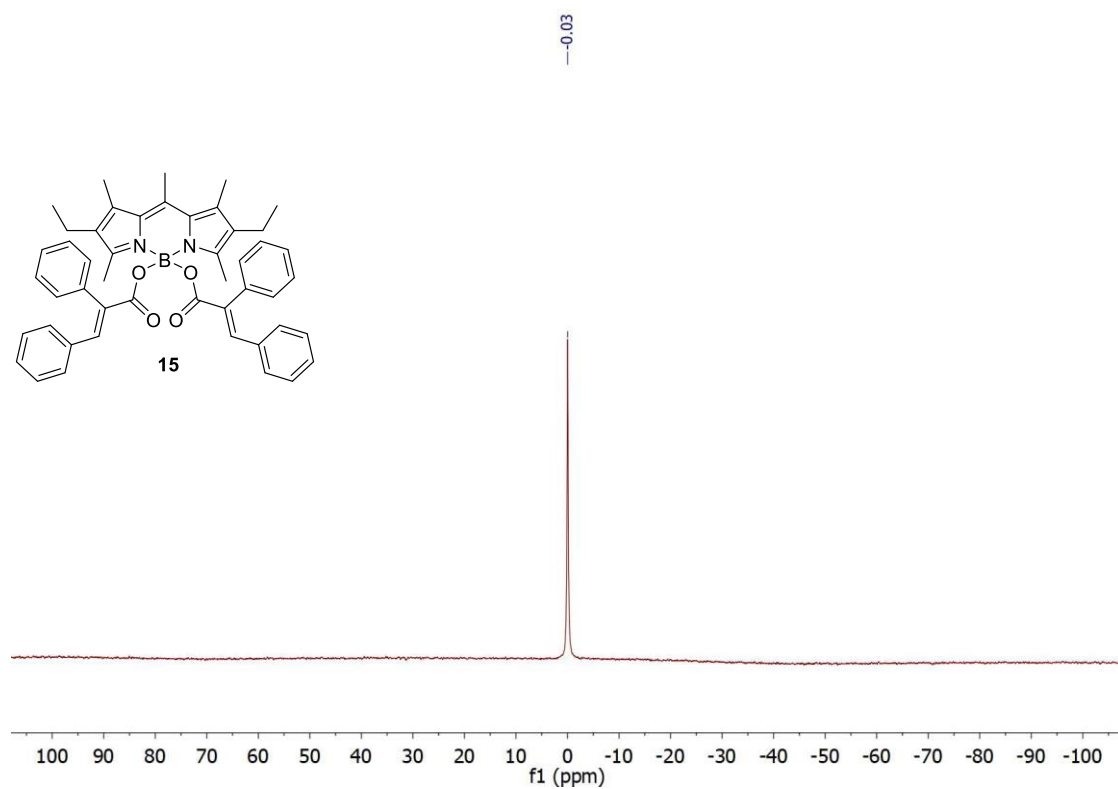
^1H NMR (300 MHz, CDCl_3)



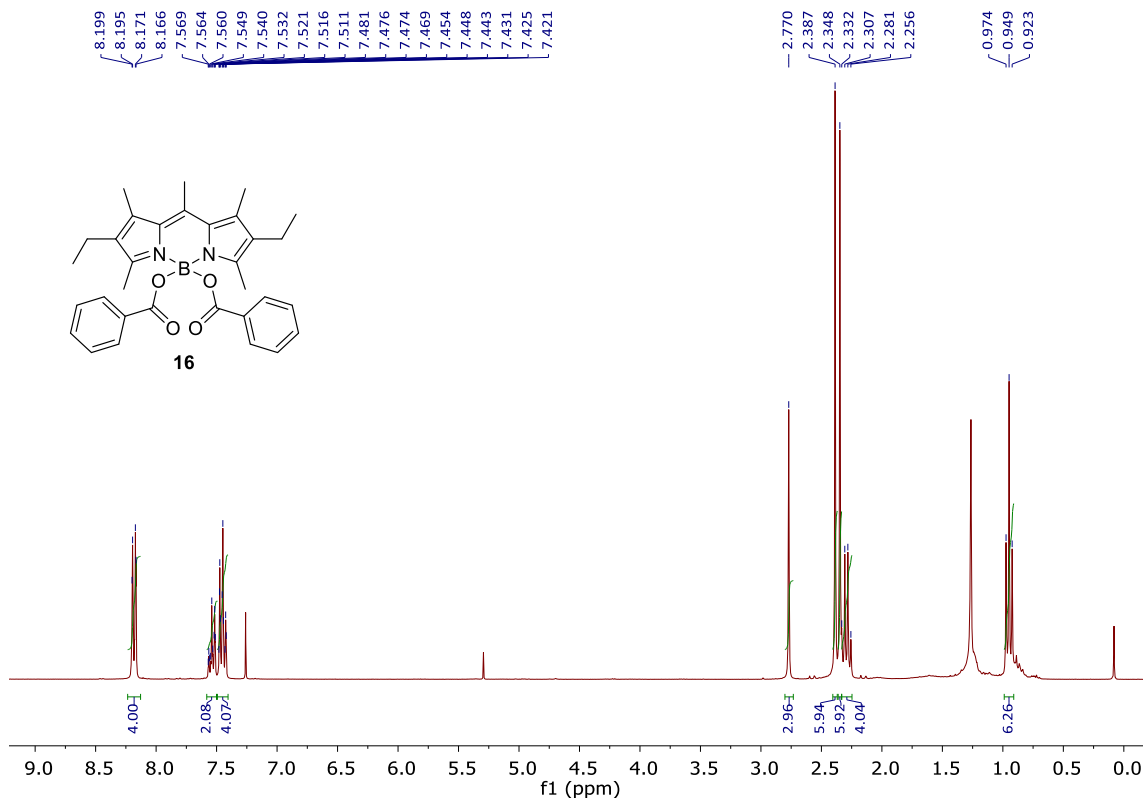
$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3)



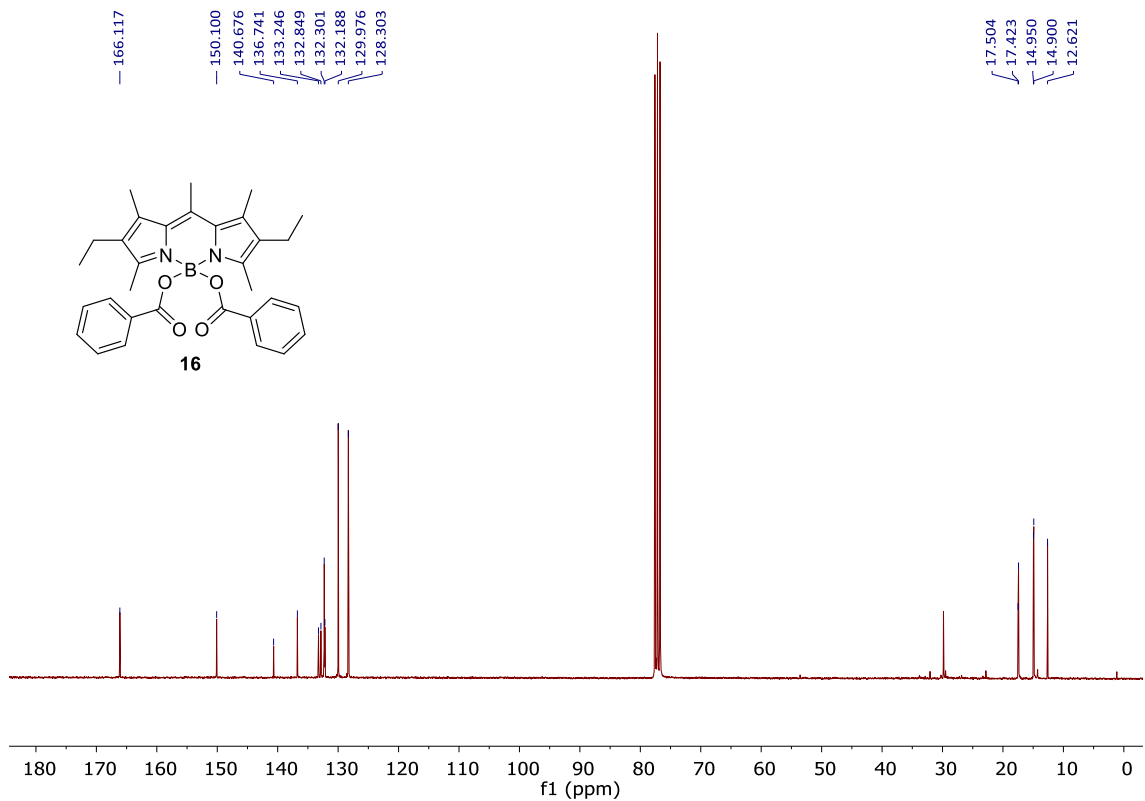
^{11}B NMR (160 MHz, CDCl_3)



