BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis of indano[60]fullerene thioketone and its application in organic solar cells

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Experimental procedures, device fabrication, method of single-crystal growth, device evaluations and characterizations

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1. General

Methods

To ensure optimal reaction conditions, all reactions that were sensitive to air or moisture were conducted in a dehydrated reaction vessel, under a carefully controlled nitrogen atmosphere. The transfer of air or moisture sensitive liquids and solutions was carried out using a syringe or Teflon cannula, which enabled accurate and precise delivery of the reagents. Prior to use, solvents were screened for their water content using the Karl-Fischer titration method with MKC-210 (Kyoto Electronics Manufacturing Co., Ltd.), and solvents should contain less than 30 ppm of water. Analytical thin-layer chromatography (TLC) was performed using a glass plate coated with 0.25mm 230–400 mesh silica gel containing a fluorescent indicator, allowing for precise detection and analysis of the reaction components. To remove the organic solutions, a diaphragm pump through a rotary evaporator was employed for evacuation. Nuclear Magnetic Resonance (NMR) was taken by ECS 400 and ECA 600 (JEOL Co., Ltd.) at room temperature reported in parts per million (ppm). ^{1}H NMR spectra were internally referenced to tetramethylsilane (0.00 ppm) or $CDCl_3$ (7.260 ppm). ^{13}C NMR spectra were internally referenced to tetramethylsilane (0.0 ppm) or $CDCl_3$ (77.16 ppm). The data were presented as following order: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, hept = heptet, m = multiplet and/or multiplet resonances), coupling constant in hertz (Hz), and signal area integration in natural numbers, assignment (italic). Matrix assisted laser desorption/ionization time-of- flight mass spectrometry (MALDI-TOF MS) was taken by AXIMA Performance (SHIMADZU Co., Ltd.). Super Photon ring-8 GeV (Spring-8) was employed to analyse the structure of single crystal of *t*-Bu-FIDS.

Materials

Unless otherwise noted, all materials including dry solvents were obtained from commercial suppliers (Sigma-Aldric, TCI, Wako) and used without further purification.

Photovoltaic device fabrication and evaluation

BHJ OPV Device fabrication

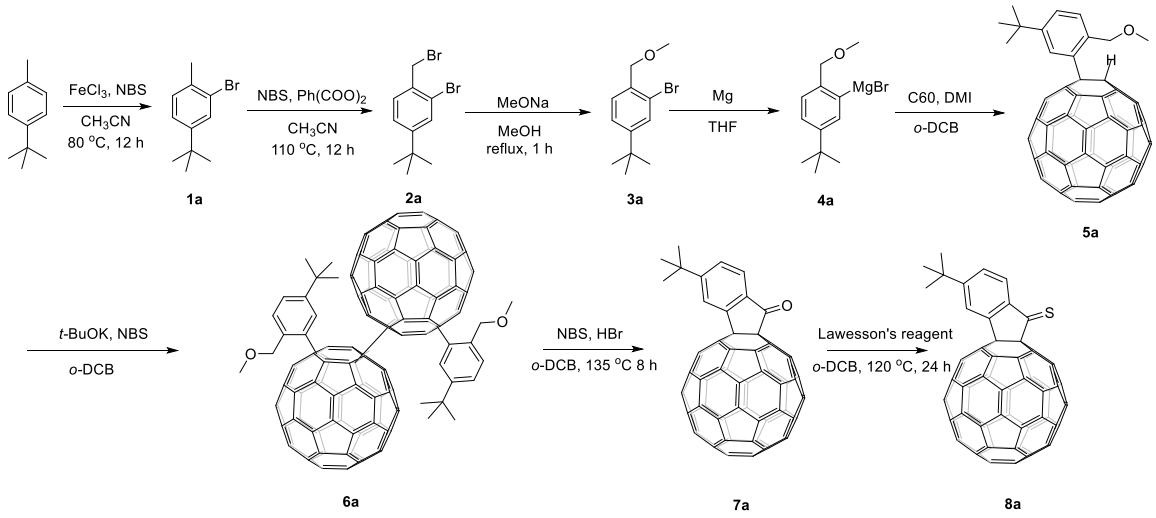
The OPV structure was fabricate using ITO/ZnO/Fullerene:P3HT (1:1, w/w)/PEDOT:PSS/Ag (ITO/ZnO/Fullerene:PNTz4T(2:1,w/w)/MoO_x/Ag). ITO-coated glass (sheet resistance ≤ 10 Ω cm^2) was cleaned consecutively in detergent, deionized water, acetone, isopropanol, and ethanol ultrasonic baths for 15 min, respectively. The ITO glass was treated with UV-Ozone for 15 min before use. BHJ solution was simply mixed P3HT and fullerene together in *o*-DCB at concentration 15 mg /ml (1:1 w/w) and keeping string 1 h at 60 ^oC before using (2:1 for fullerene: PNTz4T). The 0.5% ZnO was prepared by dilution of 40% ZnO with ethanol, then keeping ultrasound about 20 min before using. To prepare the ZnO film, 2 drops of 0.5% ZnO solution was spin-coated on the substrates at 3000 rpm for 30 s, then the film was annealed at 80 ^oC for 10 min. Blend layer was deposited by spin coating the prepared blend solutions on the top of the ZnO layer at 1000 rpm for 30 s (600 rpm for 20 s for PNTz4T device). To get the better performance of the film, the substrates then was keeping under room temperature for 20 min. HTL then was deposited on the active layer with condition 3000 rpm for 180 s (MoO_x was 7.5 nm by vacuum deposited for PNTz4T device). Finally, the Ag electrode (thickness about 100 nm) was deposited by thermal evaporation under high vacuum (10^{-4} mbar). After fabrication, the device was annealed at 150 ^oC for 5 min.

Evaluation of photovoltaic performance

The *J*–*V* measurement was performed via the solar simulator (HAL-C100, Asahi spectral) along with AM 1.5G spectra at 100 mW cm^2. The source unit (B2902A, Keysight) was used to measure the *J*–*V* curve.

2. Synthesis of FIDSs

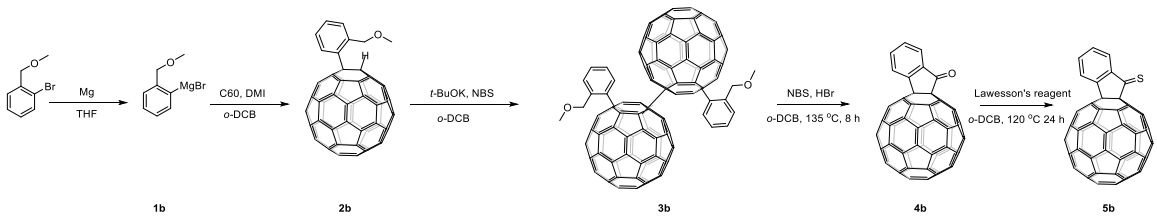
(1) *t*-Bu-FIDS



Experiment details from 1a to 7a can be found in our previous work [1].

Synthesis of *t*-Bu-FIDS (8a). A mixture of **7a** (210 mg, 0.238 mmol) and Lawesson's reagent (1350 mg, 3.341 mmol) in 15 mL *o*-DCB (dry) was stirring at 120 °C for 24 hours under N_2 atmosphere. After cooled to room temperature, the reaction solution was poured into 300 mL of methanol to settle out the crude product. The filtered crude product then was purified by column chromatography on silica gel using CS_2 as eluent to afford ***t*-Bu-FIDS** as reddish brown solid. Yield: ***t*-Bu-FIDS**, 95 mg, 45%. MALDI-TOF MS *m/z* calcd for $C_{71}H_{12}S$ $[M]^+$ 896.06, found 897.05. ^{13}C NMR (101 MHz, CHLOROFORM-D) δ 233.47, 161.69, 156.41, 156.17, 152.88, 147.92, 147.66, 147.55, 146.56, 146.51, 146.30, 146.20, 146.05, 145.87, 145.61, 145.56, 145.52, 144.86, 144.49, 143.25, 142.97, 142.92, 142.71, 142.40, 142.21, 141.99, 141.92, 140.81, 140.31, 135.80, 135.01, 128.73, 128.14, 122.80, 36.29, 31.30. ^1H NMR (400 MHz, Chloroform-d) δ 8.47 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 1.3 Hz, 1H), 7.83 (dd, *J* = 8.4, 2.1 Hz, 1H), 1.54 (s, 9H).

(2) H-FIDS

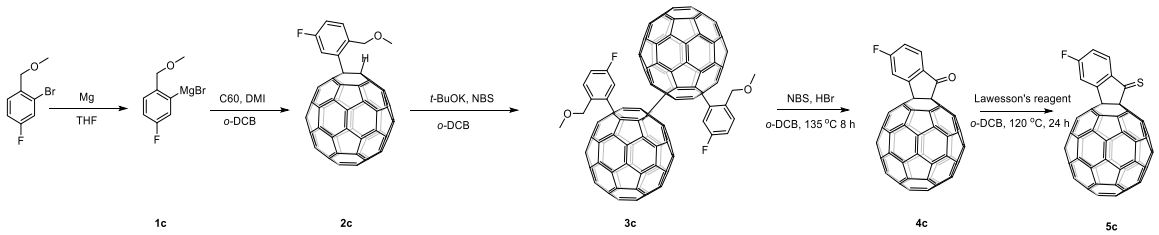


Experiment details from 1b to 4b can be found in our previous work [1].

Synthesis of H-FIDS (5b). A mixture of **4b** (130 mg, 0.157 mmol) and Lawesson's reagent (1276 mg, 3.159 mmol) in 15 mL *o*-DCB (dry) was stirring at 120 °C for 24 hours under N_2

atmosphere. After cooled to room temperature, the reaction solution was poured into 300 mL of methanol to settle out the crude product. The filtered crude product then was purified by column chromatography on silica gel using CS_2 as eluent to afford **H-FIDS** as reddish brown solid. Yield: **H-FIDS**, 50 mg, 38%. MALDI-TOF MS *m/z* calcd for $C_{67}H_4S$ $[M]^+$ 840.0, found 840.92. ^{13}C NMR (101 MHz, Chloroform-d) δ 234.56, 156.32, 155.89, 152.68, 147.83, 147.67, 147.57, 146.58, 146.32, 146.22, 146.03, 145.78, 145.64, 145.53, 144.85, 144.51, 144.33, 143.26, 142.99, 142.93, 142.72, 142.41, 142.38, 142.23, 142.02, 141.92, 140.80, 140.32, 136.65, 130.59, 128.36, 126.74. ^1H NMR (400 MHz, Chloroform-d) δ 8.55 (d, 1H, *J* = 7.9 Hz), 8.43 (d, 1H, *J* = 7.8 Hz), 8.06 (m, 1H), 7.80 (m, 1H).

