Supporting Information

Cyclopropanation of [60]Fullerobenzofurans via Electrosynthesis

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1. HPLC trace of the crude reaction mixture of dianionic fullerobenzofuran $1a^{2-}$ with diethyl dibromomalonate

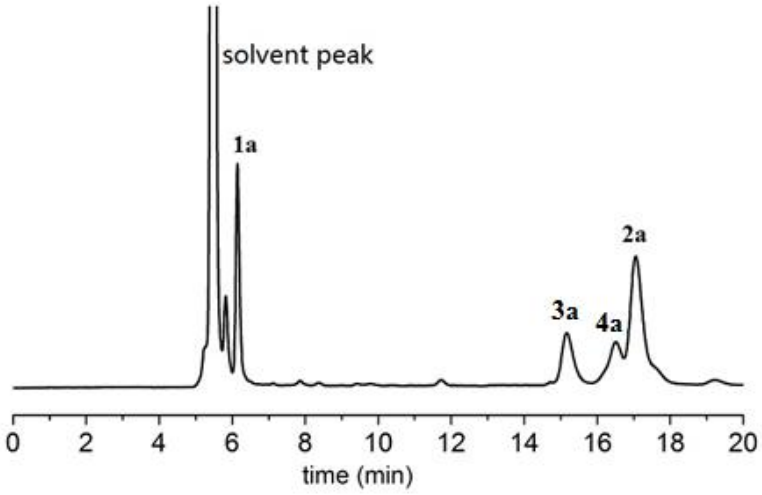
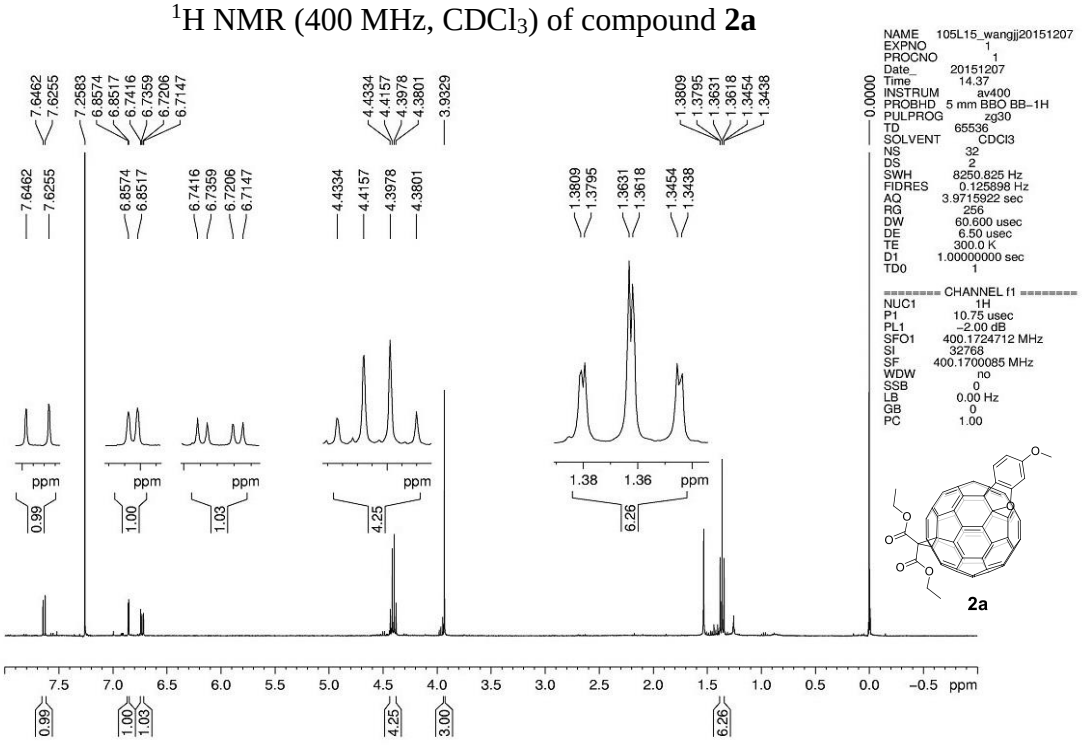


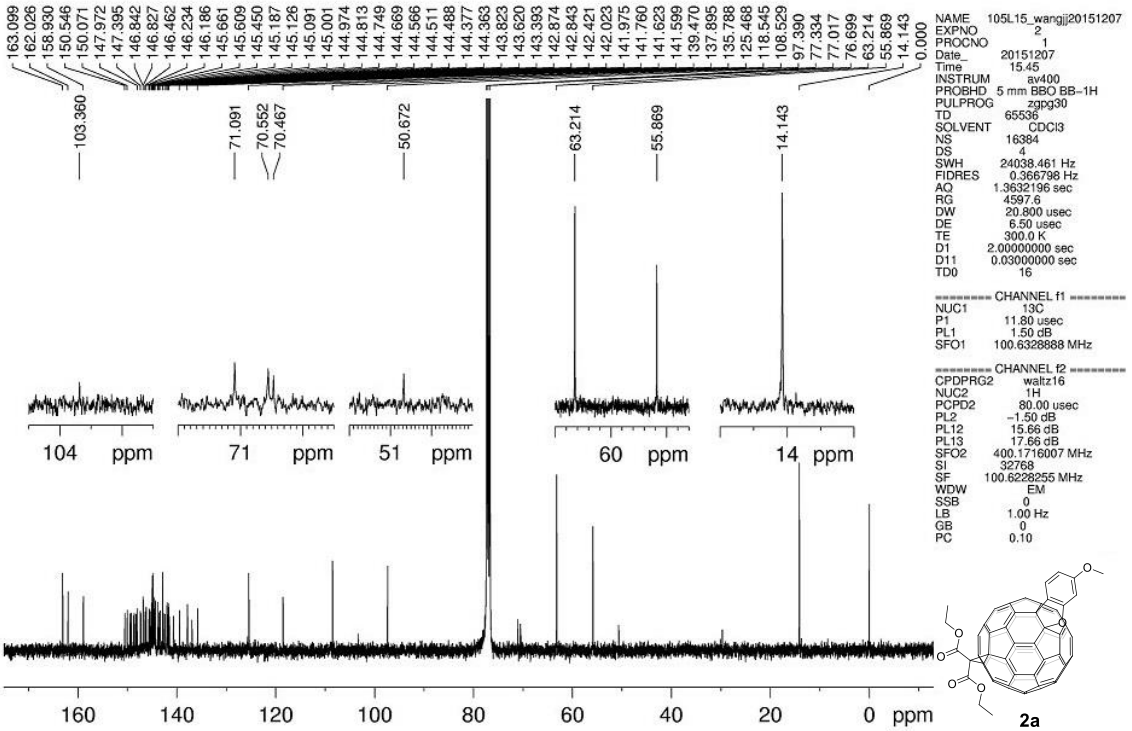
Fig. S1 HPLC trace of the crude reaction mixture of dianionic fullerobenzofuran $\mathbf{1a}^{2-}$ with diethyl dibromomalonate. The mixture was eluted on a ZARBOX SIL column (4.6×250 mm) with toluene at a flow rate of 1.0 mL/min with the detector wavelength set at 326 nm.

2. ^{1}H NMR and ^{13}C NMR spectra of compounds 2a-4a and 2b

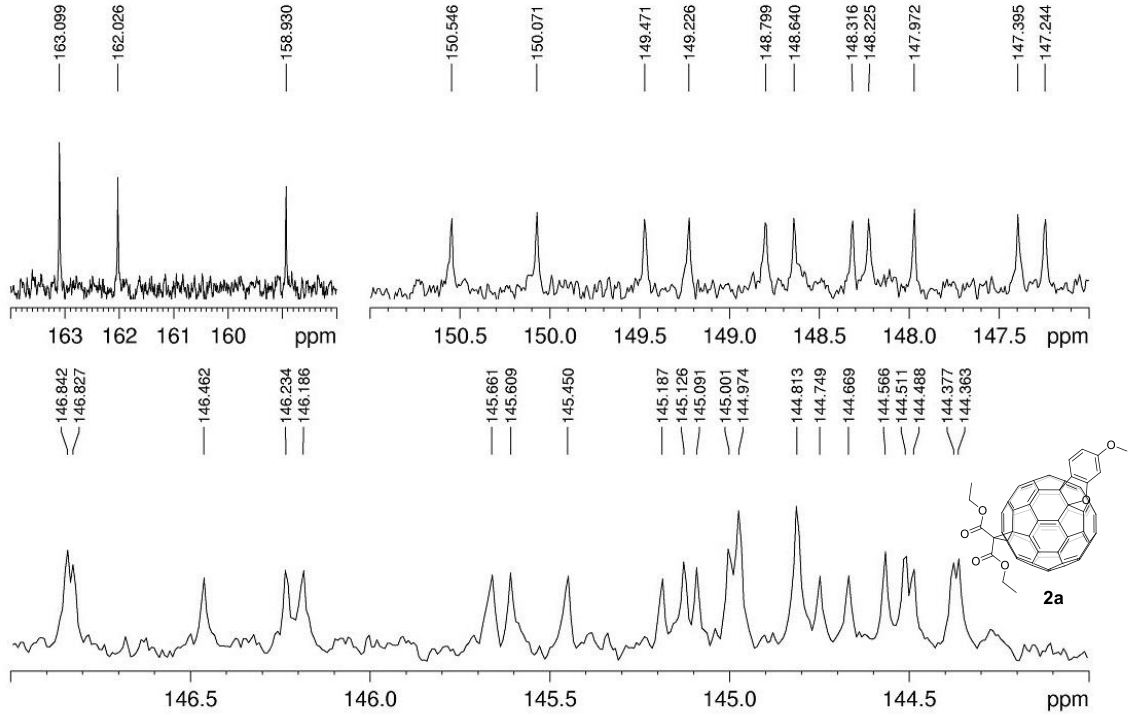
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2a**



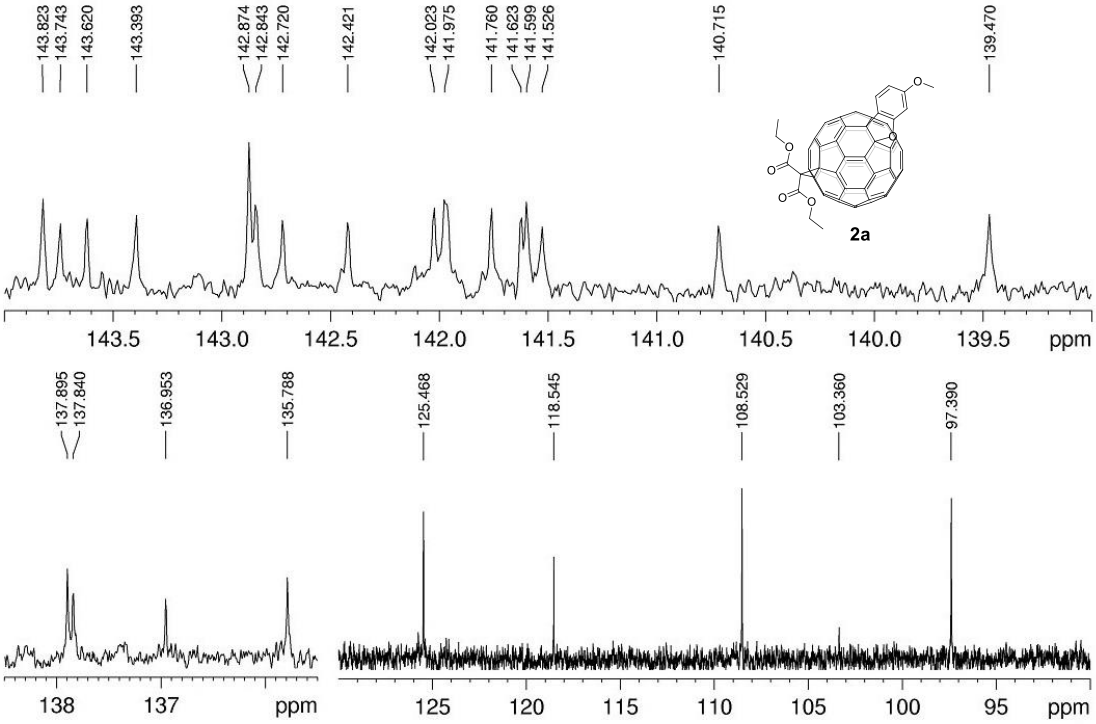
^{13}C NMR (100 MHz, $CDCl_3$) of compound **2a**



