Supporting Information for

Photoswitchable and Long-Lived Seven-Membered Cyclic Singlet Diradicals for Bioorthogonal Photoclick Reaction

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Table of Contents

1. Supporting Methods

1.1 General Information-Chemical Synthesis

Unless otherwise indicated, all solvents and starting materials were purchased from Bide Pharmatech Ltd, Leyan Shanghai, Haoyuan Chemexpress Co., Ltd, Adamas-beta® Shang Hai Titan Technology Ltd, Acros Organics, Aldrich Chemical Co., Alfa Aesar and TCI. Anhydrous solvents, purchased from Acros Organics (DMF and THF), were used as received. The ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Brüker Avance 400 or 600 or 800 spectrometers (^{1}H: 400 or 600 or 800 MHz, ^{13}C: 101 or 150 or 201 MHz, ^{19}F: 376 MHz). Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra and the chemical shifts converted to the TMS scale ($CDCl_3$, 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR; DMSO-d_6, 2.50 ppm for ^{1}H NMR and 39.5 ppm for ^{13}C NMR). Shifts multiplicity was reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, brs. = broad.

1.2 General Information–Spectra Acquisition

UV-Vis absorption spectra were recorded by using 0.2 × 1.0 cm quartz cuvettes on a Thermo NANODROP 2000C Spectrophotometer. Exact ESI mass spectra were recorded on a SHIMADZU LCMS-IT-TOF. LC-ESI-MS were obtained on a Thermo LTQ-XL mass spectrometer.

Living A549 cells were ordered from Cell bank of Chinese Academy of Sciences (Shanghai, China). Cell imaging experiments were carried out on an Olympus IX83 live cell fluorescence microscope, embedded with a digital micromirror device (DMD, Polygon 400) for patterned photo-stimulation programming with 365 or 405 or 525 nm LED as light source. The embedded DMD (Polygon 400), synchronized LED light sources, the LED controller and Polyscan 2 software were provided as whole system by Mightex, and was setup in-house into an Olympus IX83 live cell epifluorescence microscope. The living cells were stained with a commercially available NucBlue™ Live Ready Probe™ Reagent for cell nuclear fluorescent imaging and identification.

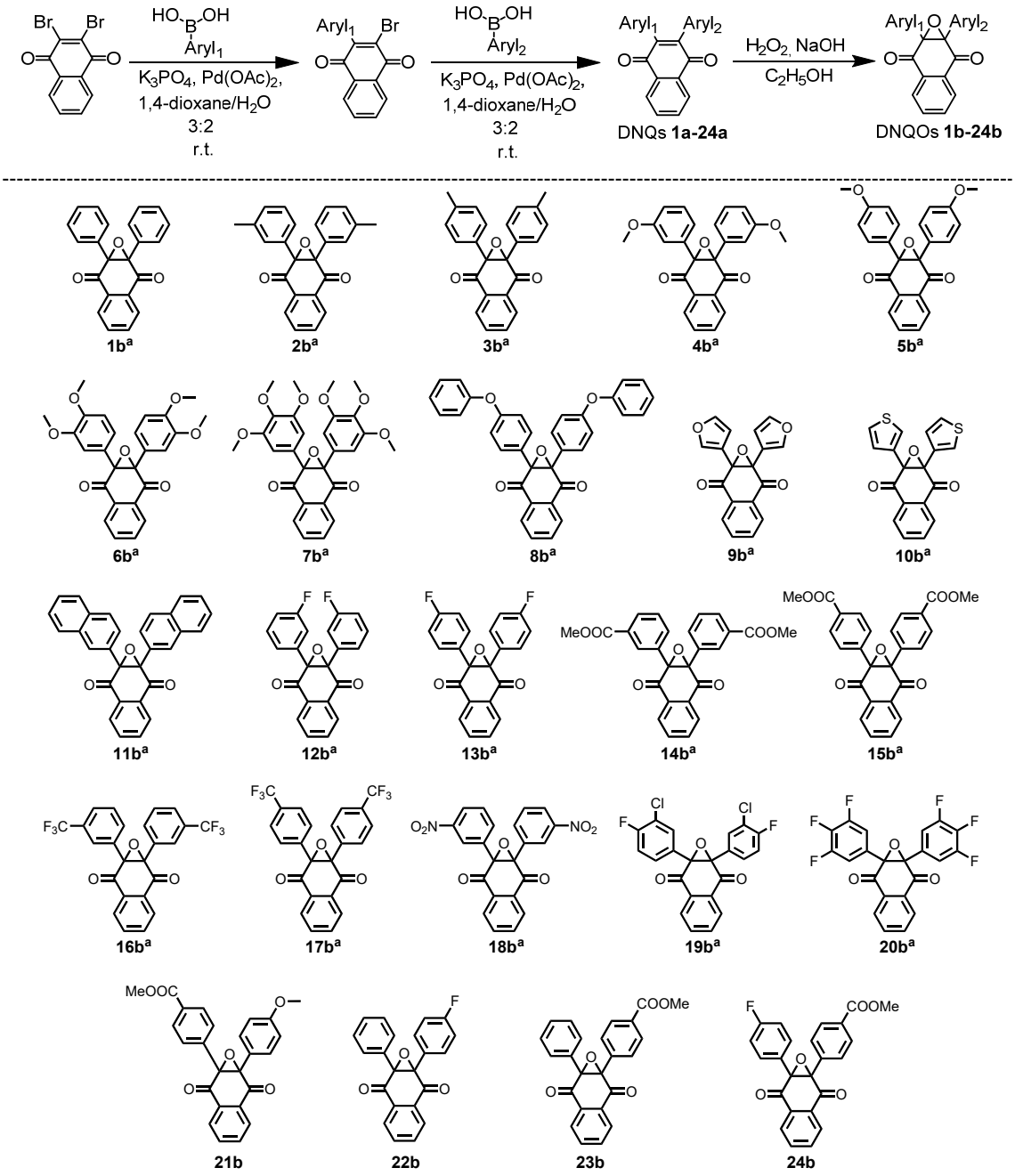
The absorption and lifetime of transient species can be fully characterized by using this transient absorption spectroscopy technique on the EOS (Ultrafast Systems, USA) system. The instrument response function (IRF) of this setup is determined to be ~ 100 ps. For this investigation, a 355 nm excitation (pulse duration 1 ns, pulse energy 7 μJ, repetition rate 1 kHz) was used to pump the molecules to the excited state and the white-light continuum (WLC) probe pulses (350-900 nm) was used for probing the excited state. The temporal and spectral profiles of the pump-induced differential absorbance of the probe light (ΔA) are visualized by an optical fiber-coupled multichannel spectrometer (with a CMOS sensor) and further analyzed by the Surface Xplorer (SX) software.

1.3 General Information–Light Sources

The photo-irradiation power density of various light sources in photo-chemical transformation experiments were measured by an optical power meter produced by Thorlabs: a 311 nm UV lamp (10.8 mW cm^{-2}), a 365 nm LED (55.0 mW cm^{-2}), a 373 nm LED array (38.5 mW·cm^{-2}).

2. Supplementary Figures and Tables

Table S1. Synthesis of DNQOs **1b-24b** via palladium(0)-catalyzed Suzuki coupling reaction between various substituted arylboronic acid and 2,3-dibromo-1,4-naphthoquinone.



[a] The two-step palladium-catalyzed coupling reactions were combined into one-step synthesis for 2,3-diaryl-1,4-naphthoquinone (DNQs) with symmetric structure, **1a-20a**.

Table S2. Spectroscopic data of DNQO, **1b**-**24b**. Compounds were dissolved in ACN:H_2O = 1:1 to derive the final concentration of 100 μM for UV-Vis spectroscopic acquisition at 298 K.

Entry	λ_{max} (nm)	ε_{max} (M^{-1} cm^{-1})	ε_{311} (M^{-1} cm^{-1})	ε_{365} (M^{-1} cm^{-1})	ε_{373} (M^{-1} cm^{-1})
1b	305	2630	2550	162	89
2b	305	2690	2570	173	100
3b	304	2670	2520	201	118
4b	302	3050	2880	197	117
5b	307	2800	2630	192	114
6b	306	3310	3030	308	228
7b	306	3060	2940	329	222
8b	306	3300	3130	315	198
9b	306	2350	2210	209	131
10b	304	2620	2480	208	122
11b	305	3920	3650	28	17
12b	308	2460	2420	133	66
13b	307	2660	2590	162	83
14b	308	2830	2780	152	81
15b	309	2810	2770	160	88
16b	308	2530	2490	1410	70
17b	308	2520	2470	136	70
18b	304	4990	4220	301	186
19b	308	2510	2460	138	70
20b	309	2850	2820	144	75
21b	306	2270	2210	213	131
22b	307	2460	2350	154	86
23b	302	2870	2610	147	78
24b	307	2280	2240	149	81

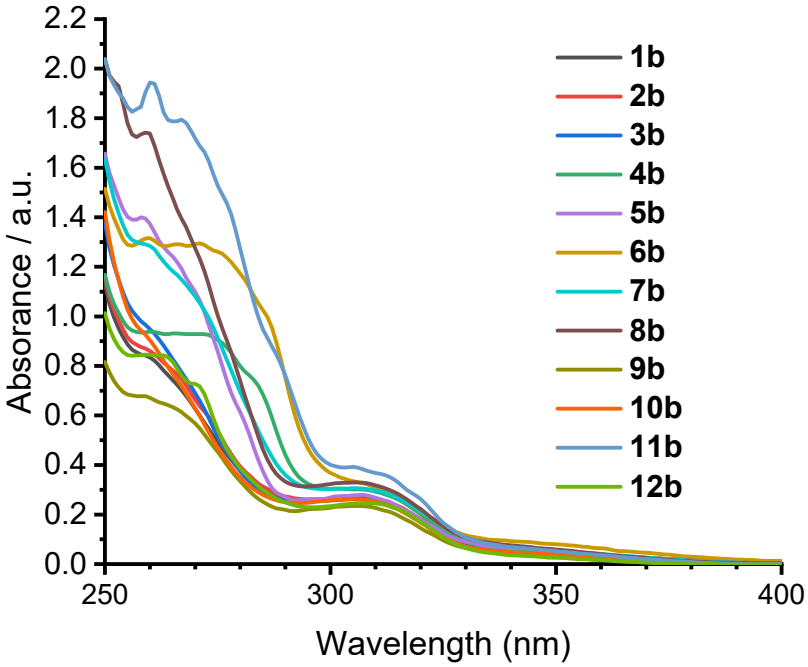


Figure S1. UV-Vis spectra of the DNQO, **1b-12b**. Compounds were dissolved in ACN:H_2O = 1:1 to derive final concentration of 100 µM at 298 K for UV-Vis spectroscopic acquisition.

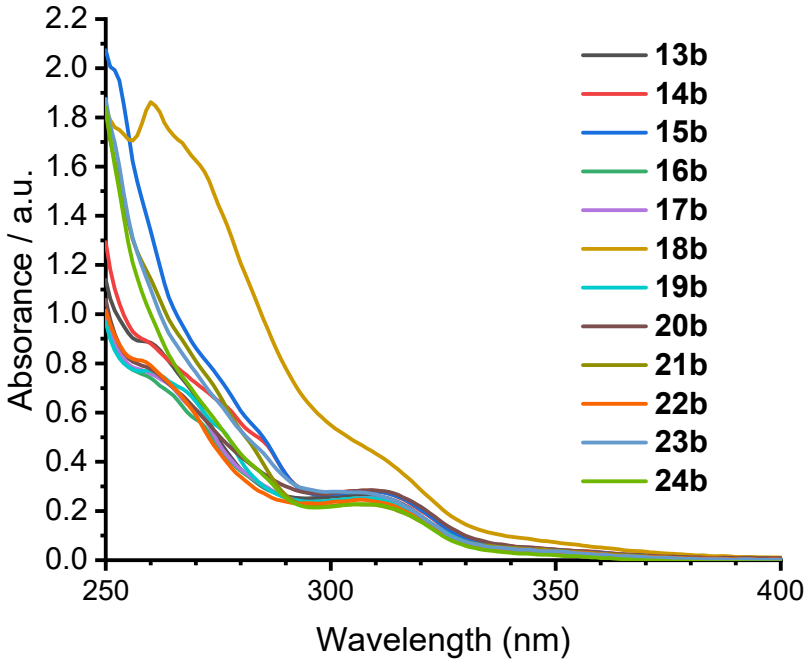
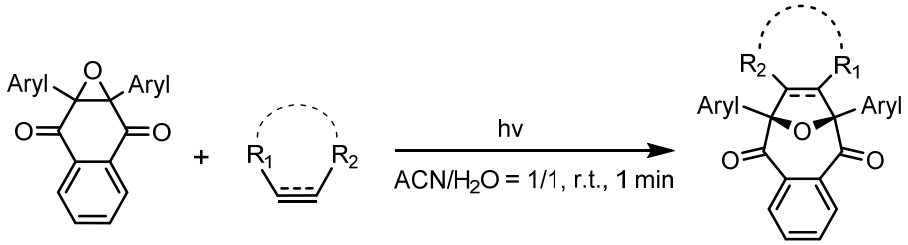


Figure S2. UV-Vis spectra of the DNQO, **13b-24b**. Compounds were dissolved in ACN:H_2O = 1:1 to derive final concentration of 100 µM at 298 K for UV-Vis spectroscopic acquisition.

Table S3. Quantitative HPLC-MS analysis the photoreaction between DNQOs (**1b**-**24b**) and dipolarophiles (**1c**-**10c**) under 311 nm irradiation, and conversion was determined by integration area of the corresponding peaks monitored via absorption at 254 nm in HPLC traces.



nb **1c-10c** **nDEBCOD**

DNQO	hν = 311 nm, conversion [%]									
	1c	**2c**	**3c**	**4c**	**5c** 	**6c**	**7c**	**8c**	**9c**	**10c** 
1b	93.55	33.53	7.96	10.65	6.60	83.61	31.23	12.51	12.61	14.49
2b	88.57	45.52	30.13	29.10	37.16	87.18	27.01	23.96	46.82	26.72
3b	90.58	12.56	11.27	10.32	11.97	84.34	19.57	10.42	45.00	7.69
4b	26.41	5.62	5.45	4.61	3.83	23.82	27.79	7.74	6.65	8.93
5b	4.61	1.02	3.46	0.15	1.61	1.56	20.80	2.87	1.27	2.15
6b	1.46	0	0.85	0.33	1.09	0	0	1.73	0	5.32
7b	0	-2.15	0.85	-0.55	-0.39	2.00	23.84	1.37	1.05	0
8b	25.81	3.17	1.94	2.40	1.67	39.22	15.32	0	2.17	2.18
9b	46.56	26.17	22.70	23.25	28.91	34.63	0	27.99	26.49	27.88
10b	63.19	23.83	18.88	22.98	22.47	32.70	25.46	24.50	23.26	23.88
11b	35.90	0	0	0	0	27.99	18.47	2.51	5.62	2.20
12b	90.8	43.62	6.30	11.33	7.8	85.12	43.17	13.00	16.07	11.67
13b	96.33	21.55	6.52	2.78	1.02	79.25	28.43	1.98	5.81	5.34
14b	99.27	55.73	8.88	15.70	7.85	85.90	45.77	16.58	27.31	14.36
15b	97.91	63.12	22.52	19.68	6.89	95.64	30.58	22.55	31.27	26.19
16b	100.00	83.28	9.03	30.74	9.19	94.87	49.61	0	22.22	12.77
17b	99.01	80.66	12.25	31.68	10.48	99.66	39.28	24.10	31.53	31.54
18b	50.01	28.46	3.2	12.62	5.93	48.80	77.47	12.59	13.04	10.96
19b	100	56.86	7.67	13.68	3.54	99.19	20.14	19.42	24.04	25.03
20b	98.70	41.34	8.08	29.71	10.86	85.27	56.68	16.75	20.85	19.74
21b	31.89	6.01	4.77	4.90	3.82	23.96	17.88	2.61	2.02	1.88
22b	100	31.26	7.67	6.61	8.28	85.32	15.05	11.56	7.14	9.97
23b	97.87	43.59	14.37	16.31	23.28	88.84	20.80	25.85	16.16	23.10
24b	14.35	53.49	29.29	26.49	18.60	20.42	31.37	21.02	18.85	17.01

Table S4. Quantitative HPLC-MS analysis the reaction between DNQOs (**1b**-**24b**) and dipolarophiles (**1c**-**10c**) under 365 nm irradiation, and conversion was determined by integration area of the corresponding peaks monitored via absorption at 254 nm in HPLC traces.

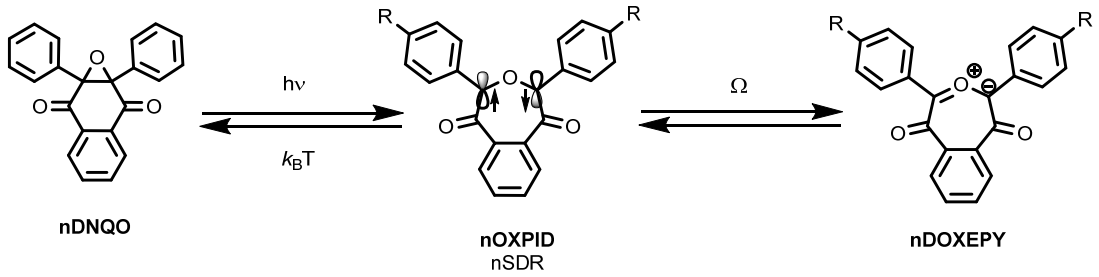
DNQO	hν = 365 nm, conversion [%]									
	1c	**2c**	**3c**	**4c**	**5c** 	**6c**	**7c**	**8c**	**9c**	**10c** 
1b	60.04	13.26	2.92	2.60	1.76	50.55	8.32	7.67	6.47	3.79
2b	25.56	5.86	2.47	0	3.35	34.08	4.09	2.05	8.72	0
3b	27.05	1.77	2.28	0	0	26.06	7.68	6.35	8.72	0.65
4b	8.71	0.84	1.17	0.42	0.44	6.50	2.08	4.28	0.17	3.27
5b	3.13	0	0	0.22	0	0.30	2.87	1.34	0.67	0.30
6b	0.56	0	2.02	0.66	0.71	0	0	0.92	0	0.29
7b	1.92	0	0	0	0	0	6.18	3.81	0	0
8b	3.90	3.58	0	0.76	3.18	9.42	4.10	0	3.45	2.58
9b	27.47	9.33	9.63	11.91	3.80	19.42	0	12.24	12.26	10.16
10b	28.48	11.91	7.78	8.54	5.36	21.21	4.27	6.18	8.55	8.06
11b	13.52	0	0	0	0	9.62	0.99	0	-1.57	2.41
12b	41.96	11.95	3.70	1.08	2.84	53.81	6.55	3.62	4.23	1.01
13b	39.11	5.50	1.33	0.66	0	48.48	3.20	0	0.49	0.79
14b	46.40	18.34	0.56	2.83	2.68	56.83	8.35	4.86	7.74	1.74
15b	50.38	12.54	1.26	4.24	1.86	37.05	18.29	12.18	3.81	0
16b	26.32	11.60	3.20	0.73	2.32	39.92	15.38	3.46	0.78	0
17b	29.04	20.92	0	6.96	0	25.89	31.34	5.83	3.87	10.67
18b	12.69	6.13	0.87	0.87	0	13.12	4.91	4.37	2.18	0.47
19b	34.57	14.55	0	1.95	0	30.43	4.41	11.79	3.60	4.57
20b	51.05	19.61	0.55	7.11	0.01	55.32	15.15	1.58	4.41	3.92
21b	7.00	2.20	0	2.64	1.31	8.63	3.14	1.90	0	1.21
22b	30.70	8.48	0	0.21	1.63	29.22	1.10	3.08	1.54	0
23b	30.96	10.10	0	1.92	2.27	30.47	11.06	0	1.14	1.59
24b	36.50	6.94	0.29	2.69	2.27	38.05	9.46	0.12	2.90	2.40

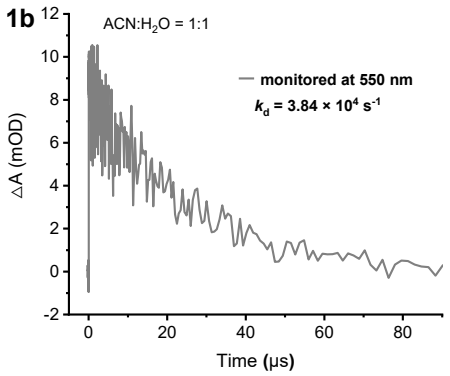
Table S5. Quantitative HPLC-MS analysis the reaction between DNQOs (**1b**-**24b**) and dipolarophiles (**1c**-**10c**) under 373 nm irradiation, and conversion was determined by integration area of the corresponding peaks monitored via absorption at 254 nm in HPLC traces.

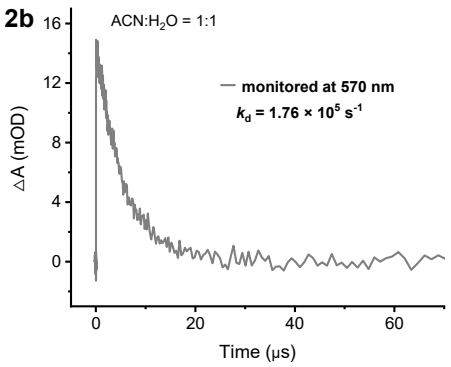
DNQO	hν = 373 nm, conversion [%]									
	1c	**2c**	**3c**	**4c**	**5c** 	**6c**	**7c**	**8c**	**9c**	**10c** 
1b	52.28	9.48	1.46	3.54	3.63	44.36	13.63	7.50	5.49	4.61
2b	29.39	10.43	9.91	8.22	11.56	24.69	7.60	0	13.94	6.88
3b	24.85	1.08	0.57	0	-0.58	18.02	1.46	1.06	4.45	0
4b	7.56	2.53	1.54	0.61	3.83	6.92	4.19	2.98	0.74	5.16
5b	0.77	2.69	0.48	1.11	2.47	0.68	2.18	0	1.41	1.51
6b	0.61	0	1.71	0.76	2.01	0.27	0	2.98	0	0.42
7b	0	2.06	0	2.06	0.45	0	7.95	0.92	0	0
8b	2.50	0.09	0	0.48	0	11.31	1.84	0	6.71	0
9b	18.36	8.98	12.02	11.62	12.89	18.60	0	9.56	15.87	13.24
10b	25.85	10.45	11.91	11.14	12.96	19.25	11.91	10.46	12.49	11.12
11b	13.45	0	0.03	0	0.18	7.57	2.17	0	1.10	0.56
12b	48.17	9.20	3.61	3.30	4.44	45.77	14.32	2.44	4.98	-0.37
13b	44.84	4.74	1.49	1.71	0.92	44.10	6.01	0.18	1.28	0.64
14b	46.09	14.83	1.25	3.96	1.47	49.76	20.43	3.92	9.00	0.32
15b	51.57	7.75	0.44	1.07	0	51.88	19.11	10.96	0.50	0
16b	23.66	10.08	0	2.01	0.34	23.17	10.12	0.41	0	0
17b	32.75	11.08	0	3.22	0	47.78	31.21	7.22	8.07	10.81
18b	11.01	3.96	1.92	1.68	1.09	9.52	7.26	2.83	1.58	2.04
19b	34.98	5.05	0	3.80	0	50.63	5.40	11.13	7.24	4.02
20b	48.49	12.69	1.28	9.06	4.54	46.55	29.08	2.16	5.21	5.65
21b	2.31	0.44	0.10	0.78	0.70	5.10	4.00	0.24	0	1.06
22b	26.10	4.38	1.96	0	0.03	22.07	3.13	1.32	2.04	0.29
23b	19.63	0	0	0	0	18.27	4.47	0	0	0
24b	31.82	5.54	0.72	0.76	0.88	29.36	7.83	3.58	1.51	1.24

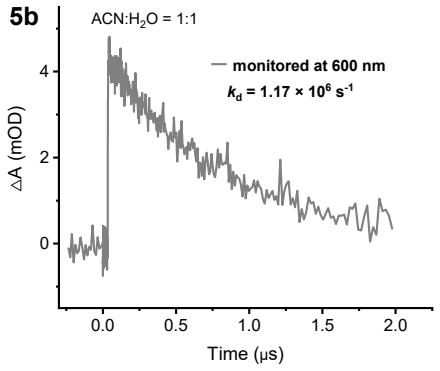
Decaying kinetics of the singlet diradicals (SDRs) measured by nanosecond transient absorption spectroscopy.

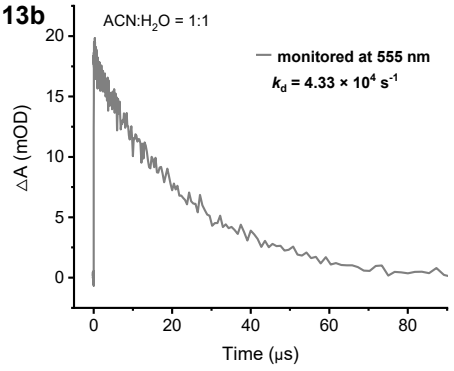
The NTAS measurements of the DNQOs compound (5.0 mM) were done in the air atmosphere at 293 K on the EOS (Ultrafast Systems, USA) system. For this investigation, a 355 nm excitation laser (Q-switched Nd:YAG laser, pulse duration 1 ns, pulse energy 7 μJ, repetition rate 1 kHz) was used to pump the molecules to the excited state and the white-light continuum (WLC) probe pulses (350-900 nm) was used for probing the absorbance spectrum of the SDRs. The temporal and spectral profiles of the pump-induced differential absorbance of the probe light (ΔA) are visualized by an optical fiber-coupled multichannel spectrometer (with a CMOS sensor) and the collected data was further plotted and analyzed by the Surface Xplorer (SX) software.











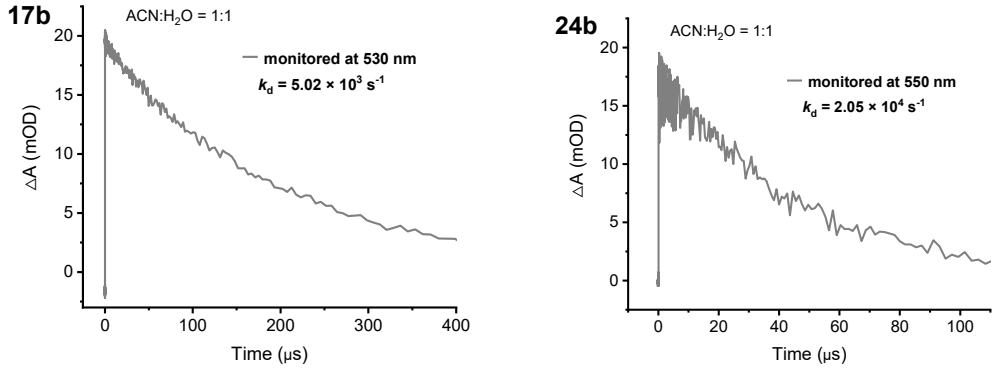


Figure S3. Kinetic tracking of the decaying process the transient SDRs back to DNQOs via NTAS by monitoring the absorbance intensity evolution at the designated wavelength, and the first order decaying curved was fitted, and the rate (k_d, SDRs to DNQOs) was determined.

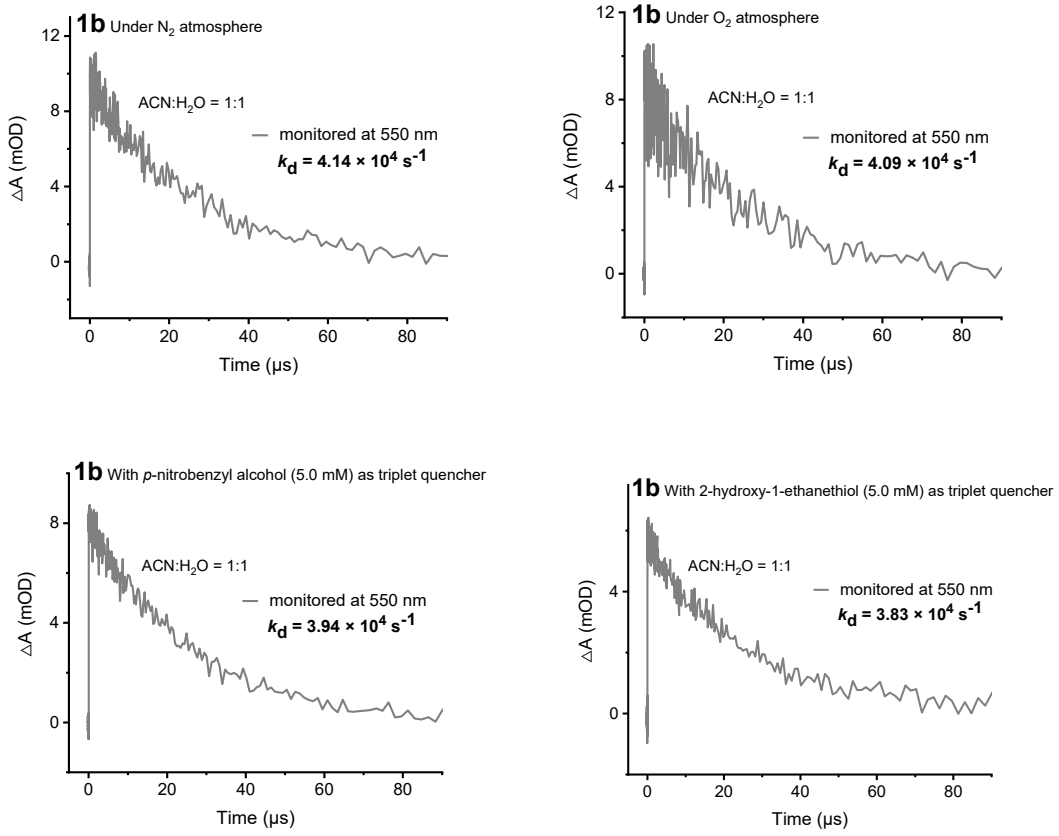
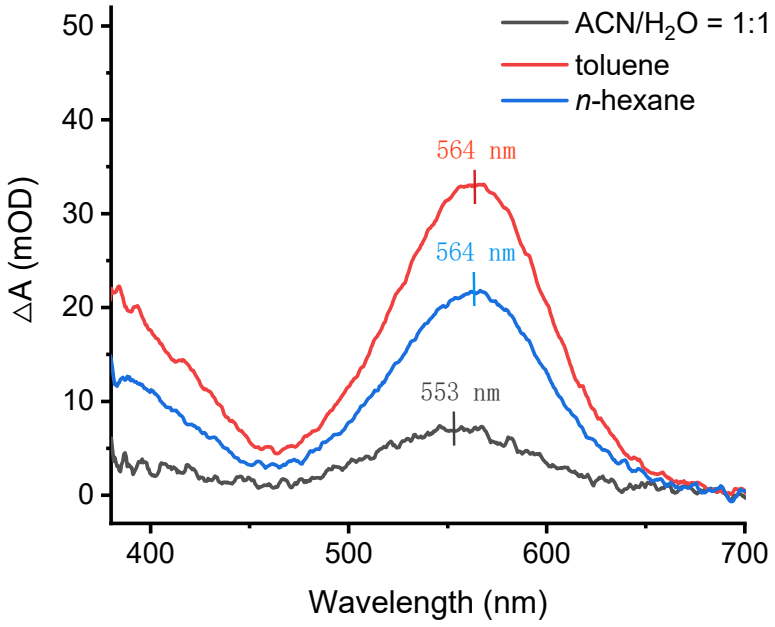


Figure S4. Comparison of the relaxation rate (k_d) of thermodynamic reversion of the transient intermediate SDR to DNQO either in the presence or absence of excited triplet quencher (including $^3O_2$) after a single 355 nm excitation pulse.

Solvent effect on the photoswitchable SDR intermediates and Gibbs free energy of the TS for the thermodynamic reversion

a)



b)

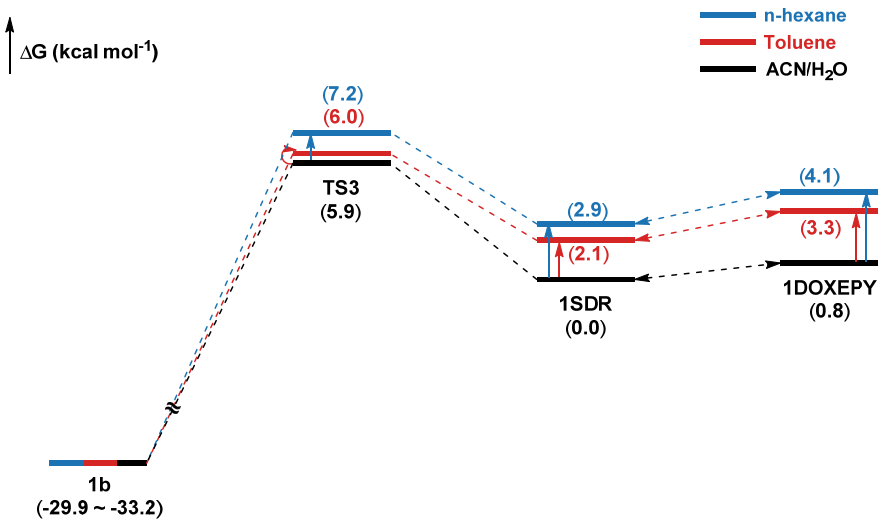


Figure S5. a) Transient absorption spectrum of the singlet diradical **1SDR**, generated from **1b** ($\lambda_{exc.}$ = 355 nm) at 0 μs delay time in various solvent with different dielectric constant, 293 K. b) The calculated Gibbs free energy profile for the solvent effect on the photoswitch intermediates and TS, **1SDR**, **1DOXEPY**, **TS3**, and DNQO **1b**, performed at M06-2X/6-311G**//M06-2X/6-31G** level of theory.

Electron paramagnetic resonance (EPR) experiments

EPR spectra were recorded at 140 K on Bruker EMX plus X-band EPR spectrometer operated at 9.43 GHz. Typical parameters are shown as follows, scan range: 300 G; center field set: 3365 G; modulation amplitude: 0.5 G; modulation frequency: 100 kHz; microwave power: 2.0 mW.

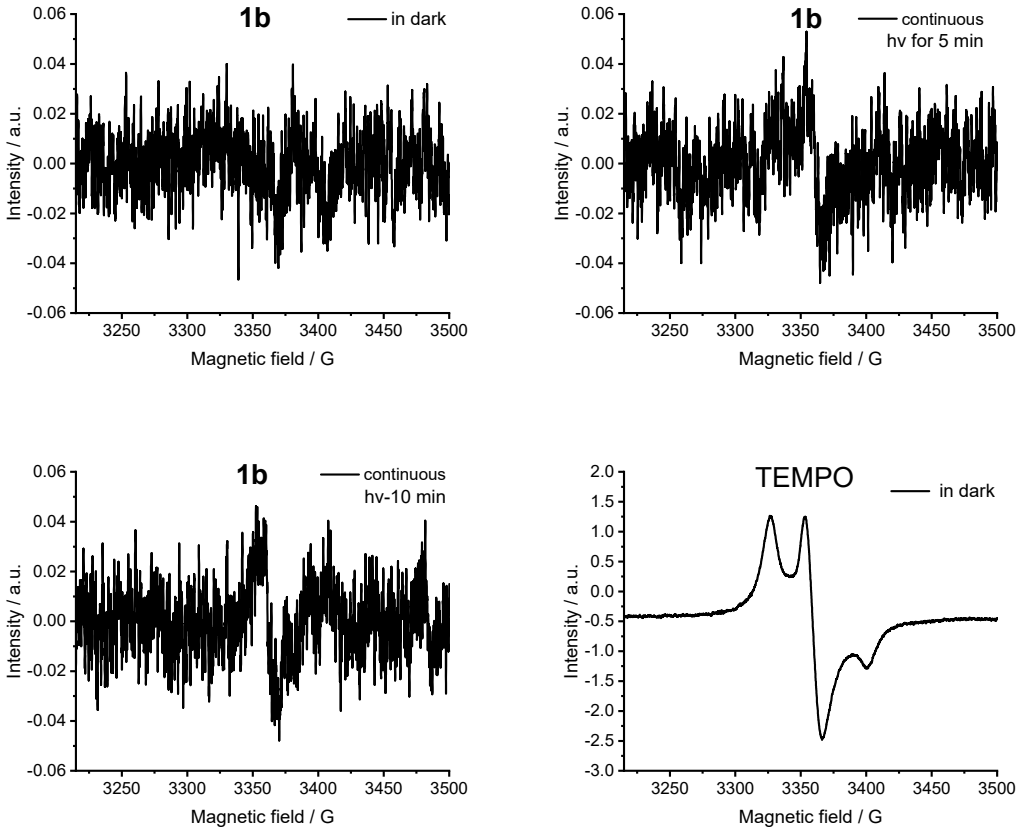
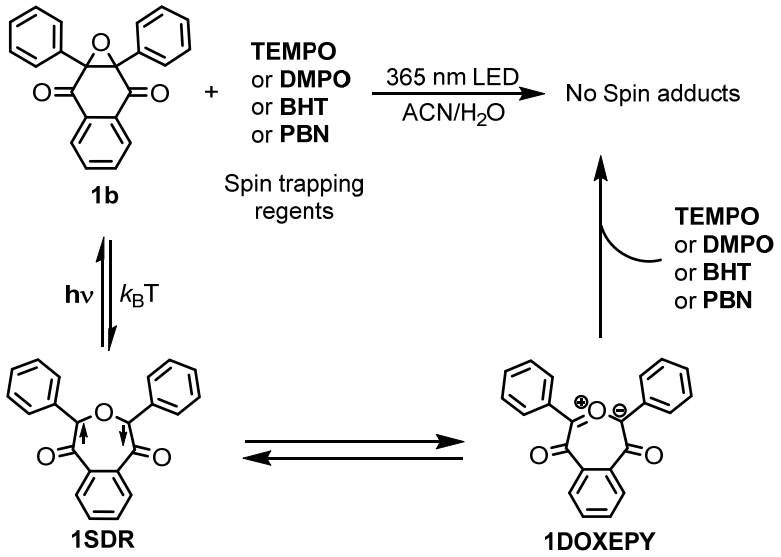
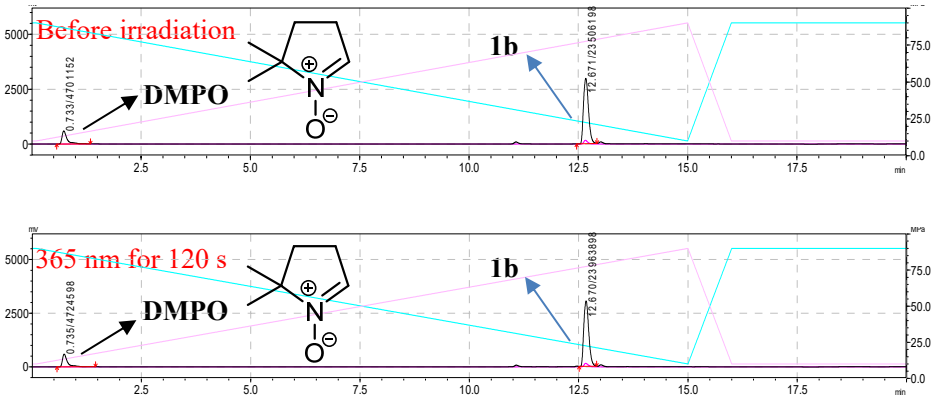


Figure S6. EPR spectrum of **1b** (5.0 mM) under continuous photoactivation by using a 100 W Hg lamp as excitation light source (> 200 nm) vs. TEMPO (1.0 mM) in methanol matrix in a sealed quartz tube at 140 K under air condition as a control (resonance frequency: 9.43 GHz).

Radical-trapping experiments

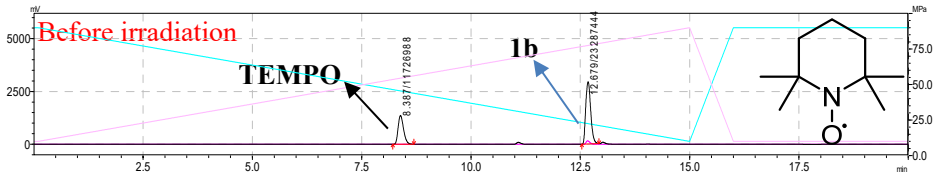


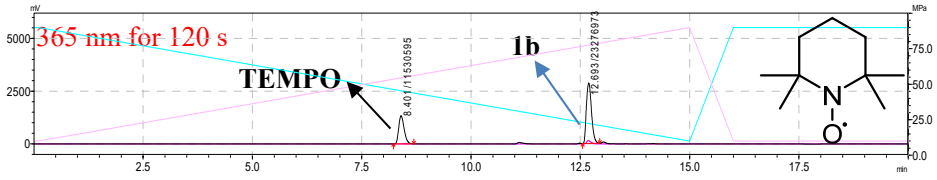
(a)



	Peak	Retention Time	Integrated Area
Before irradiation	**DMPO**	0.733	4701152
	1b	12.671	23506198
365 nm for 120 s	**DMPO**	0.735	4724598
	1b	12.670	23963898

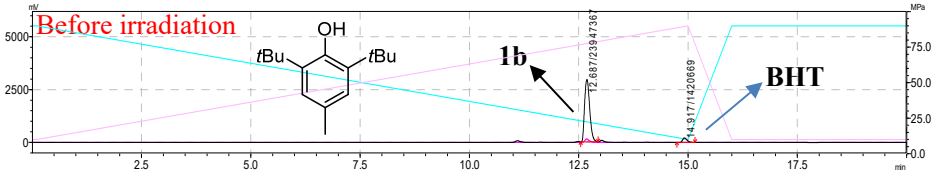
(b)

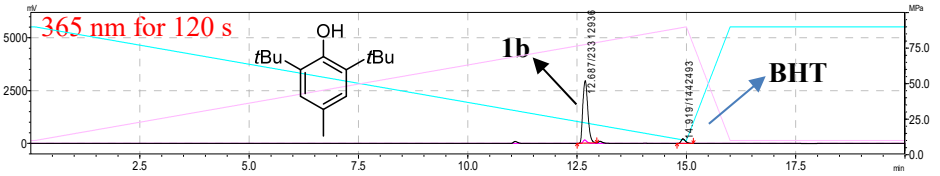




	Peak	Retention Time	Integrated Area
Before irradiation	**TEMPO**	8.387	11726988
	1b	12.679	23287444
365 nm for 120 s	**TEMPO**	8.401	11530595
	1b	12.693	23276973

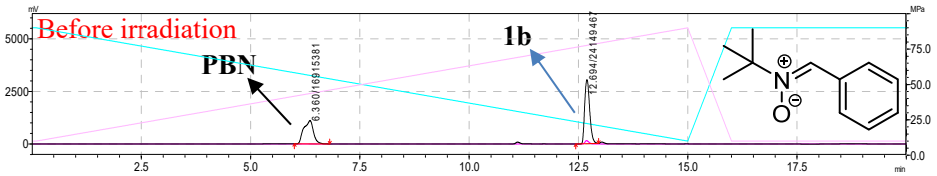
(c)

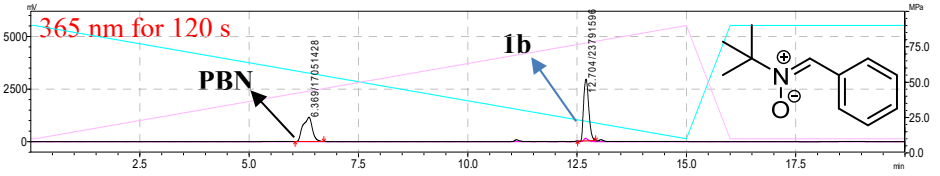




	Peak	Retention Time	Integrated Area
Before irradiation	**BHT**	12.687	23312936
	1b	14.919	1442493
365 nm for 120 s	**BHT**	12.687	23947367
	1b	14.917	1420669

(d)

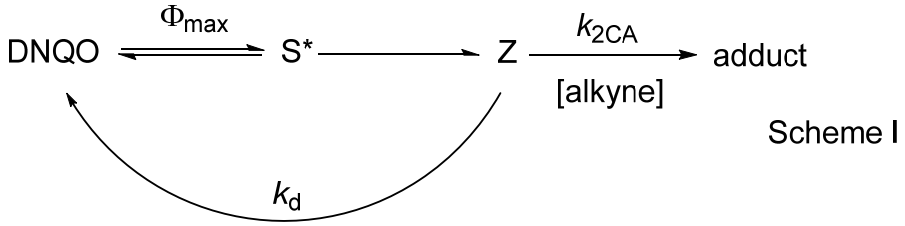




	Peak	Retention Time	Integrated Area
Before irradiation	**PBN**	6.360	16915381
	1b	12.694	24149467
365 nm for 120 s	**PBN**	6.369	17051428
	1b	12.704	23791596

Figure S7. Radical-trapping experiments for identification of the singlet diradicals by using radical-trapping reagents. A solution of 2.0 mM **1b** and various radical-trapping reagents (5.0 mM) in ACN/H_2O (1:1) were subjected to HPLC-MS analysis (monitored at 254 nm for integration of the absorbance peaks), respectively, before and after photo-irradiated for 2.0 mins at 298 K before. (a) The photo-reaction was carried out for **1b** in the presence of **DMPO**. (b) The photo-reaction was carried out for **1b** in the presence of **TEMPO**. (c) The photoreaction was carried out for **1b** in the presence of **BHT**. (d) The photo-reaction was carried out for **1b** in the presence of **PBN**.

Analysis for the photophysical and photochemical properties of the DNQO reacting with dipolarophiles



Scheme I

Scheme I is the mechanism for the photoreaction of DNQO toward alkyne through a reversible intermediate.[1] In the scheme, DNQO is the starting 2,3-diaryl-1,4-naphthoquinone epoxide, Z is considered as the transient intermediate which is capable of reversion to DNQO via a thermos-dynamic relaxation and also cycloaddition with alkyne to form adduct. The higher concentration of alkyne would lead to higher concentration of adduct because of the competitive reaction pathways of the reversible intermediate (Z) under the identical irradiation conditions. Steady state analysis of the reaction scheme gives eq. 1,

$$\Phi^{-1} = \Phi_{max}^{-1} [1 + (k_d / k_{2CA}) c_y^{-1}] \qquad \text{(eq. 1)}$$

The equation indicates the influence of alkyne concentration (c_y) upon the apparent quantum yield of the cycloaddition (Φ). In this equation, Φ_{max} is the quantum yield for formation of the intermediate Z from DNQO in a photochemical transformation, and k_d/k_{2CA} indicates the relative reactivity of the intermediate for cycloaddition with alkynes.

These values can be obtained by plotting a linear fitting to the experimental parameters, including the inverse of the alkyne concentrations (c_y^{-1} as the x axis) against the inverse of the apparent quantum yields (Φ^{-1} as the y axis). The values of k_d were experimental measured via transient absorption spectroscopy, Thus, k_{2CA} can be obtained from $\Phi_{max}^{-1} \cdot k_d/k_{2CA}$ as the slope of the linear fitting curve.

Determination of the apparent photo-quantum yields (Φ) for the photoconversion of DNQO (1b, 3b, 13b, 17b, and 24b)

The apparent quantum yields of the photoconversion of DNQO to cycloadduct were determined by using a potassium ferrioxalate-based chemical actinometer.[2] In brief, a 250 μL fresh solution of 6.0 mM potassium ferrioxalate in 0.1 N H_2SO_4 aqueous solution was irradiated with the 365 nm LED (single wavelength output after an optical filter) in a quartz cuvette (0.2 cm × 1.0 cm, 1.0 cm optical path) for specified times before quenching by addition of 4.75 mL of NaOAc/HOAc buffer (pH = 4.3) and followed by 5.0 mL of 0.1% 1,10-phenanthroline solution in water to develop the characteristic color of the Fe^{2+}-(1,10-phenanthroline)$_3$ complex at 510 nm. The mixture was stirred for 30 min till complete development of the color before UV-Vis measurement. This procedure is to calibrate the light photon flux (I_0) of the 365 nm LED light source. Then, the test samples of DNQO and BCN (excessive) in solution was exposed and the resulting adduct concentration were obtained via quantitative HPLC analysis via related calibration curves. All the workup procedures were carried out in the dark and the samples were also protected from light with aluminum foil during

handling. All the operation procedure and conditions for the photo-irradiation were also the same for both the chemical actinometer and tested samples (in ACN:H_2O = 1:1 mixed solution, and the quantitative HPLC analysis was direct measured without the color developing process), including light sources, experimental setup, volume of the solution and the cuvette. The quantum yield for a test compound was calculated based on the following equations:

The incident monochromic photon flux I_0:

$$I_0 = \frac{\mathrm{d}\,[Act]}{\mathrm{d}\,t} \times [1/(1\text{-}10^{-\mathrm{Abs}_c})]/\Phi_c = \frac{\mathrm{d}\,[DNQO]}{\mathrm{d}\,t} \times [1/(1\text{-}10^{-\mathrm{Abs}_t})]/\Phi_t \qquad \text{(eq. 2)}\ [3,4]$$

Because at the initial photo-conversion stage: $\frac{\mathrm{d}\,[Act]}{\mathrm{d}\,t} = \frac{\mathrm{d}\,Abs_{product}}{\mathrm{d}\,t}\left(\frac{1}{\varepsilon_{product} l}\right)$, therefore:

$$I_0 = (40 \times k_c/\varepsilon_{510} l) \times [1/(1\text{-}10^{-\mathrm{Abs}_c})]/\Phi_c = \frac{\mathrm{d}\,[DNQO]}{\mathrm{d}\,t} \times [1/(1\text{-}10^{-\mathrm{Abs}_t})]/\Phi_t \qquad \text{(eq. 3)}$$

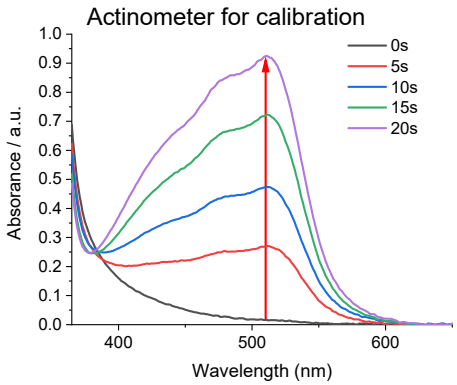
The subscript "*c*" represents to the parameters of the chemical actinometer.

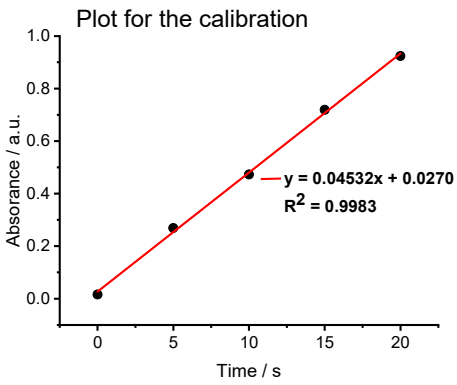
The subscript "*t*" represents to the parameters of the tested 2,3-diaryl-1,4-naphthoquinone epoxide. Therefore:

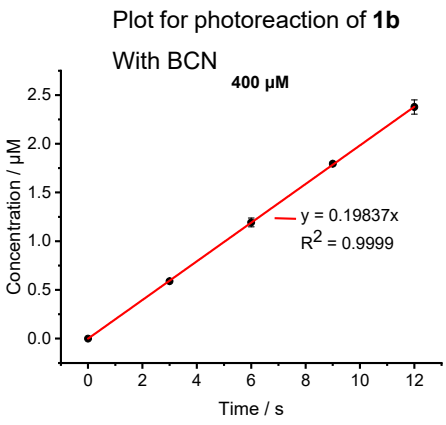
$$\Phi_{reac.} = \Phi_t = [(1\text{-}10^{-\varepsilon_c c_c l})/(1\text{-}10^{-\varepsilon_t c_t l})] \times \frac{\mathrm{d}\,[DNQO]}{\mathrm{d}\,t}\ [l\varepsilon_{510}/(40 \times k_c)] \times \Phi_c \qquad \text{(eq. 4)}$$

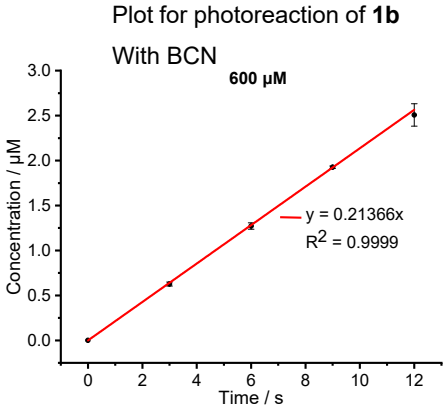
where ε_c and ε_t were extinction coefficients of the standard chemical actinometer and test samples (DNQOs) at 365 nm, respectively. l = 1.0 cm; k_c was the slopes of linear fitting line of product formation [Fe^{2+}-(1,10-phenanthroline)$_3$ complex] in the plots of absorbance changes versus time at the observing wavelength (510 nm) for the standard chemical actinometer. $\frac{\mathrm{d}\,[DNQO]}{\mathrm{d}\,t}$ were the slopes of linear fitting line of product formation in the plots of concentration changes determined by HPLC versus time for tested 2,3-diaryl-1,4-naphthoquinone epoxide. The zeroth order photo-conversion rate (k_c and $\frac{\mathrm{d}\,[DNQO]}{\mathrm{d}\,t}$) could be only applied at very low conversion (as low as possible) of the starting materials because the absorption of light by the products formed under such condition is minimal. Noteworthy, the addition of the buffer solution and the developing reagent (1,10-phenanthroline) after photoreaction of the actinometer for the absorbance 510 nm readout resulted in a 40-fold dilution, therefore the k_c need to be multiplied by a factor of 40. c_c and c_t were concentrations of the standard actinometer and the test compound for the photochemical reaction, respectively; ε_{510}[5] were extinction coefficients of the Fe^{2+}-(1,10-phenanthroline)$_3$ complex at 510 nm for the actinometer.

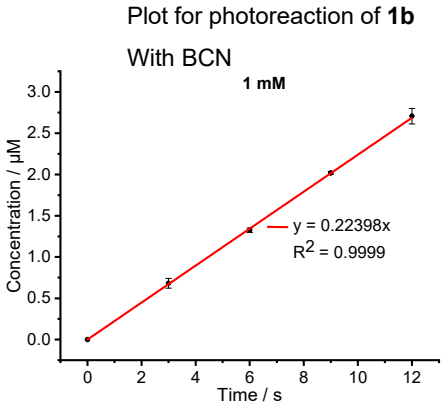
(a)

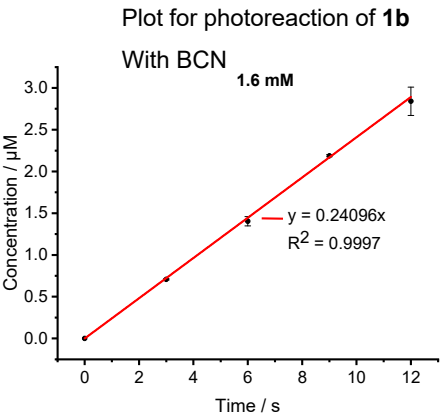

Actinometer for calibration
0s
5s
10s
15s
20s
Absorance / a.u.
Wavelength (nm)


Plot for the calibration
y = 0.04532x + 0.0270
R2 = 0.9983
Absorance / a.u.
Time / s

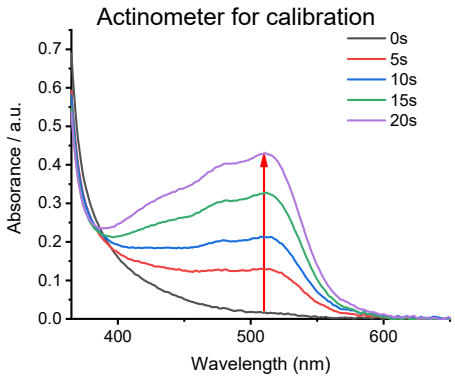

Plot for photoreaction of 1b
With BCN
400 µM
y = 0.19837x
R2 = 0.9999
Concentration / µM
Time / s

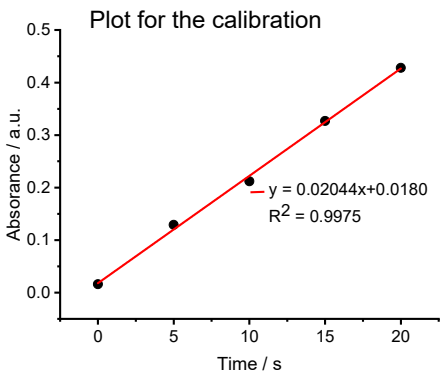

Plot for photoreaction of 1b
With BCN
600 µM
y = 0.21366x
R2 = 0.9999
Concentration / µM
Time / s

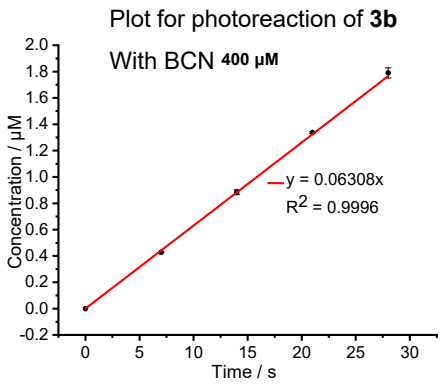

Plot for photoreaction of 1b
With BCN
1 mM
y = 0.22398x
R2 = 0.9999
Concentration / µM
Time / s

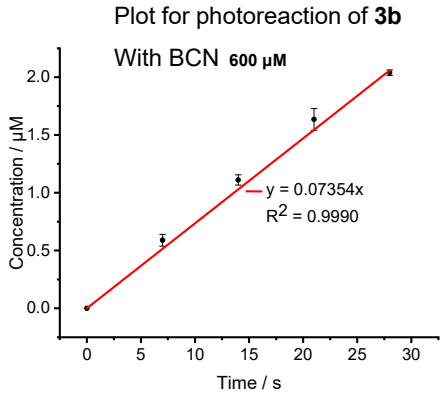

Plot for photoreaction of 1b
With BCN
1.6 mM
y = 0.24096x
R2 = 0.9997
Concentration / µM
Time / s

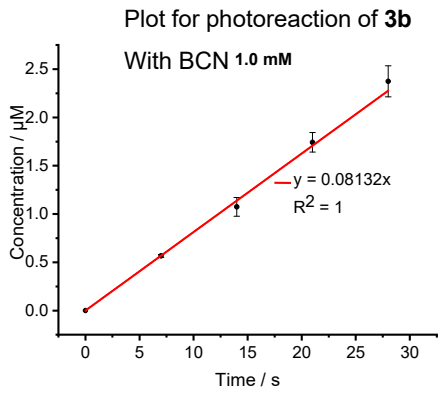
(b)

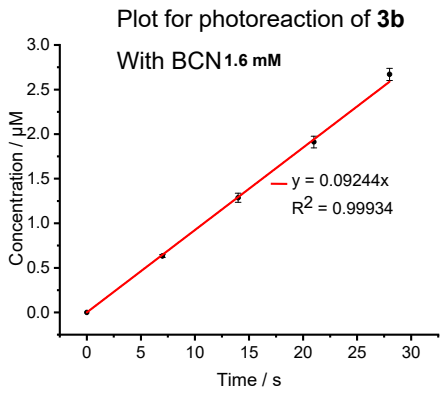

Actinometer for calibration
0s
5s
10s
15s
20s
Absorance / a.u.
Wavelength (nm)


Plot for the calibration
y = 0.02044x+0.0180
R2 = 0.9975
Absorance / a.u.
Time / s

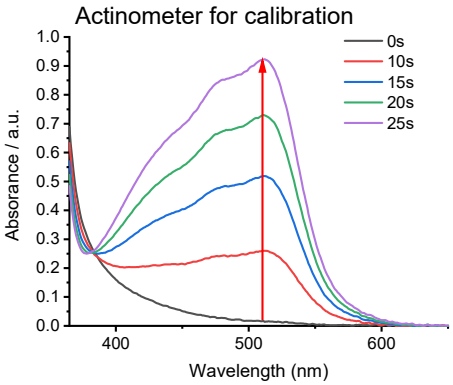

Plot for photoreaction of 3b
With BCN 400 µM
y = 0.06308x
R2 = 0.9996
Concentration / µM
Time / s

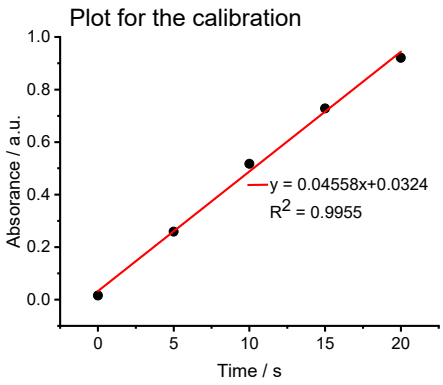

Plot for photoreaction of 3b
With BCN 600 µM
y = 0.07354x
R2 = 0.9990
Concentration / µM
Time / s

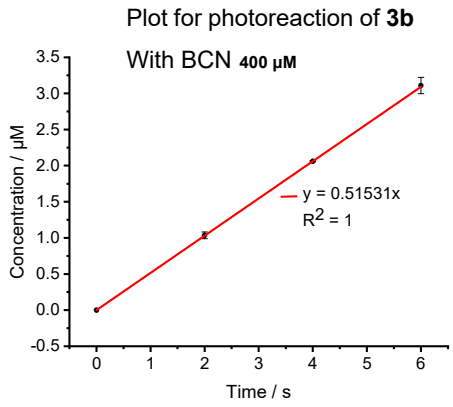

Plot for photoreaction of 3b
With BCN 1.0 mM
y = 0.08132x
R2 = 1
Concentration / µM
Time / s

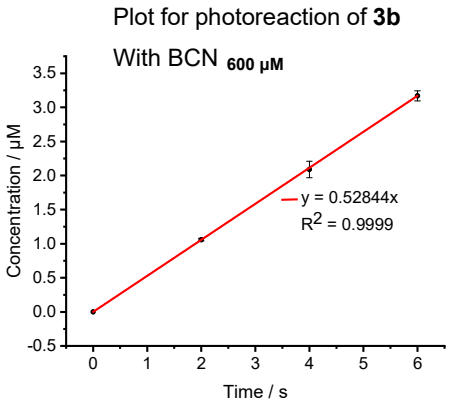

Plot for photoreaction of 3b
With BCN 1.6 mM
y = 0.09244x
R2 = 0.99934
Concentration / µM
Time / s

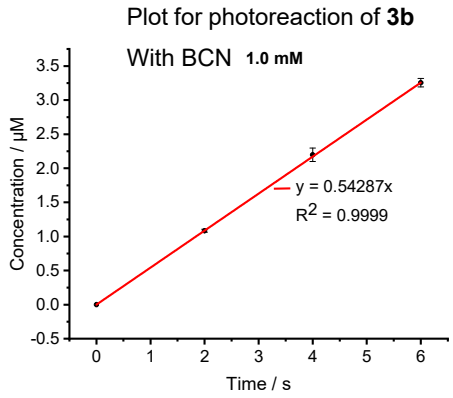
(c)

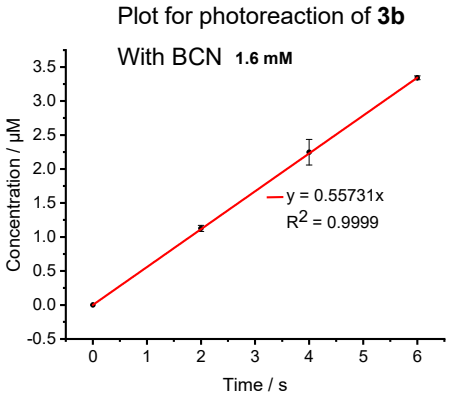

Actinometer for calibration
0s
10s
15s
20s
25s
Absorance / a.u.
Wavelength (nm)


Plot for the calibration
y = 0.04558x+0.0324
R2 = 0.9955
Absorance / a.u.
Time / s

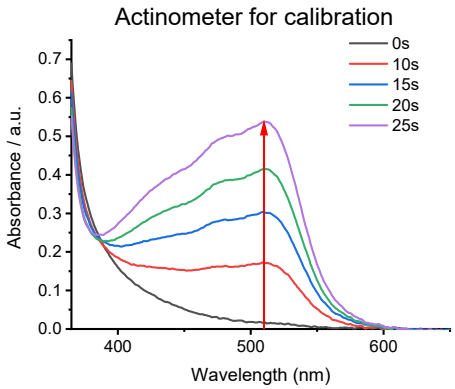

Plot for photoreaction of 3b
With BCN 400 μM
y = 0.51531x
R2 = 1
Concentration / μM
Time / s

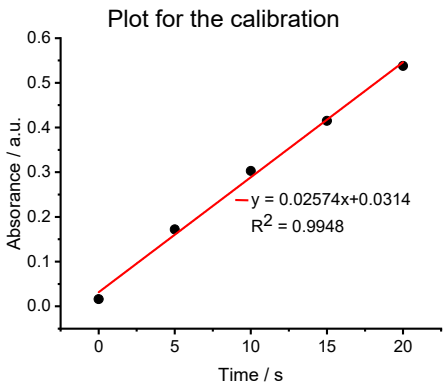

Plot for photoreaction of 3b
With BCN 600 μM
y = 0.52844x
R2 = 0.9999
Concentration / μM
Time / s

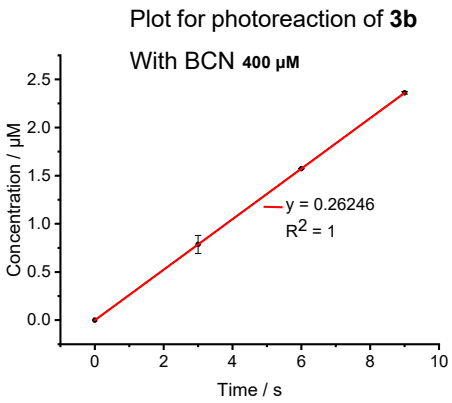

Plot for photoreaction of 3b
With BCN 1.0 mM
y = 0.54287x
R2 = 0.9999
Concentration / μM
Time / s

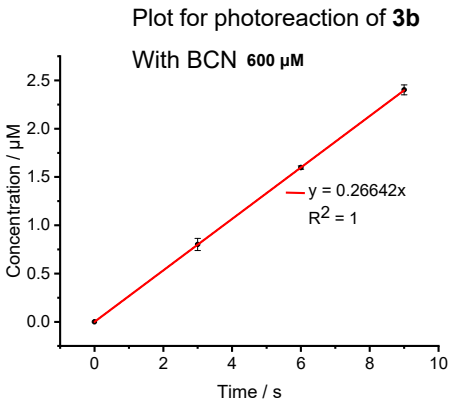

Plot for photoreaction of 3b
With BCN 1.6 mM
y = 0.55731x
R2 = 0.9999
Concentration / μM
Time / s

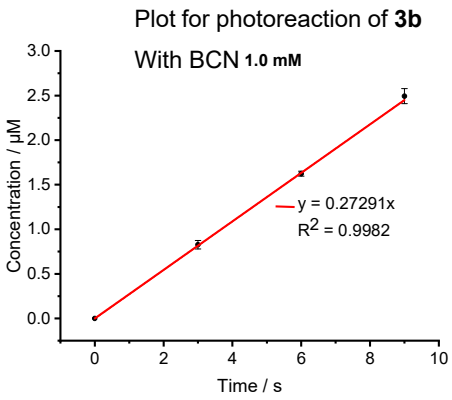
(d)

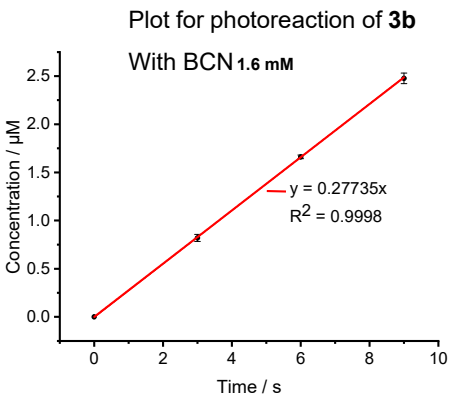

Actinometer for calibration
0s
10s
15s
20s
25s
Absorbance / a.u.
Wavelength (nm)


Plot for the calibration
Absorance / a.u.
y = 0.02574x+0.0314
R2 = 0.9948
Time / s


Plot for photoreaction of 3b
With BCN 400 μM
Concentration / μM
y = 0.26246
R2 = 1
Time / s


Plot for photoreaction of 3b
With BCN 600 μM
Concentration / μM
y = 0.26642x
R2 = 1
Time / s


Plot for photoreaction of 3b
With BCN 1.0 mM
Concentration / μM
y = 0.27291x
R2 = 0.9982
Time / s


Plot for photoreaction of 3b
With BCN 1.6 mM
Concentration / μM
y = 0.27735x
R2 = 0.9998
Time / s

(e)

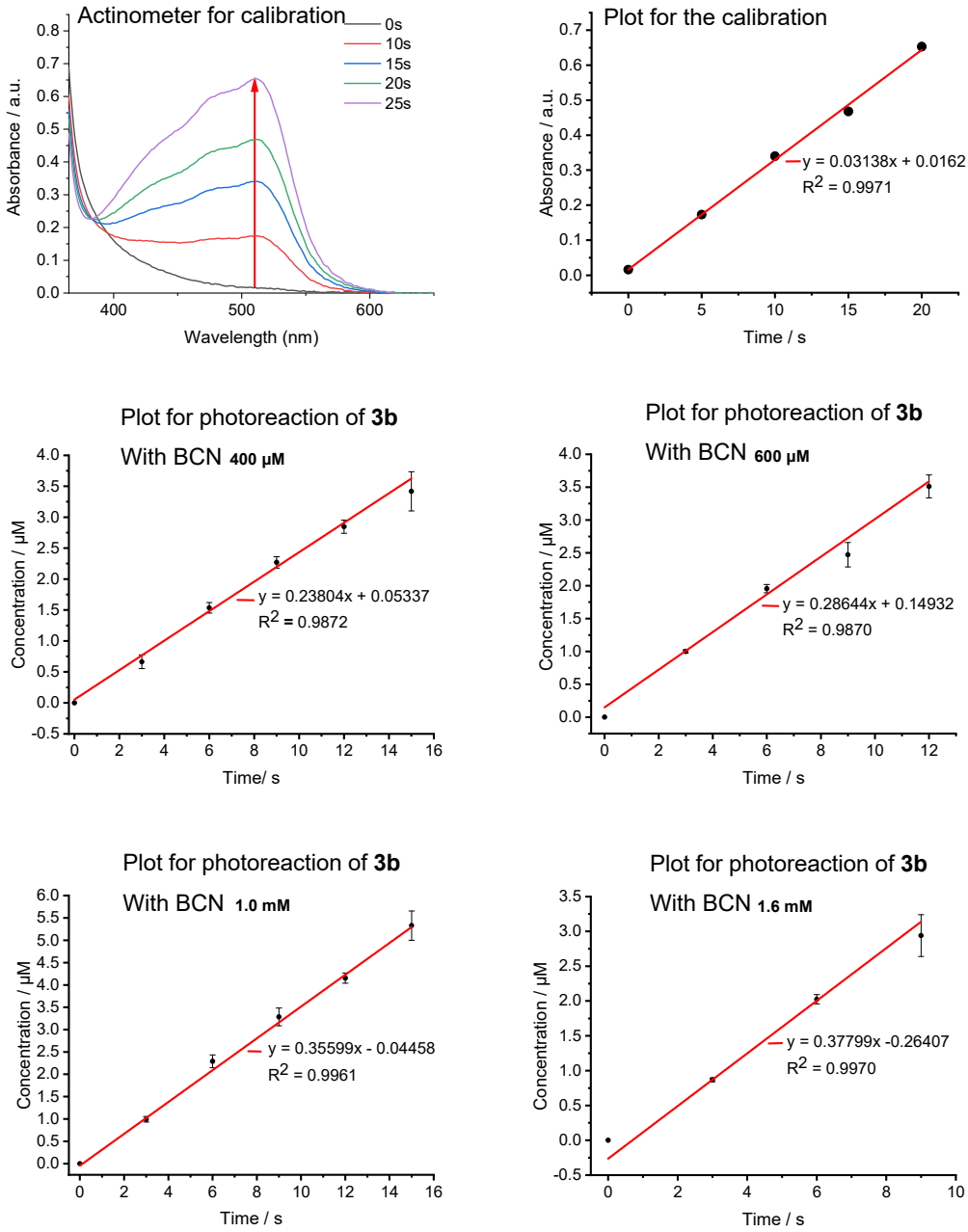


Figure S8. Determination of the apparent quantum yields using a potassium ferrioxalate-based chemical actinometer at 298 K. Time-course of absorbance change of formation of the Fe^{2+}-(1,10-phenanthroline)$_3$ complex at 510 nm was induced by the 365 nm LED to the actinometer with a linear fitting curve for calibration. And concentration changes of adduct formation from DNQO in the presence of BCN for (a) **1b**; (b) for **3b**; (c) for **13b**; (d) for **17b**; (e) for **24b** to corresponding by the same 365 nm LED with a linear fitting curve (monitored for absorbance at 254 nm in each HPLC trace). A solution of 20 μM DNQOs and various concentrations of BCN (400 μM, 600 μM, 1.0 mM, 1.6 mM) in ACN:H_2O (1:1) mixed solvent in the same quartz cuvette were photo-irradiated for a specified time before HPLC measurement, respectively. Error bars denote standard deviation from three experimental replicates (n = 3).