(3) F-FIDS



Experiment details from 1c to 4c can be found in our previous work [2].

Synthesis of F-FIDS (5c). A mixture of **4c** (70 mg, 0.083 mmol) and Lawesson's reagent (671.7 mg, 1.66 mmol) in 10 mL *o*-DCB (dry) was stirring at 120 °C for 24 hours under N_2 atmosphere. After cooled to room temperature, the reaction solution was poured into 300 mL of methanol to settle out the crude product. The filtered crude product then was purified by column chromatography on silica gel using CS_2 as eluent to afford **F-FIDS** as reddish brown solid. Yield: **F-FIDS**, 35.8 mg, 50% ^{13}C NMR (101 MHz, Chloroform-d) δ 232.46, 169.87, 167.25, 155.81, 151.93, 147.70, 147.66, 147.60, 146.61, 146.54, 146.33, 146.24, 145.98, 145.73, 145.62, 145.56, 145.53, 144.83, 144.47, 143.25, 143.00, 142.94, 142.70, 142.41, 142.23, 142.22, 142.02, 141.88, 140.87, 140.38, 135.95, 134.94, 130.74, 130.64, 119.38, 119.14, 113.60, 113.36, 89.40.^1H NMR (400 MHz, Chloroform-d) δ 8.60-8.55 (m 1H), 8.11 – 8.04 (m, 1H), 7.52-7.48 (m, 1H). MALDI-TOF MS *m/z* calcd for $C_{67}H_3FS$ $[M]^+$ 857.99, found 857.66.

3. Simulation of IR spectra by Gaussian 16

Frequency calculation was using DFT B3LYP functional with a basis set of 6-31G*. [3-5] All the calculation was conducted by Gaussian 16. [6]

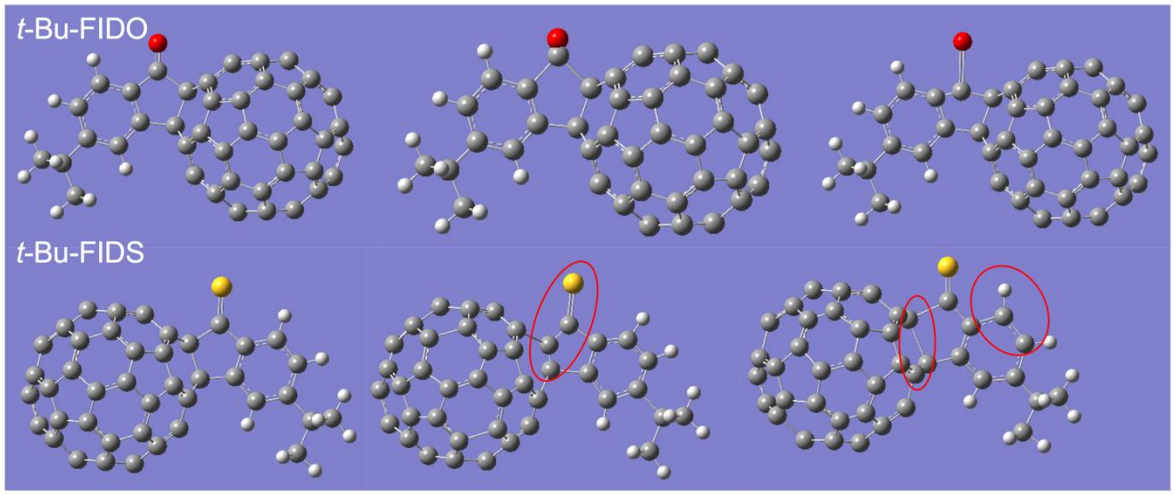


Figure S1. The simulated vibration *t*-Bu-FIDO and *t*-Bu-FIDS.

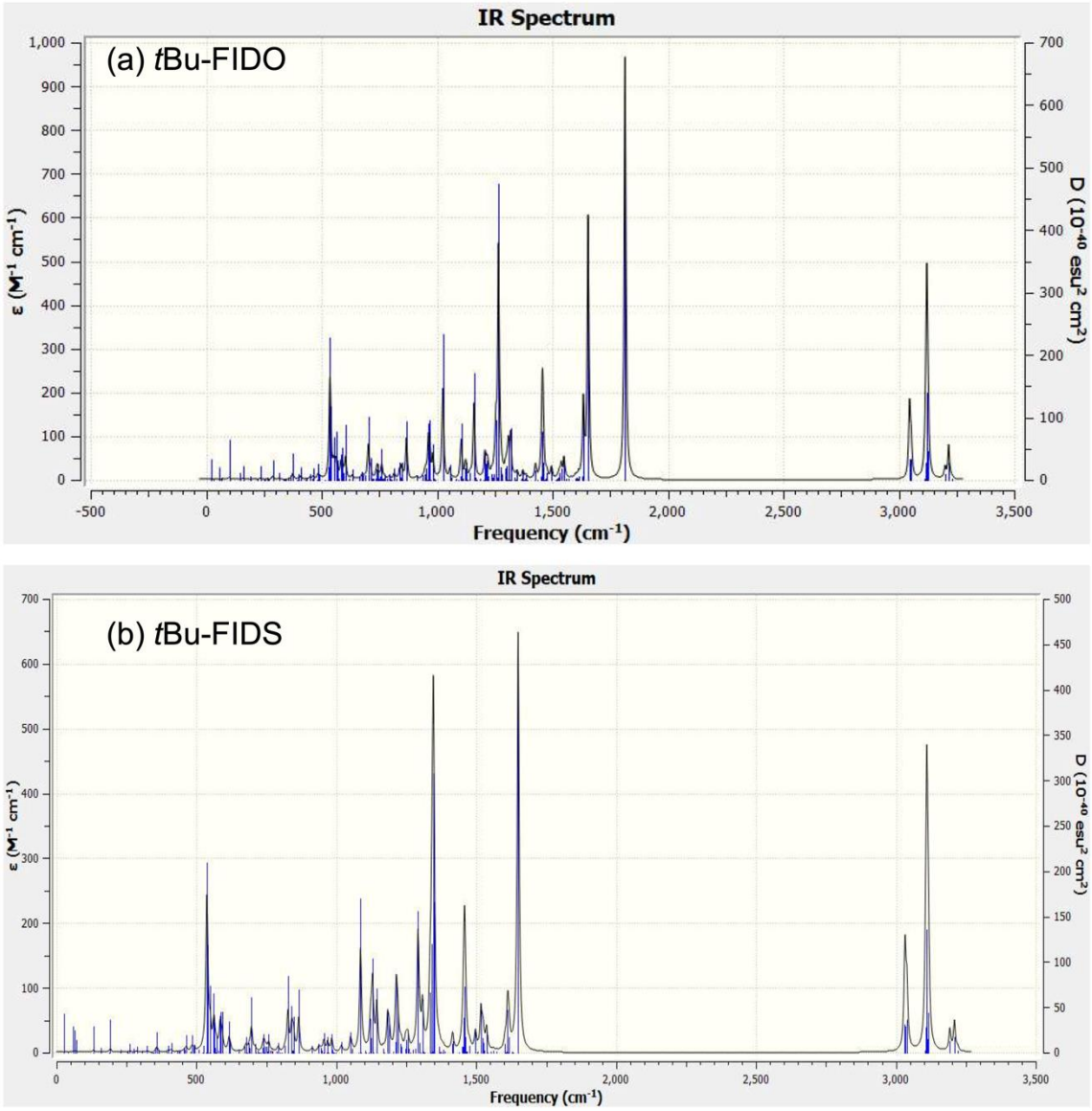


Figure S2. The simulated vibration frequency of (a) *t*-Bu-FIDO and (b) *t*-Bu-FIDS.

4. Thermal property characterized by TG-DTA

Method and procedure of TG-DTA:

Thermogravimetry Thermal Analysis (TG-DTA) is taken by DTG-60AH (SHIMADZU CO.). It is worth mentioning that the sample used for TG-DTA characterization is fullerene powder after removing the organic solvent. Under a N_2 gas flow with temperature ramp rate of 10 °C /min from rt to 800 °C.

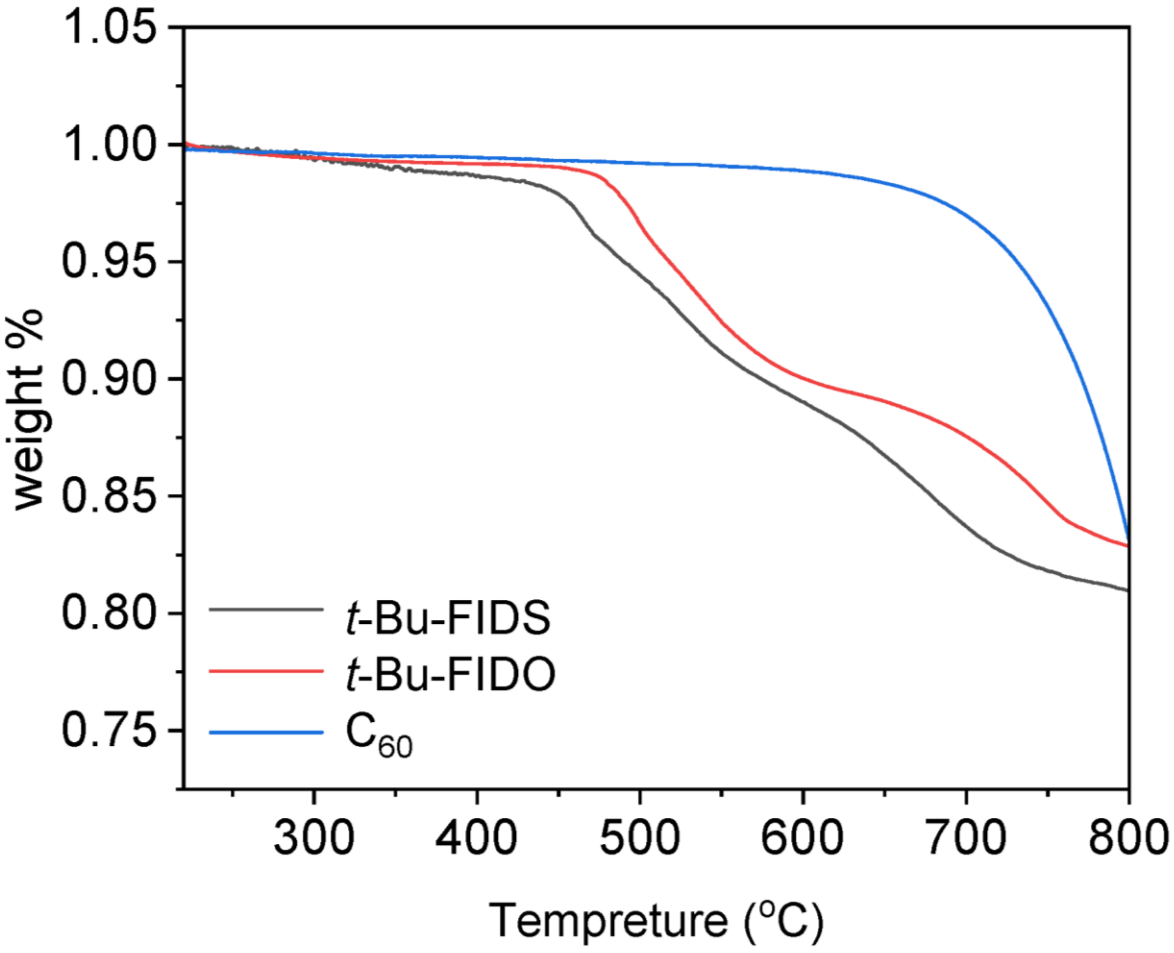


Figure S3. Normal pressure TGA of C60 (Bule), *t*-Bu-FIDO (Red) and *t*-Bu-FIDS (Black).