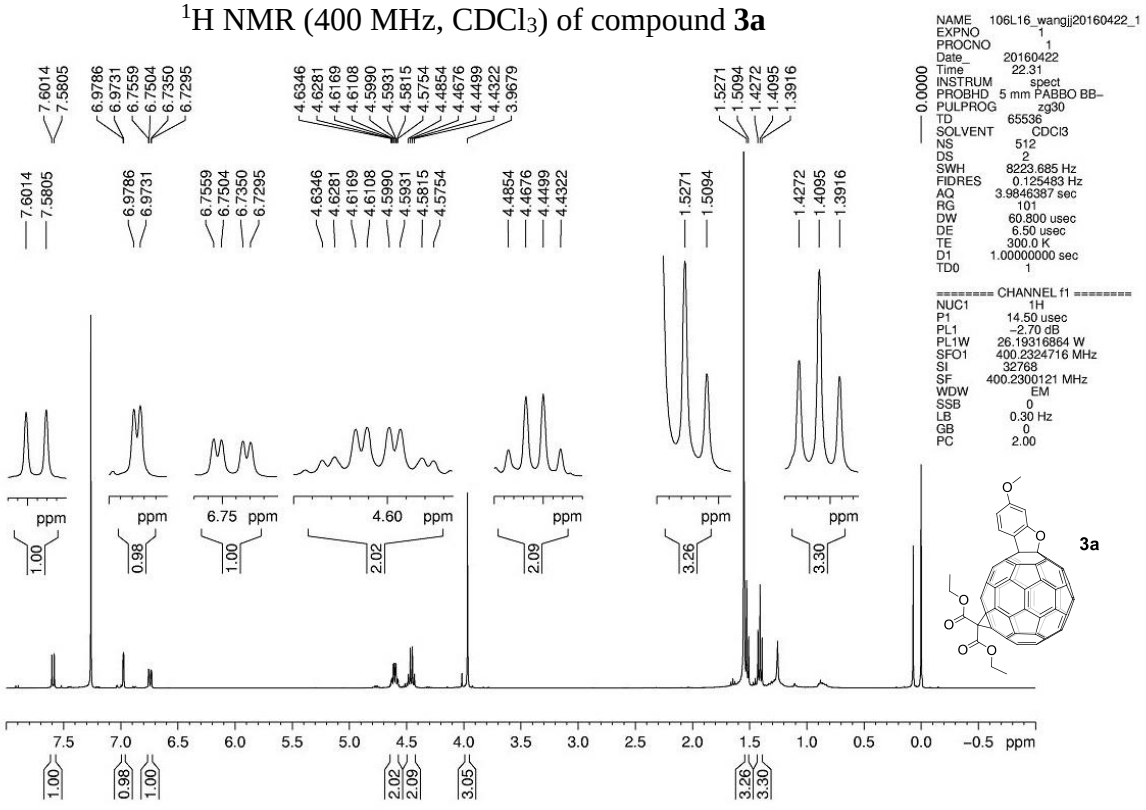
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2a**



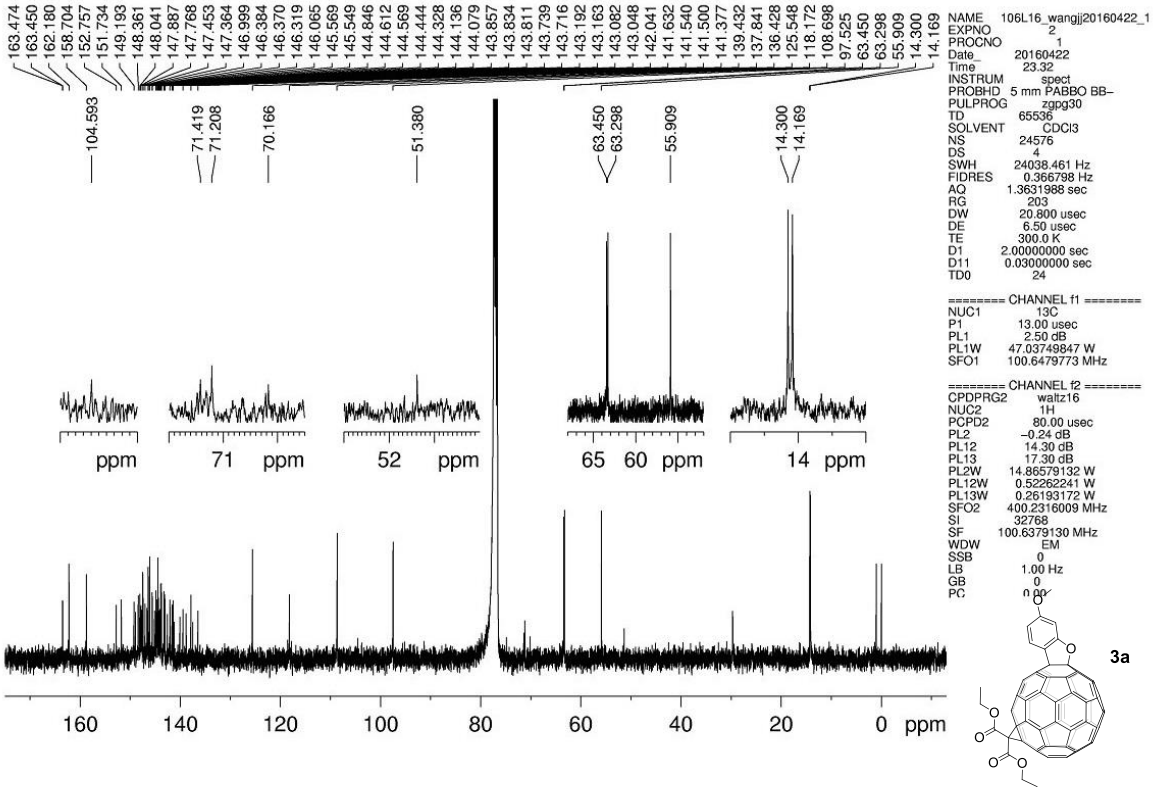
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2a**



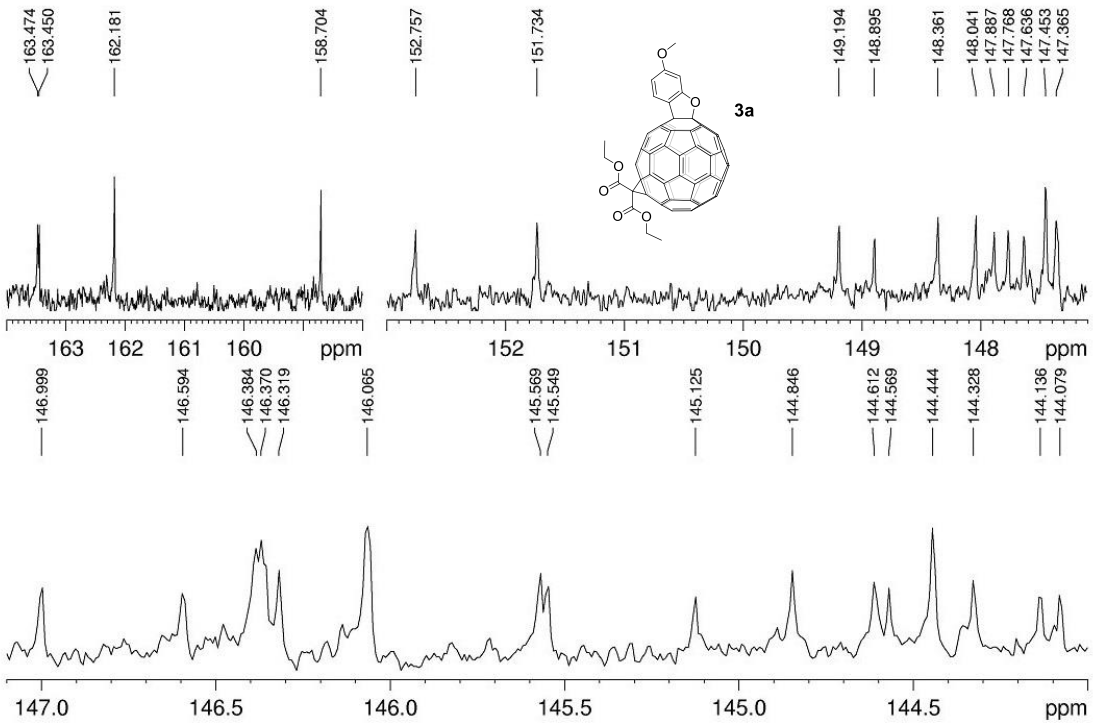
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3a**



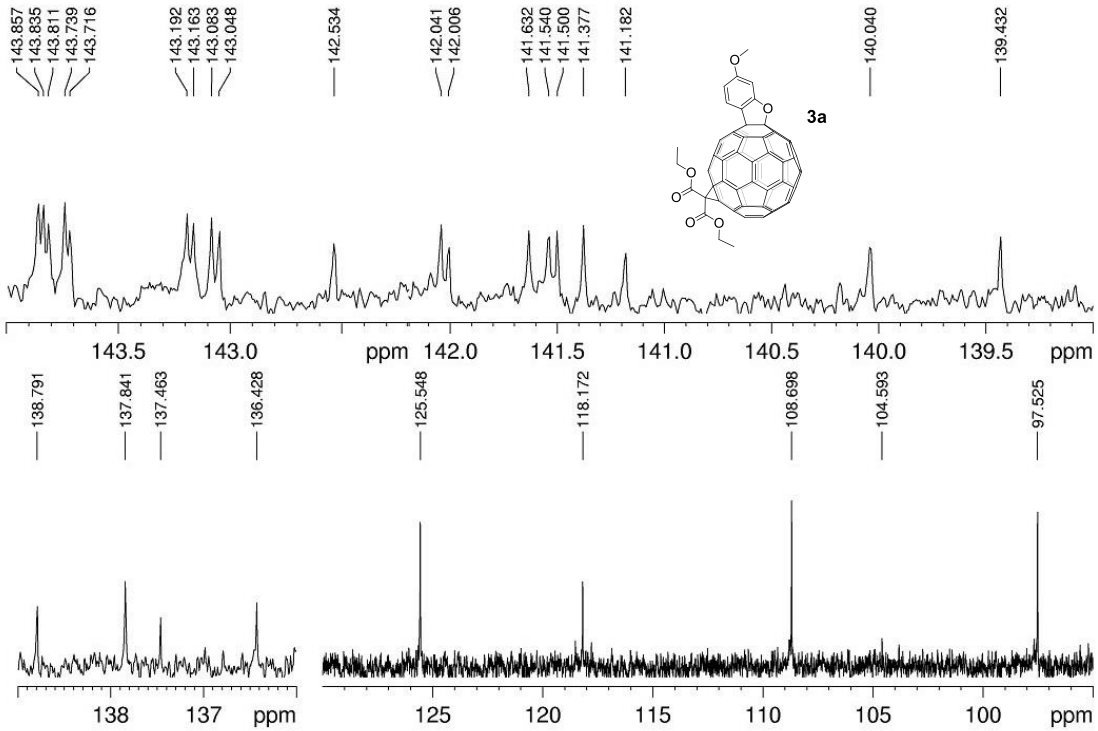
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3a**



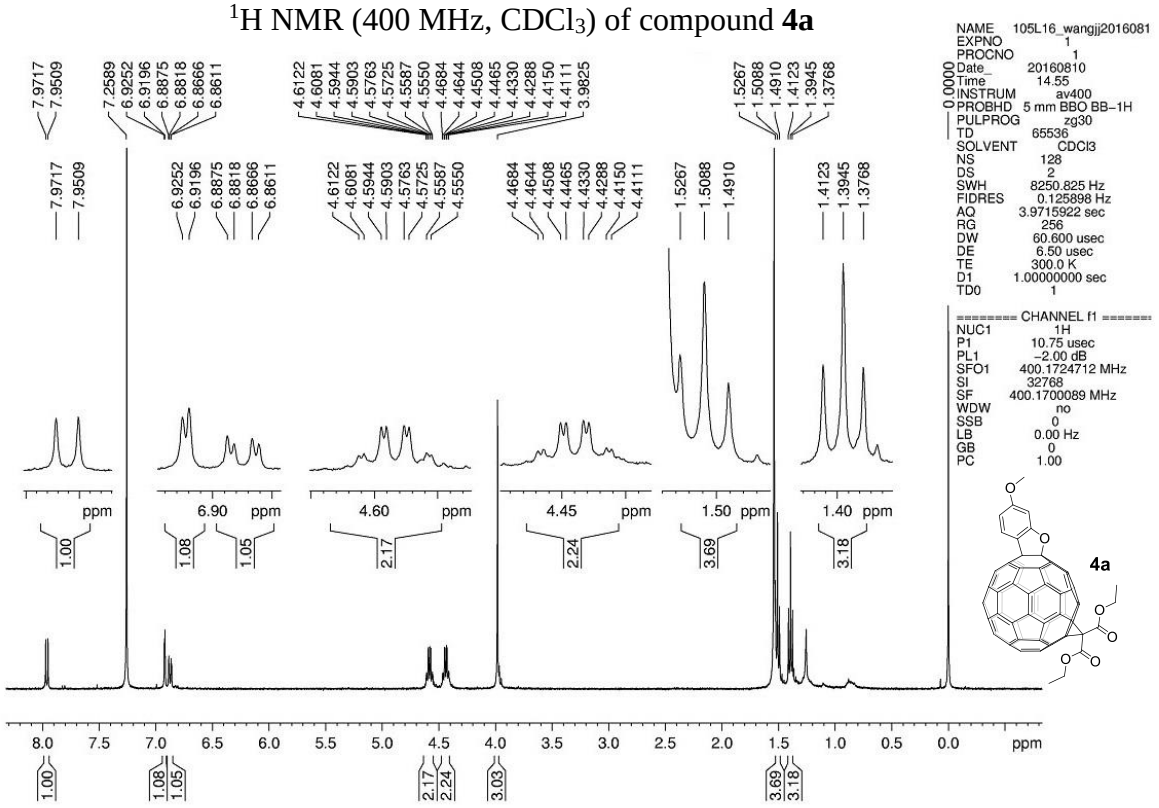
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **3a**