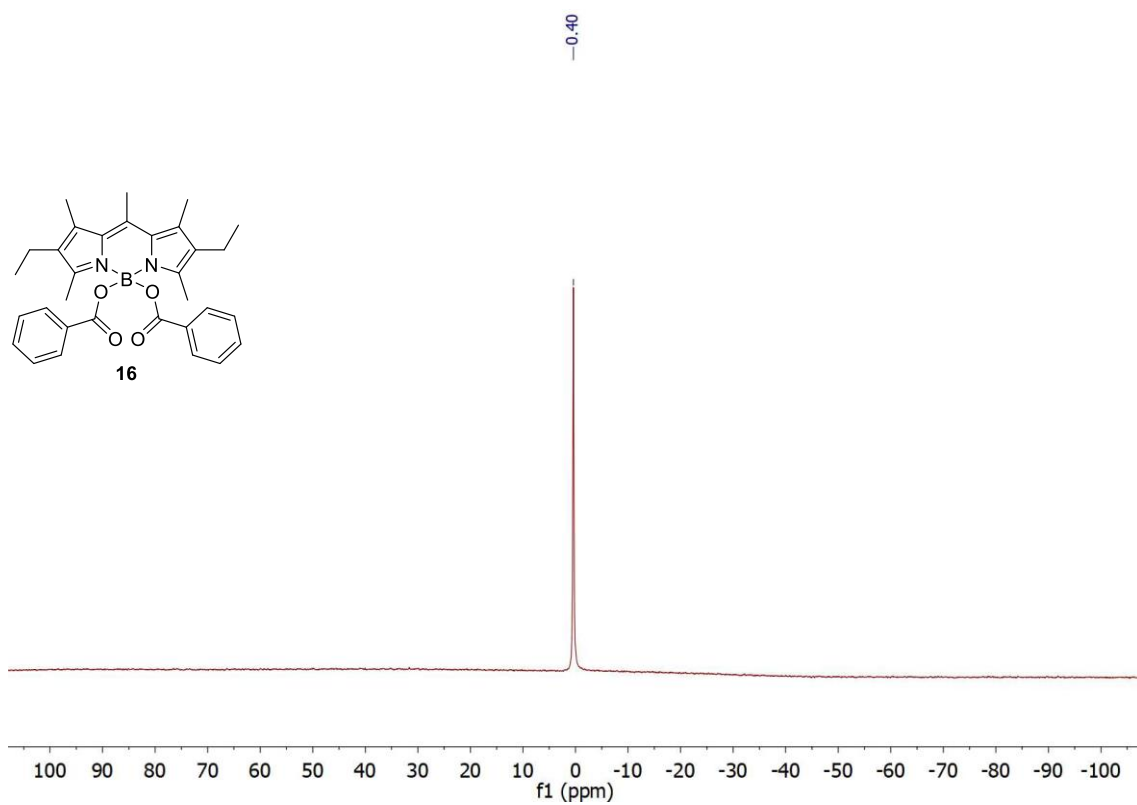
¹H NMR (300 MHz, CDCl₃)



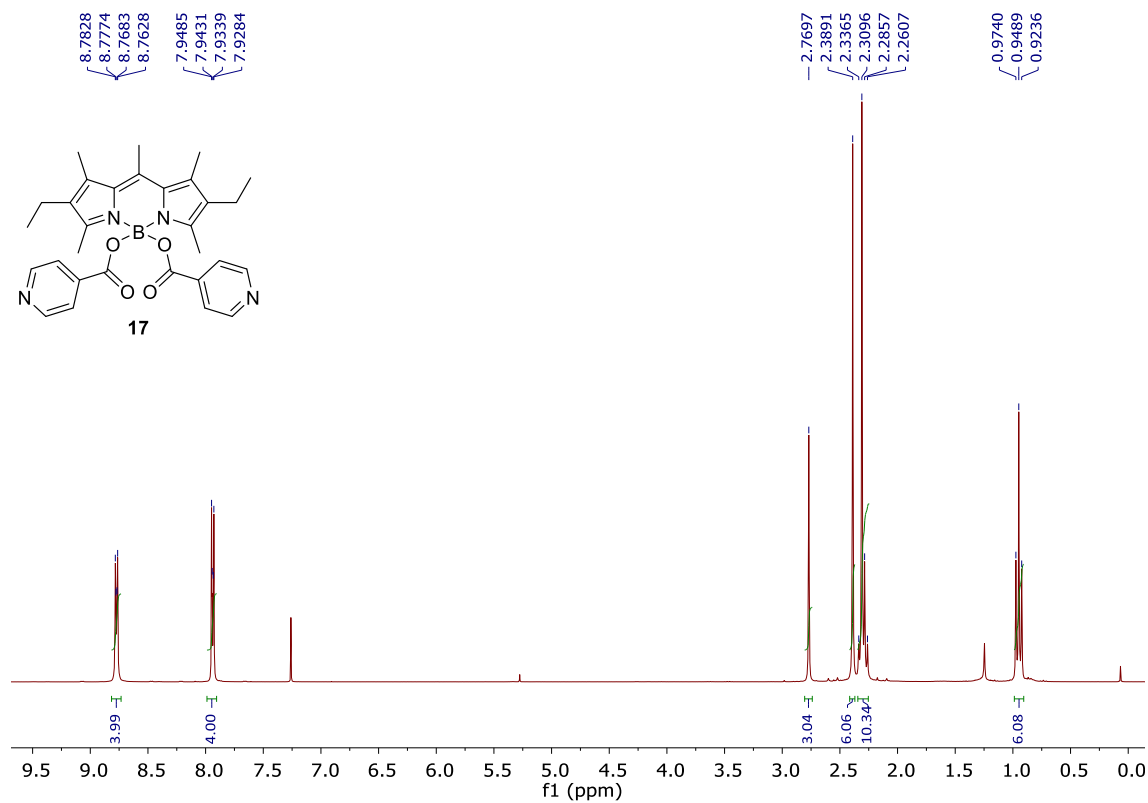
¹³C{¹H} NMR (75 MHz, CDCl₃)



^{11}B NMR (160 MHz, CDCl_3)

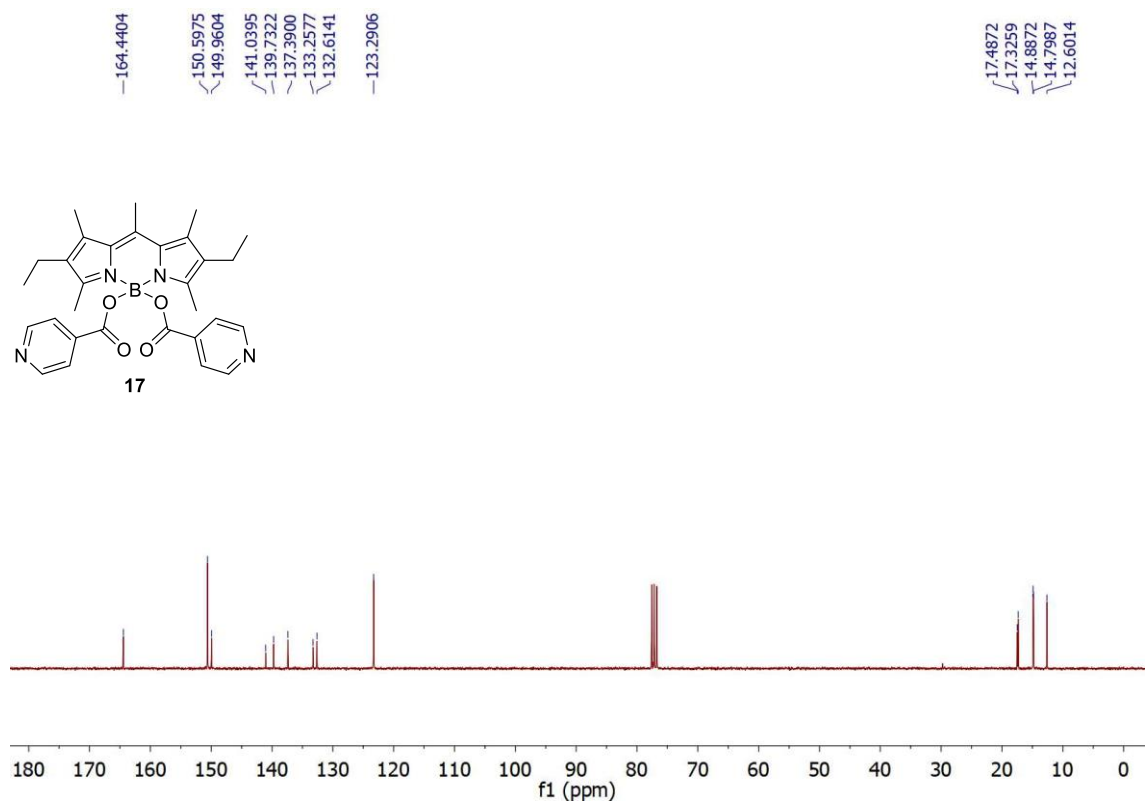


¹H NMR (300 MHz, CDCl₃)