5. Crystal growth and single-crystal structural analysis

Single crystals of *t*-Bu-FIDS were successfully grown by liquid-liquid diffusion method. *t*-Bu-FIDS was dissolved in carbon disulfide at a concentration of 1 mg/mL and then transferred into the narrow receiver. An equal volume of ethanol was slowly added to a narrow receiver via a subcutaneous syringe, resulting in the formation of clearly distinct layers. The system was then sealed and left undisturbed for a period of 14 days. Single crystal X-ray diffraction data was collected at 100 K using the diffractometer with a DECTRIS EIGER X 16M detector at beamline BL41XU of SPring-8 large synchrotron radiation facility (Hyogo, Japan). X-ray structure analysis of *t*-Bu-FIDS: $C_{71}H_{12}S$, 100 K, orthorhombic, P_{bca}, a = 17.4935(2) Å, b = 16.1506(2) Å, c = 28.4847(2) Å, V = 8047.80(15) Å^3, Z = 8, R (wR) = 0.0747 (0.1748) for 727 parameters and 19499 unique reflections. Cambridge Crystallographic Data Center (CCDC) deposition number is 2332797.

6. Photographs of films

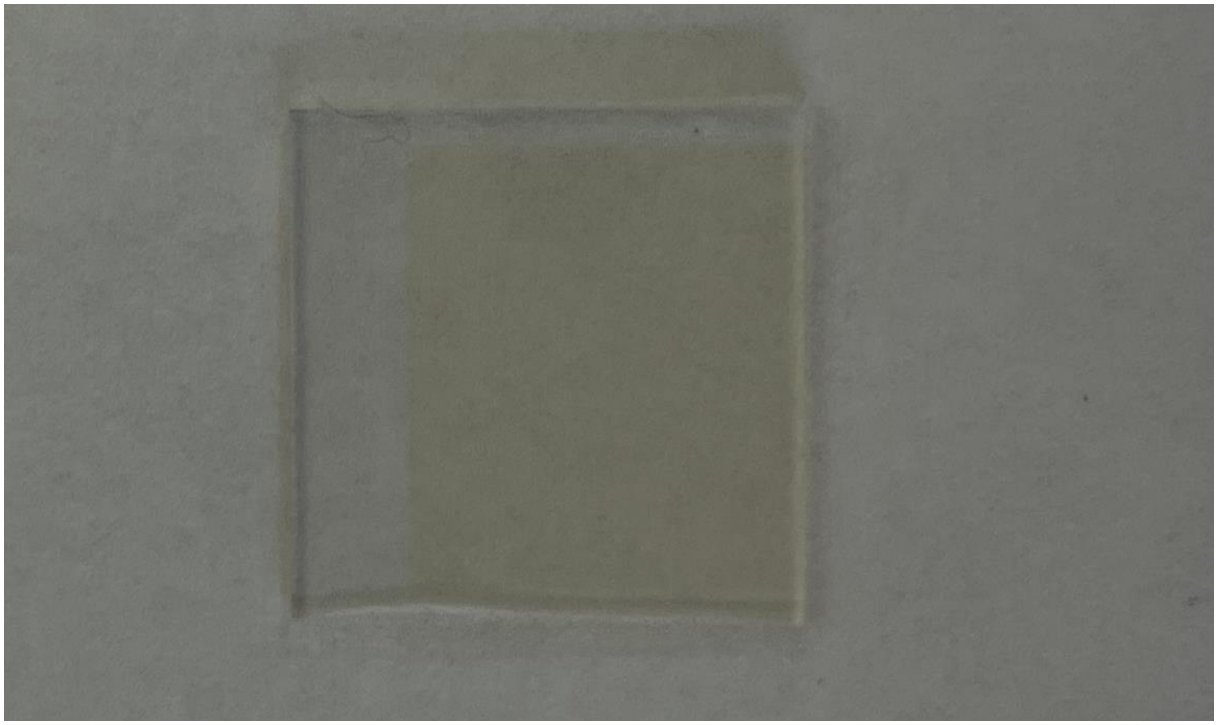
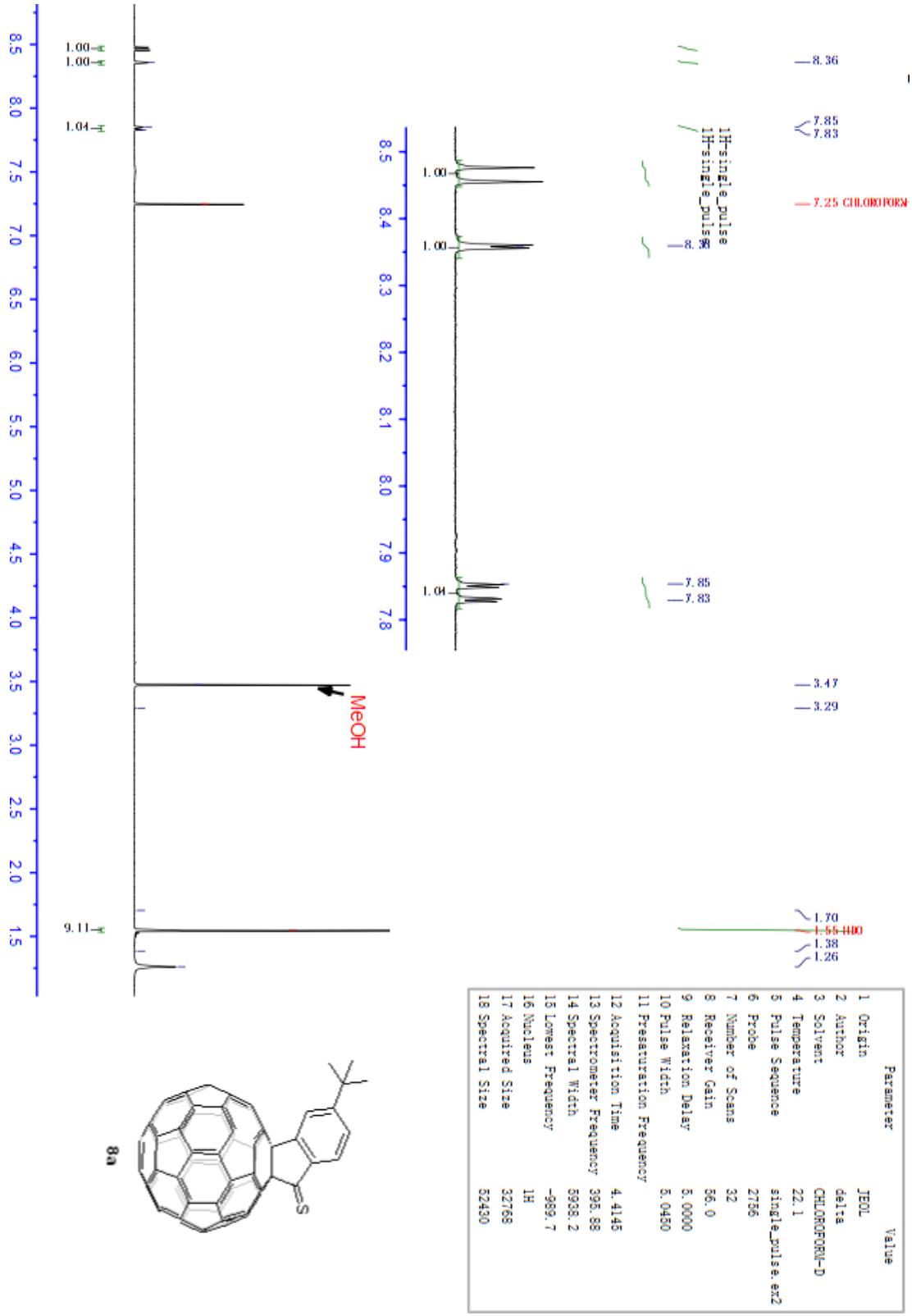


Figure S4. Photograph of evaporated *t*-Bu-FIDS film.