Table S6. Summary of the apparent for determination of the apparent quantum yields (Φ) in the photoreaction for the selected DNQOs with various concentrations of BCN under the identical 365 nm LED irradiation.

DNQO	Φ (BCN 400 μM)	Φ (BCN 600 μM)	Φ (BCN 1.0 mM)	Φ (BCN 1.6 mM)
1b	0.196	0.211	0.221	0.238
3b	0.111	0.130	0.144	0.163
13b	0.509	0.519	0.533	0.547
17b	0.543	0.551	0.565	0.574
24b	0.369	0.444	0.552	0.586

Determination of photo-quantum yields (Φ_{max}) for the cycloaddition with BCN, and corresponding k_d/k_{2CA} value for the photoconversion of DNQOs (1b, 3b, 13b, 17b, and 24b)

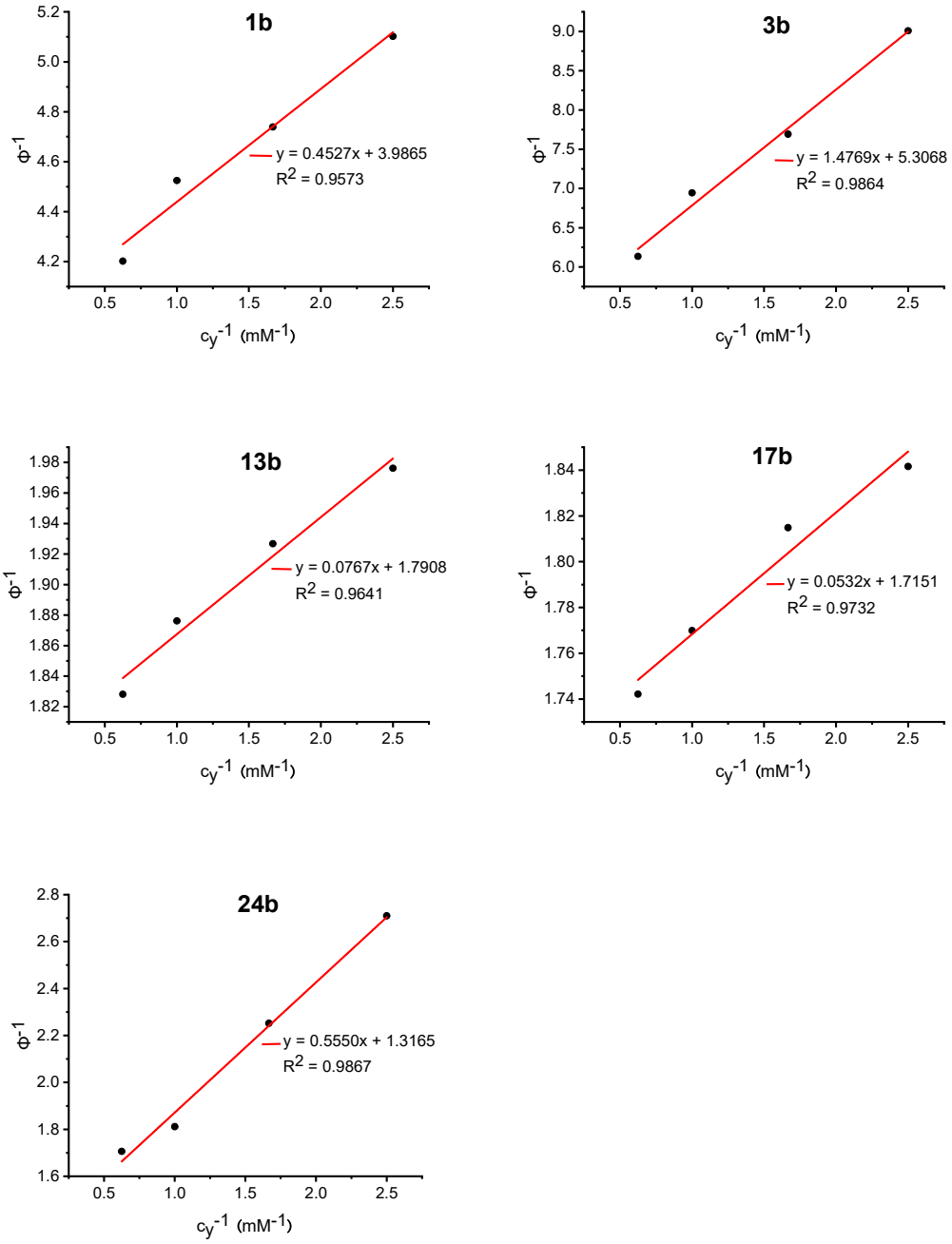
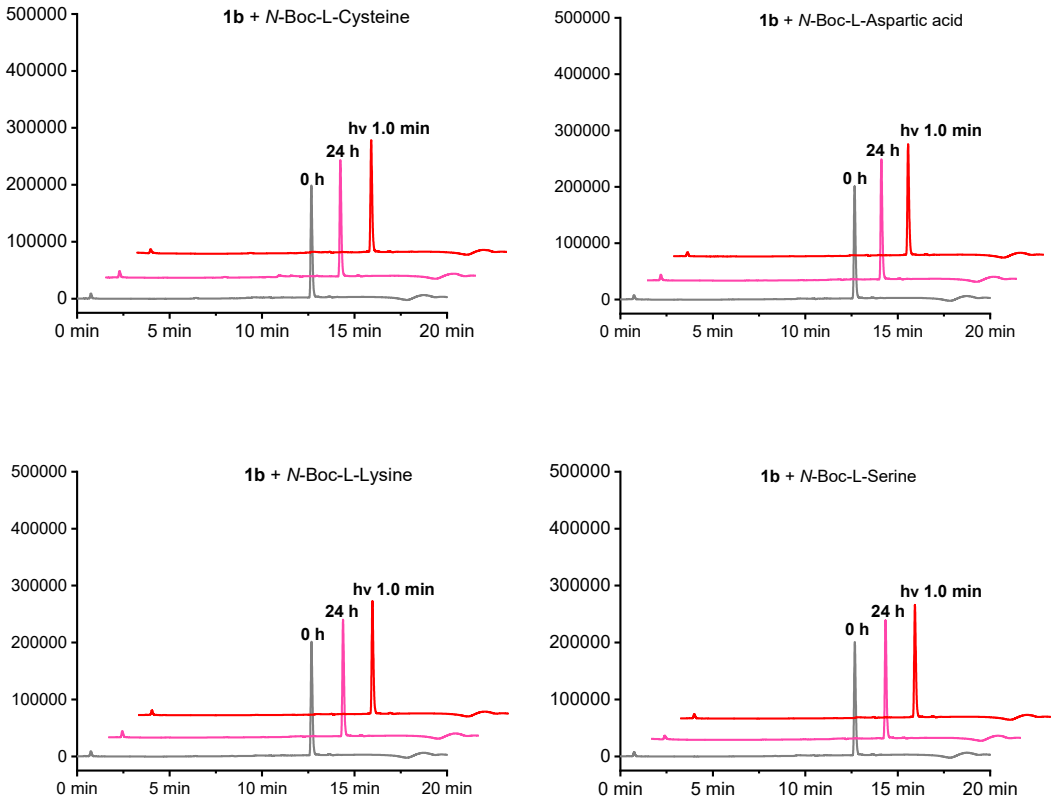


Figure S9. Determination of the quantum yields (Φ_{max}) and the k_d/k_{2CA} value by plotting the inverse of the alkyne concentrations against the inverse of the apparent quantum yields with a linear fitting curve in each plot.

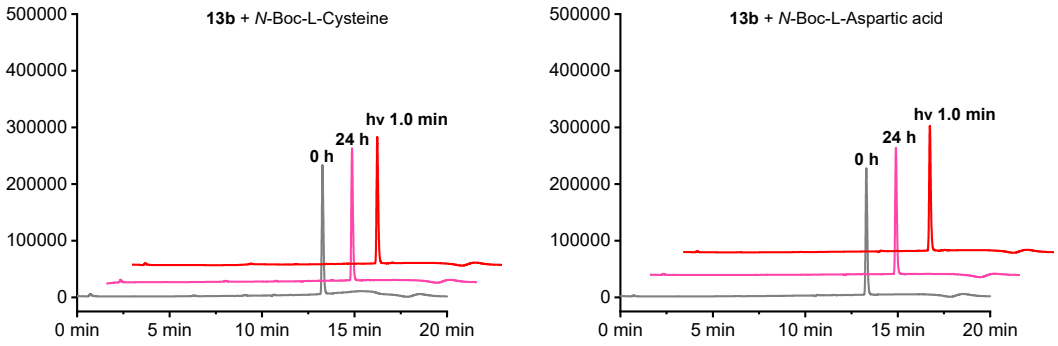
Reactivity and stability of designated DNQOs toward various bioactive species in dark or under irradiation with BCN.

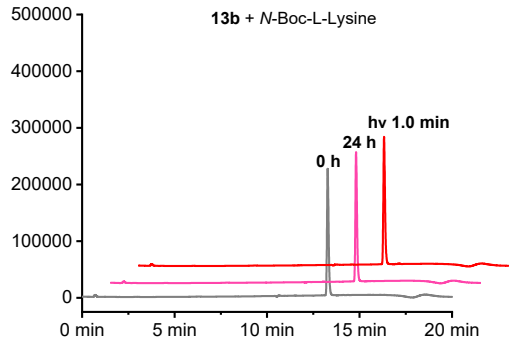
DNQO (100 μM) and *N*-Boc-L-Aspartic acid (1.0 mM), *N*-Boc-L-Cysteine (1.0 mM), *N*-Boc-L-Lysine (1.0 mM), *N*-Boc-L-Serine (1.0 mM), GSH (10.0 mM) were mixed in CH_3CN/PBS (1/1) mixed solvent, and the mixture exposed to irradiation with the 365 nm LED for 1 minute or kept in the dark for 24 hours (298 K), then subjected to quantification HPLC analysis. The results showed that all the DNQOs showed unobservable reactivity, therefore the stability of DNOQ in the presence of nucleophile upon light irradiation or in dark is robust.

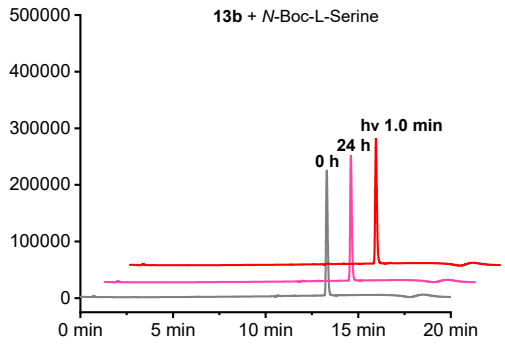
(a)



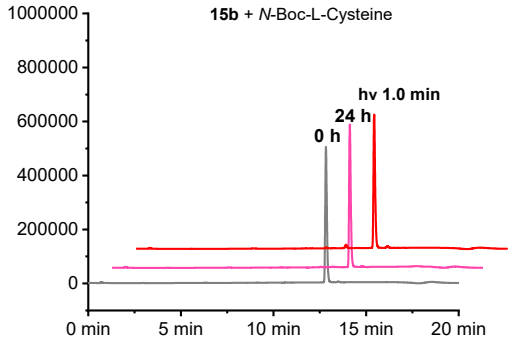
(b)

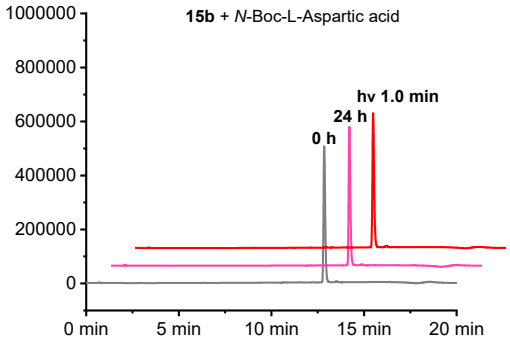


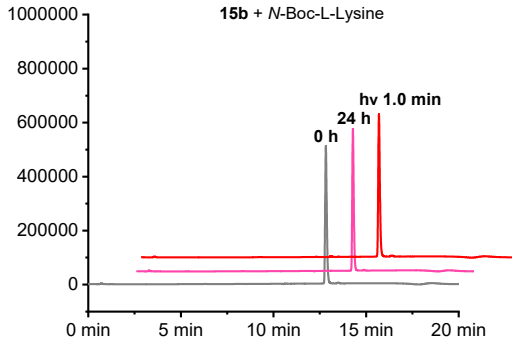

13b + N-Boc-L-Lysine
500000
400000
300000
200000
100000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min

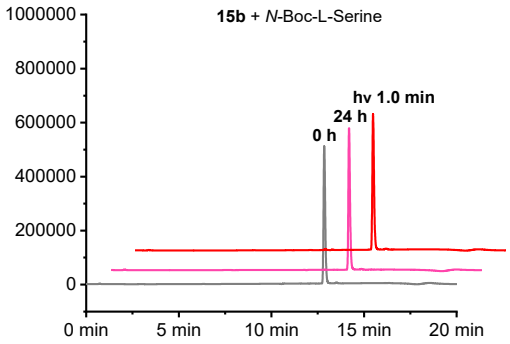

13b + N-Boc-L-Serine
500000
400000
300000
200000
100000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min

(c)

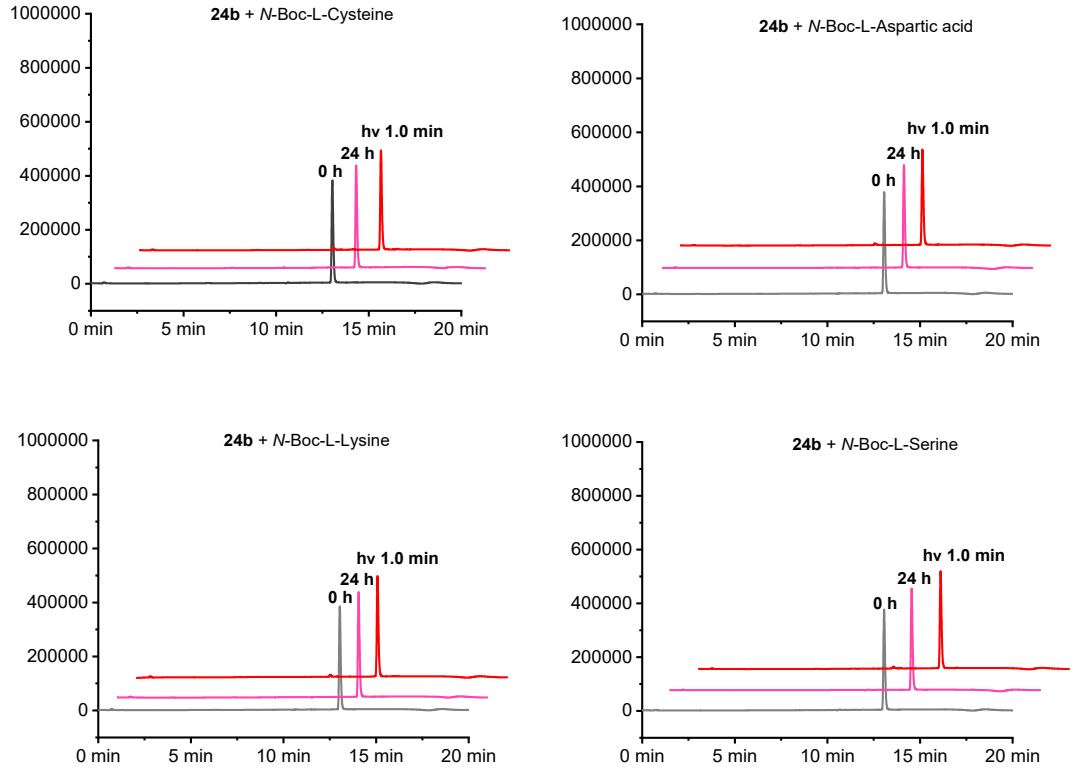

15b + N-Boc-L-Cysteine
1000000
800000
600000
400000
200000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min


15b + N-Boc-L-Aspartic acid
1000000
800000
600000
400000
200000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min

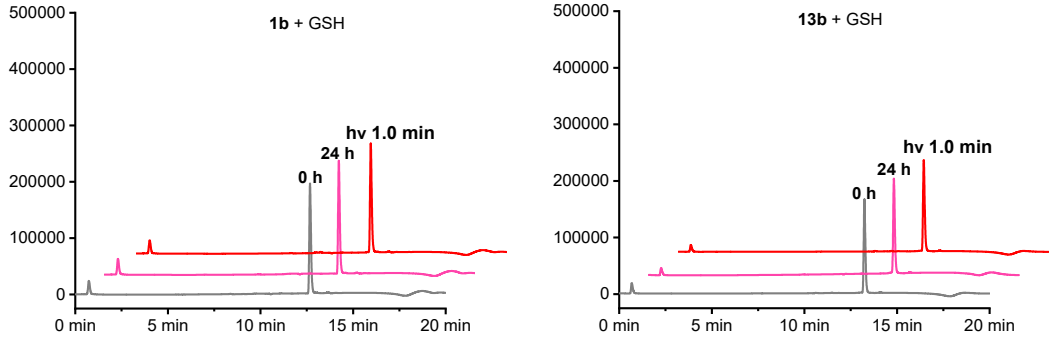

15b + N-Boc-L-Lysine
1000000
800000
600000
400000
200000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min


15b + N-Boc-L-Serine
1000000
800000
600000
400000
200000
0
hv 1.0 min
24 h
0 h
0 min
5 min
10 min
15 min
20 min

(d)


24b + N-Boc-L-Cysteine
24b + N-Boc-L-Aspartic acid
24b + N-Boc-L-Lysine
24b + N-Boc-L-Serine
hv 1.0 min
24 h
0 h
1000000
800000
600000
400000
200000
0
0 min
5 min
10 min
15 min
20 min

(e)


1b + GSH
13b + GSH
hv 1.0 min
24 h
0 h
500000
400000
300000
200000
100000
0
0 min
5 min
10 min
15 min
20 min

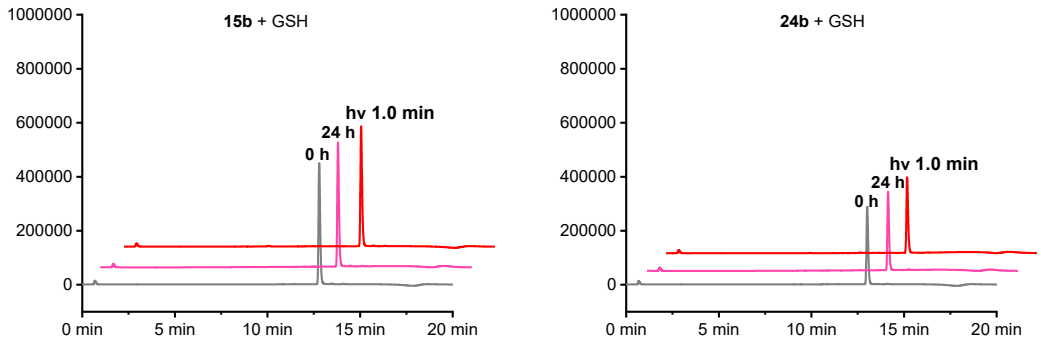
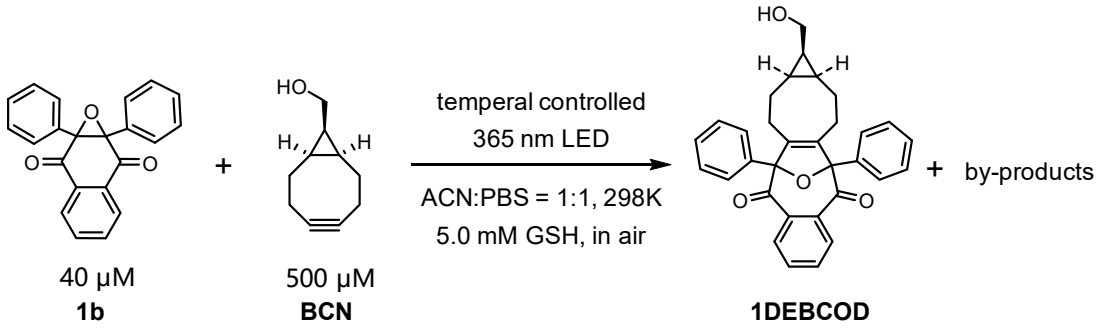
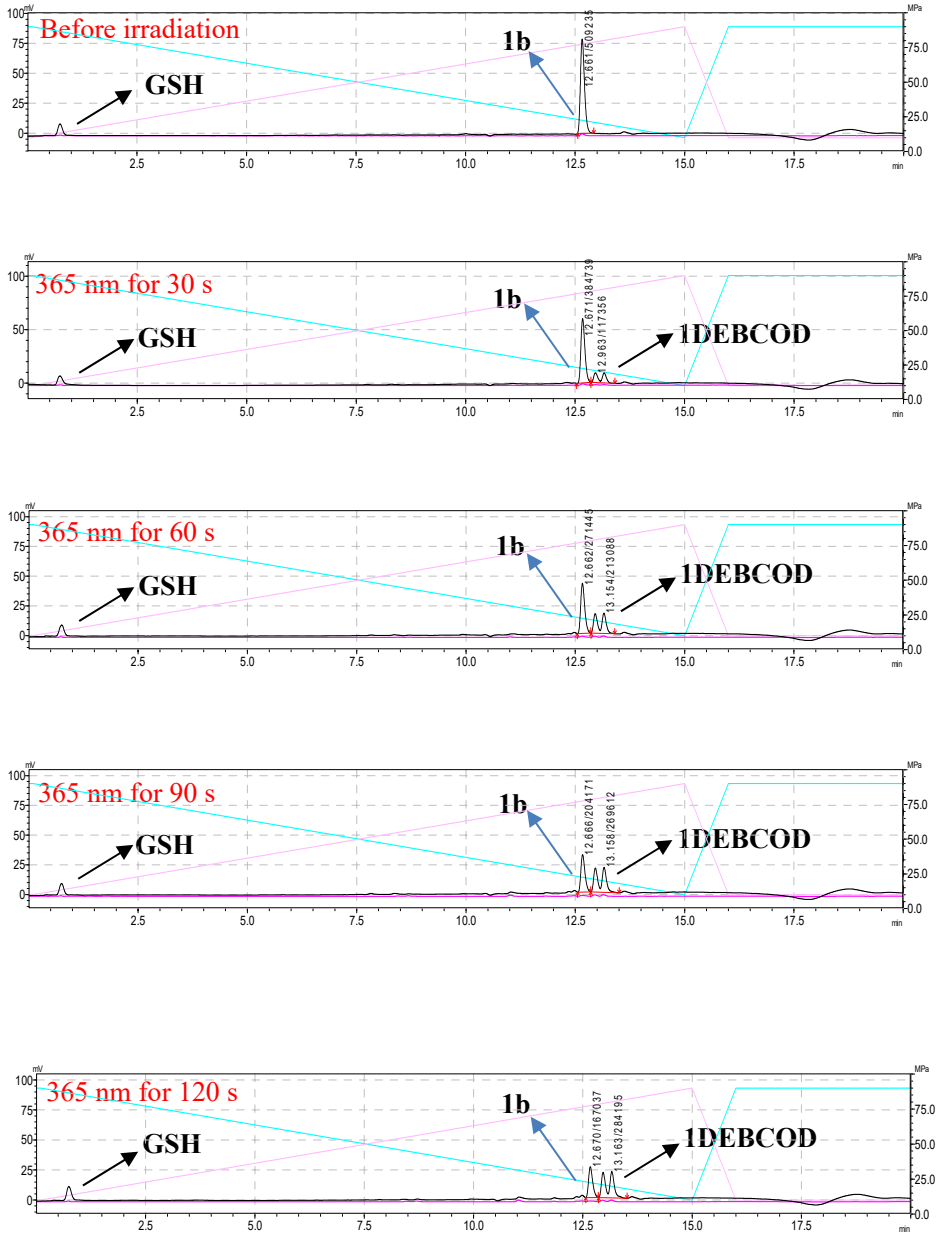
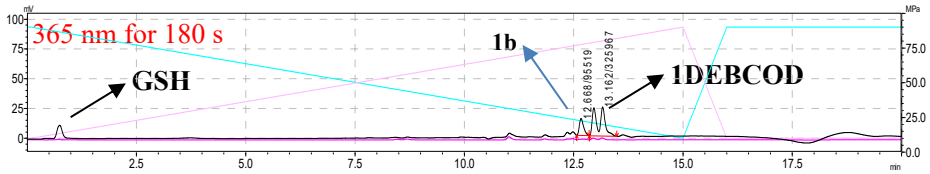


Figure S10. Reactivity and stability for DNQOs: (a) **1b**; (b) **13b**; (c) **15b**; and (d) **24b** toward various nucleophilic amino acids (including *N*-Boc-L-lysine, *N*-Boc-L-serine, *N*-Boc-L-aspartic acid, and *N*-Boc-L-cysteine, 1.0 mM each, respectively) and (e) 10.0 mM GSH.

Quantitative HPLC analysis for the temporal controlled photo-reaction of DNQO 1b with BCN in the presence 5.0 mM GSH



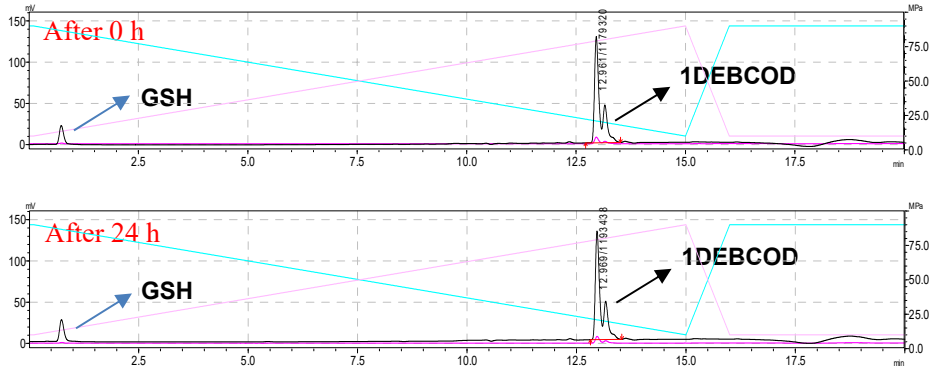




Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.661	509235
30 s	**1b**	12.671	384739
	1DEBCOD	12.963	117518
60 s	**1b**	12.662	271445
	1DEBCOD	13.154	213088
90 s	**1b**	12.666	204171
	1DEBCOD	13.158	269612
120 s	**1b**	12.670	167037
	1DEBCOD	13.163	284195
180 s	**1b**	12.668	95519
	1DEBCOD	13.162	325967

Figure S11. Chemoselectivity of the photoclick reaction of DNQO (40 μM), BCN (500 μM) and GSH (5.0 mM) mixed in CH_3CN/PBS (1/1) after exposure to controlled irradiation with 365 nm LED at 298 K for various period of time points.

Stability investigation of the cycloadduct 1DEBCOD against nucleophile additions by GSH in dark or under continuous 365 nm irradiation.



Time	Peak	Retention Time	Integrated Area
0 h	**1DEBCOD**	12.961	127866
24 h	**1DEBCOD**	12.969	130595

Figure S12. HPLC-MS analysis for testing the stability of **1DEBCOD**. **1DEBCOD** (100 µM) and GSH (10.0 mM) in ACN/PBS (v/v = 1/1) were incubated together and after 24 h incubation in dark, at 298K.

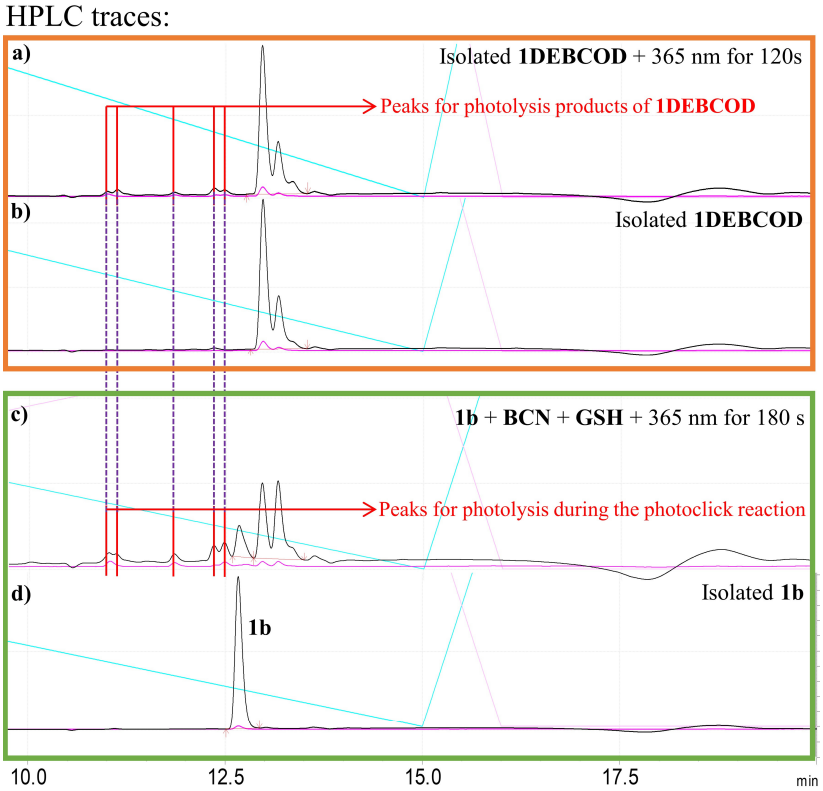
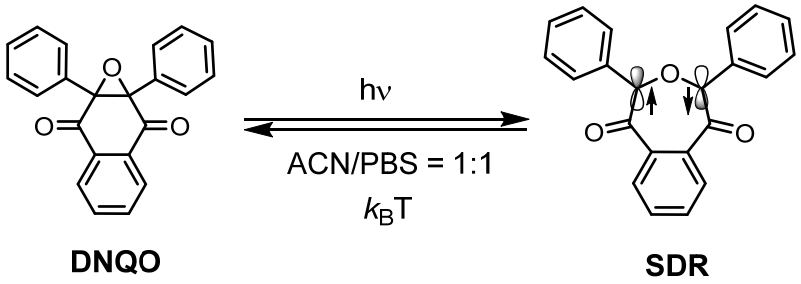
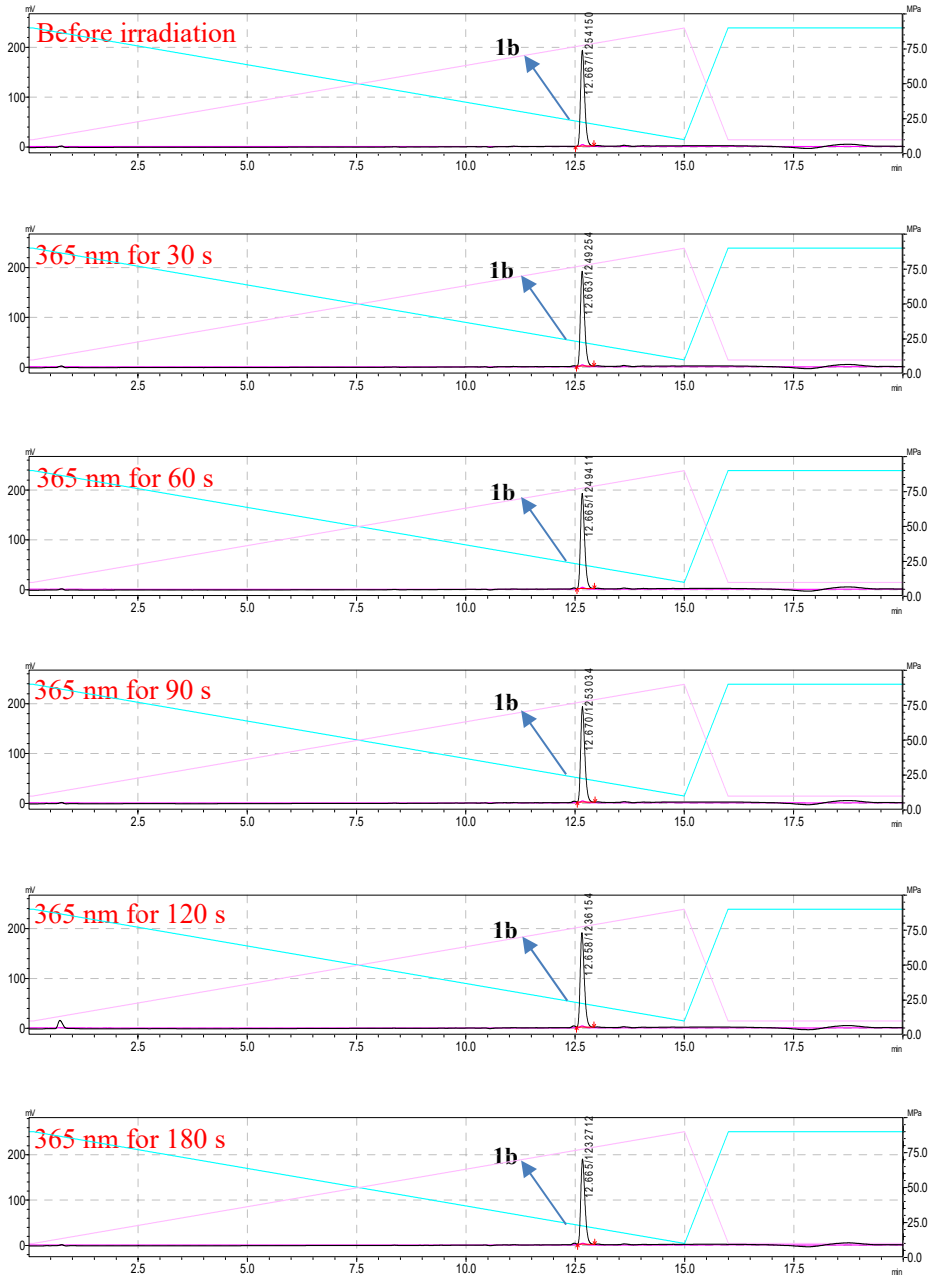


Figure S13. Quantitative HPLC-MS analysis to explain the origin of the by-products in the photoclick reaction between **1b** (40 μM) and BCN (500 μM) in the presence of GSH (5.0 mM) in CH_3CN/PBS = 1/1, at 298 K. a) The photolysis of the isolated **1DEBCOD**. b) The isolated **1DEBCOD** with both *endo*- and *exo*-isomers in unequal ratio. c) The mixture after the photoclick reaction. d) The isolated DNQO, **1b**, before irradiation. The by-products formed during the photoclick process (red lines marked peaks) were almost the same as the photolysis products from isolated **1DEBCOD**, the [3+2] cycloadduct, under 365 nm irradiation for 120 s.

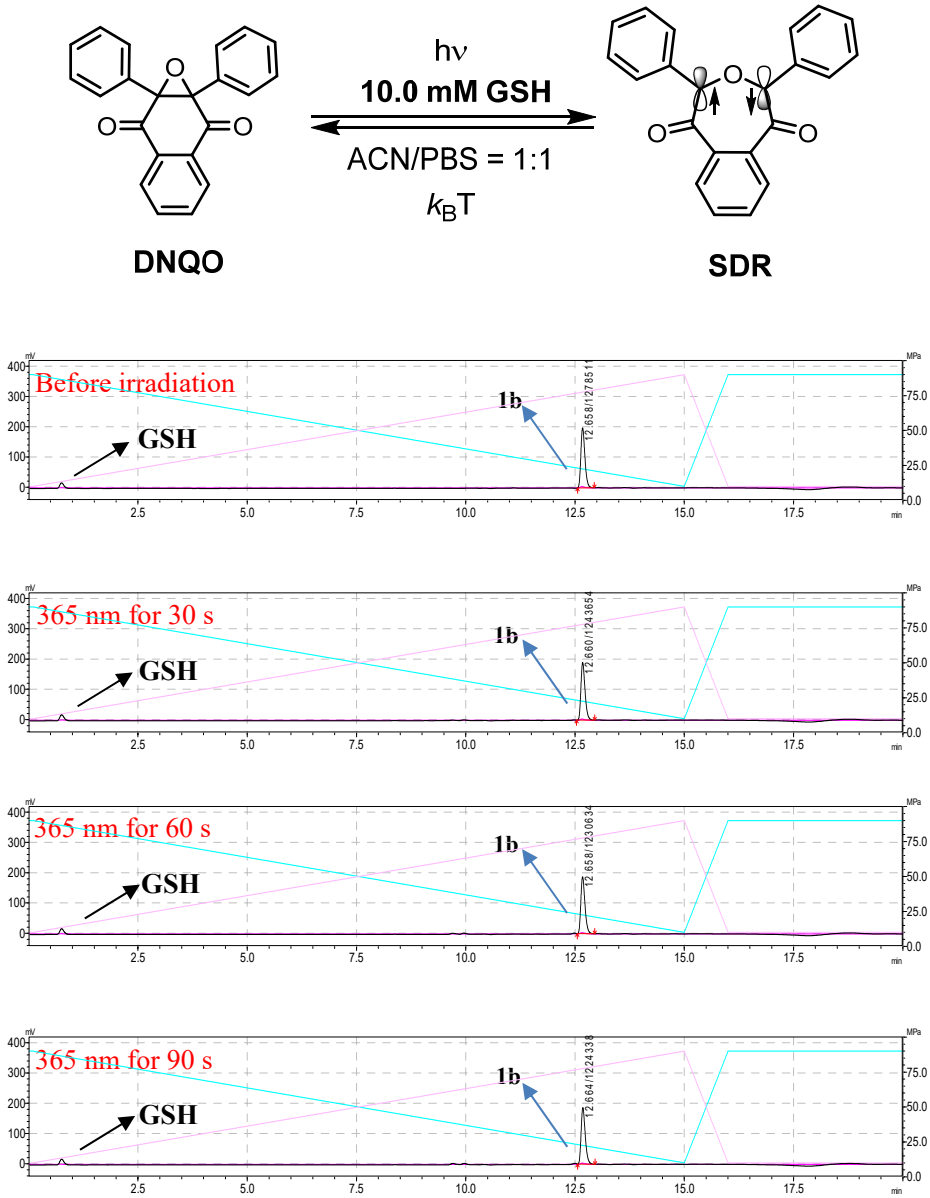
Quantitative HPLC analysis of the recovery capacity of DNQOs under continuous 365 nm irradiation with/without GSH

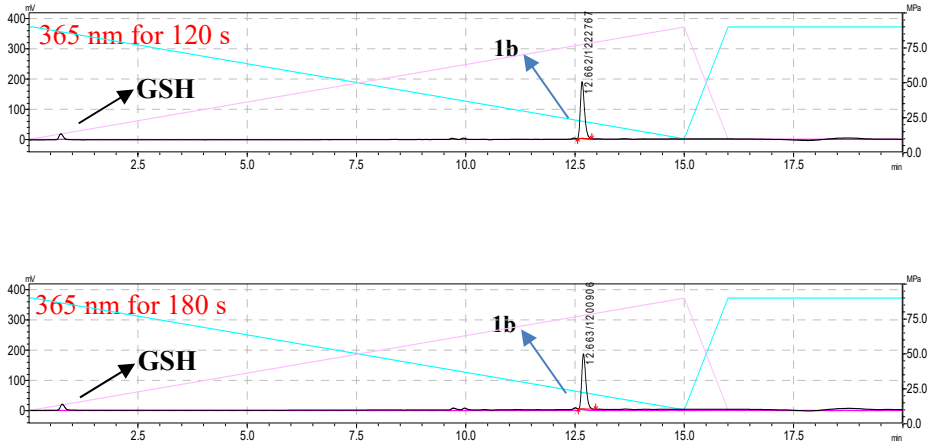




Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.667	1254150
30 s	**1b**	12.663	1249254
60 s	**1b**	12.665	1249411
90 s	**1b**	12.670	1253034
120 s	**1b**	12.658	1236154
180 s	**1b**	12.665	1232712

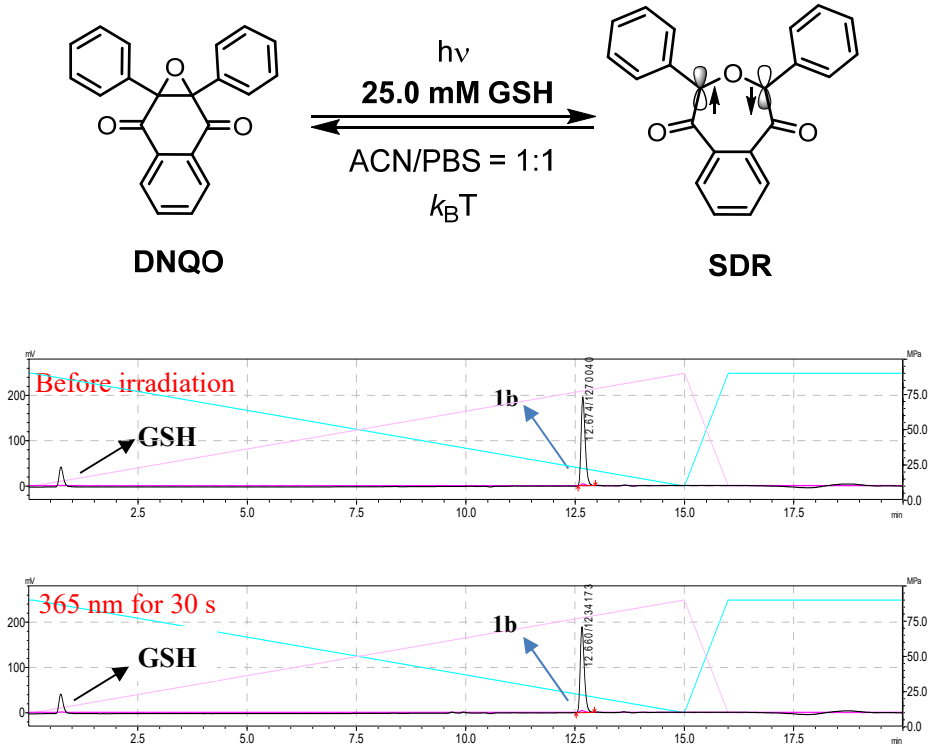
Figure S14. Photo-stability of DNQO (100 μM) in CH_3CN/PBS (1/1) after exposure to 365 nm LED irradiation for the designated period of time at 298 K.

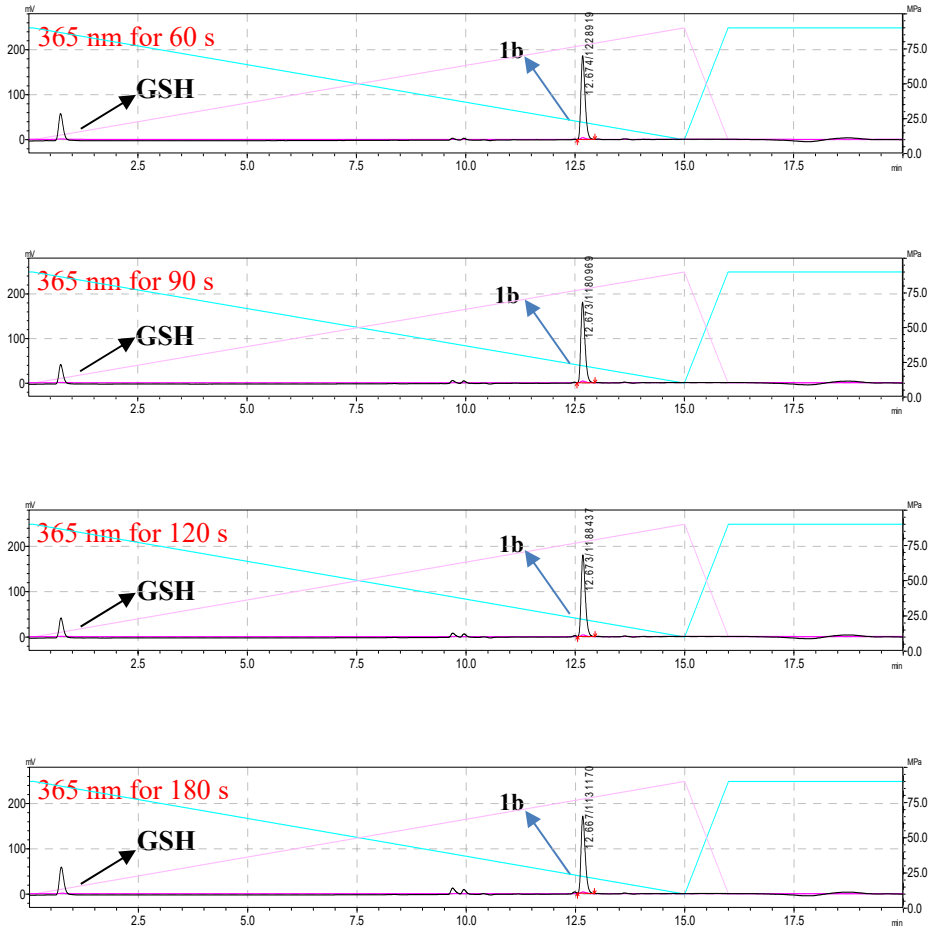




Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.658	1278511
30 s	**1b**	12.660	1243654
60 s	**1b**	12.658	1230634
90 s	**1b**	12.664	1224338
120 s	**1b**	12.662	1222767
180 s	**1b**	12.663	1200906

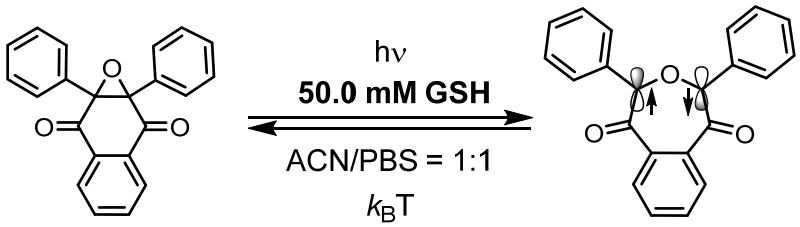
Figure S15. Photo-stability of DNQO (100 μM) with GSH (10.0 mM) mixed in CH_3CN/PBS (1/1) after exposure to the 365 nm LED irradiation at 298 K for the designated period of time.



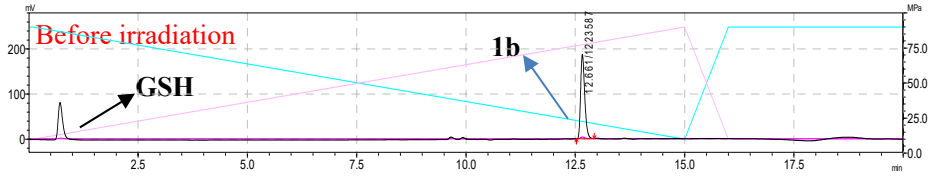


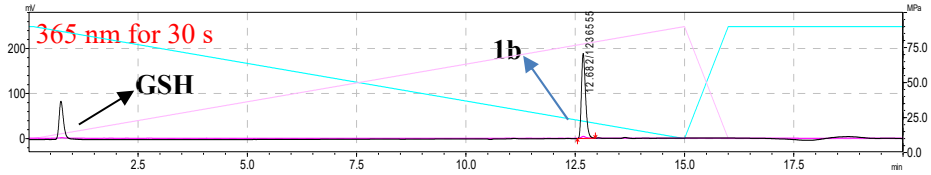
Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.674	1270040
30 s	**1b**	12.660	1234173
60 s	**1b**	12.674	1228919
90 s	**1b**	12.673	1180969
120 s	**1b**	12.673	1188437
180 s	**1b**	12.667	1131170

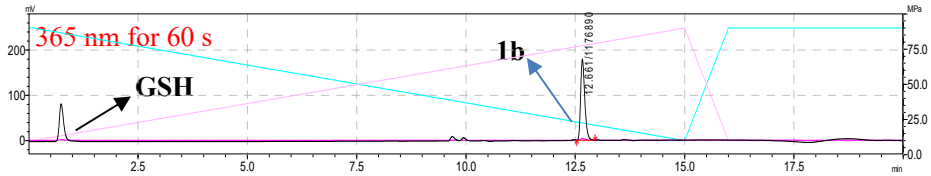
Figure S16. Photo-stability of DNQO (100 μM) with GSH (25.0 mM) mixed in CH_3CN/PBS (1/1) after exposure to the 365 nm LED irradiation at 298 K for the designated period of time.

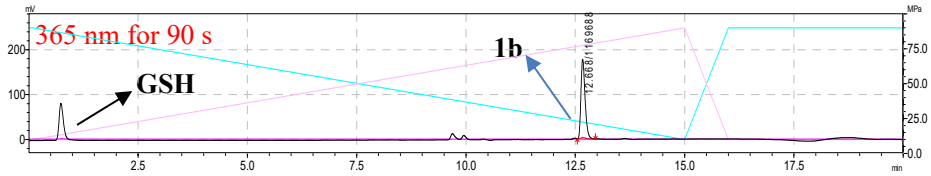


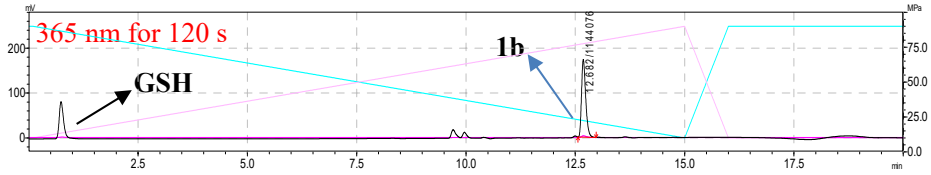
DNQO **SDR**

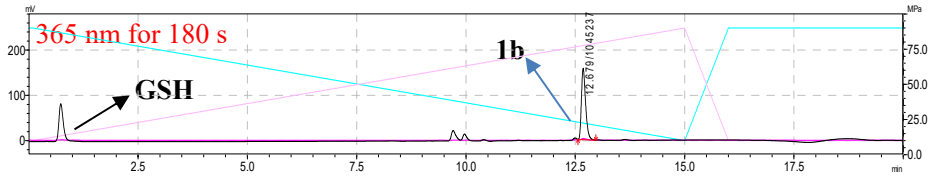








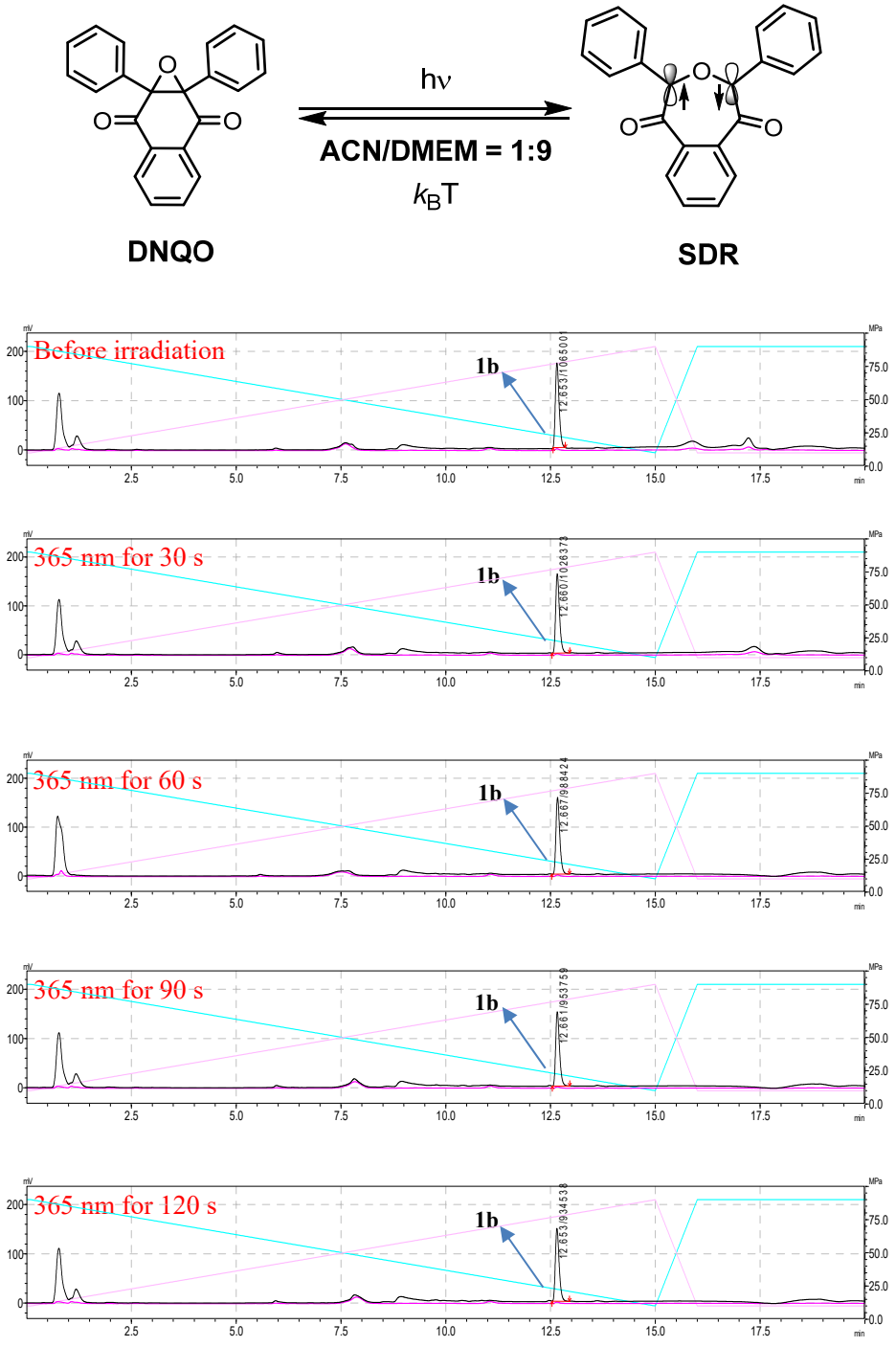


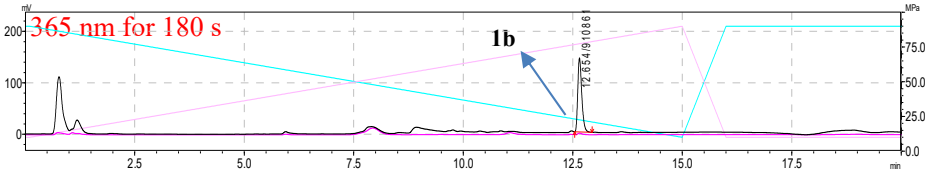


Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.682	1236555
30 s	**1b**	12.661	1223587
60 s	**1b**	12.661	1176890

90 s	**1b**	12.668	1169688
120 s	**1b**	12.682	1144076
180 s	**1b**	12.679	1045237

Figure S17. Photo-stability of DNQO (100 μM) with GSH (50.0 mM) mixed in CH_3CN/PBS (1/1) after exposure to the 365 nm LED irradiation at 298 K for the designated period of time.





Time	Peak	Retention Time /min	Integrated Area
0 s	**1b**	12.653	1065001
30 s	**1b**	12.660	1026373
60 s	**1b**	12.667	988424
90 s	**1b**	12.661	953759
120 s	**1b**	12.653	934538
180 s	**1b**	12.654	910861

Figure S18. Photo-stability of DNQO (100 μM) in CH_3CN/DMEM (v/v = 1/9, DMEM contains 10% Fetal Bovine Serum +1% Antibiotics) after exposure to the 365 nm LED irradiation at 298 K for the designated period of time.

Chemical modification of Cetuximab (a chimeric monoclonal antibody) by BCN-OCOO-PNP and FITC in sequence.

A solution of Cetuximab (1.0 mg/mL) in PBS (pH = 7.4) was mixed with 60 equivalents of BCN-OCOO-PNP at 37 °C and incubated for 30 min. Excess amount of small molecules was then removed from the modified antibody solution via a protein spin column (Millipore, Amicon Ultra 0.5, molecular weight cutoff 10 kDa, 5 times exchange with PBS). Then, 5 equivalents FITC was added into the solution of the BCN-modified Cetuximab, and further incubated for 2 h. Then the mixture was filtered again by the protein spin columns (Millipore, Amicon Ultra 0.5 molecular weight cutoff 10 kDa, 5 times exchange with PBS) to get rid of the excessive small molecule reagents. Finally, the resultant double modified antibody was stored at 4 °C. The final concentration of the Cetuximab-BCN-FITC was quantified with BCA protein assay kit.

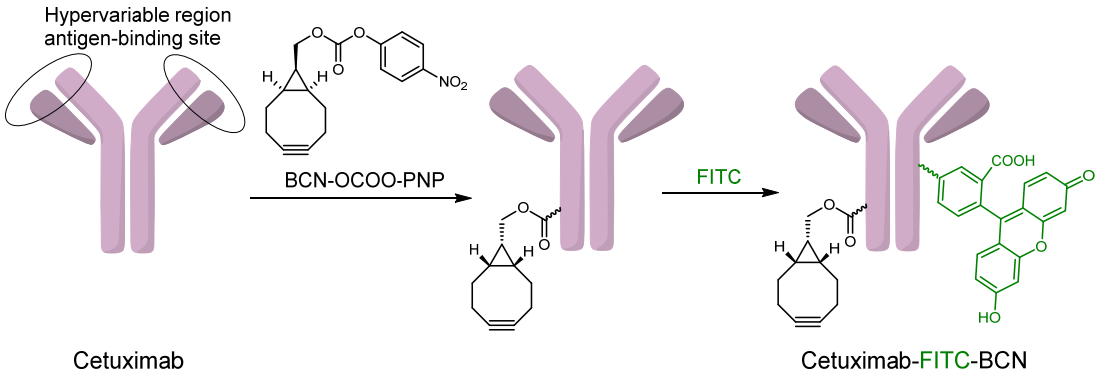


Figure S19. Chemical modification of the chimeric Cetuximab (a monoclonal antibody, mAb) with 60 eq. of BCN-OCOO-PNP (10.0 mM) and 5 eq. FITC (5.0 mM) to form the bi-conjugated Cetuximab (Cex)-FITC-BCN.

Fluorescence imaging for the photo-labeling of EGFR on living A549 cells via the DNQO-BCN photoclick reaction with the complete control experiments

Eight groups of control experiments were designed to illustrate the essential photo-labeling conditions, and the selectivity of the photoclick reaction shown in Figure S20 below. 1×10^5 A549 cells were seeded in glass-bottom 3.5 cm culture dish. When the cell confluency reached 50-60%, all groups of cells were firstly incubated with Hoechst 33342 at 37 °C for 10 min to stain the nucleus. After that, in the control groups: "2, 5, 6 and 8", cells were washed for three times and incubated with Cex-FITC-BCN (20 μg/mL in DMEM) in the CO_2 incubator at 37 °C for 60 min, and washed with PBS for three times. For the other control groups, the cells were directly washed with PBS for three times without treatment. Then, **DNQO-Cy3** (20 μM) in PBS (pH = 7.4) were added into the cell culture dishes to replace the culture medium for the control groups: "3, 5, 7 and 8". Without further incubation, the control groups: "4, 6, 7 and 8" were directly irradiated with the 365 nm LED (55.0 mW/cm^2) for 90 s, and the rest of the control groups were left in dark for 2.0 min. After washing the cells in all the control groups were washed with PBS for five times, the living cells in each group were then imaged immediately under an Olympus IX83 live cell epifluorescence microscope with corresponding excitation and filter cubes for fluorescence signal in Hoechst 33342, Cy3 and FITC channels through a 100× oil immersion objective lens. As a result, we were able to observe the desired Cy3 fluorescence signals on the cell membranes only when all the photoclick reaction conditions were fulfilled. While for all the other control conditions, the fluorescence signals in Cy3 channel on the cell membranes could not be observed or too dim to be detected.

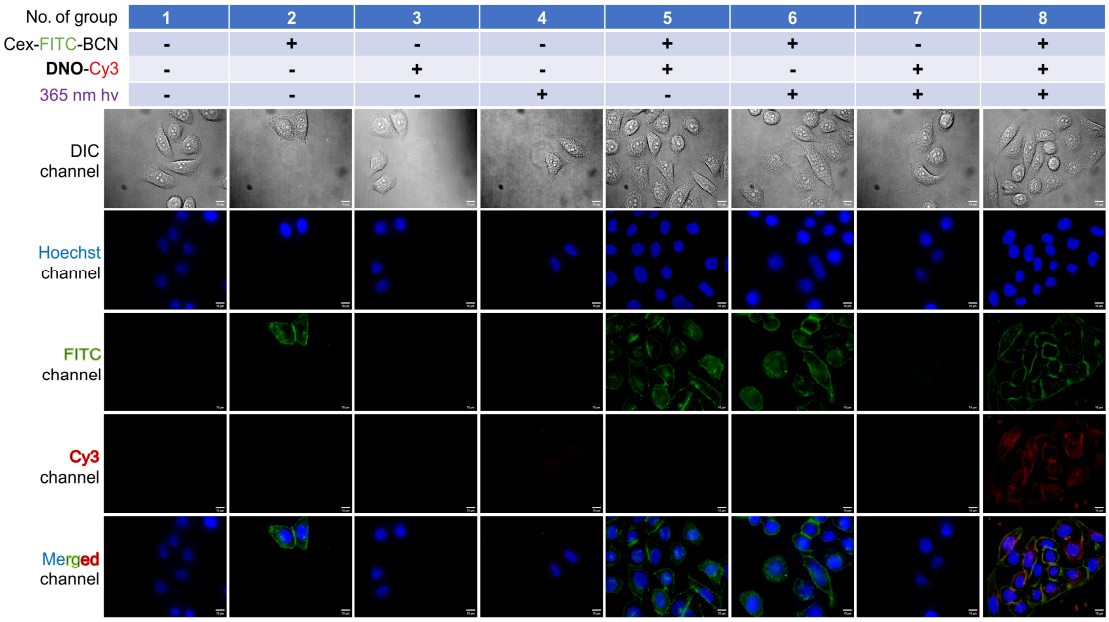


Figure S20. The fluorescence microscopic imaging for the living A549 cell in DIC, Hoechst 33342, Cy3 and FITC channels for the experimental group and the complete control groups after the treating and irradiation procedures, and a merged fluorescence image (the rightmost column) of all fluorescence channels was shown. scale bar = 10 μm.

Patterned photo-stimulation with the 365 nm LED in the microscope to test the spatial-resolving power of the DNQO-BCN photoclick reaction on the membrane of the living A549 cells.

1×10^5 A549 cells were seeded in glass-bottom 3.5 cm culture dish. When the cell confluency reached 50-60%, the cells were incubated with Hoechst 33342 (two drops per milliliter) at 37 °C for 10 min to stain the nucleus, and washed with PBS for three times. Then, the cells were incubated with Cex-BCN (120 μg/mL in DMEM) in the CO_2 incubator at 37 °C for 60 min and washed with PBS for three times to bind with the BCN-modified mAb on the cell membrane. After that, **DNQO-Cy3** (20 μM) in PBS (pH = 7.4) were added into the cell culture dish. A cluster of A549 cells of interest were irradiated by projecting a 365 nm lithographic pattern of a grid matrix (58.7×32.1 μm, 6×6 lines) with two distal-column filled via the 365 nm LED photo-stimulation (light gray regions), implemented through a digital micromirror device (DMD) embedded in the microscope. The lithographic pattern was drawn and loaded via the Polyscan 2 software (Mightex) for controlling the Polygon 400 DMD, setting the LED output wavelength to 365 nm with an output power of 25% of a 2.0 W LED (light power) via the DMD embedded in the epifluorescence microscope with a designated time sequence (continuous for 30 s). After the exposure, the cell culture medium was replaced with PBS, and washed for three times to completely remove the unreacted **DNQO-Cy3**. After the photoclick labeling procedure, the region of interest covering the irradiated living cells were imaged immediately on the microscope with corresponding excitation and filter cubes through a 100× oil immersion objective lens for fluorescence imaging in various channels: Hoechst, and Cy3 channels, respectively.