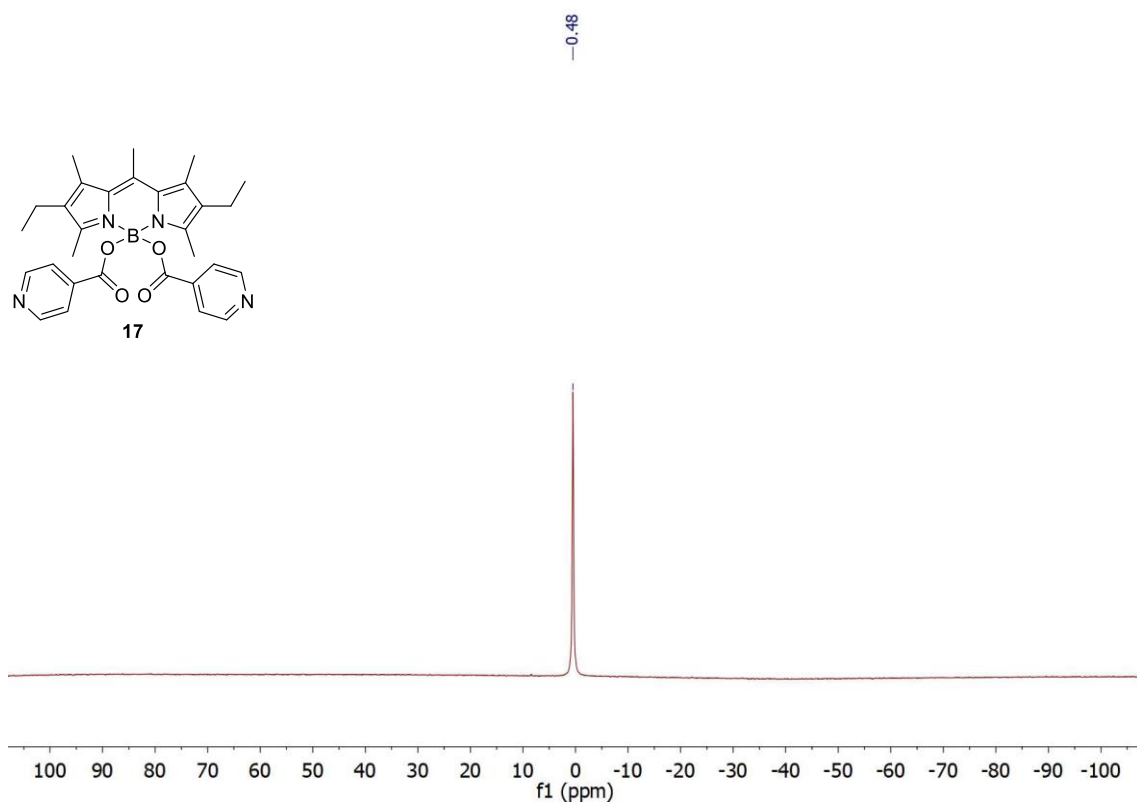


¹³C

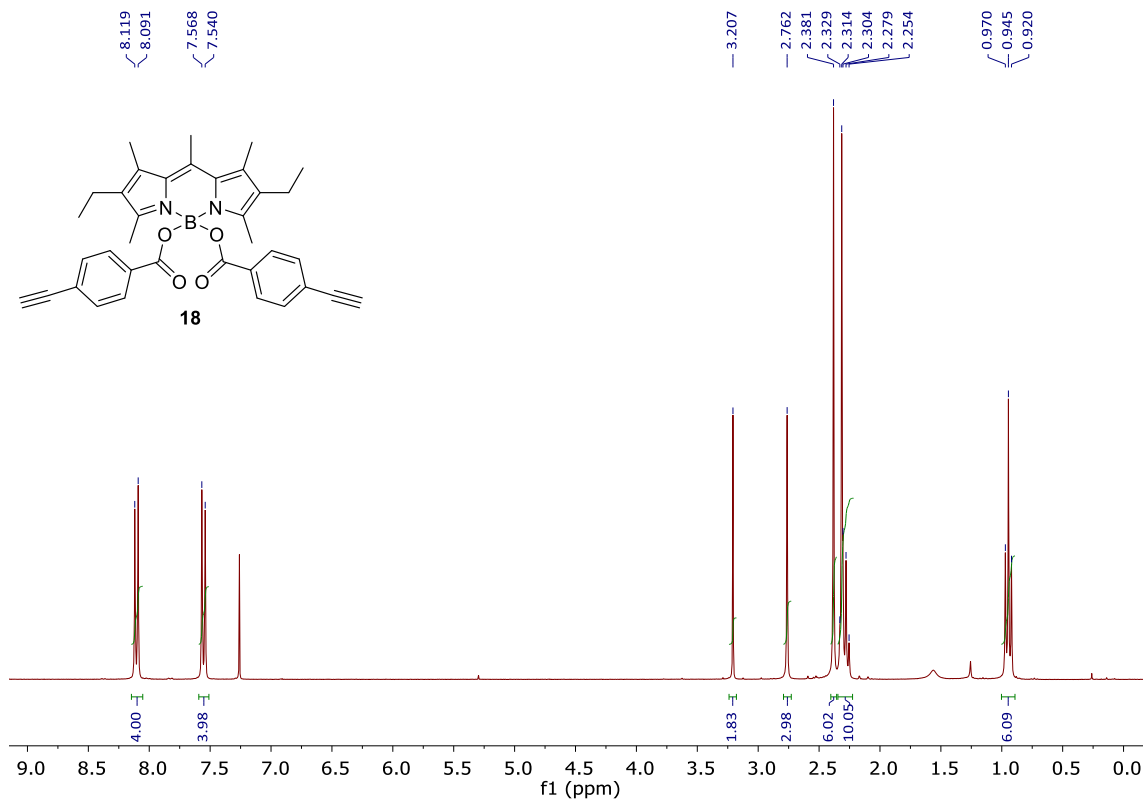
} NMR (75 MHz, CDCl₃)



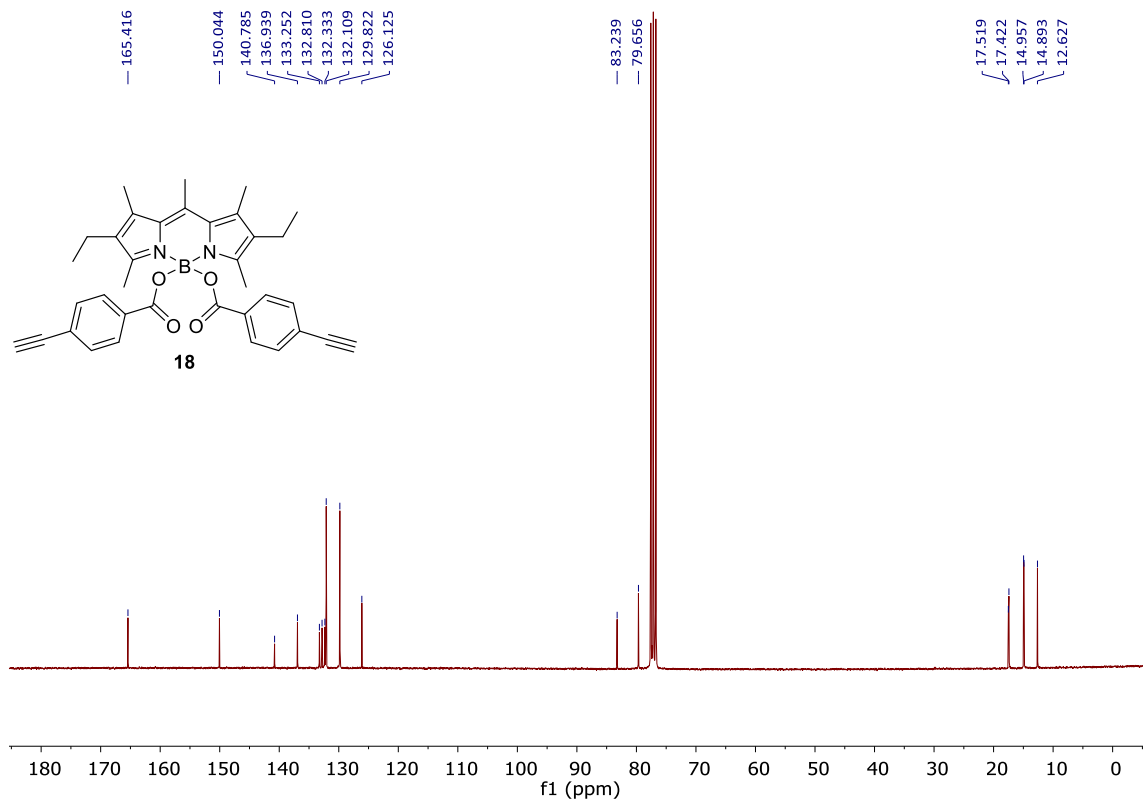
^{11}B NMR (160 MHz, CDCl_3)



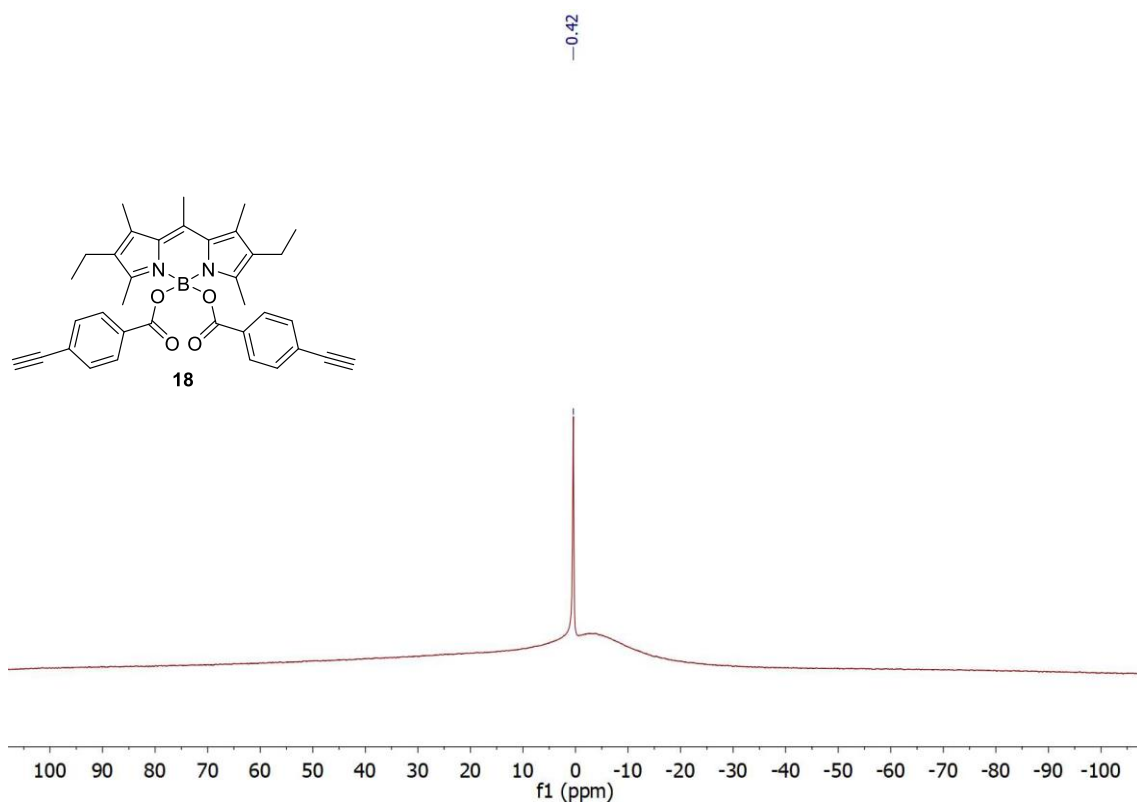
¹H NMR (300 MHz, CDCl₃)