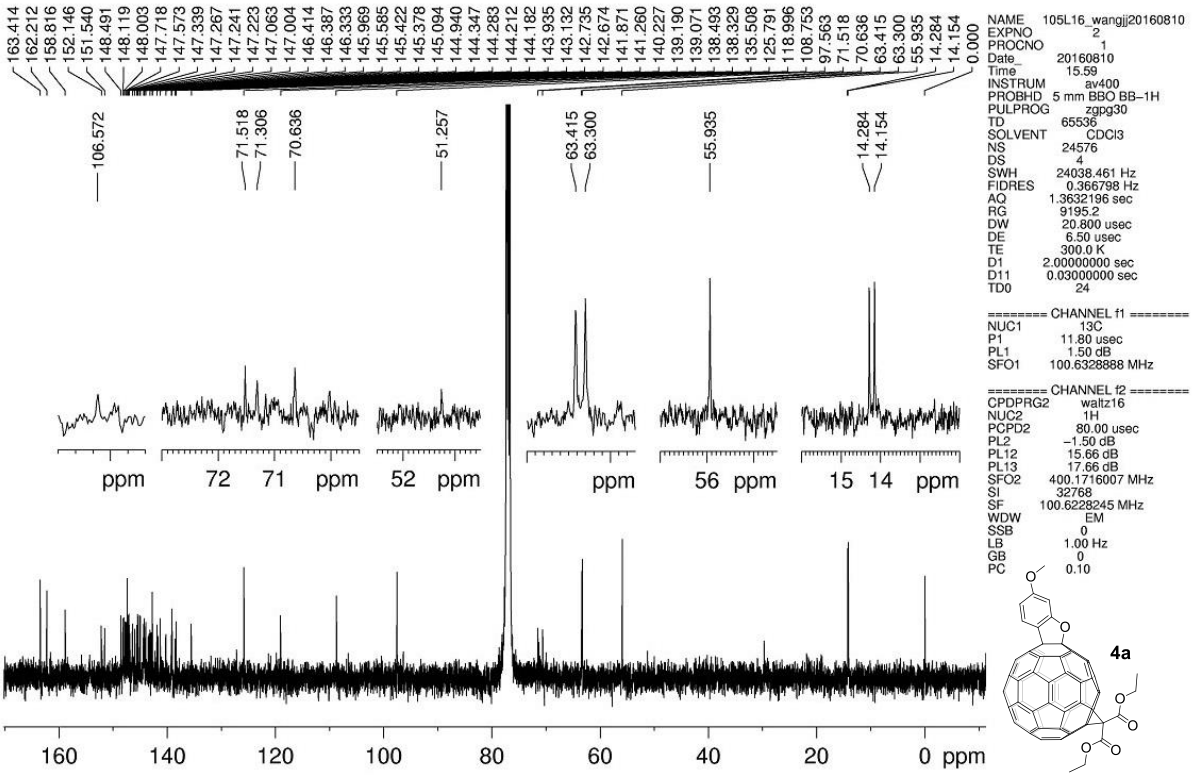
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **3a**



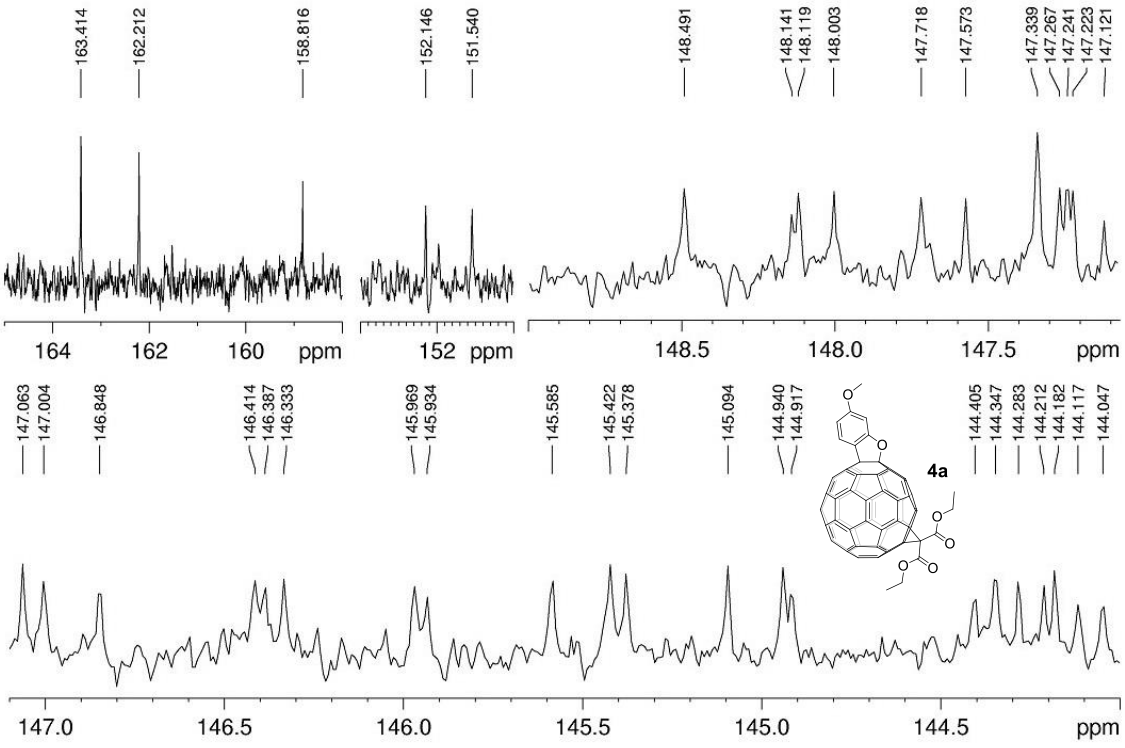
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4a**



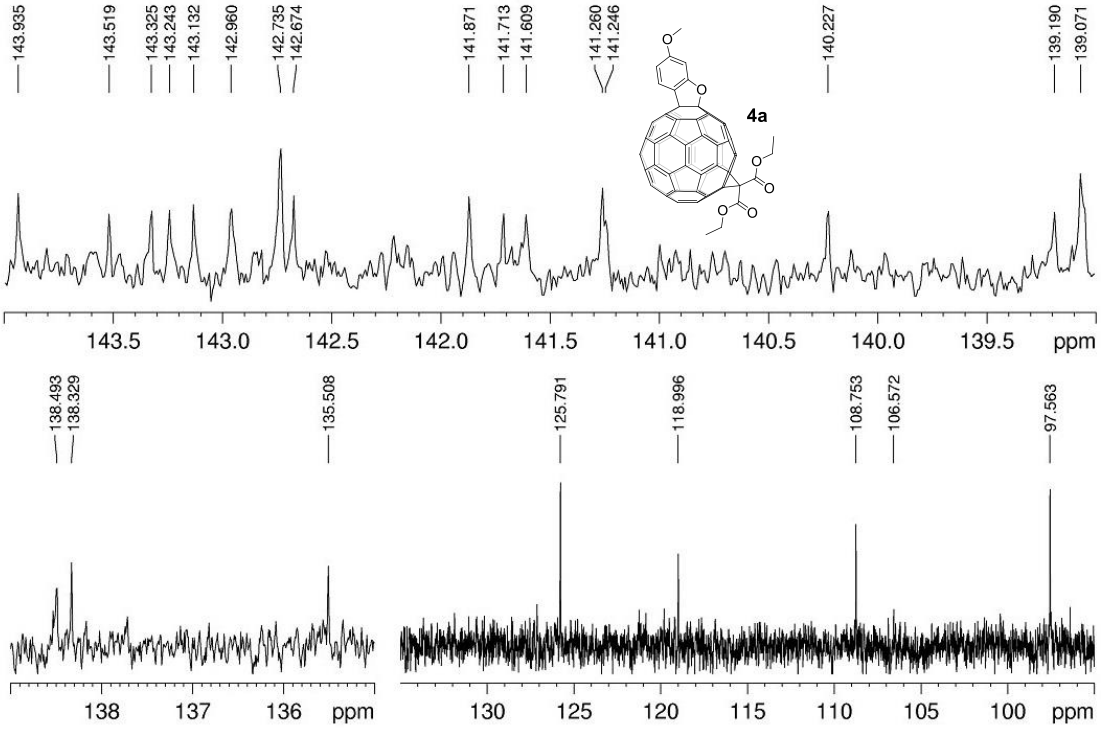
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4a**



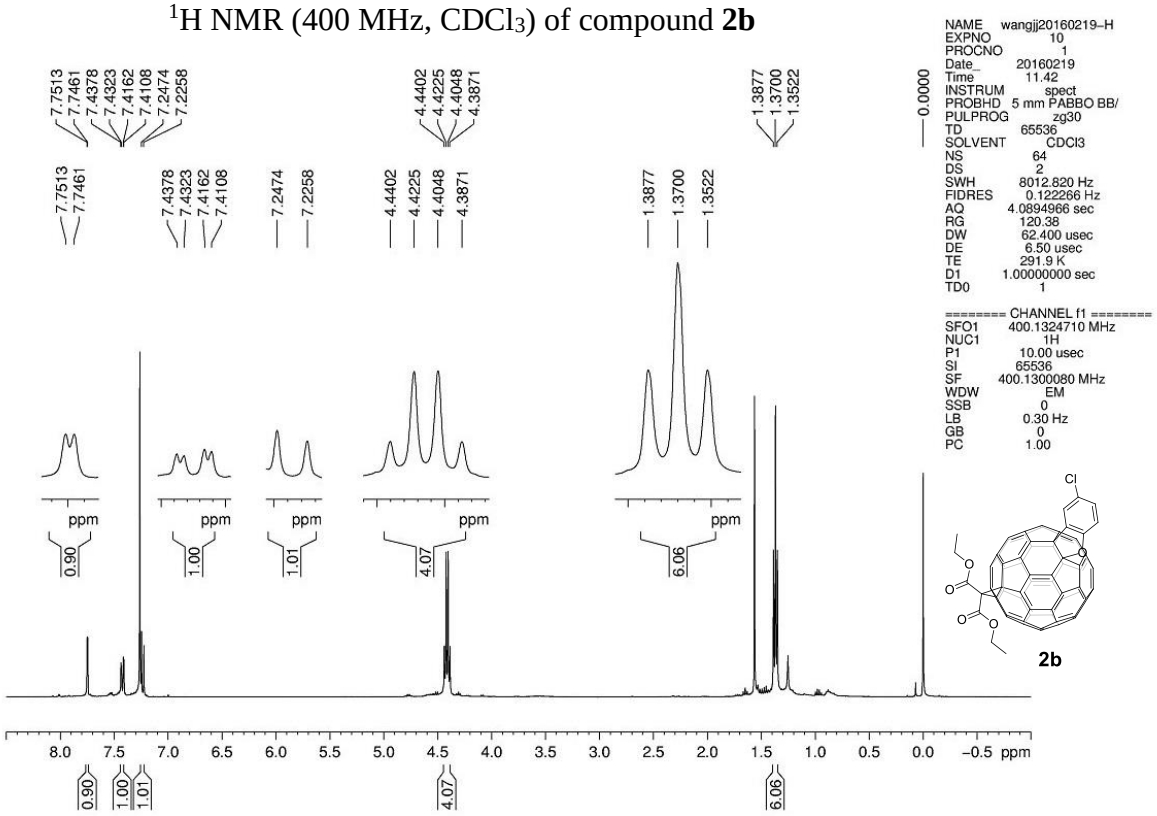
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **4a**



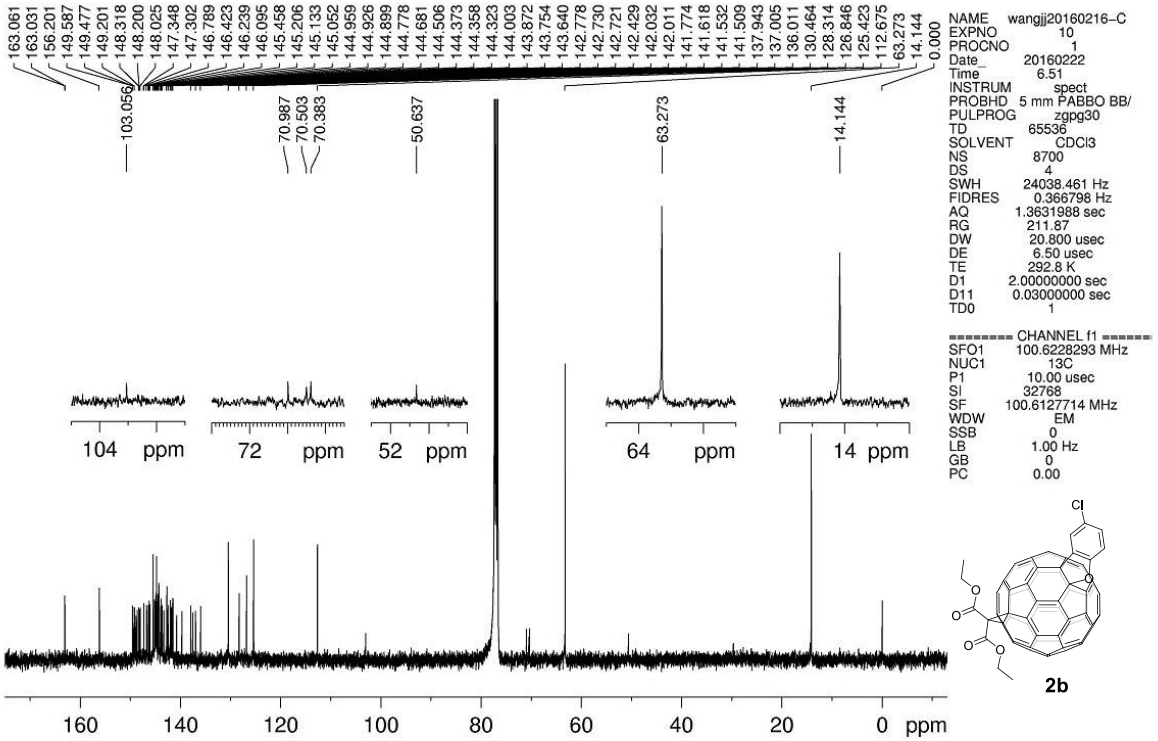
Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **4a**