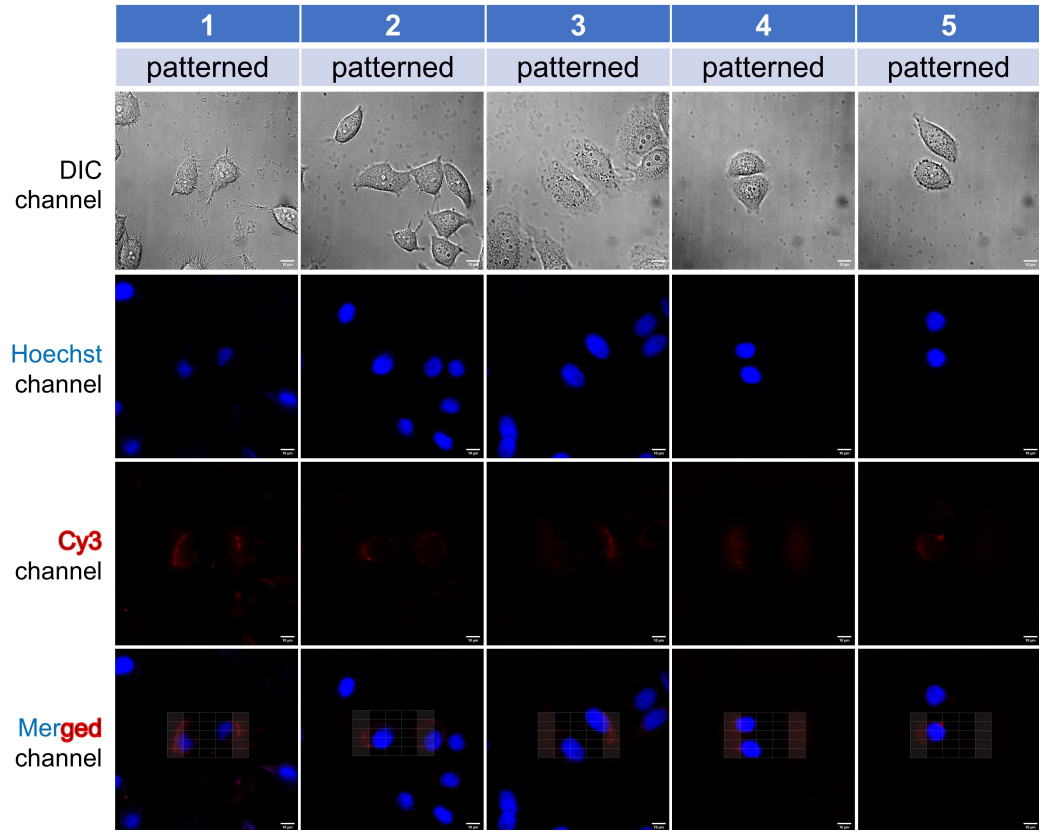


Figure S21. The fluorescence imaging of the living A549 cells after exposure to the lithographic

stimulation of 365 nm projected through the embedded DMD for 30 s in DIC, Hoechst, Cy3 channels and the merged channels, scale bar = 10 μm. The 365 nm lithographic pattern and the irradiated segments on cell membranes were highlighted in light gray color in the merged channel.

3. Crystal data and structure refinements

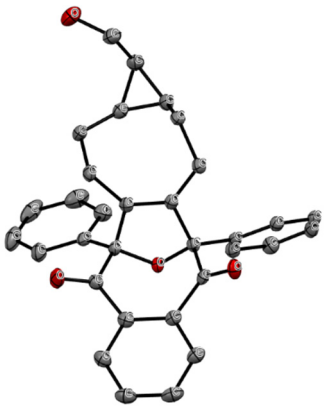


Table S7. Crystallographic Data for ***endo*-1DEBCOD (1b+6c)**.

Formula	$C_{32}H_{28}O_4$
Formula mass (amu)	476.54
Space group	P-1
a (Å)	9.1808(5)
b (Å)	10.1345(5)
c (Å)	13.7708(7)
α (deg)	80.343(1)
β (deg)	75.323(1)
γ (deg)	71.008(1)
V (Å^3)	1166.89(10)
Z	2
λ (Å)	0.71073
T (K)	173
ρ_{calcd} (g cm^{-3})	1.356
μ(mm^{-1})	0.088
Transmission factors	0.960, 1.000
θ_{max} (deg)	25.377
No. of unique data, including $F_o^2 < 0$	4260
No. of unique data, with $F_o^2 > 2\,\sigma(F_o^2)$	3873
No. of variables	334
$R(F)$ for $F_o^2 > 2\,\sigma(F_o^2)$ [a]	0.0422
$R_w(F_o^2)$ [b]	0.0950
Goodness of fit	1.126

[a] $R(F) = \sum||F_o| - |F_c|| \,/\, \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] \,/\, \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)2 + Bp]$, where $p = [\max(F_o^2,0) + 2\,F_c^2] \,/\, 3$.

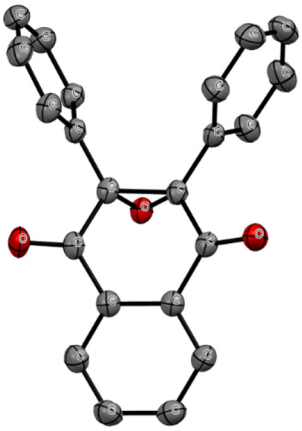


Table S8. Crystallographic Data for **1b**.

Formula	$C_{22}H_{14}O_3$
Formula mass (amu)	326.33
Space group	P 2_1/n
a (Å)	13.4416(17)
b (Å)	16.332(2)
c (Å)	15.0321(19)
α (deg)	90
β (deg)	99.607(4)
γ (deg)	90
V (Å^3)	3253.7(7)
Z	8
λ (Å)	0.71073
T (K)	173
ρ_{calcd} (g cm^{-3})	1.332
μ(mm^{-1})	0.088
Transmission factors	0.970,0.977
θ_{max} (deg)	25.387
No. of unique data, including $F_o^2 < 0$	5977
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	4819
No. of variables	451
$R(F)$ for $F_o^2 > 2\ \sigma(F_o^2)$ [a]	0.0376
$R_w(F_o^2)$ [b]	0.0880
Goodness of fit	1.063

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

4. Computational details

DFT and TD-DFT calculations were performed using Gaussian 09 program package[6]. All structures were optimized at the M06-2X level of theory[7] in experimental solvents (acetonitrile:water = 1:1, v:v) with the 6-31G** basis set[8-9], and the geometry of SDR was optimized by using broken-symmetry (BS) wavefunction method[10-11]. The self-consistent reaction field (SCRF) method based on the universal solvation model SMD[12] was adopted to evaluate the effect of solvent. The intrinsic reaction coordinate (IRC) path[13] was traced to check the energy profiles connecting each transition state to two associated minima of the proposed mechanism. All single-point energies were computed by using M06-2X density functional with the 6-311G** basis set[14-15], and Gibbs free energies were calculated by Shermo 2.3 program[16] (**Table S9**). The wavefunctions stability was tested for all the SDR structures obtained by using of BS-UDFT method. Spin density and molecular orbitals analysis of SDR or TDR and natural transition orbital (NTO) analysis[17] of **1b** were performed using Multiwfn 3.8(dev) program[18], and visualized by VMD1.9.3 software[19].

The CASSCF calculations were performed at CAS(2,2)/6-31G**(SMD, ACN:H_2O=1:1) level of theory[20]. To investigate whether the size of the active space in the CASSCF calculations as well as the dynamic correlation significantly affect the wavefunction of SDR structures (**1SDR**, **3SDR**, **5SDR**, **13SDR**, **17SDR** and **24SDR**), we firstly performed UDFT natural orbitals (UNO) analysis using the ORCA5.0.1 program[21] at the BS-UM06-2X/6-31G** (SMD, ACN : H_2O = 1:1) level (**Figure S26**). The results showed that only the two frontier UNOs (i.e., HOMO and LUMO) had electron occupation numbers between 1.98 and 0.02 (that is, 1.0 and 1.0). According to the rule of thumb that the orbitals with occupation numbers between 1.98 and 0.02 should be in the active space (see the manual of ORCA5.0.1, page 587), so the active space (2e in 2o) was used in the CASSCF calculations.

To investigate the effect of dynamic correlation, we selected the two frontier UNOs as active spaces and performed the N-electron valence state perturbation theory with a fully internally contracted wavefunction (FIC-NEVPT2) calculations for all SDR structures at the FIC-NEVPT2(2,2)/def2-TZVP (SMD, ACN : H_2O = 1:1) level[22-27] by the ORCA 5.0.1 program. Compared with BS-UDFT and CASSCF calculations, similar electron occupation numbers and orbital shapes of the natural orbitals were obtained by NEVPT2 method (NEVPT2-NOs, **Figure S27**). These results indicated that the electronic structures of the SDRs described by the BS-UDFT and CASSCF methods were reliable in this work.

Meanwhile, the electronic energies (E_e) of all SDR and TDR structures obtained at (BS)-UDFT, CASSCF and NEVPT2 theoretical levels are shown in **Table S14**. The results indicate that the SDR species is more stable than the corresponding TDR species at three theoretical levels. That is, the open-shell singlet is the ground state for diradicals species (2,7-diaryl oxepine-3,6-dione-2,7-diyl, OXPID) in this work.

We studied further the theoretical absorption wavelengths of the six DNQOs (**1b**, **3b**, **5b**, **13b**, **17b** and **24b**) and their corresponding SDR intermediates, using the DFT with the Tamm-Dancoff approximation method (TDA) at the TDA-M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level (**Table S10-S11**). The calculations were qualitatively agreement with the TD-DFT results as well as the experimental results.

Table S9. Electronic energies (E_e), enthalpies (H) and Gibbs free energies (G) for all stationary points (in Hartree), obtained at the M06-2X/6-311G** (SMD, ACN:H_2O = 1:1) theoretical level.

Structures	[a]*ZPE*	E_e	[b]H_{corr}	*H*	[c]G_{corr}	*G*
BCN	0.22074	-464.54770	0.23219	-464.31551	0.18559	-464.36210
1b	0.30180	-1072.28467	0.32149	-1071.96318	0.25680	-1072.02787
1b-S$_1$	0.29881	-1072.15339	0.31871	-1071.83468	0.25398	-1071.89941
1b-TS1-S$_1$	0.29682	-1072.14433	0.31648	-1071.82785	0.25190	-1071.89243
1SDR	0.30054	-1072.23034	0.32034	-1071.90999	0.25538	-1071.97495
1DOXEPY	0.30085	-1072.22948	0.32057	-1071.90891	0.25581	-1071.97367
1TDR	0.29996	-1072.22305	0.31982	-1071.90323	0.25363	-1071.96942
1b-IM1	0.52403	-1536.79616	0.55566	-1536.24050	0.46831	-1536.32785
1b-TS2	0.52464	-1536.79229	0.55496	-1536.23733	0.47056	-1536.32173
1DEBCOD	0.52867	-1536.91917	0.55855	-1536.36062	0.47480	-1536.44437
1b-TS3	0.30015	-1072.22119	0.31938	-1071.90181	0.25556	-1071.96563
GSH	0.29590	-1405.09068	0.31849	-1404.77219	0.24708	-1404.84360
1b-IM2	0.59840	-2477.33280	0.64159	-2476.69121	0.52982	-2476.80298
1b-TS4	0.59685	-2477.30452	0.63891	-2476.66561	0.52965	-2476.77487
GSH-P	0.60221	-2477.38556	0.64455	-2476.74101	0.53407	-2476.85149
3b	0.35690	-1150.90013	0.38012	-1150.52001	0.30838	-1150.59176
3b-S$_1$	0.35362	-1150.89006	0.37714	-1150.51291	0.30503	-1150.58502
3b-TS1-S$_1$	0.35181	-1150.87299	0.37499	-1150.49800	0.30334	-1150.56965
3SDR	0.35530	-1150.84665	0.37896	-1150.46769	0.30611	-1150.54054
3DOXEPY	0.35467	-1150.84055	0.37829	-1150.46226	0.30442	-1150.53613
3TDR	0.35557	-1150.84560	0.37916	-1150.46644	0.30639	-1150.53920
3b-IM1	0.57912	-1615.41247	0.61440	-1614.79807	0.51968	-1614.89279
3b-TS2	0.57979	-1615.40851	0.61379	-1614.79472	0.52201	-1614.88650
3DEBCOD	0.58382	-1615.53449	0.61740	-1614.91709	0.52612	-1615.00836
3b-TS3	0.35457	-1150.83855	0.37776	-1150.46079	0.30503	-1150.53353
5b	0.36762	-1301.30991	0.39245	-1300.91746	0.31746	-1300.99244
5b-S$_1$	0.36418	-1301.17979	0.38908	-1300.79071	0.31436	-1300.86543
5b-TS1-S$_1$	0.36279	-1301.18010	0.38733	-1300.79276	0.31319	-1300.86690
5SDR	0.36702	-1301.25828	0.39186	-1300.86642	0.31663	-1300.94165
5DOXEPY	0.36628	-1301.25466	0.39121	-1300.86345	0.31456	-1300.94010
5TDR	0.36712	-1301.25690	0.39193	-1300.86497	0.31679	-1300.94011
5b-IM1	0.59067	-1765.82415	0.62721	-1765.19694	0.53018	-1765.29397
5b-TS2	0.59096	-1765.82016	0.62637	-1765.19379	0.53177	-1765.28839
5DEBCOD	0.59490	-1765.94892	0.63012	-1765.31880	0.53496	-1765.41396
5b-TS3	0.36602	-1301.25301	0.39016	-1300.86284	0.31652	-1300.93649
13b	0.28517	-1270.76040	0.30652	-1270.45388	0.23836	-1270.52204
13b-S$_1$	0.28179	-1270.62868	0.30345	-1270.32523	0.23474	-1270.39394
13b-TS1-S$_1$	0.28018	-1270.62138	0.30148	-1270.31990	0.23344	-1270.38793
13SDR	0.28403	-1270.70632	0.30548	-1270.40084	0.23713	-1270.46920

13DOXEPY	0.28327	-1270.69948	0.30486	-1270.39462	0.23492	-1270.46456
13TDR	0.28431	-1270.70535	0.30569	-1270.39967	0.23747	-1270.46788
13b-IM1	0.50773	-1735.27243	0.54095	-1734.73147	0.45030	-1734.82212
13b-TS2	0.50845	-1735.26871	0.54037	-1734.72834	0.45268	-1734.81602
13DEBCOD	0.51219	-1735.39540	0.54377	-1734.85163	0.45646	-1734.93894
13b-TS3	0.28330	-1270.69754	0.30425	-1270.39329	0.23671	-1270.46083
17b	0.31192	-1746.37314	0.33881	-1746.03434	0.25869	-1746.11446
17b-S_1	0.30870	-1746.24129	0.33586	-1745.90543	0.25541	-1745.98588
17b-TS1-S_1	0.30646	-1746.22774	0.33337	-1745.89437	0.25323	-1745.97451
17SDR	0.31087	-1746.31834	0.33779	-1745.98054	0.25780	-1746.06054
17DOXEPY	0.30979	-1746.30923	0.33696	-1745.97226	0.25491	-1746.05432
17TDR	0.31119	-1746.31775	0.33805	-1745.97970	0.25819	-1746.05956
17b-IM1	0.53462	-2210.88488	0.57329	-2210.31158	0.47119	-2210.41368
17b-TS2	0.53547	-2210.88116	0.57288	-2210.30828	0.47363	-2210.40753
17DEBCOD	0.53932	-2211.00900	0.57632	-2210.43268	0.47771	-2210.53128
17b-TS3	0.31015	-1746.30764	0.33657	-1745.97107	0.25715	-1746.05049
24b	0.33698	-1399.38421	0.36195	-1399.02226	0.28619	-1399.09802
24b-S_1	0.33368	-1399.25256	0.35906	-1398.89350	0.28254	-1398.97002
24b-TS1-S_1	0.33198	-1399.24280	0.35700	-1398.88580	0.28117	-1398.96162
24SDR	0.33597	-1399.33017	0.36105	-1398.96912	0.28511	-1399.04506
24DOXEPY	0.33509	-1399.32225	0.36032	-1398.96193	0.28274	-1399.03952
24TDR	0.33629	-1399.32949	0.36131	-1398.96818	0.28544	-1399.04405
24b-IM1	0.55920	-1863.89690	0.59623	-1863.30066	0.49766	-1863.39924
24b-TS2	0.55999	-1863.89321	0.59570	-1863.29752	0.50020	-1863.39302
24DEBCOD	0.56432	-1864.01951	0.59945	-1863.42006	0.50486	-1863.51465
24b-TS3	0.33512	-1399.32144	0.35948	-1398.96197	0.28525	-1399.03619
1b*	0.30146	-1072.27898	0.32119	-1071.95779	0.25641	-1072.02258
1SDR*	0.30112	-1072.22625	0.32094	-1071.90531	0.25592	-1071.97033
1DOXEPY*	0.30166	-1072.22500	0.32138	-1071.90363	0.25657	-1071.96843
1b-TS3*	0.29977	-1072.21907	0.31889	-1071.90019	0.25549	-1071.96358
1b**	0.30141	-1072.28118	0.32116	-1071.96001	0.25632	-1072.02486
1SDR**	0.30131	-1072.22792	0.32105	-1071.90687	0.25632	-1071.97160
1DOXEPY**	0.30185	-1072.22668	0.32148	-1071.90520	0.25697	-1071.96972
1b-TS3**	0.29972	-1072.22089	0.31884	-1071.90205	0.25544	-1071.96545

[a] Zero-point correction energy;

[b] Thermal correction to enthalpy obtained at the M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level of theory;

[c] Thermal correction to Gibbs free energy obtained at the M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level of theory.

* Calculated at M06-2X/6-311G**/SMD(n-Hexane)// M06-2X/6-31G**/SMD(n-Hexane) level of theory.

** Calculated at M06-2X/6-311G**/SMD(Toluene)// M06-2X/6-31G**/SMD(Toluene) level of theory.

Table S10. TD-DFT and TDA-DFT calculated results of **1b**, **3b**, **5b**, **13b**, **17b** and **24b** at M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level of theory.

Structures	Excited state	[a]E_{ex}	[b]λ_1	[c]f	[d]λ_2	[e]E_{ex}	[f]λ_1
1b	S_1	3.65	340	0.001	375	3.74	332
	S_2	3.75	331	0.009	366	3.83	324
	S_4	4.63	268	0.211	303	4.81	258
3b	S_1	3.66	338	0.0002	373	3.74	332
	S_2	3.75	331	0.001	366	3.82	325
	S_4	4.66	266	0.003	301	4.67	265
	S_5	4.74	262	0.126	297	4.82	257
5b	S_1	3.65	340	0.0001	375	3.74	332
	S_2	3.72	333	0.015	368	3.80	326
	S_4	4.65	267	0.242	302	4.33	286
13b	S_1	3.66	339	0.001	374	3.75	331
	S_2	3.75	331	0.010	366	3.83	324
	S_4	4.63	268	0.200	303	4.79	259
17b	S_1	3.66	339	0.001	374	3.75	331
	S_2	3.76	330	0.009	365	3.84	323
	S_4	4.62	268	0.224	303	4.84	256
24b	S_1	3.65	339	0.0004	374	3.74	331
	S_2	3.75	331	0.010	366	3.83	324
	S_4	4.62	268	0.206	303	4.80	258

[a] Vertical excitation energies of $S_0 \rightarrow S_n$ excitation, showed in eV;

[b] Theoretical absorption wavelength of $S_0 \rightarrow S_n$ excitation, showed in nm;

[c] The oscillator strength of $S_0 \rightarrow S_n$ excitation;

[d] Theoretical absorption wavelength with systematic correctional value +35 nm based on experimental values;

[e] Vertical excitation energies of $S_0 \rightarrow S_n$ excitation, performed at TDA-M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory and showed in eV;

[f] Theoretical absorption wavelength of $S_0 \rightarrow S_n$ excitation performed at TDA-M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory and showed in nm.

Table S11. TD-DFT and TDA-DFT calculated results and relative Gibbs free energies of SDR, DOXEPY and TDR intermediates obtained for **1b**, **3b**, **5b**, **13b**, **17b** and **24b**, respectively.

Structures	Excited state	[a]E_{ex}	[b]λ_1	[c]f	[d]λ_2	[e]λ_{exp}	[f]ΔG_R	[g]Ω	[h]E_{ex}	[i]λ_3	[j]λ_4
1SDR	S_1	2.40	517	0.355	547	555	0.0	79%	2.61	474	554
1DOXEPY	S_1	2.37	522	0.462	552	-	0.8	21%	2.73	454	534
1TDR	-	-	-	-	-	-	3.5	-	-	-	-
3SDR	S_1	2.31	536	0.370	566	570	0.0	79%	2.52	493	573
3DOXEPY	S_1	2.29	542	0.487	572	-	0.8	21%	2.63	471	551
3TDR	-	-	-	-	-	-	2.8	-	-	-	-
5SDR	S_1	2.19	566	0.391	596	600	0.0	84%	2.37	524	604
5DOXEPY	S_1	2.18	570	0.513	600	-	1.0	16%	2.50	495	575
5TDR	-	-	-	-	-	-	1.0	-	-	-	-
13SDR	S_1	2.37	524	0.347	554	555	0.0	79%	2.58	481	561
13DOXEPY	S_1	2.34	529	0.457	559	-	0.8	21%	2.70	460	540
13TDR	-	-	-	-	-	-	2.9	-	-	-	-
17SDR	S_1	2.45	505	0.405	535	530	0.0	73%	2.69	460	540
17DOXEPY	S_1	2.43	510	0.504	540	-	0.6	27%	2.79	444	524
17TDR	-	-	-	-	-	-	3.9	-	-	-	-
24SDR	S_1	2.39	520	0.417	550	550	0.0	73%	2.61	475	555
24DOXEPY	S_1	2.36	526	0.527	556	-	0.6	27%	2.70	459	539
24TDR	-	-	-	-	-	-	3.5	-	-	-	-

[a] Vertical excitation energy of $S_0 \rightarrow S_1$ excitation, showed in eV;

[b] Theoretical absorption wavelength of $S_0 \rightarrow S_1$ excitation, calculated at TD-M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level of theory, showed in nm;

[c] The oscillator strength of $S_0 \rightarrow S_1$ excitation;

[d] Theoretical absorption wavelength with systematic correctional value +30 nm based on experimental values;

[e] Experimentally measured absorption wavelength, showed in nm;

[f] Relative Gibbs free energy of SDR, DOXEPY and TDR intermediates obtained by each structure, the values of TDR are also equal to $\Delta E_{S\text{-}T}$;

[g] The Boltzmann distribution ratio of SDR and DOXEPY intermediates of each structure under experimental environment (at 298 K).

[h] Vertical excitation energies of $S_0 \rightarrow S_n$ excitation, performed at TDA-M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory and showed in eV;

[i] Theoretical absorption wavelength of $S_0 \rightarrow S_n$ excitation performed at TDA-M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory and showed in nm;

[j] Theoretical absorption wavelength of $S_0 \rightarrow S_n$ excitation performed at TDA-M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory, with systematic correctional value +80 nm based on experimental values and showed in nm.

Table S12. Free energy barriers of the C-C bond homolytic cleavage ($\Delta G^{\ddagger}_{TS1}$), 1,3-dipolar cycloaddition ($\Delta G^{\ddagger}_{TS2}$) and radical coupling ($\Delta G^{\ddagger}_{TS3}$) in the photoreaction of **1b**, **3b**, **5b**, **13b**, **17b** and **24b** with BCN.

Structures	Free energy barriers (kcal mol^{-1})		
	$\Delta G^{\ddagger}_{TS1}$	$\Delta G^{\ddagger}_{TS2}$	[a]$\Delta G^{\ddagger}_{TS3}$
1b	4.4	3.8	5.9
3b	9.6	4.0	4.4
5b	-0.9	3.5	3.2
13b	3.8	3.8	5.3
17b	7.1	3.8	6.3
24b	5.3	3.9	5.6

[a] The same as the $\Delta G^{\ddagger}_{re.}$ in **Figure 3g**.

Table S13. Coefficients of the three electronic configurations (c) generated by CASSCF calculation at CAS(2,2)/6-31G** (SMD, ACN:H_2O = 1:1) level of theory, the occupation numbers are given by twice the square of the "c".

Structures	Coefficients of electronic configurations			Occupation numbers		[a]<**S^2**>
	c_1	c_2	c_3	$2\times c_1^2$	$2\times c_3^2$	
1SDR	0.92	0	-0.38	1.6928	0.2888	0.3157
3SDR	0.92	0	-0.39	1.6928	0.3042	0.3578
5SDR	0.92	0	-0.40	1.6928	0.32	0.4280
13SDR	0.92	0	-0.39	1.6928	0.3042	0.3460
17SDR	0.93	0	-0.38	1.7298	0.2888	0.2672
24SDR	0.92	0	-0.38	1.6928	0.2888	0.2931

[a] The expectation value of total spin operator (<**S^2**>), calculated at the BS-UM06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory.

Table S14. Electronic energies (E_e, in Hartree) and relative electronic energies (ΔE_e, in kcal mol^{-1}) for all SDR and TDR structures, obtained at three different theoretical level.

Structures	(BS)-UDFT		CASSCF		NEVPT2	
	[a]E_e	ΔE_e	[b]E_e	ΔE_e	[c]E_e	ΔE_e
1SDR	-1072.23034	0.0	-1066.18436	0.0	-1070.22812	0.0
1TDR	-1072.22305	4.6	-1066.15791	16.6	-1070.18787	25.3
3SDR	-1150.84665	0.0	-1144.28539	0.0	-1148.67247	0.0
3TDR	-1150.84560	0.7	-1144.26042	15.7	-1148.63408	24.1
5SDR	-1301.25828	0.0	-1294.04667	0.0	-1298.89181	0.0
5TDR	-1301.25690	0.9	-1294.02386	14.3	-1298.85623	22.3
13SDR	-1270.70632	0.0	-1263.97753	0.0	-1268.50164	0.0
13TDR	-1270.70535	0.6	-1263.95179	16.2	-1268.46231	24.7
17SDR	-1746.31834	0.0	-1737.71966	0.0	-1743.54248	0.0
17TDR	-1746.31775	0.4	-1737.69151	17.7	-1743.50005	26.6
24SDR	-1399.33017	0.0	-1391.82585	0.0	-1396.87862	0.0
24TDR	-1399.32949	0.4	-1391.79852	17.1	-1396.83725	26.0

[a] Calculated at the (BS)-UM06-2X/6-311G** (SMD, ACN:H_2O = 1:1) theoretical level;

[b] Calculated at the CAS(2,2)/def2-TZVP (SMD, ACN:H_2O = 1:1) theoretical level;

[c] Calculated at the FIC-NEVPT2(2,2)/def2-TZVP (SMD, ACN:H_2O = 1:1) theoretical level.

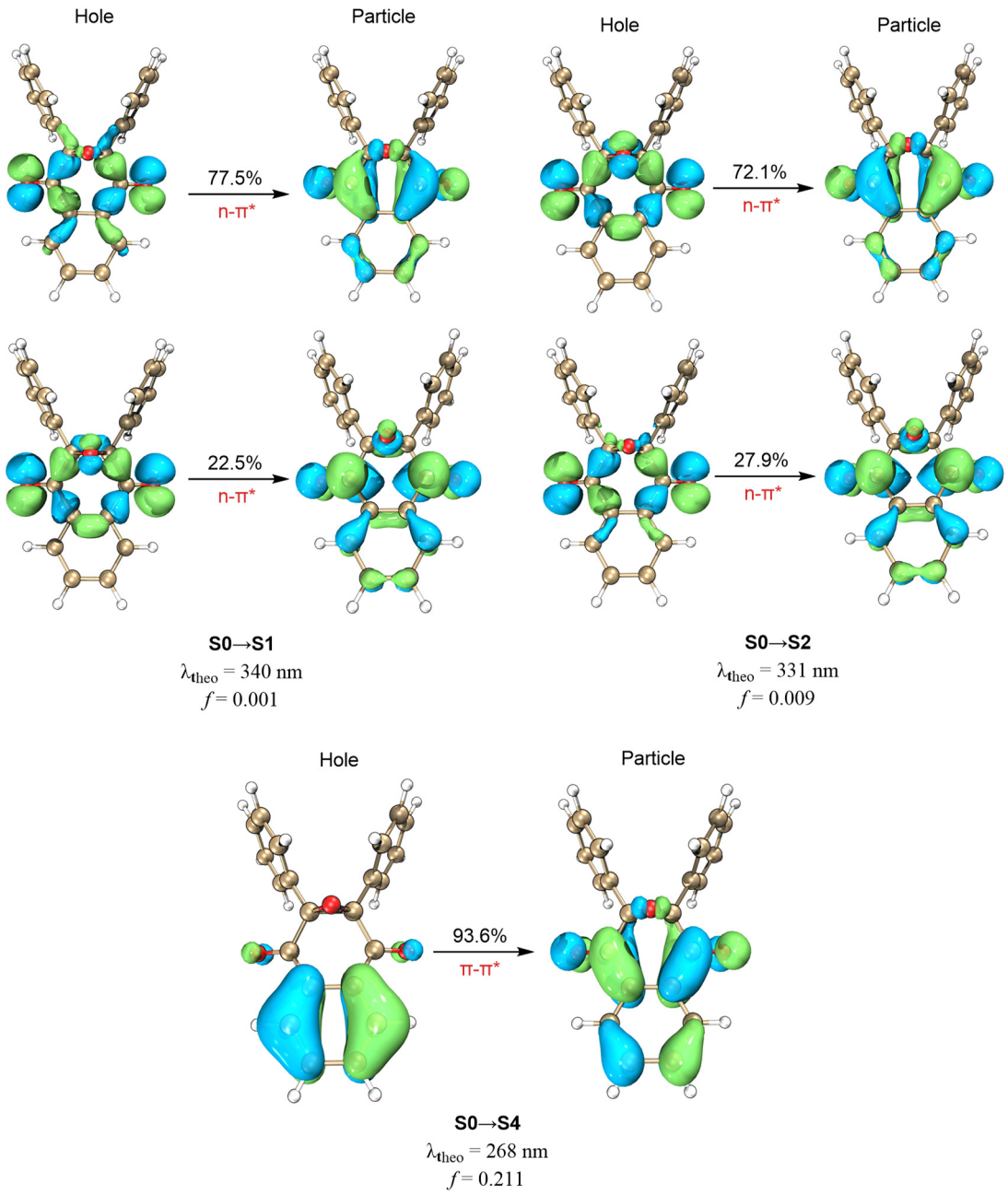


Figure S22. Theoretical absorption wavelength (λ_{theo}) and the NTOs of $S_0 \rightarrow S_1$, $S_0 \rightarrow S_2$, and $S_0 \rightarrow S_4$ transition for **1b**, calculated at the TD-M06-2X/6-31G** (SMD, ACN:H_2O = 1:1) level of theory. The oscillator strength (f) and eigenvalue of each NTO pair (in percentage) were shown. The isovalue of the NTO plots was set as 0.04.

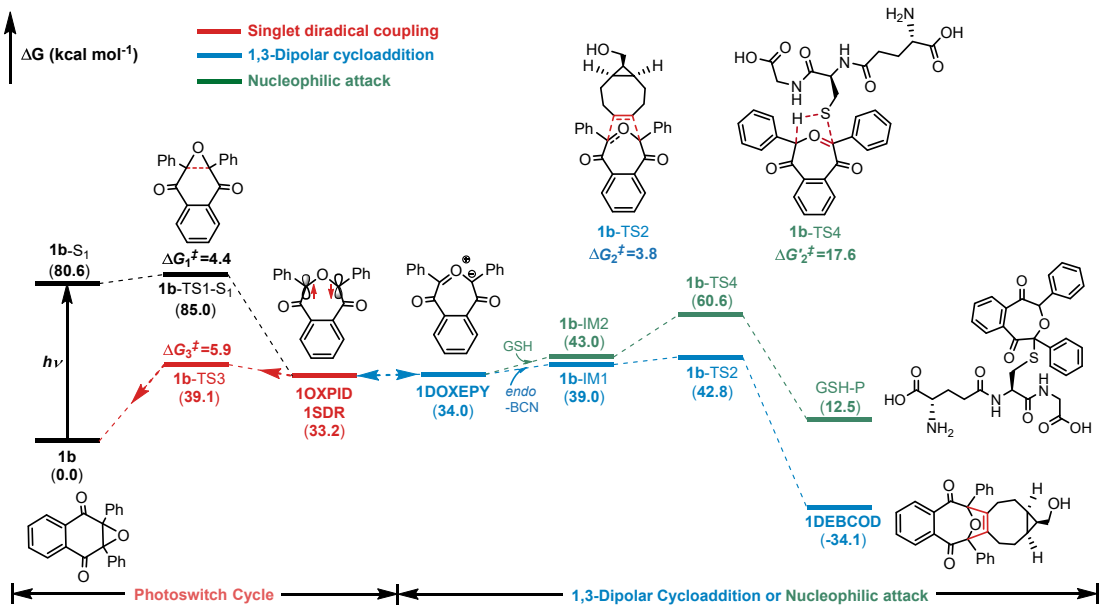


Figure S23. Gibbs free energy profile for the photoswitching cycle and the click reaction of **1b** with either BCN or GSH. The red pathway is the radical σ-coupling of **1SDR**, the blue pathway is the cycloaddition between **BCN** and **1DOXEPY**, and the green pathway is the nucleophilic reaction between GSH and **1DOXEPY**.

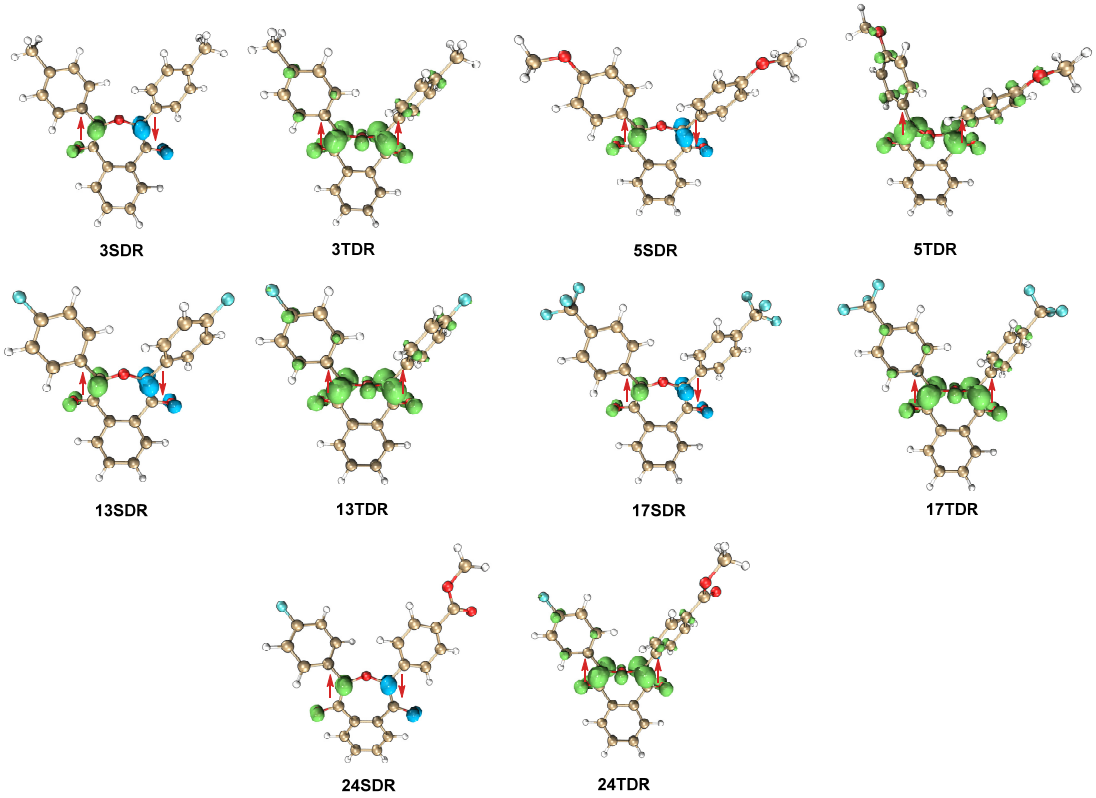


Figure S24. Visualization of the spin density analysis of SDR and TDR intermediates obtained by **3b**, **5b**, **13b**, **17b** and **24b**, the isovalue = 0.01.

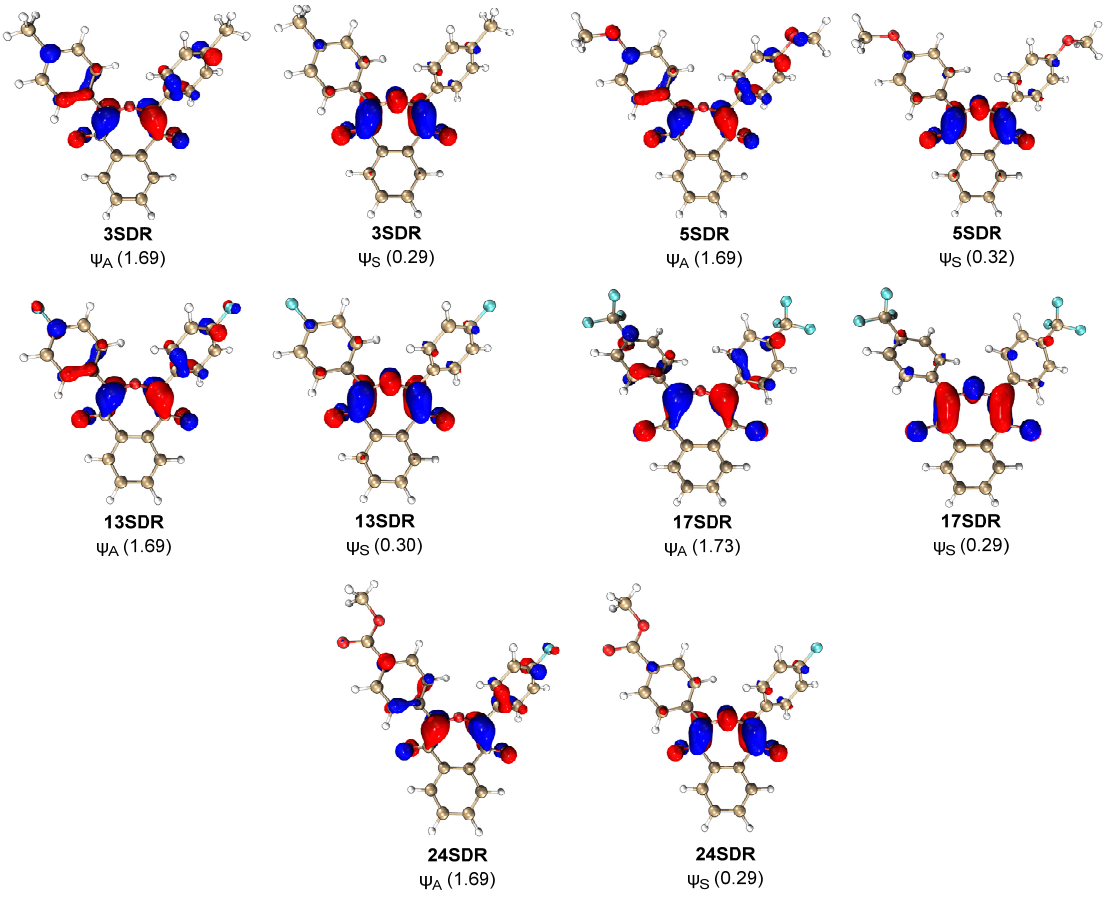


Figure S25. The molecular orbitals of the two active spaces (ψ_A and ψ_S) in the CASSCF calculation for the SDR intermediates obtained from **3b**, **5b**, **13b**, **17b** and **24b**, the isovalue = 0.05, and the values in the parenthesis are the occupation numbers of the two electrons.

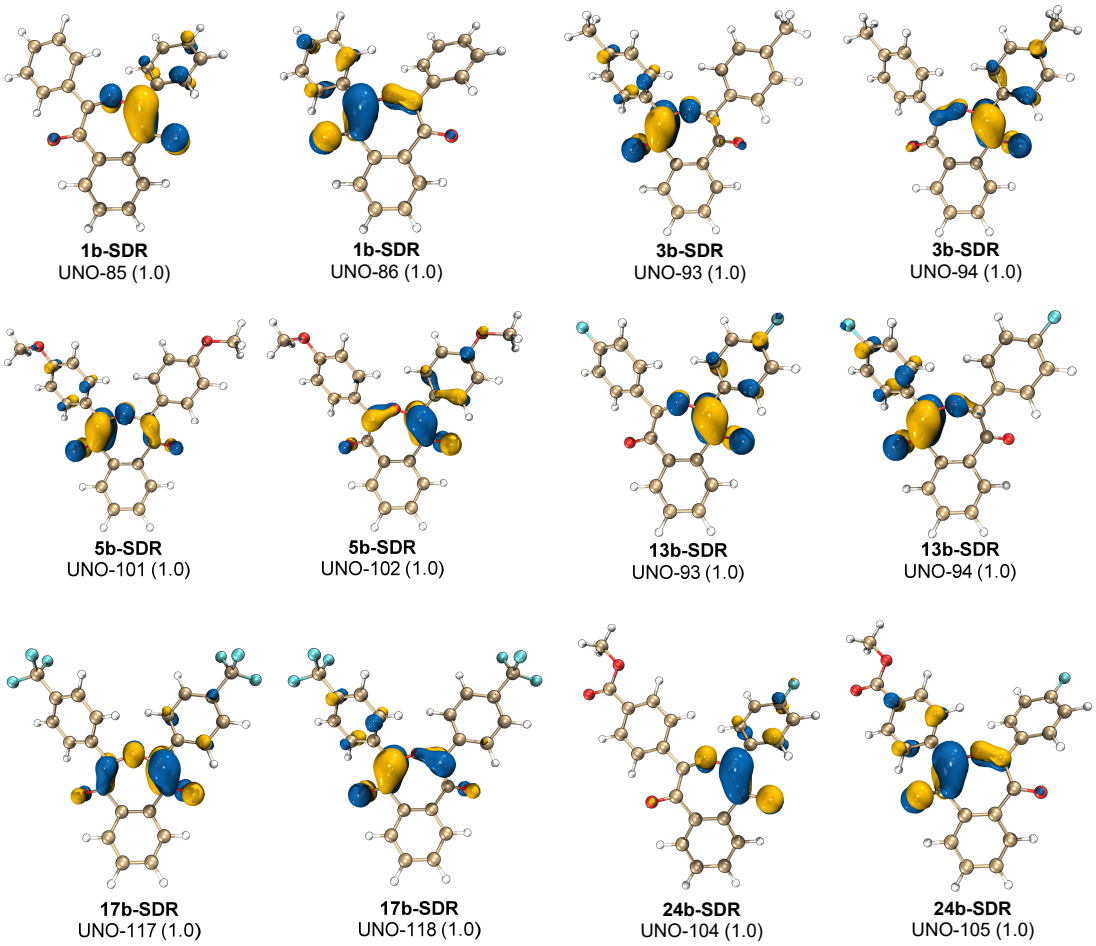


Figure S26. The UDFT natural orbitals (UNO) of the two active spaces in the NEVPT2 calculation for the SDR intermediates obtained from **1b**, **3b**, **5b**, **13b**, **17b** and **24b**, the isovalue = 0.05, and the values in the parenthesis are the occupation numbers of the two electrons.

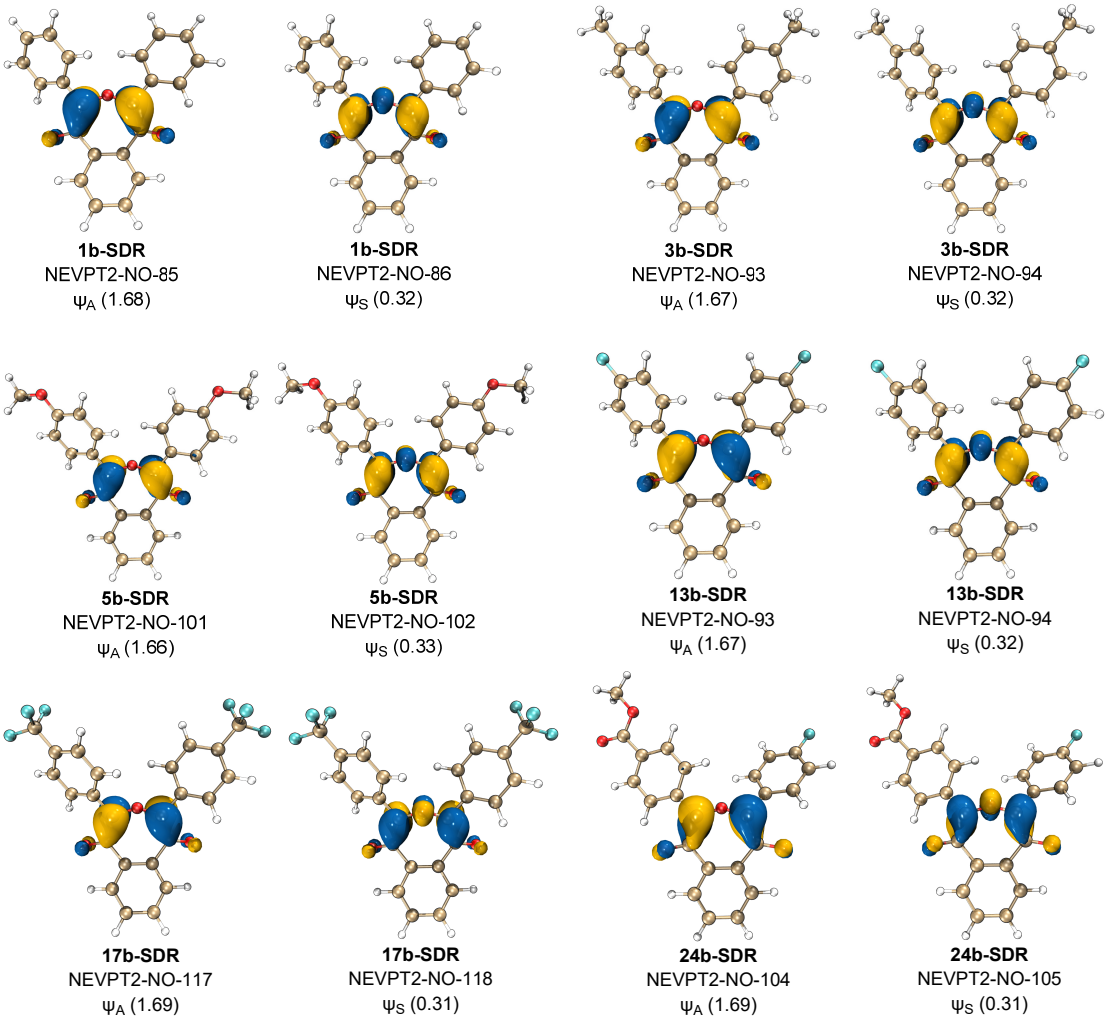


Figure S27. The frontier natural orbitals of SDR intermediates **1SDR**, **3SDR**, **5SDR**, **13SDR**, **17SDR** and **24SDR** calculated at NEVPT2(2,2)/def2-TZVP (SMD, ACN:H_2O = 1:1) level of theory (NEVPT2-NO, also marked as ψ_A and ψ_S), the isovalue = 0.05, and the values in the parenthesis are the occupation numbers of the two electrons.

Determination of the light-to-chemical-energy conversion efficiency

The calculation method for the light-to-chemical-energy conversion efficiency η is shown as follows[28], where the $\Delta G_{SDR\text{-}DNQO}$ is calculated at M06-2X/6-31G**(SMD, ACN:H_2O = 1:1) level of theory.

$$\eta = \frac{\Delta G_{SDR\text{-}DNQO}\,\Phi_{max}}{h\nu N_L}$$

Φ_{max} = the quantum yield for DNQO→SDR photo-ring-opening transformation
ν = frequency of the excitation light (s^{-1})
h = Planck's constant = 6.626070×10^{-34} J·s
N_L = Avogadro constant = 6.02214076×10^{23} mol^{-1}
$\Delta G_{SDR\text{-}DNQO}$ = the difference of the chemical energy between the metastable SDR and the staring DNQO (in kcal·mol^{-1})

Table S15. The parameters for determination of the light-to-chemical-energy conversion efficiency (η).

compounds	$\lambda_{ex.}$ [nm]	hν N_L [kcal/mol]	Φ_{max}	$\Delta G_{SDR\text{-}DNQO}$ [kcal/mol]	η [%]
1b	365	78.3	0.25	33.2	10.6
3b	365	78.3	0.19	32.1	7.8
5b	365	78.3	N.A.	31.9	N.A.
13b	365	78.3	0.56	33.2	23.7
17b	365	78.3	0.58	33.8	25.0
24b	365	78.3	0.76	33.2	33.1

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6. Cartesian coordinates of all the optimized geometries.

BCN

Charge 0 *Multiplicity* 1

O	-3.59820000	0.49620000	0.01650000
C	-0.44600000	0.55890000	-0.27270000
C	-0.17230000	-0.93530000	-0.27470000
C	-1.42490000	-0.39400000	0.36010000
C	0.27350000	1.60820000	0.55520000
C	0.87440000	-1.66210000	0.55090000
C	-2.76390000	-0.62050000	-0.28000000
C	1.57860000	2.12510000	-0.10080000
C	2.27610000	-1.67680000	-0.10930000
C	2.40590000	0.92770000	-0.28950000
C	2.62350000	-0.26280000	-0.29220000
H	-0.76020000	0.93260000	-1.24810000
H	-0.32730000	-1.39180000	-1.25270000
H	-1.43110000	-0.39400000	1.45000000
H	0.52120000	1.20200000	1.54240000
H	-0.40460000	2.45560000	0.71720000
H	0.54510000	-2.69640000	0.71110000
H	0.96390000	-1.19640000	1.53850000
H	-3.21790000	-1.54840000	0.09400000
H	-2.63330000	-0.72780000	-1.36670000
H	2.05920000	2.87030000	0.54030000
H	1.36270000	2.61020000	-1.05930000
H	2.24430000	-2.20230000	-1.07030000
H	2.99190000	-2.20550000	0.52740000
H	-4.47770000	0.31160000	-0.33800000

1b

Charge 0 *Multiplicity* 1

C	-3.85390000	1.39790000	0.00830000
C	-5.05400000	0.69750000	0.07610000
C	-5.05390000	-0.69790000	0.07590000
C	-3.85370000	-1.39810000	0.00780000
C	-2.64730000	0.70160000	-0.03660000
C	-2.64720000	-0.70170000	-0.03680000
C	-1.37580000	1.46480000	-0.14730000
C	-1.37560000	-1.46460000	-0.14800000
O	-1.34530000	2.61750000	-0.52930000
O	-1.34500000	-2.61730000	-0.53020000
C	-0.10410000	0.75310000	0.27040000
C	-0.10400000	-0.75300000	0.27020000

O	-0.27560000	-0.00010000	1.46080000
C	1.18110000	1.49450000	0.10890000
C	1.99140000	1.75340000	1.21280000
C	3.19510000	2.43490000	1.04290000
C	3.58880000	2.85290000	-0.22610000
C	2.77750000	2.59010000	-1.32990000
C	1.57400000	1.91240000	-1.16490000
C	1.18120000	-1.49430000	0.10860000
C	1.99090000	-1.75440000	1.21260000
C	3.19460000	-2.43600000	1.04270000
C	1.57470000	-1.91110000	-1.16540000
C	2.77810000	-2.58890000	-1.33040000
C	3.58880000	-2.85300000	-0.22640000
H	-3.84000000	2.48300000	-0.00600000
H	-5.99290000	1.23950000	0.12470000
H	-5.99270000	-1.24000000	0.12440000
H	-3.83960000	-2.48330000	-0.00680000
H	1.67860000	1.42190000	2.19820000
H	3.82420000	2.63930000	1.90370000
H	4.52840000	3.38100000	-0.35720000
H	3.08420000	2.91110000	-2.32050000
H	0.94020000	1.70140000	-2.02260000
H	1.67770000	-1.42370000	2.19820000
H	3.82320000	-2.64130000	1.90370000
H	0.94140000	-1.69920000	-2.02320000
H	3.08520000	-2.90910000	-2.32110000
H	4.52830000	-3.38110000	-0.35750000

1b-S_1

Charge 0 *Multiplicity* 1

C	3.84550000	1.39100000	0.07530000
C	5.03480000	0.68490000	0.09480000
C	5.03980000	-0.71690000	0.06210000
C	3.83820000	-1.40410000	0.02050000
C	2.61960000	0.69690000	0.01390000
C	2.61880000	-0.71570000	-0.00740000
C	1.37160000	1.42330000	0.00660000
C	1.36900000	-1.49370000	0.02710000
O	1.32170000	2.68650000	0.19740000
O	1.33940000	-2.67690000	0.33170000
C	0.08750000	0.72460000	-0.37310000
C	0.08460000	-0.78030000	-0.33490000
O	0.17850000	-0.03940000	-1.55630000
C	-1.17040000	1.50650000	-0.15030000

C	-2.12540000	1.61290000	-1.15920000
C	-3.29430000	2.33590000	-0.92790000
C	-3.51060000	2.94410000	0.30650000
C	-2.55470000	2.83120000	1.31550000
C	-1.38470000	2.11240000	1.09070000
C	-1.19040000	-1.51430000	-0.09270000
C	-2.05250000	-1.80830000	-1.14820000
C	-3.24240000	-2.48950000	-0.90030000
C	-1.52070000	-1.89470000	1.21070000
C	-2.71210000	-2.56960000	1.45400000
C	-3.57390000	-2.86900000	0.39840000
H	3.84160000	2.47620000	0.09750000
H	5.97420000	1.22790000	0.13500000
H	5.97860000	-1.25980000	0.07420000
H	3.81420000	-2.48970000	0.00780000
H	-1.94800000	1.14190000	-2.12070000
H	-4.03420000	2.42730000	-1.71710000
H	-4.42310000	3.50500000	0.48380000
H	-2.72140000	3.29840000	2.28100000
H	-0.64380000	2.01290000	1.87960000
H	-1.78800000	-1.50910000	-2.15800000
H	-3.91020000	-2.72240000	-1.72390000
H	-0.84560000	-1.65810000	2.02930000
H	-2.97010000	-2.86040000	2.46750000
H	-4.50380000	-3.39580000	0.58970000

1b-TS1-S_1

Charge 0 *Multiplicity* 1

C	-3.84510000	-1.39680000	0.04090000
C	-5.03270000	-0.70760000	0.09030000
C	-5.03280000	0.70700000	0.09010000
C	-3.84540000	1.39640000	0.04060000
C	-2.60730000	-0.71110000	-0.02440000
C	-2.60740000	0.71100000	-0.02460000
C	-1.40260000	-1.50060000	-0.01040000
C	-1.40280000	1.50060000	-0.01080000
O	-1.37820000	-2.72470000	0.23300000
O	-1.37870000	2.72480000	0.23250000
C	-0.09460000	-0.87360000	-0.41230000
C	-0.09470000	0.87370000	-0.41230000
O	-0.10910000	0.00000000	-1.50090000
C	1.15800000	-1.57150000	-0.15040000
C	2.17680000	-1.60340000	-1.11580000
C	3.37360000	-2.24800000	-0.83620000

C	3.57140000	-2.84490000	0.41030000
C	2.56350000	-2.80970000	1.37790000
C	1.35700000	-2.18900000	1.09950000
C	1.15780000	1.57170000	-0.15030000
C	2.17690000	1.60310000	-1.11540000
C	3.37370000	2.24770000	-0.83580000
C	1.35650000	2.18960000	1.09950000
C	2.56310000	2.81020000	1.37800000
C	3.57110000	2.84500000	0.41060000
H	-3.83220000	-2.48150000	0.04640000
H	-5.97300000	-1.24800000	0.13290000
H	-5.97320000	1.24730000	0.13260000
H	-3.83260000	2.48110000	0.04570000
H	2.01170000	-1.14460000	-2.08450000
H	4.15500000	-2.28700000	-1.58820000
H	4.51200000	-3.34140000	0.62790000
H	2.72240000	-3.27140000	2.34680000
H	0.56690000	-2.16310000	1.84290000
H	2.01200000	1.14410000	-2.08410000
H	4.15530000	2.28650000	-1.58760000
H	0.56620000	2.16380000	1.84270000
H	2.72180000	3.27210000	2.34680000
H	4.51180000	3.34150000	0.62830000

1SDR

Charge 0 *Multiplicity* 1

C	1.33790000	3.25740000	-2.48860000
C	1.56200000	3.35490000	-3.84980000
C	1.70420000	2.19140000	-4.60810000
C	1.61430000	0.95730000	-3.99010000
C	1.27360000	2.01230000	-1.83880000
C	1.40800000	0.83650000	-2.60420000
C	1.03790000	2.12330000	-0.37100000
C	1.32050000	-0.58170000	-2.13870000
O	0.51880000	3.14630000	0.08790000
O	1.07710000	-1.46680000	-2.96770000
C	1.51560000	1.11460000	0.55700000
C	1.65390000	-0.97170000	-0.78310000
O	1.78690000	-0.12320000	0.21580000
C	1.68670000	1.35140000	1.99270000
C	1.60380000	0.26450000	2.88110000
C	1.79550000	0.45390000	4.24390000
C	2.07690000	1.72480000	4.74280000
C	2.16790000	2.80650000	3.86770000

C	1.97390000	2.62870000	2.50360000
C	1.99390000	-2.34160000	-0.37820000
C	1.43220000	-3.47730000	-0.98640000
C	1.77260000	-4.74920000	-0.53770000
C	2.89600000	-2.52100000	0.68790000
C	3.23040000	-3.79560000	1.12500000
C	2.67170000	-4.91700000	0.51280000
H	1.21760000	4.15320000	-1.89020000
H	1.62900000	4.33070000	-4.32020000
H	1.88400000	2.24910000	-5.67690000
H	1.70730000	0.04880000	-4.57330000
H	1.37240000	-0.72480000	2.49840000
H	1.71850000	-0.39240000	4.91910000
H	2.22460000	1.87210000	5.80820000
H	2.39730000	3.79680000	4.24870000
H	2.05850000	3.47370000	1.83140000
H	0.71670000	-3.36250000	-1.78850000
H	1.32150000	-5.61600000	-1.01090000
H	3.34670000	-1.65340000	1.15960000
H	3.93710000	-3.91320000	1.94050000
H	2.93550000	-5.91360000	0.85300000

1DOXEPY

Charge 0 *Multiplicity* 1

C	1.33590000	3.26060000	-2.49550000
C	1.55470000	3.35640000	-3.85630000
C	1.69290000	2.19070000	-4.61420000
C	1.60340000	0.95850000	-3.99510000
C	1.27260000	2.01580000	-1.84140000
C	1.40200000	0.83700000	-2.60710000
C	1.04380000	2.13730000	-0.37520000
C	1.31520000	-0.58220000	-2.14810000
O	0.54570000	3.16680000	0.08570000
O	1.08130000	-1.46660000	-2.97850000
C	1.50780000	1.11430000	0.55220000
C	1.64190000	-0.96800000	-0.78750000
O	1.74650000	-0.11490000	0.19970000
C	1.68370000	1.34270000	1.98990000
C	1.57390000	0.25600000	2.87480000
C	1.77280000	0.43660000	4.23800000
C	2.08600000	1.69840000	4.74020000
C	2.20190000	2.78010000	3.86790000
C	2.00140000	2.61100000	2.50350000
C	1.99170000	-2.33370000	-0.37450000

C	1.44740000	-3.47610000	-0.98500000
C	1.79470000	-4.74350000	-0.52850000
C	2.88450000	-2.50120000	0.70070000
C	3.22400000	-3.77130000	1.14770000
C	2.68260000	-4.89990000	0.53340000
H	1.22000000	4.15710000	-1.89740000
H	1.62190000	4.33130000	-4.32820000
H	1.86950000	2.24720000	-5.68350000
H	1.69360000	0.04950000	-4.57760000
H	1.31540000	-0.72580000	2.48970000
H	1.67530000	-0.40950000	4.91100000
H	2.23830000	1.83910000	5.80580000
H	2.45560000	3.76350000	4.25120000
H	2.10420000	3.45590000	1.83360000
H	0.74050000	-3.37020000	-1.79600000
H	1.35750000	-5.61610000	-1.00420000
H	3.32420000	-1.62750000	1.17240000
H	3.92250000	-3.87960000	1.97160000
H	2.95170000	-5.89280000	0.87990000

1TDR

Charge 0 *Multiplicity* 3

C	1.43670000	3.27250000	-2.54110000
C	1.68240000	3.36210000	-3.90500000
C	1.83150000	2.19970000	-4.66030000
C	1.73140000	0.95930000	-4.04450000
C	1.37460000	2.02830000	-1.90530000
C	1.51920000	0.85900000	-2.66520000
C	1.06360000	2.06410000	-0.44080000
C	1.38300000	-0.53000000	-2.12520000
O	0.28790000	2.92830000	-0.01030000
O	0.92140000	-1.42080000	-2.85010000
C	1.73480000	1.15590000	0.46040000
C	1.89670000	-0.84770000	-0.81090000
O	2.49850000	0.14270000	-0.06880000
C	1.77010000	1.28400000	1.90030000
C	2.11740000	0.16350000	2.68340000
C	2.16440000	0.25520000	4.06620000
C	1.88440000	1.46640000	4.69910000
C	1.55630000	2.58750000	3.93580000
C	1.49610000	2.50640000	2.55230000
C	2.05620000	-2.19340000	-0.29660000
C	1.15480000	-3.22640000	-0.62100000
C	1.34780000	-4.50210000	-0.10750000

C	3.15060000	-2.47880000	0.54570000
C	3.33930000	-3.76070000	1.04080000
C	2.43790000	-4.77590000	0.71840000
H	1.29590000	4.17070000	-1.94830000
H	1.75170000	4.33580000	-4.37930000
H	2.01770000	2.26000000	-5.72780000
H	1.81970000	0.04710000	-4.62570000
H	2.32360000	-0.78290000	2.19840000
H	2.42000000	-0.62130000	4.65290000
H	1.92720000	1.53820000	5.78150000
H	1.35470000	3.53600000	4.42340000
H	1.25940000	3.38770000	1.97150000
H	0.29780000	-3.01560000	-1.24760000
H	0.63840000	-5.28750000	-0.34820000
H	3.85940000	-1.69210000	0.78430000
H	4.19320000	-3.97150000	1.67660000
H	2.58300000	-5.77670000	1.11290000

1b-IM1

Charge 0 *Multiplicity* 1

O	1.59450000	0.05720000	0.68130000
O	-0.20090000	-2.95470000	0.81000000
O	-0.71600000	2.66700000	1.09300000
O	-5.25630000	0.67940000	0.03510000
C	1.32300000	-1.21960000	0.66380000
C	0.02170000	-1.75780000	1.02300000
C	-1.03230000	-0.94720000	1.71230000
C	-2.02120000	-1.74770000	2.31870000
C	-3.12130000	-1.20390000	2.95380000
C	-3.27750000	0.18390000	2.99190000
C	-2.31800000	0.98900000	2.40900000
C	-1.17940000	0.45640000	1.77190000
C	-0.29640000	1.50710000	1.18700000
C	1.06400000	1.24290000	0.75550000
C	-0.18120000	0.65560000	-1.96410000
C	-0.07740000	-0.55220000	-2.03490000
C	-0.58450000	-1.92110000	-2.18880000
C	-2.05240000	-1.86270000	-1.70310000
C	-2.93530000	-0.92010000	-2.50910000
C	-3.06300000	0.59460000	-2.42720000
C	-2.34600000	1.57110000	-1.50840000
C	-0.91120000	1.92890000	-1.96460000
C	-4.18380000	-0.29280000	-1.93020000
C	-4.45310000	-0.39470000	-0.44690000

C	2.51140000	-2.02490000	0.34080000
C	3.77920000	-1.42360000	0.48080000
C	4.93720000	-2.12160000	0.16810000
C	4.86450000	-3.43660000	-0.29010000
C	3.61900000	-4.04250000	-0.42830000
C	2.45030000	-3.35400000	-0.11640000
C	1.99640000	2.29650000	0.33110000
C	2.94460000	1.98680000	-0.65920000
C	3.86290000	2.94230000	-1.07650000
C	3.84940000	4.21760000	-0.51400000
C	2.91260000	4.53120000	0.46990000
C	1.98720000	3.58330000	0.89160000
H	-4.75700000	1.49750000	-0.09280000
H	-1.90300000	-2.82320000	2.27030000
H	-3.85760000	-1.85600000	3.41290000
H	-4.13930000	0.63110000	3.47660000
H	-2.42730000	2.06640000	2.43160000
H	-0.02330000	-2.65920000	-1.60860000
H	-0.53500000	-2.22210000	-3.24160000
H	-2.48430000	-2.86990000	-1.76160000
H	-2.04220000	-1.58400000	-0.64720000
H	-3.06310000	-1.27590000	-3.53050000
H	-3.25460000	1.03350000	-3.40550000
H	-2.29110000	1.17380000	-0.49120000
H	-2.93770000	2.49510000	-1.45890000
H	-0.92450000	2.35060000	-2.97630000
H	-0.47550000	2.68020000	-1.29990000
H	-5.08810000	-0.33170000	-2.53350000
H	-5.01530000	-1.30920000	-0.22860000
H	-3.51790000	-0.44690000	0.12350000
H	3.85390000	-0.40760000	0.85450000
H	5.90140000	-1.63830000	0.29210000
H	5.77030000	-3.98320000	-0.53310000
H	3.54840000	-5.06450000	-0.78770000
H	1.49620000	-3.84490000	-0.23580000
H	2.93740000	0.99920000	-1.11230000
H	4.58340000	2.69380000	-1.84960000
H	4.56390000	4.96540000	-0.84410000
H	2.90340000	5.52090000	0.91590000
H	1.26970000	3.83150000	1.66420000

1b-TS2

Charge 0 *Multiplicity* 1

O	1.61970000	0.08010000	0.72170000

O	-0.22180000	-2.92460000	0.85330000
O	-0.73760000	2.68660000	0.99310000
O	-5.29110000	0.70910000	-0.14820000
C	1.29270000	-1.18860000	0.61130000
C	0.00290000	-1.72160000	1.02720000
C	-1.04530000	-0.90080000	1.71890000
C	-2.02020000	-1.68750000	2.36070000
C	-3.11520000	-1.12880000	2.99500000
C	-3.27330000	0.25790000	3.00040000
C	-2.32180000	1.05000000	2.38430000
C	-1.19570000	0.50060000	1.74290000
C	-0.31840000	1.52960000	1.11070000
C	1.03140000	1.24790000	0.64450000
C	-0.13070000	0.60000000	-1.54640000
C	-0.02970000	-0.62230000	-1.59570000
C	-0.53920000	-1.94410000	-1.99430000
C	-2.04700000	-1.93430000	-1.66310000
C	-2.85910000	-0.97260000	-2.51850000
C	-2.98120000	0.54530000	-2.47930000
C	-2.33630000	1.57230000	-1.56200000
C	-0.84840000	1.84410000	-1.87330000
C	-4.13270000	-0.32580000	-2.02620000
C	-4.46860000	-0.38100000	-0.55410000
C	2.47380000	-2.02270000	0.31310000
C	3.75240000	-1.43780000	0.42100000
C	4.89760000	-2.16280000	0.12250000
C	4.80380000	-3.49010000	-0.29420000
C	3.54870000	-4.08040000	-0.40170000
C	2.39280000	-3.36540000	-0.10000000
C	1.97850000	2.31030000	0.25850000
C	2.96200000	1.99420000	-0.69380000
C	3.90390000	2.94130000	-1.07510000
C	3.87760000	4.21680000	-0.51250000
C	2.90560000	4.53730000	0.43350000
C	1.95730000	3.59570000	0.81910000
H	-4.79730000	1.52390000	-0.31450000
H	-1.90040000	-2.76350000	2.33940000
H	-3.84460000	-1.77020000	3.47940000
H	-4.12890000	0.71620000	3.48590000
H	-2.43250000	2.12760000	2.38080000
H	-0.04380000	-2.77280000	-1.48260000
H	-0.38070000	-2.07850000	-3.07080000
H	-2.44870000	-2.94230000	-1.82550000
H	-2.15800000	-1.72270000	-0.59670000