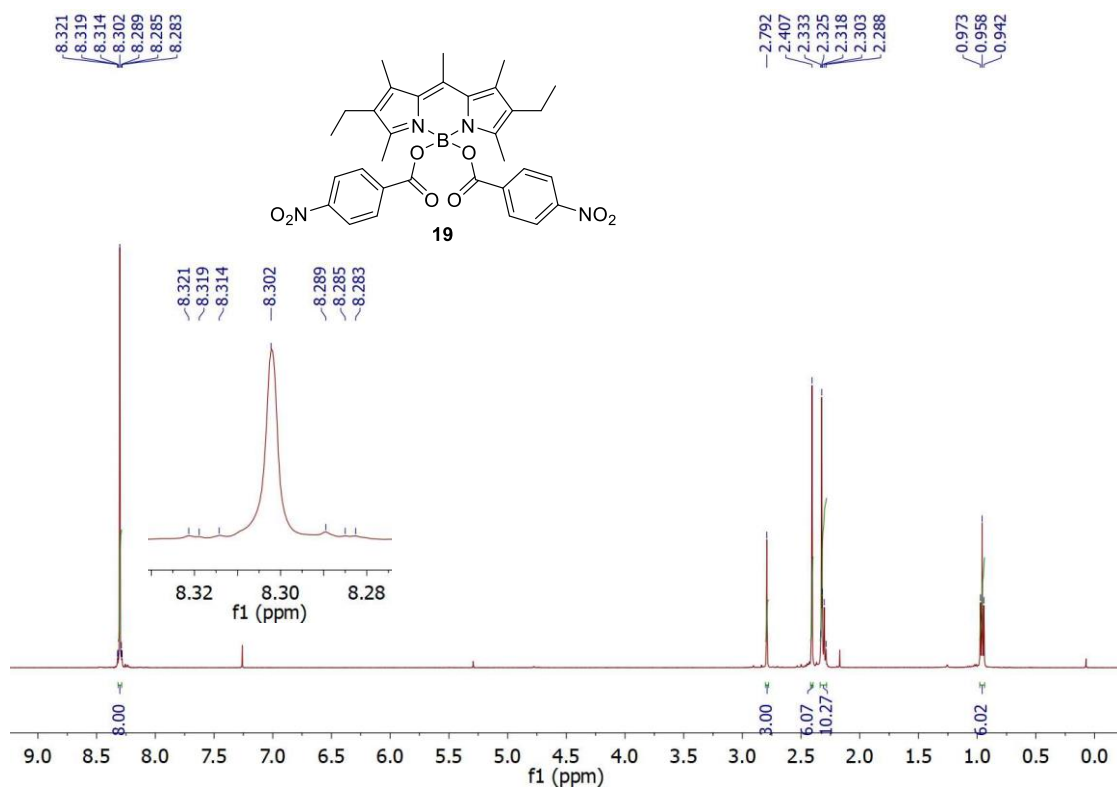
¹³C{¹H} NMR (75 MHz, CDCl₃)



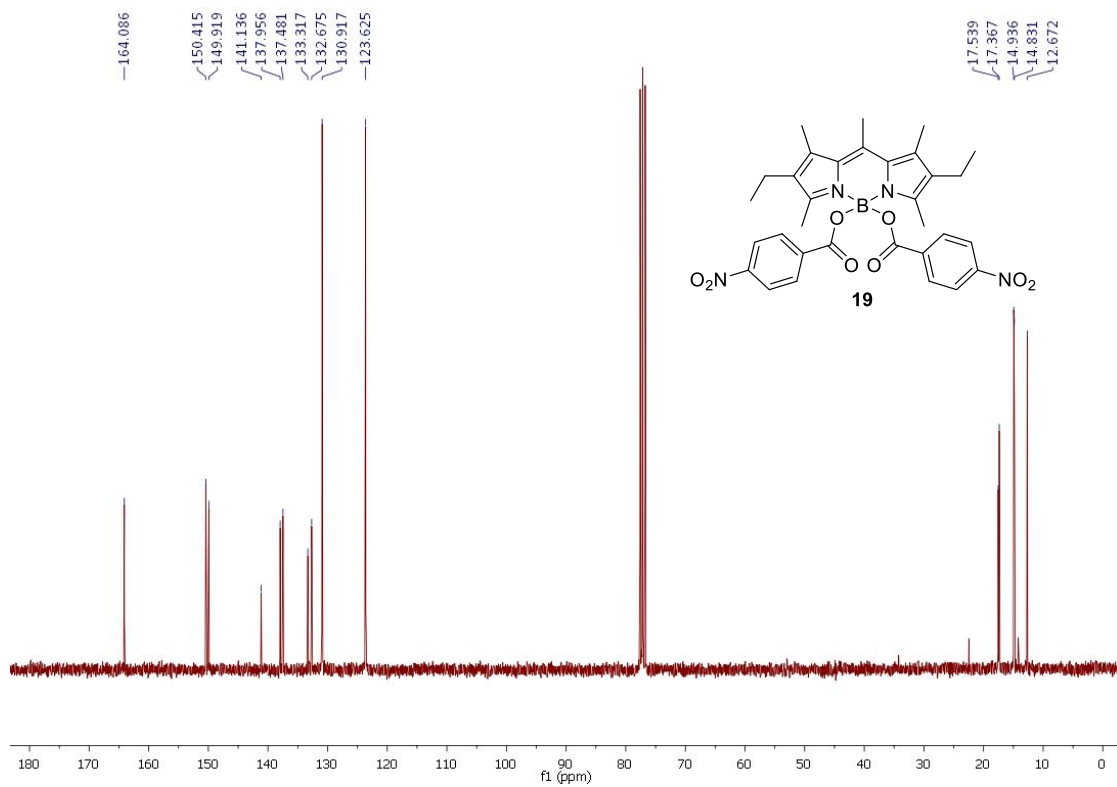
^{11}B NMR (160 MHz, CDCl_3)



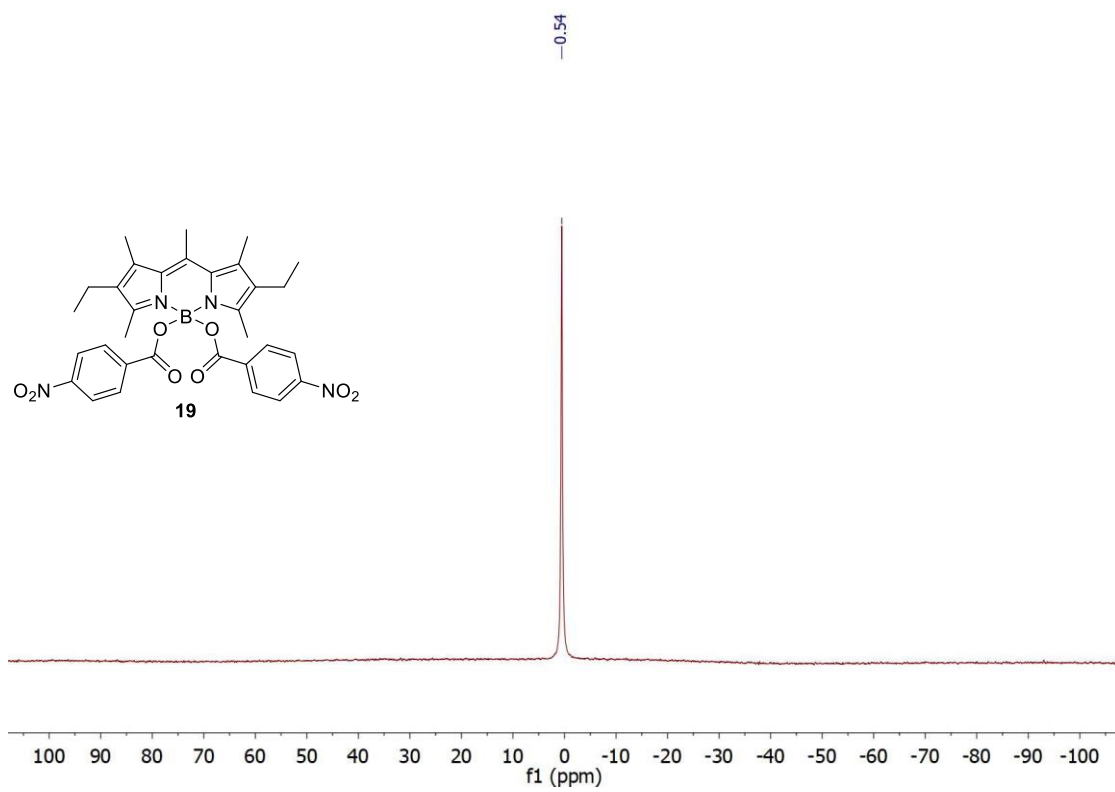
¹H NMR (500 MHz, CDCl₃)



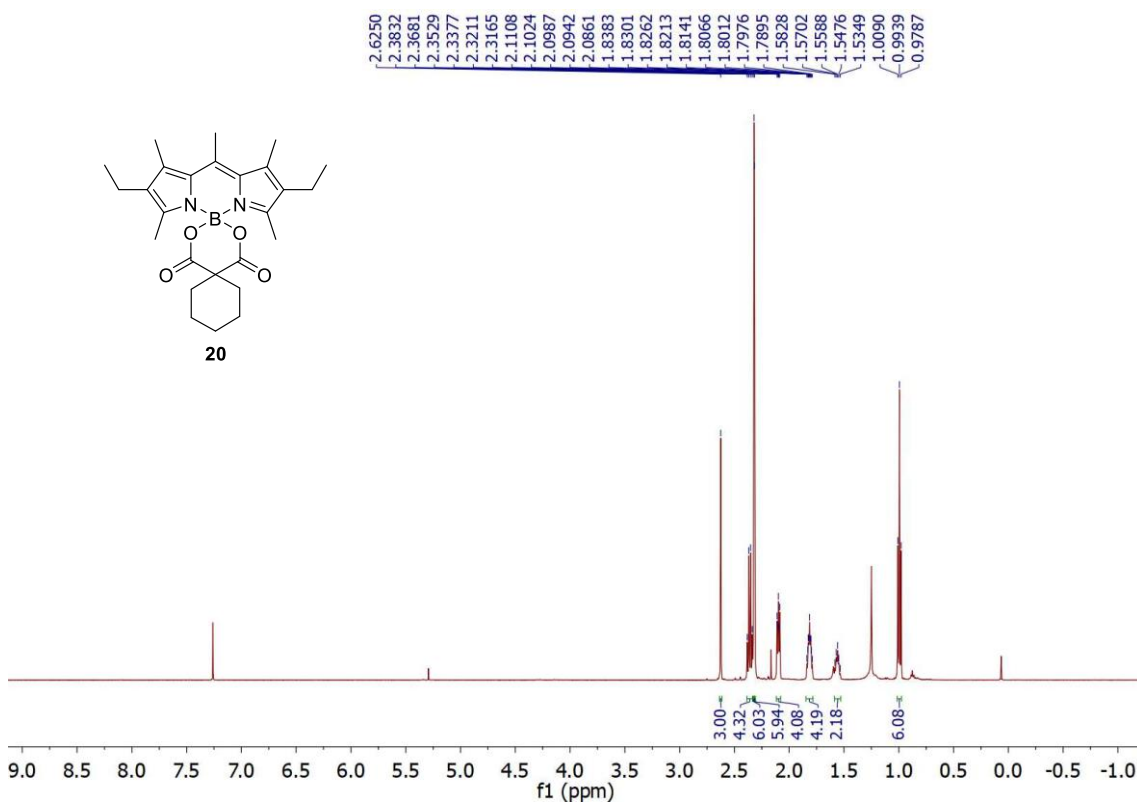
¹³C{¹H} NMR (75 MHz, CDCl₃)