7. NMR and MS spectra



Parameter	Value
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2 Author	delta
3 Solvent	CHLOROFORM-D
4 Temperature	22.1
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6 Probe	2756
7 Number of Scans	32
8 Receiver Gain	56.0
9 Relaxation Delay	5.0000
10 Pulse Width	5.0450
11 Presaturation Frequency	
12 Acquisition Time	4.4145
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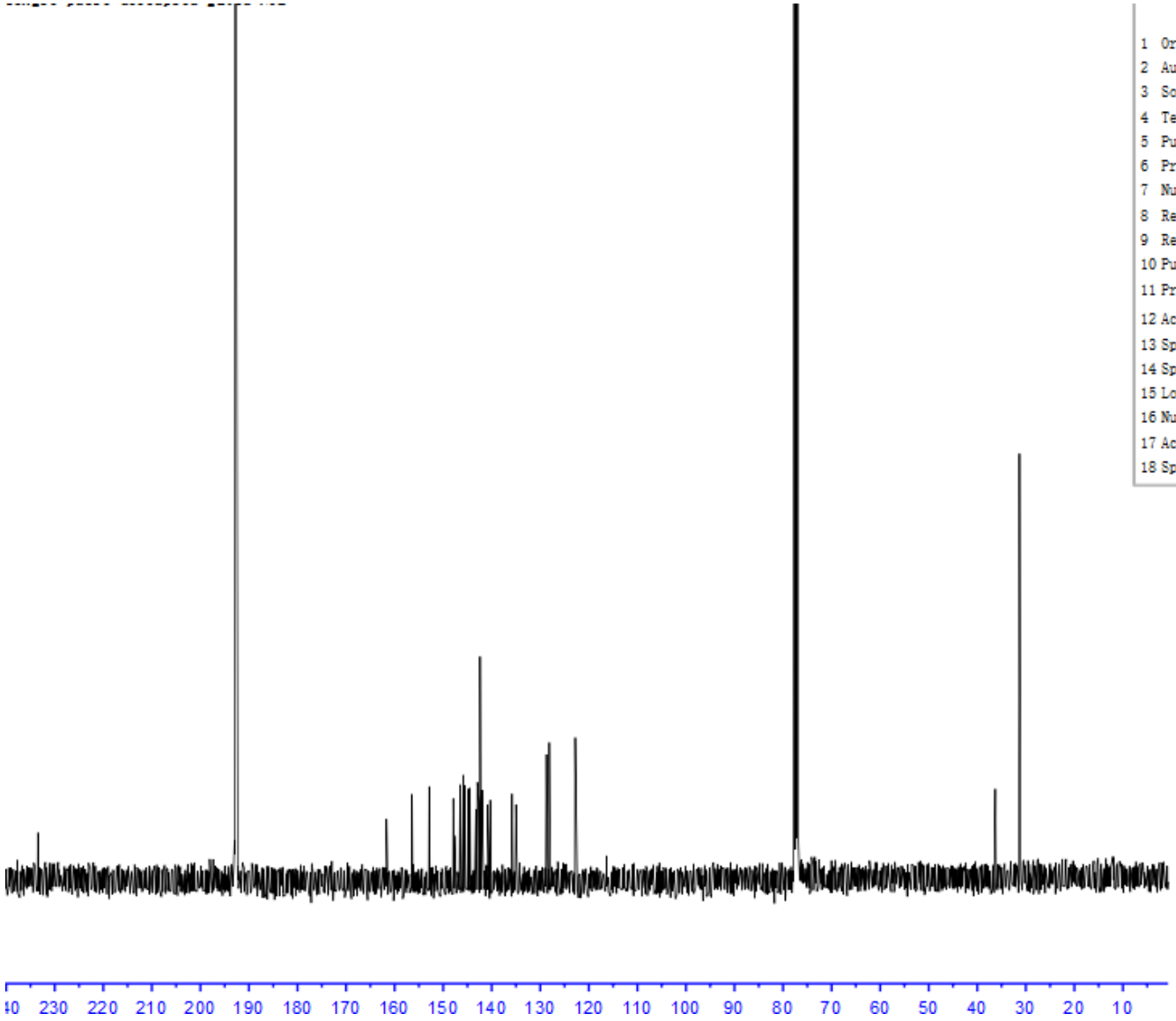
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	52430



Parameter	Value
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2 Author	delta
3 Solvent	CHLOROFORM-D
4 Temperature	21.7
5 Pulse Sequence	carbon.jxp
6 Probe	2803
7 Number of Scans	5120
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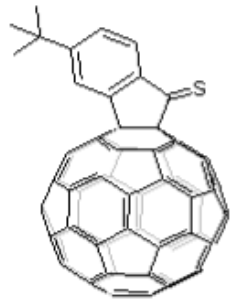
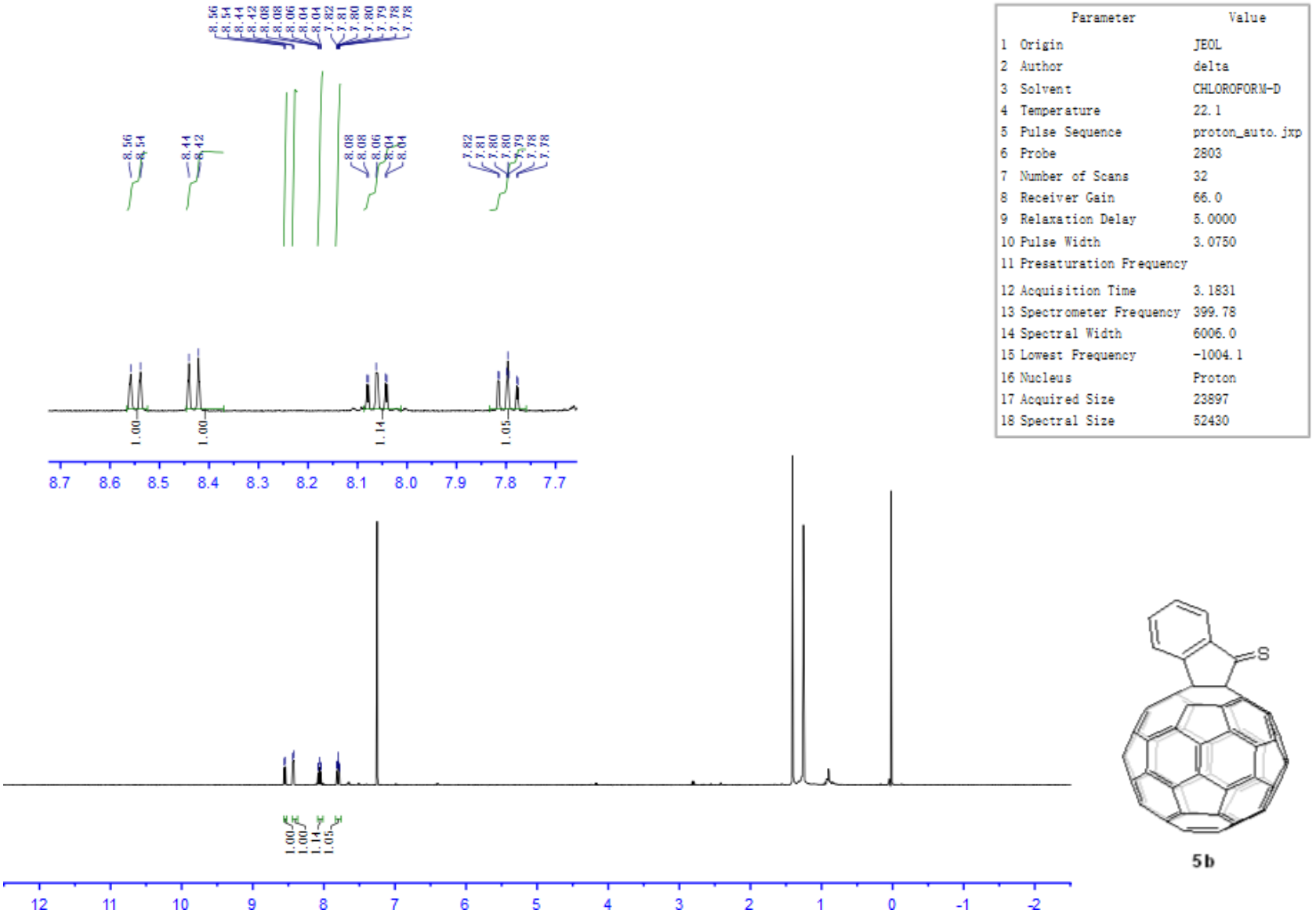
9 Relaxation Delay	2.2891
10 Pulse Width	3.3767
11 Presaturation Frequency	
12 Acquisition Time	0.7109
13 Spectrometer Frequency	100.53
14 Spectral Width	30302.6
15 Lowest Frequency	-72.5
16 Nucleus	Carbon13
17 Acquired Size	26928
18 Spectral Size	52429



8a



	Parameter	Value
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2	Author	delta
3	Solvent	CHLOROFORM-D
4	Temperature	22.1
5	Pulse Sequence	proton_auto.jxp
6	Probe	2803
7	Number of Scans	32
8	Receiver Gain	66.0
9	Relaxation Delay	5.0000
10	Pulse Width	3.0750
11	Presaturation Frequency	
12	Acquisition Time	3.1831
13	Spectrometer Frequency	399.78
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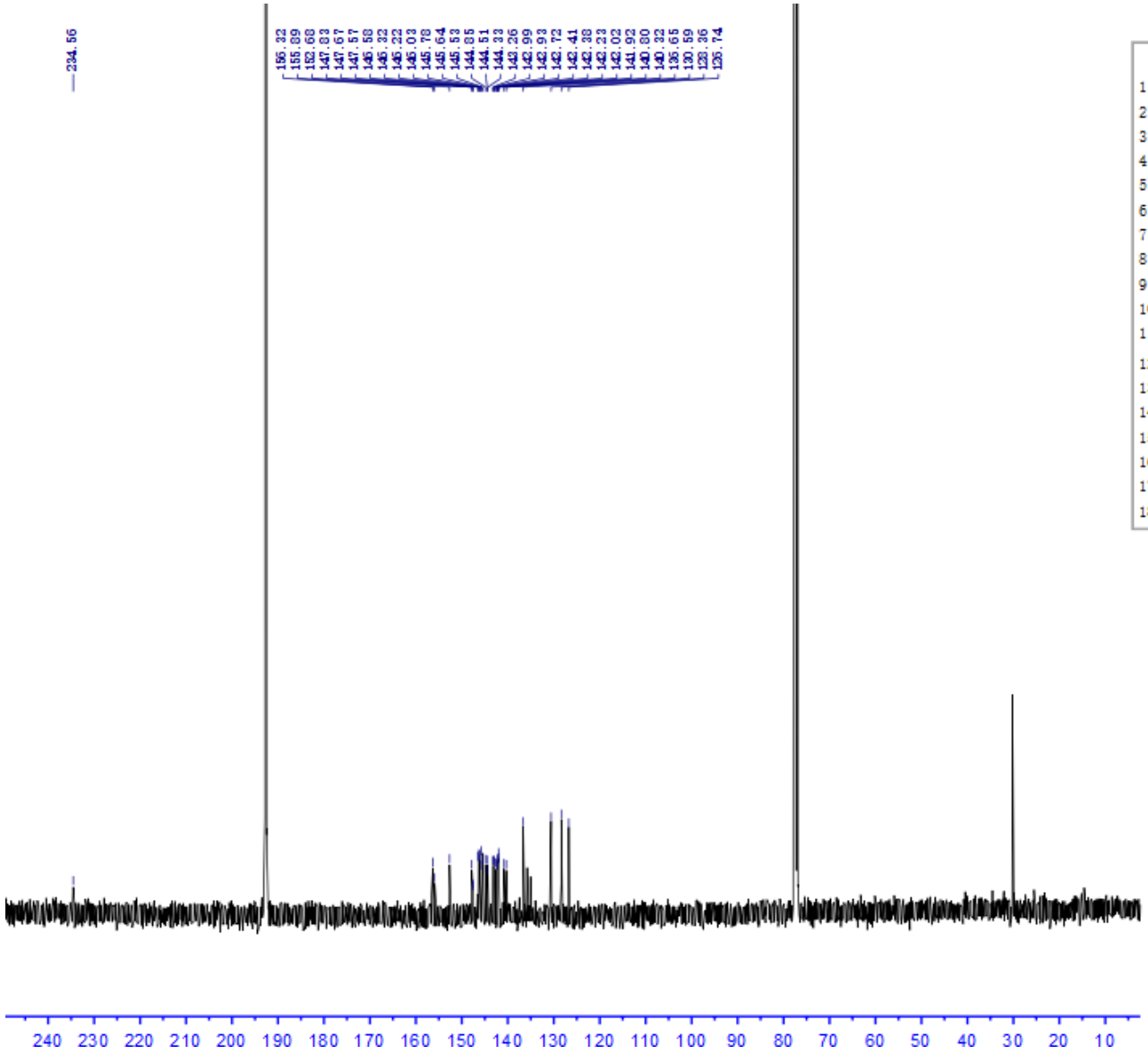
15	Lowest Frequency	-1004.1
16	Nucleus	Proton
17	Acquired Size	23897
18	Spectral Size	52430