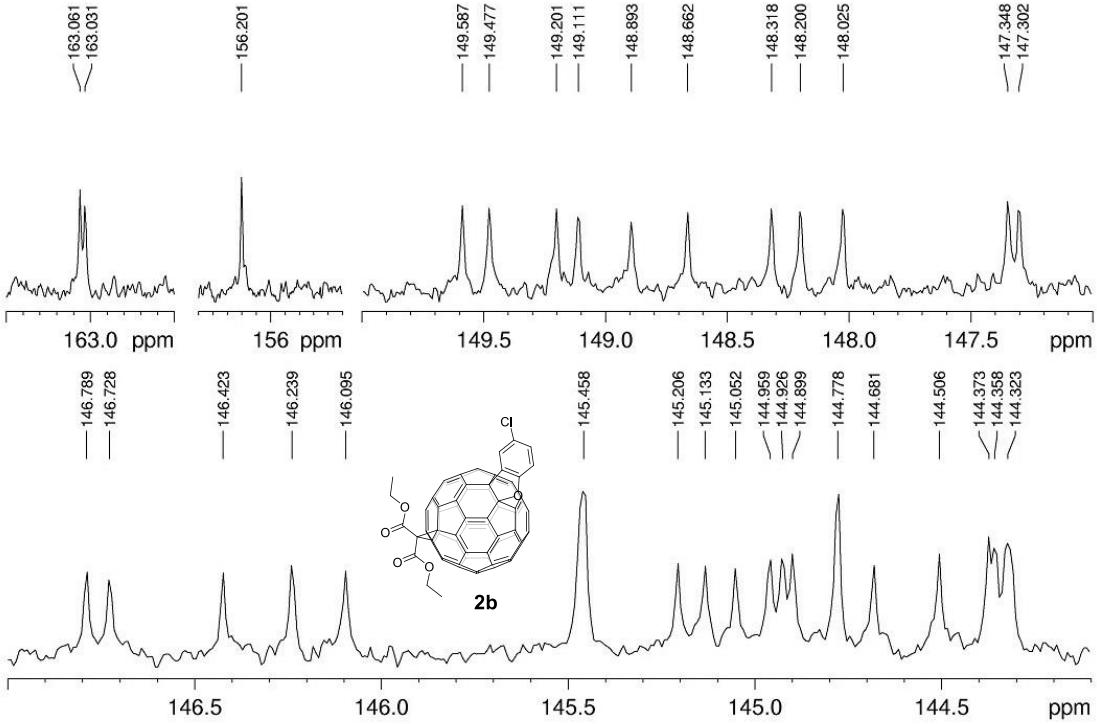
^{1}H NMR (400 MHz, $CDCl_3$) of compound **2b**



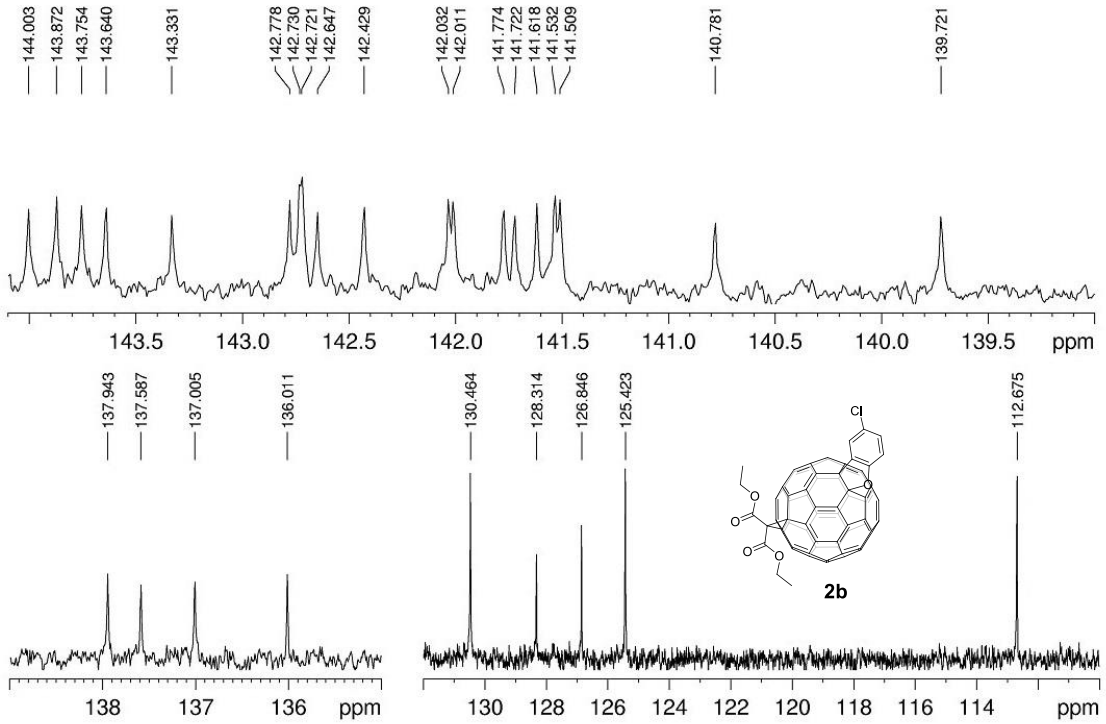
^{13}C NMR (100 MHz, $CDCl_3$) of compound **2b**



Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2b**

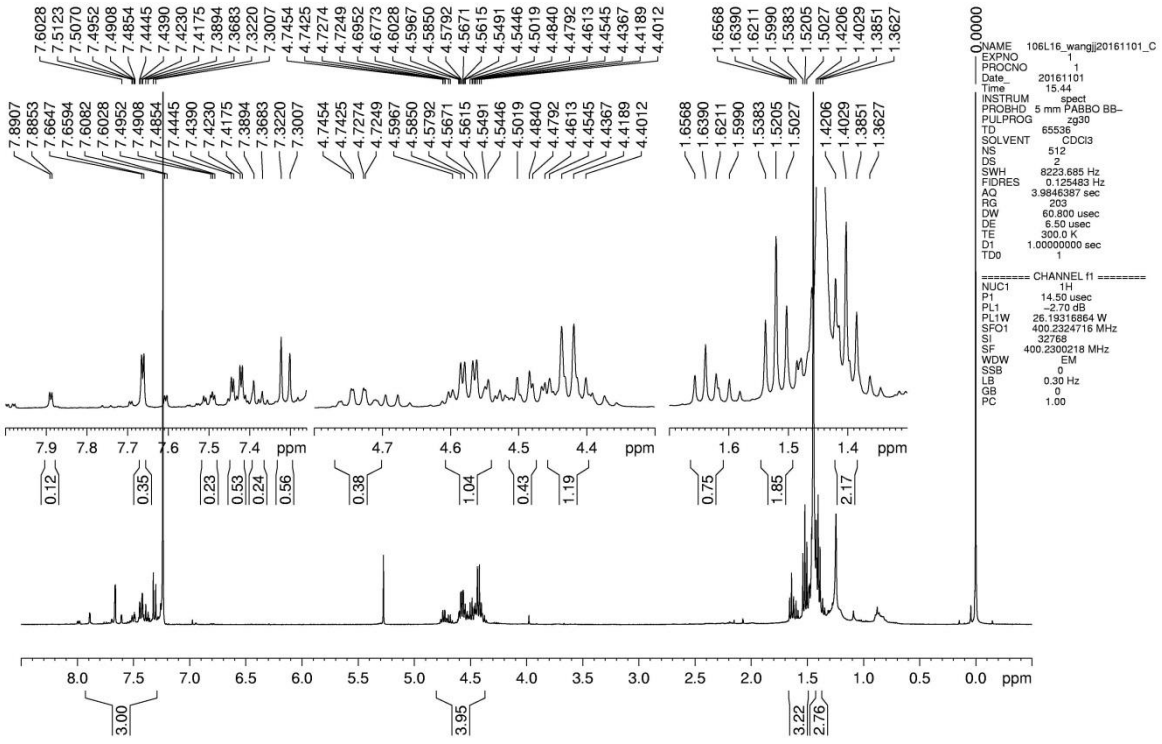


Expanded ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2b**

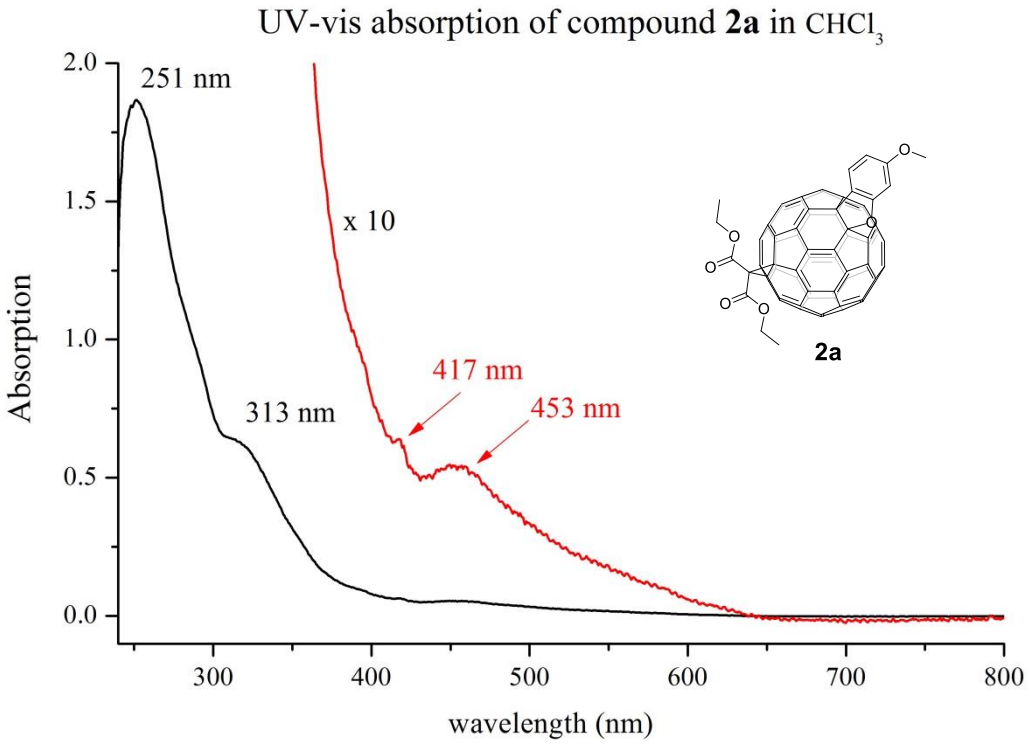


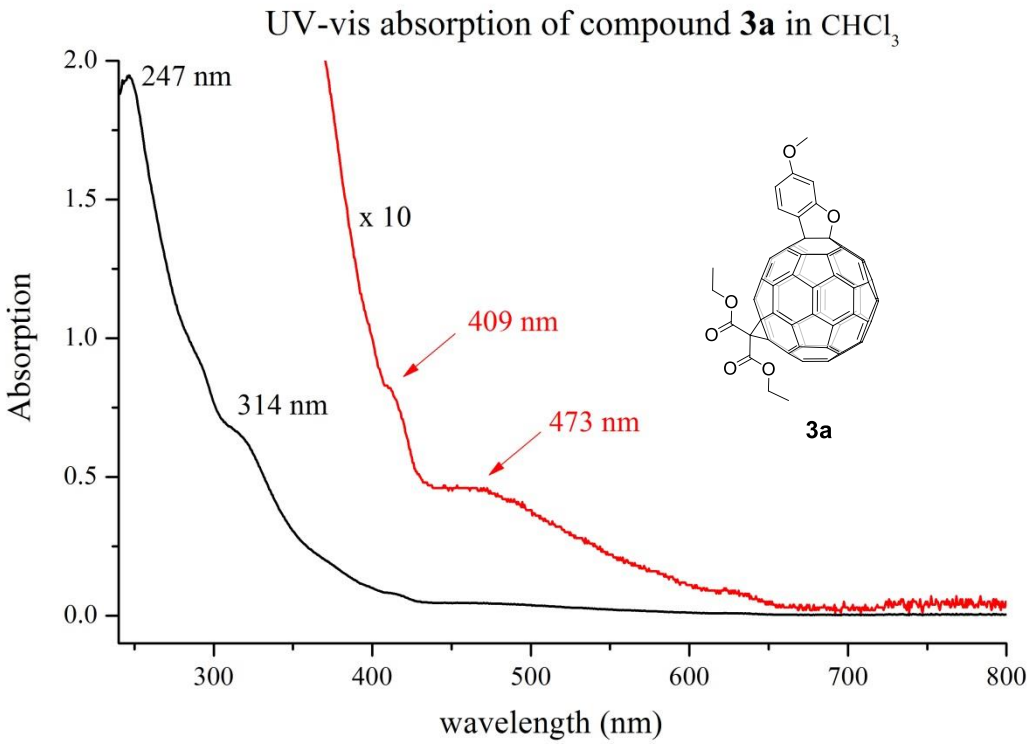
3. ^{1}H NMR spectrum of 3b and 4b mixture

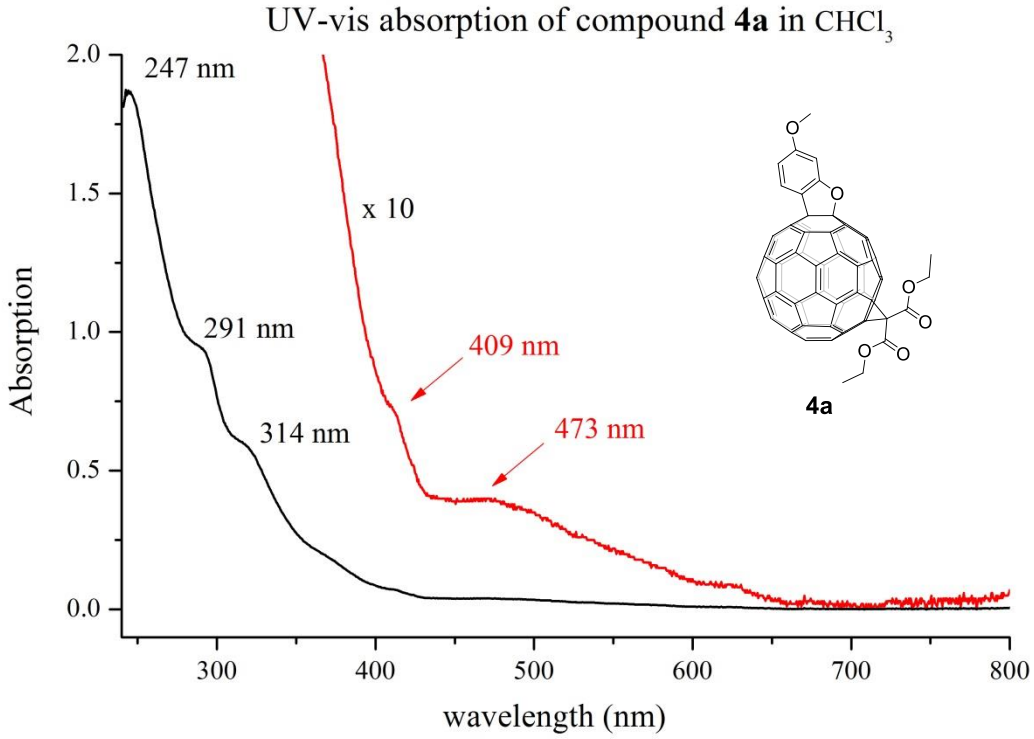
^{1}H NMR (400 MHz, $CDCl_3$) of **3b** and **4b** mixture