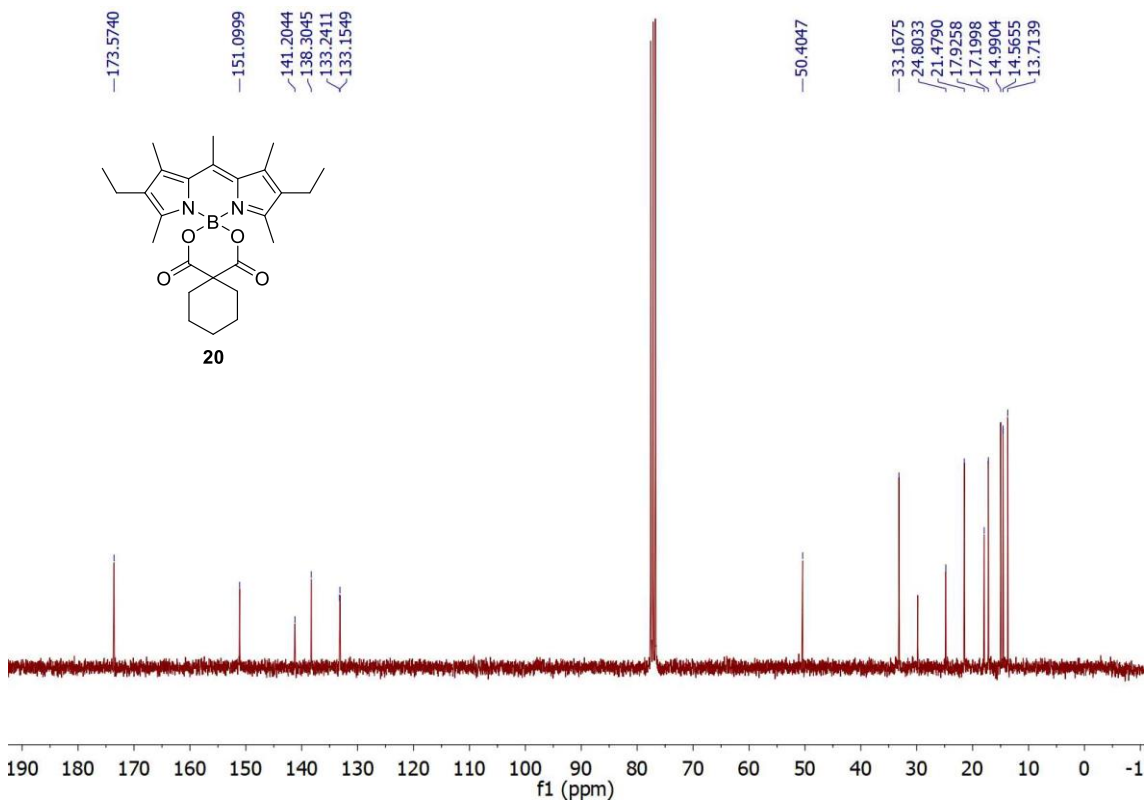
^{11}B NMR (160 MHz, CDCl_3)



¹H NMR (300 MHz, CDCl₃)

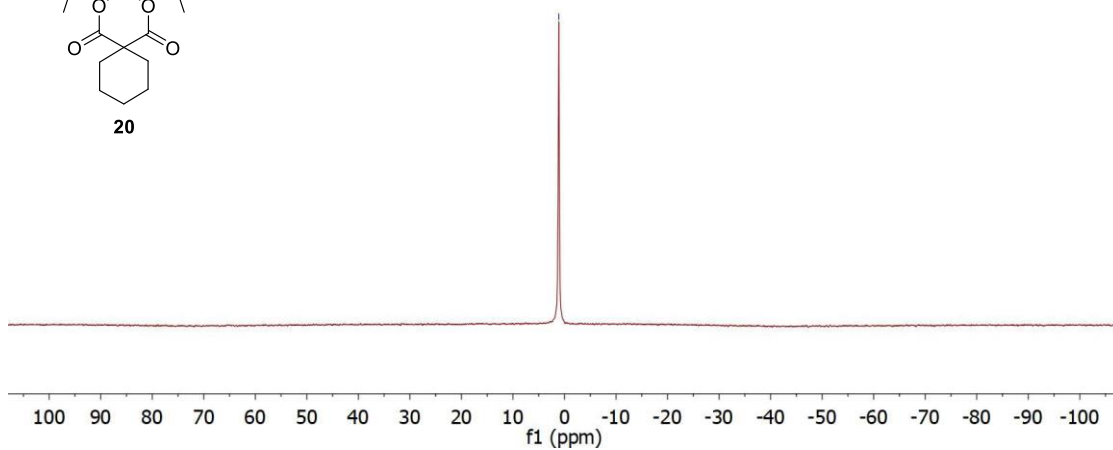
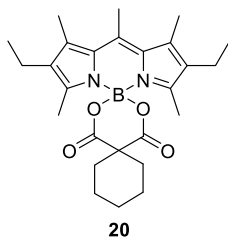


¹³C{¹H} NMR (75 MHz, CDCl₃)

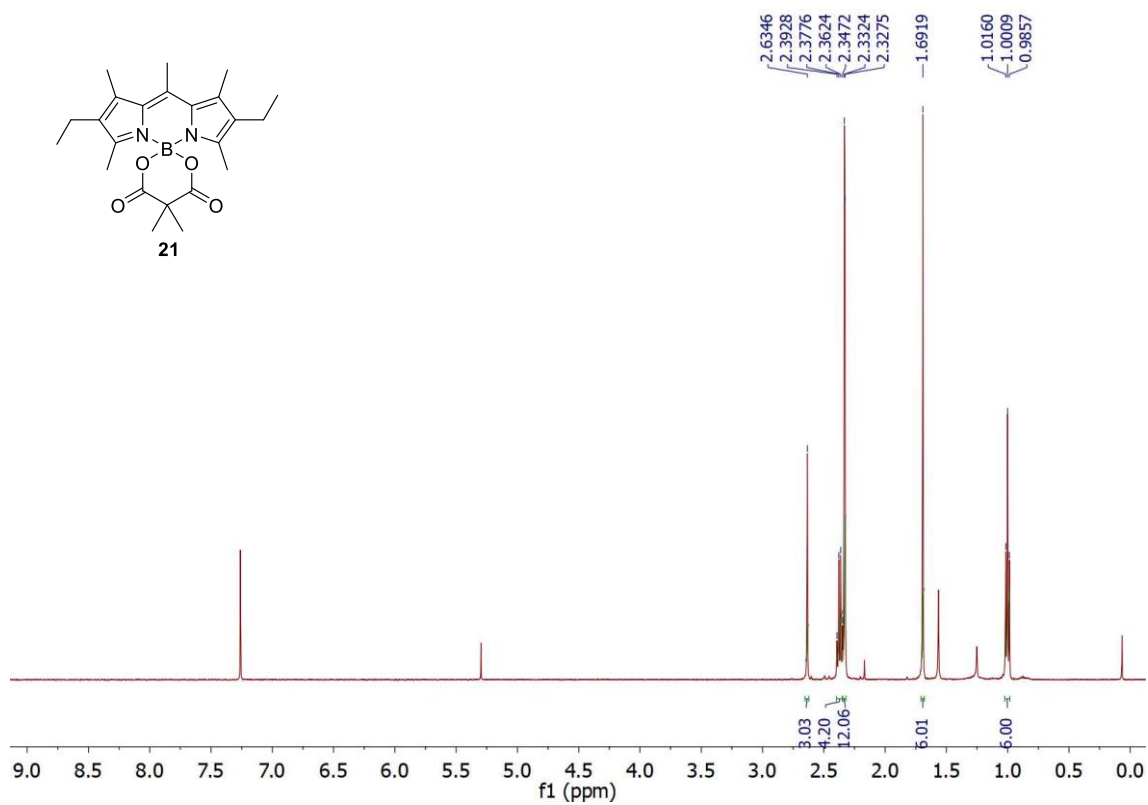


^{11}B NMR (160 MHz, CDCl_3)