H	-2.92960000	-1.33520000	-3.54280000
H	-3.11070000	0.94770000	-3.48280000
H	-2.41990000	1.28130000	-0.51040000
H	-2.89090000	2.51340000	-1.67310000
H	-0.71520000	2.06140000	-2.93940000
H	-0.49250000	2.71150000	-1.31140000
H	-5.00790000	-0.37540000	-2.67020000
H	-5.04060000	-1.28780000	-0.32950000
H	-3.55850000	-0.41310000	0.05890000
H	3.84860000	-0.41190000	0.75900000
H	5.86900000	-1.68870000	0.22380000
H	5.69970000	-4.05660000	-0.52850000
H	3.45900000	-5.11270000	-0.72610000
H	1.43350000	-3.85150000	-0.18990000
H	2.96420000	1.00470000	-1.14320000
H	4.65320000	2.68720000	-1.81830000
H	4.61040000	4.95930000	-0.81340000
H	2.88630000	5.52700000	0.87930000
H	1.21290000	3.85010000	1.56330000

1DEBCOD

Charge 0 *Multiplicity* 1

O	1.41100000	0.09780000	0.95270000
O	0.02230000	-2.67900000	1.99900000
O	-0.65720000	2.88790000	0.89170000
O	-5.06410000	0.85820000	-0.44750000
C	0.97200000	-1.14070000	0.40480000
C	-0.06760000	-1.60350000	1.44640000
C	-1.20890000	-0.66790000	1.82030000
C	-2.27510000	-1.35460000	2.41620000
C	-3.43920000	-0.71470000	2.82470000
C	-3.55750000	0.65790000	2.65110000
C	-2.51000000	1.36040000	2.06910000
C	-1.33270000	0.73560000	1.63640000
C	-0.37490000	1.70720000	0.96820000
C	0.85580000	1.18560000	0.22440000
C	0.28110000	0.56010000	-1.03670000
C	0.32190000	-0.76880000	-0.92310000
C	-0.27290000	-1.78520000	-1.84890000
C	-1.79340000	-1.94960000	-1.61300000
C	-2.63800000	-1.13570000	-2.57970000
C	-2.69730000	0.36870000	-2.70730000
C	-1.95490000	1.39750000	-1.87430000
C	-0.41790000	1.39360000	-2.07100000

C	-3.89360000	-0.39760000	-2.18000000
C	-4.26620000	-0.28960000	-0.72190000
C	2.15330000	-2.08170000	0.23570000
C	3.43920000	-1.54060000	0.15450000
C	4.53890000	-2.36410000	-0.07280000
C	4.36650000	-3.73680000	-0.23090000
C	3.08570000	-4.28070000	-0.16340000
C	1.98360000	-3.46090000	0.06810000
C	1.93920000	2.22790000	0.03140000
C	2.67610000	2.26670000	-1.15360000
C	3.73960000	3.15710000	-1.29200000
C	4.07940000	4.00670000	-0.24260000
C	3.35670000	3.96020000	0.94920000
C	2.29220000	3.07500000	1.08600000
H	-4.56150000	1.63790000	-0.72170000
H	-2.18010000	-2.42600000	2.55130000
H	-4.24350000	-1.28970000	3.27220000
H	-4.45660000	1.18320000	2.95690000
H	-2.59930000	2.43120000	1.92510000
H	0.23430000	-2.74360000	-1.71240000
H	-0.09610000	-1.47860000	-2.88620000
H	-2.06400000	-3.00210000	-1.75060000
H	-2.02720000	-1.71440000	-0.57070000
H	-2.70740000	-1.62560000	-3.54890000
H	-2.79670000	0.68650000	-3.74330000
H	-2.19060000	1.28220000	-0.81250000
H	-2.33880000	2.38370000	-2.16030000
H	-0.17890000	1.02280000	-3.07460000
H	-0.03940000	2.41890000	-2.00960000
H	-4.75270000	-0.48490000	-2.84100000
H	-4.86990000	-1.15280000	-0.42170000
H	-3.37140000	-0.28420000	-0.08840000
H	3.57740000	-0.47070000	0.27060000
H	5.53220000	-1.92900000	-0.13000000
H	5.22360000	-4.37920000	-0.40940000
H	2.93920000	-5.34920000	-0.28920000
H	0.99370000	-3.89970000	0.12530000
H	2.42360000	1.59650000	-1.97150000
H	4.30290000	3.18300000	-2.21970000
H	4.90640000	4.70190000	-0.35030000
H	3.62280000	4.61390000	1.77410000
H	1.73420000	3.04270000	2.01740000

1b-TS3

Charge 0 *Multiplicity* 1

C	-3.70310000	1.38880000	-0.02460000
C	-4.88770000	0.70960000	0.22050000
C	-4.89360000	-0.68460000	0.23880000
C	-3.71490000	-1.38000000	0.01070000
C	-2.50060000	0.69890000	-0.22370000
C	-2.50670000	-0.70570000	-0.20620000
C	-1.31490000	1.56860000	-0.50640000
C	-1.33030000	-1.59090000	-0.48070000
O	-1.48880000	2.66520000	-1.05620000
O	-1.51950000	-2.69450000	-1.01060000
C	-0.00810000	1.18800000	-0.02250000
C	-0.01390000	-1.20980000	-0.02240000
O	0.14040000	-0.01050000	0.61780000
C	1.15350000	2.05480000	0.00940000
C	2.12870000	1.86750000	1.01010000
C	3.25050000	2.68180000	1.06010000
C	3.43420000	3.68410000	0.10640000
C	2.48250000	3.86960000	-0.89570000
C	1.34680000	3.07270000	-0.94720000
C	1.15420000	-2.06590000	-0.02010000
C	2.18100000	-1.82850000	0.91710000
C	3.30990000	-2.63330000	0.94510000
C	1.30860000	-3.12310000	-0.94200000
C	2.45210000	-3.90970000	-0.91440000
C	3.45210000	-3.67630000	0.02910000
H	-3.68950000	2.47300000	-0.06140000
H	-5.80460000	1.26420000	0.39270000
H	-5.81500000	-1.22690000	0.42550000
H	-3.71090000	-2.46480000	0.00050000
H	1.97960000	1.10530000	1.76610000
H	3.98450000	2.53630000	1.84610000
H	4.31670000	4.31520000	0.14270000
H	2.62760000	4.63820000	-1.64810000
H	0.62230000	3.21370000	-1.73740000
H	2.06890000	-1.03060000	1.64100000
H	4.08210000	-2.44860000	1.68500000
H	0.54740000	-3.30280000	-1.68820000
H	2.56550000	-4.70860000	-1.64030000
H	4.33980000	-4.30090000	0.04810000

GSH

Charge 0 *Multiplicity* 1

O	-0.10227000	-3.25586800	-2.97036100

C	-0.00505100	-2.03768600	-2.81929700
N	-1.07695700	-1.27675800	-2.52608200
C	-1.14594600	0.16301300	-2.45299700
C	-2.52152200	0.62353300	-2.87022000
O	-2.60025400	1.95059100	-2.87370800
O	-3.44167000	-0.11379500	-3.14635200
C	1.34851300	-1.33101900	-2.96825500
C	2.44252600	-2.33431600	-3.31706700
S	2.80438000	-3.51487300	-1.95982400
N	1.67082600	-0.55020000	-1.79178100
C	1.95179500	0.77337500	-1.83130900
C	2.30936700	1.39891500	-0.50242300
C	1.02999700	1.79221300	0.25048000
C	1.31775800	2.44584100	1.60289300
N	2.06497700	3.68578600	1.45467900
C	1.94191000	1.41964700	2.54610900
O	2.79162900	1.95896300	3.42091300
O	1.68144200	0.23276200	2.53176400
O	1.86183100	1.43947000	-2.86515200
H	-1.95996200	-1.77418400	-2.46148200
H	-0.96887400	0.54179800	-1.43864600
H	-0.41632000	0.64330200	-3.11224800
H	-3.50188400	2.21665600	-3.12683300
H	1.26759700	-0.62443700	-3.80273200
H	2.13742100	-2.91440100	-4.18811300
H	3.35919000	-1.79561800	-3.55909000
H	3.99598500	-3.00140000	-1.61806400
H	1.79302000	-1.04522500	-0.91519000
H	2.90169700	0.69853000	0.09649900
H	2.91474800	2.28279700	-0.71824000
H	0.45243800	2.49706900	-0.35596500
H	0.41469100	0.90254800	0.41468300
H	0.35180600	2.68899300	2.06465000
H	2.10697900	4.15712900	2.35505200
H	3.03170200	3.47085500	1.21692600
H	3.12638700	1.25429200	4.00348200

1b-IM2

Charge 0 *Multiplicity* 1

O	-0.95738200	1.34145500	0.55031200
C	-0.62743700	0.47942400	-0.26520500
N	0.64385300	0.02936000	-0.33488900
C	1.18661400	-1.12376900	-1.02088800
C	2.67621400	-0.93234500	-1.18487000

O	3.21798400	-1.94799700	-1.84719400
O	3.29996700	0.01038600	-0.74840300
C	-1.67591600	-0.09359900	-1.21908500
C	-2.06136600	-1.53250000	-0.83781700
S	-2.84521100	-1.63114600	0.80550400
N	-1.21685600	-0.00494000	-2.59895700
C	-2.09775900	-0.10062800	-3.62664200
C	-1.52515200	0.14393800	-5.00624800
C	-0.32531700	-0.75799700	-5.32144700
C	0.14729300	-0.60691600	-6.76962100
N	0.57259100	0.75558500	-7.05099300
C	-0.90862800	-1.17274900	-7.71658600
O	-1.01549900	-0.49292600	-8.85858400
O	-1.57274500	-2.16147200	-7.47655700
O	-3.28147800	-0.38013000	-3.43710200
C	-2.92853600	-0.43564500	4.30590700
C	-4.05562500	0.36006900	4.39870200
C	-3.93883300	1.74444500	4.24641300
C	-2.69748400	2.30364700	4.00711300
C	-1.54414900	1.50882000	3.87932400
C	-1.66204400	0.11251800	4.02958700
C	-0.30066000	2.28743100	3.63465100
C	0.82603900	1.72709600	2.90117000
O	1.01473200	0.45636300	2.68564400
C	0.54337400	-0.71953000	3.02353500
C	-0.58314300	-0.90887400	3.92441800
O	-0.25040700	3.48042200	3.94608700
O	-0.71596100	-1.99902100	4.48758300
C	1.27623100	-1.83877300	2.41657900
C	1.82309600	2.57841600	2.23764800
C	1.44016300	3.76442100	1.59313000
C	2.38058000	4.50484000	0.88712900
C	3.70613100	4.07617600	0.81265100
C	4.09236400	2.90052800	1.45319600
C	3.15748200	2.15503300	2.16285200
C	2.59659000	-1.66218500	1.97250300
C	3.27383000	-2.69511600	1.33334700
C	2.64335500	-3.91779200	1.10778300
C	1.32889700	-4.09969100	1.53627400
C	0.64891100	-3.07627200	2.18771900
H	1.28971300	0.47978800	0.30845400
H	1.04110100	-2.05442600	-0.45430600
H	0.74562200	-1.27084800	-2.00961000
H	4.17971000	-1.81024000	-1.91617000

H	-2.56077400	0.53804900	-1.09375900
H	-2.81784300	-1.88312900	-1.54226100
H	-1.20921400	-2.21289000	-0.88766200
H	-0.31484500	0.41521200	-2.79116800
H	-2.33987600	-0.02872900	-5.71543700
H	-1.23248600	1.19885300	-5.07098800
H	0.52037700	-0.51015700	-4.67309000
H	-0.59134800	-1.80338400	-5.14065500
H	1.01416200	-1.26649700	-6.90465700
H	1.01275000	0.78377500	-7.96760200
H	-0.24665900	1.35581700	-7.12684100
H	-1.67903200	-0.93165200	-9.42042900
H	-3.00496600	-1.51026400	4.43104800
H	-5.02389900	-0.09283400	4.58633700
H	-4.81564300	2.38030600	4.31318600
H	-2.59248000	3.37725900	3.90061900
H	-1.79054300	-1.17945700	1.51131700
H	0.40633900	4.08999000	1.63183500
H	2.07498900	5.41606700	0.38240800
H	4.43563500	4.65863400	0.25844300
H	5.12403100	2.56606700	1.40834300
H	3.46157800	1.25590800	2.68937000
H	3.09403000	-0.71060400	2.12237100
H	4.29610200	-2.53676100	1.00203300
H	3.16996900	-4.72037700	0.60113900
H	0.82411500	-5.04433700	1.35907900
H	-0.37379600	-3.23416100	2.50927500

1b-TS4

Charge 0 *Multiplicity* 1

O	-0.43212000	1.22909800	-2.47583200
C	0.41166000	1.08582700	-1.59291300
N	0.62467400	2.03137300	-0.65219000
C	1.69189400	2.11136300	0.32413800
C	1.27740900	2.97329600	1.49169800
O	2.26474400	3.06507500	2.37756200
O	0.20508500	3.52199500	1.60639700
C	1.13495700	-0.25810500	-1.49437700
C	0.57770400	-1.05070000	-0.29500900
S	-1.13706900	-1.59943600	-0.58064100
N	2.57657500	-0.12351100	-1.39092700
C	3.37973800	-1.19472900	-1.62827300
C	4.86474200	-0.90916700	-1.63809500
C	5.35091700	-0.26238500	-0.33504500

C	6.86815900	-0.06877500	-0.31308400
N	7.31108200	0.79704600	-1.39658700
C	7.57046300	-1.42208700	-0.23697100
O	8.77355800	-1.41967200	-0.81349500
O	7.11199200	-2.40038900	0.31818100
O	2.91113000	-2.31804800	-1.80454700
C	-4.73198500	-3.54505200	0.26644600
C	-5.53143600	-4.06120100	-0.73913700
C	-5.79245300	-3.27778500	-1.86034000
C	-5.26480800	-1.99787100	-1.95079000
C	-4.44803000	-1.44765200	-0.95138600
C	-4.17872200	-2.25745400	0.17529600
C	-4.04317300	-0.00607100	-1.22680400
C	-3.13782800	0.73527800	-0.42578400
O	-2.67136200	0.32554800	0.82325900
C	-2.19776600	-0.86998000	1.16977600
C	-3.29697500	-1.92325700	1.32181300
O	-4.51238000	0.50731700	-2.27158600
O	-3.41199900	-2.47185400	2.39877900
C	-1.17937800	-0.78509600	2.25426600
C	-2.99348400	2.19878900	-0.55402600
C	-2.96323200	2.84565000	-1.80277700
C	-2.82298000	4.22708200	-1.88586000
C	-2.71054400	5.00453600	-0.73384000
C	-2.73952000	4.37728400	0.50883500
C	-2.87739000	2.99482500	0.59837700
C	-0.70514700	0.46688500	2.65854400
C	0.31319900	0.55102700	3.60574400
C	0.87760800	-0.60832900	4.13170100
C	0.41974800	-1.85750500	3.71220600
C	-0.60539200	-1.95060500	2.77935900
H	0.06083500	2.87091400	-0.76817200
H	1.95798200	1.13007300	0.72437600
H	2.60560000	2.55525600	-0.09247700
H	1.98369000	3.64161600	3.11032000
H	0.89141600	-0.79128500	-2.41840500
H	1.14772200	-1.97291700	-0.17301400
H	0.61939700	-0.47599400	0.63267400
H	2.99399200	0.79784700	-1.44435500
H	5.36532600	-1.86598400	-1.80964800
H	5.07776500	-0.25023100	-2.48811800
H	4.89427400	0.72345900	-0.20555900
H	5.05691800	-0.88233500	0.51678900
H	7.12408800	0.42259000	0.63466900

H	8.28929800	1.03575200	-1.25301000
H	7.28521300	0.28071100	-2.27408900
H	9.17656800	-2.29776900	-0.69299900
H	-4.50413800	-4.14059800	1.14365900
H	-5.93916000	-5.06279300	-0.65170100
H	-6.41016200	-3.66173800	-2.66632600
H	-5.48591400	-1.38297000	-2.81345400
H	-1.74583900	-0.43267100	-1.11366200
H	-3.02783700	2.25840400	-2.70828400
H	-2.79426500	4.69811300	-2.86438000
H	-2.60159400	6.08235600	-0.80512800
H	-2.65583700	4.96313300	1.41979700
H	-2.91583800	2.52875000	1.57771700
H	-1.12167400	1.37000200	2.22629900
H	0.66811100	1.52561300	3.92693100
H	1.67666800	-0.54095700	4.86343500
H	0.86409800	-2.76337600	4.11164400
H	-0.94682900	-2.92714100	2.45080000

GSH-P

Charge 0 *Multiplicity* 1

O	-0.31948000	0.80090800	-2.77944600
C	0.42957600	0.77246100	-1.80159500
N	0.45634500	1.78940800	-0.91578600
C	1.36032300	2.03735400	0.18681800
C	0.72066200	3.02839500	1.13106200
O	1.47757500	3.22205600	2.20482300
O	-0.33128700	3.59123400	0.92374000
C	1.27331900	-0.47642600	-1.55540400
C	0.77427500	-1.28235600	-0.34314800
S	-0.96249300	-1.82139600	-0.53077700
N	2.68714900	-0.16429500	-1.41429000
C	3.62501200	-1.11802800	-1.63458000
C	5.06218700	-0.65526200	-1.54812000
C	5.42084900	-0.14835100	-0.14543100
C	6.89627600	0.24263600	-0.03212300
N	7.23758500	1.30873100	-0.96191000
C	7.77112700	-1.00576100	-0.12147800
O	8.93370000	-0.79230300	-0.73864700
O	7.46493000	-2.08464400	0.34567800
O	3.31267300	-2.28593700	-1.86885600
C	-4.35096300	-3.69658600	0.02585700
C	-5.22069900	-4.16887800	-0.94820200
C	-5.74706100	-3.28582600	-1.88708500

C	-5.40183800	-1.94184700	-1.83811600
C	-4.49772900	-1.45523800	-0.88583200
C	-3.96258600	-2.35214300	0.05735300
C	-4.26581200	0.02957900	-0.95007900
C	-2.91109300	0.65116300	-0.58656600
O	-2.41248000	0.22974000	0.67093500
C	-1.85075500	-1.04015500	0.90622500
C	-3.02076600	-2.01376200	1.17645600
O	-5.13592800	0.73955600	-1.41683100
O	-3.16282300	-2.53842800	2.25962800
C	-0.94114100	-0.90441400	2.11343200
C	-3.00802600	2.15800700	-0.52940300
C	-2.64741800	2.92662900	-1.63532700
C	-2.73799400	4.31715000	-1.58014000
C	-3.20627800	4.94090300	-0.42601200
C	-3.58920700	4.17156300	0.67229200
C	-3.49474000	2.78381000	0.62078800
C	-0.63958900	0.35315300	2.63584800
C	0.23817100	0.47062900	3.71574300
C	0.81818700	-0.66242300	4.27551400
C	0.51965500	-1.92099000	3.75192500
C	-0.35139200	-2.04269100	2.67660500
H	-0.15115700	2.56977100	-1.15553800
H	1.59138800	1.13438200	0.75655900
H	2.30994100	2.48226300	-0.13957300
H	1.05589800	3.88530000	2.78040600
H	1.14577400	-1.08514000	-2.45525400
H	1.38452400	-2.18338300	-0.25933700
H	0.87598200	-0.71777100	0.58361400
H	2.99315000	0.79764700	-1.33842500
H	5.68424300	-1.51186900	-1.82271300
H	5.21777900	0.14032300	-2.28583400
H	4.82393900	0.73506900	0.10023400
H	5.19743900	-0.92202200	0.59474900
H	7.06129900	0.61794800	0.98586600
H	8.17103300	1.65064100	-0.74673500
H	7.30051800	0.92875200	-1.90464400
H	9.44668600	-1.61987100	-0.72921900
H	-3.94818300	-4.37148200	0.77420800
H	-5.48965700	-5.21992800	-0.96965700
H	-6.43167700	-3.63982300	-2.65104300
H	-5.82907900	-1.24297500	-2.54884900
H	-2.22689100	0.34983400	-1.39371100
H	-2.27190500	2.43641200	-2.52961600

H	-2.44123900	4.91066500	-2.43950900
H	-3.27459000	6.02365400	-0.38140300
H	-3.96041600	4.65398900	1.57149700
H	-3.79003100	2.18287000	1.47623600
H	-1.08879200	1.23969100	2.20023600
H	0.46606100	1.45457400	4.11350500
H	1.50244400	-0.56939500	5.11317800
H	0.97038300	-2.81090700	4.18009400
H	-0.56475400	-3.02501200	2.26517600

3b

Charge 0 *Multiplicity* 1

C	-4.29520000	1.39790000	-0.03800000
C	-5.49630000	0.69760000	0.01220000
C	-5.49630000	-0.69770000	0.01220000
C	-4.29510000	-1.39790000	-0.03810000
C	-3.08810000	0.70160000	-0.06470000
C	-3.08810000	-0.70160000	-0.06470000
C	-1.81400000	1.46300000	-0.15780000
C	-1.81400000	-1.46300000	-0.15780000
O	-1.77570000	2.61240000	-0.54950000
O	-1.77560000	-2.61240000	-0.54960000
C	-0.55140000	0.75390000	0.29010000
C	-0.55140000	-0.75390000	0.29000000
O	-0.75010000	0.00000000	1.47590000
C	0.73570000	1.49630000	0.16110000
C	1.52670000	1.74610000	1.27840000
C	2.73600000	2.42520000	1.13720000
C	3.17520000	2.86050000	-0.11420000
C	2.36930000	2.59900000	-1.23020000
C	1.16230000	1.92550000	-1.09930000
C	0.73570000	-1.49630000	0.16100000
C	1.52660000	-1.74630000	1.27840000
C	2.73590000	-2.42550000	1.13720000
C	1.16240000	-1.92530000	-1.09940000
C	2.36940000	-2.59880000	-1.23030000
C	3.17510000	-2.86050000	-0.11420000
H	-4.28120000	2.48300000	-0.05260000
H	-6.43560000	1.24000000	0.04660000
H	-6.43560000	-1.24020000	0.04650000
H	-4.28110000	-2.48310000	-0.05270000
H	1.19690000	1.40980000	2.25680000
H	3.34680000	2.62020000	2.01480000
H	2.69770000	2.92790000	-2.21310000

H	0.54970000	1.72540000	-1.97480000
H	1.19670000	-1.41010000	2.25690000
H	3.34660000	-2.62060000	2.01480000
H	0.54990000	-1.72500000	-1.97490000
H	2.69790000	-2.92750000	-2.21320000
C	4.48340000	3.58800000	-0.27610000
H	5.16510000	3.02350000	-0.92060000
H	4.33170000	4.56620000	-0.74330000
H	4.97330000	3.74100000	0.68820000
C	4.48340000	-3.58810000	-0.27620000
H	4.33160000	-4.56630000	-0.74330000
H	5.16510000	-3.02360000	-0.92070000
H	4.97330000	-3.74100000	0.68810000

3b-S_1

Charge 0 *Multiplicity* 1

C	-4.25050000	1.41730000	-0.18430000
C	-5.44700000	0.72590000	-0.23000000
C	-5.47110000	-0.67500000	-0.16470000
C	-4.28130000	-1.37540000	-0.06340000
C	-3.03580000	0.70990000	-0.06430000
C	-3.05390000	-0.70200000	-0.00870000
C	-1.78290000	1.42200000	-0.02950000
C	-1.81510000	-1.49670000	0.02100000
O	-1.70770000	2.68200000	-0.22720000
O	-1.79890000	-2.69300000	-0.23030000
C	-0.51340000	0.71890000	0.39920000
C	-0.52660000	-0.79070000	0.38670000
O	-0.63900000	-0.02300000	1.59150000
C	0.74910000	1.50010000	0.20440000
C	1.65250000	1.66840000	1.24900000
C	2.81940000	2.40380000	1.04450000
C	3.10340000	2.97730000	-0.19580000
C	2.18400000	2.79670000	-1.23770000
C	1.01890000	2.06660000	-1.04560000
C	0.74320000	-1.54450000	0.19060000
C	1.66660000	-1.67190000	1.22640000
C	2.85480000	-2.36970000	1.02000000
C	1.02370000	-2.11670000	-1.05570000
C	2.21190000	-2.80540000	-1.25290000
C	3.14680000	-2.94530000	-0.21780000
H	-4.23120000	2.50160000	-0.23210000
H	-6.37780000	1.27850000	-0.31660000
H	-6.41600000	-1.20660000	-0.19820000

H	-4.27280000	-2.46050000	-0.02420000
H	1.43990000	1.23640000	2.22180000
H	3.51730000	2.53740000	1.86670000
H	2.38850000	3.23230000	-2.21250000
H	0.31880000	1.93070000	-1.86600000
H	1.45220000	-1.23210000	2.19540000
H	3.56640000	-2.46790000	1.83550000
H	0.30950000	-2.01880000	-1.86870000
H	2.42220000	-3.24510000	-2.22480000
C	4.36010000	3.77510000	-0.42020000
H	4.96110000	3.33830000	-1.22400000
H	4.12250000	4.80250000	-0.71410000
H	4.97210000	3.81190000	0.48390000
C	4.42850000	-3.70050000	-0.44710000
H	4.22380000	-4.73480000	-0.74160000
H	5.01230000	-3.24410000	-1.25280000
H	5.04470000	-3.71810000	0.45460000

3b-TS1-S_1

Charge 0 *Multiplicity* 1

C	-4.27600000	1.39690000	-0.13940000
C	-5.46000000	0.70760000	-0.23700000
C	-5.45990000	-0.70790000	-0.23710000
C	-4.27590000	-1.39710000	-0.13960000
C	-3.04070000	0.71120000	-0.02560000
C	-3.04070000	-0.71130000	-0.02570000
C	-1.83670000	1.49770000	0.01620000
C	-1.83650000	-1.49770000	0.01590000
O	-1.80090000	2.72510000	-0.20800000
O	-1.80060000	-2.72510000	-0.20850000
C	-0.54250000	0.85490000	0.45560000
C	-0.54240000	-0.85490000	0.45550000
O	-0.60390000	0.00000000	1.56260000
C	0.71480000	1.56030000	0.24100000
C	1.70000000	1.60200000	1.23830000
C	2.89940000	2.25770000	1.00330000
C	3.15640000	2.86830000	-0.23070000
C	2.16620000	2.81740000	-1.22740000
C	0.95900000	2.18710000	-0.99770000
C	0.71490000	-1.56030000	0.24100000
C	1.69990000	-1.60220000	1.23850000
C	2.89930000	-2.25790000	1.00350000
C	0.95930000	-2.18670000	-0.99790000
C	2.16650000	-2.81710000	-1.22750000

C	3.15660000	-2.86820000	-0.23060000
H	-4.26260000	2.48160000	-0.14270000
H	-6.39830000	1.24720000	-0.31660000
H	-6.39820000	-1.24760000	-0.31680000
H	-4.26240000	-2.48190000	-0.14320000
H	1.50880000	1.14080000	2.20120000
H	3.65180000	2.30090000	1.78550000
H	2.35590000	3.28560000	-2.18930000
H	0.19890000	2.15990000	-1.77210000
H	1.50860000	-1.14130000	2.20140000
H	3.65160000	-2.30130000	1.78580000
H	0.19940000	-2.15940000	-1.77240000
H	2.35640000	-3.28500000	-2.18950000
C	4.45780000	3.56520000	-0.49840000
H	4.99190000	3.07460000	-1.31920000
H	4.28340000	4.60220000	-0.80360000
H	5.10080000	3.56360000	0.38380000
C	4.45800000	-3.56510000	-0.49820000
H	4.28350000	-4.60210000	-0.80330000
H	4.99210000	-3.07470000	-1.31910000
H	5.10090000	-3.56350000	0.38400000

3SDR

Charge 0 *Multiplicity* 1

C	1.33060000	3.25990000	-2.48780000
C	1.57080000	3.36240000	-3.84580000
C	1.72860000	2.20160000	-4.60540000
C	1.63760000	0.96530000	-3.99190000
C	1.26350000	2.01240000	-1.84270000
C	1.41350000	0.83970000	-2.60920000
C	1.00940000	2.11600000	-0.37770000
C	1.32300000	-0.57900000	-2.14620000
O	0.46680000	3.12960000	0.07680000
O	1.08120000	-1.46290000	-2.97850000
C	1.49960000	1.11570000	0.55160000
C	1.65540000	-0.96940000	-0.79180000
O	1.79150000	-0.11990000	0.20920000
C	1.67220000	1.35670000	1.98370000
C	1.64170000	0.26850000	2.87500000
C	1.83760000	0.46300000	4.23390000
C	2.07620000	1.74010000	4.75520000
C	2.10860000	2.81870000	3.86530000
C	1.91140000	2.64040000	2.50270000
C	1.99430000	-2.33830000	-0.38930000

C	1.43590000	-3.47670000	-0.99640000
C	1.77460000	-4.74660000	-0.54670000
C	2.89560000	-2.52610000	0.67500000
C	3.22660000	-3.80160000	1.10910000
C	2.67180000	-4.93680000	0.50890000
H	1.19920000	4.15330000	-1.88800000
H	1.63880000	4.33980000	-4.31250000
H	1.92100000	2.26350000	-5.67170000
H	1.74310000	0.05880000	-4.57630000
H	1.44400000	-0.72960000	2.49620000
H	1.79700000	-0.38970000	4.90660000
H	2.29600000	3.81850000	4.24800000
H	1.95300000	3.49500000	1.83860000
H	0.72380000	-3.36540000	-1.80220000
H	1.32350000	-5.61310000	-1.02390000
H	3.35360000	-1.66300000	1.14830000
H	3.93710000	-3.91990000	1.92300000
C	2.31380000	1.93920000	6.22670000
H	1.67690000	1.27990000	6.82260000
H	3.35400000	1.70760000	6.48260000
H	2.12070000	2.97310000	6.52270000
C	3.00670000	-6.31870000	0.99900000
H	2.24210000	-6.67480000	1.69870000
H	3.04940000	-7.03180000	0.17140000
H	3.96600000	-6.33180000	1.52220000

3DOXEPY

Charge 0 *Multiplicity* 1

C	1.33530000	3.26380000	-2.49520000
C	1.56820000	3.36320000	-3.85320000
C	1.71410000	2.19940000	-4.61280000
C	1.61910000	0.96570000	-3.99790000
C	1.26400000	2.01690000	-1.84530000
C	1.40260000	0.84000000	-2.61220000
C	1.01740000	2.13350000	-0.38210000
C	1.31060000	-0.57940000	-2.15630000
O	0.50230000	3.15700000	0.07460000
O	1.07770000	-1.46230000	-2.98990000
C	1.48840000	1.11550000	0.54680000
C	1.63590000	-0.96590000	-0.79670000
O	1.73850000	-0.11220000	0.19250000
C	1.66700000	1.34690000	1.98140000
C	1.60130000	0.25850000	2.86950000
C	1.80640000	0.44370000	4.22900000

C	2.08690000	1.71080000	4.75260000
C	2.15190000	2.78980000	3.86490000
C	1.94640000	2.62090000	2.50220000
C	1.98800000	-2.32990000	-0.38560000
C	1.45370000	-3.47690000	-0.99700000
C	1.80350000	-4.74130000	-0.53920000
C	2.87820000	-2.50300000	0.69010000
C	3.21800000	-3.77300000	1.13440000
C	2.68690000	-4.91710000	0.53010000
H	1.21450000	4.15850000	-1.89550000
H	1.64080000	4.33960000	-4.32150000
H	1.90130000	2.25900000	-5.68010000
H	1.71620000	0.05820000	-4.58180000
H	1.36870000	-0.73160000	2.48890000
H	1.73900000	-0.40870000	4.90010000
H	2.37100000	3.78260000	4.24930000
H	2.01190000	3.47550000	1.83980000
H	0.75270000	-3.37750000	-1.81420000
H	1.37160000	-5.61500000	-1.02110000
H	3.32060000	-1.63220000	1.16490000
H	3.91860000	-3.87930000	1.95860000
C	3.03350000	-6.29310000	1.02940000
H	2.27440000	-6.65010000	1.73470000
H	3.07950000	-7.01200000	0.20710000
H	3.99460000	-6.29510000	1.54970000
C	2.33340000	1.89980000	6.22410000
H	1.69950000	1.23750000	6.81960000
H	3.37510000	1.66680000	6.47250000
H	2.14300000	2.93210000	6.52790000

3TDR

Charge 0 *Multiplicity* 3

C	1.45080000	3.27720000	-2.55090000
C	1.68930000	3.35880000	-3.91640000
C	1.81870000	2.19150000	-4.66810000
C	1.70740000	0.95480000	-4.04680000
C	1.37690000	2.03630000	-1.90990000
C	1.50330000	0.86220000	-2.66550000
C	1.07070000	2.08040000	-0.44480000
C	1.35720000	-0.52400000	-2.11920000
O	0.30300000	2.95470000	-0.01760000
O	0.87840000	-1.41010000	-2.84010000
C	1.73290000	1.16720000	0.45600000
C	1.88410000	-0.84280000	-0.81110000

O	2.49240000	0.15050000	-0.07640000
C	1.76840000	1.29400000	1.89240000
C	2.12430000	0.17760000	2.68070000
C	2.17460000	0.27120000	4.05960000
C	1.89130000	1.47780000	4.71550000
C	1.55610000	2.58970000	3.93470000
C	1.49100000	2.51110000	2.55210000
C	2.05230000	-2.18510000	-0.30030000
C	1.17010000	-3.23470000	-0.63430000
C	1.37700000	-4.50590000	-0.12570000
C	3.14000000	-2.46790000	0.55040000
C	3.33970000	-3.75020000	1.03880000
C	2.46340000	-4.79110000	0.71360000
H	1.32360000	4.17860000	-1.95980000
H	1.76800000	4.32990000	-4.39480000
H	1.99810000	2.24560000	-5.73710000
H	1.77950000	0.03920000	-4.62470000
H	2.33560000	-0.76930000	2.19890000
H	2.43840000	-0.60540000	4.64550000
H	1.35250000	3.53930000	4.42210000
H	1.24900000	3.39490000	1.97740000
H	0.31450000	-3.03750000	-1.26680000
H	0.67830000	-5.29990000	-0.37710000
H	3.84130000	-1.67860000	0.80120000
H	4.19290000	-3.95150000	1.68060000
C	1.94220000	1.56130000	6.21440000
H	1.11490000	0.99650000	6.65840000
H	2.87110000	1.12940000	6.59860000
H	1.86950000	2.59550000	6.55750000
C	2.66630000	-6.18100000	1.24780000
H	1.80600000	-6.49240000	1.84930000
H	2.76450000	-6.90070000	0.42880000
H	3.56180000	-6.24070000	1.87010000

3b-IM1

Charge 0 *Multiplicity* 1

O	-1.23470000	0.01670000	-0.76270000
O	0.56050000	-3.00070000	-0.79160000
O	1.10230000	2.61350000	-1.11840000
O	5.58470000	0.66850000	0.09060000
C	-0.96390000	-1.26080000	-0.71750000
C	0.34720000	-1.80540000	-1.02580000
C	1.42210000	-1.00640000	-1.69420000
C	2.42570000	-1.81570000	-2.26450000

C	3.54250000	-1.28120000	-2.87780000
C	3.70160000	0.10610000	-2.92960000
C	2.72890000	0.91930000	-2.38120000
C	1.57320000	0.39600000	-1.76700000
C	0.67830000	1.45480000	-1.21660000
C	-0.69670000	1.20120000	-0.82990000
C	0.47030000	0.63800000	1.92480000
C	0.36540000	-0.56920000	2.00590000
C	0.86740000	-1.93560000	2.19430000
C	2.34950000	-1.88400000	1.75270000
C	3.20780000	-0.93290000	2.57540000
C	3.33580000	0.58110000	2.48430000
C	2.64920000	1.54860000	1.53300000
C	1.20050000	1.91110000	1.93900000
C	4.47300000	-0.30870000	2.03040000
C	4.78800000	-0.41760000	0.55670000
C	-2.16060000	-2.06220000	-0.42560000
C	-3.42650000	-1.46730000	-0.61430000
C	-4.59070000	-2.16270000	-0.33310000
C	-4.55330000	-3.47830000	0.14680000
C	-3.30170000	-4.06730000	0.32890000
C	-2.12160000	-3.38430000	0.04890000
C	-1.64070000	2.26340000	-0.46390000
C	-2.64760000	1.97610000	0.47360000
C	-3.58100000	2.94170000	0.82470000
C	-3.54600000	4.21940000	0.25660000
C	-2.53850000	4.50080000	-0.67320000
C	-1.59630000	3.54650000	-1.03170000
H	5.07040000	1.47850000	0.21090000
H	2.30440000	-2.89040000	-2.20580000
H	4.28910000	-1.93990000	-3.30980000
H	4.57610000	0.54600000	-3.39790000
H	2.84030000	1.99630000	-2.41400000
H	0.32330000	-2.68200000	1.60830000
H	0.78630000	-2.22130000	3.24950000
H	2.77870000	-2.89050000	1.83580000
H	2.37220000	-1.61740000	0.69370000
H	3.30460000	-1.27890000	3.60360000
H	3.49600000	1.02940000	3.46390000
H	2.62580000	1.14110000	0.51860000
H	3.24280000	2.47190000	1.49320000
H	1.18040000	2.34100000	2.94710000
H	0.78750000	2.65650000	1.25360000
H	5.35790000	-0.34070000	2.66210000

H	5.37300000	-1.32290000	0.36160000
H	3.87110000	-0.49100000	-0.04070000
H	-3.49300000	-0.45620000	-1.00270000
H	-5.55140000	-1.68080000	-0.49710000
H	-3.24210000	-5.08620000	0.70240000
H	-1.17490000	-3.87900000	0.20700000
H	-2.67580000	0.99580000	0.94170000
H	-4.34490000	2.70550000	1.56110000
H	-2.49380000	5.48740000	-1.12720000
H	-0.83430000	3.78880000	-1.76230000
C	-5.82610000	-4.21880000	0.45240000
H	-6.36840000	-3.73650000	1.27250000
H	-6.49240000	-4.22500000	-0.41600000
H	-5.62370000	-5.25330000	0.73880000
C	-4.57550000	5.25490000	0.61680000
H	-4.15820000	6.26360000	0.56130000
H	-5.42300000	5.21100000	-0.07690000
H	-4.96590000	5.09170000	1.62440000

3b-TS2

Charge 0 *Multiplicity* 1

O	1.25260000	0.03980000	0.81520000
O	-0.58640000	-2.97080000	0.82000000
O	-1.12240000	2.63580000	1.04420000
O	-5.61110000	0.67110000	-0.26830000
C	0.93280000	-1.22770000	0.66760000
C	-0.36980000	-1.77070000	1.02510000
C	-1.44110000	-0.96480000	1.69680000
C	-2.43470000	-1.76410000	2.29380000
C	-3.54880000	-1.21840000	2.90520000
C	-3.70850000	0.16810000	2.93240000
C	-2.73990000	0.97200000	2.36030000
C	-1.59390000	0.43590000	1.74270000
C	-0.70070000	1.47850000	1.15650000
C	0.66490000	1.20950000	0.73370000
C	-0.42230000	0.59540000	-1.50620000
C	-0.31600000	-0.62560000	-1.57310000
C	-0.80610000	-1.94090000	-2.01510000
C	-2.32500000	-1.94350000	-1.73880000
C	-3.11250000	-0.96630000	-2.59960000
C	-3.23970000	0.55040000	-2.53660000
C	-2.62830000	1.56350000	-1.58140000
C	-1.13120000	1.84350000	-1.83590000
C	-4.40200000	-0.33080000	-2.13320000

C	-4.77980000	-0.41310000	-0.67240000
C	2.12400000	-2.05470000	0.40000000
C	3.39920000	-1.47520000	0.56400000
C	4.55320000	-2.19670000	0.30070000
C	4.49640000	-3.52330000	-0.14140000
C	3.23480000	-4.09900000	-0.29910000
C	2.06670000	-3.39150000	-0.03380000
C	1.62100000	2.27870000	0.40070000
C	2.65230000	1.98310000	-0.50660000
C	3.60260000	2.93980000	-0.83370000
C	3.55960000	4.21970000	-0.26950000
C	2.52900000	4.50960000	0.63070000
C	1.57010000	3.56170000	0.96500000
H	-5.10600000	1.48650000	-0.39150000
H	-2.31260000	-2.83950000	2.25610000
H	-4.29150000	-1.86950000	3.35530000
H	-4.57850000	0.61650000	3.40110000
H	-2.85120000	2.04940000	2.37420000
H	-0.32630000	-2.77770000	-1.50140000
H	-0.60820000	-2.05450000	-3.08750000
H	-2.71550000	-2.94930000	-1.93820000
H	-2.47580000	-1.75730000	-0.67270000
H	-3.15190000	-1.30900000	-3.63240000
H	-3.34070000	0.97020000	-3.53620000
H	-2.74690000	1.25460000	-0.53840000
H	-3.18150000	2.50500000	-1.69570000
H	-0.96120000	2.08050000	-2.89250000
H	-0.79780000	2.70100000	-1.24590000
H	-5.25800000	-0.37110000	-2.80310000
H	-5.35970000	-1.32270000	-0.48180000
H	-3.88790000	-0.45940000	-0.03420000
H	3.48570000	-0.45520000	0.92250000
H	5.52050000	-1.72360000	0.44960000
H	3.15830000	-5.12930000	-0.63730000
H	1.11440000	-3.88220000	-0.16520000
H	2.68640000	1.00010000	-0.96930000
H	4.38610000	2.69620000	-1.54660000
H	2.47790000	5.49760000	1.08110000
H	0.79060000	3.81240000	1.67360000
C	5.75130000	-4.29140000	-0.45350000
H	6.07330000	-4.10160000	-1.48380000
H	6.57140000	-3.99380000	0.20540000
H	5.59250000	-5.36780000	-0.34980000
C	4.60590000	5.24710000	-0.60410000

H	4.20070000	6.26010000	-0.53960000
H	5.44500000	5.18240000	0.09800000
H	5.00560000	5.09230000	-1.60950000

3DEBCOD

Charge 0 *Multiplicity* 1

O	-1.05480000	0.08670000	-1.00840000
O	0.36480000	-2.68930000	-2.01880000
O	1.01060000	2.87920000	-0.89970000
O	5.38540000	0.84900000	0.54850000
C	-0.62660000	-1.15140000	-0.45020000
C	0.43870000	-1.61280000	-1.46570000
C	1.58700000	-0.67580000	-1.81410000
C	2.66850000	-1.36170000	-2.38290000
C	3.84080000	-0.72050000	-2.76480000
C	3.95220000	0.65280000	-2.59160000
C	2.89000000	1.35430000	-2.03570000
C	1.70390000	0.72800000	-1.62970000
C	0.72950000	1.69860000	-0.98370000
C	-0.51740000	1.17640000	-0.26840000
C	0.02970000	0.55120000	1.00560000
C	-0.00870000	-0.77760000	0.89240000
C	0.56120000	-1.79230000	1.83560000
C	2.08680000	-1.95890000	1.63800000
C	2.90790000	-1.14250000	2.62280000
C	2.96360000	0.36220000	2.75080000
C	2.24150000	1.39200000	1.90100000
C	0.70010000	1.38630000	2.05730000
C	4.17230000	-0.40430000	2.25280000
C	4.57920000	-0.29730000	0.80390000
C	-1.80830000	-2.09530000	-0.31160000
C	-3.10100000	-1.56450000	-0.26900000
C	-4.19990000	-2.39290000	-0.07210000
C	-4.04510000	-3.77220000	0.09900000
C	-2.75070000	-4.29400000	0.06700000
C	-1.64390000	-3.47200000	-0.13480000
C	-1.60400000	2.21700000	-0.09410000
C	-2.38590000	2.23190000	1.06080000
C	-3.45540000	3.11760000	1.17910000
C	-3.77480000	4.00120000	0.14710000
C	-2.99580000	3.96800000	-1.01640000
C	-1.92620000	3.09010000	-1.13800000
H	4.87510000	1.62960000	0.80540000
H	2.57870000	-2.43360000	-2.51770000

H	4.65670000	-1.29510000	-3.19150000
H	4.85710000	1.17930000	-2.87730000
H	2.97380000	2.42540000	-1.89170000
H	0.05590000	-2.75030000	1.68910000
H	0.35940000	-1.48220000	2.86730000
H	2.35320000	-3.01110000	1.78560000
H	2.34560000	-1.72740000	0.60080000
H	2.95440000	-1.63110000	3.59410000
H	3.03800000	0.67980000	3.78890000
H	2.50410000	1.27970000	0.84530000
H	2.61720000	2.37780000	2.19910000
H	0.43510000	1.01640000	3.05460000
H	0.32140000	2.41090000	1.98460000
H	5.01560000	-0.49110000	2.93390000
H	5.18830000	-1.16160000	0.51790000
H	3.69920000	-0.29070000	0.14990000
H	-3.24560000	-0.49620000	-0.39410000
H	-5.19780000	-1.96120000	-0.04810000
H	-2.60200000	-5.36270000	0.19900000
H	-0.65310000	-3.91240000	-0.16200000
H	-2.16690000	1.54390000	1.87390000
H	-4.05230000	3.11810000	2.08730000
H	-3.23460000	4.63940000	-1.83760000
H	-1.33980000	3.08280000	-2.05240000
C	-5.24260000	-4.65730000	0.32230000
H	-5.72040000	-4.43280000	1.28200000
H	-5.99530000	-4.50460000	-0.45720000
H	-4.95990000	-5.71260000	0.32430000
C	-4.91450000	4.97610000	0.27810000
H	-4.53820000	5.99460000	0.42270000
H	-5.53210000	4.98320000	-0.62480000
H	-5.55050000	4.72840000	1.13120000

3b-TS3

Charge 0 *Multiplicity* 1

C	-3.68810000	1.38940000	-0.00220000
C	-4.86760000	0.70870000	0.26210000
C	-4.87250000	-0.68580000	0.27460000
C	-3.69820000	-1.37950000	0.02140000
C	-2.48900000	0.70050000	-0.22620000
C	-2.49410000	-0.70350000	-0.21460000
C	-1.30810000	1.57040000	-0.52540000
C	-1.32230000	-1.58630000	-0.51420000
O	-1.49250000	2.66710000	-1.07360000

O	-1.52310000	-2.68240000	-1.05700000
C	0.00350000	1.19250000	-0.05450000
C	-0.00170000	-1.21510000	-0.06120000
O	0.16980000	-0.01240000	0.56800000
C	1.15300000	2.07130000	-0.01110000
C	2.13920000	1.88200000	0.97970000
C	3.24440000	2.71340000	1.04340000
C	3.42790000	3.74870000	0.11660000
C	2.45510000	3.92770000	-0.87290000
C	1.33230000	3.11610000	-0.94060000
C	1.15320000	-2.08410000	-0.04740000
C	2.20160000	-1.83270000	0.86450000
C	3.31470000	-2.65320000	0.90690000
C	1.28530000	-3.18090000	-0.92570000
C	2.41710000	-3.98140000	-0.88100000
C	3.44790000	-3.74170000	0.03370000
H	-3.67550000	2.47370000	-0.03490000
H	-5.78120000	1.26220000	0.45390000
H	-5.79000000	-1.22950000	0.47620000
H	-3.69400000	-2.46430000	0.00620000
H	2.00730000	1.10590000	1.72470000
H	3.98100000	2.56400000	1.82840000
H	2.58240000	4.71760000	-1.60810000
H	0.60430000	3.26990000	-1.72520000
H	2.11560000	-1.00980000	1.56330000
H	4.09850000	-2.45320000	1.63280000
H	0.51270000	-3.38490000	-1.65340000
H	2.50460000	-4.81230000	-1.57580000
C	4.64980000	4.62170000	0.17350000
H	5.49760000	4.12480000	-0.31170000
H	4.48260000	5.57200000	-0.33890000
H	4.93960000	4.82600000	1.20780000
C	4.67670000	-4.60580000	0.06940000
H	4.50680000	-5.55910000	-0.43610000
H	5.51230000	-4.10350000	-0.43100000
H	4.98680000	-4.80430000	1.09920000

5b

Charge 0 *Multiplicity* 1

C	4.66800000	-1.39770000	-0.19080000
C	5.87010000	-0.69760000	-0.20790000
C	5.87010000	0.69770000	-0.20790000
C	4.66790000	1.39780000	-0.19080000
C	3.46130000	-0.70160000	-0.14900000

C	3.46130000	0.70160000	-0.14900000
C	2.18390000	-1.46340000	-0.16850000
C	2.18390000	1.46340000	-0.16850000
O	2.12470000	-2.61250000	-0.55860000
O	2.12460000	2.61250000	-0.55860000
C	0.94890000	-0.75510000	0.35110000
C	0.94890000	0.75510000	0.35110000
O	1.21590000	0.00000000	1.52320000
C	-0.34390000	-1.49510000	0.29970000
C	-1.08690000	-1.71340000	1.46210000
C	-2.30310000	-2.37580000	1.40070000
C	-2.79400000	-2.82740000	0.17030000
C	-2.05830000	-2.61360000	-0.99840000
C	-0.83740000	-1.94750000	-0.92240000
C	-0.34400000	1.49500000	0.29970000
C	-1.08690000	1.71330000	1.46220000
C	-2.30310000	2.37570000	1.40070000
C	-0.83740000	1.94740000	-0.92240000
C	-2.05840000	2.61360000	-0.99830000
C	-2.79400000	2.82740000	0.17040000
H	4.65320000	-2.48290000	-0.20500000
H	6.80980000	-1.24020000	-0.22620000
H	6.80970000	1.24040000	-0.22620000
H	4.65310000	2.48300000	-0.20490000
H	-0.70890000	-1.36050000	2.41660000
H	-2.89140000	-2.55550000	2.29500000
H	-2.42130000	-2.95330000	-1.96080000
H	-0.26880000	-1.77460000	-1.83250000
H	-0.70900000	1.36040000	2.41660000
H	-2.89150000	2.55540000	2.29500000
H	-0.26890000	1.77460000	-1.83250000
H	-2.42140000	2.95330000	-1.96080000
O	-3.99550000	-3.46140000	0.21040000
C	-4.53940000	-3.92510000	-1.01840000
H	-3.88170000	-4.66550000	-1.48620000
H	-5.49170000	-4.39260000	-0.76750000
H	-4.71110000	-3.09560000	-1.71260000
O	-3.99560000	3.46130000	0.21040000
C	-4.53920000	3.92540000	-1.01830000
H	-4.71140000	3.09610000	-1.71260000
H	-5.49130000	4.39330000	-0.76740000
H	-3.88120000	4.66550000	-1.48600000

5b-S_1

Charge 0 *Multiplicity* 1

C	4.57240000	-1.45020000	-0.42340000
C	5.76700000	-0.77400000	-0.56590000
C	5.81730000	0.62750000	-0.46800000
C	4.65450000	1.33820000	-0.23740000
C	3.37990000	-0.73280000	-0.17320000
C	3.42480000	0.67890000	-0.08170000
C	2.13960000	-1.44370000	-0.04080000
C	2.21270000	1.48630000	0.09020000
O	2.02430000	-2.69820000	-0.20960000
O	2.19820000	2.70020000	-0.08170000
C	0.89940000	-0.73690000	0.48960000
C	0.94010000	0.78280000	0.50490000
O	1.09940000	-0.01920000	1.68290000
C	-0.38560000	-1.48980000	0.36000000
C	-1.14690000	-1.80800000	1.48630000
C	-2.33650000	-2.50670000	1.34750000
C	-2.77720000	-2.89590000	0.07770000
C	-2.01940000	-2.58190000	-1.05470000
C	-0.82760000	-1.87930000	-0.90230000
C	-0.33450000	1.52950000	0.38400000
C	-1.27450000	1.51910000	1.42400000
C	-2.47500000	2.19120000	1.28870000
C	-0.63330000	2.21670000	-0.79780000
C	-1.83950000	2.88860000	-0.94960000
C	-2.76620000	2.87710000	0.10000000
H	4.53120000	-2.53230000	-0.49830000
H	6.67750000	-1.33430000	-0.75620000
H	6.76310000	1.14690000	-0.57790000
H	4.66650000	2.42180000	-0.16960000
H	-0.80340000	-1.50940000	2.47200000
H	-2.93990000	-2.76550000	2.21180000
H	-2.34480000	-2.87170000	-2.04640000
H	-0.23770000	-1.63140000	-1.78130000
H	-1.05140000	0.98840000	2.34350000
H	-3.20900000	2.20070000	2.08810000
H	0.08140000	2.22300000	-1.61510000
H	-2.04760000	3.40940000	-1.87630000
O	-3.95350000	-3.57400000	0.04220000
C	-4.42030000	-4.02270000	-1.22360000
H	-3.70450000	-4.71000000	-1.68660000
H	-5.35450000	-4.54970000	-1.02900000
H	-4.61170000	-3.18070000	-1.89710000
O	-3.96770000	3.49530000	0.05870000

C	-4.30420000	4.22290000	-1.11770000
H	-4.34060000	3.56380000	-1.99100000
H	-5.29360000	4.64220000	-0.93710000
H	-3.58980000	5.03320000	-1.29420000

5b-TS1-S_1

Charge 0 *Multiplicity* 1

C	4.56040000	-1.48290000	-0.41900000
C	5.75720000	-0.82580000	-0.56520000
C	5.81460000	0.58570000	-0.47070000
C	4.66650000	1.30440000	-0.23920000
C	3.36300000	-0.76250000	-0.16840000
C	3.41900000	0.65600000	-0.07520000
C	2.13950000	-1.49960000	-0.05950000
C	2.24240000	1.47260000	0.10920000
O	2.02770000	-2.72700000	-0.28260000
O	2.23430000	2.70750000	-0.03800000
C	0.89450000	-0.80760000	0.49520000
C	0.96540000	0.79970000	0.54550000
O	1.08120000	-0.06420000	1.66760000
C	-0.39370000	-1.51770000	0.36630000
C	-1.19210000	-1.77380000	1.48740000
C	-2.40330000	-2.42810000	1.34730000
C	-2.83950000	-2.82990000	0.07690000
C	-2.04660000	-2.58180000	-1.05160000
C	-0.82800000	-1.93580000	-0.89460000
C	-0.28890000	1.52840000	0.41410000
C	-1.28010000	1.45850000	1.41750000
C	-2.47150000	2.12470000	1.26490000
C	-0.54820000	2.27500000	-0.75580000
C	-1.74890000	2.93220000	-0.93050000
C	-2.72000000	2.86420000	0.08640000
H	4.50720000	-2.56430000	-0.49170000
H	6.66480000	-1.39030000	-0.75590000
H	6.76550000	1.09620000	-0.58380000
H	4.69170000	2.38720000	-0.16980000
H	-0.85350000	-1.46310000	2.47090000
H	-3.03230000	-2.64150000	2.20530000
H	-2.36840000	-2.88510000	-2.04040000
H	-0.20910000	-1.74370000	-1.76710000
H	-1.08350000	0.89500000	2.32240000
H	-3.23990000	2.10010000	2.03030000
H	0.20350000	2.32430000	-1.53630000
H	-1.93280000	3.48720000	-1.84180000

O	-4.03950000	-3.45170000	0.03740000
O	-3.90860000	3.46560000	0.02670000
C	-4.53610000	-3.86610000	-1.23100000
H	-5.50350000	-4.32830000	-1.03620000
H	-4.66650000	-3.00910000	-1.89990000
H	-3.86630000	-4.59810000	-1.69340000
C	-4.23320000	4.24040000	-1.12990000
H	-4.23790000	3.61170000	-2.02450000
H	-5.23180000	4.63410000	-0.94780000
H	-3.52400000	5.06400000	-1.25040000

5SDR

Charge 0 *Multiplicity* 1

C	1.45500000	3.25650000	-2.54030000
C	1.66770000	3.31370000	-3.90560000
C	1.70720000	2.13000000	-4.64590000
C	1.53000000	0.91680000	-4.00560000
C	1.30210000	2.03050000	-1.86920000
C	1.33550000	0.83670000	-2.61490000
C	1.08120000	2.17380000	-0.40310000
C	1.14590000	-0.55870000	-2.11610000
O	0.60940000	3.22960000	0.04060000
O	0.76260000	-1.42750000	-2.91090000
C	1.52970000	1.16300000	0.53040000
C	1.55220000	-0.95100000	-0.78230000
O	1.77990000	-0.08990000	0.19710000
C	1.72710000	1.41080000	1.95460000
C	1.64840000	0.33510000	2.86350000
C	1.86160000	0.52960000	4.21380000
C	2.16720000	1.80840000	4.70050000
C	2.25740000	2.88690000	3.81490000
C	2.03800000	2.68350000	2.45850000
C	1.87250000	-2.32130000	-0.38480000
C	1.31330000	-3.45610000	-0.99460000
C	1.63620000	-4.73920000	-0.56420000
C	2.77670000	-2.52390000	0.68210000
C	3.10360000	-3.79410000	1.11060000
C	2.53480000	-4.91540000	0.48990000
H	1.41310000	4.16780000	-1.95480000
H	1.80380000	4.27350000	-4.39350000
H	1.87490000	2.15670000	-5.71780000
H	1.54480000	-0.00580000	-4.57400000
H	1.39820000	-0.65690000	2.50050000
H	1.78750000	-0.29300000	4.91780000

H	2.50340000	3.88110000	4.16740000
H	2.12330000	3.52540000	1.78260000
H	0.60110000	-3.34020000	-1.79890000
H	1.17230000	-5.58840000	-1.05150000
H	3.24030000	-1.66890000	1.16330000
H	3.80940000	-3.94660000	1.92070000
O	2.35530000	1.90300000	6.03740000
C	2.66800000	3.18300000	6.57550000
H	1.86230000	3.89820000	6.38080000
H	2.77490000	3.03680000	7.65010000
H	3.60780000	3.56380000	6.16270000
O	2.91610000	-6.11930000	0.97920000
C	2.36940000	-7.28450000	0.37220000
H	2.63010000	-7.33340000	-0.69000000
H	2.81410000	-8.13060000	0.89580000
H	1.28090000	-7.31350000	0.48710000

5DOXEPY

Charge 0 *Multiplicity* 1

C	1.37470000	3.27820000	-2.52940000
C	1.57610000	3.36600000	-3.89280000
C	1.66920000	2.19510000	-4.65060000
C	1.55570000	0.96740000	-4.02780000
C	1.28450000	2.03610000	-1.87140000
C	1.37150000	0.85240000	-2.63590000
C	1.07520000	2.16710000	-0.40450000
C	1.25610000	-0.56180000	-2.17180000
O	0.60120000	3.20910000	0.05780000
O	0.98580000	-1.44350000	-2.99760000
C	1.53670000	1.14100000	0.51880000
C	1.60090000	-0.95070000	-0.81950000
O	1.75000000	-0.09540000	0.16510000
C	1.74830000	1.37520000	1.94560000
C	1.67210000	0.29360000	2.84630000
C	1.90810000	0.47560000	4.19520000
C	2.23200000	1.74750000	4.68700000
C	2.31690000	2.83190000	3.80870000
C	2.07480000	2.64090000	2.45390000
C	1.92490000	-2.32080000	-0.41260000
C	1.35460000	-3.45490000	-1.00900000
C	1.66710000	-4.73680000	-0.56520000
C	2.82790000	-2.51710000	0.65370000
C	3.14330000	-3.78610000	1.09800000
C	2.56420000	-4.90840000	0.49050000

H	1.29530000	4.17800000	-1.93060000
H	1.66470000	4.33810000	-4.36710000
H	1.83030000	2.24520000	-5.72270000
H	1.61220000	0.05550000	-4.61000000
H	1.40700000	-0.69340000	2.47970000
H	1.83720000	-0.35210000	4.89360000
H	2.57510000	3.82170000	4.16480000
H	2.15430000	3.48830000	1.78390000
H	0.64170000	-3.33970000	-1.81360000
H	1.19600000	-5.58770000	-1.04270000
H	3.29760000	-1.65860000	1.12400000
H	3.84780000	-3.93570000	1.90990000
O	2.44070000	1.83050000	6.02230000
C	2.77230000	3.10380000	6.56430000
H	1.97010000	3.82760000	6.38700000
H	2.89420000	2.94940000	7.63620000
H	3.70900000	3.47980000	6.14000000
O	2.93520000	-6.11180000	0.99380000
C	2.36510000	-7.27660000	0.40920000
H	2.61940000	-7.34880000	-0.65340000
H	2.79650000	-8.12210000	0.94480000
H	1.27660000	-7.28400000	0.52910000

5TDR

Charge 0 *Multiplicity* 3

C	2.11510000	3.18960000	-2.88680000
C	1.89350000	3.04420000	-4.24940000
C	1.33170000	1.86380000	-4.73350000
C	1.00870000	0.83970000	-3.85280000
C	1.81960000	2.15480000	-1.99360000
C	1.26270000	0.95910000	-2.48070000
C	1.98030000	2.47000000	-0.53980000
C	0.88340000	-0.24870000	-1.66870000
O	1.88780000	3.64590000	-0.15980000
O	-0.09690000	-0.92250000	-2.01370000
C	2.24780000	1.38990000	0.38110000
C	1.78160000	-0.68830000	-0.62270000
O	2.71910000	0.21780000	-0.18700000
C	2.15580000	1.44230000	1.80590000
C	2.64350000	0.36500000	2.59010000
C	2.55140000	0.38290000	3.96220000
C	1.96050000	1.47770000	4.61710000
C	1.45720000	2.54960000	3.86700000
C	1.55410000	2.52870000	2.48700000

C	1.94550000	-2.03890000	-0.16310000
C	0.95640000	-3.03340000	-0.32660000
C	1.16050000	-4.33010000	0.12000000
C	3.16680000	-2.41520000	0.45280000
C	3.37730000	-3.70420000	0.88640000
C	2.37220000	-4.67430000	0.73110000
H	2.51780000	4.11570000	-2.48950000
H	2.14690000	3.85110000	-4.92960000
H	1.14290000	1.74140000	-5.79540000
H	0.56210000	-0.07790000	-4.22130000
H	3.10740000	-0.48270000	2.10290000
H	2.93150000	-0.43800000	4.56160000
H	0.98150000	3.39390000	4.35090000
H	1.14540000	3.35570000	1.92300000
H	0.01270000	-2.77970000	-0.78940000
H	0.37270000	-5.06260000	-0.00720000
H	3.96080000	-1.68360000	0.55630000
H	4.31590000	-3.99620000	1.34650000
O	1.91770000	1.40520000	5.96030000
C	1.34600000	2.49800000	6.67520000
H	0.29180000	2.62780000	6.41120000
H	1.43030000	2.23880000	7.73010000
H	1.89610000	3.42310000	6.47750000
O	2.66790000	-5.90420000	1.19770000
C	1.68580000	-6.92770000	1.06160000
H	1.45150000	-7.10590000	0.00750000
H	2.12880000	-7.82380000	1.49480000
H	0.77310000	-6.66810000	1.60720000

5b-IM1

Charge 0 *Multiplicity* 1

O	-0.94250000	0.04430000	-0.81840000
O	0.75540000	-3.02910000	-0.89950000
O	1.48050000	2.57850000	-1.05910000
O	5.86250000	0.46270000	0.19790000
C	-0.71240000	-1.24260000	-0.80230000
C	0.58610000	-1.81970000	-1.10070000
C	1.69980000	-1.03660000	-1.72050000
C	2.69210000	-1.86150000	-2.28990000
C	3.83830000	-1.34650000	-2.86330000
C	4.04110000	0.03640000	-2.87380000
C	3.08160000	0.86460000	-2.32530000
C	1.89510000	0.36250000	-1.75210000
C	1.02190000	1.43510000	-1.19410000

C	-0.36500000	1.21450000	-0.83870000
C	0.71420000	0.53240000	1.93580000
C	0.56990000	-0.67240000	1.98040000
C	1.02610000	-2.05970000	2.12820000
C	2.51650000	-2.03850000	1.71270000
C	3.38860000	-1.14310000	2.58200000
C	3.56550000	0.36780000	2.54040000
C	2.92760000	1.38220000	1.60380000
C	1.48400000	1.78050000	1.99440000
C	4.68400000	-0.54340000	2.08220000
C	5.02810000	-0.61580000	0.61300000
C	-1.93530000	-2.01320000	-0.55000000
C	-3.18230000	-1.37150000	-0.72860000
C	-4.36950000	-2.02800000	-0.47640000
C	-4.36040000	-3.35790000	-0.03390000
C	-3.14240000	-4.01550000	0.14200000
C	-1.94750000	-3.34900000	-0.11680000
C	-1.27920000	2.29230000	-0.45430000
C	-2.31330000	2.01000000	0.46090000
C	-3.22250000	2.98400000	0.82560000
C	-3.12520000	4.27320000	0.28390000
C	-2.10510000	4.57270000	-0.62390000
C	-1.19250000	3.58730000	-0.98270000
H	5.36960000	1.28260000	0.34010000
H	2.53640000	-2.93290000	-2.26270000
H	4.57440000	-2.01650000	-3.29600000
H	4.93960000	0.46070000	-3.31010000
H	3.22680000	1.93800000	-2.32580000
H	0.46940000	-2.76580000	1.50510000
H	0.91750000	-2.38130000	3.17050000
H	2.91380000	-3.06010000	1.76670000
H	2.56460000	-1.73580000	0.66440000
H	3.45330000	-1.52400000	3.60030000
H	3.71930000	0.78270000	3.53560000
H	2.90850000	1.00180000	0.57900000
H	3.55050000	2.28670000	1.59830000
H	1.45970000	2.18690000	3.01220000
H	1.10740000	2.55530000	1.32070000
H	5.55320000	-0.62250000	2.73150000
H	5.59410000	-1.52970000	0.40230000
H	4.12350000	-0.64670000	-0.00570000
H	-3.21500000	-0.34780000	-1.08660000
H	-5.32410000	-1.53320000	-0.62450000
H	-3.10410000	-5.04260000	0.48480000

H	-1.01890000	-3.87960000	0.03150000
H	-2.38230000	1.01810000	0.89890000
H	-4.01400000	2.77610000	1.53850000
H	-2.01540000	5.56060000	-1.05940000
H	-0.41470000	3.82670000	-1.69730000
O	-5.57470000	-3.91570000	0.18900000
O	-4.05890000	5.16080000	0.70280000
C	-5.61220000	-5.27080000	0.62100000
H	-5.11000000	-5.39000000	1.58670000
H	-6.66760000	-5.52200000	0.72610000
H	-5.15020000	-5.93200000	-0.11950000
C	-4.01160000	6.47740000	0.16580000
H	-4.14040000	6.46260000	-0.92140000
H	-4.84020000	7.01650000	0.62460000
H	-3.06810000	6.97200000	0.41940000

5b-TS2

Charge 0 *Multiplicity* 1

O	0.96530000	0.06690000	0.86270000
O	-0.75570000	-3.01320000	0.88170000
O	-1.50850000	2.57750000	1.01320000
O	-5.89600000	0.42860000	-0.34780000
C	0.69790000	-1.21490000	0.72920000
C	-0.58980000	-1.80130000	1.06930000
C	-1.70290000	-1.02590000	1.70670000
C	-2.67770000	-1.85330000	2.29750000
C	-3.81950000	-1.34110000	2.88580000
C	-4.02790000	0.03940000	2.89560000
C	-3.08000000	0.87050000	2.32800000
C	-1.90580000	0.36940000	1.73380000
C	-1.04410000	1.43750000	1.14670000
C	0.33400000	1.21330000	0.74490000
C	-0.69220000	0.51700000	-1.49600000
C	-0.53930000	-0.69990000	-1.54110000
C	-0.97160000	-2.03920000	-1.97000000
C	-2.49360000	-2.09410000	-1.71760000
C	-3.30260000	-1.16090000	-2.60720000
C	-3.48680000	0.35080000	-2.57260000
C	-2.92980000	1.40070000	-1.62380000
C	-1.44010000	1.73260000	-1.85780000
C	-4.62310000	-0.56570000	-2.17430000
C	-5.02470000	-0.63590000	-0.71930000
C	1.92260000	-1.99820000	0.49700000
C	3.17430000	-1.36040000	0.65640000