5b



	Parameter	Value
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3	Solvent	CHLOROFORM-D
4	Temperature	22.1
5	Pulse Sequence	carbon.jxp
6	Probe	2803
7	Number of Scans	10240
8	Receiver Gain	50.0
9	Relaxation Delay	2.2891
10	Pulse Width	3.3767
11	Presaturation Frequency	
12	Acquisition Time	0.7109
13	Spectrometer Frequency	100.53
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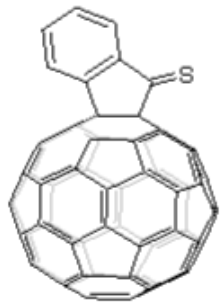
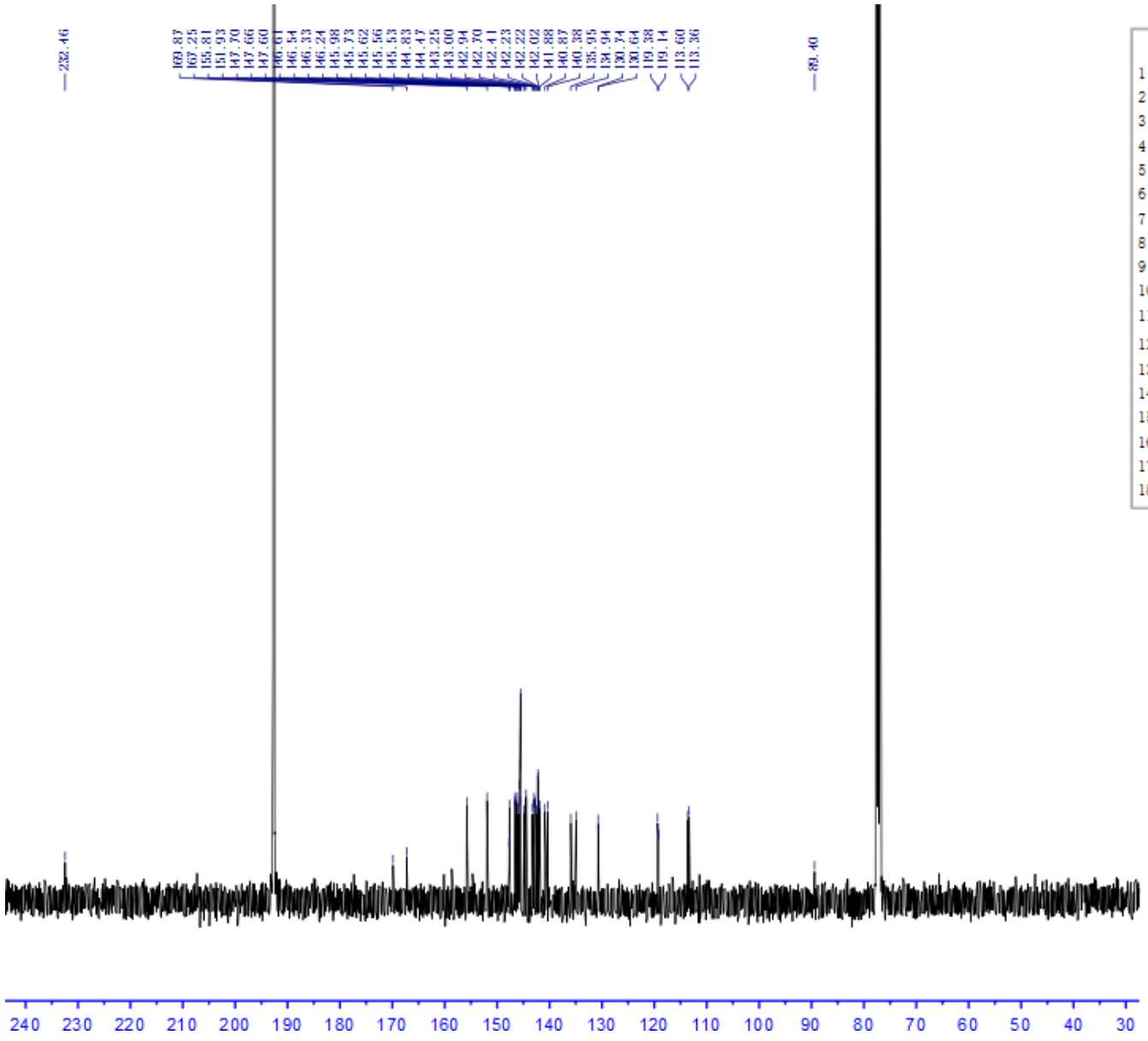
15	Lowest Frequency	-72.5
16	Nucleus	Carbon13
17	Acquired Size	26928
18	Spectral Size	52429



5b



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2	Author	delta
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4	Temperature	21.5
5	Pulse Sequence	carbon.jxp
6	Probe	2803
7	Number of Scans	10240
8	Receiver Gain	50.0
9	Relaxation Delay	2.2891
10	Pulse Width	3.3767
11	Presaturation Frequency	
12	Acquisition Time	0.7109
13	Spectrometer Frequency	100.53
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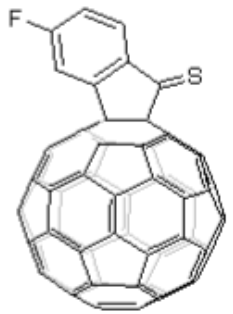
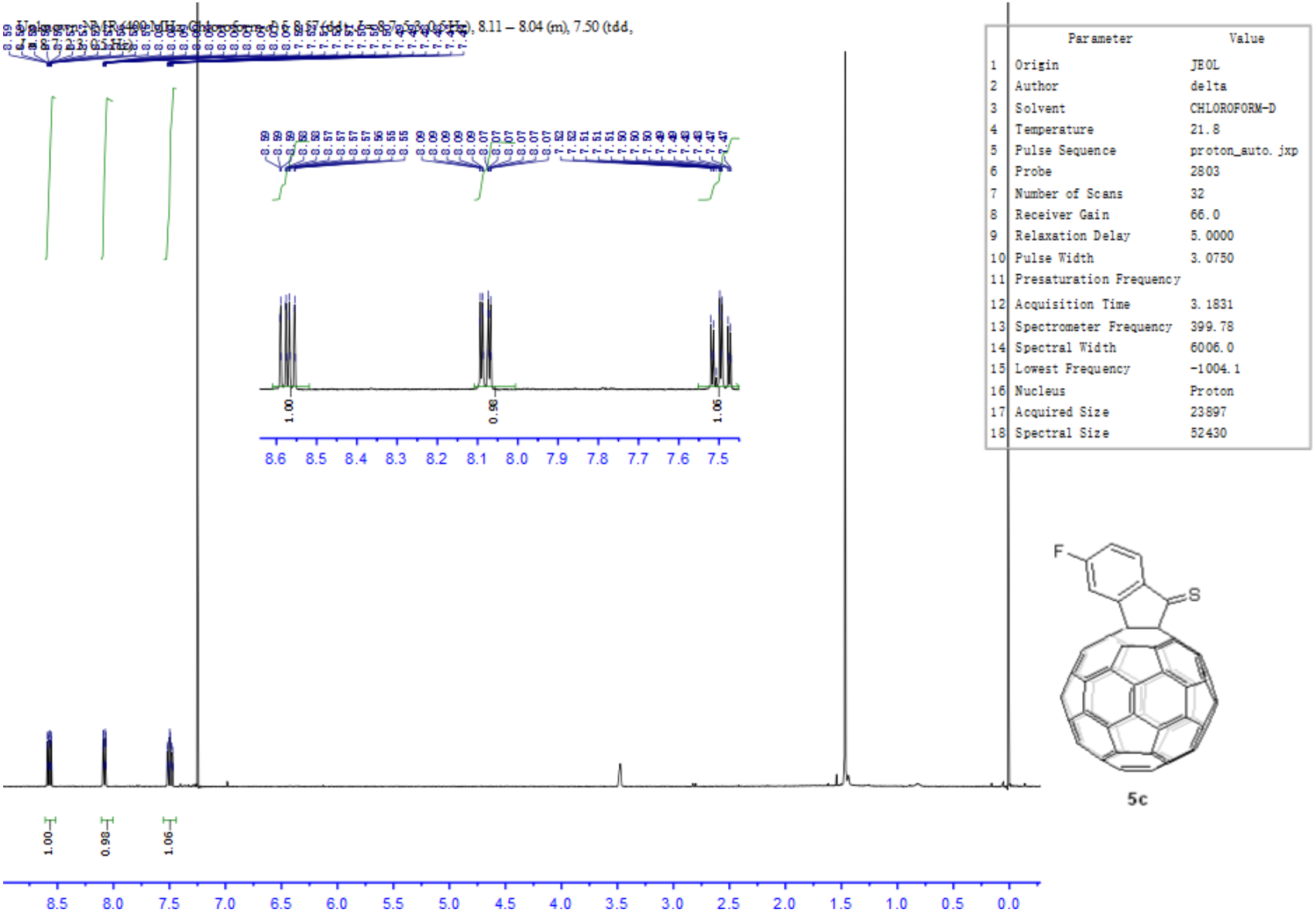
16	Nucleus	Carbon13
17	Acquired Size	26928
18	Spectral Size	52429