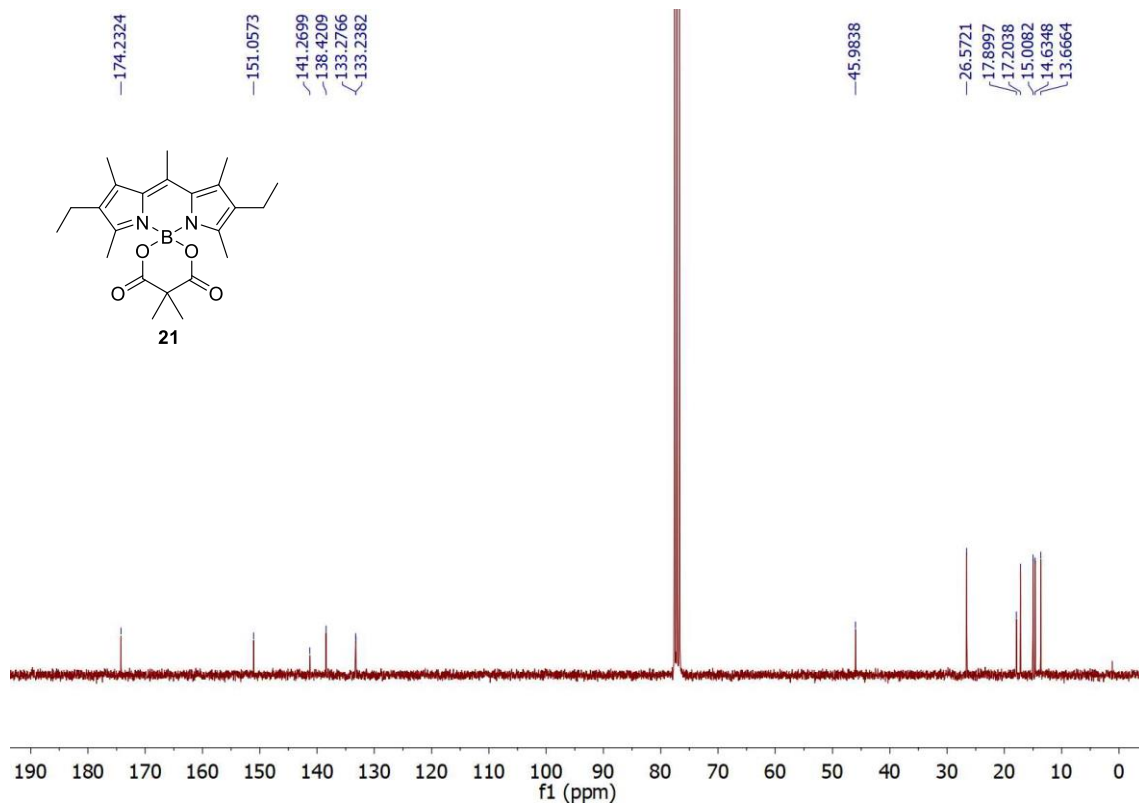
-1.11



^1H NMR (300 MHz, CDCl_3)

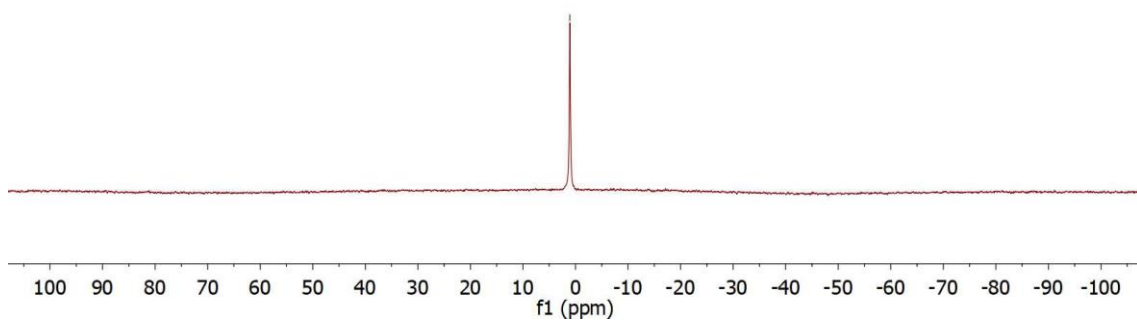
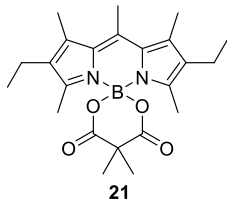


$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3)



^{11}B NMR (160 MHz, CDCl_3)

-1.07



4. Cartesian coordinates and computed energies. Tables S2-S3

Table S2. Cartesian coordinates and total computed energies (in hartrees) in the ground state (B3LYP/6-311g*) and first singlet excited state (TD-B3LYP/6-311g*) for **12**, **20** and **21**.

	S_0 (ground state)				S_1 (excited state)			
12	N	1.28894100	-0.09287800	0.38226100	N	1.22284900	0.21921700	-0.46828100
	C	1.42241300	0.95773700	1.29092900	C	1.50919200	-0.93464400	-1.23430200
	C	0.30250000	1.72098100	1.66494600	C	0.54500100	-1.90091800	-1.45625600
	C	-0.98680500	1.34400400	1.26354500	C	-0.85355600	-1.54788300	-1.17648100
	N	-1.18281800	0.26498700	0.38742700	N	-1.16946400	-0.43760000	-0.33772700
	C	-2.27317200	1.77412100	1.71989100	C	-2.01347200	-2.02779300	-1.70157500
	C	-3.21133300	0.92560500	1.13654400	C	-3.10945600	-1.19841800	-1.12972900
	C	-2.50751300	0.00816600	0.31835900	C	-2.52006400	-0.23112400	-0.32217700
	C	2.50408100	-0.63808400	0.17394300	C	2.35200400	0.97173700	-0.39648900
	C	3.45918400	0.00761400	0.99160200	C	3.37926900	0.35702800	-1.15315500
	C	2.79281800	1.01782600	1.68945000	C	2.87530900	-0.83683700	-1.67006900
	B	-0.01065000	-0.34822200	-0.43188100	B	-0.03801500	0.33696400	0.41043400
	C	0.49372900	2.94786900	2.52070500	C	0.88169300	-3.28257500	-1.93929300
	C	-3.11762000	-1.11741100	-0.44820800	C	-3.22848300	0.84930300	0.42939600
	C	-2.60780900	2.86588500	2.69408100	C	-2.27258600	-3.09303300	-2.71381400
	C	3.43863800	1.91501600	2.70506300	C	3.59694900	-1.76532500	-2.59900500
	C	2.76386600	-1.75243100	-0.78809400	C	2.47611200	2.22033900	0.41094800
	C	-4.70534700	0.95388700	1.31382700	C	-4.56136600	-1.44453700	-1.33142100
	C	-5.42399400	1.88150600	0.31876500	C	-5.14092700	-2.48685300	-0.34220500
	C	4.92045200	-0.34357400	1.06776900	C	4.77035700	0.89736300	-1.33394800
	C	5.81288200	0.51408100	0.15406900	C	5.79296200	0.31466800	-0.34198200
	O	0.25157700	0.38085100	-1.70420900	O	0.33075300	-0.33429500	1.69030100
	C	-0.55210400	0.52876200	-2.75779100	C	-0.44490700	-0.54504800	2.75341100
	C	-0.33917600	-2.73021000	0.16512300	C	-0.70054700	2.65576200	-0.18353300
	O	-0.21241400	-1.76231800	-0.75414900	O	-0.40475900	1.71891200	0.72772000
	O	-1.67758000	0.09110700	-2.85235900	O	-1.62743700	-0.28815700	2.82122500
	O	-0.30819500	-2.55083500	1.36035400	O	-0.73899900	2.46678700	-1.37743800
	C	-0.52957500	-4.08745400	-0.49064000	C	-0.99129700	3.99165000	0.47912400
	C	0.11068100	1.34486000	-3.85536200	C	0.33020600	-1.17714400	3.89793300
	C	-0.66710500	-5.24164000	0.50052200	C	-1.33599700	5.11072200	-0.50188100
	C	-0.85846700	-6.59216100	-0.19263600	C	-1.62214400	6.43976400	0.20019700
	C	0.43695600	2.78421300	-3.42521600	C	0.93465400	-2.54487500	3.54250300
	C	1.08006000	3.59988800	-4.54842900	C	1.69685900	-3.16991500	4.71251800
	H	-0.26958800	3.69389400	2.31948200	H	0.21201100	-4.02013200	-1.48870000
	H	0.44873100	2.70876700	3.58884700	H	0.80401700	-3.40583900	-3.02837200
	H	1.45737400	3.41243600	2.33096000	H	1.89777600	-3.56070700	-1.06425900
	H	-2.62614100	-1.25949800	-1.40598500	H	-2.80919100	0.97708100	1.42391400
	H	-3.05179200	-2.04608200	0.13052200	H	-3.18423100	1.80312900	-0.10672800
	H	-4.17438600	-0.92135600	-0.63130800	H	-4.28302600	0.59035600	0.53943500
	H	-3.66410200	2.82740900	2.96224600	H	-2.84671700	-2.68828700	-3.55512000
	H	-2.03621200	2.79012300	3.62185900	H	-1.36446800	-3.52814300	-3.11920800
	H	-2.42392100	3.86354600	2.28149200	H	-2.87614700	-3.90726300	-2.29413500
H	2.85886700	1.98847300	3.62739400	H	2.95601700	-2.11131800	-3.41349800	
H	4.42611800	1.53704400	2.97445900	H	4.45705800	-1.26832700	-3.05305500	
H	3.58437200	2.93504700	2.33219300	H	3.98280000	-2.65948300	-2.09439700	
H	3.81415400	-1.76414200	-1.08187400	H	3.52610500	2.48401400	0.54072300	
H	2.54000900	-2.72608600	-0.33844800	H	1.98593300	3.07105300	-0.07678600	
H	2.15471400	-1.65963300	-1.68564400	H	2.02577800	2.11156500	1.39877500	
H	-5.10617500	-0.05926300	1.21673500	H	-5.11672200	-0.50918400	-1.22177500	
H	-4.95276700	1.26164300	2.33481100	H	-4.74197200	-1.79636500	-2.35309400	
H	-6.50697500	1.86344400	0.47368700	H	-6.20687300	-2.63726600	-0.53322900	
H	-5.08596200	2.91556700	0.42893900	H	-4.63951900	-3.45225400	-0.44202100	
H	-5.22573400	1.58342500	-0.71407300	H	-5.01872900	-2.15374900	0.69021700	
H	5.27038400	-0.24727100	2.10107400	H	5.11120000	0.69360700	-2.35483700	
H	5.05860900	-1.39988500	0.81807800	H	4.76121800	1.98774500	-1.24534600	
H	6.86374600	0.22198400	0.24075700	H	6.79052600	0.72958700	-0.51508800	
H	5.52096200	0.41143500	-0.89467800	H	5.51162600	0.53411300	0.69150800	
H	5.73720200	1.57440900	0.40958900	H	5.85952800	-0.77219100	-0.43776900	
H	-1.40821900	-4.01919800	-1.14306200	H	-1.80232800	3.83273800	1.19969900	
H	0.31307700	-4.25111800	-1.17309500	H	-0.12124800	4.25764300	1.09130300	
H	1.03662700	0.83843900	-4.15171200	H	1.13559600	-0.49101100	4.18541500	
H	-0.56305100	1.34268900	-4.71480900	H	-0.35331800	-1.26381400	4.74525300	
H	0.21756900	-5.27210000	1.14396300	H	-0.51448800	5.23224900	-1.21453900	
H	-1.50813500	-5.04215000	1.17145600	H	-2.20020100	4.81078300	-1.10240100	
H	-0.95504300	-7.40170100	0.53593000	H	-1.86680000	7.22452900	-0.52076900	
H	-1.75941900	-6.60110200	-0.81458800	H	-2.46588800	6.35549500	0.89276300	
H	-0.01134500	-6.83497700	-0.84247200	H	-0.75853600	6.78356300	0.77880700	
H	-0.48460300	3.27735100	-3.09476900	H	0.13190300	-3.22057300	3.22484100	
H	1.10000900	2.75308800	-2.55656100	H	1.59777600	-2.42647400	2.68172300	
H	1.29937000	4.62073200	-4.22293500	H	2.11385800	-4.14363000	4.44025200	
H	2.02172800	3.14983700	-4.87874800	H	2.52816500	-2.53320500	5.03170700	
H	0.42379900	3.66635800	-5.42177300	H	1.04684400	-3.32064000	5.58011900	
E	-1450.054860				-1449.953099			
20	N	-0.56806700	1.36574600	0.45013400	N	0.85911700	1.27377200	-0.36010900
	C	-1.71274500	1.78781200	-0.23520100	C	2.03727200	1.31786000	0.44019700
	C	-2.60909100	0.84623800	-0.76774100	C	2.49954600	0.09757700	1.12743900
	C	-2.45595800	-0.52114200	-0.47949700	C	2.07371700	-1.11269600	0.60686800