C	4.35800000	-2.03050000	0.42240000
C	4.34270000	-3.37090000	0.01360000
C	3.12120000	-4.02410000	-0.14750000
C	1.92990000	-3.34450000	0.09680000
C	1.24990000	2.30850000	0.39750000
C	2.30100000	2.03500000	-0.50000000
C	3.21500000	3.01200000	-0.84250000
C	3.10430000	4.29780000	-0.29440000
C	2.06910000	4.58830000	0.59850000
C	1.15210000	3.59780000	0.93480000
H	-5.41270000	1.25750000	-0.47010000
H	-2.51680000	-2.92400000	2.27380000
H	-4.54580000	-2.01330000	3.33140000
H	-4.92030000	0.46170000	3.34620000
H	-3.22960000	1.94340000	2.32740000
H	-0.46970000	-2.84930000	-1.43480000
H	-0.75160000	-2.16230000	-3.03700000
H	-2.84360000	-3.11680000	-1.90610000
H	-2.66750000	-1.89600000	-0.65720000
H	-3.31170000	-1.52170000	-3.63460000
H	-3.58480000	0.75050000	-3.58070000
H	-3.05350000	1.10280000	-0.57810000
H	-3.51640000	2.31870000	-1.76160000
H	-1.26070000	1.95980000	-2.91510000
H	-1.14850000	2.61070000	-1.27590000
H	-5.46400000	-0.64910000	-2.85910000
H	-5.57980000	-1.55970000	-0.52370000
H	-4.14340000	-0.64380000	-0.06560000
H	3.21640000	-0.32850000	0.98650000
H	5.31480000	-1.53660000	0.55870000
H	3.07610000	-5.05940000	-0.46380000
H	1.00040000	-3.87760000	-0.03290000
H	2.37910000	1.04500000	-0.94150000
H	4.01950000	2.81010000	-1.54240000
H	1.97000000	5.57290000	1.03960000
H	0.36200000	3.83180000	1.63730000
O	5.55470000	-3.94160000	-0.19240000
O	4.04140000	5.19060000	-0.69350000
C	5.58410000	-5.30910000	-0.58300000
H	5.08570000	-5.45410000	-1.54710000
H	6.63800000	-5.57150000	-0.67500000
H	5.11360000	-5.94420000	0.17480000
C	3.97850000	6.50550000	-0.15390000
H	4.09080000	6.48860000	0.93510000

H	4.81090000	7.05060000	-0.59860000
H	3.03620000	6.99540000	-0.42060000

5DEBCOD

Charge 0 *Multiplicity* 1

O	0.89890000	0.14330000	0.74470000
O	-0.75800000	-2.95920000	1.07950000
O	-1.81580000	2.37960000	1.06400000
O	-6.36200000	-0.11090000	-0.99510000
C	0.50010000	-1.12490000	0.23570000
C	-0.47130000	-1.78350000	1.21550000
C	-1.10170000	-0.97140000	2.31760000
C	-1.48750000	-1.73190000	3.42590000
C	-2.09880000	-1.14930000	4.53060000
C	-2.36940000	0.21430000	4.52570000
C	-2.02630000	0.97850000	3.41570000
C	-1.37850000	0.41570000	2.31180000
C	-1.10660000	1.39960000	1.20260000
C	0.04230000	1.15360000	0.22240000
C	-0.61950000	0.51040000	-0.99310000
C	-0.35590000	-0.79860000	-0.98640000
C	-0.89250000	-1.89360000	-1.86090000
C	-2.40770000	-2.14690000	-1.65060000
C	-3.25060000	-1.47630000	-2.71660000
C	-3.54730000	0.00090000	-2.72850000
C	-3.03540000	0.95530000	-1.66890000
C	-1.53860000	1.30320000	-1.87600000
C	-4.66110000	-0.99210000	-2.48100000
C	-5.34290000	-1.09690000	-1.14010000
C	1.73660000	-1.95420000	-0.04740000
C	2.46210000	-1.68720000	-1.21540000
C	3.64550000	-2.35190000	-1.48610000
C	4.13400000	-3.30400000	-0.58200000
C	3.42810000	-3.57610000	0.59040000
C	2.23710000	-2.89630000	0.84750000
C	0.85620000	2.39960000	-0.05750000
C	1.50970000	2.53590000	-1.28790000
C	2.33570000	3.61920000	-1.53730000
C	2.53000000	4.59220000	-0.54920000
C	1.88940000	4.46910000	0.68520000
C	1.06030000	3.37310000	0.91820000
H	-5.93480000	0.75520000	-1.04580000
H	-1.28920000	-2.79850000	3.41360000
H	-2.36470000	-1.76070000	5.38680000

H	-2.85000000	0.68460000	5.37740000
H	-2.25240000	2.03950000	3.39520000
H	-0.32960000	-2.80800000	-1.65180000
H	-0.70750000	-1.64410000	-2.91290000
H	-2.59870000	-3.22540000	-1.68500000
H	-2.69470000	-1.81540000	-0.64840000
H	-3.08440000	-1.90700000	-3.70220000
H	-3.55380000	0.44910000	-3.72030000
H	-3.18090000	0.54930000	-0.66240000
H	-3.62440000	1.87850000	-1.71840000
H	-1.27050000	1.13340000	-2.92600000
H	-1.37350000	2.36600000	-1.67760000
H	-5.35290000	-1.13450000	-3.30830000
H	-5.84970000	-2.06380000	-1.05400000
H	-4.62870000	-1.03080000	-0.31110000
H	2.09230000	-0.94520000	-1.91920000
H	4.20980000	-2.15130000	-2.39140000
H	3.78960000	-4.30340000	1.30730000
H	1.70500000	-3.11930000	1.76740000
H	1.36900000	1.78460000	-2.06120000
H	2.84130000	3.73430000	-2.49090000
H	2.02520000	5.20890000	1.46480000
H	0.57190000	3.28840000	1.88530000
O	5.29980000	-3.90800000	-0.93130000
O	3.35680000	5.61750000	-0.88250000
C	5.82150000	-4.89220000	-0.04750000
H	5.11910000	-5.72370000	0.07360000
H	6.73960000	-5.25500000	-0.50970000
H	6.05160000	-4.45980000	0.93220000
C	3.58600000	6.62420000	0.09510000
H	4.04730000	6.20300000	0.99470000
H	4.27000000	7.33800000	-0.36380000
H	2.65360000	7.13250000	0.36340000

5b-TS3

Charge 0 *Multiplicity* 1

C	-3.43230000	1.35530000	-0.68110000
C	-4.68210000	0.98070000	-0.20600000
C	-4.84560000	-0.25610000	0.41730000
C	-3.75850000	-1.10930000	0.54330000
C	-2.31890000	0.52000000	-0.52280000
C	-2.48890000	-0.73220000	0.09310000
C	-1.03180000	1.09770000	-1.04050000
C	-1.42830000	-1.78590000	0.15070000

O	-1.05380000	1.82010000	-2.04570000
O	-1.76380000	-2.97830000	0.11610000
C	0.15550000	0.95090000	-0.22400000
C	-0.04400000	-1.38230000	0.23930000
O	0.18880000	-0.08720000	0.66730000
C	1.19040000	1.93430000	-0.06880000
C	2.06830000	1.85640000	1.04370000
C	3.04590000	2.80450000	1.24580000
C	3.19220000	3.87370000	0.34590000
C	2.33500000	3.97640000	-0.75620000
C	1.34710000	3.02440000	-0.95320000
C	1.10370000	-2.20140000	0.02030000
C	2.40500000	-1.65170000	0.17610000
C	3.53100000	-2.40820000	-0.04640000
C	1.01210000	-3.55550000	-0.39120000
C	2.14280000	-4.31870000	-0.61630000
C	3.41400000	-3.75360000	-0.43900000
H	-3.29730000	2.31300000	-1.17290000
H	-5.52660000	1.65250000	-0.32230000
H	-5.81880000	-0.55820000	0.79090000
H	-3.87750000	-2.09110000	0.99010000
H	1.95150000	1.05460000	1.76460000
H	3.70920000	2.75150000	2.10310000
H	2.42990000	4.79150000	-1.46330000
H	0.69450000	3.11600000	-1.81010000
H	2.51810000	-0.61700000	0.47420000
H	4.52330000	-1.98650000	0.07620000
H	0.04080000	-4.00600000	-0.53700000
H	2.03010000	-5.34870000	-0.93210000
O	4.17750000	4.74950000	0.63040000
O	4.57050000	-4.41510000	-0.62330000
C	4.34410000	5.87390000	-0.22820000
H	5.17200000	6.44600000	0.18970000
H	4.59330000	5.55660000	-1.24560000
H	3.44040000	6.49110000	-0.24230000
C	4.50890000	-5.78830000	-1.00310000
H	4.01740000	-5.90280000	-1.97400000
H	5.54340000	-6.12210000	-1.07400000
H	3.98240000	-6.37740000	-0.24610000

13b

Charge 0 *Multiplicity* 1

C	-4.26370000	1.39790000	-0.02480000
C	-5.46450000	0.69760000	0.03100000

C	-5.46450000	-0.69770000	0.03090000
C	-4.26360000	-1.39800000	-0.02490000
C	-3.05680000	0.70170000	-0.05700000
C	-3.05680000	-0.70170000	-0.05700000
C	-1.78380000	1.46370000	-0.15590000
C	-1.78380000	-1.46370000	-0.15600000
O	-1.74590000	2.61310000	-0.54660000
O	-1.74570000	-2.61300000	-0.54690000
C	-0.51900000	0.75380000	0.28540000
C	-0.51900000	-0.75370000	0.28540000
O	-0.70960000	0.00000000	1.47190000
C	0.76800000	1.49580000	0.15090000
C	1.56940000	1.72630000	1.26780000
C	2.78050000	2.39990000	1.13460000
C	3.16040000	2.82620000	-0.12760000
C	2.38520000	2.60970000	-1.25760000
C	1.17830000	1.93680000	-1.11010000
C	0.76800000	-1.49570000	0.15080000
C	1.56930000	-1.72660000	1.26780000
C	2.78030000	-2.40020000	1.13460000
C	1.17840000	-1.93640000	-1.11020000
C	2.38540000	-2.60940000	-1.25770000
C	3.16040000	-2.82620000	-0.12760000
H	-4.24980000	2.48310000	-0.03940000
H	-6.40360000	1.24000000	0.06970000
H	-6.40360000	-1.24020000	0.06960000
H	-4.24960000	-2.48320000	-0.03960000
H	1.24580000	1.37910000	2.24380000
H	3.42260000	2.59570000	1.98650000
H	2.73040000	2.96060000	-2.22390000
H	0.55540000	1.74890000	-1.98030000
H	1.24560000	-1.37960000	2.24390000
H	3.42230000	-2.59630000	1.98660000
H	0.55570000	-1.74830000	-1.98040000
H	2.73060000	-2.96010000	-2.22400000
F	4.33090000	3.47560000	-0.26530000
F	4.33090000	-3.47570000	-0.26540000

13b-S_1

Charge 0 *Multiplicity* 1

C	-4.22750000	1.41830000	-0.17410000
C	-5.42430000	0.72620000	-0.20970000
C	-5.44750000	-0.67430000	-0.14160000
C	-4.25670000	-1.37450000	-0.04760000

C	-3.01250000	0.71120000	-0.06100000
C	-3.02960000	-0.70050000	-0.00260000
C	-1.75870000	1.42320000	-0.03460000
C	-1.79020000	-1.49450000	0.02010000
O	-1.68200000	2.68210000	-0.24040000
O	-1.77150000	-2.68930000	-0.23650000
C	-0.48970000	0.72170000	0.39320000
C	-0.50200000	-0.78710000	0.38420000
O	-0.61050000	-0.01800000	1.58740000
C	0.77600000	1.49600000	0.19280000
C	1.66540000	1.68450000	1.24900000
C	2.84270000	2.40050000	1.05070000
C	3.10070000	2.90840000	-0.21220000
C	2.23340000	2.73620000	-1.28150000
C	1.06040000	2.02190000	-1.07040000
C	0.77000000	-1.53710000	0.18510000
C	1.69450000	-1.65570000	1.22380000
C	2.89160000	-2.33670000	1.02480000
C	1.04800000	-2.10120000	-1.06450000
C	2.24140000	-2.77870000	-1.27850000
C	3.13910000	-2.88120000	-0.22500000
H	-4.20890000	2.50250000	-0.22370000
H	-6.35570000	1.27840000	-0.29050000
H	-6.39240000	-1.20630000	-0.16690000
H	-4.24760000	-2.45960000	-0.00620000
H	1.43470000	1.27940000	2.22890000
H	3.55060000	2.56750000	1.85500000
H	2.48260000	3.15080000	-2.25210000
H	0.36660000	1.86930000	-1.89260000
H	1.47530000	-1.21930000	2.19270000
H	3.62470000	-2.44650000	1.81640000
H	0.33080000	-2.00710000	-1.87440000
H	2.48250000	-3.22130000	-2.23880000
F	4.23880000	3.59630000	-0.41160000
F	4.29690000	-3.53470000	-0.42790000

13b-TS1-S_1

Charge 0 *Multiplicity* 1

C	-4.24720000	1.39680000	-0.11400000
C	-5.43240000	0.70740000	-0.19770000
C	-5.43230000	-0.70770000	-0.19790000
C	-4.24710000	-1.39710000	-0.11440000
C	-3.01130000	0.71120000	-0.01340000
C	-3.01130000	-0.71130000	-0.01350000

C	-1.80690000	1.49930000	0.00930000
C	-1.80670000	-1.49940000	0.00900000
O	-1.77220000	2.72330000	-0.23290000
O	-1.77190000	-2.72320000	-0.23340000
C	-0.51220000	0.86450000	0.44900000
C	-0.51210000	-0.86450000	0.44890000
O	-0.56400000	-0.00010000	1.54610000
C	0.74570000	1.56550000	0.22930000
C	1.73400000	1.59850000	1.22710000
C	2.93950000	2.24130000	0.99720000
C	3.14450000	2.82940000	-0.24560000
C	2.19080000	2.81400000	-1.25930000
C	0.98310000	2.18860000	-1.01210000
C	0.74580000	-1.56550000	0.22930000
C	1.73400000	-1.59860000	1.22720000
C	2.93950000	-2.24140000	0.99740000
C	0.98340000	-2.18840000	-1.01220000
C	2.19110000	-2.81380000	-1.25930000
C	3.14470000	-2.82930000	-0.24550000
H	-4.23390000	2.48160000	-0.11840000
H	-6.37140000	1.24710000	-0.26690000
H	-6.37130000	-1.24750000	-0.26720000
H	-4.23370000	-2.48180000	-0.11890000
H	1.54110000	1.14070000	2.19080000
H	3.71440000	2.29680000	1.75360000
H	2.40740000	3.28810000	-2.20990000
H	0.21870000	2.16540000	-1.78170000
H	1.54100000	-1.14090000	2.19090000
H	3.71430000	-2.29700000	1.75390000
H	0.21910000	-2.16500000	-1.78190000
H	2.40790000	-3.28770000	-2.20990000
F	4.30940000	3.44170000	-0.47830000
F	4.30960000	-3.44150000	-0.47810000

13SDR

Charge 0 *Multiplicity* 1

C	1.33760000	3.25540000	-2.48610000
C	1.56070000	3.35390000	-3.84740000
C	1.70530000	2.19100000	-4.60600000
C	1.61920000	0.95650000	-3.98800000
C	1.27440000	2.01010000	-1.83680000
C	1.41210000	0.83470000	-2.60240000
C	1.03840000	2.12070000	-0.36900000
C	1.32770000	-0.58350000	-2.13670000

O	0.51960000	3.14400000	0.09070000
O	1.09040000	-1.47100000	-2.96570000
C	1.51690000	1.11360000	0.55890000
C	1.65770000	-0.97230000	-0.78090000
O	1.79270000	-0.12510000	0.22020000
C	1.68680000	1.35270000	1.99280000
C	1.61850000	0.26460000	2.88170000
C	1.81010000	0.44520000	4.24390000
C	2.07460000	1.72460000	4.70910000
C	2.15660000	2.82250000	3.86480000
C	1.96130000	2.63360000	2.50420000
C	1.99420000	-2.34240000	-0.37800000
C	1.42850000	-3.47630000	-0.98740000
C	1.75880000	-4.75230000	-0.54770000
C	2.89600000	-2.52580000	0.68790000
C	3.23220000	-3.79640000	1.13050000
C	2.65560000	-4.88910000	0.49990000
H	1.21730000	4.15070000	-1.88710000
H	1.62570000	4.33010000	-4.31720000
H	1.88390000	2.24950000	-5.67490000
H	1.71510000	0.04850000	-4.57160000
H	1.39700000	-0.72760000	2.50180000
H	1.74830000	-0.38260000	4.94170000
H	2.37580000	3.80230000	4.27500000
H	2.03400000	3.48140000	1.83460000
H	0.71380000	-3.36010000	-1.78960000
H	1.32070000	-5.63520000	-1.00030000
H	3.35130000	-1.66220000	1.16170000
H	3.93600000	-3.94760000	1.94150000
F	2.25630000	1.90800000	6.02700000
F	2.97780000	-6.12350000	0.92170000

13DOXEPY

Charge 0 *Multiplicity* 1

C	1.33900000	3.25860000	-2.49280000
C	1.55730000	3.35510000	-3.85350000
C	1.69470000	2.18970000	-4.61200000
C	1.60670000	0.95740000	-3.99320000
C	1.27370000	2.01360000	-1.83930000
C	1.40460000	0.83480000	-2.60520000
C	1.04270000	2.13550000	-0.37360000
C	1.32010000	-0.58420000	-2.14660000
O	0.54540000	3.16580000	0.08720000
O	1.09260000	-1.47100000	-2.97680000

C	1.50550000	1.11320000	0.55430000
C	1.64260000	-0.96840000	-0.78530000
O	1.74590000	-0.11650000	0.20340000
C	1.68090000	1.34350000	1.99040000
C	1.58700000	0.25520000	2.87570000
C	1.78830000	0.42670000	4.23800000
C	2.08590000	1.69750000	4.70620000
C	2.19090000	2.79560000	3.86490000
C	1.98630000	2.61560000	2.50430000
C	1.99060000	-2.33400000	-0.37390000
C	1.44390000	-3.47530000	-0.98580000
C	1.78260000	-4.74660000	-0.53820000
C	2.88380000	-2.50450000	0.70070000
C	3.22620000	-3.77040000	1.15330000
C	2.66790000	-4.87090000	0.52050000
H	1.22550000	4.15490000	-1.89400000
H	1.62500000	4.33040000	-4.32460000
H	1.87010000	2.24680000	-5.68150000
H	1.69770000	0.04870000	-4.57620000
H	1.33800000	-0.72990000	2.49380000
H	1.70800000	-0.40120000	4.93380000
H	2.43440000	3.76880000	4.27710000
H	2.07550000	3.46380000	1.83710000
H	0.73800000	-3.36890000	-1.79730000
H	1.35950000	-5.63550000	-0.99330000
H	3.32730000	-1.63430000	1.17430000
H	3.92280000	-3.91150000	1.97240000
F	2.27630000	1.87240000	6.02440000
F	2.99800000	-6.10120000	0.95020000

13TDR

Charge 0 *Multiplicity* 3

C	1.46130000	3.27210000	-2.54220000
C	1.70080000	3.35270000	-3.90780000
C	1.82750000	2.18510000	-4.65920000
C	1.71290000	0.94870000	-4.03790000
C	1.38390000	2.03150000	-1.90130000
C	1.50790000	0.85700000	-2.65680000
C	1.07670000	2.07710000	-0.43670000
C	1.35960000	-0.52820000	-2.11040000
O	0.31330000	2.95390000	-0.00880000
O	0.88230000	-1.41580000	-2.82950000
C	1.73410000	1.16140000	0.46580000
C	1.88300000	-0.84730000	-0.80060000

O	2.49140000	0.14140000	-0.06130000
C	1.76590000	1.28830000	1.90350000
C	2.11930000	0.16930000	2.68780000
C	2.16990000	0.25100000	4.06880000
C	1.87900000	1.46840000	4.66950000
C	1.54130000	2.59980000	3.93840000
C	1.48490000	2.50960000	2.55770000
C	2.04860000	-2.19240000	-0.29230000
C	1.15700000	-3.23240000	-0.62710000
C	1.35250000	-4.51180000	-0.13060000
C	3.14300000	-2.47650000	0.55210000
C	3.35030000	-3.75590000	1.04050000
C	2.44720000	-4.75030000	0.68890000
H	1.33650000	4.17400000	-1.95140000
H	1.78230000	4.32350000	-4.38620000
H	2.00760000	2.23860000	-5.72810000
H	1.78330000	0.03280000	-4.61560000
H	2.33030000	-0.77710000	2.20570000
H	2.42760000	-0.60650000	4.68050000
H	1.33910000	3.53250000	4.45330000
H	1.24240000	3.39060000	1.97970000
H	0.29960000	-3.02730000	-1.25410000
H	0.66820000	-5.32050000	-0.36240000
H	3.84680000	-1.68890000	0.80000000
H	4.19590000	-3.99390000	1.67610000
F	1.93240000	1.55660000	6.00550000
F	2.63920000	-5.99020000	1.16130000

13b-IM1

Charge 0 *Multiplicity* 1

O	-1.26240000	0.02220000	-0.74860000
O	0.52000000	-3.00150000	-0.78860000
O	1.07840000	2.61200000	-1.12270000
O	5.56870000	0.65780000	0.06520000
C	-0.99520000	-1.25520000	-0.70660000
C	0.31240000	-1.80530000	-1.02140000
C	1.38810000	-1.01030000	-1.69320000
C	2.38660000	-1.82340000	-2.26670000
C	3.50250000	-1.29270000	-2.88520000
C	3.66570000	0.09390000	-2.93910000
C	2.69790000	0.91090000	-2.38720000
C	1.54360000	0.39160000	-1.76780000
C	0.65370000	1.45340000	-1.21550000
C	-0.71940000	1.20310000	-0.81980000

C	0.46240000	0.63720000	1.92080000
C	0.35600000	-0.56990000	2.00230000
C	0.85700000	-1.93650000	2.19260000
C	2.33750000	-1.88850000	1.74550000
C	3.20040000	-0.93680000	2.56280000
C	3.33030000	0.57700000	2.47000000
C	2.64110000	1.54630000	1.52230000
C	1.19440000	1.90940000	1.93460000
C	4.46400000	-0.31480000	2.01130000
C	4.77070000	-0.42530000	0.53600000
C	-2.19440000	-2.05280000	-0.41040000
C	-3.45570000	-1.44840000	-0.59350000
C	-4.62870000	-2.13000000	-0.30890000
C	-4.54050000	-3.43190000	0.16120000
C	-3.32440000	-4.06630000	0.35040000
C	-2.15150000	-3.37740000	0.06300000
C	-1.65620000	2.27010000	-0.44680000
C	-2.65130000	1.98530000	0.50500000
C	-3.58410000	2.94680000	0.86770000
C	-3.50840000	4.19550000	0.26930000
C	-2.54040000	4.51530000	-0.67140000
C	-1.61080000	3.54810000	-1.02740000
H	5.05830000	1.46990000	0.18810000
H	2.26230000	-2.89760000	-2.20650000
H	4.24530000	-1.95410000	-3.31950000
H	4.53960000	0.53070000	-3.41150000
H	2.81250000	1.98750000	-2.42160000
H	0.31010000	-2.68430000	1.61120000
H	0.77930000	-2.21860000	3.24900000
H	2.76530000	-2.89550000	1.83030000
H	2.35700000	-1.62540000	0.68560000
H	3.30160000	-1.28170000	3.59090000
H	3.49580000	1.02510000	3.44880000
H	2.61360000	1.14050000	0.50730000
H	3.23530000	2.46910000	1.48180000
H	1.17870000	2.33680000	2.94390000
H	0.77960000	2.65730000	1.25310000
H	5.35220000	-0.34770000	2.63820000
H	5.35140000	-1.33270000	0.33790000
H	3.85020000	-0.49560000	-0.05620000
H	-3.51900000	-0.43690000	-0.98000000
H	-5.60060000	-1.67160000	-0.45590000
H	-3.29940000	-5.08470000	0.72250000
H	-1.20380000	-3.87150000	0.21450000

H	-2.67600000	1.00670000	0.97600000
H	-4.35160000	2.74760000	1.60740000
H	-2.52800000	5.50460000	-1.11570000
H	-0.85800000	3.77930000	-1.77030000
F	-5.67420000	-4.09940000	0.43580000
F	-4.40430000	5.13370000	0.61790000

13b-TS2

Charge 0 *Multiplicity* 1

O	1.28070000	0.04440000	0.79680000
O	-0.54670000	-2.97200000	0.81990000
O	-1.09730000	2.63440000	1.04730000
O	-5.59550000	0.66360000	-0.24090000
C	0.96280000	-1.22330000	0.65550000
C	-0.33550000	-1.77090000	1.02210000
C	-1.40650000	-0.96820000	1.69820000
C	-2.39440000	-1.77040000	2.30000000
C	-3.50720000	-1.22770000	2.91680000
C	-3.67110000	0.15820000	2.94420000
C	-2.70790000	0.96510000	2.36690000
C	-1.56350000	0.43210000	1.74430000
C	-0.67550000	1.47690000	1.15490000
C	0.68760000	1.21070000	0.72240000
C	-0.41250000	0.59530000	-1.51340000
C	-0.30470000	-0.62540000	-1.58110000
C	-0.79630000	-1.94230000	-2.01670000
C	-2.31300000	-1.94610000	-1.72850000
C	-3.10750000	-0.97100000	-2.58530000
C	-3.23680000	0.54540000	-2.52200000
C	-2.62090000	1.55940000	-1.57070000
C	-1.12630000	1.84260000	-1.83620000
C	-4.39540000	-0.33740000	-2.11190000
C	-4.76510000	-0.41980000	-0.64910000
C	2.15550000	-2.04760000	0.38260000
C	3.42760000	-1.45880000	0.54010000
C	4.58910000	-2.16640000	0.27170000
C	4.48070000	-3.47920000	-0.16190000
C	3.25460000	-4.09920000	-0.32740000
C	2.09350000	-3.38500000	-0.05220000
C	1.63700000	2.28460000	0.38350000
C	2.65580000	1.99270000	-0.53980000
C	3.60680000	2.94520000	-0.87670000
C	3.52440000	4.19460000	-0.27960000
C	2.53410000	4.52160000	0.63430000

C	1.58670000	3.56110000	0.96410000
H	-5.09320000	1.47990000	-0.36980000
H	-2.26930000	-2.84550000	2.26210000
H	-4.24570000	-1.88090000	3.37050000
H	-4.54040000	0.60410000	3.41680000
H	-2.82250000	2.04220000	2.38100000
H	-0.31180000	-2.77780000	-1.50540000
H	-0.60630000	-2.05750000	-3.09030000
H	-2.70390000	-2.95260000	-1.92320000
H	-2.45580000	-1.75810000	-0.66160000
H	-3.15220000	-1.31450000	-3.61760000
H	-3.34400000	0.96500000	-3.52110000
H	-2.73170000	1.25010000	-0.52690000
H	-3.17670000	2.49990000	-1.68080000
H	-0.96470000	2.08070000	-2.89390000
H	-0.79010000	2.70040000	-1.24820000
H	-5.25490000	-0.37920000	-2.77720000
H	-5.34280000	-1.33000000	-0.45490000
H	-3.86960000	-0.46470000	-0.01590000
H	3.51090000	-0.43800000	0.89540000
H	5.56780000	-1.71760000	0.40220000
H	3.21150000	-5.12760000	-0.66910000
H	1.14020000	-3.87410000	-0.17960000
H	2.68510000	1.01250000	-1.00760000
H	4.39310000	2.73940000	-1.59460000
H	2.51740000	5.51060000	1.07890000
H	0.81660000	3.79960000	1.68650000
F	5.60350000	-4.17080000	-0.42300000
F	4.43720000	5.12530000	-0.60320000

13DEBCOD

Charge 0 *Multiplicity* 1

O	1.07850000	0.08540000	0.99910000
O	-0.33800000	-2.70430000	1.99060000
O	-0.99380000	2.87320000	0.90520000
O	-5.36430000	0.84460000	-0.52680000
C	0.65020000	-1.15040000	0.43780000
C	-0.41250000	-1.62060000	1.45210000
C	-1.55820000	-0.68590000	1.81320000
C	-2.63490000	-1.37500000	2.38700000
C	-3.80540000	-0.73660000	2.77900000
C	-3.91990000	0.63700000	2.61060000
C	-2.86250000	1.34180000	2.04970000
C	-1.67820000	0.71860000	1.63410000

C	-0.71000000	1.69330000	0.98600000
C	0.53620000	1.17620000	0.26530000
C	-0.01260000	0.55550000	-1.01010000
C	0.02890000	-0.77360000	-0.90240000
C	-0.54310000	-1.78540000	-1.84730000
C	-2.06770000	-1.95530000	-1.64340000
C	-2.89480000	-1.13620000	-2.62100000
C	-2.95350000	0.36890000	-2.74300000
C	-2.22890000	1.39670000	-1.89280000
C	-0.68800000	1.39330000	-2.05630000
C	-4.15830000	-0.40130000	-2.24130000
C	-4.55810000	-0.29980000	-0.79000000
C	1.83440000	-2.09140000	0.29620000
C	3.12320000	-1.55310000	0.25960000
C	4.23310000	-2.36890000	0.06200000
C	4.03000000	-3.72810000	-0.10790000
C	2.76680000	-4.29700000	-0.09000000
C	1.66690000	-3.46920000	0.11330000
C	1.61970000	2.22030000	0.09140000
C	2.40460000	2.22650000	-1.06390000
C	3.47030000	3.11250000	-1.19700000
C	3.73700000	3.97970000	-0.15070000
C	2.99030000	3.99120000	1.01820000
C	1.92810000	3.10180000	1.13200000
H	-4.85690000	1.62680000	-0.78460000
H	-2.54290000	-2.44730000	2.51750000
H	-4.61740000	-1.31360000	3.20970000
H	-4.82360000	1.16130000	2.90400000
H	-2.94900000	2.41320000	1.90960000
H	-0.03600000	-2.74350000	-1.70810000
H	-0.34630000	-1.47010000	-2.87830000
H	-2.33280000	-3.00740000	-1.79440000
H	-2.32260000	-1.72880000	-0.60420000
H	-2.94570000	-1.62110000	-3.59380000
H	-3.03390000	0.69040000	-3.77950000
H	-2.48690000	1.28030000	-0.83650000
H	-2.60670000	2.38310000	-2.18580000
H	-0.42720000	1.02610000	-3.05570000
H	-0.31020000	2.41810000	-1.98240000
H	-5.00500000	-0.48680000	-2.91850000
H	-5.16470000	-1.16590000	-0.50400000
H	-3.67490000	-0.29440000	-0.14020000
H	3.26290000	-0.48520000	0.38940000
H	5.23950000	-1.96530000	0.03610000

H	2.65350000	-5.36660000	-0.23080000
H	0.67620000	-3.90850000	0.13530000
H	2.19020000	1.53110000	-1.87110000
H	4.08610000	3.13430000	-2.08940000
H	3.24320000	4.68320000	1.81410000
H	1.33650000	3.09890000	2.04220000
F	5.09760000	-4.52600000	-0.29900000
F	4.76210000	4.84310000	-0.27060000

13b-TS3

Charge 0 *Multiplicity* 1

C	-3.69080000	1.38930000	-0.02500000
C	-4.87390000	0.70980000	0.22590000
C	-4.87960000	-0.68460000	0.24250000
C	-3.70240000	-1.37970000	0.00690000
C	-2.48940000	0.69930000	-0.23160000
C	-2.49530000	-0.70490000	-0.21580000
C	-1.30520000	1.56870000	-0.51900000
C	-1.32060000	-1.58920000	-0.49750000
O	-1.48160000	2.66550000	-1.06840000
O	-1.51290000	-2.69080000	-1.03140000
C	0.00300000	1.18980000	-0.03850000
C	-0.00300000	-1.21240000	-0.04010000
O	0.16270000	-0.01130000	0.59310000
C	1.15560000	2.06570000	0.00260000
C	2.13740000	1.87290000	0.99690000
C	3.25210000	2.69190000	1.06530000
C	3.39200000	3.69920000	0.11960000
C	2.45720000	3.91600000	-0.88270000
C	1.33570000	3.10310000	-0.93690000
C	1.15580000	-2.07810000	-0.02850000
C	2.19210000	-1.83220000	0.89760000
C	3.31540000	-2.64020000	0.94320000
C	1.29490000	-3.15800000	-0.92800000
C	2.42480000	-3.96010000	-0.89740000
C	3.41120000	-3.69130000	0.04080000
H	-3.67740000	2.47350000	-0.06060000
H	-5.78980000	1.26420000	0.40410000
H	-5.80000000	-1.22710000	0.43380000
H	-3.69850000	-2.46450000	-0.00480000
H	2.00120000	1.09940000	1.74310000
H	4.00470000	2.56520000	1.83560000
H	2.61800000	4.70530000	-1.60860000
H	0.60840000	3.25220000	-1.72250000

H	2.09490000	-1.02060000	1.60750000
H	4.10800000	-2.47210000	1.66380000
H	0.52840000	-3.34880000	-1.66540000
H	2.55280000	-4.78130000	-1.59390000
F	4.47280000	4.49090000	0.17670000
F	4.49970000	-4.47330000	0.07560000

17b

Charge 0 *Multiplicity* 1

C	-5.27790000	1.39810000	-0.08820000
C	-6.47960000	0.69750000	-0.05980000
C	-6.47950000	-0.69780000	-0.05990000
C	-5.27770000	-1.39820000	-0.08840000
C	-4.07070000	0.70190000	-0.09300000
C	-4.07060000	-0.70190000	-0.09310000
C	-2.79650000	1.46420000	-0.15910000
C	-2.79640000	-1.46410000	-0.15950000
O	-2.74520000	2.61400000	-0.54580000
O	-2.74510000	-2.61400000	-0.54590000
C	-1.54410000	0.75250000	0.31650000
C	-1.54410000	-0.75250000	0.31640000
O	-1.76380000	-0.00010000	1.49820000
C	-0.25330000	1.49520000	0.21340000
C	0.51840000	1.72090000	1.35080000
C	1.72790000	2.40100000	1.24380000
C	2.15510000	2.84450000	-0.00380000
C	1.38980000	2.61750000	-1.14700000
C	0.18230000	1.94110000	-1.03720000
C	-0.25320000	-1.49510000	0.21330000
C	0.51820000	-1.72120000	1.35080000
C	1.72770000	-2.40140000	1.24380000
C	0.18270000	-1.94050000	-1.03740000
C	1.39020000	-2.61700000	-1.14720000
C	2.15520000	-2.84450000	-0.00390000
H	-5.26380000	2.48320000	-0.10160000
H	-7.41920000	1.24000000	-0.04200000
H	-7.41910000	-1.24030000	-0.04220000
H	-5.26350000	-2.48340000	-0.10200000
H	0.17300000	1.36590000	2.31610000
H	2.33270000	2.58280000	2.12590000
H	1.73830000	2.96270000	-2.11510000
H	-0.41920000	1.75170000	-1.92150000
H	0.17260000	-1.36670000	2.31620000
H	2.33230000	-2.58360000	2.12600000

H	-0.41870000	-1.75080000	-1.92170000
H	1.73880000	-2.96180000	-2.11530000
C	3.42830000	-3.62890000	-0.12080000
C	3.42830000	3.62890000	-0.12080000
F	3.20210000	-4.95550000	-0.09230000
F	4.28190000	-3.36200000	0.87890000
F	4.07090000	-3.37670000	-1.27290000
F	4.28190000	3.36200000	0.87900000
F	4.07080000	3.37660000	-1.27290000
F	3.20210000	4.95550000	-0.09240000

17b-S_1

Charge 0 *Multiplicity* 1

C	-5.24880000	1.37920000	-0.23390000
C	-6.43490000	0.67060000	-0.30710000
C	-6.43990000	-0.73040000	-0.26420000
C	-5.24120000	-1.41600000	-0.15750000
C	-4.02770000	0.68730000	-0.10570000
C	-4.02610000	-0.72510000	-0.07430000
C	-2.78120000	1.41610000	-0.03940000
C	-2.77550000	-1.50120000	-0.03500000
O	-2.72560000	2.67800000	-0.24000000
O	-2.72250000	-2.68460000	-0.33200000
C	-1.52420000	0.72310000	0.42690000
C	-1.51730000	-0.78190000	0.40480000
O	-1.68900000	-0.03050000	1.60890000
C	-0.25300000	1.50180000	0.28300000
C	0.64420000	1.57560000	1.34460000
C	1.82910000	2.29280000	1.20090000
C	2.10540000	2.92490000	-0.00600000
C	1.21220000	2.84970000	-1.07520000
C	0.03080000	2.13530000	-0.93080000
C	-0.23060000	-1.52370000	0.26180000
C	0.55070000	-1.79770000	1.38270000
C	1.75020000	-2.48800000	1.23880000
C	0.18640000	-1.93270000	-1.00760000
C	1.38530000	-2.61720000	-1.15470000
C	2.15980000	-2.89220000	-0.02810000
H	-5.24520000	2.46420000	-0.26310000
H	-7.37210000	1.21150000	-0.39720000
H	-7.37660000	-1.27460000	-0.31820000
H	-5.21680000	-2.50140000	-0.13430000
H	0.41400000	1.08230000	2.28250000
H	2.52760000	2.35990000	2.02770000

H	1.43990000	3.34230000	-2.01580000
H	-0.66400000	2.06240000	-1.76260000
H	0.22010000	-1.47380000	2.36420000
H	2.36180000	-2.70710000	2.10760000
H	-0.42410000	-1.70830000	-1.87770000
H	1.71920000	-2.93210000	-2.13810000
C	3.35830000	3.73380000	-0.17260000
C	3.42640000	-3.68110000	-0.18140000
F	4.23010000	3.53700000	0.82590000
F	3.09750000	5.05310000	-0.21280000
F	3.99300000	3.43900000	-1.32010000
F	4.29880000	-3.43220000	0.80720000
F	3.19510000	-5.00700000	-0.16740000
F	4.04940000	-3.41470000	-1.34060000

17b-TS1-S_1

Charge 0 *Multiplicity* 1

C	5.28910000	-1.39690000	-0.18400000
C	6.47600000	-0.70620000	-0.27190000
C	6.47610000	0.70550000	-0.27170000
C	5.28940000	1.39640000	-0.18360000
C	4.05830000	-0.71060000	-0.07400000
C	4.05850000	0.71040000	-0.07380000
C	2.84760000	-1.50020000	-0.05300000
C	2.84790000	1.50020000	-0.05240000
O	2.80700000	-2.70970000	-0.35300000
O	2.80760000	2.70990000	-0.35210000
C	1.57970000	-0.89060000	0.46220000
C	1.57980000	0.89080000	0.46240000
O	1.67650000	-0.00010000	1.52700000
C	0.30860000	-1.59320000	0.32140000
C	-0.61080000	-1.60780000	1.37930000
C	-1.83690000	-2.24200000	1.22720000
C	-2.14610000	-2.84350000	0.01140000
C	-1.24030000	-2.83480000	-1.05340000
C	-0.01050000	-2.22240000	-0.89780000
C	0.30880000	1.59340000	0.32160000
C	-0.61080000	1.60770000	1.37930000
C	-1.83690000	2.24180000	1.22710000
C	-0.01000000	2.22310000	-0.89740000
C	-1.23980000	2.83550000	-1.05310000
C	-2.14590000	2.84380000	0.01150000
H	5.27600000	-2.48150000	-0.18970000
H	7.41420000	-1.24670000	-0.34500000

H	7.41450000	1.24580000	-0.34460000
H	5.27660000	2.48110000	-0.18900000
H	-0.35250000	-1.14480000	2.32480000
H	-2.54410000	-2.26640000	2.04850000
H	-1.50030000	-3.30800000	-1.99530000
H	0.70200000	-2.21270000	-1.71540000
H	-0.35280000	1.14430000	2.32470000
H	-2.54440000	2.26580000	2.04830000
H	0.70260000	2.21370000	-1.71490000
H	-1.49960000	3.30910000	-1.99490000
C	-3.47390000	-3.51470000	-0.19590000
C	-3.47380000	3.51470000	-0.19600000
F	-3.32270000	-4.78240000	-0.61290000
F	-4.20010000	-2.88650000	-1.13570000
F	-4.21190000	-3.54660000	0.92080000
F	-3.32290000	4.78240000	-0.61290000
F	-4.21210000	3.54630000	0.92060000
F	-4.19970000	2.88640000	-1.13600000

17SDR

Charge 0 *Multiplicity* 1

C	1.34230000	3.25550000	-2.47770000
C	1.59030000	3.35680000	-3.83470000
C	1.74800000	2.19580000	-4.59340000
C	1.64920000	0.95920000	-3.98100000
C	1.26720000	2.00830000	-1.83420000
C	1.41750000	0.83480000	-2.60010000
C	1.00810000	2.11310000	-0.37070000
C	1.31980000	-0.58400000	-2.13900000
O	0.47610000	3.12670000	0.08720000
O	1.08460000	-1.46740000	-2.96890000
C	1.48400000	1.10230000	0.56200000
C	1.63780000	-0.97630000	-0.77700000
O	1.75180000	-0.13350000	0.22530000
C	1.65580000	1.34490000	1.99690000
C	1.59420000	0.25820000	2.88650000
C	1.79170000	0.44930000	4.24610000
C	2.05500000	1.72860000	4.72970000
C	2.12370000	2.81590000	3.86100000
C	1.92330000	2.62880000	2.50130000
C	1.98300000	-2.34560000	-0.37490000
C	1.43790000	-3.47980000	-0.99940000
C	1.78610000	-4.75190000	-0.56310000
C	2.87760000	-2.52220000	0.69760000

C	3.22440000	-3.79320000	1.12800000
C	2.67990000	-4.90750000	0.49210000
H	1.21170000	4.14950000	-1.87860000
H	1.66460000	4.33400000	-4.30080000
H	1.94680000	2.25720000	-5.65850000
H	1.75530000	0.05280000	-4.56530000
H	1.37230000	-0.73500000	2.51020000
H	1.73060000	-0.39220000	4.92830000
H	2.33590000	3.80840000	4.24500000
H	1.98600000	3.47580000	1.83010000
H	0.73120000	-3.36710000	-1.80880000
H	1.35500000	-5.62290000	-1.04580000
H	3.31890000	-1.65580000	1.17890000
H	3.92820000	-3.91740000	1.94460000
C	2.32400000	1.93080000	6.19120000
C	3.02300000	-6.28110000	0.98460000
F	1.68160000	1.03130000	6.95210000
F	1.94730000	3.14980000	6.60850000
F	3.63340000	1.81370000	6.47890000
F	2.21060000	-6.67460000	1.98310000
F	2.91850000	-7.20560000	0.01740000
F	4.27550000	-6.34420000	1.46440000

17DOXEPY

Charge 0 *Multiplicity* 1

C	1.34570000	3.25760000	-2.48100000
C	1.59120000	3.35710000	-3.83750000
C	1.74160000	2.19410000	-4.59640000
C	1.63830000	0.95910000	-3.98370000
C	1.26610000	2.01070000	-1.83490000
C	1.40940000	0.83450000	-2.60120000
C	1.00940000	2.12300000	-0.37310000
C	1.30820000	-0.58460000	-2.14490000
O	0.49170000	3.14130000	0.08590000
O	1.07460000	-1.46650000	-2.97520000
C	1.47560000	1.10120000	0.55870000
C	1.62500000	-0.97390000	-0.77990000
O	1.71970000	-0.12690000	0.21200000
C	1.65290000	1.33690000	1.99490000
C	1.57560000	0.24930000	2.88160000
C	1.78090000	0.43370000	4.24130000
C	2.06520000	1.70740000	4.72730000
C	2.14770000	2.79570000	3.86090000
C	1.94070000	2.61520000	2.50140000

C	1.97910000	-2.33930000	-0.37170000
C	1.45210000	-3.47950000	-1.00030000
C	1.80700000	-4.74770000	-0.55790000
C	2.86450000	-2.50620000	0.70990000
C	3.21640000	-3.77320000	1.14790000
C	2.68920000	-4.89380000	0.50840000
H	1.22140000	4.15230000	-1.88180000
H	1.66980000	4.33350000	-4.30440000
H	1.93880000	2.25430000	-5.66190000
H	1.73900000	0.05210000	-4.56780000
H	1.33500000	-0.73900000	2.50380000
H	1.70870000	-0.40850000	4.92150000
H	2.37560000	3.78400000	4.24690000
H	2.01310000	3.46300000	1.83210000
H	0.75470000	-3.37480000	-1.81900000
H	1.38990000	-5.62330000	-1.04460000
H	3.29470000	-1.63480000	1.19270000
H	3.91220000	-3.88920000	1.97260000
C	2.34030000	1.90370000	6.18830000
C	3.03930000	-6.26280000	1.00770000
F	1.69920000	1.00310000	6.94900000
F	1.96740000	3.12220000	6.61110000
F	3.65070000	1.78400000	6.47090000
F	2.22100000	-6.66120000	1.99970000
F	2.95240000	-7.19110000	0.04230000
F	4.28750000	-6.31370000	1.50030000

17TDR

Charge 0 *Multiplicity* 3

C	1.43700000	3.26900000	-2.52740000
C	1.68680000	3.36120000	-3.89050000
C	1.83380000	2.20060000	-4.64860000
C	1.72870000	0.95820000	-4.03710000
C	1.36950000	2.02310000	-1.89630000
C	1.51350000	0.85530000	-2.65880000
C	1.05680000	2.05700000	-0.43310000
C	1.37310000	-0.53400000	-2.12310000
O	0.28650000	2.92000000	0.00210000
O	0.91640000	-1.42410000	-2.84850000
C	1.72530000	1.14380000	0.47000000
C	1.87940000	-0.85720000	-0.80410000
O	2.48010000	0.12300000	-0.05110000
C	1.76690000	1.28060000	1.91090000
C	2.11350000	0.16360000	2.69550000

C	2.17500000	0.25950000	4.07690000
C	1.90830000	1.47960000	4.69260000
C	1.57800000	2.60310000	3.93410000
C	1.50490000	2.50960000	2.55440000
C	2.04030000	-2.20890000	-0.29930000
C	1.14200000	-3.23790000	-0.63300000
C	1.33340000	-4.51950000	-0.13240000
C	3.13450000	-2.49480000	0.54330000
C	3.32780000	-3.77630000	1.02810000
C	2.42430000	-4.78480000	0.68920000
H	1.29720000	4.16520000	-1.93130000
H	1.76080000	4.33610000	-4.36160000
H	2.02250000	2.26380000	-5.71550000
H	1.81480000	0.04730000	-4.62040000
H	2.31290000	-0.78760000	2.21810000
H	2.43250000	-0.61100000	4.67010000
H	1.39050000	3.55460000	4.42180000
H	1.26900000	3.38930000	1.97160000
H	0.28570000	-3.02710000	-1.25950000
H	0.62980000	-5.30690000	-0.37880000
H	3.84140000	-1.71020000	0.79100000
H	4.18060000	-3.99580000	1.66340000
C	1.94040000	1.59640000	6.18830000
F	0.70400000	1.57990000	6.71680000
F	2.50930000	2.74630000	6.58470000
F	2.62280000	0.59470000	6.76040000
C	2.66000000	-6.16020000	1.24060000
F	1.74220000	-7.04470000	0.83030000
F	2.64180000	-6.16320000	2.58520000
F	3.86360000	-6.63630000	0.87780000

17b-IM1

Charge 0 *Multiplicity* 1

O	-0.36170000	-0.05820000	-0.86050000
O	1.35600000	-3.11840000	-0.82430000
O	2.05150000	2.47380000	-1.12510000
O	6.42190000	0.44530000	0.26260000
C	-0.12280000	-1.33990000	-0.80930000
C	1.18650000	-1.92020000	-1.06730000
C	2.31080000	-1.15130000	-1.69050000
C	3.31510000	-1.98710000	-2.21660000
C	4.47110000	-1.48110000	-2.78140000
C	4.66870000	-0.09920000	-2.82480000
C	3.69470000	0.74030000	-2.31760000

C	2.50170000	0.24620000	-1.75520000
C	1.60960000	1.32650000	-1.24230000
C	0.21110000	1.10660000	-0.91080000
C	1.25300000	0.51830000	1.87150000
C	1.11670000	-0.68630000	1.94730000
C	1.57860000	-2.06220000	2.16810000
C	3.07950000	-2.04740000	1.79330000
C	3.92350000	-1.11370000	2.65030000
C	4.08940000	0.39700000	2.56740000
C	3.46830000	1.38320000	1.59030000
C	2.01030000	1.77450000	1.93000000
C	5.22400000	-0.51780000	2.15840000
C	5.59480000	-0.63080000	0.69800000
C	-1.35120000	-2.11100000	-0.56240000
C	-2.58940000	-1.48260000	-0.80490000
C	-3.78370000	-2.14520000	-0.56870000
C	-3.76350000	-3.45270000	-0.08900000
C	-2.55200000	-4.09250000	0.15340000
C	-1.35220000	-3.43320000	-0.08240000
C	-0.72200000	2.19760000	-0.59500000
C	-1.77110000	1.93820000	0.30210000
C	-2.70350000	2.92280000	0.59900000
C	-2.58990000	4.17550000	0.00250000
C	-1.55120000	4.44990000	-0.88600000
C	-0.61730000	3.46830000	-1.18280000
H	5.91420000	1.26200000	0.36570000
H	3.16380000	-3.05830000	-2.16320000
H	5.21790000	-2.15900000	-3.18180000
H	5.57420000	0.31720000	-3.25390000
H	3.83640000	1.81400000	-2.34370000
H	1.04430000	-2.80210000	1.56540000
H	1.44350000	-2.33500000	3.22110000
H	3.48100000	-3.06310000	1.89880000
H	3.15510000	-1.78670000	0.73530000
H	3.97030000	-1.46120000	3.68140000
H	4.21970000	0.84010000	3.55370000
H	3.48430000	0.98100000	0.57380000
H	4.08220000	2.29380000	1.58400000
H	1.95130000	2.19620000	2.94010000
H	1.64640000	2.53550000	1.23420000
H	6.08160000	-0.57060000	2.82540000
H	6.17590000	-1.54340000	0.52600000
H	4.70140000	-0.69320000	0.06520000
H	-2.61540000	-0.47320000	-1.20030000

H	-4.72720000	-1.64910000	-0.77110000
H	-2.53870000	-5.11150000	0.52670000
H	-0.42210000	-3.94550000	0.11060000
H	-1.83950000	0.96580000	0.78050000
H	-3.50680000	2.71930000	1.29900000
H	-1.47340000	5.42840000	-1.34950000
H	0.18070000	3.67960000	-1.88270000
C	-3.61950000	5.23310000	0.26750000
C	-5.04750000	-4.16600000	0.20930000
F	-3.07420000	6.45850000	0.33230000
F	-4.54660000	5.28020000	-0.70660000
F	-4.27690000	5.02620000	1.41800000
F	-6.06850000	-3.69890000	-0.52530000
F	-5.40880000	-4.03390000	1.49910000
F	-4.95460000	-5.48440000	-0.02790000

17b-TS2

Charge 0 *Multiplicity* 1

O	-0.37750000	-0.03760000	-0.90960000
O	1.35800000	-3.10610000	-0.81520000
O	2.08560000	2.47320000	-1.08790000
O	6.44480000	0.40620000	0.42330000
C	-0.10300000	-1.31130000	-0.74440000
C	1.19460000	-1.90410000	-1.04440000
C	2.32060000	-1.14350000	-1.67980000
C	3.31140000	-1.98290000	-2.22140000
C	4.46480000	-1.48060000	-2.79770000
C	4.66700000	-0.10070000	-2.84250000
C	3.70210000	0.74240000	-2.32100000
C	2.51830000	0.25090000	-1.74120000
C	1.63680000	1.32910000	-1.20280000
C	0.24730000	1.10760000	-0.82230000
C	1.21450000	0.50030000	1.46550000
C	1.06950000	-0.71600000	1.54640000
C	1.50310000	-2.03970000	2.02150000
C	3.03050000	-2.09180000	1.80290000
C	3.81530000	-1.12790000	2.68080000
C	3.99060000	0.38320000	2.60420000
C	3.44690000	1.39900000	1.61230000
C	1.95120000	1.73030000	1.80530000
C	5.14010000	-0.53710000	2.25510000
C	5.57060000	-0.65010000	0.81090000
C	-1.33330000	-2.09580000	-0.52130000
C	-2.57530000	-1.47650000	-0.76830000

C	-3.76650000	-2.15060000	-0.54960000
C	-3.74210000	-3.46100000	-0.07870000
C	-2.52800000	-4.09210000	0.16990000
C	-1.33110000	-3.42200000	-0.05210000
C	-0.68790000	2.21420000	-0.54100000
C	-1.76080000	1.95450000	0.32680000
C	-2.69840000	2.93910000	0.60520000
C	-2.56540000	4.19460000	0.01750000
C	-1.50510000	4.46900000	-0.84380000
C	-0.56600000	3.48520000	-1.12180000
H	5.95580000	1.23640000	0.50760000
H	3.15530000	-3.05350000	-2.16990000
H	5.20440000	-2.16140000	-3.20680000
H	5.56790000	0.31300000	-3.28380000
H	3.84760000	1.81570000	-2.34740000
H	1.01830000	-2.86890000	1.50090000
H	1.26120000	-2.13270000	3.08680000
H	3.38080000	-3.10650000	2.02940000
H	3.22730000	-1.92480000	0.74110000
H	3.80650000	-1.45840000	3.71820000
H	4.06710000	0.81380000	3.60140000
H	3.59490000	1.06720000	0.58030000
H	4.02530000	2.32460000	1.73190000
H	1.74870000	1.98680000	2.85160000
H	1.66780000	2.59020000	1.19320000
H	5.96820000	-0.59460000	2.95790000
H	6.13300000	-1.57720000	0.65560000
H	4.70280000	-0.68240000	0.13980000
H	-2.60890000	-0.46390000	-1.15340000
H	-4.71150000	-1.65910000	-0.75700000
H	-2.50910000	-5.11420000	0.53450000
H	-0.40080000	-3.93370000	0.13970000
H	-1.84370000	0.97890000	0.79680000
H	-3.52000000	2.73410000	1.28310000
H	-1.41290000	5.44920000	-1.30100000
H	0.24970000	3.69920000	-1.79980000
C	-3.59760000	5.25480000	0.26290000
C	-5.02350000	-4.18490000	0.20360000
F	-3.05120000	6.47910000	0.33560000
F	-4.50710000	5.30180000	-0.72760000
F	-4.27540000	5.05060000	1.40190000
F	-6.04080000	-3.72180000	-0.53900000
F	-5.39860000	-4.06110000	1.49030000
F	-4.91920000	-5.50160000	-0.03850000

17DEBCOD

Charge 0 *Multiplicity* 1

O	-0.19470000	0.08240000	-1.06130000
O	1.26130000	-2.70300000	-2.03370000
O	1.86820000	2.86860000	-0.87070000
O	6.19880000	0.80270000	0.65510000
C	0.21710000	-1.16120000	-0.50800000
C	1.31280000	-1.62000000	-1.49170000
C	2.46470000	-0.67810000	-1.81090000
C	3.55800000	-1.35800000	-2.36340000
C	4.73820000	-0.71310000	-2.71380000
C	4.84650000	0.65810000	-2.52410000
C	3.77250000	1.35450000	-1.98440000
C	2.57810000	0.72450000	-1.61100000
C	1.59230000	1.68900000	-0.97600000
C	0.32970000	1.15860000	-0.29660000
C	0.83800000	0.51980000	0.98560000
C	0.79540000	-0.80770000	0.85860000
C	1.33780000	-1.83270000	1.80690000
C	2.86720000	-2.00420000	1.64360000
C	3.66850000	-1.20020000	2.65450000
C	3.72630000	0.30300000	2.79930000
C	3.02760000	1.34480000	1.94470000
C	1.48270000	1.34170000	2.06310000
C	4.94300000	-0.46230000	2.31990000
C	5.38250000	-0.34230000	0.88130000
C	-0.97190000	-2.10270000	-0.41500000
C	-2.25960000	-1.56130000	-0.42400000
C	-3.37140000	-2.38110000	-0.26920000
C	-3.19670000	-3.75090000	-0.09680000
C	-1.91930000	-4.30400000	-0.07680000
C	-0.80970000	-3.48140000	-0.23740000
C	-0.76580000	2.19680000	-0.14110000
C	-1.58420000	2.17810000	0.98860000
C	-2.66030000	3.05510000	1.09520000
C	-2.91740000	3.94760000	0.06090000
C	-2.11600000	3.96780000	-1.08040000
C	-1.04340000	3.09200000	-1.17900000
H	5.68050000	1.58420000	0.89230000
H	3.47190000	-2.42860000	-2.51020000
H	5.56280000	-1.28380000	-3.12880000
H	5.75730000	1.18700000	-2.78520000
H	3.85330000	2.42410000	-1.82770000

H	0.83240000	-2.78780000	1.64430000
H	1.11340000	-1.52680000	2.83500000
H	3.12500000	-3.05900000	1.78820000
H	3.15160000	-1.76520000	0.61490000
H	3.69180000	-1.69850000	3.62160000
H	3.77840000	0.60930000	3.84220000
H	3.31440000	1.24420000	0.89440000
H	3.39800000	2.32600000	2.26310000
H	1.19080000	0.96090000	3.04850000
H	1.10880000	2.36830000	1.99240000
H	5.77080000	-0.55930000	3.01850000
H	5.99400000	-1.20660000	0.60060000
H	4.51710000	-0.32580000	0.20810000
H	-2.39280000	-0.49340000	-0.55640000
H	-4.36910000	-1.95410000	-0.28400000
H	-1.78670000	-5.37270000	0.05740000
H	0.18080000	-3.92100000	-0.23120000
H	-1.38960000	1.47250000	1.79150000
H	-3.29050000	3.04180000	1.97800000
H	-2.32920000	4.66410000	-1.88560000
H	-0.42130000	3.10670000	-2.06810000
C	-4.09830000	4.86920000	0.13160000
C	-4.39140000	-4.62710000	0.12910000
F	-3.80020000	6.10020000	-0.31670000
F	-5.12070000	4.42740000	-0.62340000
F	-4.56700000	5.00270000	1.38090000
F	-5.48520000	-4.15810000	-0.49220000
F	-4.70440000	-4.72300000	1.43530000
F	-4.19170000	-5.88090000	-0.30720000

17b-TS3

Charge 0 *Multiplicity* 1

C	-3.72070000	1.38840000	-0.03830000
C	-4.91000000	0.70700000	0.18030000
C	-4.91560000	-0.68680000	0.19550000
C	-3.73200000	-1.38230000	-0.00890000
C	-2.51540000	0.69870000	-0.21300000
C	-2.52120000	-0.70630000	-0.19830000
C	-1.32250000	1.56520000	-0.47400000
C	-1.33660000	-1.58610000	-0.45240000
O	-1.47710000	2.66000000	-1.02810000
O	-1.50410000	-2.68770000	-0.98850000
C	-0.02310000	1.17610000	0.03140000
C	-0.02820000	-1.19520000	0.02950000

O	0.08920000	-0.00970000	0.70850000
C	1.15360000	2.02190000	0.04290000
C	2.11920000	1.84290000	1.05120000
C	3.25350000	2.64040000	1.09090000
C	3.44160000	3.61390000	0.11360000
C	2.50300000	3.79690000	-0.90240000
C	1.36170000	3.01350000	-0.93900000
C	1.15450000	-2.03040000	0.01310000
C	2.16370000	-1.80830000	0.96970000
C	3.30350000	-2.59780000	0.99060000
C	1.33010000	-3.05470000	-0.94230000
C	2.47760000	-3.82970000	-0.92570000
C	3.45630000	-3.60660000	0.04330000
H	-3.70730000	2.47270000	-0.07250000
H	-5.83080000	1.26050000	0.33370000
H	-5.84080000	-1.22940000	0.36100000
H	-3.72750000	-2.46710000	-0.02100000
H	1.95790000	1.10190000	1.82490000
H	3.98510000	2.50810000	1.88020000
H	2.66570000	4.55010000	-1.66720000
H	0.64260000	3.14770000	-1.73480000
H	2.03330000	-1.03700000	1.71810000
H	4.06610000	-2.43320000	1.74370000
H	0.58020000	-3.22180000	-1.70240000
H	2.61370000	-4.60850000	-1.66980000
C	4.67250000	4.47120000	0.11230000
C	4.69320000	-4.45510000	0.02220000
F	4.36770000	5.77540000	0.00400000
F	5.40080000	4.32250000	1.22660000
F	5.47610000	4.18200000	-0.92650000
F	5.43600000	-4.30250000	1.12650000
F	4.39620000	-5.76100000	-0.08380000
F	5.48080000	-4.15830000	-1.02680000

24b

Charge 0 *Multiplicity* 1

C	4.24520000	-2.57420000	0.00790000
C	5.61370000	-2.32730000	0.05410000
C	6.09200000	-1.01660000	0.04420000
C	5.20360000	0.05240000	-0.01190000
C	3.34990000	-1.50660000	-0.02560000
C	3.83080000	-0.18830000	-0.03560000
C	1.89320000	-1.78770000	-0.11750000
C	2.89850000	0.96490000	-0.13590000

O	1.46220000	-2.86100000	-0.48800000
O	3.26020000	2.05770000	-0.52300000
C	0.94860000	-0.67950000	0.30530000
C	1.46340000	0.73640000	0.29880000
O	1.37380000	-0.02780000	1.49070000
C	-0.51400000	-0.93440000	0.15390000
C	-1.36490000	-0.82860000	1.25300000
C	-2.72920000	-1.05010000	1.09800000
C	-3.23920000	-1.37440000	-0.16000000
C	-2.38570000	-1.47600000	-1.26170000
C	-1.02460000	-1.25680000	-1.10630000
C	0.51270000	1.87540000	0.14750000
C	-0.17280000	2.37530000	1.25360000
C	-1.07130000	3.42810000	1.10380000
C	0.29930000	2.42700000	-1.11860000
C	-0.59560000	3.47740000	-1.28260000
C	-1.26180000	3.95520000	-0.16320000
H	3.86040000	-3.58900000	0.00080000
H	6.31030000	-3.15850000	0.09280000
H	7.16030000	-0.82870000	0.07520000
H	5.56160000	1.07670000	-0.03430000
H	-0.95770000	-0.57600000	2.22660000
H	-3.39310000	-0.97260000	1.95190000
H	-2.79810000	-1.72390000	-2.23430000
H	-0.35680000	-1.33050000	-1.95970000
H	-0.00490000	1.94090000	2.23400000
H	-1.61660000	3.83790000	1.94690000
H	0.83080000	2.03160000	-1.97970000
H	-0.78230000	3.92280000	-2.25370000
F	-2.13120000	4.97070000	-0.31610000
C	-4.69160000	-1.62070000	-0.37860000
O	-5.17530000	-1.91380000	-1.45500000
O	-5.41670000	-1.48640000	0.73140000
C	-6.82610000	-1.70950000	0.58450000
H	-7.01180000	-2.73000000	0.24300000
H	-7.25320000	-1.55530000	1.57360000
H	-7.24700000	-0.99860000	-0.12930000

24b-S_1

Charge 0 *Multiplicity* 1

C	4.14660000	-2.66390000	-0.10630000
C	5.51300000	-2.45380000	-0.15350000
C	6.04300000	-1.15590000	-0.12950000
C	5.18750000	-0.06870000	-0.06790000

C	3.27160000	-1.56110000	-0.02590000
C	3.79970000	-0.25060000	-0.01190000
C	1.84370000	-1.76820000	0.00890000
C	2.93150000	0.93830000	-0.02430000
O	1.31570000	-2.91780000	-0.17240000
O	3.33860000	2.04780000	-0.33390000
C	0.92320000	-0.64140000	0.41390000
C	1.48030000	0.75830000	0.36880000
O	1.31500000	0.03040000	1.59000000
C	-0.53940000	-0.90090000	0.22620000
C	-1.43290000	-0.67380000	1.27080000
C	-2.78990000	-0.91690000	1.08400000
C	-3.24780000	-1.38330000	-0.14940000
C	-2.34980000	-1.60550000	-1.19630000
C	-0.99590000	-1.36410000	-1.01120000
C	0.56580000	1.91580000	0.15710000
C	-0.17000000	2.43910000	1.22050000
C	-1.03430000	3.51030000	1.01540000
C	0.43220000	2.46240000	-1.12320000
C	-0.43080000	3.52860000	-1.34290000
C	-1.14570000	4.03010000	-0.26430000
H	3.73720000	-3.66900000	-0.12120000
H	6.18020000	-3.30860000	-0.20740000
H	7.11630000	-1.00380000	-0.16270000
H	5.57260000	0.94650000	-0.05910000
H	-1.06450000	-0.31790000	2.22690000
H	-3.48850000	-0.75040000	1.89650000
H	-2.72110000	-1.96140000	-2.15150000
H	-0.29540000	-1.52650000	-1.82530000
H	-0.06210000	2.01230000	2.21250000
H	-1.61380000	3.93980000	1.82540000
H	1.00150000	2.05040000	-1.95150000
H	-0.55660000	3.96900000	-2.32590000
F	-1.98370000	5.06150000	-0.47150000
C	-4.69040000	-1.65890000	-0.39860000
O	-5.12410000	-2.10330000	-1.44390000
O	-5.46580000	-1.36520000	0.64410000
C	-6.86920000	-1.60070000	0.46090000
H	-7.05230000	-2.66220000	0.28180000
H	-7.34420000	-1.28270000	1.38710000
H	-7.24180000	-1.01450000	-0.38160000

24b-TS1-S_1

Charge 0 *Multiplicity* 1

C	4.23810000	-2.56410000	-0.11060000
C	5.59350000	-2.33320000	-0.13630000
C	6.09070000	-1.01140000	-0.09610000
C	5.21840000	0.05080000	-0.03710000
C	3.32270000	-1.48750000	-0.02980000
C	3.82110000	-0.15680000	0.01020000
C	1.91570000	-1.79370000	-0.06580000
C	2.96400000	1.01130000	-0.00640000
O	1.44640000	-2.91420000	-0.36620000
O	3.36650000	2.14760000	-0.31640000
C	0.92780000	-0.77190000	0.42090000
C	1.54110000	0.86640000	0.43210000
O	1.29190000	0.00400000	1.51230000
C	-0.50870000	-1.01340000	0.23510000
C	-1.40120000	-0.84700000	1.30070000
C	-2.76190000	-1.04110000	1.10300000
C	-3.23350000	-1.38810000	-0.16490000
C	-2.34360000	-1.55750000	-1.23130000
C	-0.98540000	-1.38140000	-1.03320000
C	0.58200000	1.92880000	0.22080000
C	-0.41430000	2.18670000	1.18630000
C	-1.36050000	3.17000000	0.97240000
C	0.60620000	2.68350000	-0.97610000
C	-0.34830000	3.65380000	-1.20620000
C	-1.31230000	3.87930000	-0.22540000
H	3.84520000	-3.57470000	-0.14690000
H	6.28440000	-3.16870000	-0.18990000
H	7.16140000	-0.83550000	-0.11450000
H	5.58620000	1.07120000	-0.01420000
H	-1.02470000	-0.58480000	2.28390000
H	-3.45440000	-0.92260000	1.92870000
H	-2.72900000	-1.82640000	-2.20900000
H	-0.28870000	-1.51140000	-1.85500000
H	-0.41810000	1.62380000	2.11180000
H	-2.12870000	3.39730000	1.70270000
H	1.36720000	2.48750000	-1.72210000
H	-0.36510000	4.23660000	-2.11990000
C	-4.68590000	-1.59300000	-0.43230000
O	-5.13340000	-1.91690000	-1.51490000
O	-5.44690000	-1.38320000	0.63950000
C	-6.85720000	-1.56510000	0.44680000
H	-7.06400000	-2.58910000	0.12930000
H	-7.31360000	-1.36660000	1.41480000
H	-7.22790000	-0.86250000	-0.30230000