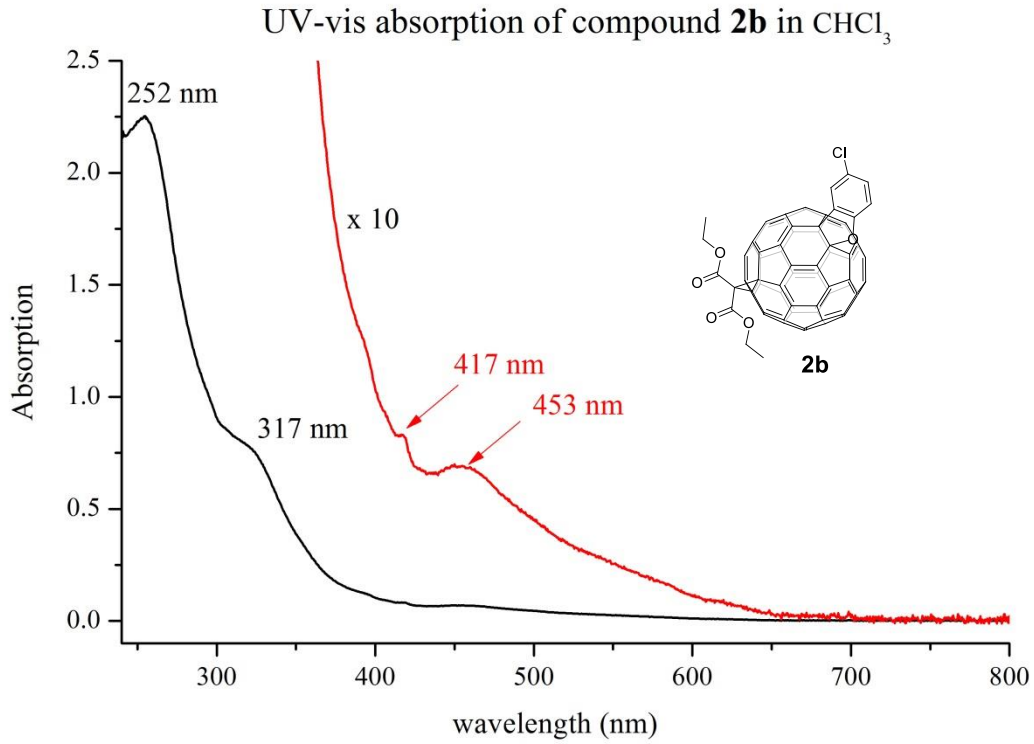


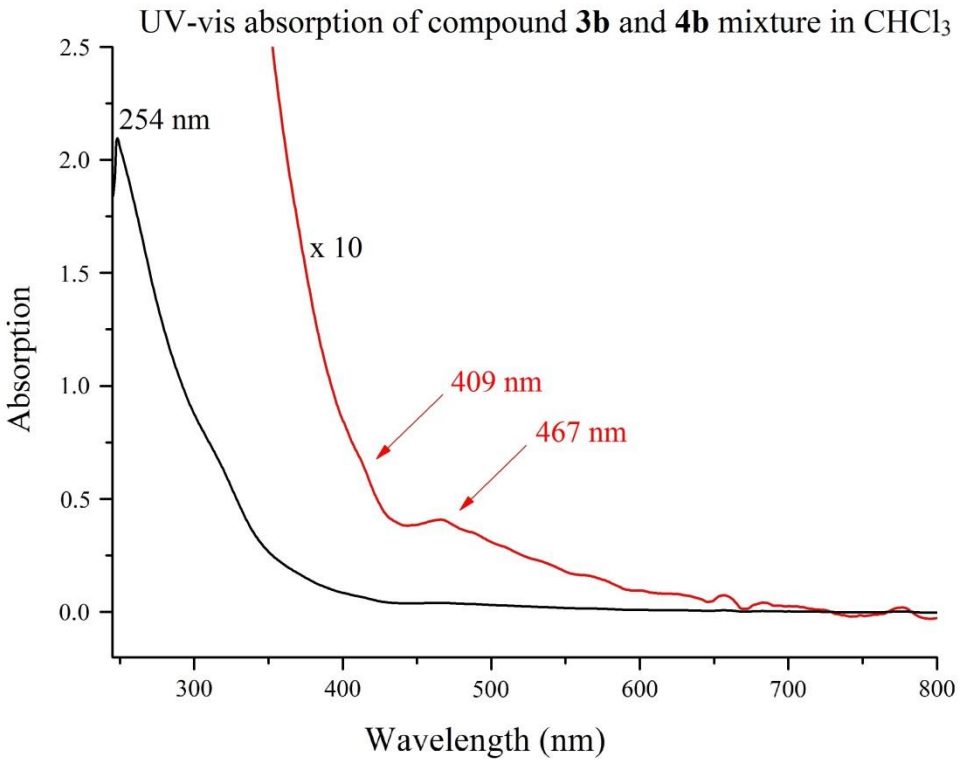
4. UV-vis spectra of compounds 2a-4b






UV-vis absorption of compound 4a in CHCl3
247 nm
x 10
291 nm
409 nm
314 nm
473 nm
4a
Absorption
wavelength (nm)


UV-vis absorption of compound 2b in CHCl3
252 nm
x 10
417 nm
453 nm
317 nm
Cl
2b
Absorption
wavelength (nm)



5. Single-crystal X-ray crystallography of compound 2a

Brown block crystals of **2a** were obtained by slow diffusion of $CHCl_3$/methanol solution at 4 ^oC in a refrigerator. Single-crystal X-ray diffraction data were collected on a diffractometer equipped with a CCD area detector using graphite-monochromated Cu Kα radiation (λ= 1.54184 Å) in the scan range 8.68°< 2θ< 139.93°. Using Olex2, the structure was solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXL refinement package using Least Squares minimisation.

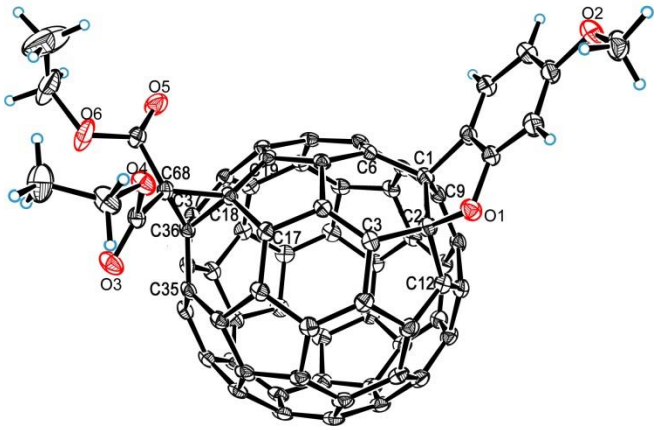


Fig. S2 ORTEP diagram for one enantiomer of **2a** with thermal ellipsoids shown at 50%

probability. The chloroform molecule was omitted for clarity.

Empirical formula	$C_{74}H_{16}O_6$•$3CHCl_3$
Formula weight	1358.97
Temperature/K	289(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	21.0174(6)
b/Å	9.9144(2)
c/Å	26.3443(8)
α/°	90
β/°	104.108(3)
γ/°	90
Volume/Å^3	5323.9(3)
Z	4
ρ_{calc} g/cm^3	1.695
μ/mm^{-1}	4.878
F(000)	2728.0
Crystal size/mm^3	0.350 × 0.320 × 0.210
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	8.676 to 139.928
Index ranges	$-24 \leq h \leq 25$, $-3 \leq k \leq 11$, $-32 \leq l \leq 30$
Reflections collected	19282
Independent reflections	9762 [R_{int} = 0.0298, R_{sigma} = 0.0511]
Data/restraints/parameters	9762/18/852
Goodness-of-fit on F^2	1.093
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0977, wR_2 = 0.2206
Final *R* indexes [all data]	R_1 = 0.1249, wR_2 = 0.2410
Largest diff. peak/hole/e Å^{-3}	1.19/-0.75

6. Optimized xyz coordinates of compounds 2a-4a

Cartesian coordinates for **2a**, **3a**, and **4a** obtained at the B3LYP/6-31G* level.

2a

0 1

C	-0.21255200	1.94672900	0.77436800
C	-0.31064900	1.95402000	-0.69686100
C	-1.46900800	1.52537300	-1.31803600
C	-2.79949000	1.27711600	-0.58925600
C	-2.67835200	1.26391100	1.01426800
C	-1.27178000	1.52920000	1.55589900
C	1.14362400	1.63191000	1.13024300
C	1.97232900	1.59473600	-0.11403200
C	0.98315400	1.64010200	-1.23504800
C	1.08565000	0.81818700	-2.35004200
C	-1.36432900	0.67909800	-2.45989100
C	-3.18815400	-0.07840600	-1.20402300
C	-3.64751300	-1.15065200	-0.47143600
C	-3.54028100	-1.15028200	1.00664300
C	-2.99350900	-0.07990900	1.67707600
C	-2.07195400	-0.31498600	2.75541600
C	-1.01179600	0.67838900	2.67306700
C	0.30015400	0.33398100	3.02147000
C	1.39968200	0.81479200	2.22467400
C	3.06550600	0.44109900	-0.18107700
C	3.13377900	-0.47385100	0.99971300
C	2.40765200	-0.25607900	2.15975700
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C	-1.77739300	-1.61180900	3.18279300
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C	-3.83595900	2.37519700	-0.78608300
C	-4.40011800	2.90402900	-1.94550800
C	-4.22253200	2.87672400	0.44793800
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H	-5.80061600	4.35857500	-2.72443300
H	-5.42614900	4.25101800	1.58119100
O	-3.60104200	2.28451400	1.50629600
O	-6.64759100	5.41704900	-0.59962300
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H	-7.80740200	6.73412400	0.38678200
H	-7.55365600	5.20307800	1.27037800
H	-6.24291100	6.41879800	1.18826500
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C	4.09254600	2.45148200	1.11446800
O	5.24730300	3.06705200	-1.14328700
O	3.66078000	3.70337000	1.33843600
C	5.95555400	3.64548300	-2.27060200

H	6.10342600	2.86456900	-3.02254300
H	5.32455700	4.42198300	-2.71368600
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H	7.09500600	4.97274700	-0.99506200
H	7.87161800	3.40399100	-1.29489900
H	7.83653700	4.63696100	-2.57280900
C	4.22056700	4.36536500	2.50106000
H	4.00019900	3.75866900	3.38464200
H	5.30828800	4.40590400	2.38564400
C	3.59767300	5.74534200	2.58149700
H	3.82257500	6.33019300	1.68396000
H	2.51034600	5.67769000	2.68638600
H	3.99591300	6.27987800	3.45066600
O	3.56502800	2.45920700	-2.52337800
O	4.87103100	1.85036600	1.81608000

3a

0 1

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C	-1.92820500	3.16125400	-2.24779000
C	0.08052300	1.69167700	-3.63640700
C	0.39139900	2.99356500	-3.06555300
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C	3.06802900	0.97076500	-1.83536700
C	3.39304400	1.65443500	-0.59756800
C	2.90087900	2.94281500	-0.36250800
C	2.40750400	3.28585500	0.94896600
C	0.17944400	3.02952100	2.70447200
C	0.16099100	4.02726500	1.64464400
C	1.25392500	4.15215300	0.78462600
C	1.03680800	4.34358500	-0.64027800
C	2.05648300	3.59368200	-1.35082400
C	1.73987500	2.93522500	-2.53897400
C	2.25900900	1.59774300	-2.78907000
C	1.24388800	0.83615200	-3.47005500
C	1.08123100	-0.52107500	-3.16856500
C	0.18052600	-2.40862600	0.79160100
C	-0.23017400	-2.05122900	-1.97565100
C	2.95418800	0.99443200	1.70835900
C	-4.54312500	-2.00401800	0.11369900
C	-4.77354500	-3.37146200	-0.02579500
C	-5.60907800	-1.15857300	0.38295200
C	-6.06912300	-3.86204800	0.10662600
H	-3.95429200	-4.05366400	-0.23578700
C	-6.91982100	-1.60886600	0.52125700
C	-7.13714800	-2.98629400	0.37796500
H	-6.28445400	-4.91992000	0.00454000
H	-7.71579400	-0.90608900	0.73063500
O	-5.26034900	0.15401600	0.50037100

O	-8.36087900	-3.57569600	0.48609900
C	-9.48589200	-2.75237100	0.75312700
H	-10.34473700	-3.42501000	0.79547500
H	-9.38465300	-2.23107500	1.71443300
H	-9.64187200	-2.01343600	-0.04379300
C	3.92179900	-2.00477600	0.35281400
C	4.97001900	-2.11904900	1.44007300
C	4.21653100	-3.07287000	-0.70189900
O	5.77719700	-3.02523900	1.44971300
O	4.90658500	-1.15551100	2.36407700
O	5.22171800	-2.66918100	-1.48998400
O	3.63614600	-4.12783000	-0.79349100
C	5.87801100	-1.24541200	3.44155100
H	5.75417800	-2.21373500	3.93600700
H	6.88017200	-1.21921800	3.00288200
C	5.62873600	-0.08144300	4.38075100
H	5.74126400	0.87480600	3.85995800
H	4.62099900	-0.12805800	4.80548800
H	6.35204700	-0.11469900	5.20272000
C	5.68167000	-3.63366200	-2.47069700
H	5.94065300	-4.55881400	-1.94768500
H	4.85578000	-3.85188800	-3.15485700
C	6.87186600	-3.02186300	-3.18286500
H	7.67960400	-2.80684200	-2.47617400
H	7.25026500	-3.72004600	-3.93790700
H	6.59232000	-2.08994900	-3.68436100