	N	-1.32226300	-0.97866000	0.20139800	N	0.97523600	-1.16161600	-0.29205100
	C	-3.35312900	-1.62285400	-0.62277400	C	2.61183600	-2.43807700	0.69770500
	C	-2.74482000	-2.72046000	-0.00901400	C	1.87219200	-3.23632400	-0.18065100
	C	-1.49064300	-2.28974300	0.48276200	C	0.87183100	-2.43101100	-0.77608400
	C	0.05692600	2.45403600	0.94902600	C	0.69733500	2.44640900	-1.03505700
	C	-0.68002900	3.61707800	0.61995400	C	1.74634600	3.28950400	-0.67617300
	C	-1.78200600	3.21132800	-0.13666700	C	2.62291200	2.53130600	0.26119400
	B	-0.04233600	-0.10012900	0.28783700	B	-0.04150400	-0.00951100	-0.29408000
	C	-3.76053500	1.30618900	-1.62449300	C	3.40743800	0.20452000	2.31706100
	C	-0.49019700	-3.12835400	1.20972200	C	-0.15518200	-2.87239900	-1.76667600
	C	-4.72276700	-1.64150000	-1.23662700	C	3.81606400	-2.86818000	1.47922400
	C	-2.84263300	4.13308500	-0.66284200	C	3.91327600	3.08230600	0.76991400
	C	1.33382800	2.40220300	1.72356100	C	-0.44882800	2.75194100	-1.94766400
	C	-3.31479000	-4.10487800	0.15024000	C	2.10720000	-4.69041700	-0.48466000
	C	-4.12399300	-4.29832600	1.44430900	C	3.07144100	-4.92511300	-1.66188700
	C	-0.31295900	5.02320400	1.01024500	C	1.93523100	4.71535300	-1.05261800
	C	0.58515800	5.73350100	-0.01703400	C	1.30125200	5.70073700	-0.03941700
	O	0.77836900	-0.48170100	1.41806700	O	-0.93137600	-0.07622000	-1.42904600
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	C	2.81399400	-0.76124700	0.02055200	C	-2.96372700	-0.01784700	-0.01345600
	C	1.99256600	-0.14959500	-1.12463600	C	2.03099300	0.36432000	1.14763000
	O	0.66241500	-0.19559200	-0.99654800	O	-0.73836500	0.05199900	0.99779200
	C	3.08856600	-2.25240000	-0.37807800	C	-3.39175200	-1.50634700	0.23436400
	C	4.00500100	-2.41874700	-1.60177600	C	-4.24569700	-1.70088800	1.49954900
	C	5.22594200	-1.46593500	-1.57961700	C	-5.32479500	-0.60404200	1.67817700
	C	5.41015300	-0.82245000	-0.20256000	C	-5.52581800	0.19748000	0.38900500
	C	4.17572400	-0.00325300	0.20148300	C	-4.22959500	0.89889100	-0.04613100
	O	2.64594400	-1.15413600	2.37938500	O	-2.90053000	0.01183100	-2.41680500
	O	2.51057100	0.26519600	-2.13234100	O	-2.44185500	0.83583800	2.17874800
	H	-3.50143000	2.20266600	-2.18119900	H	3.14880300	1.08185900	2.91645800
	H	-4.03994000	0.54510400	-2.34782700	H	3.31288600	-0.66611900	2.96483700
	H	-4.64916200	1.53499400	-1.02590400	H	4.47143700	0.29686500	2.05848300
	H	-0.93722200	-4.07586000	1.50936600	H	0.12917000	-3.83056700	-2.20275100
	H	0.37467400	-3.36289100	0.58160500	H	-1.14361600	-3.00657900	-1.31271600
	H	-0.11153700	-2.62534900	2.09888400	H	-0.27853600	-2.14842600	-2.57207900
	H	-4.69152100	-1.53180500	-2.32578800	H	3.61333600	-2.94670400	2.55354500
	H	-5.22517100	-2.58620400	-1.02755600	H	4.16781100	-3.84761500	1.15101700
	H	-5.36371300	-0.84500400	-0.85156500	H	4.65015900	-2.17034900	1.36447300
	H	-2.72024700	5.13533500	-0.25089600	H	4.57709100	3.34410300	-0.06240100
	H	-2.80019100	4.23308000	-1.75264400	H	3.75671900	4.00482600	1.34119800
	H	-3.85136400	3.79991600	-0.40888100	H	4.44860200	2.38537200	1.40804800
	H	2.18471000	2.14219200	1.08521300	H	-1.39902700	2.83165500	-1.40903500
	H	1.55197600	3.37627500	2.16037500	H	-0.28311700	3.70861000	-2.44494000
	H	1.29221700	1.66468200	2.52517700	H	-0.58114000	1.98773400	-2.71375900
	H	-3.94799300	-4.34197100	-0.71003200	H	2.49879200	-5.19054300	0.40632300
	H	-2.50630100	-4.84177200	0.11781600	H	1.15398300	-5.18424900	-0.69771000
	H	-4.51570800	-5.31721200	1.51583700	H	3.21441200	-5.99413400	-1.84525100
	H	-3.50893000	-4.11282900	2.32892300	H	2.69130900	-4.47428300	-2.58233900
	H	-4.97130500	-3.60869900	1.48843600	H	4.05153300	-4.48309200	-1.46426700
	H	-1.22172300	5.61428500	1.16087100	H	3.00466400	4.93903200	-1.13297400
	H	2.18471200	5.01954000	1.98345600	H	1.50267100	4.90244300	-0.93961900
	H	0.82619900	6.75012700	0.30724600	H	1.48446700	6.73226100	-0.35128700
	H	1.52549700	5.19517000	-0.16151200	H	0.22225400	5.54945300	0.02933500
	H	0.09508200	5.79849100	-0.99206700	H	1.72002800	5.56936100	0.06069900
	H	3.53852400	-2.72528500	0.49761900	H	-3.95324200	-1.81889600	-0.64977100
	H	2.14037400	-2.76747100	-0.55829900	H	-2.50610000	-2.14549200	0.28604300
	H	3.43281100	-2.26362600	-2.51879700	H	-3.60066300	-1.73234800	-2.03892100
	H	4.33543400	-3.46289000	-1.61825900	H	-4.71251900	-2.68896200	1.42719400
	H	6.13342400	-2.00300100	-1.87219100	H	-6.27027100	-1.05117100	2.00024700
	H	5.07607700	-0.67230700	-2.31568100	H	5.01350600	0.08316900	2.46841500
	H	5.61460600	-1.58940000	0.55327400	H	-5.88551000	-0.45841300	-0.41257100
	H	6.28328400	-0.16164900	-0.20654600	H	-6.30448300	0.95396400	0.53076900
	H	4.14440500	0.89966500	-0.41197700	H	-4.05071000	1.74537300	0.61951000
	H	4.27603300	0.30126000	1.24392300	H	-4.35386400	1.28495200	-1.05786600
E		-1447.621486				-1447.522958		
21	N	1.23627600	-0.36955400	-0.15783900	N	1.21733400	-0.33167200	-0.12180200
	C	1.21919000	-1.63994200	0.42905900	C	1.21326200	-1.58997400	0.54839200
	C	0.00076300	-2.23571500	0.79705100	C	0.00064200	-2.12317500	1.06716300
	C	-1.21801200	-1.64070400	0.42897900	C	-1.21233200	-1.59062400	0.54837500
	N	-1.23580900	-0.37039400	-0.15802800	N	-1.21710100	-0.33229600	-0.12177500
	C	-2.55044700	-2.15406100	0.40068600	C	-2.49735500	-2.14566100	0.43948000
	C	-3.34282600	-1.18389900	-0.21712900	C	-3.27663800	-1.22368200	-0.30906700
	C	-2.50133200	-0.09376100	-0.54093500	C	-2.44792600	-0.12280400	-0.64382400
	C	2.50165200	-0.09220100	-0.54070500	C	2.44806500	-0.12152800	-0.64382400
	C	3.34374900	-1.18188700	-0.21699000	C	3.27740200	-1.22192200	-0.30898600
	C	2.55192100	-2.15257000	0.40066800	C	2.49866900	-2.14427200	0.43957300
	B	-0.00010800	0.57428900	-0.02420500	B	-0.00011900	0.61618300	0.01224500
	C	0.00111000	-3.53840500	1.55466800	C	0.00091800	-3.23548300	2.07520300
	C	-2.91787800	1.17942500	-1.20272300	C	-2.84786900	1.09826600	-1.40343300
	C	-3.04736200	-3.49263600	0.86329000	C	-2.97203400	-3.48043200	0.93306400
	C	3.04957700	-3.49095700	0.86301600	C	2.97406400	-3.47876200	0.93322800
	C	2.91764000	1.18136300	-1.20214000	C	2.84735400	1.09972400	-1.40348100
	C	-4.81282900	-1.27376300	-0.52958400	C	-4.71365100	-1.38459100	-0.69675900
	C	-5.11792700	-1.87078500	-1.91425600	C	-4.90349000	-2.08859600	-2.05783600
	C	4.81381500	-1.27085000	-0.52933900	C	4.71451400	-1.38202600	-0.69668900
	C	5.11947500	-1.86751700	-1.91401600	C	4.90475100	-2.08586600	-2.05778700