5c



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7	Number of Scans	32
8	Receiver Gain	66.0
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10	Pulse Width	3.0750
11	Presaturation Frequency	
12	Acquisition Time	3.1831
13	Spectrometer Frequency	399.78
14	Spectral Width	6006.0
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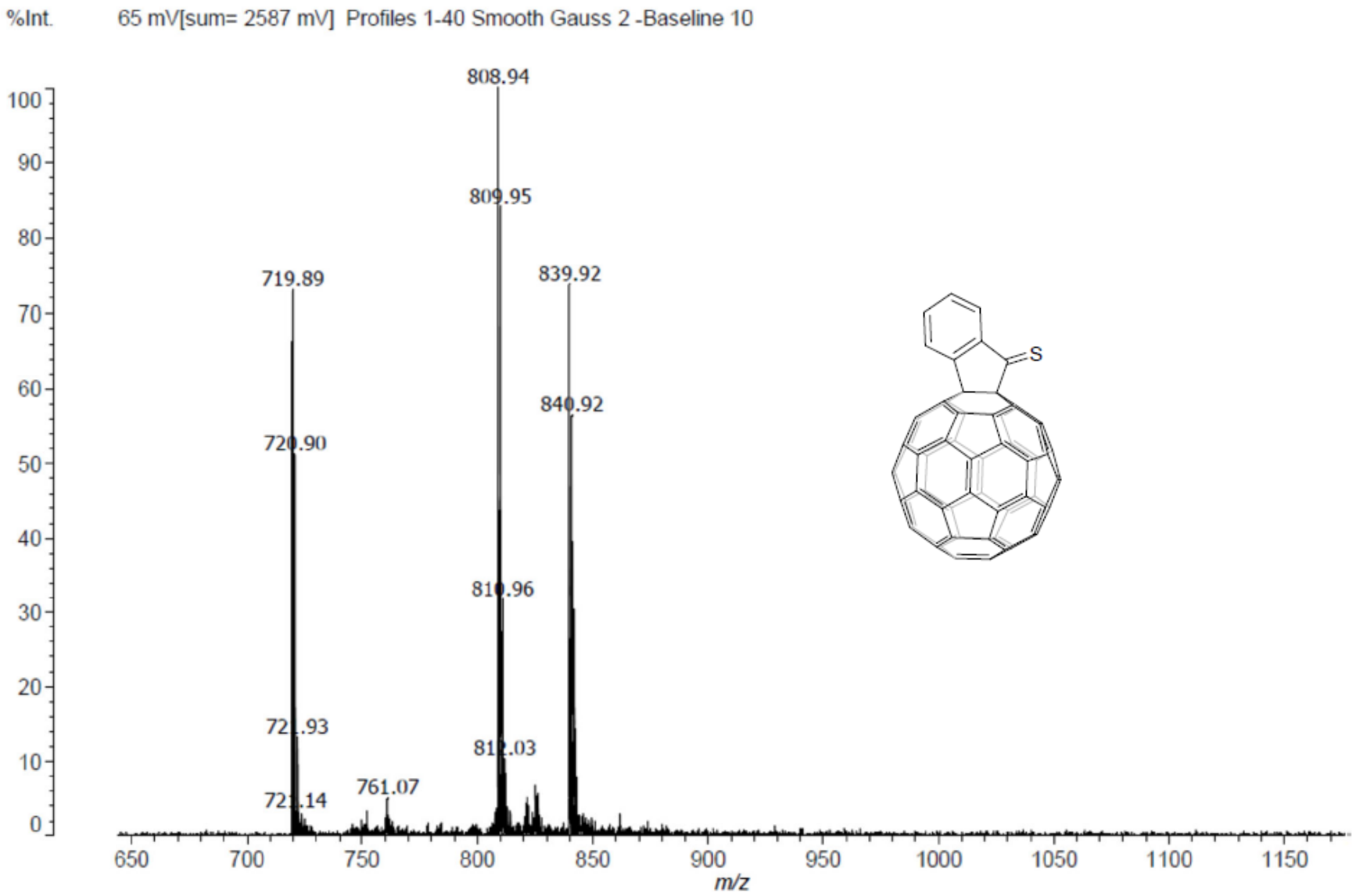
16	Nucleus	Proton
17	Acquired Size	23897
18	Spectral Size	52430

5c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m/z
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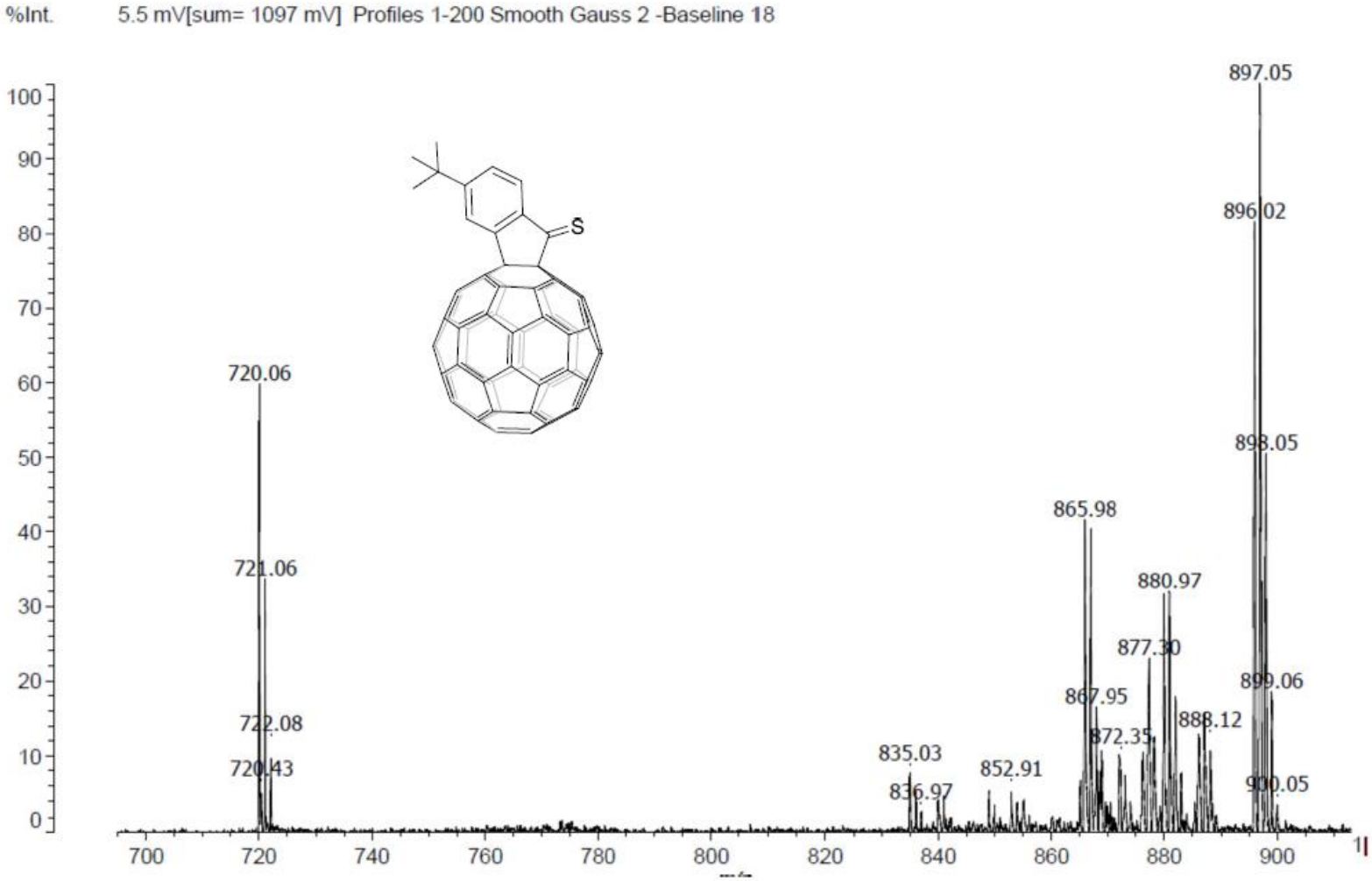
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722.08
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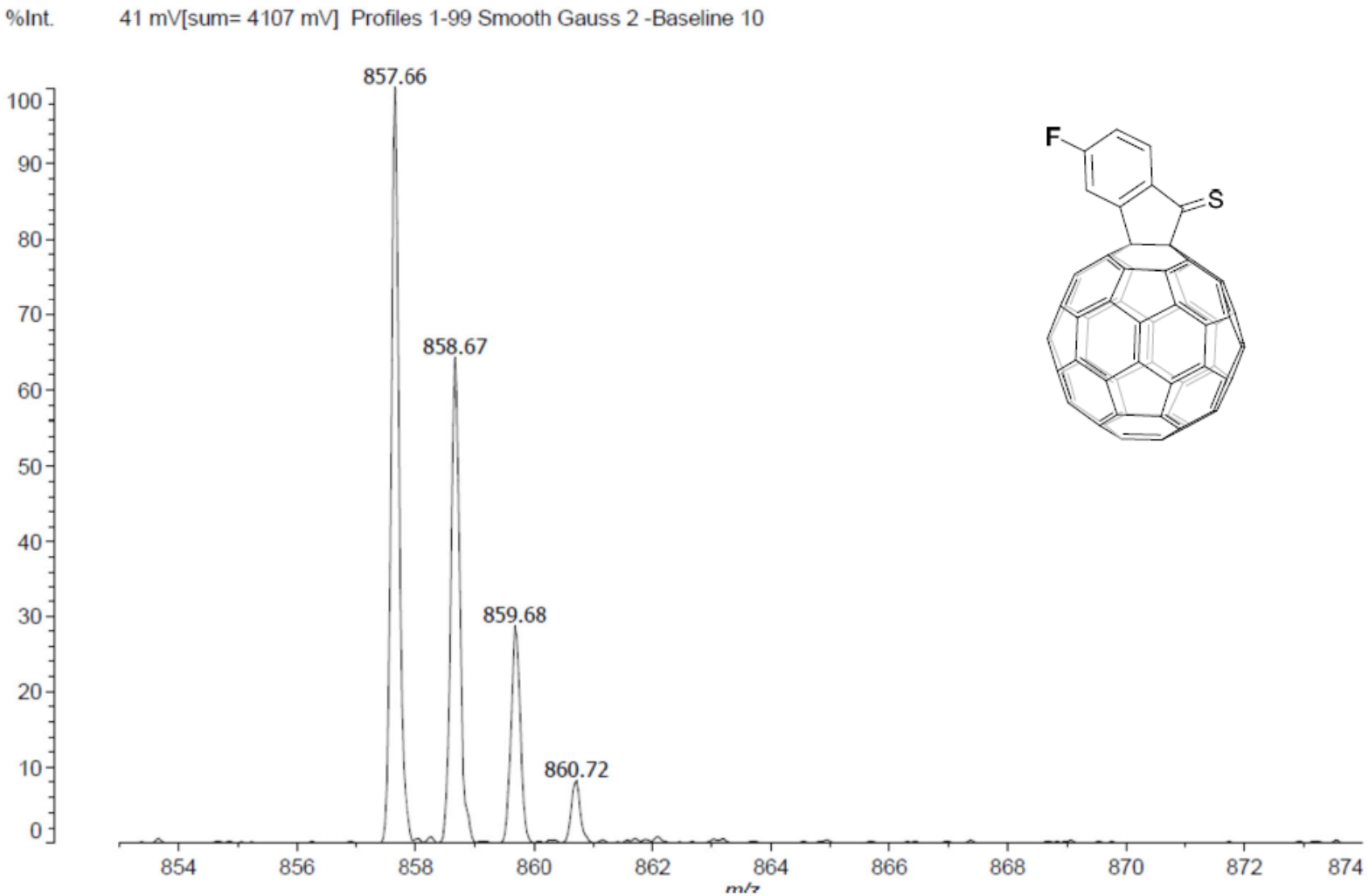
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856
858
860
862
864
866
868
870
872
874
m/z
F
S