4a

0 1

C	-2.34448700	-0.60139600	2.37537500
C	-3.13456000	0.59135000	1.99835800
C	-3.66762800	0.70344600	0.73322500
C	-3.74568800	-0.45819200	-0.27049800
C	-2.87922200	-1.74999300	0.14696600
C	-2.13988800	-1.62906500	1.48354400
C	-1.26769900	-0.15666300	3.23540300
C	-1.37843600	1.28248300	3.39962700
C	-2.52268700	1.73854800	2.63449100
C	-2.47305100	2.97398700	1.97662000
C	-3.57396200	1.95508100	0.03508600
C	-3.24654800	0.25323300	-1.53963100
C	-2.31757700	-0.28110100	-2.40611700
C	-1.53131300	-1.47278000	-2.01613000
C	-1.71890200	-2.07891900	-0.79654900

C	-0.57465200	-2.48574100	-0.02714300
C	-0.83202300	-2.21487700	1.36889800
C	0.22295100	-1.80776700	2.19495400
C	-0.00509700	-0.75174700	3.15103200
C	-0.22979100	2.06904900	3.48357600
C	1.08088400	1.44740100	3.39070700
C	1.19246800	0.06195800	3.22325100
C	2.17334900	-0.49016100	2.31261000
C	1.56738200	-1.66812900	1.66536200
C	1.81718100	-1.95912100	0.33548000
C	0.72565200	-2.33992300	-0.52701300
C	0.92146900	-1.73368700	-1.82141100
C	-0.19544400	-1.30277900	-2.54947600
C	-3.31272300	1.67665600	-1.36657000
C	0.92708300	2.16890600	-3.03303400
C	-0.32393000	2.78215500	-2.95905400
C	-0.54988600	3.85293400	-1.99967700
C	0.48749200	4.27191700	-1.16445800
C	1.79004600	3.63688800	-1.25327000
C	2.78795100	1.43619300	-1.79399700
C	2.17523500	0.26413200	-2.43672700
C	1.02691300	0.72678100	-3.18706800
C	-0.13730300	-0.04381900	-3.24870000
C	-1.44124100	0.58764500	-3.16059600
C	-1.53206600	1.97784300	-3.02638900
C	-1.89091200	3.69871000	-1.46980400
C	-2.14712800	3.96755400	-0.12502400
C	-1.07190400	4.40521300	0.74674800
C	0.22073500	4.55353700	0.23737900
C	1.36018200	4.09148200	1.00866900
C	2.32694600	3.52628200	0.08135800
C	3.06099100	2.38953700	0.43588200
C	3.34293000	1.35040700	-0.52606900
C	2.13999200	-0.96476500	-1.79818900
C	2.82100400	-1.21252200	-0.48704900
C	3.47683100	0.05492700	0.21483400
C	3.01248000	0.35485700	1.60485200
C	2.86202300	1.77960700	1.73723700
C	1.93468300	2.32452600	2.63273100
C	1.16492900	3.50201400	2.25750200
C	-0.17424400	3.34646500	2.78826400
C	-1.27409600	3.78792000	2.04859300
C	-2.49051200	2.53517700	-2.10804600
C	-3.00985600	3.08329600	0.64264300

C	2.00590200	2.59987600	-2.16761100
C	-5.13049500	-1.07690800	-0.40140800
C	-6.35800300	-0.50878200	-0.73741200
C	-5.06314800	-2.43303800	-0.11822500
C	-7.49319800	-1.31272200	-0.78157700
H	-6.43522900	0.55121100	-0.96361500
C	-6.17465300	-3.27166600	-0.15122500
C	-7.40306900	-2.68666400	-0.48960700
H	-8.46433100	-0.90388500	-1.03847300
H	-6.06737100	-4.32357000	0.07948400
O	-3.81202400	-2.87266700	0.19674500
O	-8.57682800	-3.37568800	-0.56156900
C	-8.56317300	-4.76521300	-0.27263300
H	-9.59441500	-5.10389600	-0.38674000
H	-7.92054900	-5.31608500	-0.97188600
H	-8.22843400	-4.95959300	0.75476500
C	4.30797100	-1.15920100	-0.17541700
C	5.30049400	-1.01094100	-1.30805500
C	4.81193000	-2.05113100	0.95368200
C	5.19557800	-4.30491600	1.56462300
H	6.25495000	-4.10366200	1.75274400
C	7.56286800	-1.37217200	-1.92572400
H	7.25652300	-1.91127000	-2.82731700
O	4.71121300	-3.34131800	0.59534900
O	6.50350200	-1.48664400	-0.94013300
O	5.06544100	-0.51247700	-2.38514400
O	5.24451100	-1.65604200	2.01040400
H	4.65425500	-4.15359000	2.50343500
C	4.96576800	-5.68688600	0.98472500
H	5.31883400	-6.44685700	1.69013000
H	3.90150700	-5.85927200	0.79614400
H	5.50843600	-5.81222000	0.04239700
H	7.67620400	-0.31624400	-2.18897300
C	8.82082400	-1.94967700	-1.30733300
H	9.64865800	-1.87564000	-2.02070100
H	9.09669400	-1.40390300	-0.39976700
H	8.68222200	-3.00430400	-1.04906000

7. Comparison of calculated and experimental ^{1}H NMR spectra of compounds 2a-4a

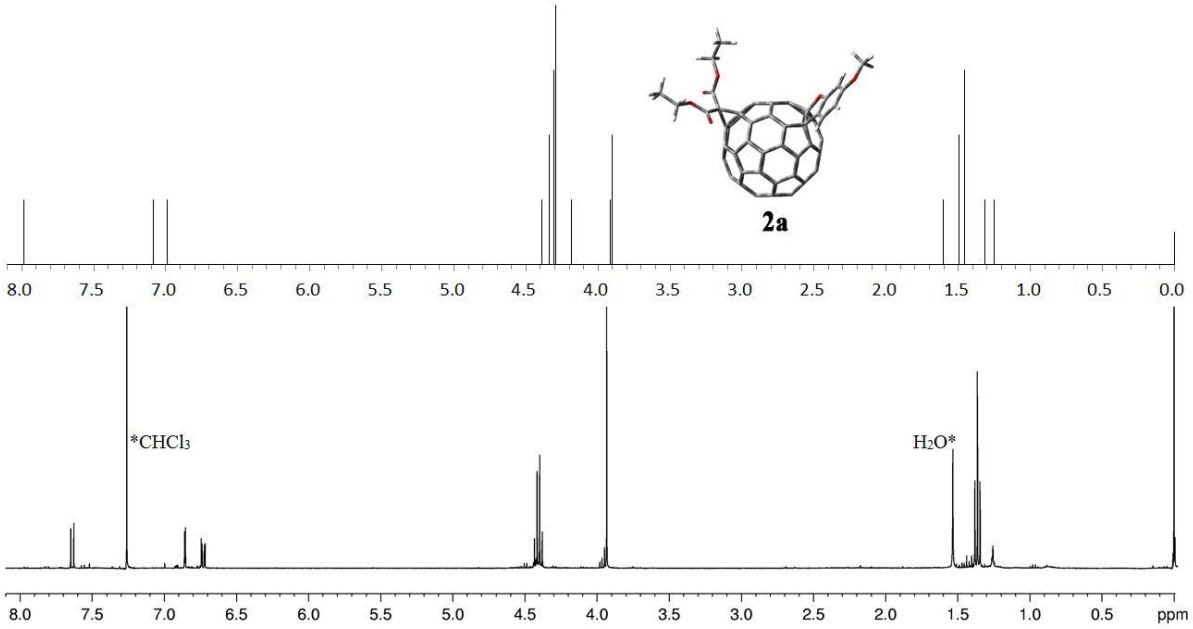


Fig. S3 Comparison of the calculated ^{1}H NMR spectrum at the B97-2/def2-TZVP level with the experimental ^{1}H NMR spectrum of compound **2a**

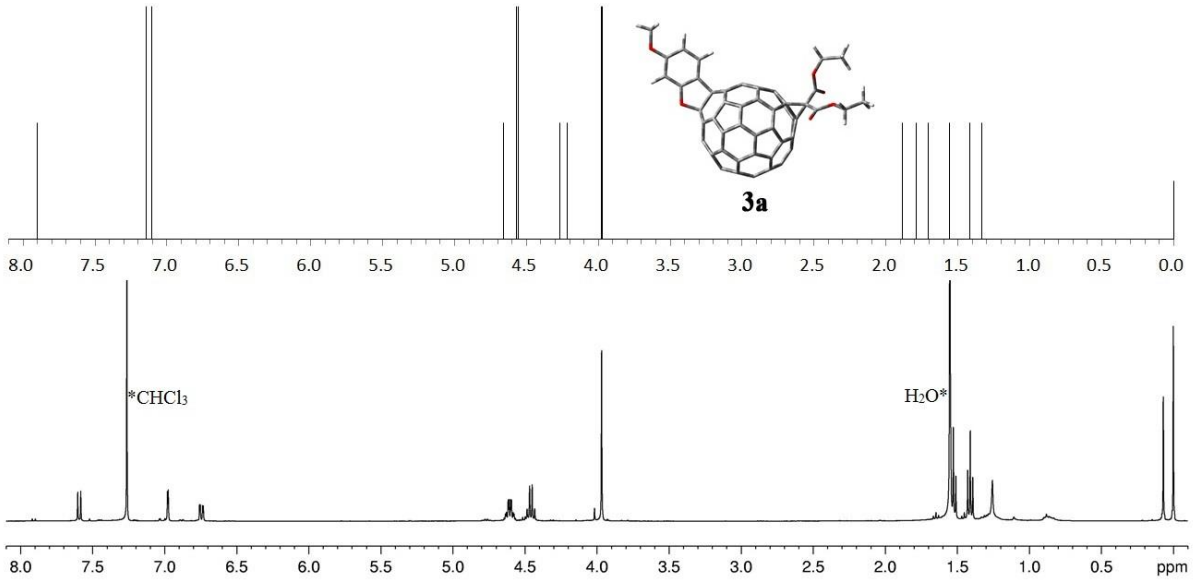


Fig. S4 Comparison of the calculated ^{1}H NMR spectrum at the B97-2/def2-TZVP level with the experimental ^{1}H NMR spectrum of compound **3a**

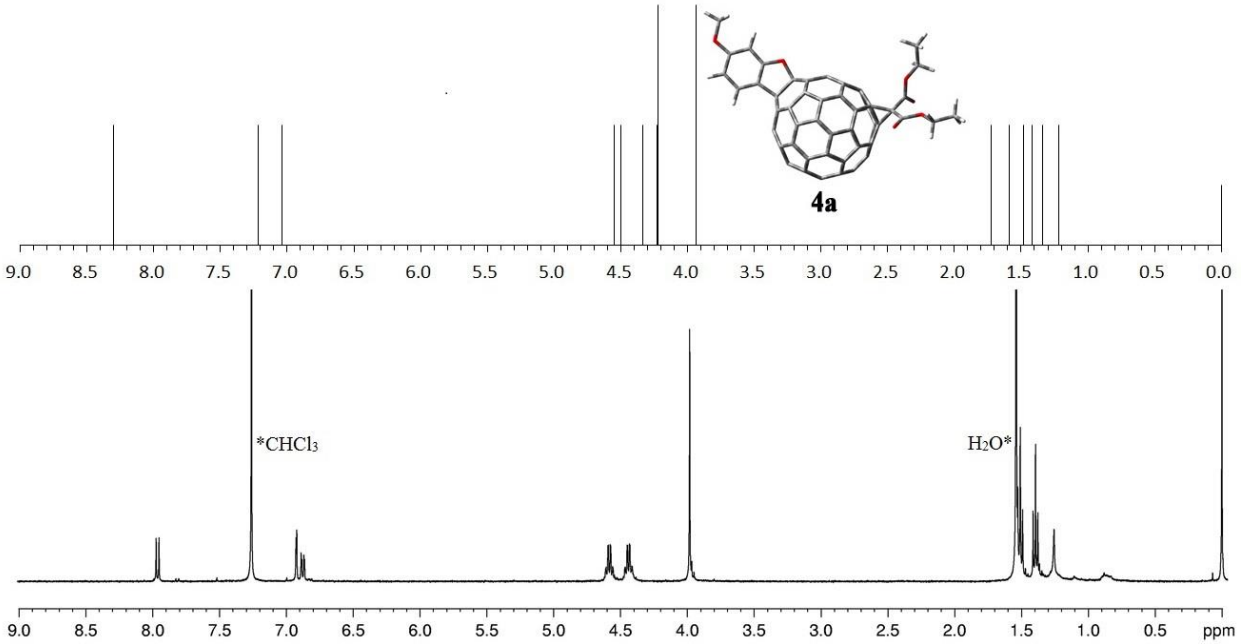


Fig. S5 Comparison of the calculated ^{1}H NMR spectrum at the B97-2/def2-TZVP level with experimental ^{1}H NMR spectrum of compound **4a**