	O	-0.00044100	1.58227000	-1.06153300	O	-0.00040500	1.61671400	-1.03268900
	C	-0.00104200	2.91197800	-0.87834800	C	-0.00085300	2.94665100	-0.86078600
	C	-0.00136400	3.46526200	0.55671500	C	-0.00109000	3.51026100	0.56940800
	C	-0.00123600	2.41244900	1.68013600	C	-0.00090500	2.46831400	1.70267300
	O	-0.00034100	1.12496300	1.33717300	O	-0.00028100	1.17675100	1.37225100
	C	-1.25602500	4.35316000	0.73182900	C	-1.25944100	4.39426100	0.73461200
	C	1.25301200	4.35355000	0.73208700	C	1.25685900	4.39481700	0.73478800
	O	-0.00132900	3.65022100	-1.83112300	O	-0.00109400	3.67755500	-1.81951900
	O	-0.00186100	2.75205600	2.83731400	O	-0.00117100	2.81834400	2.85687000
	H	0.00094700	-4.40259100	0.88119100	H	0.00106700	-4.23900800	1.62939100
	H	0.87675200	-3.62084300	2.19275300	H	0.87919400	-3.17390200	2.71951400
	H	-0.87416800	-3.62096000	2.19325000	H	-0.87730500	-3.17422200	2.71962400
	H	-3.92422400	1.08367500	-1.60937300	H	-3.83341700	0.96164400	-1.84879800
	H	-2.93445300	2.01503300	-0.49594300	H	-2.90366300	1.98473100	-0.76044400
	H	-2.24175500	1.45594100	-2.01114700	H	-2.13929700	1.33466700	-2.19859400
	H	-3.04012500	-3.58351700	1.95460000	H	-3.18471800	-3.47739600	2.00801800
	H	-4.07530100	-3.65497400	0.53836500	H	-3.89303300	-3.77851100	0.42912400
	H	-2.45132500	-4.31843600	0.46792300	H	-2.23861200	-4.26934200	0.75412800
	H	4.07731400	-3.65303300	0.53729500	H	3.89522200	-3.77637300	0.42930100
	H	3.04322400	-3.58171800	1.95435000	H	3.18674800	-3.47555900	2.00818300
	H	2.45349700	-4.31696500	0.46818600	H	2.24106200	-4.26807300	0.75433500
	H	2.93538900	2.01639200	-0.49466200	H	2.90262100	1.98625300	-0.76053700
	H	3.92345300	1.08565200	-1.61013400	H	3.83299700	0.96363200	-1.84879600
	H	2.24058600	1.45864300	-2.00948400	H	2.13868100	1.33568600	-2.19868300
	H	-5.31502600	-1.86931400	0.23869300	H	-5.24095000	-1.95323000	0.07544200
	H	-5.26605800	-0.28018700	-0.45800000	H	-5.20392000	-0.40696200	-0.73214200
	H	-6.19577300	-1.91533000	-2.09565800	H	-5.96650800	-2.18942500	-2.29483400
	H	-4.66819900	-1.27390200	-2.71224300	H	-4.42877700	-1.52442000	-2.86414300
	H	-4.71969800	-2.88505100	-2.00455600	H	-4.46138400	-3.08796100	-2.05214700
	H	5.26645800	-0.27700800	-0.45761000	H	5.20424400	-0.40412300	-0.73202100
	H	5.31628100	-1.86617600	0.23895000	H	5.24212500	-1.95039600	0.07549700
	H	6.19737700	-1.91113000	-2.09532000	H	5.96782400	-2.18609300	-2.29479800
	H	4.72211400	-2.88211100	-2.00444600	H	4.46320400	-3.08547900	-2.05213700
	H	4.66932000	-1.27092500	-2.71197800	H	4.42972000	-1.52192900	-2.86407500
	H	-1.26512000	5.13241200	-0.03054300	H	-1.26783600	5.17040400	-0.03091400
	H	-2.18069300	3.77689300	0.64310200	H	-2.18004000	3.81091600	0.64084900
	H	-1.24014300	4.80785000	1.72214500	H	-1.25241200	4.85281400	1.72332300
	H	2.17786100	3.77756700	0.64343600	H	2.17773100	3.81187500	0.64119900
	H	1.26197400	5.13285000	-0.03024000	H	1.26503600	5.17094300	-0.03075900
	H	1.23682600	4.80818500	1.72242400	H	1.24946300	4.85340500	1.72348200
E		-1330.872310				-1330.772813		

Table S3. Cartesian coordinates and total computed energy (in hartrees) in the ground state (B3LYP/6-311g*) for **19**.

19	N	0.03509900	-1.47055600	1.24707900	
	C	0.06385300	-2.86730100	1.22124400	
	C	0.04326500	-3.56094300	0.00027400	
	C	0.06364900	-2.86735500	-1.22073300	
	N	0.03518000	-1.47061800	-1.24673000	
	C	0.10631200	-3.31932000	-2.57570300	
	C	0.08680700	-2.18094600	-3.38728200	
	C	0.03478300	-1.05840700	-2.53315100	
	C	0.03468700	-1.05819300	2.53344200	
	C	0.08705800	-2.18061400	3.38771100	
	C	0.10676700	-3.31909300	2.57627400	
	B	0.03980400	-0.57181100	0.00011800	
	C	-0.02777000	-5.06543900	0.00017300	
	C	-0.04664200	0.37811000	-2.93810700	
	C	0.20149700	-4.72301700	-3.09814200	
	C	0.20259900	-4.72270300	3.09885900	
	C	-0.04706400	0.37836100	2.93817300	
	C	0.08766200	-2.13091400	-4.89060400	
	C	-1.31679200	-2.22017200	-5.51208400	
	C	0.08812800	-2.13027200	4.89102500	
	C	-1.31636300	-2.21774700	5.51266500	
	O	-1.09382000	0.38808800	0.00009100	
	C	-2.36281100	-0.01489400	-0.00007000	
	C	2.46647500	-0.09179700	0.00002300	
	O	1.21079900	0.35465700	0.00014500	
	O	-2.72849000	-1.16982100	-0.00014700	
	O	2.79186400	-1.25844800	0.00003700	
	C	3.48030800	1.01944200	-0.00012800	
	C	-3.33735900	1.13114300	-0.00013000	
	C	-2.91732600	2.46563300	-0.00010300	
	C	-3.85144500	3.49484200	-0.00018000	
	C	-5.20324700	3.16869900	-0.00024300	
	C	-5.64748200	1.84996000	-0.00025200	
	C	-4.70398600	0.83180400	-0.00021800	
	C	3.10927000	2.36837000	0.00001400	
	C	4.07985700	3.36327000	-0.00002000	
	C	5.41891800	2.98858900	-0.00030200	
	C	5.81499300	1.65460900	-0.00052300	
	C	4.83530200	0.67131600	-0.00036700	
	N	-6.20313800	4.26165900	-0.00029000	
	N	6.45754300	4.04470100	-0.00039300	
	O	-7.38508500	3.94684800	0.00059300	
	O	-5.78495200	5.41128900	-0.00119200	
	O	7.62736700	3.68747300	-0.00269700	
	O	6.08113300	5.20870800	0.00182300	
	H	-0.55396800	-5.43888900	-0.87248500	
	H	0.97403300	-5.50955700	-0.00153900	
	H	-0.55123200	-5.43931300	0.87423700	
	H	0.43587700	1.03367100	-2.21598400	
	H	0.42208700	0.52965500	-3.91172900	
	H	-1.08933200	0.70249300	-3.02721900	
	H	0.44699500	-4.71791300	-4.16082200	
	H	0.97293800	-5.30597200	-2.59128600	
	H	-0.74146200	-5.27138100	-2.99708500	
	H	0.97412800	-5.30540600	2.59184900	
	H	0.44842300	-4.71739400	4.16146100	
	H	-0.74019100	-5.27143400	2.99819800	
	H	0.41972300	0.52979300	3.91273200	
	H	0.43714600	1.03372200	2.21697000	
	H	-1.08980600	0.70314900	3.02507400	
	H	0.56977500	-1.20848800	-5.22905500	
	H	0.70791700	-2.94037600	-5.28844900	
	H	-1.26745000	-2.17739900	-6.60402200	
	H	-1.81382800	-3.15340000	-5.23440400	
	H	-1.95319300	-1.39853200	-5.17288100	
	H	0.70741700	-2.94040800	5.28896700	
	H	0.57143500	-1.20838000	5.22925200	
	H	-1.26686000	-2.17486300	6.60459200	
	H	-1.95184600	-1.39541500	5.17341600	
	H	-1.81450600	-3.15043900	5.23516400	
	H	-1.85861200	2.68915900	-0.00002800	
	H	-3.55308300	4.53443500	-0.00020500	
	H	-6.70903000	1.64317400	-0.00027000	
	H	-5.00773000	-0.20778400	-0.00025400	
	H	2.05969500	2.63193400	0.00014500	
	H	3.81918000	4.41293300	0.00023800	
	H	6.86833800	1.40944300	-0.00084500	
	H	5.10125800	-0.37853000	-0.00043500	
	E	-2085.445092			