F	-2.23090000	4.81950000	-0.44360000

24SDR

Charge 0 *Multiplicity* 1

C	1.36070000	3.25870000	-2.46340000
C	1.60060000	3.36230000	-3.82160000
C	1.74380000	2.20260000	-4.58540000
C	1.64000000	0.96540000	-3.97570000
C	1.27970000	2.01060000	-1.82210000
C	1.41660000	0.83880000	-2.59310000
C	1.02780000	2.11450000	-0.35620000
C	1.31640000	-0.57970000	-2.13540000
O	0.50470000	3.13510000	0.10140000
O	1.07390000	-1.46180000	-2.96460000
C	1.49650000	1.10050000	0.57040000
C	1.64130000	-0.97880000	-0.77500000
O	1.75950000	-0.14050000	0.22830000
C	1.66650000	1.33110000	2.00630000
C	1.61920000	0.23540000	2.88780000
C	1.81040000	0.41460000	4.24910000
C	2.05600000	1.69360000	4.75520000
C	2.11270000	2.78630000	3.88670000
C	1.91950000	2.61350000	2.52590000
C	1.98190000	-2.35070000	-0.38410000
C	1.41600000	-3.48090000	-1.00010000
C	1.74940000	-4.75880000	-0.56900000
C	2.88770000	-2.53830000	0.67750000
C	3.22700000	-3.81090000	1.11120000
C	2.64950000	-4.90020000	0.47540000
H	1.24090000	4.15190000	-1.86110000
H	1.67970000	4.34050000	-4.28500000
H	1.93530000	2.26590000	-5.65170000
H	1.73560000	0.05970000	-4.56310000
H	1.41360000	-0.75730000	2.50110000
H	1.76070000	-0.43730000	4.91850000
H	2.31490000	3.77400000	4.28820000
H	1.97600000	3.46740000	1.86320000
H	0.69840000	-3.36080000	-1.79910000
H	1.31130000	-5.63960000	-1.02560000
H	3.34350000	-1.67640000	1.15410000
H	3.93370000	-3.96630000	1.91880000
F	2.97440000	-6.13630000	0.88850000
C	2.25980000	1.94240000	6.20740000
O	2.46910000	3.04140000	6.68490000

O	2.18740000	0.83290000	6.94270000
C	2.36960000	1.01050000	8.35450000
H	1.60820000	1.68570000	8.75020000
H	2.26520000	0.01930000	8.79160000
H	3.36330000	1.41570000	8.55720000

24DOXEPY

Charge 0 *Multiplicity* 1

C	1.37220000	3.25970000	-2.47330000
C	1.60540000	3.35700000	-3.83210000
C	1.73160000	2.19340000	-4.59490000
C	1.61860000	0.96010000	-3.98170000
C	1.28150000	2.01420000	-1.82550000
C	1.40230000	0.83820000	-2.59620000
C	1.03730000	2.13200000	-0.35970000
C	1.29320000	-0.57790000	-2.14060000
O	0.54130000	3.16670000	0.09460000
O	1.04260000	-1.46050000	-2.96290000
C	1.48670000	1.10730000	0.56580000
C	1.62500000	-0.97210000	-0.77420000
O	1.72100000	-0.13010000	0.21330000
C	1.66160000	1.32590000	2.00360000
C	1.59940000	0.22640000	2.87950000
C	1.79980000	0.39440000	4.24110000
C	2.06750000	1.66600000	4.75440000
C	2.13650000	2.76260000	3.89150000
C	1.93510000	2.60090000	2.53050000
C	1.97980000	-2.33990000	-0.37950000
C	1.42510000	-3.47700000	-0.99210000
C	1.76940000	-4.75000000	-0.55510000
C	2.88710000	-2.51400000	0.68270000
C	3.23580000	-3.78180000	1.12360000
C	2.66850000	-4.87870000	0.49180000
H	1.26600000	4.15560000	-1.87290000
H	1.69290000	4.33310000	-4.29840000
H	1.91780000	2.25240000	-5.66230000
H	1.70200000	0.05190000	-4.56680000
H	1.37520000	-0.76070000	2.48860000
H	1.73980000	-0.46080000	4.90530000
H	2.35490000	3.74500000	4.29760000
H	2.00000000	3.45810000	1.87290000
H	0.70810000	-3.36650000	-1.79330000
H	1.34050000	-5.63690000	-1.00860000
H	3.33610000	-1.64540000	1.15380000

H	3.94330000	-3.92770000	1.93220000
F	3.00370000	-6.11020000	0.91070000
C	2.28150000	1.90280000	6.20640000
O	2.51310000	2.99490000	6.68970000
O	2.19150000	0.79060000	6.93640000
C	2.38270000	0.95730000	8.34820000
H	1.63490000	1.64330000	8.75100000
H	2.26330000	-0.03430000	8.78060000
H	3.38400000	1.34410000	8.54900000

24TDR

Charge 0 *Multiplicity* 3

C	1.48090000	3.26780000	-2.55270000
C	1.70580000	3.33630000	-3.92150000
C	1.80730000	2.16280000	-4.66740000
C	1.68380000	0.93180000	-4.03700000
C	1.39400000	2.03260000	-1.90290000
C	1.49400000	0.85240000	-2.65310000
C	1.09570000	2.09120000	-0.43650000
C	1.33850000	-0.52700000	-2.09610000
O	0.34570000	2.98040000	-0.01210000
O	0.84510000	-1.41590000	-2.79810000
C	1.74220000	1.17000000	0.46890000
C	1.88290000	-0.84220000	-0.78890000
O	2.49660000	0.14560000	-0.06060000
C	1.76900000	1.28690000	1.90630000
C	2.14270000	0.16830000	2.68310000
C	2.18820000	0.23940000	4.06450000
C	1.87150000	1.44580000	4.67460000
C	1.51340000	2.57640000	3.95200000
C	1.46230000	2.49730000	2.57060000
C	2.06500000	-2.19090000	-0.28580000
C	1.16510000	-3.22940000	-0.59640000
C	1.37990000	-4.50320000	-0.09560000
C	3.17950000	-2.46920000	0.53170000
C	3.39370000	-3.74810000	1.01810000
C	2.49180000	-4.77010000	0.70690000
H	1.37500000	4.17500000	-1.96660000
H	1.79480000	4.30300000	-4.40670000
H	1.97530000	2.20740000	-5.73860000
H	1.73630000	0.01160000	-4.60960000
H	2.37580000	-0.76940000	2.19450000
H	2.46100000	-0.61800000	4.66960000
H	1.29140000	3.50030000	4.47450000

H	1.20370000	3.37800000	1.99990000
H	0.29220000	-3.02610000	-1.20180000
H	0.67960000	-5.30190000	-0.31710000
H	3.88700000	-1.67900000	0.75970000
H	4.26160000	-3.95560000	1.63390000
F	1.91930000	1.52360000	6.01120000
C	2.67300000	-6.15880000	1.21440000
O	1.92330000	-7.07910000	0.95200000
O	3.74650000	-6.29170000	1.99130000
C	3.97720000	-7.60730000	2.51530000
H	4.11700000	-8.31900000	1.69910000
H	4.88300000	-7.53070000	3.11390000
H	3.13360000	-7.91720000	3.13540000

24b-IM1

Charge 0 *Multiplicity* 1

O	-0.50620000	0.60750000	-0.83970000
O	0.15240000	-2.84210000	-1.01150000
O	2.58200000	2.25520000	-0.96610000
O	6.06380000	-1.12180000	0.30070000
C	-0.68370000	-0.69230000	-0.85480000
C	0.36910000	-1.63490000	-1.17280000
C	1.68610000	-1.22320000	-1.75920000
C	2.38110000	-2.29900000	-2.34590000
C	3.64870000	-2.15370000	-2.87840000
C	4.27950000	-0.90860000	-2.82810000
C	3.61460000	0.16340000	-2.26490000
C	2.31490000	0.04130000	-1.73410000
C	1.80490000	1.31530000	-1.15360000
C	0.39880000	1.53280000	-0.82930000
C	1.15880000	0.52020000	1.95320000
C	0.63920000	-0.57720000	1.96050000
C	0.63300000	-2.04100000	2.06740000
C	2.06350000	-2.47570000	1.66880000
C	3.15030000	-1.93200000	2.58510000
C	3.79830000	-0.55530000	2.59510000
C	3.53560000	0.63060000	1.67920000
C	2.28370000	1.45700000	2.06050000
C	4.58200000	-1.76340000	2.12770000
C	4.92960000	-1.90500000	0.66410000
C	-2.08900000	-1.04340000	-0.60820000
C	-3.06530000	-0.03460000	-0.75310000
C	-4.40230000	-0.29150000	-0.50150000
C	-4.80550000	-1.56830000	-0.09980000

C	-3.85260000	-2.57750000	0.03690000
C	-2.51070000	-2.32840000	-0.21550000
C	-0.13450000	2.84310000	-0.44060000
C	-1.19760000	2.88510000	0.47820000
C	-1.76430000	4.09530000	0.85220000
C	-1.25450000	5.25920000	0.29610000
C	-0.20470000	5.25810000	-0.61130000
C	0.35890000	4.04380000	-0.97660000
H	5.84230000	-0.19570000	0.47050000
H	1.89550000	-3.26700000	-2.36450000
H	4.14700000	-3.00670000	-3.32770000
H	5.27820000	-0.77760000	-3.23160000
H	4.09030000	1.13590000	-2.22040000
H	-0.10430000	-2.52000000	1.41690000
H	0.40820000	-2.34070000	3.09750000
H	2.11810000	-3.57170000	1.68150000
H	2.23000000	-2.16130000	0.63610000
H	3.06200000	-2.34130000	3.59050000
H	4.05070000	-0.23490000	3.60490000
H	3.42280000	0.29830000	0.64340000
H	4.41220000	1.29180000	1.70960000
H	2.36620000	1.82480000	3.08960000
H	2.18770000	2.32840000	1.40640000
H	5.36190000	-2.13020000	2.79120000
H	5.19830000	-2.94270000	0.43930000
H	4.07650000	-1.64680000	0.02470000
H	-2.77210000	0.95620000	-1.08200000
H	-5.13450000	0.49860000	-0.62570000
H	-4.16860000	-3.56740000	0.35030000
H	-1.79190000	-3.12520000	-0.09980000
H	-1.56350000	1.96040000	0.91500000
H	-2.57820000	4.14820000	1.56690000
H	0.15300000	6.19590000	-1.02170000
H	1.17050000	4.02600000	-1.69320000
F	-1.79630000	6.43470000	0.65180000
C	-6.22650000	-1.89460000	0.18790000
O	-6.61600000	-2.99410000	0.53330000
O	-7.04280000	-0.85170000	0.03190000
C	-8.42990000	-1.10090000	0.29780000
H	-8.93470000	-0.15000000	0.13650000
H	-8.81490000	-1.85890000	-0.38740000
H	-8.56240000	-1.43350000	1.32940000

24b-TS2

Charge 0 *Multiplicity* 1

O	-0.51570000	0.64210000	-0.87620000
O	0.14150000	-2.82540000	-0.97580000
O	2.62520000	2.22910000	-0.92370000
O	6.08490000	-1.17760000	0.43390000
C	-0.66700000	-0.66430000	-0.77900000
C	0.36860000	-1.62010000	-1.13300000
C	1.68260000	-1.22500000	-1.74220000
C	2.35340000	-2.30310000	-2.34900000
C	3.61540000	-2.16690000	-2.90040000
C	4.25750000	-0.92890000	-2.85440000
C	3.61220000	0.14650000	-2.27180000
C	2.32470000	0.02980000	-1.71530000
C	1.83460000	1.29880000	-1.10200000
C	0.44050000	1.51840000	-0.72420000
C	1.14260000	0.50670000	1.51760000
C	0.61810000	-0.60270000	1.53220000
C	0.59740000	-2.02210000	1.91570000
C	2.02870000	-2.54600000	1.67090000
C	3.07210000	-1.94190000	2.59920000
C	3.72130000	-0.56390000	2.61790000
C	3.54300000	0.63300000	1.69710000
C	2.23060000	1.41390000	1.92380000
C	4.52160000	-1.77990000	2.20320000
C	4.91870000	-1.93180000	0.75290000
C	-2.08010000	-1.01840000	-0.55590000
C	-3.05660000	-0.00970000	-0.70050000
C	-4.39620000	-0.27040000	-0.46700000
C	-4.80340000	-1.54990000	-0.07870000
C	-3.85080000	-2.55830000	0.06100000
C	-2.50660000	-2.30620000	-0.17750000
C	-0.08230000	2.84940000	-0.37360000
C	-1.17020000	2.90990000	0.51390000
C	-1.74050000	4.12660000	0.85850000
C	-1.20750000	5.28110000	0.30340000
C	-0.13440000	5.26240000	-0.57500000
C	0.43170000	4.03950000	-0.91080000
H	5.87730000	-0.24410000	0.57850000
H	1.85740000	-3.26580000	-2.36680000
H	4.09850000	-3.02240000	-3.36140000
H	5.24980000	-0.80400000	-3.27560000
H	4.09810000	1.11400000	-2.22880000
H	-0.12510000	-2.61520000	1.34970000
H	0.33130000	-2.10160000	2.97630000

H	2.03560000	-3.63210000	1.82540000
H	2.27320000	-2.37870000	0.61920000
H	2.94560000	-2.31710000	3.61360000
H	3.91720000	-0.24360000	3.64010000
H	3.58810000	0.33860000	0.64440000
H	4.38620000	1.31480000	1.86970000
H	2.11030000	1.65980000	2.98510000
H	2.24300000	2.35340000	1.36520000
H	5.27700000	-2.14280000	2.89650000
H	5.16900000	-2.97600000	0.53720000
H	4.09480000	-1.65180000	0.08310000
H	-2.76300000	0.98520000	-1.01440000
H	-5.12720000	0.52070000	-0.59260000
H	-4.16840000	-3.55150000	0.36200000
H	-1.79170000	-3.10680000	-0.06670000
H	-1.55440000	1.99110000	0.94790000
H	-2.57380000	4.19220000	1.54940000
H	0.24030000	6.19300000	-0.98690000
H	1.26230000	4.00980000	-1.60440000
F	-1.75090000	6.46400000	0.63200000
C	-6.22740000	-1.87950000	0.18970000
O	-6.61950000	-2.98060000	0.52700000
O	-7.04350000	-0.83780000	0.02510000
C	-8.43380000	-1.09030000	0.27030000
H	-8.93820000	-0.14010000	0.10400000
H	-8.80740000	-1.84740000	-0.42210000
H	-8.58050000	-1.42570000	1.29910000

24DEBCOD

Charge 0 *Multiplicity* 1

O	-0.29510000	0.67300000	-1.02140000
O	-0.12940000	-2.49430000	-1.96970000
O	2.74740000	2.33710000	-0.83940000
O	5.80730000	-1.31690000	0.59580000
C	-0.44000000	-0.63140000	-0.47730000
C	0.36110000	-1.51050000	-1.45900000
C	1.79090000	-1.12160000	-1.80910000
C	2.49310000	-2.18550000	-2.39110000
C	3.82470000	-2.08060000	-2.77480000
C	4.49380000	-0.87850000	-2.58800000
C	3.81610000	0.19240000	-2.01930000
C	2.47730000	0.10760000	-1.61390000
C	1.99630000	1.38710000	-0.94980000
C	0.63440000	1.42940000	-0.25510000

C	0.84130000	0.62170000	1.01610000
C	0.24360000	-0.56390000	0.88560000
C	0.32240000	-1.73300000	1.81920000
C	1.63620000	-2.52750000	1.62120000
C	2.71420000	-2.15090000	2.62380000
C	3.39610000	-0.81150000	2.77530000
C	3.18690000	0.43210000	1.93180000
C	1.78900000	1.08370000	2.08420000
C	4.17740000	-2.00970000	2.27520000
C	4.61620000	-2.06280000	0.83200000
C	-1.91400000	-0.98760000	-0.37910000
C	-2.85670000	0.04420000	-0.38390000
C	-4.21050000	-0.23280000	-0.23600000
C	-4.63620000	-1.55210000	-0.07350000
C	-3.69930000	-2.58620000	-0.05450000
C	-2.34680000	-2.30840000	-0.20590000
C	0.08200000	2.82870000	-0.07470000
C	-0.64990000	3.14720000	1.07130000
C	-1.25540000	4.39370000	1.20740000
C	-1.12010000	5.30480000	0.17310000
C	-0.41270000	5.01960000	-0.98520000
C	0.18790000	3.77130000	-1.10220000
H	5.63500000	-0.39930000	0.84920000
H	1.97080000	-3.12410000	-2.53570000
H	4.32860000	-2.93590000	-3.21330000
H	5.53460000	-0.76950000	-2.87530000
H	4.33410000	1.13210000	-1.86570000
H	-0.54050000	-2.38570000	1.66500000
H	0.26600000	-1.37310000	2.85270000
H	1.43120000	-3.59610000	1.74600000
H	1.98070000	-2.40640000	0.59030000
H	2.53730000	-2.62470000	3.58720000
H	3.58460000	-0.56370000	3.81790000
H	3.37600000	0.22310000	0.87530000
H	3.94660000	1.16210000	2.23480000
H	1.38010000	0.85180000	3.07440000
H	1.88440000	2.17250000	2.02200000
H	4.89540000	-2.44930000	2.96350000
H	4.84680000	-3.09440000	0.54540000
H	3.81800000	-1.71200000	0.16740000
H	-2.52750000	1.06990000	-0.50750000
H	-4.93200000	0.57690000	-0.24670000
H	-4.03720000	-3.60920000	0.07620000
H	-1.63340000	-3.12370000	-0.19660000

H	-0.75860000	2.41610000	1.86790000
H	-1.82400000	4.65910000	2.09200000
H	-0.33910000	5.76410000	-1.77050000
H	0.74150000	3.53410000	-2.00530000
F	-1.70010000	6.51290000	0.29410000
C	-6.07370000	-1.90260000	0.08400000
O	-6.48570000	-3.03750000	0.23100000
O	-6.87680000	-0.83910000	0.04570000
C	-8.27800000	-1.11020000	0.18890000
H	-8.77220000	-0.14270000	0.12190000
H	-8.61820000	-1.76940000	-0.61240000
H	-8.47460000	-1.57400000	1.15770000

24b-TS3

Charge 0 *Multiplicity* 1

C	-3.53650000	1.37070000	-0.41990000
C	-4.77900000	0.90480000	-0.00610000
C	-4.91090000	-0.40010000	0.46440000
C	-3.79890000	-1.23190000	0.50760000
C	-2.40280000	0.55520000	-0.34360000
C	-2.54050000	-0.76400000	0.12240000
C	-1.12680000	1.20350000	-0.80720000
C	-1.42960000	-1.76370000	0.09550000
O	-1.16490000	2.02540000	-1.72630000
O	-1.67730000	-2.96120000	-0.08400000
C	0.08920000	0.97720000	-0.04000000
C	-0.07370000	-1.29410000	0.28680000
O	0.05460000	-0.04320000	0.87880000
C	1.23440000	1.85420000	0.00800000
C	2.04390000	1.84610000	1.16550000
C	3.13920000	2.68590000	1.26620000
C	3.45780000	3.54360000	0.20840000
C	2.66500000	3.56060000	-0.94250000
C	1.55920000	2.73410000	-1.04710000
C	1.12470000	-2.02640000	-0.00270000
C	2.35680000	-1.60040000	0.54320000
C	3.53020000	-2.28060000	0.27060000
C	1.11320000	-3.16410000	-0.84630000
C	2.28440000	-3.84600000	-1.12320000
C	3.47140000	-3.39340000	-0.55880000
H	-3.42820000	2.38170000	-0.79900000
H	-5.64340000	1.55940000	-0.05310000
H	-5.87830000	-0.77100000	0.78720000
H	-3.89180000	-2.26080000	0.84030000

H	1.78460000	1.19840000	1.99560000
H	3.74560000	2.67970000	2.16480000
H	2.92730000	4.22560000	-1.75880000
H	0.95710000	2.74680000	-1.94440000
H	2.38120000	-0.74090000	1.20070000
H	4.48040000	-1.96820000	0.68940000
H	0.18600000	-3.49510000	-1.29520000
H	2.29510000	-4.71320000	-1.77400000
F	4.60420000	-4.05450000	-0.82890000
C	4.63240000	4.45700000	0.26510000
O	4.94560000	5.21290000	-0.63400000
O	5.30950000	4.36140000	1.40790000
C	6.45380000	5.21840000	1.52790000
H	6.14820000	6.26470000	1.46360000
H	6.87920000	5.00520000	2.50680000
H	7.17600000	4.99470000	0.74010000

1b*

Charge 0 *Multiplicity* 1

C	3.84733100	-1.40879600	0.00750100
C	5.05003600	-0.71745100	0.09215600
C	5.05729000	0.67802700	0.11071200
C	3.86196400	1.38421700	0.04495200
C	2.64453500	-0.70549200	-0.03245100
C	2.65152100	0.69530400	-0.01355200
C	1.36870400	-1.46507600	-0.17155600
C	1.38375600	1.47286600	-0.13164400
O	1.34282200	-2.60443200	-0.58010300
O	1.37383100	2.62661100	-0.49876000
C	0.09591900	-0.75119700	0.24933600
C	0.10101600	0.76026600	0.26309800
O	0.26217700	-0.00740700	1.44494700
C	-1.18671500	-1.49791900	0.08626400
C	-2.00151800	-1.74419300	1.18878500
C	-3.20084700	-2.43237000	1.02641100
C	-3.58712900	-2.87270800	-0.23584200
C	-2.77062400	-2.62773200	-1.33831900
C	-1.57132500	-1.94378800	-1.17901900
C	-1.17919900	1.51311800	0.10737100
C	-2.05623700	1.63678100	1.18270500
C	-3.26047000	2.31681500	1.02367200
C	-1.50842900	2.07475600	-1.12757300
C	-2.71295800	2.75067300	-1.28350500
C	-3.59115000	2.87224900	-0.20841000

H	3.81934900	-2.49274600	-0.03127900
H	5.98589400	-1.26494200	0.13627100
H	5.99890800	1.21417100	0.16939100
H	3.84620100	2.46901100	0.03552800
H	-1.68953200	-1.39583800	2.16806100
H	-3.83286800	-2.62480200	1.88755000
H	-4.52395200	-3.40612800	-0.36234400
H	-3.06921600	-2.97035700	-2.32376700
H	-0.93074100	-1.75536400	-2.03569400
H	-1.78827500	1.19836100	2.13825600
H	-3.94096600	2.41058200	1.86394400
H	-0.82026900	1.98632100	-1.96266300
H	-2.96613400	3.18412600	-2.24576500
H	-4.53185200	3.39932000	-0.33269900

1SDR*

Charge 0 *Multiplicity* 1

C	1.46219700	3.24794300	-2.51737800
C	1.65598600	3.30574700	-3.88531000
C	1.68353800	2.12392400	-4.62741400
C	1.51588800	0.91042900	-3.98598000
C	1.32060600	2.02239700	-1.84540600
C	1.34510200	0.83153500	-2.59325300
C	1.10436400	2.17496500	-0.37205900
C	1.17063600	-0.57199200	-2.09803600
O	0.66865800	3.23877700	0.06470600
O	0.78355000	-1.43583900	-2.88173600
C	1.51939400	1.14593900	0.56905200
C	1.60223500	-0.96085600	-0.76176900
O	1.78070800	-0.10118400	0.22555200
C	1.68009400	1.36872400	2.00788800
C	1.62925500	0.26524700	2.87988500
C	1.81615900	0.43219600	4.24489800
C	2.05656100	1.69995000	4.76962500
C	2.10653700	2.79935000	3.91536500
C	1.91918500	2.64449700	2.54831000
C	1.97540200	-2.32428700	-0.37319800
C	1.47494600	-3.46701200	-1.02248800
C	1.85085900	-4.73411500	-0.59171400
C	2.86445600	-2.49893600	0.70610400
C	3.23239300	-3.76916500	1.12452200
C	2.72639700	-4.89527600	0.47818800
H	1.41241200	4.15440200	-1.92567500
H	1.78143000	4.26619900	-4.37446100

H	1.83083300	2.15212100	-5.70211400
H	1.50950300	-0.01638600	-4.54727500
H	1.42577300	-0.72328600	2.48138900
H	1.76518800	-0.43036400	4.90145900
H	2.19944700	1.83142200	5.83745500
H	2.29463500	3.79010300	4.31652700
H	1.95641300	3.50612700	1.89593400
H	0.78749800	-3.35394300	-1.84784100
H	1.44653700	-5.60496600	-1.09788400
H	3.28162400	-1.62923300	1.20284100
H	3.92650800	-3.87895600	1.95156800
H	3.01582700	-5.88902400	0.80442200

1DOXEPY*

Charge 0 *Multiplicity* 1

C	1.44846300	3.25195600	-2.52265400
C	1.64004200	3.31331400	-3.88939200
C	1.67493100	2.13194900	-4.63383000
C	1.51631700	0.91770200	-3.99435900
C	1.31500800	2.02438900	-1.84917500
C	1.34660000	0.83288500	-2.60023900
C	1.10397500	2.18519800	-0.37675100
C	1.18314200	-0.57502000	-2.11705900
O	0.68947400	3.25375500	0.06160500
O	0.82408800	-1.44198600	-2.90735800
C	1.50503800	1.14266100	0.56326800
C	1.59490500	-0.95778700	-0.76892800
O	1.72609300	-0.09583400	0.20792200
C	1.67378300	1.35661200	2.00396900
C	1.59889000	0.25333700	2.87357200
C	1.79942300	0.41254300	4.23801900
C	2.07423400	1.67239900	4.76405000
C	2.14480900	2.77204000	3.91159600
C	1.94524600	2.62469600	2.54528200
C	1.97452700	-2.31727800	-0.36877400
C	1.48600800	-3.46546800	-1.01588900
C	1.86418700	-4.72806600	-0.57366200
C	2.85469400	-2.47960500	0.71867400
C	3.22273300	-3.74560700	1.15092000
C	2.72879900	-4.87806700	0.50677700
H	1.39557200	4.15706700	-1.92936400
H	1.75968900	4.27524600	-4.37707900
H	1.82193100	2.16271600	-5.70849900
H	1.51693700	-0.00840700	-4.55667500

H	1.36599500	-0.72903200	2.47528600
H	1.73067700	-0.44998900	4.89308400
H	2.22616600	1.79801600	5.83130700
H	2.35823300	3.75744000	4.31341900
H	1.99672200	3.48694600	1.89445900
H	0.80688100	-3.36030400	-1.84943900
H	1.47024000	-5.60428000	-1.07883600
H	3.26526500	-1.60416000	1.21166400
H	3.90895000	-3.84655800	1.98569000
H	3.02006700	-5.86823900	0.84209400

1b-TS3*

Charge 0 *Multiplicity* 1

C	-3.62479300	1.33476100	-0.42065700
C	-4.87336700	0.81122500	-0.11079800
C	-4.99295900	-0.52290100	0.27297900
C	-3.86083600	-1.32415900	0.33693100
C	-2.47358000	0.54840100	-0.31994100
C	-2.59792200	-0.79698400	0.06024300
C	-1.18980300	1.24741800	-0.68840600
C	-1.45333100	-1.76252500	0.04007700
O	-1.20890700	2.12683500	-1.54942600
O	-1.64909100	-2.94966800	-0.21133300
C	0.00669800	0.98137500	0.09629900
C	-0.11883900	-1.25497100	0.32557600
O	-0.06894900	-0.04686100	1.01215800
C	1.17686600	1.82566000	0.15139500
C	1.95558600	1.83275000	1.32849800
C	3.06829800	2.65202900	1.43274500
C	3.43699300	3.47007600	0.36461100
C	2.67602900	3.47126000	-0.80375800
C	1.55114400	2.66733500	-0.91628700
C	1.11683200	-1.93510100	0.04172800
C	2.30911600	-1.51863400	0.66962600
C	3.50943700	-2.15649500	0.40052000
C	1.17363300	-3.01561000	-0.86789300
C	2.38068600	-3.64365400	-1.12845100
C	3.55205000	-3.22077000	-0.49911200
H	-3.51915200	2.36339800	-0.74838200
H	-5.75429400	1.44173500	-0.17613900
H	-5.96721700	-0.94017700	0.50623200
H	-3.93359100	-2.37668000	0.58992100
H	1.65181700	1.21432300	2.16657200
H	3.64889300	2.65735700	2.34945200

H	4.31309600	4.10590200	0.44329100
H	2.96306800	4.10382300	-1.63735600
H	0.95909000	2.67217200	-1.82065500
H	2.27516600	-0.70301100	1.37959700
H	4.41562000	-1.82580000	0.89751900
H	0.26971500	-3.34628000	-1.36167700
H	2.41076700	-4.46874800	-1.83260400
H	4.49308800	-3.71931100	-0.70848700

1b**

Charge 0 *Multiplicity* 1

C	3.84767100	-1.40912500	0.00453000
C	5.05070900	-0.71812100	0.08902900
C	5.05828000	0.67728600	0.10860600
C	3.86296000	1.38382000	0.04406100
C	2.64492500	-0.70565600	-0.03486700
C	2.65222400	0.69540900	-0.01488600
C	1.36894800	-1.46469100	-0.17258600
C	1.38460900	1.47319000	-0.13023400
O	1.34154200	-2.60423600	-0.58122100
O	1.37381000	2.62814000	-0.49422300
C	0.09709200	-0.75080300	0.25043900
C	0.10233100	0.76006000	0.26475400
O	0.26439400	-0.00774400	1.44659000
C	-1.18644200	-1.49590200	0.08730700
C	-1.99827100	-1.74797200	1.19080200
C	-3.19845700	-2.43482000	1.02777200
C	-3.58852500	-2.86771800	-0.23602800
C	-2.77528200	-2.61606100	-1.33962600
C	-1.57523000	-1.93331800	-1.17977000
C	-1.17870300	1.51149900	0.10894600
C	-2.05388400	1.63944500	1.18540900
C	-3.25901200	2.31795900	1.02523200
C	-1.51113000	2.06579000	-1.12855000
C	-2.71657200	2.74006700	-1.28559500
C	-3.59255600	2.86687700	-0.20913800
H	3.82070600	-2.49313900	-0.03371200
H	5.98636500	-1.26599800	0.13259900
H	5.99997400	1.21328800	0.16756000
H	3.84876700	2.46866400	0.03676700
H	-1.68410600	-1.40551000	2.17150200
H	-3.82806200	-2.63200400	1.88964300
H	-4.52592100	-3.40009000	-0.36297400
H	-3.07718700	-2.95223500	-2.32633800

H	-0.93790400	-1.73840600	-2.03753100
H	-1.78464600	1.20555900	2.14276100
H	-3.93807700	2.41529400	1.86630500
H	-0.82550300	1.97190300	-1.96522800
H	-2.97248100	3.16758400	-2.24984200
H	-4.53399200	3.39251100	-0.33431600

1SDR**

Charge 0 *Multiplicity* 1

C	1.47402400	3.24637500	-2.51560300
C	1.67467800	3.30308300	-3.88281200
C	1.69606700	2.12131900	-4.62539300
C	1.51633400	0.90877100	-3.98518100
C	1.32021400	2.02169300	-1.84499600
C	1.34040200	0.83072600	-2.59319600
C	1.09708700	2.17349700	-0.37289300
C	1.16139100	-0.57137600	-2.09684400
O	0.65130200	3.23404700	0.06218600
O	0.76855700	-1.43587600	-2.87730800
C	1.51883700	1.14730500	0.56775600
C	1.60029900	-0.95827200	-0.76289700
O	1.78545700	-0.09825700	0.22267600
C	1.67725300	1.36770200	2.00696400
C	1.63207300	0.26127000	2.87578600
C	1.81344000	0.42644200	4.24184200
C	2.04353000	1.69466400	4.77042800
C	2.08914600	2.79665400	3.91901700
C	1.90756900	2.64361200	2.55091700
C	1.97785500	-2.32092700	-0.37585800
C	1.44868900	-3.46461700	-0.99961300
C	1.82698700	-4.73098500	-0.56837500
C	2.89470300	-2.49183900	0.68015500
C	3.26592500	-3.76132600	1.09857200
C	2.73263200	-4.88897700	0.47700500
H	1.42833300	4.15361800	-1.92461900
H	1.80990700	4.26254700	-4.37138000
H	1.84866700	2.14893000	-5.69939400
H	1.50766600	-0.01772200	-4.54701100
H	1.43613400	-0.72792700	2.47502600
H	1.76609900	-0.43788800	4.89630100
H	2.18144100	1.82430600	5.83914100
H	2.26968600	3.78761700	4.32312200
H	1.94283700	3.50693700	1.90059600
H	0.73752100	-3.35251100	-1.80499200

H	1.40046400	-5.60332300	-1.05333700
H	3.32892600	-1.62032600	1.15903100
H	3.98245000	-3.86970000	1.90644900
H	3.02415300	-5.88209000	0.80342900

1DOXEPY**

Charge 0 *Multiplicity* 1

C	1.46582600	3.24958200	-2.52105100
C	1.66506000	3.30898600	-3.88701000
C	1.69032500	2.12743900	-4.63178100
C	1.51586200	0.91470400	-3.99334500
C	1.31640800	2.02339400	-1.84872300
C	1.34059000	0.83163600	-2.59998100
C	1.09671200	2.18414200	-0.37786500
C	1.16864400	-0.57389800	-2.11498600
O	0.67171000	3.25010200	0.05744100
O	0.79866600	-1.44072600	-2.90066000
C	1.50378000	1.14468700	0.56233300
C	1.59049100	-0.95489100	-0.76977200
O	1.72918400	-0.09282000	0.20562400
C	1.67064400	1.35605900	2.00342100
C	1.60932400	0.24840200	2.86894500
C	1.80470400	0.40555200	4.23441800
C	2.06097400	1.66721000	4.76584700
C	2.11868800	2.77084100	3.91741700
C	1.92490600	2.62557600	2.54994700
C	1.97560000	-2.31350100	-0.37203700
C	1.45662800	-3.46282000	-0.99230700
C	1.83801100	-4.72456500	-0.55007400
C	2.88619900	-2.47175200	0.69035600
C	3.25840900	-3.73688000	1.12222500
C	2.73528700	-4.87102100	0.50425100
H	1.41917900	4.15572200	-1.92867600
H	1.79745800	4.26951100	-4.37425000
H	1.84286600	2.15705200	-5.70573200
H	1.51139000	-0.01128400	-4.55590500
H	1.38987200	-0.73590100	2.46778300
H	1.74601000	-0.46022900	4.88612900
H	2.20812800	1.79082500	5.83401100
H	2.31787200	3.75762500	4.32317900
H	1.96798600	3.49086600	1.90258300
H	0.75152400	-3.35875500	-1.80436100
H	1.42019600	-5.60236600	-1.03282000
H	3.31524400	-1.59443900	1.16424800

H	3.96916800	-3.83642900	1.93634300
H	3.02921600	-5.86045800	0.83953300

1b-TS3**

Charge 0 *Multiplicity* 1

C	-3.61329100	1.33071400	-0.44026500
C	-4.86350000	0.81646900	-0.12104100
C	-4.98779100	-0.51191900	0.28079000
C	-3.85870800	-1.31685800	0.35256200
C	-2.46480900	0.54112800	-0.33221200
C	-2.59417700	-0.79897700	0.06563600
C	-1.17896600	1.23255400	-0.70904900
C	-1.45368800	-1.76934500	0.05441800
O	-1.19530000	2.09832900	-1.58406900
O	-1.65439000	-2.95903900	-0.18187700
C	0.01367000	0.97828400	0.08544300
C	-0.11721100	-1.26210800	0.32852200
O	-0.06190000	-0.04782600	1.00276400
C	1.17708700	1.83085300	0.14946300
C	1.95175800	1.83709500	1.32958600
C	3.05792400	2.66411700	1.44232400
C	3.42438800	3.49121600	0.38029600
C	2.66767000	3.49323900	-0.79092200
C	1.54932600	2.68142400	-0.91212900
C	1.11630500	-1.94464900	0.04217500
C	2.31357200	-1.52126800	0.65620300
C	3.51196200	-2.16132100	0.38347000
C	1.16647200	-3.03345000	-0.85803900
C	2.37168500	-3.66351200	-1.12247300
C	3.54786400	-3.23424300	-0.50636700
H	-3.50526800	2.35523700	-0.77996000
H	-5.74179500	1.45004800	-0.19238500
H	-5.96312500	-0.92186500	0.52248100
H	-3.93608400	-2.36532100	0.62075300
H	1.65092800	1.21164300	2.16348300
H	3.63531500	2.66822600	2.36109200
H	4.29533600	4.13325200	0.46594100
H	2.95302300	4.13249000	-1.62004200
H	0.96150800	2.68660300	-1.81922200
H	2.28596900	-0.69851700	1.35838500
H	4.42207600	-1.82527900	0.86965700
H	0.25928400	-3.36856300	-1.34287300
H	2.39647700	-4.49502000	-1.81929200
H	4.48746300	-3.73434700	-0.71862300

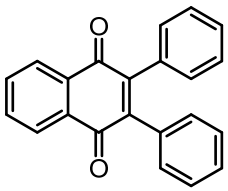
7. Synthetic procedure and spectroscopic data for all the compound characterization

General procedure 1 (GP1): K_3PO_4 (6 equiv.) and the corresponding $ArB(OH)_2$ (2.4 equiv.) were stirred in distilled H_2O for 30 min to form a homogeneous solution. A solution of 2,3-dibromo-1,4-naphthoquinone in 1,4-dioxane was added at room temperature. Then, the $Pd(OAc)_2$ (6 mol%) in 1,4-dioxane was added, and the reaction mixture was vigorously stirred at r.t. until full consumption of the starting dibromide observed by TLC. 1,4-Dioxane was evaporated, dichloromethane and H_2O were added to the formed suspension with formation of two clear layers. The organic layer was combined with two additional dichloromethane extracts and evaporated with silica gel. The crude product was separated by flash chromatography on silica gel (eluting with petroleum ether/ethyl acetate = 2/1) and recrystallized from *n*-hexane/$CHCl_3$ to give pure product.

General procedure 2 (GP2): K_3PO_4 (6.0 equiv.) and the corresponding $ArB(OH)_2$ (1.0 equiv.) were stirred in distilled H_2O for 30 min to form a homogeneous solution. A solution of 2,3-dibromo-1,4-naphthoquinone in 1,4-dioxane was added at room temperature. Then, the $Pd(OAc)_2$ (6 mol%) in 1,4-dioxane was added, and the reaction mixture was vigorously stirred at r.t. until full consumption of the starting dibromide observed by TLC. 1,4-Dioxane was evaporated, dichloromethane and H_2O were added to the formed suspension with formation of two clear layers. The organic layer was combined with two additional dichloromethane extracts and evaporated with silica gel. The crude product was purified by flash chromatography on silica gel (eluting with petroleum ether/ethyl acetate = 2/1).

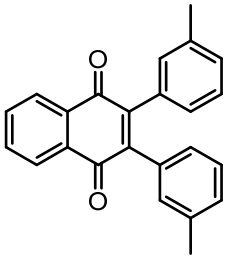
General procedure 3 (GP3): K_3PO_4 (6 equiv.) and the corresponding $ArB(OH)_2$ (1.2 equiv.) were stirred in distilled H_2O for 30 min to form a homogeneous solution. A solution of monobromide in 1,4-dioxane was added at room temperature. Then, the $Pd(OAc)_2$ (6 mol%) in 1,4-dioxane was added, and the reaction mixture was vigorously stirred at r.t. until full consumption of the starting dibromide observed by TLC. 1,4-Dioxane was evaporated, dichloromethane and H_2O were added to the formed suspension with formation of two clear layers. The organic layer was combined with two additional dichloromethane extracts and evaporated with silica gel. The crude product was purified by flash chromatography on silica gel (eluting with petroleum ether/ethyl acetate = 2/1).

General procedure 4 (GP4): To a stirred solution of diaryl naphthoquinone (**na**) in ethanol were added H_2O_2 (15% in H_2O), and NaOH (4.0 M in H_2O) successively at room temperature. The reaction mixture was vigorously stirred at r.t. until full consumption of the starting **na** observed by TLC. The solvent was removed under reduced pressure, and the residue was purified on silica gel by using a flash chromatography column (eluting with petroleum ether/ethyl acetate = 1/1).



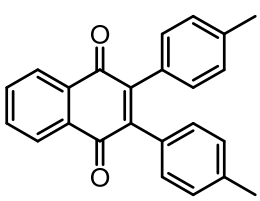
2,3-Diphenyl-1,4-naphthoquinone (1a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), benzeneboronic acid (859 mg, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **1a** as a yellow solid (687 mg, 75%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.93 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.23 – 7.19 (m, 6H), 7.12 – 7.08 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.30, 145.34, 134.17, 133.66, 131.78, 130.23, 127.74, 127.26, 126.06. HRMS (ESI) calcd. for $C_{22}H_{15}O_2^+$ 311.1067 [M+H$^+$], found 311.1065.



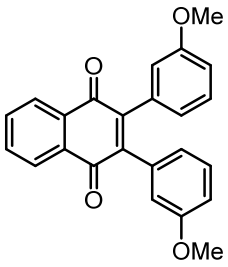
2,3-Di-*m*-tolyl-1,4-naphthoquinone (2a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-tolylboronic acid (957 mg, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **2a** as a yellow solid (312 mg, 31%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.79 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 2H), 7.06 – 7.03 (m, 2H), 6.92 (tt, *J* = 1.6, 0.8 Hz, 2H), 6.84 (dt, *J* = 7.6, 1.7 Hz, 2H), 2.25 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.10, 146.01, 137.19, 133.92, 133.32, 132.33, 131.21, 129.10, 127.64, 127.61, 126.73, 21.50. HRMS (ESI) calcd. for $C_{24}H_{19}O_2^+$ 339.1380 [M+H$^+$], found 339.1379.



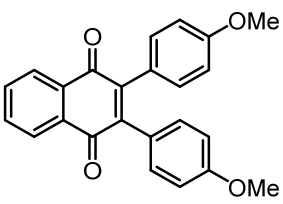
2,3-Di-*p*-tolyl-1,4-naphthoquinone (3a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-tolylboronic acid (957 mg, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **3a** as a yellow solid (280mg, 28%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.77 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 4H), 6.98 (d, *J* = 7.9 Hz, 4H), 2.31 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.13, 145.61, 138.20, 133.85, 132.37, 130.64, 130.53, 128.56, 126.71, 21.50. HRMS (ESI) calcd. for $C_{24}H_{19}O_2^+$ 339.1380 [M+H$^+$], found 339.1382.



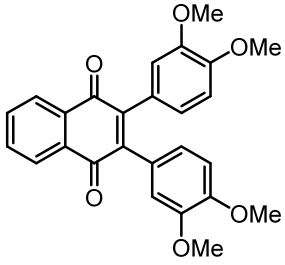
2,3-Bis(3-methoxyphenyl)-1,4-naphthoquinone (4a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-methoxyphenylboronic acid (1.07 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **4a** as a yellow solid (756 mg, 69%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.79 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.19 – 7.15 (m, 2H), 6.80 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 2H), 6.71 (ddd, *J* = 7.6, 1.6, 1.0 Hz, 2H), 6.61 (dd, *J* = 2.6, 1.5 Hz, 2H), 3.65 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.78, 159.01, 145.77, 134.59, 134.01, 132.26, 128.86, 126.78, 123.08, 115.85, 114.55, 55.32. HRMS (ESI) calcd. for $C_{24}H_{19}O_4^+$ 371.1278 [M+H$^+$], found 371.1278.



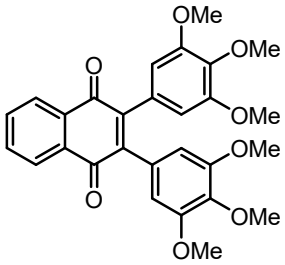
2,3-Bis(4-methoxyphenyl)-1,4-naphthoquinone (5a)

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-methoxyphenylboronic acid (1.07 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **5a** as a dark-red solid (730 mg, 67%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.77 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.05 – 7.01 (m, 4H), 6.80 – 6.76 (m, 4H), 3.78 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.20, 159.54, 144.89, 133.81, 132.41, 132.38, 126.67, 125.84, 113.41, 55.31. HRMS (ESI) calcd. for $C_{24}H_{19}O_4^+$ 371.1278 [M+H$^+$], found 371.1277.



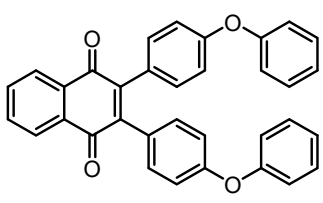
2,3-Bis(3,4-dimethoxyphenyl)-1,4-naphthoquinone (6a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3,4-dimethoxyphenylboronic acid (1.28 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **6a** as a red solid (598 mg, 47%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.79 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.79 – 6.73 (m, 4H), 6.59 (d, *J* = 1.8 Hz, 2H), 3.86 (s, 6H), 3.64 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.97, 149.09, 148.25, 144.81, 133.78, 132.23, 126.60, 125.97, 124.00, 114.13, 110.44, 55.83, 55.79. HRMS (ESI) calcd. for $C_{26}H_{23}O_6^+$ 431.1489 [M+H$^+$], found 431.1489.



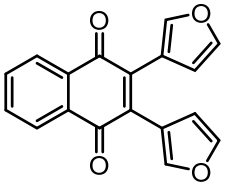
2,3-Bis(3,4,5-trimethoxyphenyl)-1,4-naphthoquinone (7a):

2,3-Dibromo-1,4-naphthoquinone (697 mg, 2.22 mmol), 3,4,5,-trimethoxyphenylboronic acid (1.0 g, 4.72 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP1** affording **7a** as a red solid (517mg, 22%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.34 (s, 4H), 3.82 (s, 6H), 3.66 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.79, 152.86, 145.38, 138.48, 134.11, 132.20, 128.77, 126.79, 108.47, 61.03, 56.30. HRMS (ESI) calcd. for $C_{28}H_{27}O_8^+$ 491.1700 [M+H$^+$], found 491.1701.



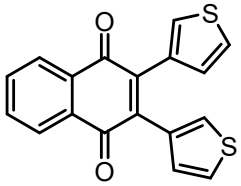
2,3-Bis(4-phenoxyphenyl)-1,4-naphthoquinone (8a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-phenoxyphenyl boronic acid (1.51 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording 8a as a brick-red solid (517 mg, 22%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.37 – 7.32 (m, 4H), 7.15 – 7.11 (m, 2H), 7.04 – 7.00 (m, 4H), 7.04 – 7.00 (m, 4H), 6.91 – 6.87 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.91, 157.63, 156.61, 145.10, 134.00, 132.56, 132.29, 129.95, 128.05, 126.76, 123.86, 119.53, 117.80. HRMS (ESI) calcd. for $C_{34}H_{23}O_4^+$ 495.1591 [M+H$^+$], found 495.1595.



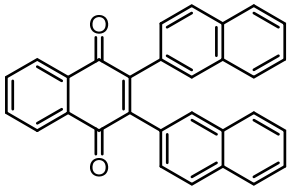
2,3-Di(furan-3-yl)-1,4-naphthoquinone (9a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-furanboronic acid (1.51 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **9a** as a red solid (619 mg, 72%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.86 (dd, *J* = 1.5, 0.8 Hz, 2H), 7.75 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.39 (t, *J* = 1.7 Hz, 2H), 6.22 (dd, *J* = 1.9, 0.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.95, 145.47, 142.36, 136.47, 133.93, 132.26, 126.73, 117.52, 111.97. HRMS (ESI) calcd. for $C_{18}H_{11}O_4^+$ 291.0652 [M+H$^+$], found 291.0681.



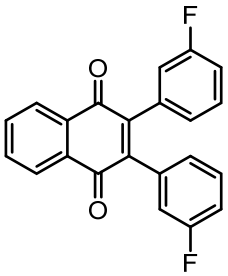
2,3-Di(thiophen-3-yl)-1,4-naphthoquinone (10a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-thiopheneboronic acid (1.51 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **10a** as a red solid (505 mg, 54%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.78 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.37 (dd, *J* = 3.0, 1.2 Hz, 2H), 7.20 (dd, *J* = 5.1, 3.0 Hz, 2H), 6.78 (dd, *J* = 5.0, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.58, 139.95, 133.97, 133.21, 132.28, 129.59, 128.85, 126.75, 124.58. HRMS (ESI) calcd. for $C_{18}H_{11}O_2S_2^+$ 323.0195 [M+H$^+$], found 323.0199.



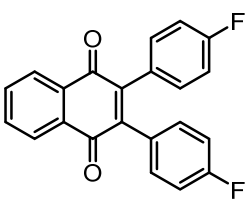
[2,2':3',2''-Ternaphthalene]-1',4'-dione (11a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 2-naphthaleneboronic acid (1.21 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **11a** as an orange-yellow solid (836 mg, 69%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.83 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.72 – 7.68 (m, 6H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.38 (m, 4H), 7.16 (dd, *J* = 8.5, 1.7 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.05, 145.89, 134.08, 132.94, 132.73, 132.39, 130.89, 130.79, 128.53, 127.96, 127.73, 127.39, 126.85, 126.79, 126.21. HRMS (ESI) calcd. for $C_{30}H_{19}O_2^+$ 411.1380 [M+H$^+$], found 411.1379.



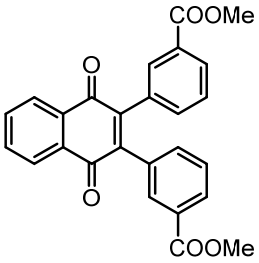
2,3-Bis(3-fluorophenyl)-1,4-naphthoquinone (12a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-fluorophenylboronic acid (986 mg, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **12a** as a yellow solid (678 mg, 66%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.82 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.27 – 7.16 (m, 2H), 6.97 (tdd, *J* = 8.5, 2.4, 1.2 Hz, 2H), 6.85 – 6.81 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.26, 162.26 (d, *J* = 246.4 Hz), 145.04 (d, *J* = 2.0 Hz), 134.99 (d, *J* = 8.3 Hz), 134.31, 132.07, 129.57 (d, *J* = 8.4 Hz), 126.92, 126.30 (d, *J* = 3.1 Hz), 117.65 (d, *J* = 22.4 Hz), 115.72 (d, *J* = 21.2 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -113.09. HRMS (ESI) calcd. for $C_{22}H_{13}F_2O_2^+$ 347.0878 [M+H$^+$], found 347.0878.



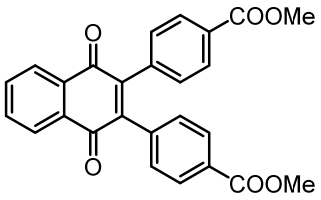
2,3-Bis(4-fluorophenyl)-1,4-naphthoquinone (13a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-fluorophenylboronic acid (986 mg, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **13a** as a yellow solid (441 mg, 43%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.08 – 7.03 (m, 4H), 6.98 – 6.92 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.65, 162.69 (d, *J* = 249.3 Hz), 145.06, 134.19, 132.68 (d, *J* = 8.6 Hz), 132.17, 129.11 (d, *J* = 3.6 Hz), 126.86, 115.20 (d, *J* = 21.8 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.26. HRMS (ESI) calcd. for $C_{22}H_{13}F_2O_2^+$ 347.0878 [M+H$^+$], found 347.0878.



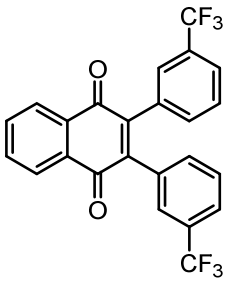
Dimethyl 3,3'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)di-benzoate (14a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-methoxycarbonylphenylboronic acid (1.27 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **14a** as a yellow solid (865 mg, 69%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.93 (dt, *J* = 7.8, 1.5 Hz, 2H), 7.85 – 7.81 (m, 4H), 7.29 (td, *J* = 7.7, 0.6 Hz, 2H), 7.22 (dt, *J* = 7.7, 1.5 Hz, 2H), 3.87 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.39, 166.58, 145.40, 134.93, 134.32, 133.30, 132.11, 131.87, 129.97, 129.76, 128.15, 126.94, 52.34. HRMS (ESI) calcd. for $C_{26}H_{19}O_6^+$ 427.1176 [M+H$^+$], found 427.1176.



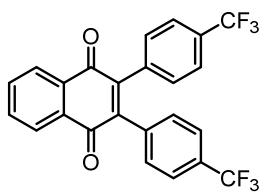
Dimethyl 4,4'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)di-benzoate (15a):

2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-methoxycarbonylphenylboronic acid (1.27 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **15a** as a yellow solid (1.03g, 81%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.91 – 7.88 (m, 4H), 7.82 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.16 – 7.13 (m, 4H), 3.89 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.13, 166.62, 145.47, 137.63, 134.35, 132.05, 130.65, 130.16, 129.13, 126.93, 52.34. HRMS (ESI) calcd. for $C_{26}H_{19}O_6^+$ 427.1176 [M+H$^+$], found 427.1142.

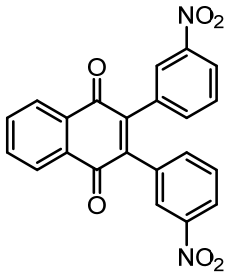


2,3-Bis(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (16a):

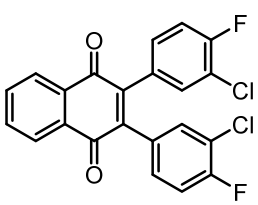
2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-(trifluoro-methyl)phenylboronic acid (1.34 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **16a** as a yellow solid (685 mg, 52%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.19 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.50 (ddt, *J* = 7.8, 1.8, 0.9 Hz, 2H), 7.39 – 7.35 (m, 2H), 7.26 – 7.23 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.05, 145.21, 134.51, 133.91, 133.59, 132.00, 130.59 (q, *J* = 32.7 Hz), 128.56, 127.65 (q, *J* = 3.8 Hz), 127.01, 125.45 (q, *J* = 3.9 Hz), 123.76 (q, *J* = 272.5 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -63.05. HRMS (ESI) calcd. for $C_{24}H_{13}F_6O_2^+$ 447.0814 [M+H$^+$], found 447.0793.



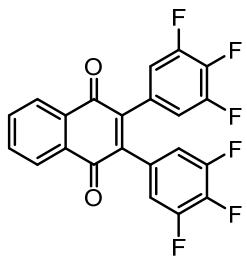
2,3-Bis(4-(trifluoromethyl)phenyl)-1,4-naphthoquinone (17a): 2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-(trifluoromethyl)phenylboronic acid (1.34 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **17a** as a yellow solid (537 mg, 41%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.84 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.54 – 7.52 (m, 4H), 7.22 – 7.19 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.05, 145.12, 136.46, 134.50, 131.99, 130.97, 130.79 (q, *J* = 32.7 Hz), 127.00, 125.02 (q, *J* = 3.8 Hz), 123.91 (q, *J* = 272.1 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.85. HRMS (ESI) calcd. for $C_{24}H_{13}F_6O_2^+$ 447.0814 [M+H$^+$], found 447.0811.



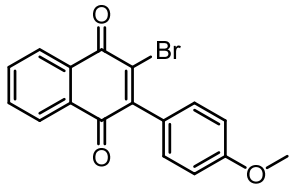
2,3-Bis(3-nitrophenyl)-1,4-naphthoquinone (18a): 2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3-nitrophenyl-boronic acid (1.18 g, 7.04 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP1** affording **18a** as a yellow solid (487 mg, 41%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.24 (dd, *J* = 5.8, 3.3 Hz, 2H), 8.16 (ddd, *J* = 8.0, 2.3, 1.3 Hz, 2H), 8.01 (t, *J* = 1.9 Hz, 2H), 7.88 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.49 – 7.40 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 183.56, 147.94, 144.50, 136.52, 134.82, 134.14, 131.84, 129.35, 127.20, 125.71, 123.93. HRMS (ESI) calcd. for $C_{22}H_{13}N_2O_6^+$ 401.0768 [M+H$^+$], found 401.0760.



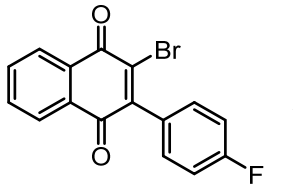
2,3-Bis(3-chloro-4-fluorophenyl)-1,4-naphthoquinone (19a): 2,3-Dibromo-1,4-naphthoquinone (697 mg, 2.22 mmol), 3-chloro-4-fluorophenylboronic acid (921 g, 5.28 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP1** affording **19a** as a yellow solid (383 mg, 42%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.83 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.21 (dd, *J* = 7.0, 2.2 Hz, 2H), 7.05 (t, *J* = 8.7 Hz, 2H), 6.91 (ddd, *J* = 8.5, 4.5, 2.2 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.01, 158.20 (d, *J* = 252.7 Hz), 144.20, 134.50, 133.01, 131.94, 130.63 (d, *J* = 7.5 Hz), 129.78 (d, *J* = 4.0 Hz), 127.02, 121.17 (d, *J* = 18.0 Hz), 116.54 (d, *J* = 21.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -113.93. HRMS (ESI) calcd. for $C_{22}H_{11}Cl_2F_2O_2^+$ 415.0099 [M+H$^+$], found 415.0099.



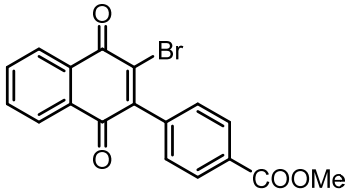
2,3-Bis(3,4,5-trifluorophenyl)-1,4-naphthoquinone (20a): 2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 3,4,5-trifluoro-phenylboronic acid (1.24 g, 7.04 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP1** affording **20a** as a yellow solid (564 mg, 46%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.85 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.78 – 6.70 (m, 4H). Due to multiple conformers harboring $^1J_{CF}$, $^2J_{CF}$, $^3J_{CF}$ and $^4J_{CF}$ coupling with fluorine atoms, the signal peaks in the ^{13}C NMR spectrum were highly overlapped and is not reported herein. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -133.12, -133.18, -157.98, -158.04, -158.09. HRMS (ESI) calcd. for $C_{22}H_9F_6O_2^+$ 419.0501 [M+H$^+$], found 419.0505.



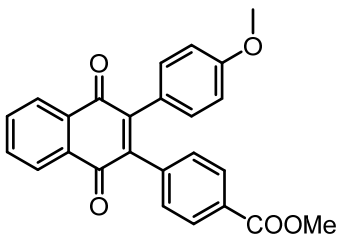
2-Bromo-3-(4-methoxyphenyl)-1,4-naphthoquinone (S1):
2,3-Dibromo-1,4-naphthoquinone (697 mg, 2.22 mmol), 4-methoxyphenylboronic acid (337 mg, 2.22 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP2** affording **S1** as a yellow solid (390 mg, 51%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25 – 8.20 (m, 1H), 8.18 – 8.13 (m, 1H), 7.82 – 7.75 (m, 2H), 7.34 – 7.31 (m, 2H), 7.03 – 7.00 (m, 2H), 3.88 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 181.96, 178.50, 160.61, 149.45, 138.64, 134.45, 134.17, 131.78, 131.35, 127.65, 127.57, 126.22, 113.66, 55.48. HRMS (ESI) calcd. for $C_{17}H_{12}BrO_3^+$ 342.9964 [M+H$^+$], found 343.0027.



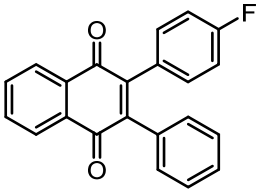
2-Bromo-3-(4-fluorophenyl)-1,4-naphthoquinone (S2):
2,3-Dibromo-1,4-naphthoquinone (697 mg, 2.22 mmol), 4-fluorophenyl-boronic acid (310 mg, 2.22 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP2** affording **S2** as a yellow solid (502 mg, 69%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.27 – 8.21 (m, 1H), 8.18 – 8.13 (m, 1H), 7.83 – 7.77 (m, 2H), 7.37 – 7.32 (m, 2H), 7.22 – 7.16 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 181.62, 178.20, 163.31 (d, *J* = 249.9 Hz), 148.95, 139.51, 134.61, 134.32, 131.59 (d, *J* = 8.4 Hz), 131.25, 129.98 (d, *J* = 3.6 Hz), 127.76, 127.57, 115.49 (d, *J* = 21.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.94. HRMS (ESI) calcd. for $C_{16}H_8BrFO_2^+$ 330.9764 [M+H$^+$], found 330.9739.



Methyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (S3):
2,3-Dibromo-1,4-naphthoquinone (929 mg, 2.96 mmol), 4-methoxycarbonylphenylboronic acid (532 mg, 2.96 mmol), and $Pd(OAc)_2$ (40 mg) were subjected to the **GP2** affording **S3** as a yellow solid (550 mg, 67%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25 – 8.20 (m, 1H), 8.17 – 8.12 (m, 3H), 7.83 – 7.77 (m, 2H), 7.42 – 7.39 (m, 2H), 3.95 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 181.32, 178.01, 166.63, 149.17, 139.60, 138.64, 134.70, 134.40, 131.58, 131.18, 130.95, 129.53, 129.45, 129.42, 127.82, 127.56, 52.46, 52.43. HRMS (ESI) calcd. for $C_{18}H_{12}BrO_4^+$ 370.9913 [M+H$^+$], found 370.9881.

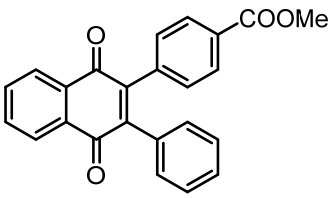


Methyl 4-(3-(4-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (21a):
2-Bromo-3-(4-methoxyphenyl)-1,4-naphthoquinone (408 mg, 1.19 mmol), 4-methoxycarbonylphenylboronic acid (258 mg, 1.43 mmol), and $Pd(OAc)_2$ (16 mg) were subjected to the **GP3** affording **21a** as an orange solid (190 mg, 25%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.23 – 8.16 (m, 2H), 7.94 – 7.91 (m, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.20 – 7.17 (m, 2H), 7.01 – 6.98 (m, 2H), 6.76 – 6.73 (m, 2H), 3.90 (s, 3H), 3.77 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.95, 184.46, 166.90, 159.97, 145.96, 144.32, 138.71, 134.11, 134.08, 132.40, 132.29, 132.21, 130.87, 129.67, 129.09, 126.89, 126.75, 124.92, 113.52, 55.32, 52.33. HRMS (ESI) calcd. for $C_{25}H_{19}O_5^+$ 399.1227 [M+H$^+$], found 399.1227.



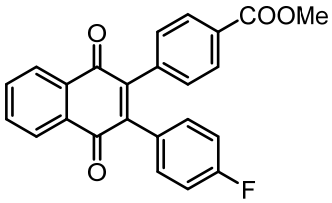
2-(4-Fluorophenyl)-3-phenyl-1,4-naphthoquinone (22a):

2-Bromo-3-(4-fluorophenyl)-1,4-naphthoquinone (521 mg, 1.58 mmol), benzeneboronic acid (231 mg, 1.89 mmol), and $Pd(OAc)_2$ (22 mg) were subjected to the **GP3** affording **22a** as a yellow solid (71 mg, 14%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.17 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.78 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.26 – 7.23 (m, 3H), 7.08 – 7.03 (m, 4H), 6.94 – 6.88 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.78, 184.68, 162.58 (d, *J* = 248.8 Hz), 146.07, 144.83, 134.08, 134.03, 133.23, 132.72, 132.64, 132.19 (d, *J* = 6.8 Hz), 130.60, 129.22 (d, *J* = 3.7 Hz), 128.48, 127.90, 126.77, 126.75, 114.97 (d, *J* = 21.7 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.58. HRMS (ESI) calcd. for $C_{22}H_{14}FO_2^+$ 329.0972 [M+H$^+$], found 329.0972.



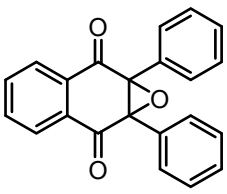
Methyl 4-(1,4-dioxo-3-phenyl-1,4-dihydronaphthalen-2-yl)benzoate (23a)

Methyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzo-ate (548 mg, 1.48 mmol), benzeneboronic acid (217 mg, 1.78 mmol), and $Pd(OAc)_2$ (20 mg) were subjected to the **GP3** affording **23a** as a yellow solid (267 mg, 49%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.23 – 8.17 (m, 2H), 7.92 – 7.89 (m, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.26 – 7.20 (m, 3H), 7.18 – 7.15 (m, 2H), 7.08 – 7.04 (m, 2H), 3.89 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.61, 184.46, 166.80, 146.38, 144.99, 138.23, 134.20, 134.17, 132.85, 132.21, 132.15, 130.77, 130.56, 129.81, 128.99, 128.73, 127.95, 126.90, 126.82, 52.31. HRMS (ESI) calcd. for $C_{24}H_{17}O_4^+$ 369.1121 [M+H$^+$], found 369.1120.



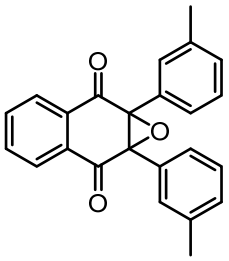
Methyl 4-(3-(4-fluorophenyl)-1,4-dioxo-1,4-dihydro-naphthalen-2-yl)benzoate (24a):

Methyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benz-oate (320 mg, 0.87 mmol), 4-fluorophenylboronic acid (121 mg, 0.87 mmol), and $Pd(OAc)_2$ (12 mg) were subjected to the **GP3** affording **24a** as a yellow solid (200 mg, 60%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.22 – 8.17 (m, 2H), 7.94 – 7.91 (m, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.17 – 7.14 (m, 2H), 7.07 – 7.02 (m, 2H), 6.95 – 6.89 (m, 2H), 3.90 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.51, 184.25, 166.70, 162.79 (d, *J* = 249.4 Hz), 145.24 (d, *J* = 15.1 Hz), 138.07, 134.26, 132.68, 132.60, 132.10, 130.73, 129.98, 129.12, 128.73 (d, *J* = 3.5 Hz), 126.91, 126.85, 115.22 (d, *J* = 21.8 Hz), 52.35, 29.84. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.85. HRMS (ESI) calcd. for $C_{24}H_{16}FO_4^+$ 387.1027 [M+H$^+$], found 387.0993.



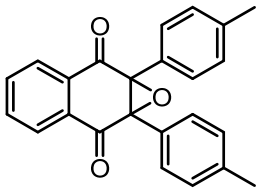
2,3-Diphenyl-1,4-naphthoquinone epoxide (1b):

2,3-Diphenyl-1,4-naphthoquinone (285 mg) were subjected to the **GP4** affording **1b** as a colorless solid (247 mg, 83%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.20 (tdd, *J* = 7.7, 3.9, 2.4 Hz, 10H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.16, 134.62, 132.64, 129.25, 128.74, 128.43, 127.82, 127.64, 71.03. HRMS (ESI) calcd. for $C_{22}H_{15}O_3^+$ 327.1016 [M+H$^+$], found 327.1023.



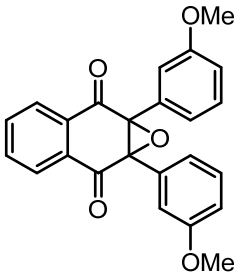
2,3-Di-*m*-tolyl-1,4-naphthoquinone epoxide (2b):

2,3-Di-*m*-tolyl-1,4-naphthoquinone (150 mg) were subjected to the **GP4** affording **2b** as a colorless solid (132 mg, 84%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.08 (t, *J* = 7.5 Hz, 2H), 7.03 (dd, *J* = 1.7, 0.9 Hz, 2H), 7.01 – 6.97 (m, 4H), 2.23 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.33, 137.33, 134.56, 132.63, 129.51, 129.15, 129.02, 127.62, 125.56, 71.01, 21.45. HRMS (ESI) calcd. for $C_{24}H_{19}O_3^+$ 355.1329 [M+H$^+$], found 355.1332.



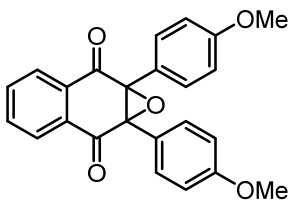
2,3-Di-*p*-tolyl-1,4-naphthoquinone epoxide (3b):

2,3-Di-*p*-tolyl-1,4-naphthoquinone (138 mg) were subjected to the **GP4** affording **3b** as a colorless solid (132 mg, 91%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.08 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.79 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.12 – 7.09 (m, 4H), 7.03 – 6.99 (m, 4H), 2.25 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.52, 138.47, 134.50, 132.66, 128.63, 128.28, 127.59, 126.27, 71.14, 21.44. HRMS (ESI) calcd. for $C_{24}H_{19}O_3^+$ 355.1329 [M+H$^+$], found 355.1335.



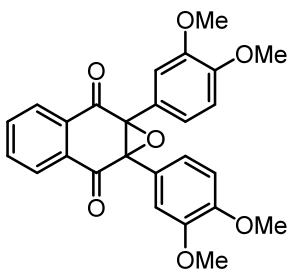
2,3-Dis(3-methoxyphenyl)-1,4-naphthoquinone epoxide (4b):

2,3-Bis(3-methoxyphenyl)-1,4-naphthoquinone (262 mg) were subjected to the **GP4** affording **4b** as a colorless solid (197 mg, 72%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.13 (td, *J* = 7.7, 1.0 Hz, 2H), 6.83 (dt, *J* = 7.6, 1.1 Hz, 2H), 6.76 – 6.73 (m, 4H), 3.69 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.86, 159.07, 134.64, 132.56, 130.66, 128.93, 127.68, 121.02, 114.73, 113.90, 70.88, 55.34. HRMS (ESI) calcd. for $C_{24}H_{19}O_5^+$ 387.1227 [M+H$^+$], found 387.1234.