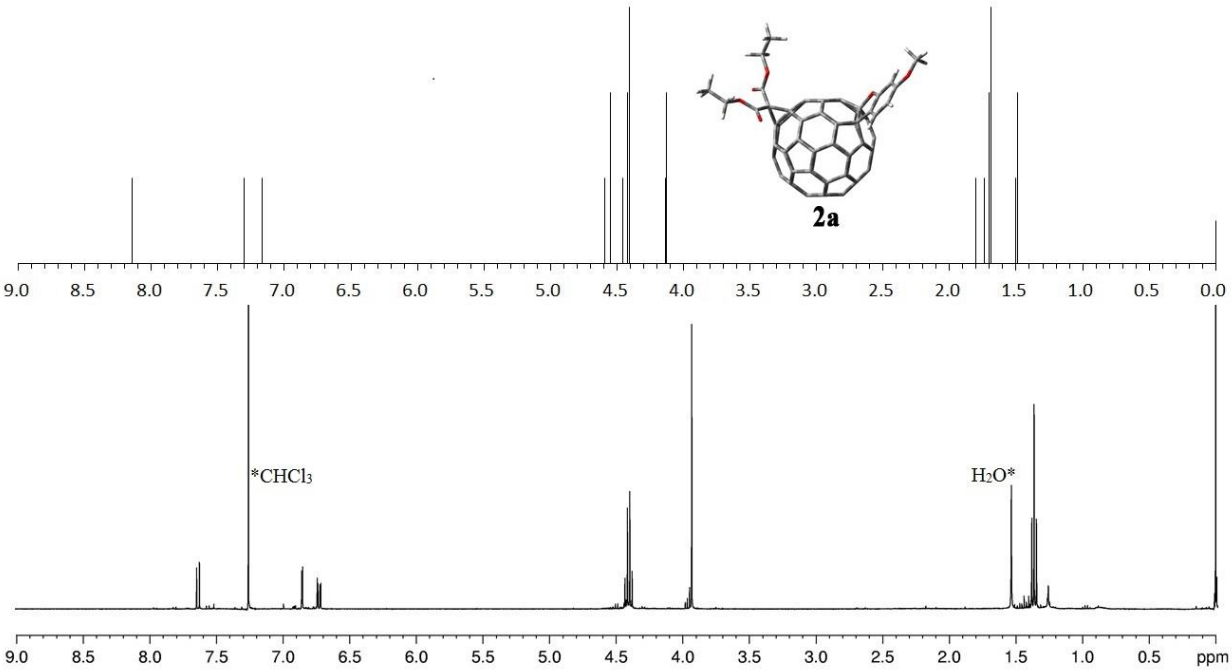


Fig. S6 Comparison of the calculated ^{1}H NMR spectrum at the B3LYP/6-311++G level with the experimental ^{1}H NMR spectrum of compound **2a**

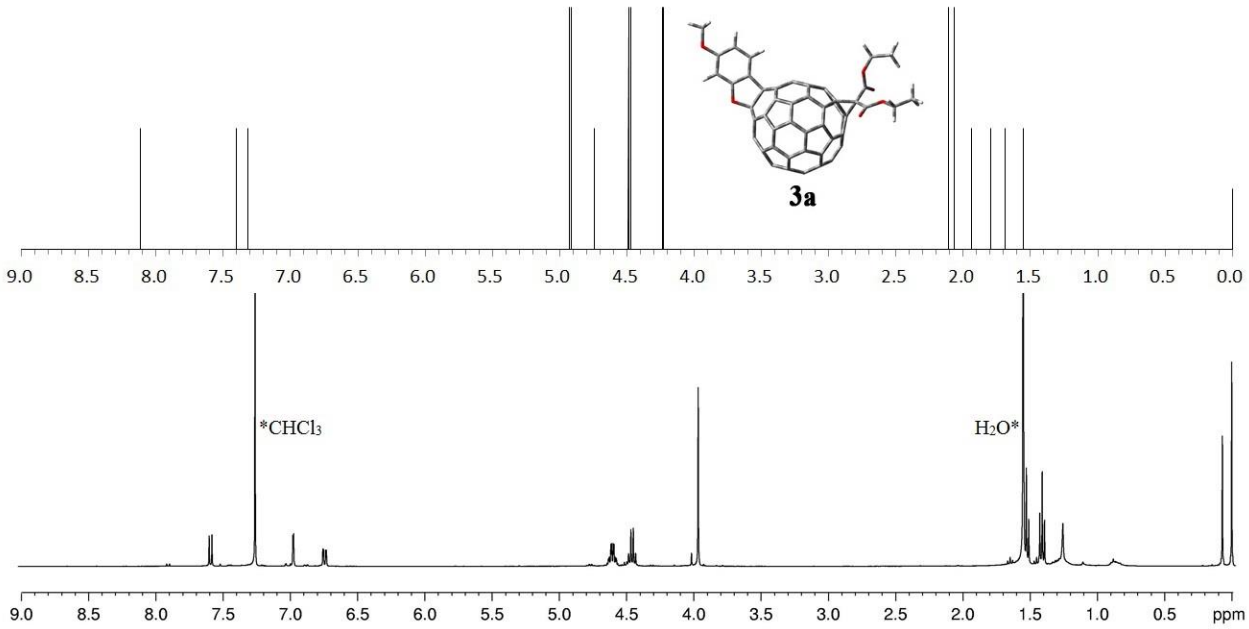


Fig. S7 Comparison of the calculated ^{1}H NMR spectrum at the B3LYP/6-311++G level with the experimental ^{1}H NMR spectrum of compound **3a**

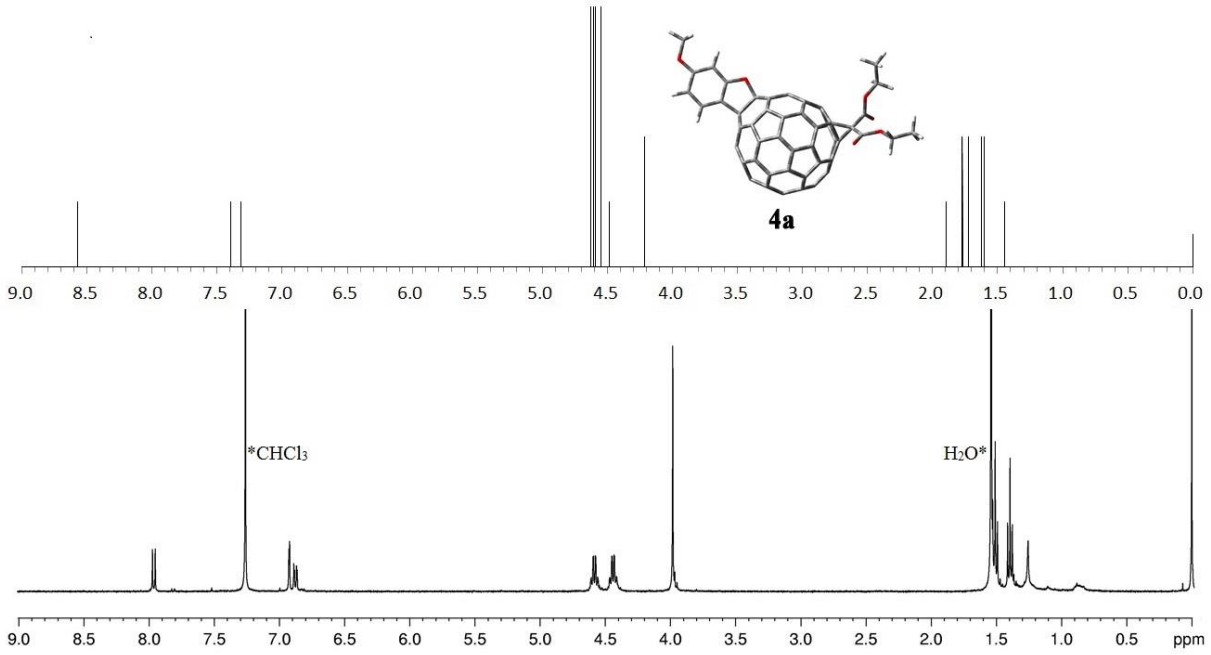


Fig. S8 Comparison of the calculated ^{1}H NMR spectrum at the B3LYP/6-311++G level with the experimental ^{1}H NMR spectrum of compound **4a**

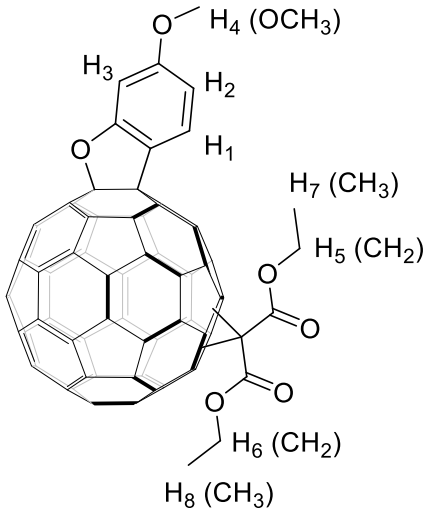


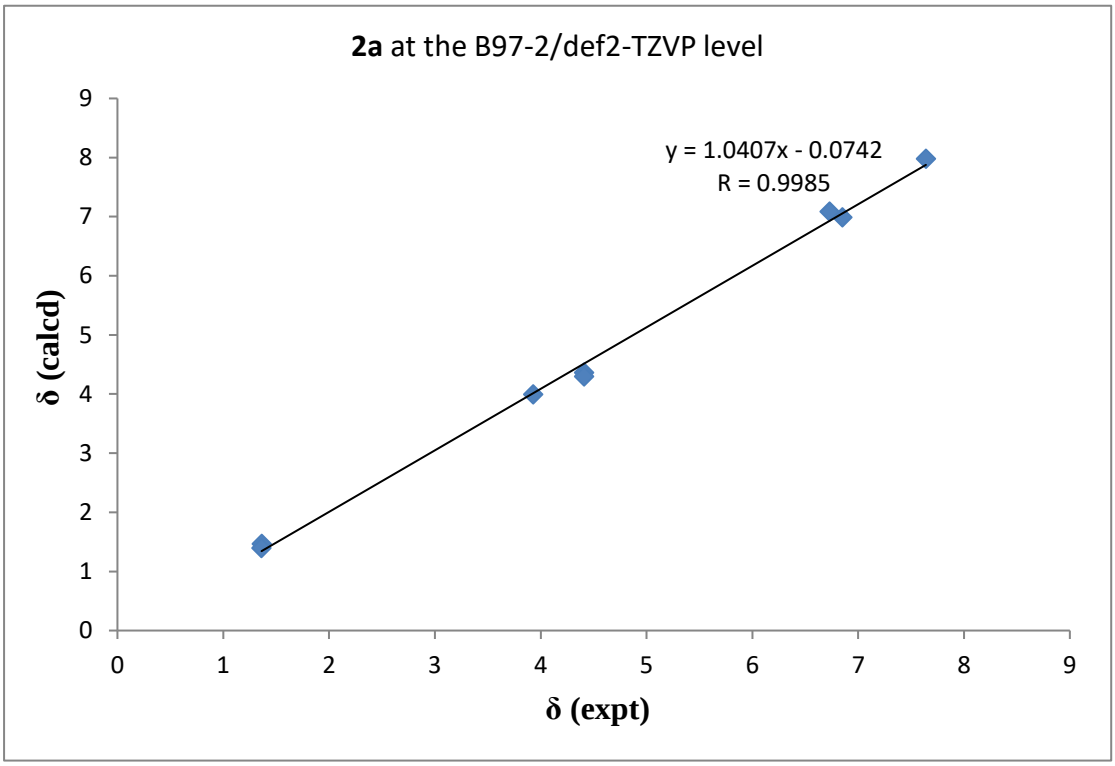
Table S1. Calculated ^{1}H NMR data at the B97-2/def2-TZVP level

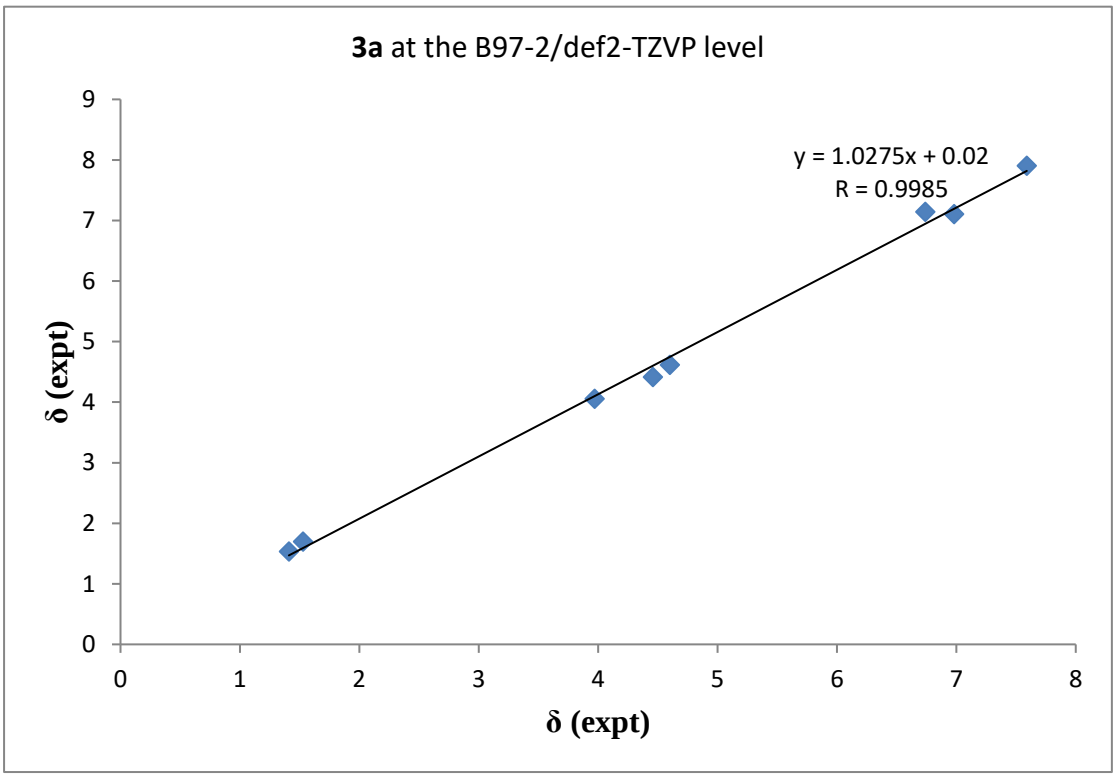
Structure	Chemical shifts	H_1	H_2	H_3	H_4 (OCH_3)	H_5 (CH_2)	H_6 (CH_2)	H_7 (CH_3)	H_8 (CH_3)
2a	δ (calcd)	7.98	7.09	6.99	4.18 3.92 3.90	4.39 4.34	4.30 4.29	1.61 1.49 1.31	1.50 1.45 1.25
	δ (expt)	7.64	6.73	6.85	3.93	4.41	4.41	1.363	1.362
3a	δ (calcd)	7.90	7.14	7.10	4.22 3.98 3.97	4.66 4.57	4.55 4.27	1.88 1.79 1.42	1.70 1.56 1.33
	δ (expt)	7.59	6.74	6.98	3.97	4.65-4.55	4.46	1.53	1.41
4a	δ (calcd)	8.30	7.22	7.04	4.22 3.94 3.93	4.55 4.50	4.34 4.23	1.72 1.59 1.42	1.49 1.34 1.22
	δ (expt)	7.96	6.87	6.92	3.98	4.62-4.49	4.48-4.40	1.51	1.39