8. Computational data

Table S1. Simulation for vibration of *t*-Bu-FIDO (left) and *t*-Bu-FIDS (right)

t-Bu-FIDO vibration		*t*-Bu-FIDS vibration	
Frequency (cm^{-1})	Epsilon (M^{-1} cm^{-1})	Frequency (cm^{-1})	Epsilon (M^{-1} cm^{-1})
34.4656	0.20835	41.28579	0.00626
56.3838	20.62488	58.52742	29.00104
65.7884	3.01986	63.87735	24.46495
99.9959	63.89282	70.05813	14.2865
144.8204	11.71583	132.75737	28.53075
162.2506	22.83968	158.74273	5.73898
189.4856	5.06345	188.8313	0.52435
221.7946	1.29326	192.0298	36.5428
236.4787	21.73363	228.08132	3.27663
237.7582	0.74668	251.52542	1.61157
252.5937	0.01895	251.95696	0.21967
255.2707	0.23442	254.35761	0.06112
266.532	3.7195	262.38045	9.1858
269.2064	0.02519	269.3761	0.05319
273.5868	1.51068	274.9394	3.82632
288.5923	31.20964	286.39565	5.96694
313.9002	11.52845	304.0532	2.24385
333.7379	0.60964	323.09418	7.03449
336.0422	0.63751	336.39034	0.05494
337.6815	0.43121	338.53739	0.01082
338.6451	0.16021	342.54908	1.22797E-4
343.0459	0.01047	344.23011	0.24717
346.7	0.10126	346.88503	0.02133
353.506	3.67221	352.3317	5.37233
363.7724	6.47257	358.46175	22.91525
365.0149	0.05574	365.14683	2.937
375.3216	42.83918	365.33463	0.02175
394.7179	0.01314	392.84381	0.76831
398.865	9.74483	398.7671	7.24512
399.1133	0.07597	398.88119	0.24263
408.6214	0.03027	408.61395	0.04027
409.1693	0.00585	409.49255	11.16948
410.1316	19.52913	409.64008	5.31111E-4
432.509	0.51192	431.06157	0.94002

436.0605	2.56988	431.99684	0.77895
436.2287	0.29722	436.0308	1.00493
436.3337	0.14629	436.19932	0.06819
449.0373	9.95312	441.52508	2.40651
457.7539	1.83454	454.14473	5.3597
463.4829	18.33555	458.79326	2.7921
466.5332	1.54947	463.01867	18.71205
478.781	0.63076	477.49423	0.9309
484.5471	25.39546	483.22954	19.53456
490.9428	6.93553	491.08159	6.32465
491.9362	9.06327	491.95567	8.05106
516.5557	0.40623	508.84357	2.73087
529.0155	0.02112	522.36119	0.11093
531.8753	19.53838	524.05413	7.41189
535.8619	25.33697	533.30862	0.04924
536.2392	227.41176	536.15021	147.58175
537.1045	43.23532	536.57173	65.34471
537.3417	114.28852	536.75984	209.64682
539.05	116.81633	538.95917	118.11785
553.0171	67.59042	546.70616	0.52437
554.7822	1.48493	548.60761	73.43171
562.24	77.74727	561.69214	65.02186
566.0357	0.65969	563.85878	33.03154
566.6802	0.01126	566.24946	5.05945
568.2463	0.12637	566.45243	0.00655
570.475	30.86901	568.21119	0.11525
574.2364	1.07266	571.0099	17.75748
576.6103	1.57677	572.7756	0.67991
583.727	40.67671	576.93525	1.82331
584.2997	22.06562	583.69417	41.01059
591.0987	50.87286	585.66665	45.28047
596.7081	10.6222	591.22818	45.39996
604.025	88.94535	592.35014	2.87654
619.3688	1.56776	615.77004	34.09666
633.4068	16.05315	618.71206	1.36311
634.6143	0	620.13343	13.10797
662.0056	3.77302	652.48313	2.26757
675.3925	13.40367	672.72386	6.29867
679.7063	8.17182	677.54019	16.596
681.1937	0.02694	680.887	0.00596

687.895	8.20271	687.52862	10.21058
702.5326	100.65137	689.39241	5.50143
703.2299	26.9965	696.48417	61.067
712.7053	34.92978	709.18293	9.34816
714.7594	2.70254	713.37075	0.0312
717.7472	1.47515	717.5434	1.88587
719.4021	0.38153	718.82625	0.12911
721.7596	1.01758	721.28877	0.08192
722.1129	0.03591	721.96621	0.19473
724.0543	0.28761	723.79134	1.46113E-4
732.4877	2.61752	731.38967	0.0749
736.9883	0.7849	735.50808	5.65425
737.3125	0.00433	736.83549	0.38684
737.3806	17.02545	737.85305	0.26679
741.5694	26.27753	739.66199	5.66448
742.0347	0.02258	740.59789	20.6912
743.121	18.09056	742.44542	0.00178
743.461	1.1553	744.04772	2.7942
746.8782	0.98549	746.42849	6.59843
751.4609	0.03238	749.68531	6.64097
752.0669	0.72036	751.47457	0.08557
753.2589	4.55419	752.91723	0.17868
754.2125	4.90071	753.69742	0.17463
754.4455	0.36856	754.11866	0.69648
754.6922	0.32615	754.19521	0.01152
756.1601	0.26801	756.69209	0.16388
761.121	49.65669	757.80127	20.78293
763.5864	0.98013	763.15219	2.02657
767.5159	0.00104	767.57334	2.60685
767.8726	1.76955	767.7029	0.05099
772.0587	2.86057	771.10901	0.32745
773.3048	6.49505	771.47546	0.61095
785.0952	1.03	785.02251	0.87989
792.0691	9.34002	791.62032	11.12073
798.1055	1.15017	797.7365	0.10413
804.0706	0.22376	803.82974	0.10327
805.2351	0.8249	805.11066	0.06613
815.2576	18.26762	815.46969	0.71979
823.1936	1.43255	816.19809	7.88643
838.3503	27.71092	826.42431	84.66891

841.9506	4.57718	840.42441	51.28321
847.9782	9.8392	841.46528	1.92907
848.0155	28.07252	843.79723	1.83559
867.7	93.44394	846.66486	39.08205
868.9886	33.70144	865.08163	69.30077
912.5097	7.573	913.21227	7.79143
939.1106	7.93707	936.76408	9.28281
948.824	8.29604	943.34956	5.29226
950.299	18.41766	946.81901	1.86084
959.2558	0.29278	954.25024	0.1182
962.5802	90.38123	955.1276	21.3777
965.2645	0.00992	964.81967	0.11082
968.7203	95.69082	968.52894	16.92122
973.907	0.35023	970.70561	0.41589
982.9752	56.62287	983.10566	20.51405
986.2878	2.25501	986.18243	3.42829
986.9184	0.14067	989.95564	0.13441
989.7071	0.12617	991.26591	0.02474
991.8686	4.0221E-4	996.68687	2.0753E-4
1025.5851	233.74062	1018.23772	11.29818
1055.348	24.45847	1050.63694	22.93456
1060.5345	0.0158	1055.58632	0.02235
1062.897	3.04883	1056.09692	3.80002
1080.6198	0.99973	1078.20953	0.26896
1093.2175	0.48681	1086.41534	169.46892
1100.8299	5.84115	1089.2816	0.02322
1104.7458	90.15838	1101.6556	2.50371
1105.8245	0.13493	1105.3423	5.84236E-4
1113.9864	1.22799	1114.10584	0.37644
1122.8568	18.2349	1121.95498	37.1422
1125.2728	27.94099	1124.22693	15.94856
1131.4563	0.14104	1129.23097	103.57075
1143.2387	11.53683	1131.71816	0.11944
1160.4013	170.99451	1144.31035	71.04546
1168.6398	3.49018	1168.00616	4.10097
1172.6174	0.01973	1169.553	0.01456
1186.9139	2.12828	1183.04375	47.96023
1202.5067	0.771	1188.53237	31.39894
1207.4678	43.53333	1202.82529	0.70654
1211.5489	25.39216	1211.4575	11.74819

1218.8862	32.04286	1213.91615	83.68797
1220.1317	5.86215	1219.1053	43.24274
1236.6499	9.30177	1220.5232	5.10268
1239.9628	3.01112	1229.57257	9.20185
1245.3991	0.42668	1233.62481	6.30956
1246.4254	4.66754	1245.4504	0.96634
1248.44	8.7624	1246.41231	3.80799
1255.2237	95.62169	1248.43749	14.36907
1259.6281	4.13943	1254.57413	20.61309
1263.8601	6.31304E-4	1259.32182	3.85244
1266.6712	474.86908	1263.472	0.01439
1274.7113	21.03655	1274.49411	3.16
1283.4757	8.97266	1283.08415	3.92479
1296.7947	17.54598	1291.83885	155.77012
1298.191	3.0795	1296.72811	11.20417
1303.1737	22.87613	1298.13628	3.06741
1303.8642	0.01622	1303.6513	0.00973
1309.4025	61.74688	1307.34485	58.30849
1315.3392	0.00364	1312.6777	1.29569
1318.5228	82.85791	1315.28882	5.69789E-4
1333.7322	2.33968	1333.48261	4.03485
1333.7483	0.34398	1333.49493	0.3242
1335.838	3.8767	1335.19114	66.16436
1337.8745	0.00567	1337.90325	0.01349
1342.7421	0.68097	1341.86135	120.05132
1343.5121	1.00543	1343.27221	0.69388
1347.4341	13.76535	1345.90846	307.21881
1367.434	1.60721	1348.32225	165.46625
1368.2717	0.03382	1366.15354	6.6771
1372.5239	14.67346	1368.35367	0.02873
1373.1734	0.18913	1369.17737	0.33446
1373.5059	0.75634	1373.16945	0.09429
1379.0043	0.06972	1373.69794	0.9426
1381.0723	1.72191	1379.36664	0.13854
1386.4264	8.01893	1381.29118	3.24336
1388.6081	0.02385	1387.11984	0.5905
1426.6652	14.46755	1388.74846	0.00247
1427.8279	12.6226	1415.12424	9.34811
1436.7483	0.08413	1415.6553	12.38831
1451.3532	5.02168	1436.49387	0.03444