2,3-Dis(4-methoxyphenyl)-1,4-naphthoquinone epoxide (5b):

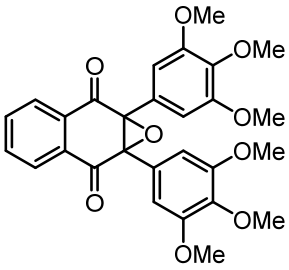
2,3-Bis(4-methoxyphenyl)-1,4-naphthoquinone (733 mg) were subjected to the **GP4** affording **5b** as a colorless solid (338 mg, 72%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.07 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.78 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.15 – 7.12 (m, 4H), 6.76 – 6.72 (m, 4H), 3.73 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.73, 159.70, 134.48, 132.66, 129.70, 127.55, 121.32, 113.43, 71.11, 55.24. HRMS (ESI) calcd. for $C_{24}H_{19}O_5^+$ 387.1227 [M+H$^+$], found 387.1228.



2,3-Bis(3,4-dimethoxyphenyl)-1,4-naphthoquinone epoxide (6b):

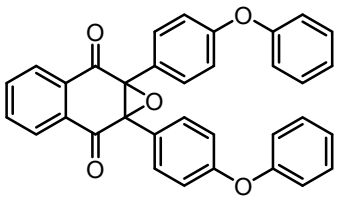
2,3-Bis(3,4-dimethoxyphenyl)-1,4-naphthoquinone (491 mg) were subjected to the **GP4** affording **6b** as a colorless solid (427 mg, 84%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.81 (dd, *J* = 8.3, 2.0 Hz, 2H), 6.72 – 6.70 (m, 4H), 3.81 (s, 6H), 3.75 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.44, 149.27, 148.38, 134.58, 132.60, 127.63, 121.67, 121.41,

111.55, 110.50, 71.09, 55.97, 55.86. HRMS (ESI) calcd. for $C_{26}H_{23}O_7^+$ 447.1438 [M+H$^+$], found 447.1437.



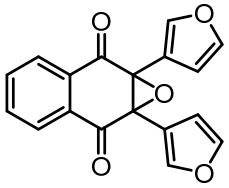
2,3-Bis(3,4,5-trimethoxyphenyl)-1,4-naphthoquinone epoxide (7b):

2,3-Bis(3,4,5-trimethoxyphenyl)-1,4-naphthoquinone (240 mg) were subjected to the **GP4** affording **7b** as a colorless solid (212 mg, 85%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.83 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.44 (s, 4H), 3.78 (s, 6H), 3.72 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.86, 152.85, 138.54, 134.77, 132.48, 127.73, 124.73, 106.09, 71.06, 60.97, 56.27. HRMS (ESI) calcd. for $C_{28}H_{27}O_9^+$ 507.1650 [M+H$^+$], found 507.1652.



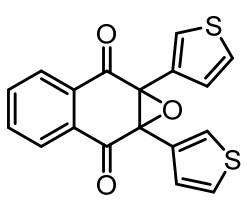
2,3-Bis(4-phenoxyphenyl)-1,4-naphthoquinone epoxide (8b):

2,3-Bis(4-phenoxyphenyl)-1,4-naphthoquinone (883 mg) were subjected to the **GP4** affording **8b** as a colorless solid (778 mg, 85%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.82 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.35 – 7.30 (m, 4H), 7.19 – 7.16 (m, 4H), 7.13 – 7.09 (m, 2H), 6.95 – 6.91 (m, 4H), 6.87 – 6.84 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.29, 157.65, 156.84, 134.66, 132.60, 130.06, 129.94, 127.64, 123.91, 123.72, 119.24, 118.12, 70.90. HRMS (ESI) calcd. for $C_{34}H_{23}O_5^+$ 511.1540 [M+H$^+$], found 511.1514.



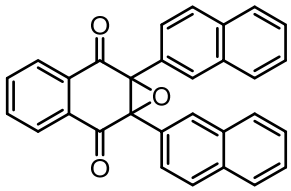
2,3-Di(furan-3-yl)-1,4-naphthoquinone epoxide (9b):

2,3-Di(furan-3-yl)-1,4-naphthoquinone (402 mg) were subjected to the **GP4** affording **9b** as a colorless solid (243 mg, 57%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.46 (dd, *J* = 1.6, 0.8 Hz, 2H), 7.35 (t, *J* = 1.7 Hz, 2H), 6.33 (dd, *J* = 1.9, 0.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.80, 143.38, 142.84, 134.69, 132.26, 127.58, 114.82, 110.75, 66.69. HRMS (ESI) calcd. for $C_{18}H_{11}O_5^+$ 307.0601 [M+H$^+$], found 307.0611.



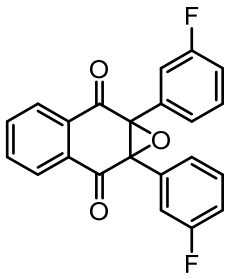
2,3-Di(thiophen-3-yl)-1,4-naphthoquinone epoxide (10b):

2,3-Di(thiophen-3-yl)-1,4-naphthoquinone (230 mg) were subjected to the **GP4** affording **10b** as a colorless solid (173 mg, 72%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.06 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.80 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.20 – 7.17 (m, 4H), 6.95 (dd, *J* = 4.7, 1.6 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.96, 134.63, 132.36, 129.93, 127.56, 127.49, 126.06, 125.37, 68.83. HRMS (ESI) calcd. for $C_{18}H_{11}O_3S_2^+$ 339.0144 [M+H$^+$], found 339.0150.



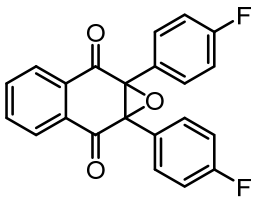
[2,2':3',2''-Ternaphthalene]-1',4'-dione epoxide (11b):

[2,2':3',2''-ternaphthalene]-1',4'-dione (743 mg) were subjected to the **GP4** affording **11b** as a colorless solid (720 mg, 93%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.85 – 7.81 (m, 4H), 7.72 – 7.61 (m, 6H), 7.39 – 7.35 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.29, 134.70, 133.27, 132.65, 132.61, 128.19, 128.11, 127.77, 127.70, 127.62, 126.79, 126.58, 126.24, 125.39, 71.47. HRMS (ESI) calcd. for $C_{30}H_{19}O_3^+$ 427.1329 [M+H$^+$], found 427.1335.



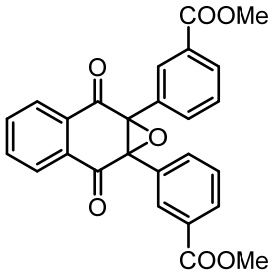
2,3-Bis(3-fluorophenyl)-1,4-naphthoquinone epoxide (12b):

2,3-Bis(3-fluorophenyl)-1,4-naphthoquinone (225 mg) were subjected to the **GP4** affording **12b** as a colorless solid (194 mg, 82%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.83 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.23 – 7.17 (m, 2H), 7.01 (ddd, *J* = 7.7, 1.6, 1.0 Hz, 2H), 6.96 – 6.89 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.15, 162.30 (d, *J* = 247.0 Hz), 134.91, 132.35, 131.39 (d, *J* = 8.0 Hz), 129.67 (d, *J* = 8.1 Hz), 127.78, 124.20 (d, *J* = 3.0 Hz), 116.13 (d, *J* = 21.1 Hz), 115.60 (d, *J* = 23.3 Hz), 70.37 (d, *J* = 2.2 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.67. HRMS (ESI) calcd. for $C_{22}H_{13}F_2O_3^+$ 363.0827 [M+H$^+$], found 363.0837.



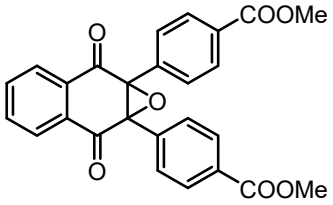
2,3-Bis(4-fluorophenyl)-1,4-naphthoquinone epoxide (13b):

2,3-Bis(4-fluorophenyl)-1,4-naphthoquinone (522 mg) were subjected to the **GP4** affording **13b** as a colorless solid (441 mg, 81%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.82 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.21 – 7.16 (m, 4H), 6.94 – 6.88 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.83, 162.84 (d, *J* = 248.0 Hz), 134.79, 132.45, 130.25 (d, *J* = 8.2 Hz), 127.69, 124.98 (d, *J* = 3.0 Hz), 115.20 (d, *J* = 21.9 Hz), 70.63. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.97. HRMS (ESI) calcd. for $C_{22}H_{13}F_2O_3^+$ 363.0827 [M+H$^+$], found 363.0838.



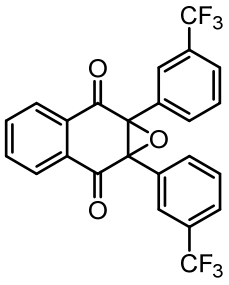
Dimethyl 3,3'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)dibenzoate epoxide (14b):

Dimethyl 3,3'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)dibenzoate (655 mg) were subjected to the **GP4** affording **14b** as a colorless solid (322 mg, 47%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.93 (td, *J* = 1.8, 0.5 Hz, 2H), 7.87 – 7.81 (m, 4H), 7.40 (ddd, *J* = 7.7, 1.8, 1.2 Hz, 2H), 7.29 – 7.25 (m, 2H), 3.86 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.28, 166.43, 134.88, 132.66, 132.36, 130.11, 130.00, 129.66, 129.60, 128.18, 127.76, 70.57, 52.31. HRMS (ESI) calcd. for $C_{26}H_{19}O_7^+$ 443.1125 [M+H$^+$], found 443.1127.



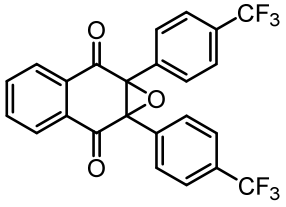
Dimethyl 4,4'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)-dibenzoate epoxide (15b):

Dimethyl 4,4'-(1,4-dioxo-1,4-dihydronaphthalene-2,3-diyl)dibenzoate (185 mg) were subjected to the **GP4** affording **15b** as a colorless solid (133 mg, 69%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.88 – 7.82 (m, 6H), 7.31 – 7.28 (m, 4H), 3.86 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.10, 166.54, 134.97, 133.84, 132.36, 130.68, 129.23, 128.43, 127.81, 70.63, 52.34. HRMS (ESI) calcd. for $C_{26}H_{19}O_7^+$ 443.1125 [M+H$^+$], found 443.1132.



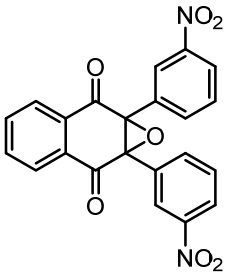
2,3-Bis(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone epoxide (16b):

2,3-Bis(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (600 mg) were subjected to the **GP4** affording **16b** as a colorless solid (520 mg, 84%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.86 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.47 – 7.44 (m, 4H), 7.41 (dt, *J* = 7.8, 1.5 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 2H). **^{13}C NMR** (101 MHz, CDCl3) δ 189.86, 135.08, 132.29, 131.78, 130.62 (q, *J* = 32.9 Hz), 130.08, 128.57, 127.85, 125.84 (q, *J* = 3.7 Hz), 125.23 (q, *J* = 3.8 Hz), 123.71 (q, *J* = 272.4 Hz), 70.37. **^{19}F NMR** (376 MHz, CDCl3) δ -63.12. HRMS (ESI) calcd. for $C_{24}H_{13}F_6O_3^+$ 463.0763 [M+H$^+$], found 463.0770.



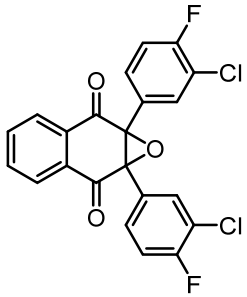
2,3-Bis(4-(trifluoromethyl)phenyl)-1,4-naphthoquinone epoxide (17b):

2,3-Bis(3-(trifluoromethyl)phenyl)-1,4-naphthoquinone (327 mg) were subjected to the **GP4** affording **17b** as a colorless solid (72 mg, 22%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.86 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.50 – 7.48 (m, 4H), 7.36 – 7.34 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 189.91, 135.07, 132.85, 132.24, 131.24 (q, *J* = 32.7 Hz), 128.79, 127.85, 125.14 (q, *J* = 272.4 Hz), 125.12 (q, *J* = 3.6 Hz), 70.42. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.92. HRMS (ESI) calcd. for $C_{24}H_{13}F_6O_3^+$ 463.0763 [M+H$^+$], found 463.0768.



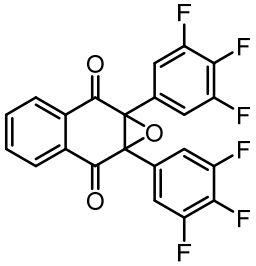
2,3-Bis(3-nitrophenyl)-1,4-naphthoquinone epoxide (18b):

2,3-Bis(3-nitrophenyl)-1,4-naphthoquinone (428 mg) were subjected to the **GP4** affording **18b** as a colorless solid (108 mg, 24%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.16 – 8.07 (m, 6H), 7.89 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.60 (ddd, *J* = 7.7, 1.7, 1.1 Hz, 2H), 7.46 – 7.42 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 189.14, 147.97, 135.36, 134.23, 132.05, 130.95, 129.45, 128.02, 124.31, 123.46, 70.08. HRMS (ESI) calcd. for $C_{22}H_{13}N_2O_7^+$ 417.0717 [M+H$^+$], found 417.0722.

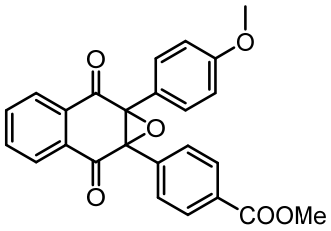


2,3-Bis(3-chloro-4-fluorophenyl)-1,4-naphthoquinone epoxide (19b):

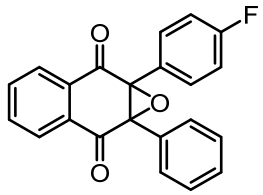
2,3-Bis(3-chloro-4-fluorophenyl)-1,4-naphthoquinone (383 mg) were subjected to the **GP4** affording **19b** as a colorless solid (360 mg, 91%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.85 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.30 (dd, *J* = 6.8, 2.2 Hz, 2H), 7.09 (ddd, *J* = 8.5, 4.5, 2.1 Hz, 2H), 7.03 (t, *J* = 8.6 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 189.86, 158.38 (d, *J* = 251.6 Hz), 135.08, 132.18, 130.74, 128.28 (d, *J* = 7.7 Hz), 127.84, 125.98 (d, *J* = 4.1 Hz), 121.32 (d, *J* = 18.3 Hz), 116.56 (d, *J* = 21.8 Hz), 70.02. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -113.51. HRMS (ESI) calcd. for $C_{22}H_{11}Cl_2F_2O_3^+$ 431.0048 [M+H$^+$], found 431.0054.



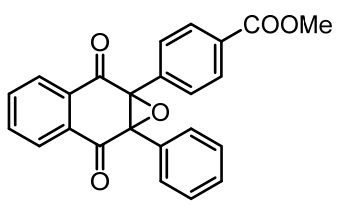
2,3-Bis(3,4,5-trifluorophenyl)-1,4-naphthoquinone epoxide (20b): 2,3-Bis(3,4,5-trifluorophenyl)-1,4-naphthoquinone (374 mg) were subjected to the **GP4**. Purification procedure of **20b**: After the reaction is complete, the reaction mixture was diluted with plenty of water, and the mixture was allowed to stand in the dark for sedimentation. The solid was washed with water and collected by filtration and dried in air overnight affording **20b** as a colorless solid (356 mg, 92%). **^{1}H NMR** (400 MHz, Chloroform-d) δ 8.09 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.86 (dd, *J* = 5.8, 3.3 Hz, 2H), 6.89 (dd, *J* = 7.6, 6.3 Hz, 4H). Due to multiple conformers harboring $^1J_{CF}$, $^2J_{CF}$, $^3J_{CF}$ and $^4J_{CF}$ coupling with fluorine atoms, the signal peaks in the ^{13}C NMR spectrum were highly overlapped and is not reported herein. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -132.36, -132.42, -157.35, -157.40, -157.46. HRMS (ESI) calcd. for $C_{22}H_9F_6O_3^+$ 435.0450 [M+H$^+$], found 435.0453.



Methyl 4-(3-(4-methoxyphenyl)-1,4-dioxo-1,4-dihydro-naphthalen-2-yl)benzoate epoxide (21b): Methyl 4-(3-(4-methoxyphenyl)-1,4-dioxo-1,4-dihydronaphtha-len-2-yl)benzoate (89 mg) were subjected to the **GP4** affording **21b** as a colorless solid (28 mg, 30%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.08 (ddd, *J* = 8.9, 4.6, 2.3 Hz, 2H), 7.88 (d, *J* = 8.1 Hz, 2H), 7.81 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.10 (m, 2H), 6.72 – 6.70 (m, 2H), 3.87 (s, 3H), 3.71 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.00, 190.77, 166.73, 159.86, 134.74, 134.65, 134.55, 132.53, 132.44, 130.34, 129.58, 129.08, 128.54, 127.71, 127.59, 120.62, 113.54, 70.88, 55.22, 52.28. HRMS (ESI) calcd. for $C_{25}H_{19}O_6^+$ 415.1176 [M+H$^+$], found 415.1180.

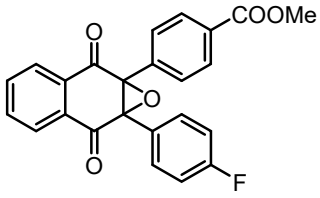


2-(4-Fluorophenyl)-3-phenyl-1,4-naphthoquinone epoxide (22b): 2-(4-Fluorophenyl)-3-phenylnaphthalene-1,4-dione (68 mg) were subjected to the **GP4** affording **22b** as a colorless solid (38 mg, 53%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 – 8.07 (m, 2H), 7.82 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.23 – 7.17 (m, 7H), 6.92 – 6.86 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.08, 190.92, 162.77 (d, *J* = 247.8 Hz), 134.73, 134.68, 132.54 (d, *J* = 10.1 Hz), 130.34, 130.25, 129.08, 128.90, 128.36, 127.97, 127.69, 127.65, 125.15 (d, *J* = 3.5 Hz), 115.04 (d, *J* = 21.9 Hz), 71.13, 70.53. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.33. HRMS (ESI) calcd. for $C_{22}H_{14}FO_3^+$ 345.0921 [M+H$^+$], found 345.0930.



Methyl 4-(1,4-dioxo-3-phenyl-1,4-dihydronaphthalen-2-yl)ben-zoate epoxide (23b): Methyl 4-(3-bromo-1,4-dioxo-1,4-dihydronaphthalen-2-yl)ben-zoate (209 mg) were subjected to the **GP4** affording **23b** as a colorless solid (147 mg, 67%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 – 8.07 (m, 2H), 7.88 – 7.85 (m, 2H), 7.84 – 7.80 (m, 2H), 7.32 – 7.29 (m, 2H), 7.22 – 7.16 (m, 5H), 3.85 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.63, 190.58, 166.67, 134.81, 134.73, 134.34, 132.53, 132.41, 130.38, 129.05, 128.99, 128.79,

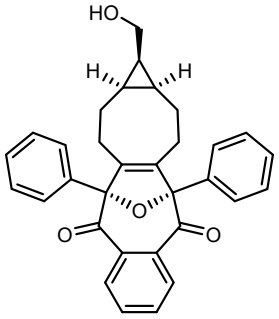
128.53, 128.30, 127.99, 127.74, 127.66, 70.99, 70.65, 52.28. HRMS (ESI) calcd. for $C_{24}H_{17}O_5^+$ 385.1071 [M+H$^+$], found 385.1078.



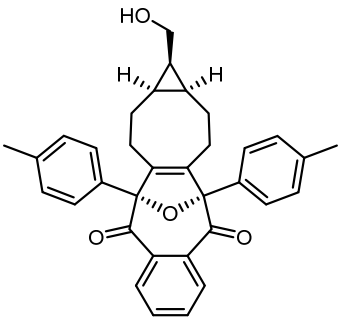
Methyl 4-(3-(4-fluorophenyl)-1,4-dioxo-1,4-dihydro-naphthalen-2-yl)benzoate epoxide (24b):
Methyl 4-(3-(4-fluorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (200 mg) were subjected to the **GP4** affording **24b** as a colorless solid (84 mg, 40%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 – 8.07 (m, 2H), 7.90 – 7.87 (m, 2H), 7.85 – 7.81 (m, 2H), 7.31 – 7.28 (m, 2H), 7.21 – 7.17 (m, 2H), 6.91 – 6.86 (m, 2H), 3.87 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.56, 190.35, 166.59, 162.86 (d, *J* = 248.6 Hz), 134.89, 134.86, 134.14, 132.40, 130.59, 130.21 (d, *J* = 8.2 Hz), 129.19, 128.48, 127.77, 127.73, 124.71 (d, *J* = 3.5 Hz), 115.26 (d, *J* = 22.0 Hz), 70.77, 70.50, 52.35. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.75. HRMS (ESI) calcd. for $C_{24}H_{16}FO_5^+$ 403.0976 [M+H$^+$], found 403.0983.

General conditions for the photoclick reactions:

The photoclick reaction: a solution of DNQOs (2.5 eq.) with corresponding dipolarophiles in ethyl acetate was vigorously stirred and irradiated simultaneously with a 365 nm LED in a quartz flask at room temperature. The solvent was then evaporated, and the residue was purified by silica gel flash chromatography to give the corresponding cycloaddition products, ***endo*-DEBCOD** and ***exo*-DEBCOD**, respectively.

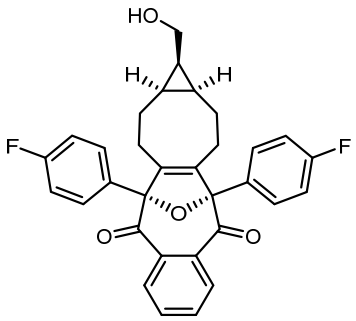


***endo*-1DEBCOD (1b+6c):** 2,3-Diphenyl-1,4-naphthoquinone epoxide **1b** (391 mg, 1.2 mmol) and BCN (**6c**, 72 mg, 0.48 mmol) in 200 mL ethyl acetate were subjected to the general condition affording the desired cycloadduct as a white solid (162 mg, 71%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.72 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.64 – 7.61 (m, 4H), 7.43 – 7.34 (m, 6H), 3.57 (d, *J* = 7.7 Hz, 2H), 2.57 (ddd, *J* = 16.1, 7.8, 3.9 Hz, 2H), 2.38 (ddd, *J* = 16.2, 8.7, 4.1 Hz, 2H), 1.90 – 1.82 (m, 2H), 1.42 – 1.34 (m, 2H), 1.17 – 1.09 (m, 2H), 1.05 – 0.97 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.14, 138.52, 138.33, 134.15, 133.32, 129.68, 128.74, 128.66, 127.96, 99.59, 59.98, 29.84, 25.07, 23.30, 21.76, 19.64. HRMS (ESI) calcd. for $C_{32}H_{31}O_4^+$ 479.2217 [M+H$^+$], found 479.2249.

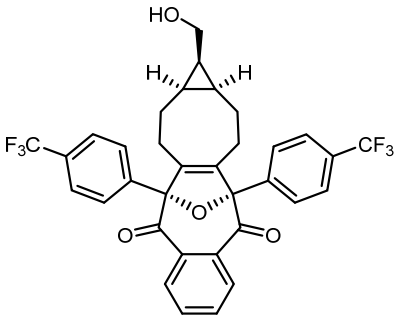


***endo*-3DEBCOD (3b+6c):** 2,3-Di-*p*-tolyl-1,4-naphthoquinone epoxide **3b** (425 mg, 1.2 mmol) and BCN **6c** (72 mg, 0.48 mmol) in 200 mL ethyl acetate were subjected to the general condition affording the desired cycloadduct as a white solid (155 mg, 64%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.70 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.50 – 7.48 (m, 4H), 7.20 (d, *J* = 8.1 Hz, 4H), 3.57 (d, *J* = 7.6 Hz, 2H), 2.55 (ddd, *J* = 16.2, 7.8, 3.9 Hz, 2H), 2.40 – 2.33 (s, 8H), 1.90 – 1.82 (m, 2H), 1.41

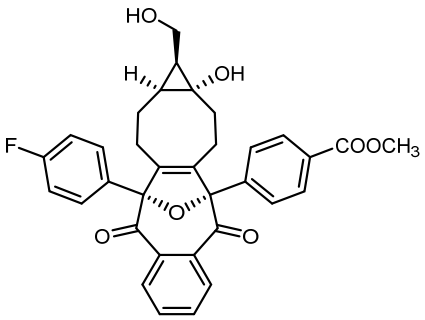
– 1.33 (m, 2H), 1.16 – 1.18 (m, 2H), 1.04 – 0.96 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.33, 138.49, 138.47, 135.50, 134.18, 133.23, 129.65, 129.30, 127.87, 99.47, 59.99, 29.84, 25.10, 23.35, 21.78, 21.27, 19.71. HRMS (ESI) calcd. for $C_{34}H_{35}O_4^+$ 507.2530 [M+H$^+$], found 507.2452.



***endo*-13DEBCOD (13b+6c):** 2,3-Bis(4-fluorophenyl)-1,4-naphthoquinone epoxide **13b** (434 mg, 1.2 mmol) and BCN (72 mg, 0.48 mmol) in 200 mL ethyl acetate were subjected to the general condition affording the desired cycloadduct as a white solid (149 mg, 61%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.73 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.62–7.58 (m, 4H), 7.12–7.07 (m, 4H), 3.57 (d, *J* = 7.7 Hz, 2H), 2.54 (ddd, *J* = 16.1, 7.8, 3.9 Hz, 2H), 2.34 (ddd, *J* = 16.3, 8.7, 4.2 Hz, 2H), 1.90 – 1.82 (m, 2H), 1.43–1.33 (m, 2H), 1.18–1.09 (m, 2H), 1.02 – 0.93 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.58, 162.93 (d, *J* = 248.1 Hz), 138.45, 134.09 (d, *J* = 3.1 Hz), 133.74, 133.51, 129.79 (d, *J* = 8.8 Hz), 115.62 (d, *J* = 21.4 Hz), 98.99, 59.88,29.84, 24.97, 23.26, 21.74, 19.57. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -117.79. HRMS (ESI) calcd. for $C_{32}H_{29}F_2O_4^+$ 515.2028 [M+H$^+$], found 515.1948.



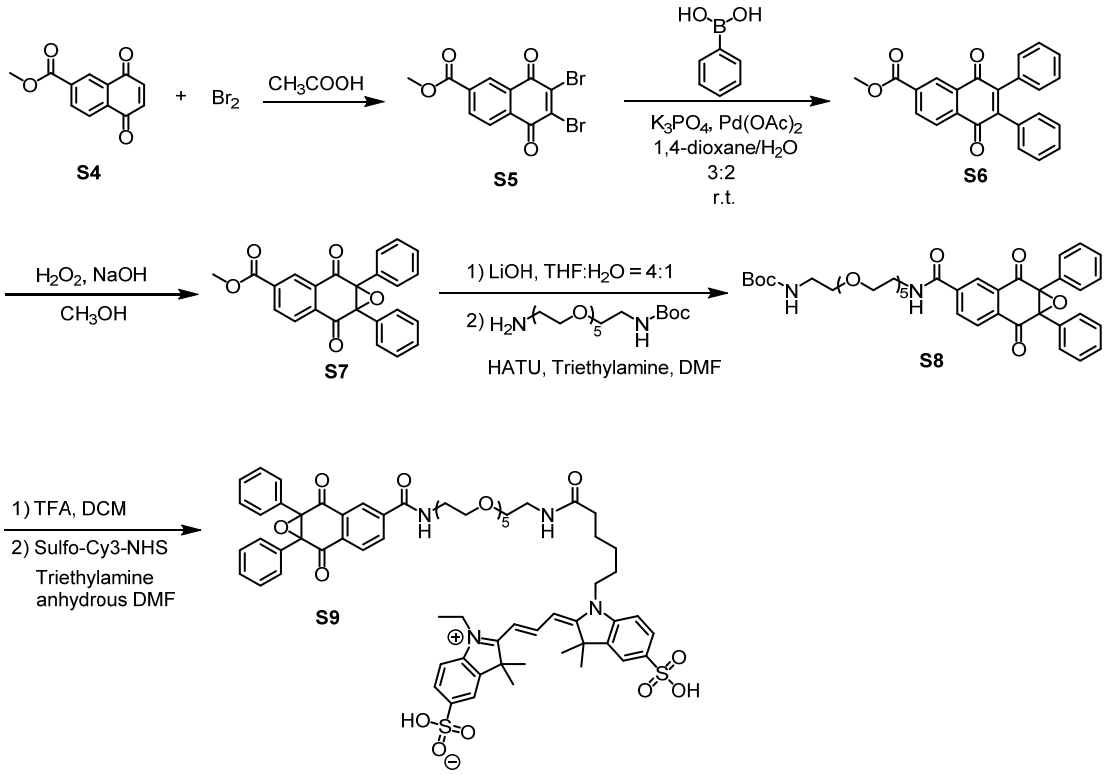
***endo*-17DEBCOD (17b+6c):** 2,3-Bis(4-(trifluoro-methyl)phenyl)-1,4-naphthoquinone epoxide **17b** (555 mg, 1.2 mmol) and BCN (72 mg, 0.48 mmol) in 200 mL ethyl acetate were subjected to the general condition affording the desired cycloadduct as a white solid (166 mg, 56%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.81 – 7.78 (m, 4H), 7.75 (dd, *J* = 5.8, 3.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 5H), 3.57 (d, *J* = 7.7 Hz, 2H), 2.57 (ddd, *J* = 16.2, 7.8, 4.1 Hz, 2H), 2.36 (ddd, *J* = 16.3, 8.6, 4.3 Hz, 2H), 1.89 – 1.81 (m, 2H), 1.46 – 1.36 (m, 2H), 1.18 – 1.09 (m, 2H), 0.99 – 0.90 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.79, 141.81, 138.49, 133.73, 133.46, 131.04 (q, *J* = 32.7 Hz), 130.03, 128.25, 125.68 (q, *J* = 3.8 Hz), 124.03 (q, *J* = 272.1 Hz), 98.99, 59.79, 29.83, 24.88, 23.15, 21.69, 19.41. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.73. HRMS (ESI) calcd. for $C_{34}H_{29}F_6O_4^+$ 615.1965 [M+H$^+$], found 615.1926.

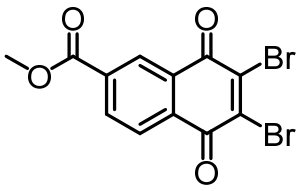


e*ndo*-DEBCOD 24b+6c: Methyl 4-(3-(4-fluorophenyl)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate epoxide **24b** (483 mg, 1.2 mmol) and BCN **6c** (72 mg, 0.48 mmol) in 200 mL ethyl acetate were subjected to the general condition affording **24b-6c** as a white solid (144 mg, 54%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.09 – 8.06 (m, 2H), 7.94 (dd, *J* = 5.7, 3.5 Hz, 2H), 7.76 – 7.71 (m, 4H), 7.63 – 7.58 (m, 2H), 7.13 – 7.07 (m, 2H), 3.92 (s, 3H), 3.55 (d, *J* = 7.7 Hz, 2H), 2.53 (m, 2H), 2.34 (dddd, *J* = 16.1, 8.8, 4.3, 2.5 Hz, 2H), 1.89 – 1.76 (m, 2H), 1.43 – 1.34 (m, 2H), 1.16 – 1.07 (m, 2H), 0.97-0,91 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.41, 203.16, 166.77, 162.95 (d, *J* = 248.6 Hz), 142.92, 138.55, 138.22, 133.92 (d, *J* = 3.1 Hz), 133.69 (d, *J* = 10.2 Hz), 133.54, 130.44, 129.88, 129.84, 129.76,

127.82, 115.64 (d, J = 21.4 Hz), 99.23, 98.83, 59.85, 52.38, 29.83, 24.99, 24.77, 23.12, 21.65, 19.51, 19.30. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.90. HRMS (ESI) calcd. for $C_{34}H_{32}FO_6^+$ 555.2177 [$M+H^+$], found 555.2088.

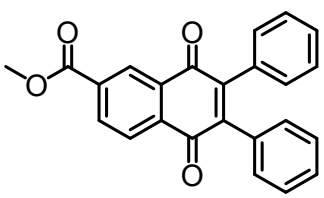
The synthesis of DNQO-Cy3 and the corresponding characterization





S5:

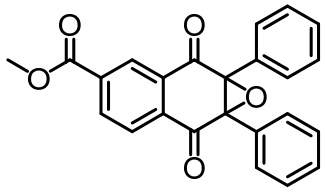
To a solution of **S4** (1.5g, 6.94 mmol) was dissolved in glacial acetic acid, liquid bromine (0.716 mL) diluted with glacial acetic acid was added dropwise. The resulting solution was stirred at 25 °C for 1h and then heated to 110 °C for 8h. The mixture was poured into ice-water, the precipitate was formed, filtered and washed with water and dried under vacuum. The residue was dissolved with dichloromethane and purified on silica gel by using a flash chromatography column (eluting with petroleum ether/dichloromethane = 1/1) to give pure product as a yellow solid (1.6 g, 62.0%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.79 (d, *J* = 1.6 Hz, 2H), 8.41 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.26 (d, *J* = 8.1 Hz, 1H), 4.01 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.47, 175.22, 165.03, 143.21, 142.81, 135.73, 135.15, 133.42, 131.01, 129.51, 128.65, 53.13. HRMS (ESI) calcd. for $C_{12}H_7BrO_4^+$ 372.8706 [M+H$^+$], found 372.8704.



S6:

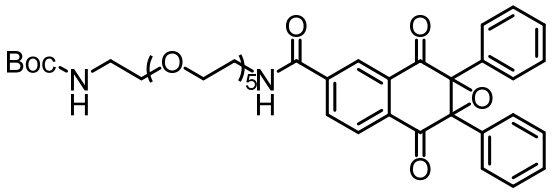
S5 (825.54 mg, 2.22 mmol), phenylboronic acid (576.09 mg, 4.72 mmol), and $Pd(OAc)_2$ (30 mg) were subjected to the **GP1** affording **S6** as a yellow solid (506 mg, 61.9%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.83 (dd, *J* = 1.7, 0.5 Hz, 1H), 8.43 (dd, *J* = 8.1, 1.7 Hz, 1H), 8.27 (dd, *J* = 8.0, 0.6 Hz, 1H), 7.25 – 7.21 (m, 6H), 7.09 – 7.06 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.38, 184.08, 165.70, 146.35, 146.14, 135.12,

134.87, 134.51, 133.07, 133.06, 132.28, 130.69, 130.63, 128.59, 128.56, 128.19, 127.87, 127.85, 127.14, 52.95. HRMS (ESI) calcd. for $C_{24}H_{16}O_4^+$ 369.1121 [M+H$^+$], found 369.1120.



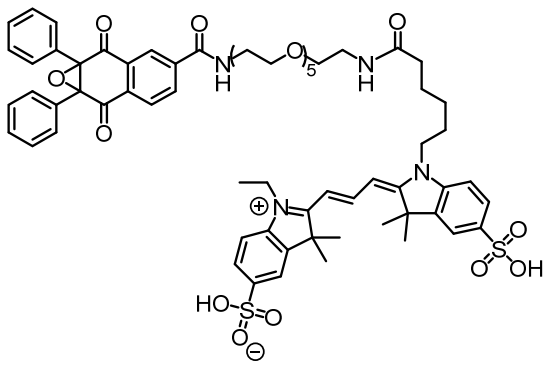
S7:

S6 (504 mg, 1.37 mmol), were subjected to the **GP4** affording as **S7** a colorless solid (436 mg, 82.9%). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 1.7 Hz, 1H), 8.42 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.23-7.19 (m, 10H), 4.00 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 190.80, 190.37, 165.36, 135.67, 135.41, 135.02, 132.77, 128.89, 128.82, 128.77, 128.42, 127.96, 127.88, 71.29, 71.26, 52.98. HRMS (ESI) calcd. for $C_{24}H_{17}O_5^+$ 385.1071 [M+H$^+$], found 385.1070.



S8:

A mixture of **S7** (96 mg, 0.25 mmol) and LiOH·H_2O (31.47 mg, 0.75 mmol) in a solution of THF/ H_2O = 4/1 (20 mL), It was stirred vigorously at room temperature and was traced with TLC till the conversion was completed. The residue was purified by silica gel flash chromatography (MeOH/EtOAc = 9/1) affording product as a colorless solid. The colorless solid (60.0 mg， 0.16 mmol), HATU 1.22 eq. (75.3 mg, 0.198 mmol), TEA (49.1 mg, 0.49 mmol) and tert-butyl (17-amino-3,6,9,12,15-pentaoxaheptadecyl)-carbamate (Boc-NH-PEG_5-$CH_2CH_2NH_2$, 75.33 mg, 0.198 mmol) was added to react until the raw material was converted completely. Then the mixture was extracted by EtOAc and the crude product was purified by flash chromatography on silica gel (eluting with 10% EtOH in DCM) to yield a yellow oil (116.0 mg, 99.0%). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.00 (t, *J* = 5.6 Hz, 1H), 8.45 (d, *J* = 1.7 Hz, 1H), 8.34 (dd, *J* = 8.1, 1.7 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.32 (m, 3H), 7.20 – 7.13 (m, 6H), 6.73 (t, *J* = 5.8 Hz, 1H), 3.60 – 3.35 (m, 20H), 3.36 (t, *J* = 6.0 Hz, 2H), 3.05 (q, *J* = 6.1 Hz, 2H). 1.37 (s, 9H). **^{13}C NMR** (101 MHz, DMSO-d_6) δ 190.02, 164.63, 155.57, 139.38, 133.89, 132.92, 132.31, 129.96, 129.89, 128.35, 128.15, 127.26, 127.24, 127.15, 125.47, 77.56, 70.60, 70.56, 69.77, 69.72, 69.62, 69.49, 69.15, 68.67, 38.24, 28.22. HRMS (ESI) calcd. for $C_{35}H_{41}N_2O_9^+$ 633.2807 [M+H$^+$], found 633.2804.



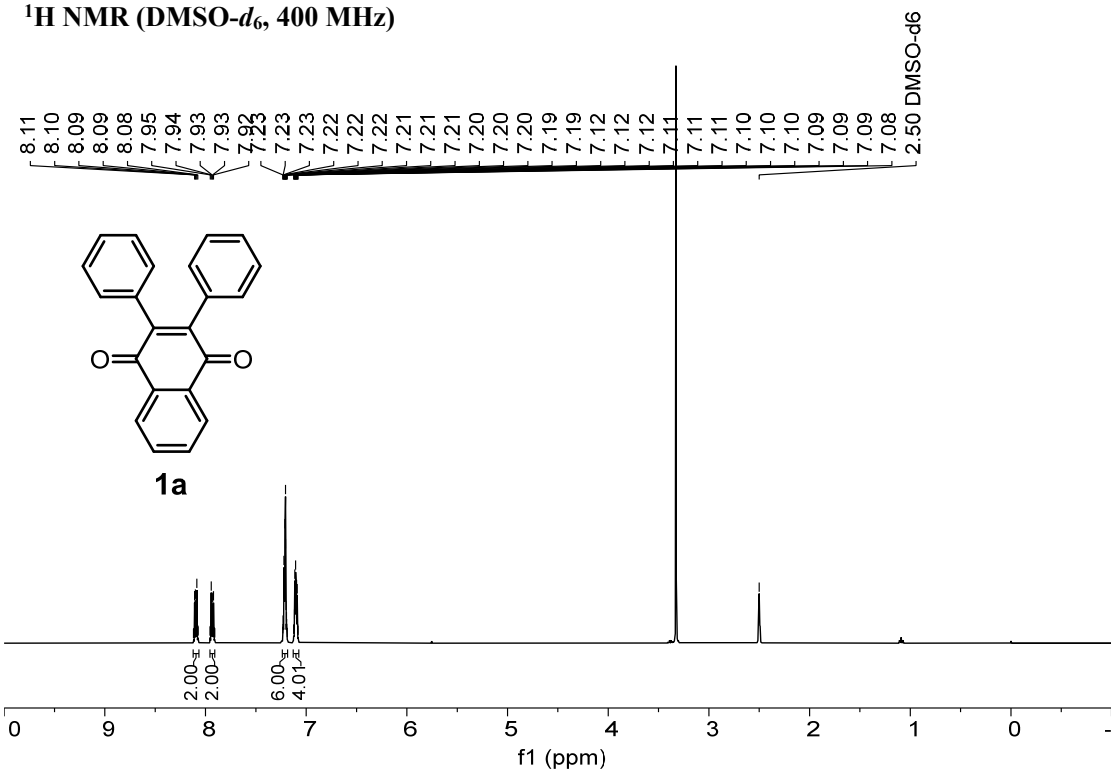
S9:

To a stirring suspension of **S8** (50.0 mg, 0.068 mmol) in DCM (10 mL), the TFA (5 mL) was added at 0 ºC, then the mixture reacted at room temperature for 2 h. After getting rid of the TFA by air flow, the residual TFA was neutralized by $NaHCO_3$ aqueous solution, the organic layer was extracted by DCM and purified by flash chromatography on silica gel (eluting with 60% EtOH in DCM) to get a yellow oil crude primary amine product (42.3 mg, 98.0%). Then, the crude product (7.58 mg, 0.012 mmol) was dissolved in anhydrous DMF, the Sulfo-Cy3-NHS (8.82 mg, 0.012 mmol) and TEA (10

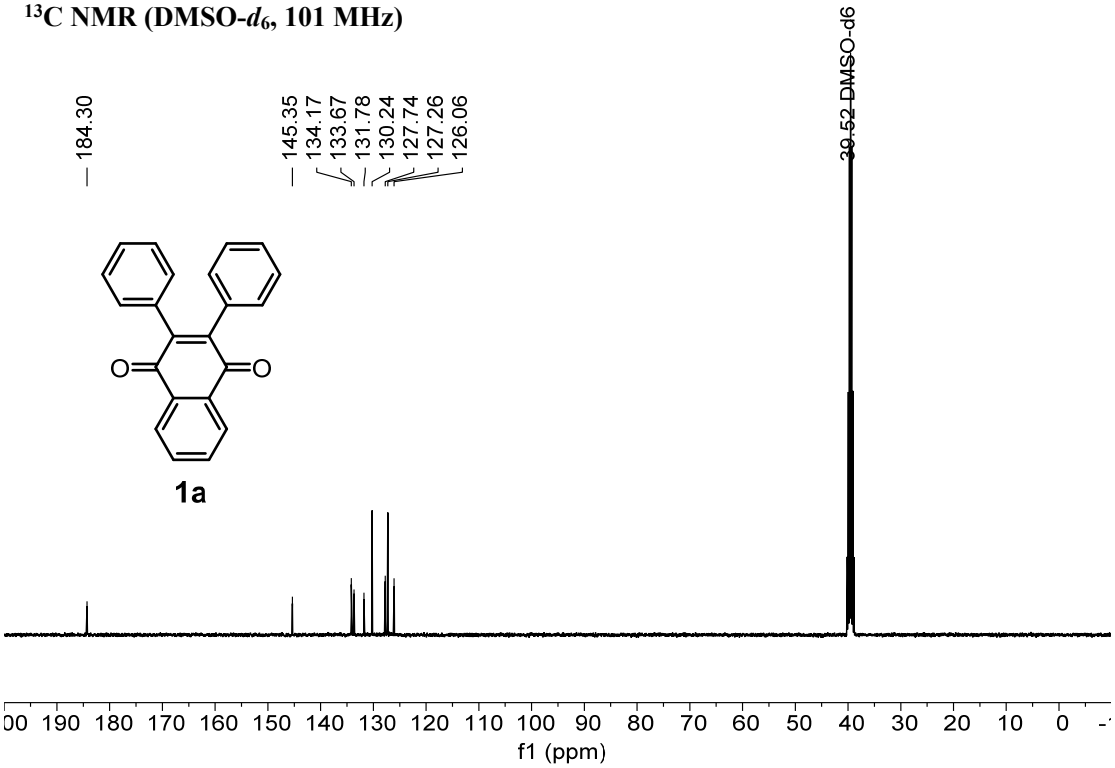
μL) were added under N_2 atmosphere, after the reaction was reacted for 24 h at room temperature, the mixture was concentrated and purified by reversed phase HPLC via a Gemini C18 HPLC Column to yield a red solid (12.6 mg, 80.0%). HRMS (ESI) calcd. for $C_{66}H_{78}N_4O_{16}S_2^-$ 1244.4703 [M-H^+], found 1244.4692.

8. ^{1}H, ^{13}C and ^{19}F NMR Spectra

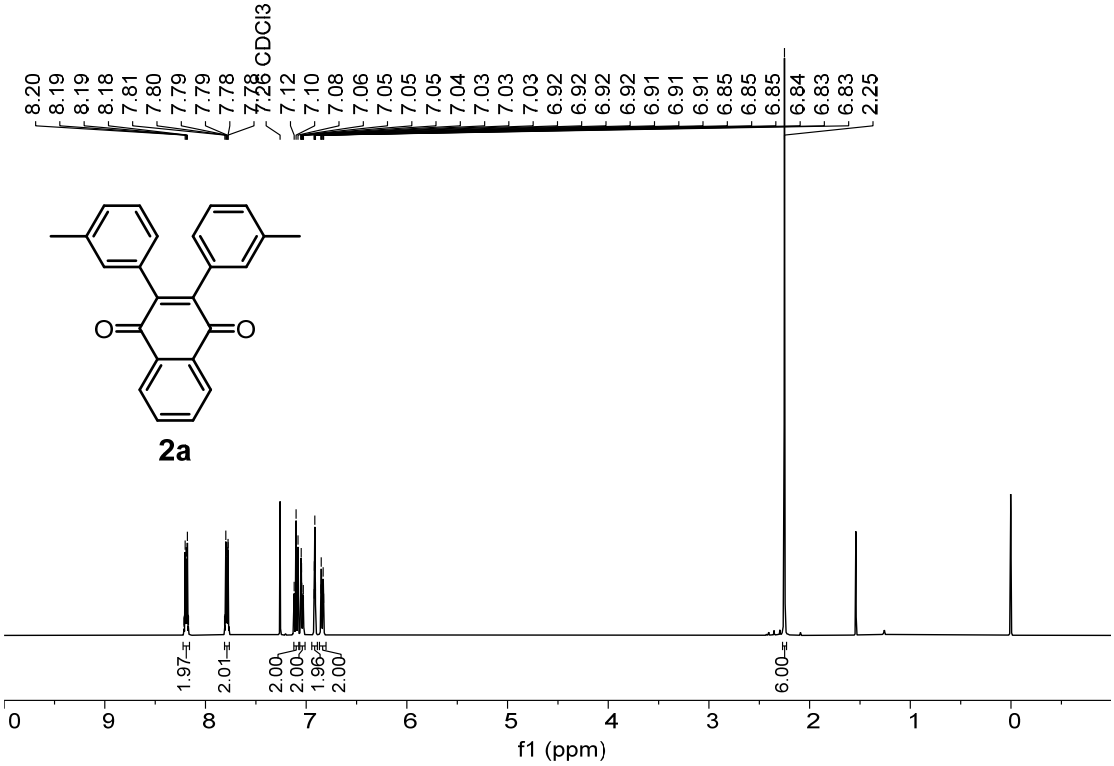
^{1}H NMR (DMSO-d_6, 400 MHz)



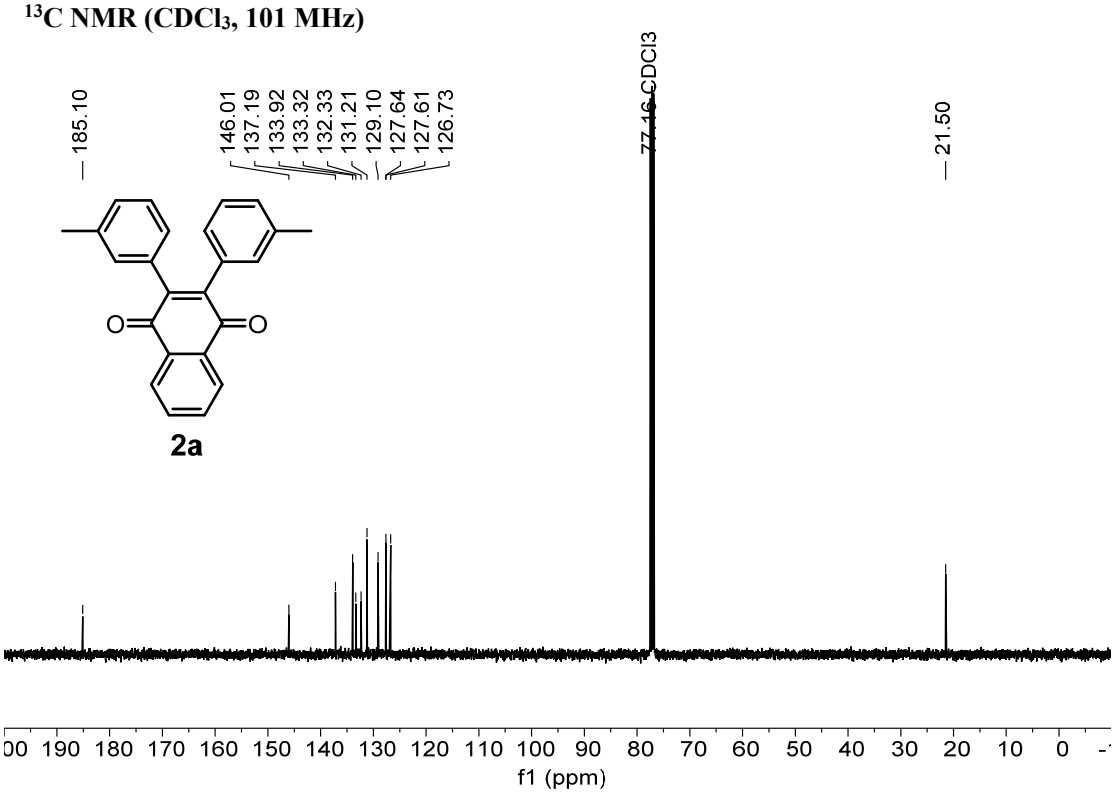
^{13}C NMR (DMSO-d_6, 101 MHz)



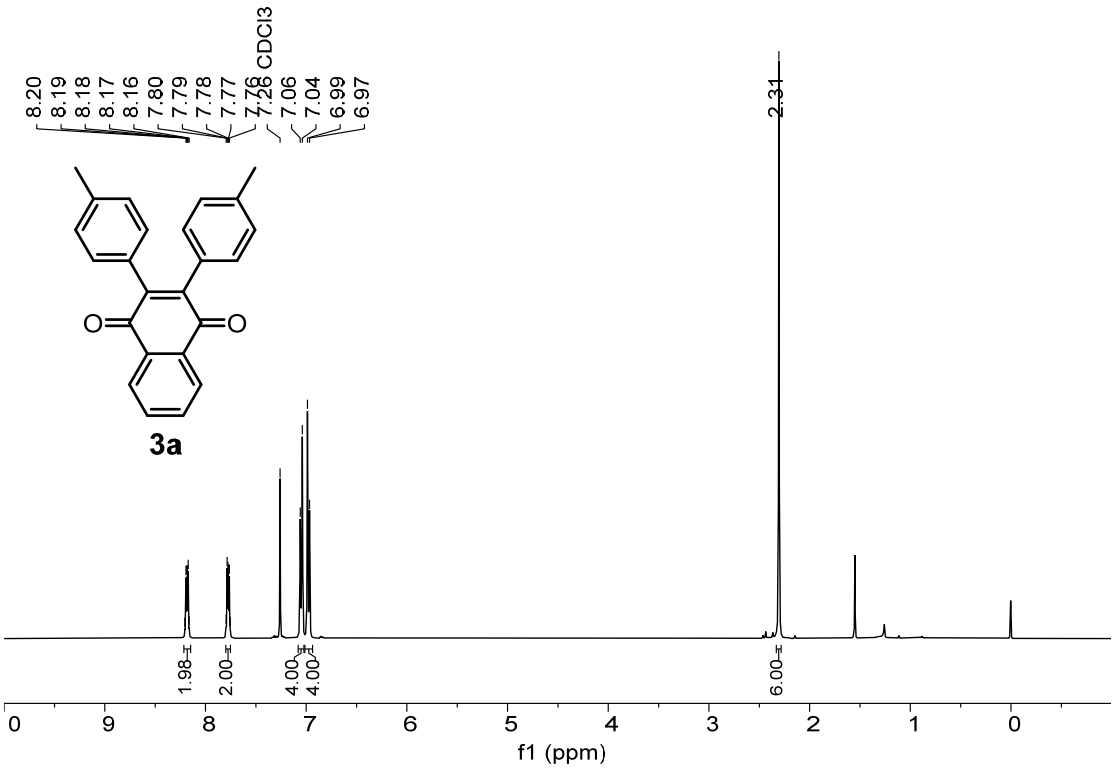
^{1}H NMR ($CDCl_3$, 400 MHz)



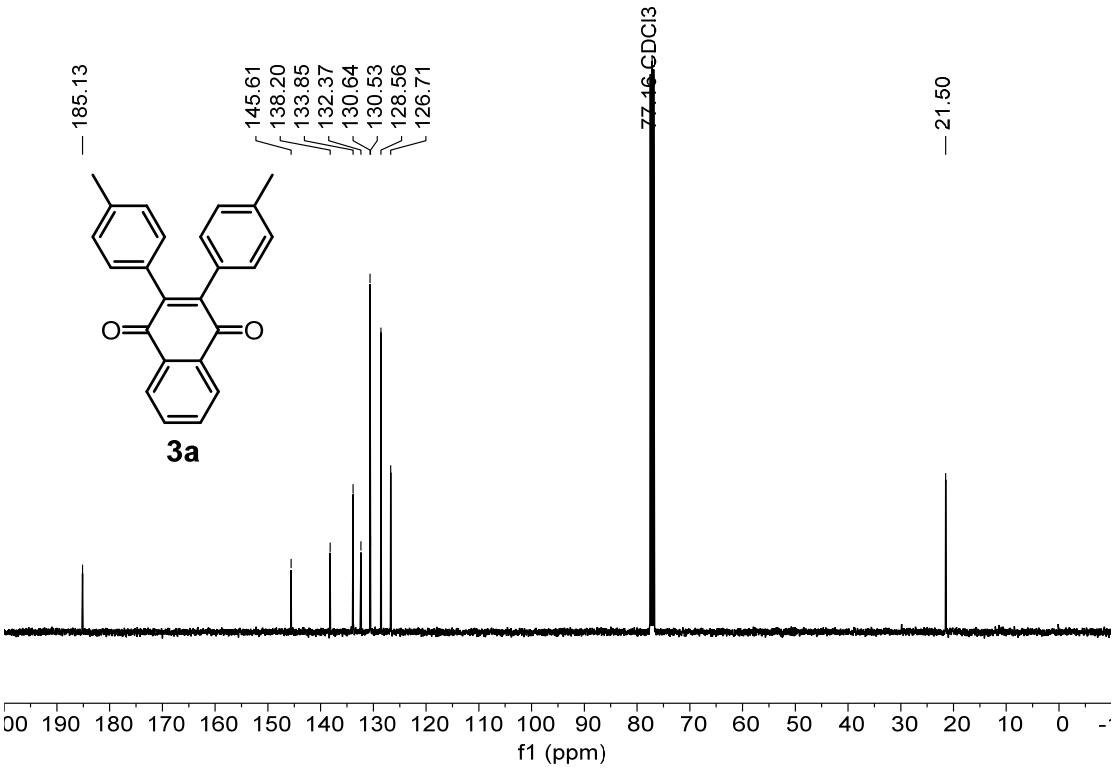
^{13}C NMR ($CDCl_3$, 101 MHz)



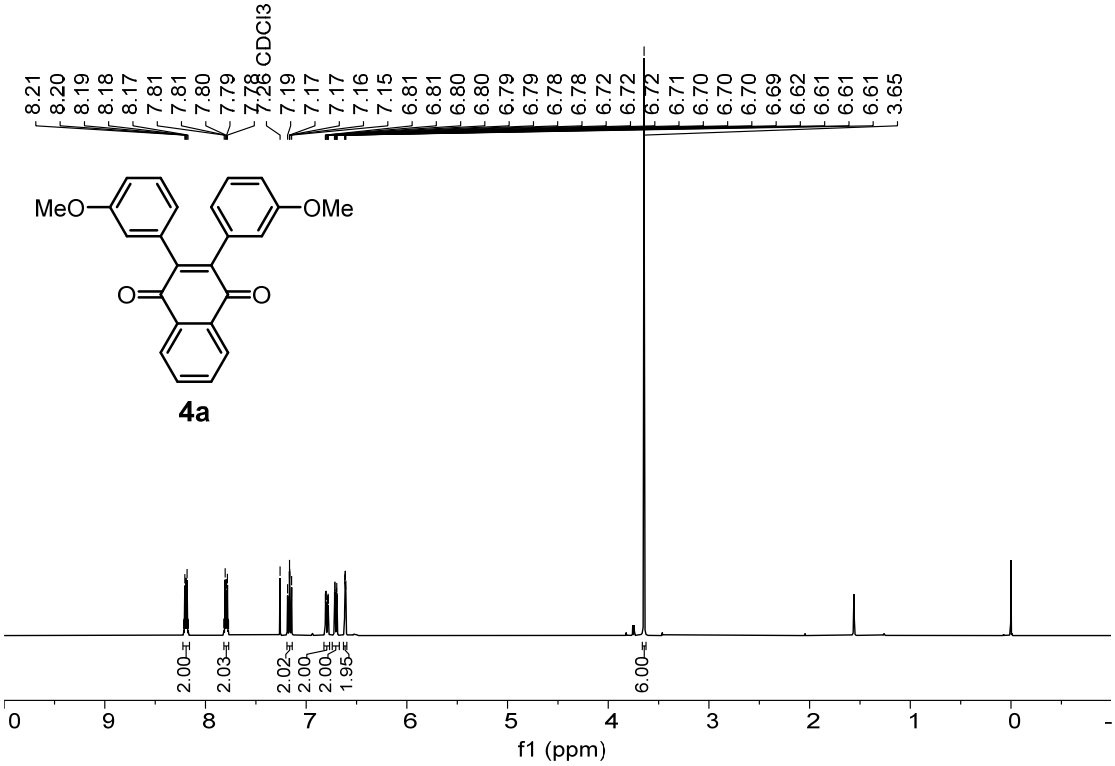
^{1}H NMR ($CDCl_3$, 400 MHz)



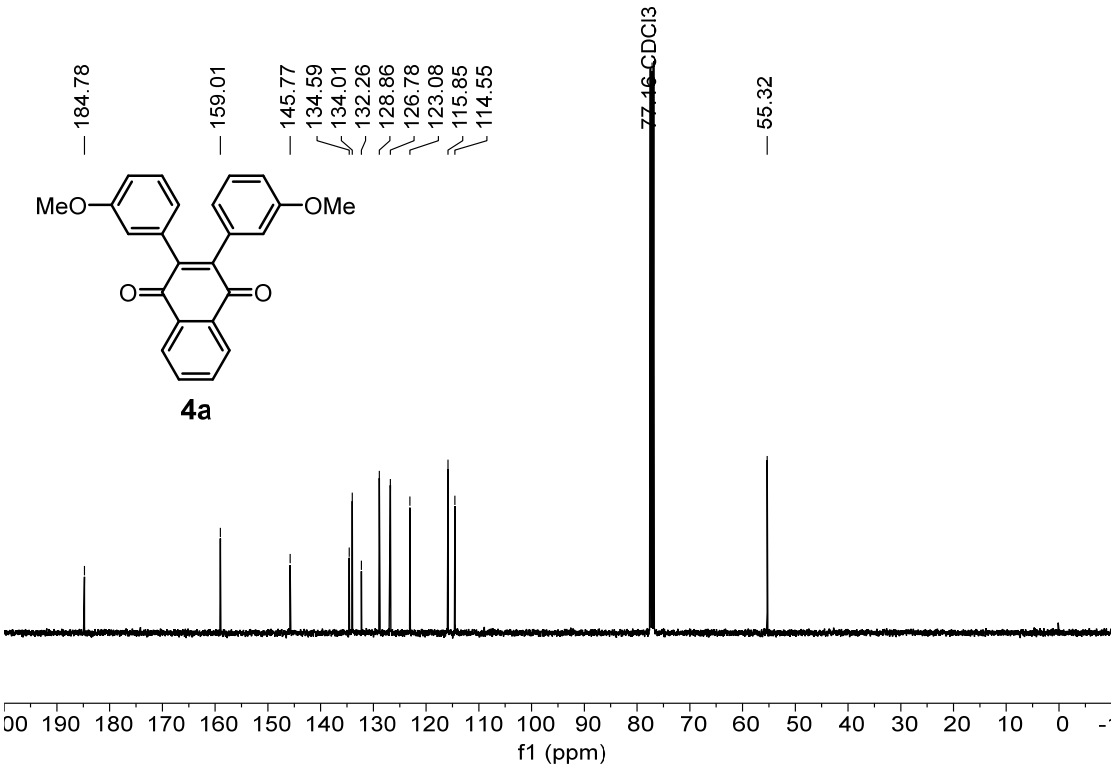
^{13}C NMR ($CDCl_3$, 101 MHz)



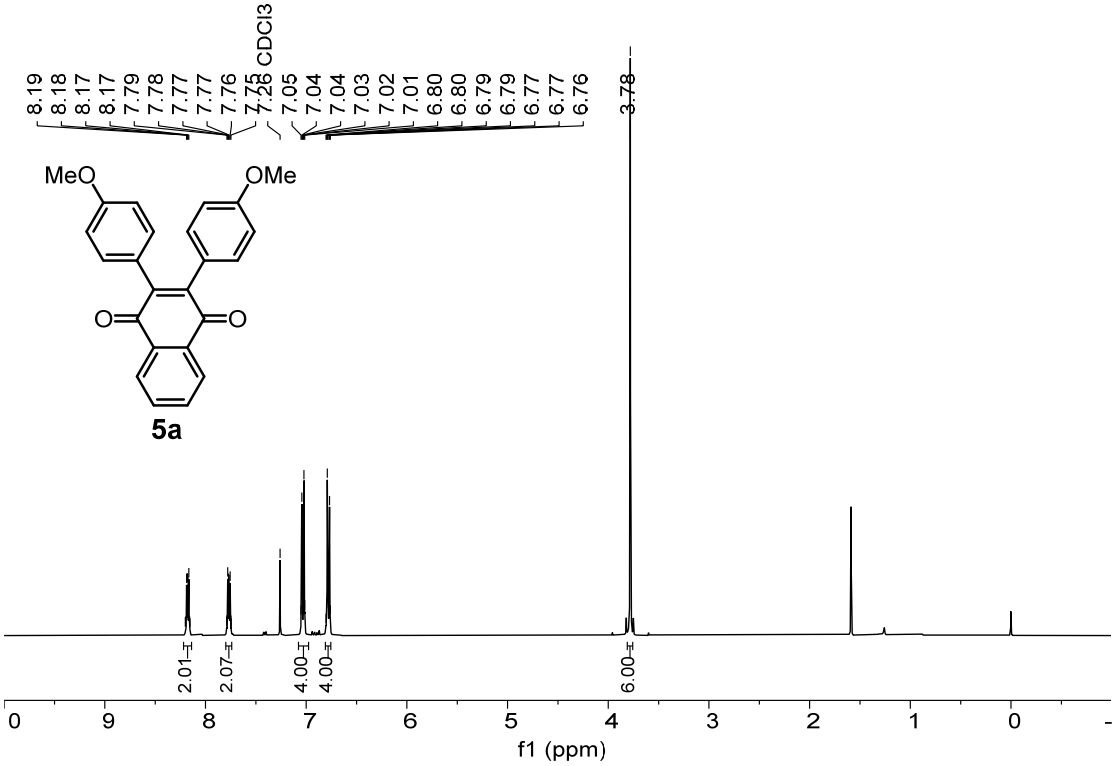
^{1}H NMR ($CDCl_3$, 400 MHz)



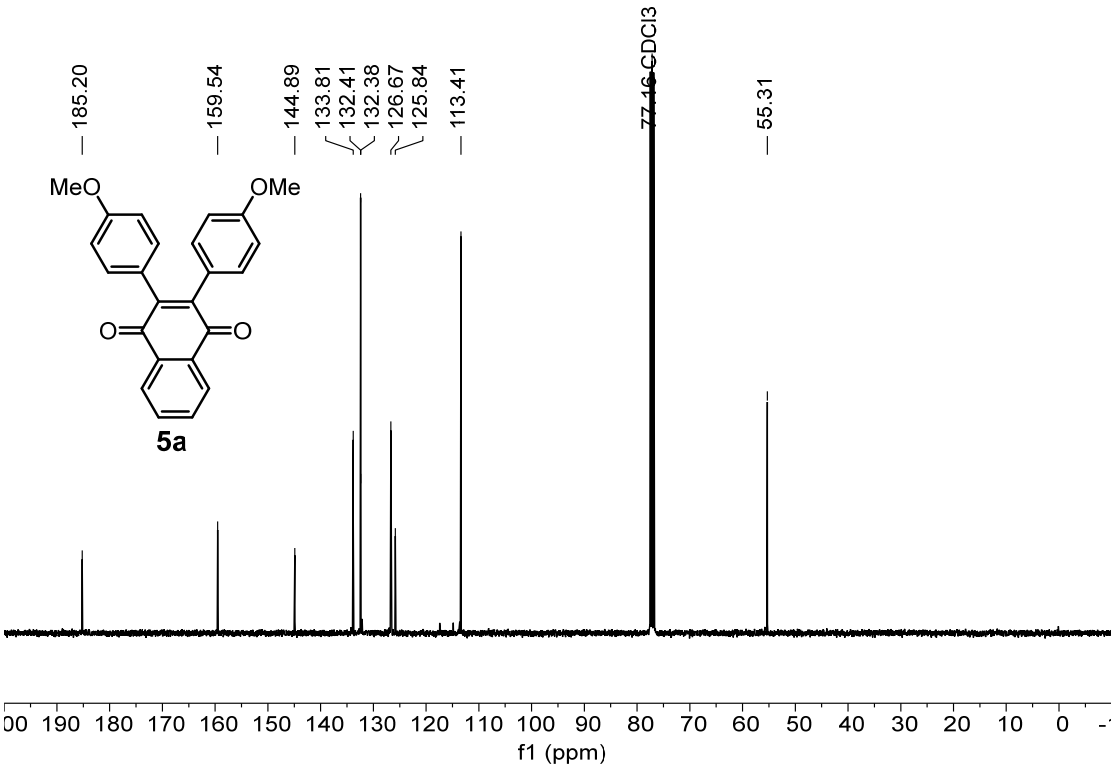
^{13}C NMR ($CDCl_3$, 101 MHz)



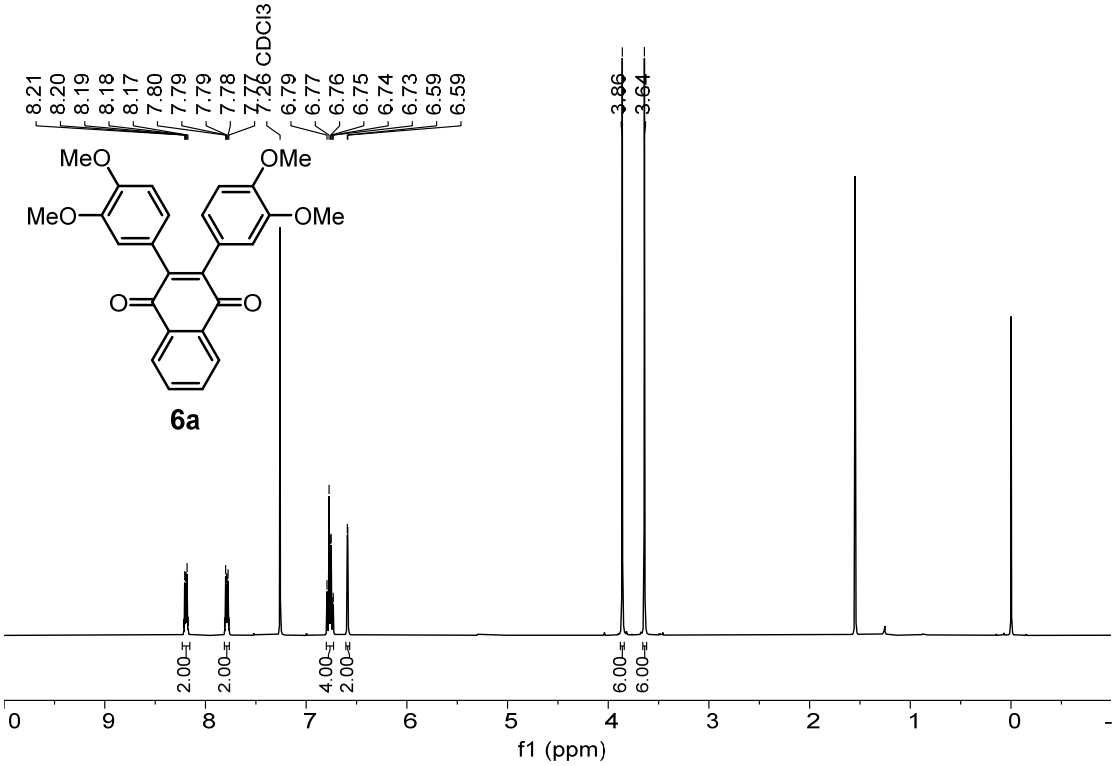
^{1}H NMR ($CDCl_3$, 400 MHz)