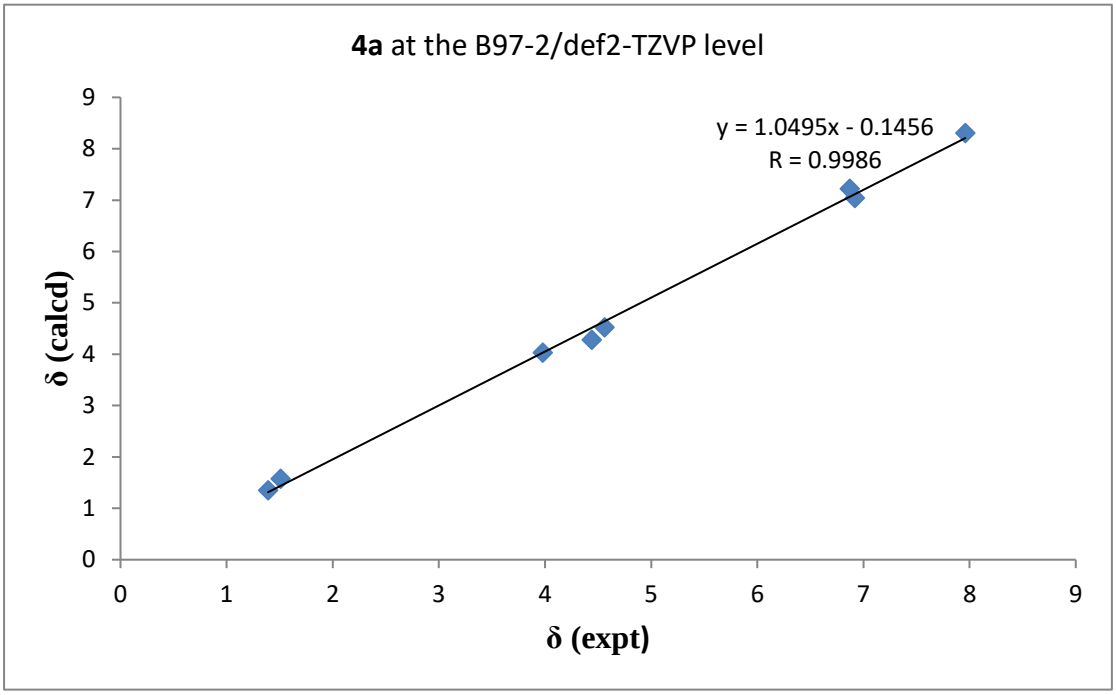
Table S2. Calculated ^{1}H NMR data at the B3LYP/6-311++G level

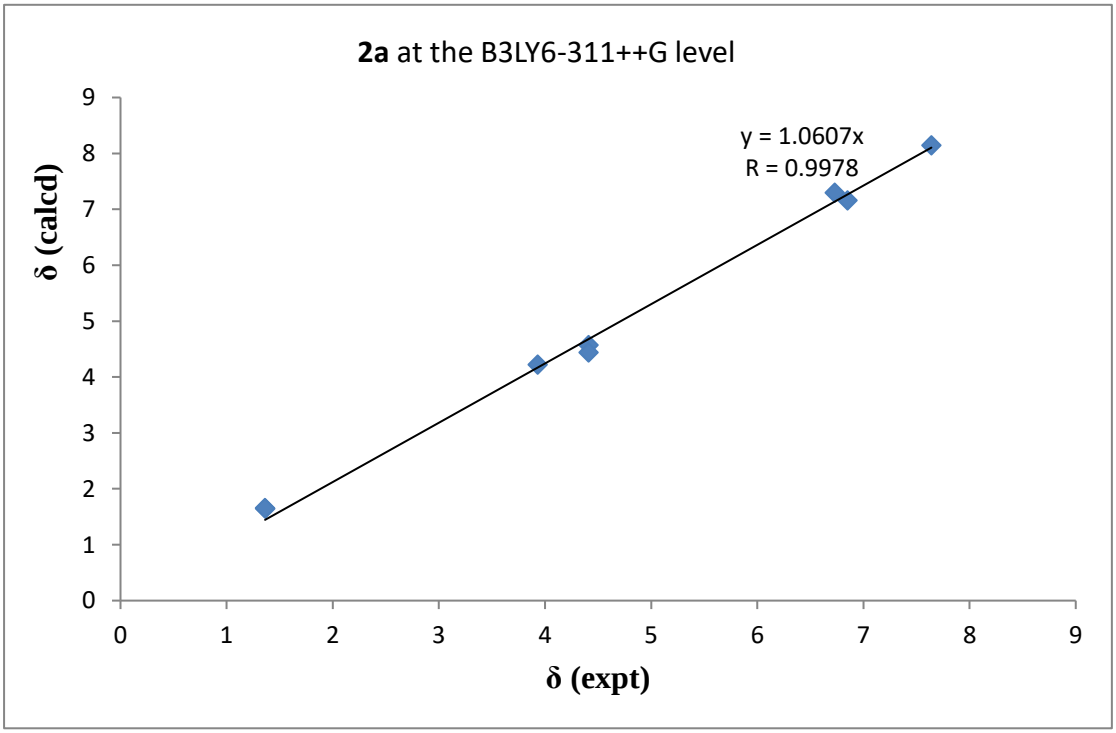
Structure	Chemical shifts	H_1	H_2	H_3	H_4 (OCH_3)	H_5 (CH_2)	H_6 (CH_2)	H_7 (CH_3)	H_8 (CH_3)
2a	δ (calcd)	8.15	7.30	7.16	4.41 4.13 4.13	4.59 4.55	4.46 4.42	1.74 1.70 1.50	1.80 1.69 1.49
	δ (expt)	7.64	6.73	6.85	3.93	4.41	4.41	1.363	1.362
3a	δ (calcd)	8.12	7.32	7.40	4.47 4.23 4.23	4.93 4.91	4.74 4.49	2.11 2.07 1.69	1.94 1.79 1.55
	δ (expt)	7.59	6.74	6.98	3.97	4.65-4.55	4.46	1.53	1.41
4a	δ (calcd)	8.57	7.40	7.32	4.55 4.21 4.21	4.63 4.61	4.59 4.49	1.90 1.77 1.62	1.72 1.61 1.45
	δ (expt)	7.96	6.87	6.92	3.98	4.62-4.49	4.48-4.40	1.51	1.39

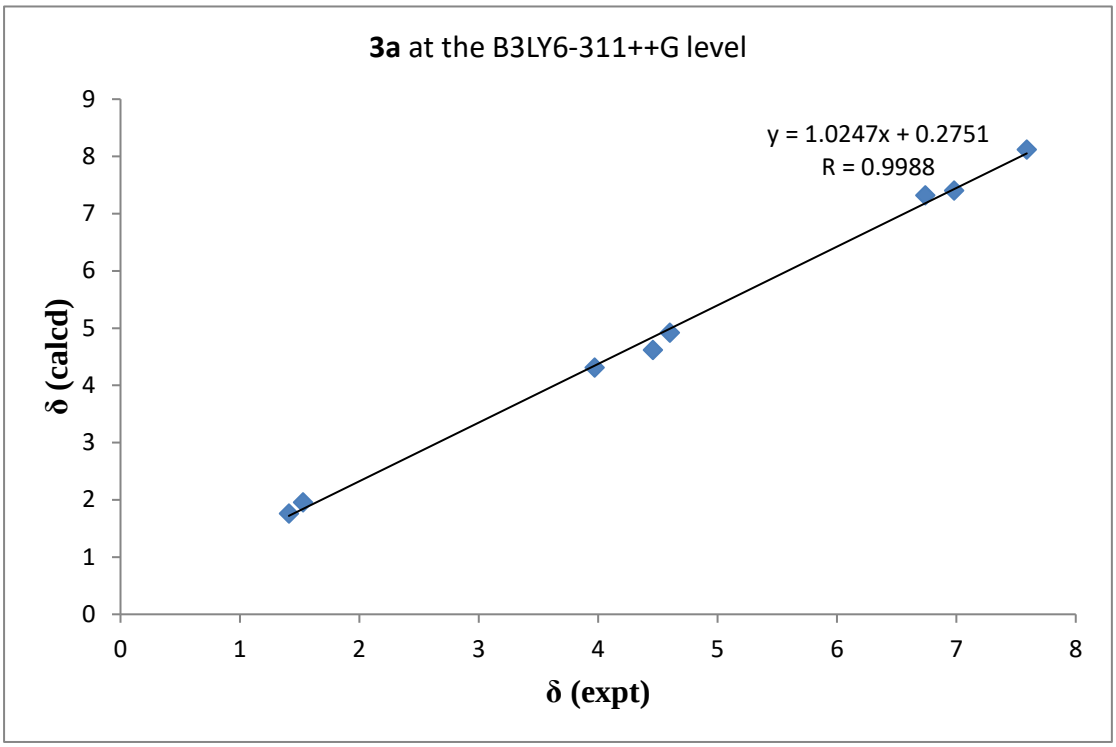
Linear correlations between the experimental and calculated chemical shifts of **2a-4a** (Note: the calculated chemical shifts for the protons in the OCH_3 and OCH_2CH_3 moieties had been averaged for comparison).

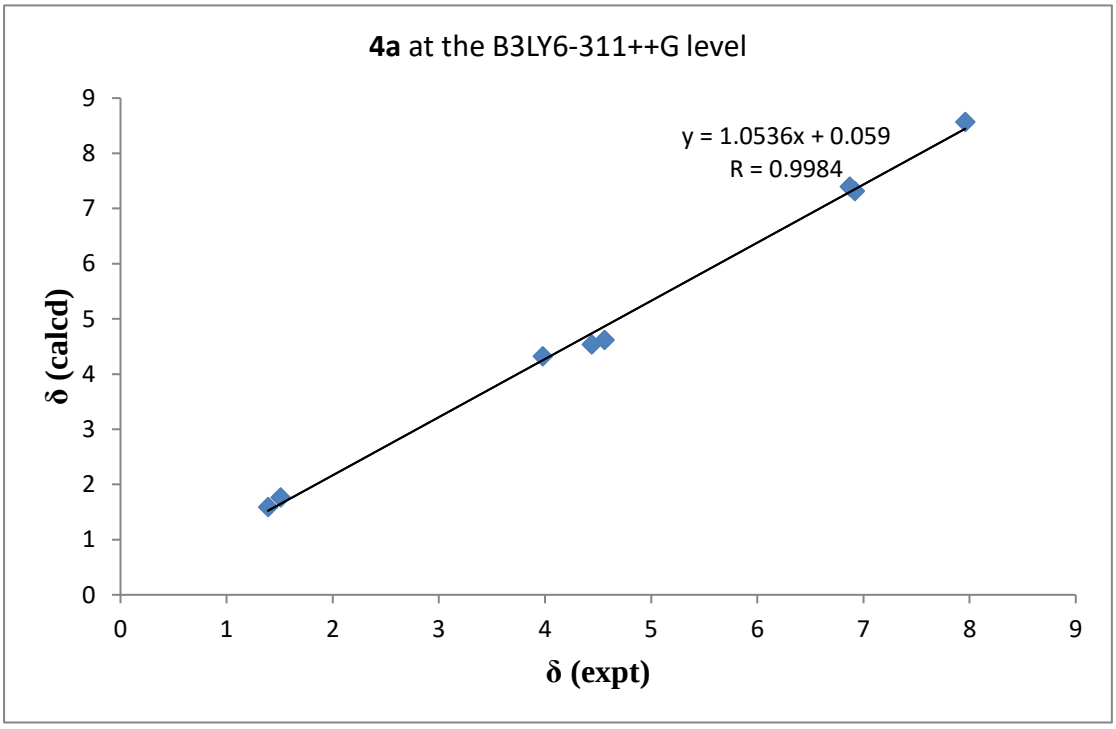





4a at the B97-2/def2-TZVP level
y = 1.0495x - 0.1456
R = 0.9986
δ (calcd)
δ (expt)
0
1
2
3
4
5
6
7
8
9


2a at the B3LY6-311++G level
y = 1.0607x
R = 0.9978
δ (calcd)
δ (expt)
0
1
2
3
4
5
6
7
8
9


3a at the B3LY6-311++G level
y = 1.0247x + 0.2751
R = 0.9988
δ (calcd)
δ (expt)
0
1
2
3
4
5
6
7
8
9


4a at the B3LY6-311++G level
y = 1.0536x + 0.059
R = 0.9984
δ (calcd)
δ (expt)
0
1
2
3
4
5
6
7
8
9