1454.6627	12.6149	1448.14378	6.34423
1455.3865	1.39606	1451.37584	5.94539
1455.9282	62.40207	1454.64825	11.88606
1457.3597	76.94078	1455.44523	0.4632
1458.7668	26.70124	1456.0986	38.46669
1458.9789	13.09766	1457.86654	72.50502
1460.6141	15.64251	1459.11353	25.75798
1461.2177	24.70082	1459.53921	35.72259
1464.7273	0.1528	1462.19523	16.94767
1468.0678	1.02556	1465.38925	0.82301
1476.2893	11.72507	1468.04619	1.05406
1496.4393	20.94299	1476.47797	7.38818
1512.9674	0	1496.92738	21.94074
1516.3255	0.30756	1497.60019	9.54358E-4
1518.3553	2.1524	1501.32198	0.26821
1526.6318	3.22495	1503.90582	0.68072
1529.7162	10.83753	1516.92132	46.87178
1537.9635	7.869	1523.37056	16.53529
1538.8749	17.61181	1525.19024	10.58319
1539.9691	0.05129	1527.84125	1.94138
1540.0296	0.05854	1536.61572	25.86335
1550.6765	34.6692	1539.87697	0.16849
1551.3752	1.08698	1540.18518	0.01695
1559.7021	2.23372	1551.4227	0.96224
1571.1207	1.04412	1559.93265	2.02574
1600.1226	1.79335	1571.5715	1.04617
1602.7298	4.58646	1601.56017	1.18594
1604.1443	0.00124	1602.95591	9.51132
1605.7697	0.14062	1604.22586	0.02599
1608.4171	0.94054	1605.93331	0.25764
1609.5966	0.05701	1608.47635	1.15701
1613.3207	5.95694	1609.45965	0.05502
1614.6035	0.27821	1611.82438	46.9399
1615.965	0.67026	1614.67171	0.20164
1628.1804	4.63973	1615.07738	12.37073
1629.8741	0.08812	1617.16958	16.66188
1634.2198	121.37195	1629.38957	1.4689
1654.8836	418.24265	1630.36492	5.42714E-4
1814.8508	614.91736	1649.81408	453.02441
3046.1957	32.5758	3031.97582	31.32994

3047.1271	30.0478	3032.89263	29.11754
3053.974	33.02894	3039.3623	35.87596
3113.3712	2.09761	3103.02384	1.84308
3113.7136	2.04754	3103.26496	1.67925
3117.5306	28.00843	3106.85484	27.34062
3121.3846	138.81686	3110.55311	136.00149
3124.0959	16.55779	3113.68148	15.05937
3126.4785	46.05364	3116.05243	43.87036
3200.5443	9.90985	3192.95871	12.39887
3216.3872	27.91473	3209.0889	16.86476
3229.2964	1.92496	3220.4556	2.30941

Table S2. Cartesian coordinates of optimized structures

t-Bu-FIDS

C	1.00598	2.1391	1.17689
C	-0.03928	3.01582	0.72509
C	-1.24547	3.12311	1.42498
C	-1.45971	2.30445	2.59331
C	-0.4555	1.42043	3.00295
C	0.79638	1.34402	2.28151
C	1.00597	2.13912	-1.17688
C	-0.03928	3.01583	-0.72506
C	-1.24548	3.12313	-1.42494
C	-2.50113	3.21691	0.69702
C	-2.8478	1.88073	2.59866
C	-3.18407	0.59466	3.02687
C	-2.1433	-0.31997	3.46816
C	-0.80864	0.08469	3.44868
C	0.22594	-0.83133	3.00326
C	1.22464	-0.07303	2.28198
C	1.84298	-0.61701	1.1783
C	0.79636	1.34405	-2.28151
C	1.22462	-0.073	-2.282
C	1.84297	-0.617	-1.17833
C	1.45793	-1.92571	-0.72598
C	1.45793	-1.92572	0.72593
C	0.51337	-2.68585	1.42538
C	-0.11868	-2.12444	2.5939

C	-1.50871	-2.54327	2.59956
C	-2.50137	-1.65884	3.02641
C	-3.49371	2.44585	1.42455
C	-4.60927	-1.79648	0.
C	-5.01333	-0.46053	0.00001
C	-4.79646	0.366	-1.17545
C	-4.17695	-0.17553	-2.30386
C	-3.75495	-1.56892	-2.30373
C	-2.93816	-3.2815	-0.7271
C	-2.93815	-3.2815	0.72707
C	-3.96996	-2.36338	1.17541
C	-3.75493	-1.56895	2.30373
C	-4.17693	-0.17556	2.30388
C	-4.79645	0.36598	1.17548
C	-4.44809	1.7025	-0.72698
C	-3.49372	2.44586	-1.4245
C	-2.84782	1.88077	-2.59862
C	-3.1841	0.5947	-3.02684
C	-2.14333	-0.31993	-3.46816
C	-2.5014	-1.6588	-3.02642
C	-1.50873	-2.54324	-2.59959
C	-1.73227	-3.37127	-1.42536
C	-1.73226	-3.37129	1.42532
C	-0.47868	-3.46078	0.69705
C	-0.47868	-3.46077	-0.6971
C	0.51336	-2.68583	-1.42543
C	-0.1187	-2.12441	-2.59393
C	0.22592	-0.83129	-3.00328
C	-0.80866	0.08473	-3.44868
C	-0.45552	1.42046	-3.00294
C	-1.45973	2.30448	-2.59328
C	-4.44808	1.70249	0.72703
C	-2.50114	3.21692	-0.69697
C	-3.96997	-2.36336	-1.17542
C	1.91315	1.75312	0.
C	3.23846	2.57724	0.
C	2.38106	0.2137	-0.00001
C	4.34594	1.64316	-0.00002
C	3.90512	0.31702	-0.00003
C	5.72291	1.92241	-0.00003
C	4.814	-0.73938	-0.00003

C	6.61988	0.86839	-0.00002
H	6.06049	2.95436	-0.00004
C	6.19186	-0.48229	-0.00002
H	4.44511	-1.75829	-0.00001
H	7.6827	1.08941	-0.00003
S	3.32203	4.21586	0.00002
C	7.24049	-1.6069	0.00001
C	8.12577	-1.47908	1.26382
C	6.60141	-3.00847	0.00002
C	8.1258	-1.47911	-1.26379
H	8.65073	-0.51918	1.30301
H	7.52506	-1.57071	2.1757
H	8.88213	-2.27269	1.27413
H	5.98217	-3.17634	-0.88837
H	7.38906	-3.76967	0.00003
H	5.98215	-3.17633	0.88839
H	8.88216	-2.27274	-1.27405
H	7.52511	-1.57077	-2.17567
H	8.65077	-0.51922	-1.30299

t-Bu-FIDO

C	0.99156	2.24653	1.17583
C	-0.07749	3.0951	0.72516
C	-1.28687	3.1639	1.42562
C	-1.47522	2.33851	2.59391
C	-0.44394	1.48588	3.00429
C	0.80936	1.44812	2.28348
C	0.99156	2.24652	-1.17584
C	-0.07749	3.09509	-0.72518
C	-1.28687	3.16389	-1.42564
C	-2.54451	3.21796	0.69714
C	-2.84925	1.87091	2.59862
C	-3.14523	0.57504	3.0269
C	-2.07641	-0.30677	3.46815
C	-0.75508	0.13926	3.44932
C	0.30755	-0.74374	3.0031
C	1.28213	0.04541	2.28162
C	1.92007	-0.47928	1.1788
C	0.80936	1.44811	-2.28349
C	1.28212	0.0454	-2.28163

C	1.92006	-0.47929	-1.1788
C	1.57421	-1.7992	-0.72602
C	1.57421	-1.7992	0.72603
C	0.65337	-2.58817	1.42522
C	0.00374	-2.04684	2.59365
C	-1.37244	-2.50902	2.59943
C	-2.39238	-1.65614	3.02631
C	-3.51252	2.4156	1.42463
C	-4.49504	-1.85983	0.00001
C	-4.94048	-0.53711	0.00001
C	-4.74945	0.29581	-1.17545
C	-4.11343	-0.22604	-2.30385
C	-3.64819	-1.60561	-2.30374
C	-2.77819	-3.29176	-0.72709
C	-2.77819	-3.29176	0.72711
C	-3.83825	-2.40636	1.17545
C	-3.64819	-1.6056	2.30375
C	-4.11343	-0.22603	2.30386
C	-4.74945	0.29581	1.17546
C	-4.44265	1.64248	-0.72704
C	-3.51252	2.4156	-1.42464
C	-2.84926	1.8709	-2.59863
C	-3.14524	0.57502	-3.0269
C	-2.07641	-0.30678	-3.46815
C	-2.39239	-1.65615	-3.02631
C	-1.37245	-2.50903	-2.59942
C	-1.56996	-3.34365	-1.4252
C	-1.56995	-3.34364	1.42521
C	-0.31413	-3.39387	0.69701
C	-0.31414	-3.39387	-0.697
C	0.65337	-2.58817	-1.42521
C	0.00374	-2.04685	-2.59365
C	0.30754	-0.74376	-3.0031
C	-0.75509	0.13925	-3.44932
C	-0.44395	1.48586	-3.00429
C	-1.47523	2.33849	-2.59392
C	-4.44265	1.64248	0.72704
C	-2.54451	3.21796	-0.69715
C	-3.83825	-2.40636	-1.17544
C	1.89602	1.8776	-0.00001
C	3.19726	2.76483	0.00001

C	2.43033	0.36846	-0.00001
C	4.35492	1.86332	0.00001
C	3.95696	0.53105	-0.00001
C	5.71146	2.20723	0.
C	4.90787	-0.48977	-0.00001
C	6.65175	1.18823	-0.00002
H	6.00494	3.25293	-0.00002
C	6.2745	-0.17643	-0.00001
H	4.58119	-1.52307	0.00002
H	7.70552	1.44922	-0.00005
C	7.36702	-1.26026	0.
C	8.24658	-1.09905	1.2637
C	6.78296	-2.68569	0.00005
C	8.24654	-1.09908	-1.26373
H	8.73441	-0.11971	1.30309
H	7.64959	-1.21343	2.17548
H	9.0329	-1.86303	1.27457
H	6.1707	-2.87771	-0.88829
H	7.5997	-3.41564	0.00007
H	6.1707	-2.87765	0.88841
H	9.03283	-1.8631	-1.27464
H	7.64951	-1.21344	-2.17549
H	8.7344	-0.11977	-1.30313
O	3.19067	3.97694	0.00001

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