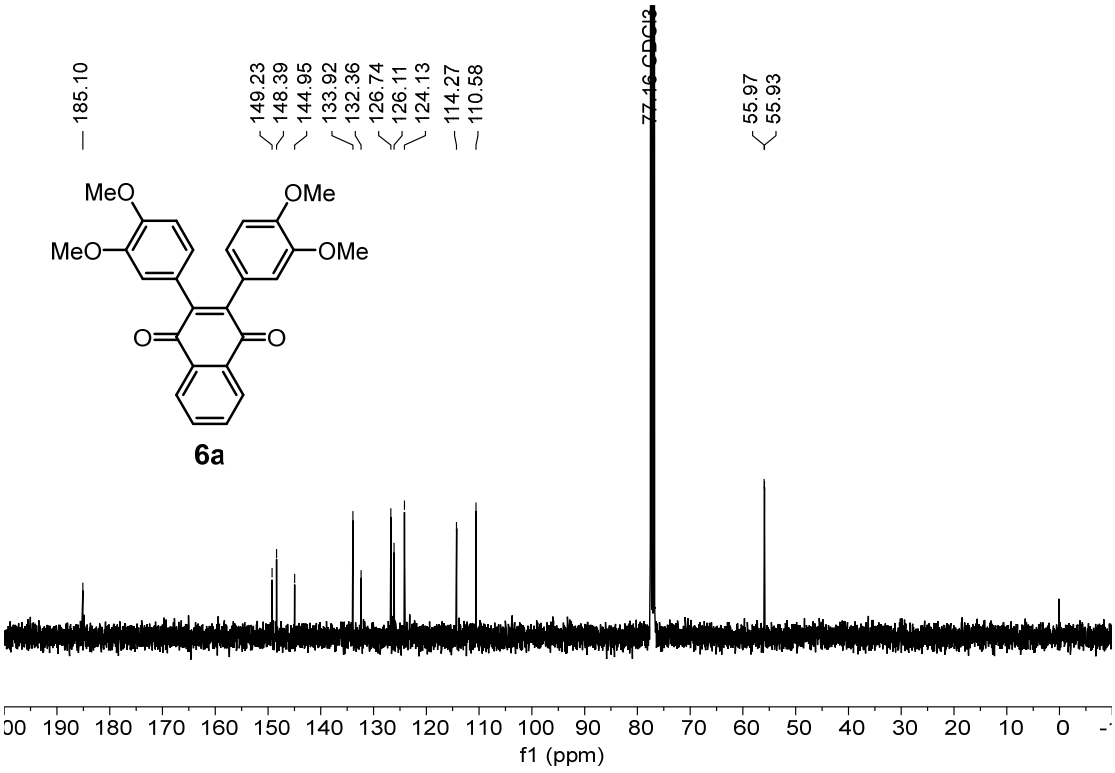
^{13}C NMR ($CDCl_3$, 101 MHz)

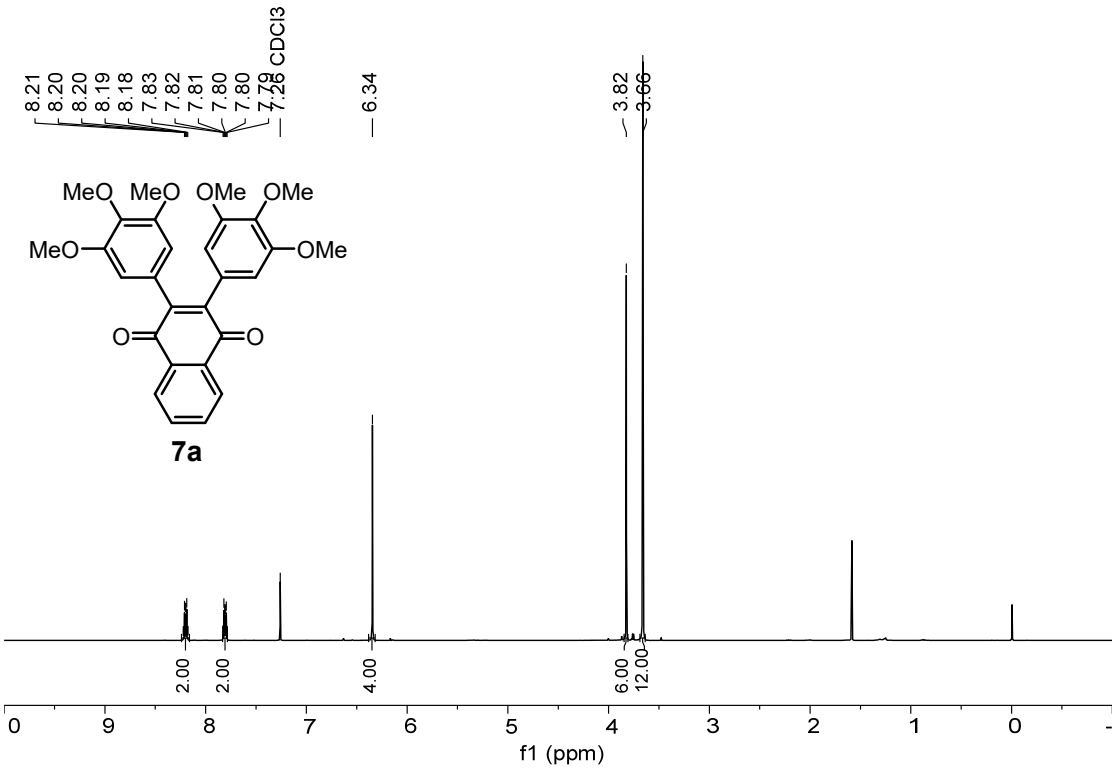


^{1}H NMR ($CDCl_3$, 400 MHz)

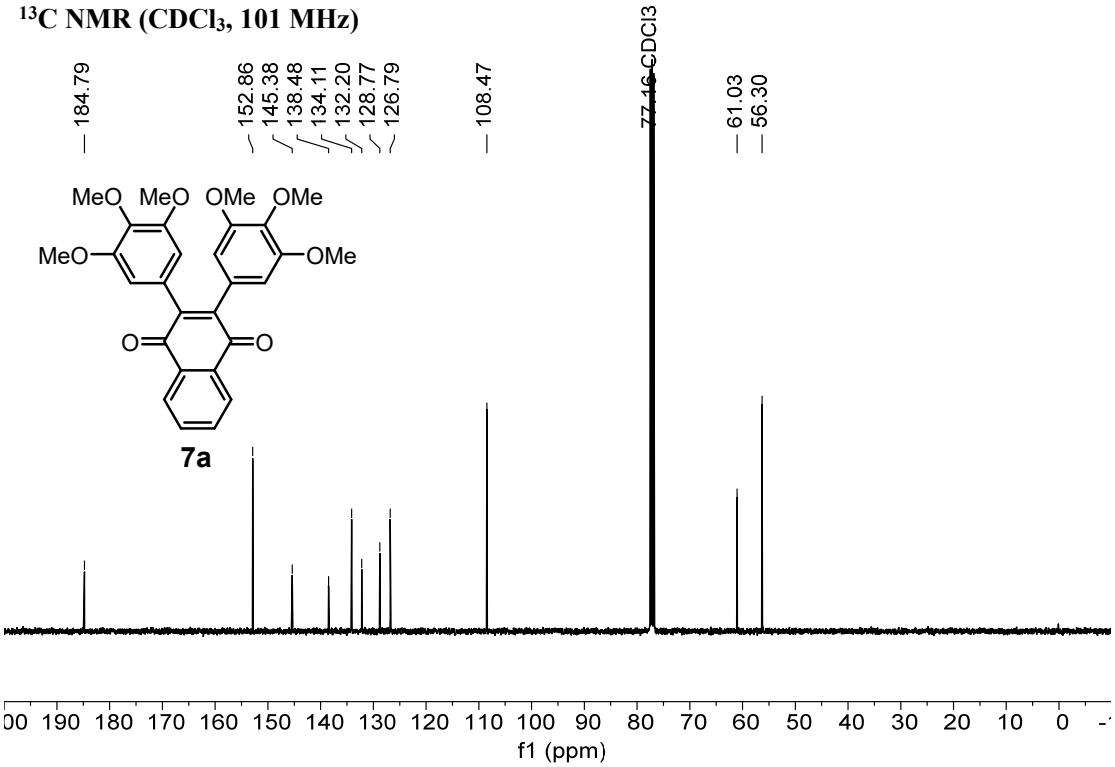


^{13}C NMR ($CDCl_3$, 101 MHz)

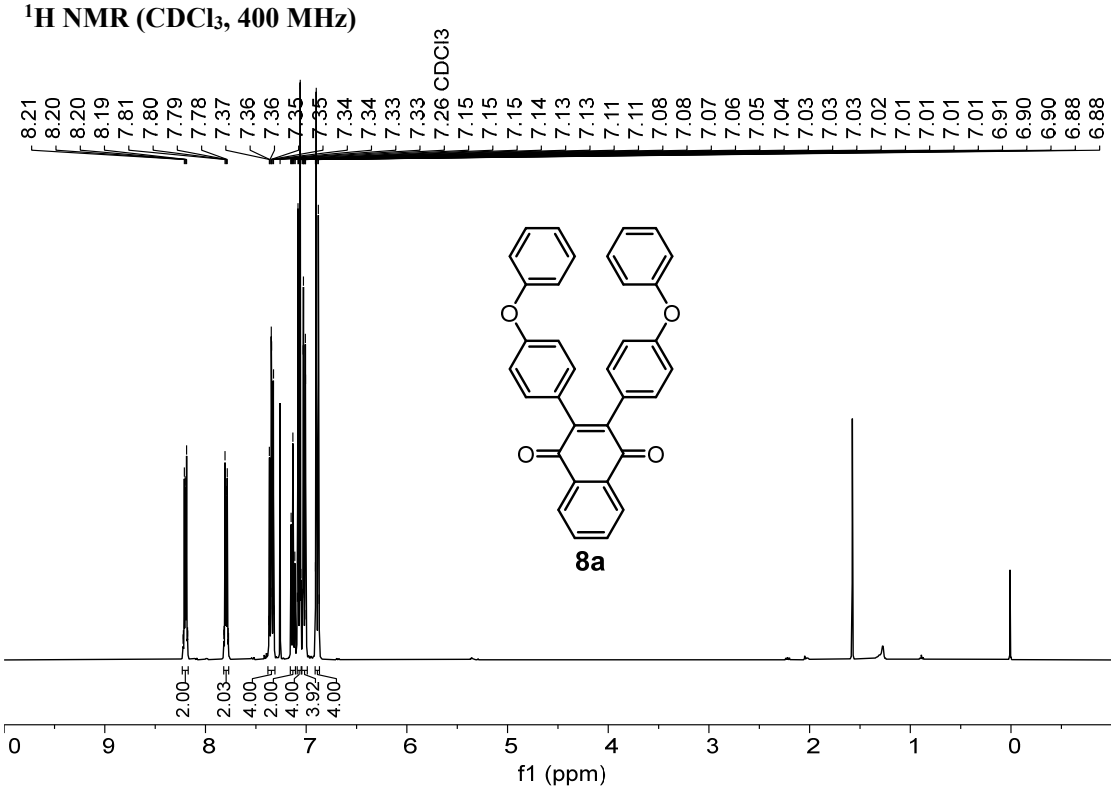




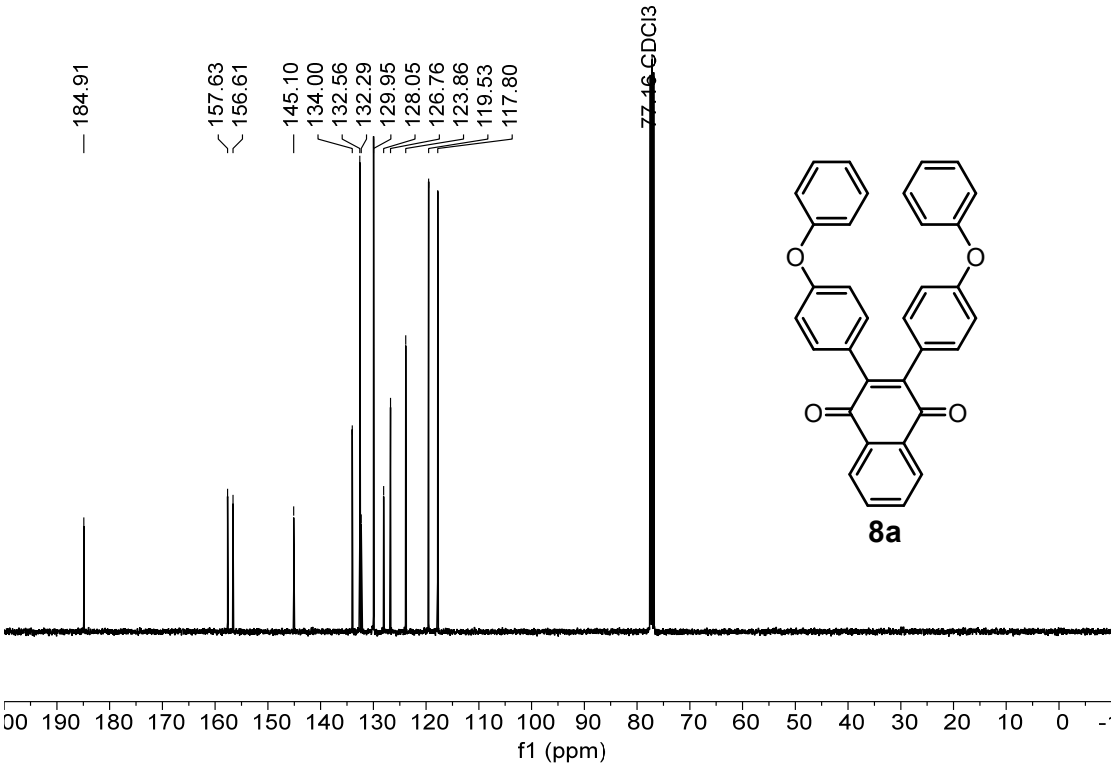
^{13}C NMR ($CDCl_3$, 101 MHz)



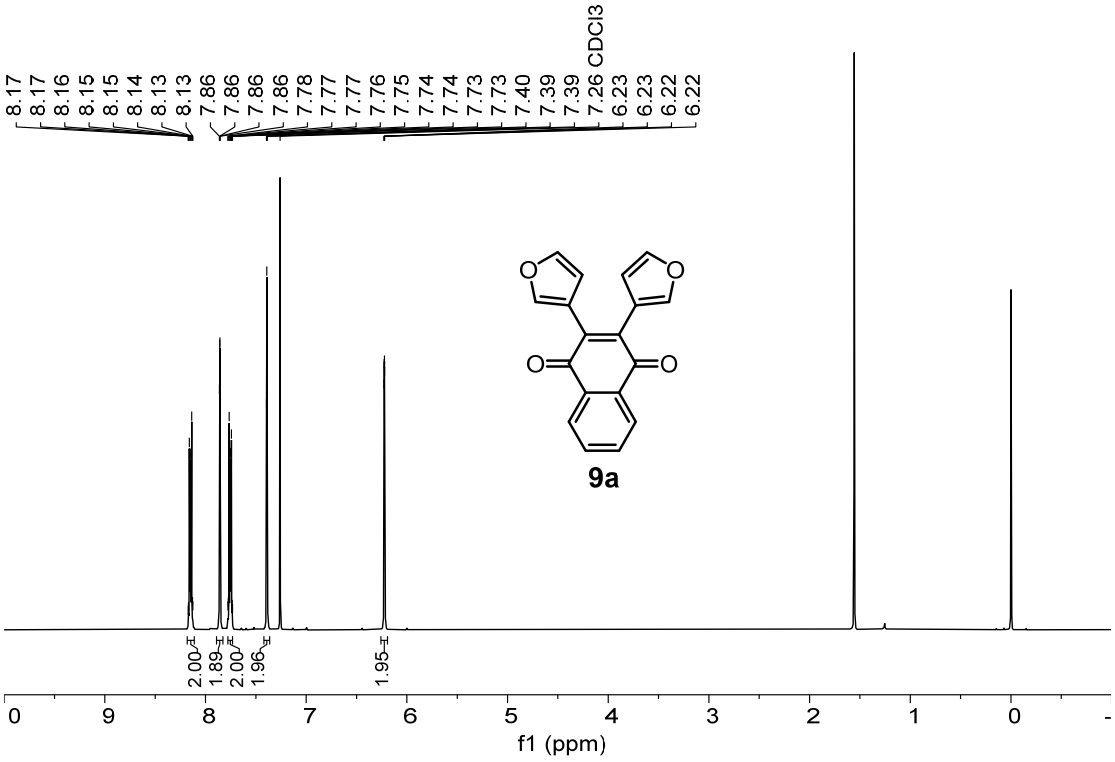
^{1}H NMR ($CDCl_3$, 400 MHz)



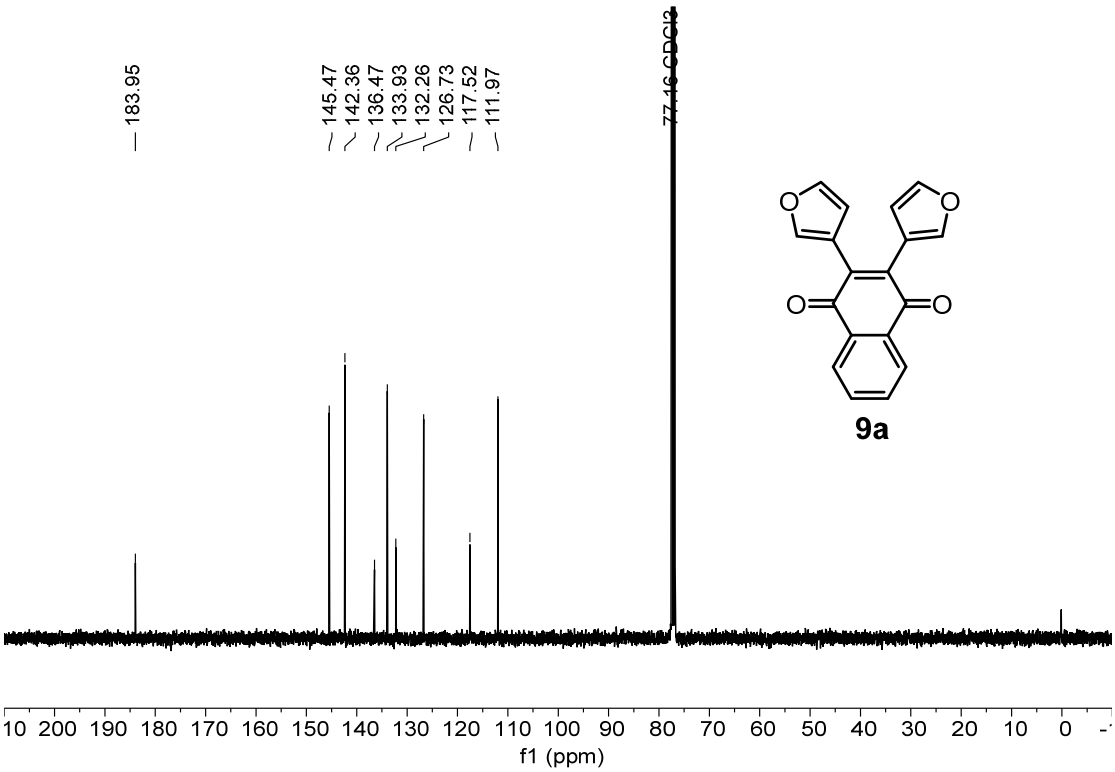
^{13}C NMR ($CDCl_3$, 101 MHz)



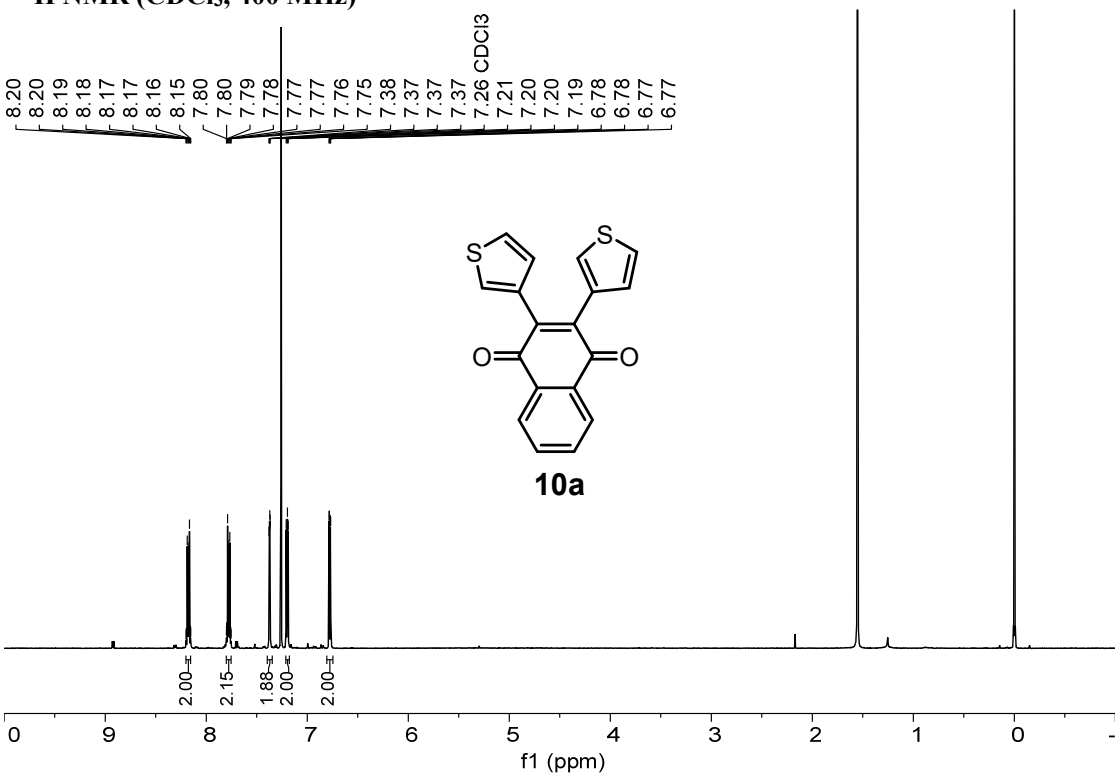
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)

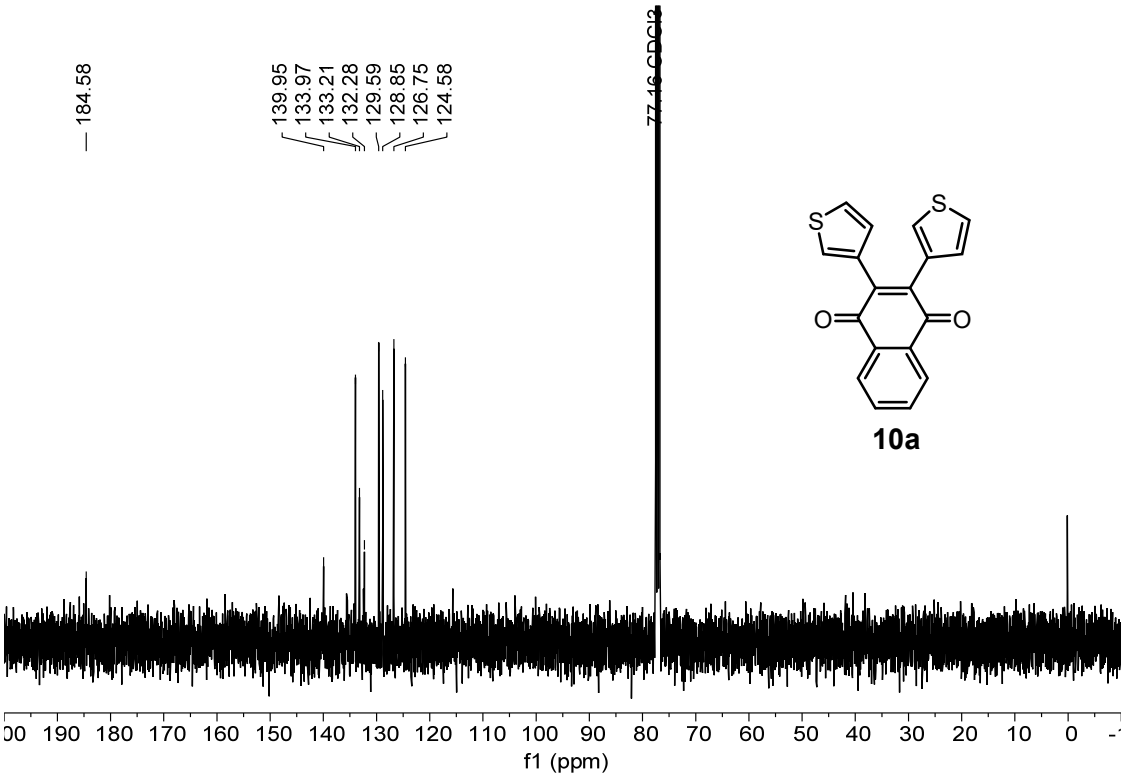


^{1}H NMR ($CDCl_3$, 400 MHz)



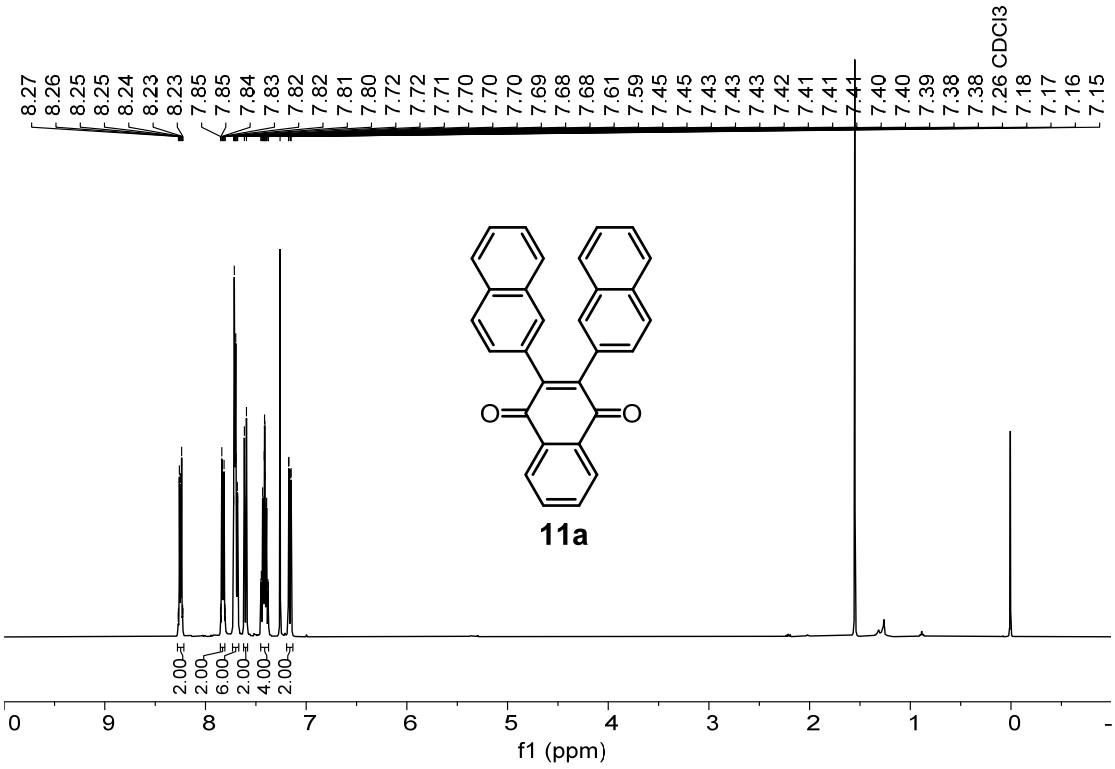
10a

^{13}C NMR ($CDCl_3$, 101 MHz)

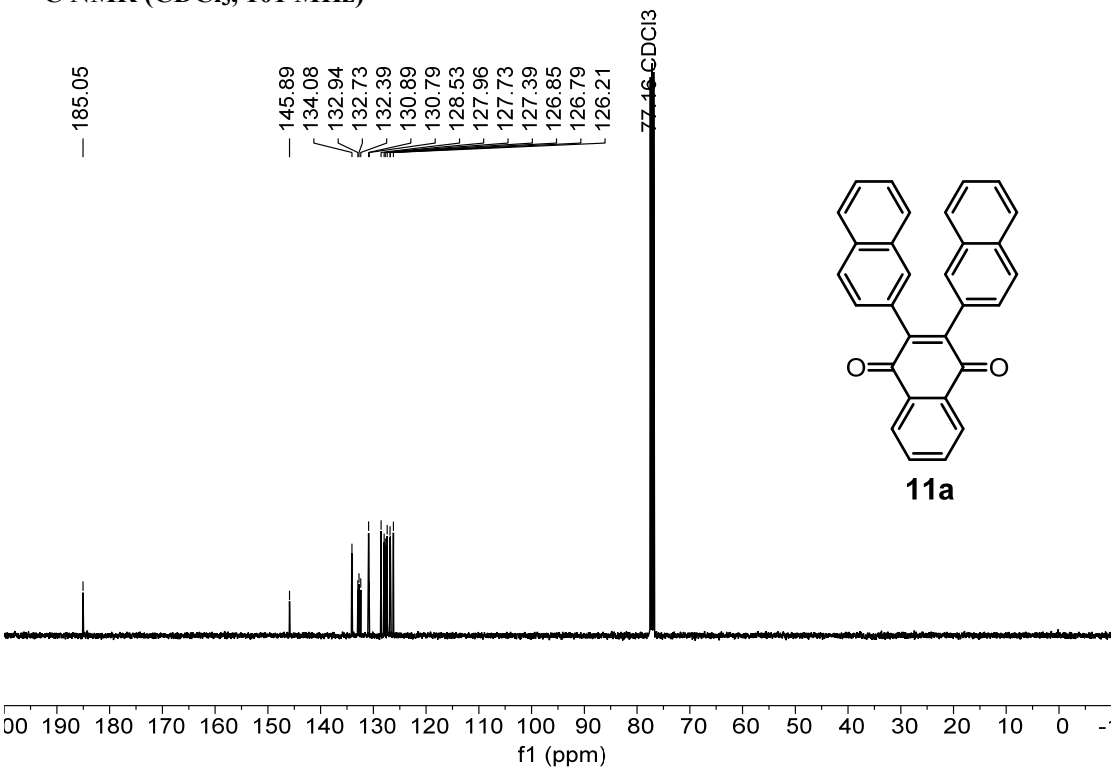


10a

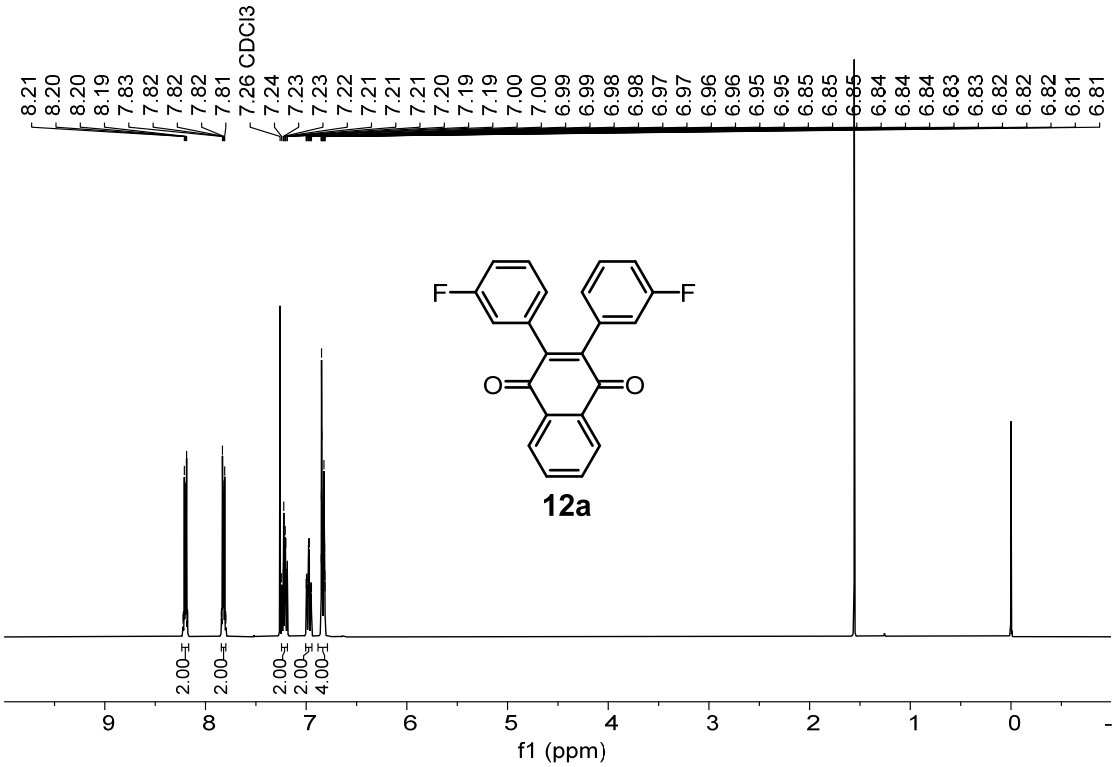
^{1}H NMR ($CDCl_3$, 400 MHz)



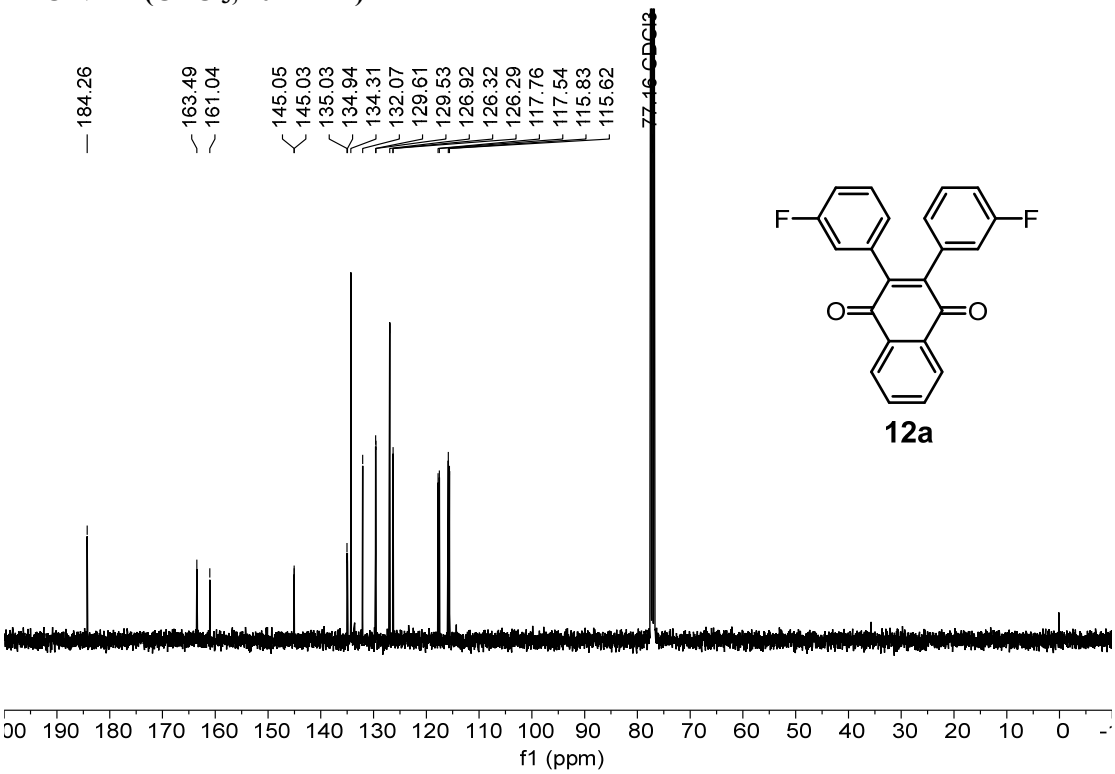
^{13}C NMR ($CDCl_3$, 101 MHz)



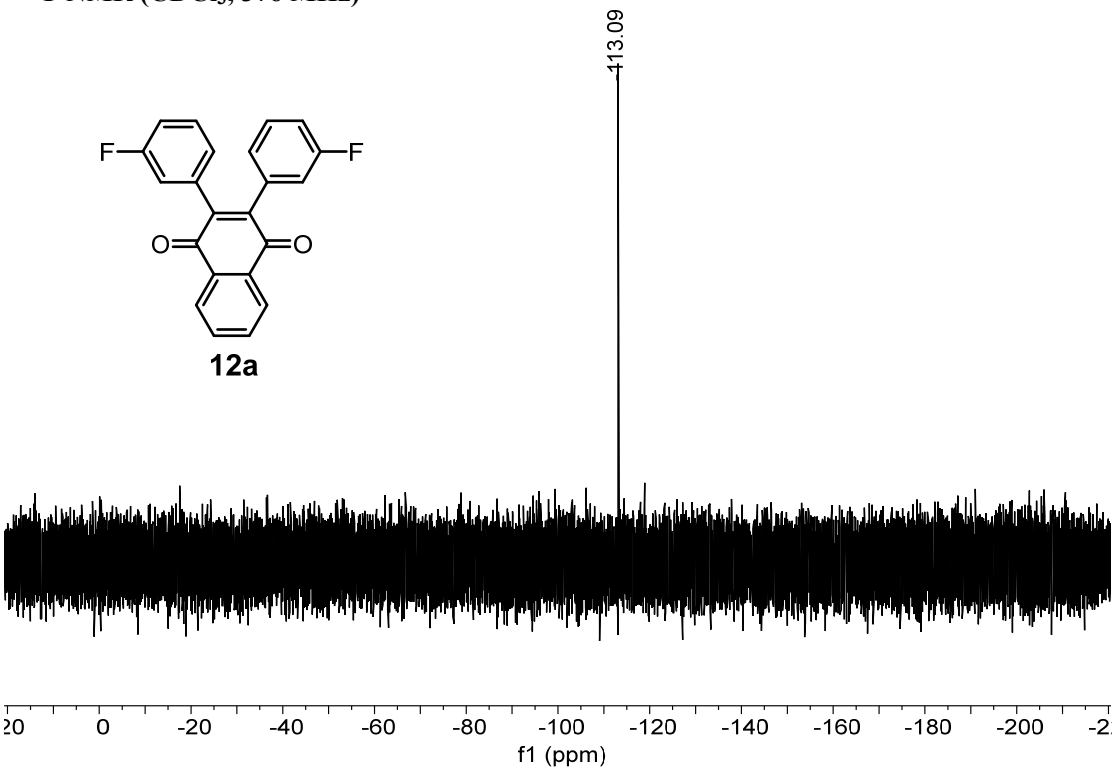
^{1}H NMR ($CDCl_3$, 400 MHz)



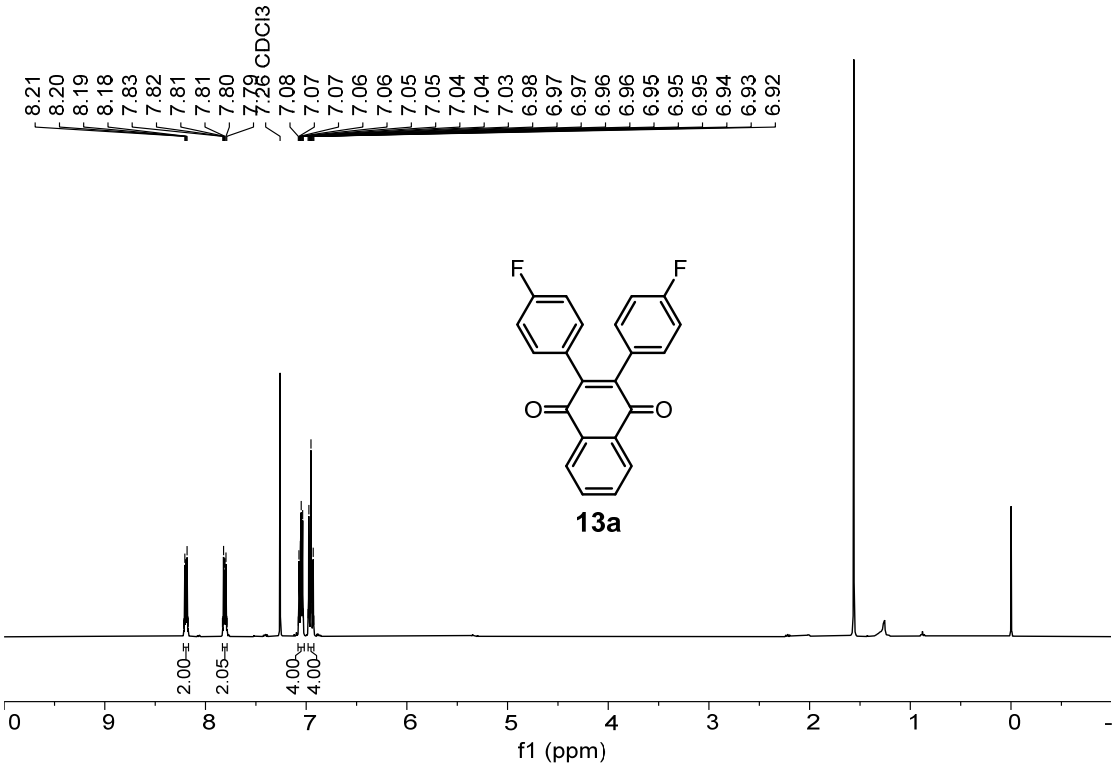
^{13}C NMR ($CDCl_3$, 101 MHz)



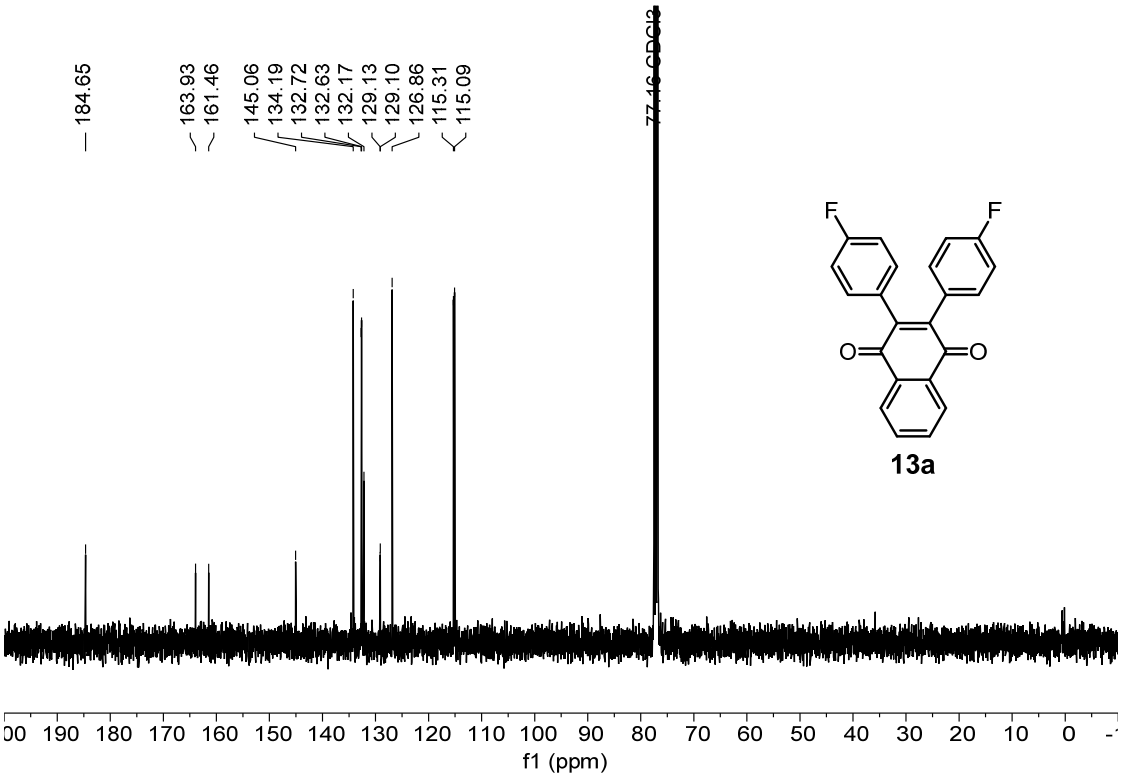
^{19}F NMR ($CDCl_3$, 376 MHz)



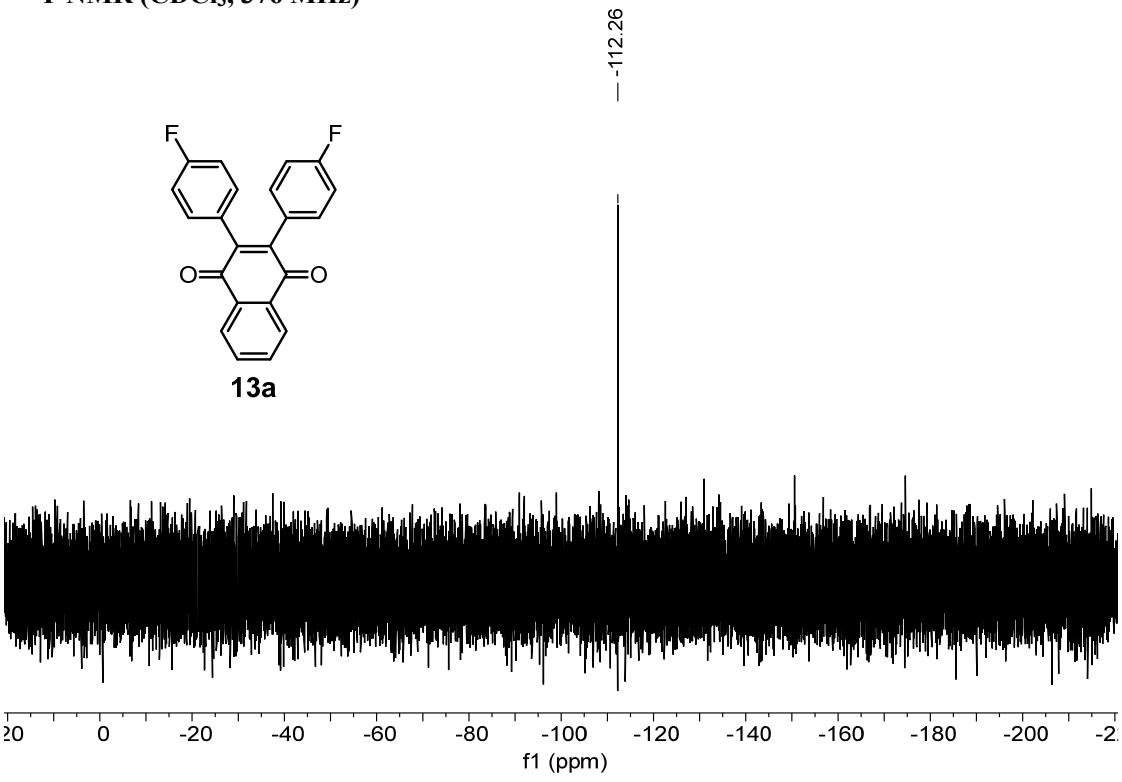
^{1}H NMR ($CDCl_3$, 400 MHz)



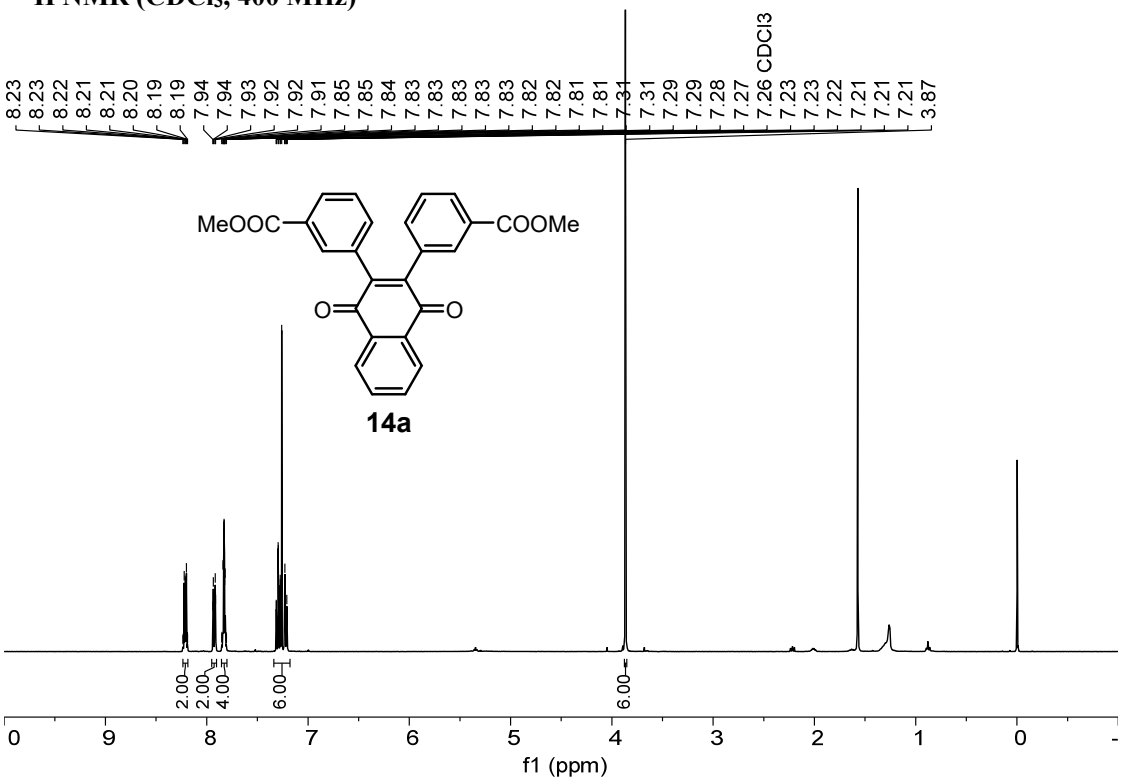
^{13}C NMR ($CDCl_3$, 101 MHz)



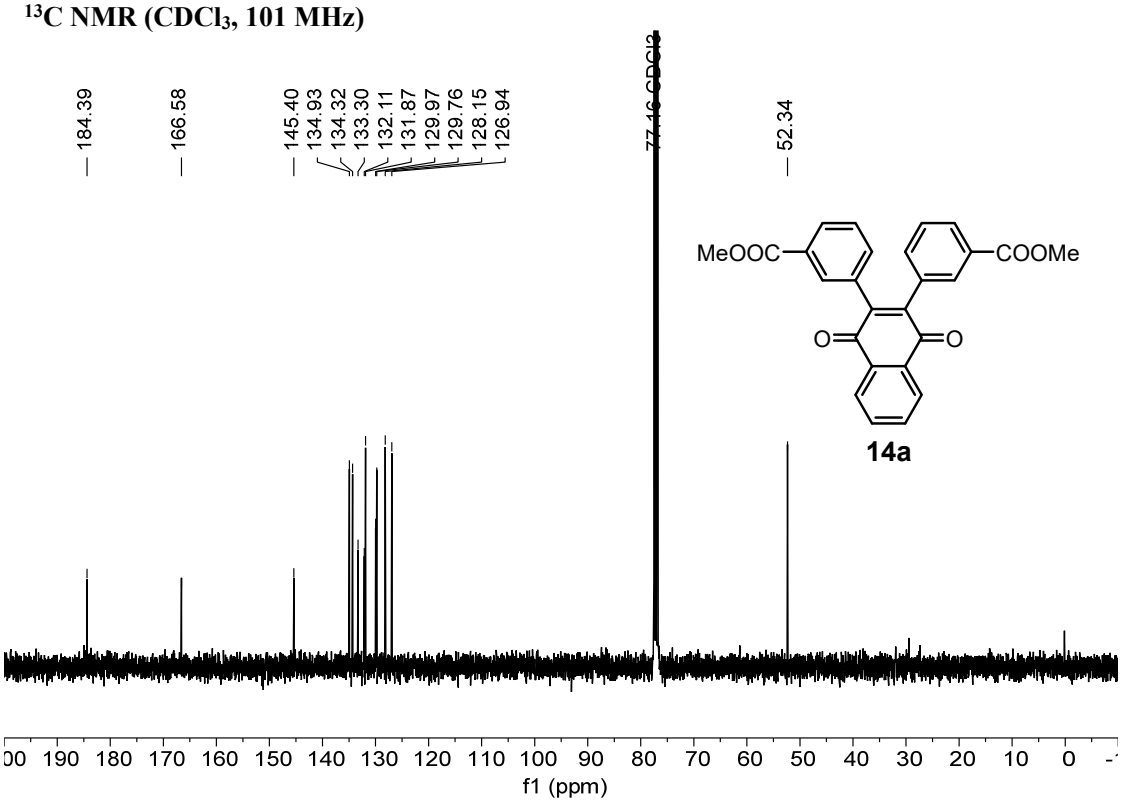
^{19}F NMR ($CDCl_3$, 376 MHz)



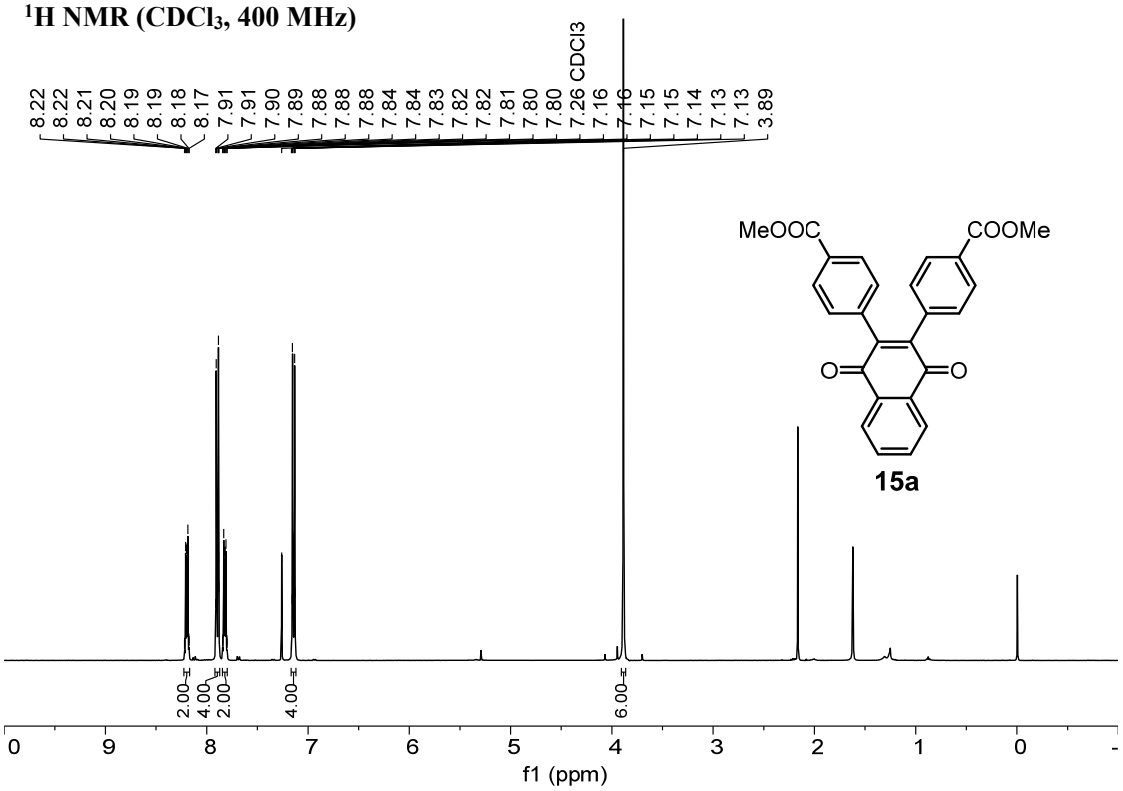
^{1}H NMR ($CDCl_3$, 400 MHz)



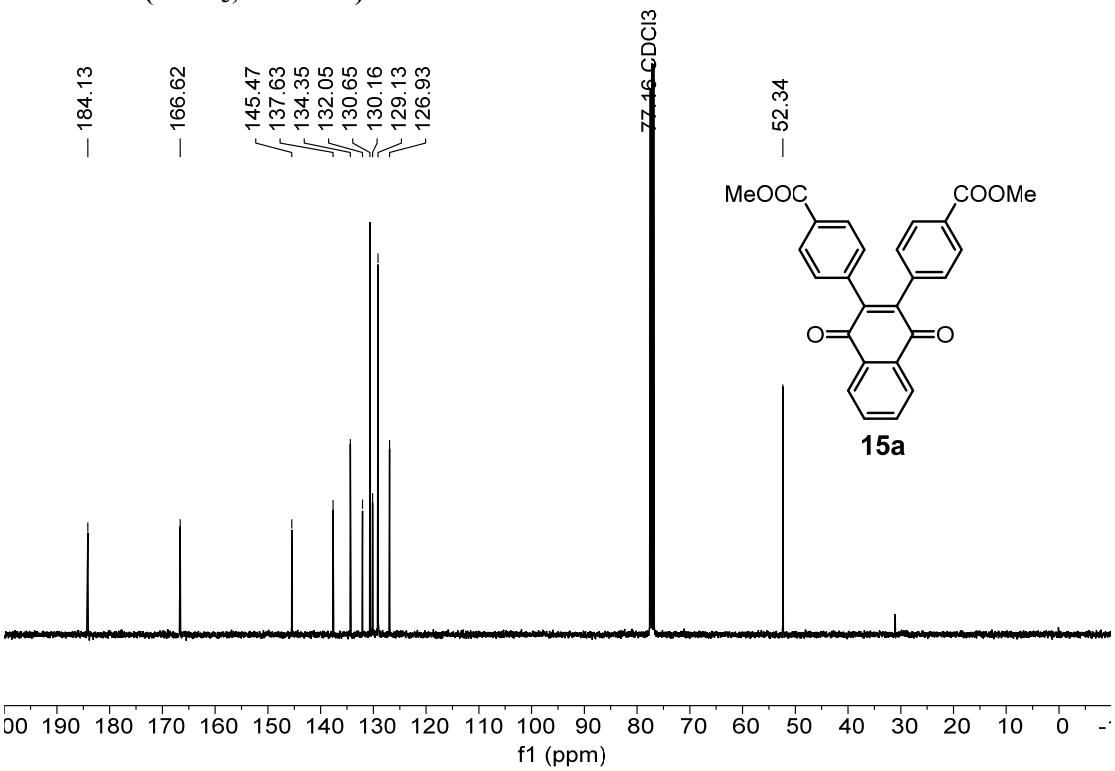
^{13}C NMR ($CDCl_3$, 101 MHz)



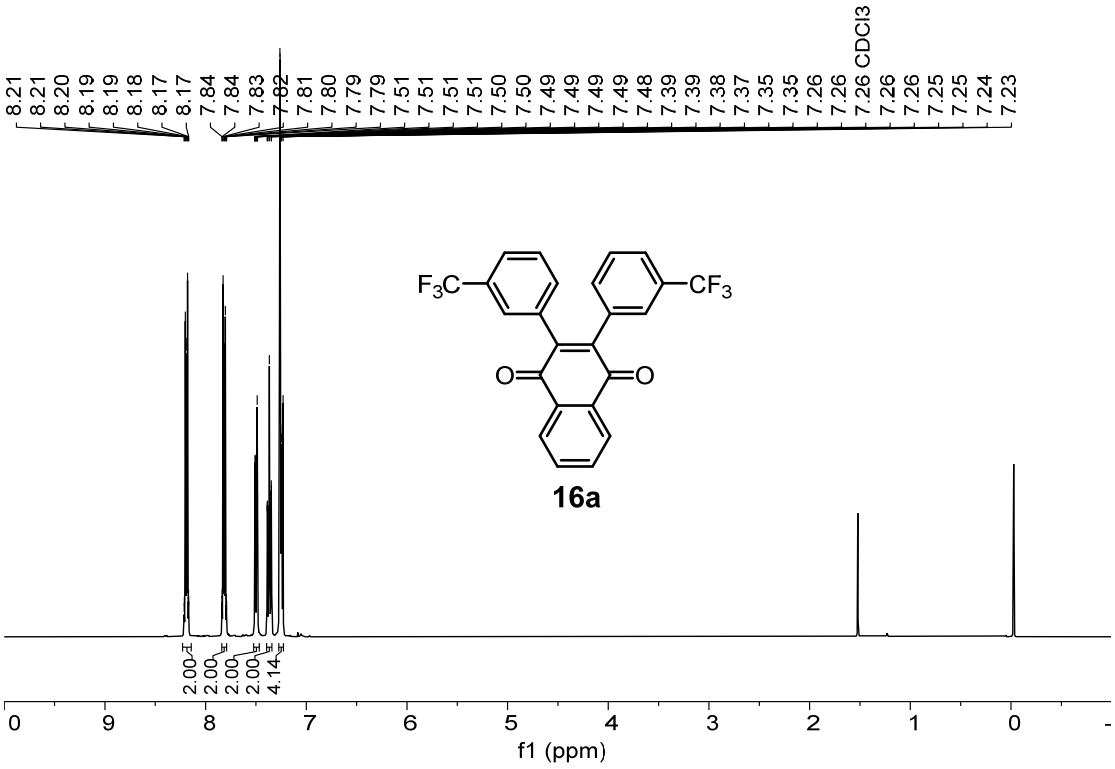
^{1}H NMR ($CDCl_3$, 400 MHz)



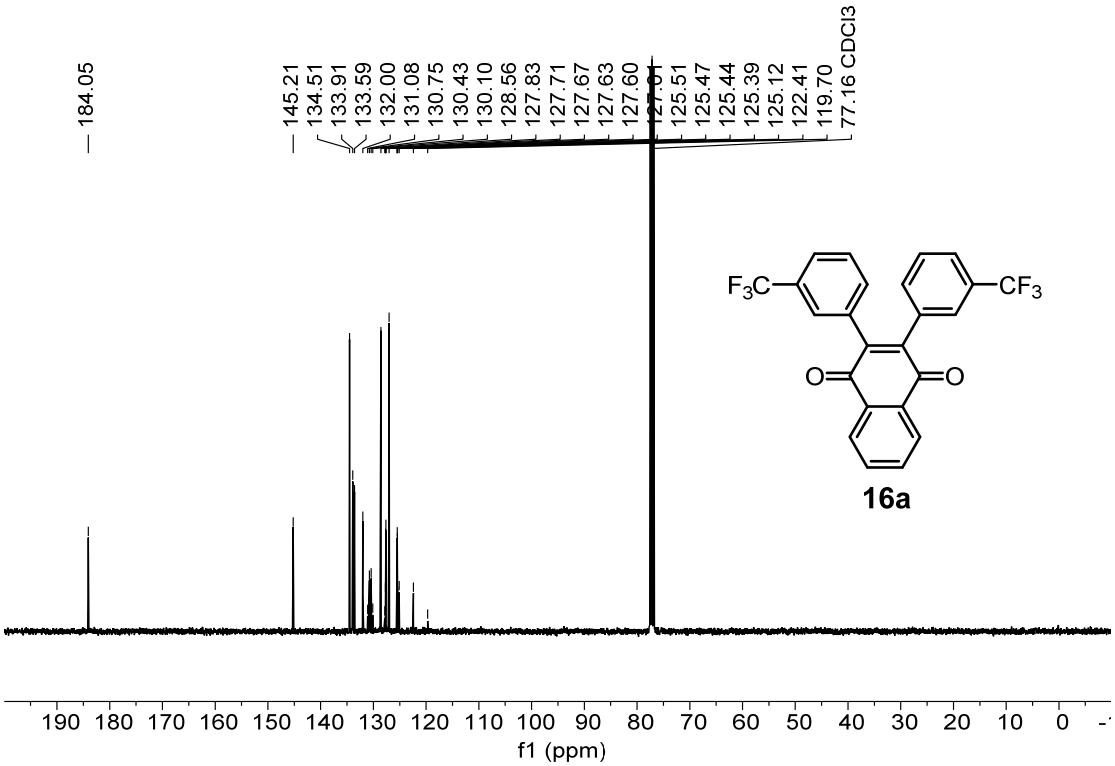
^{13}C NMR ($CDCl_3$, 101 MHz)



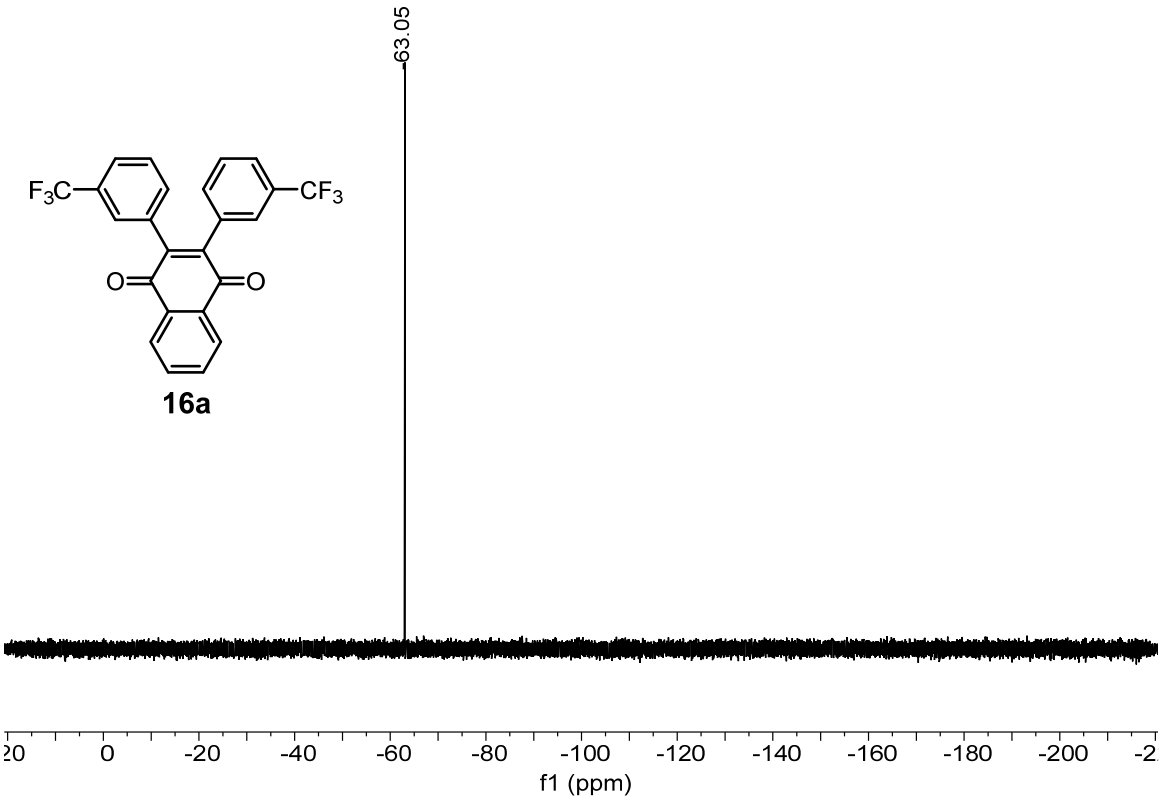
^{1}H NMR ($CDCl_3$, 400 MHz)



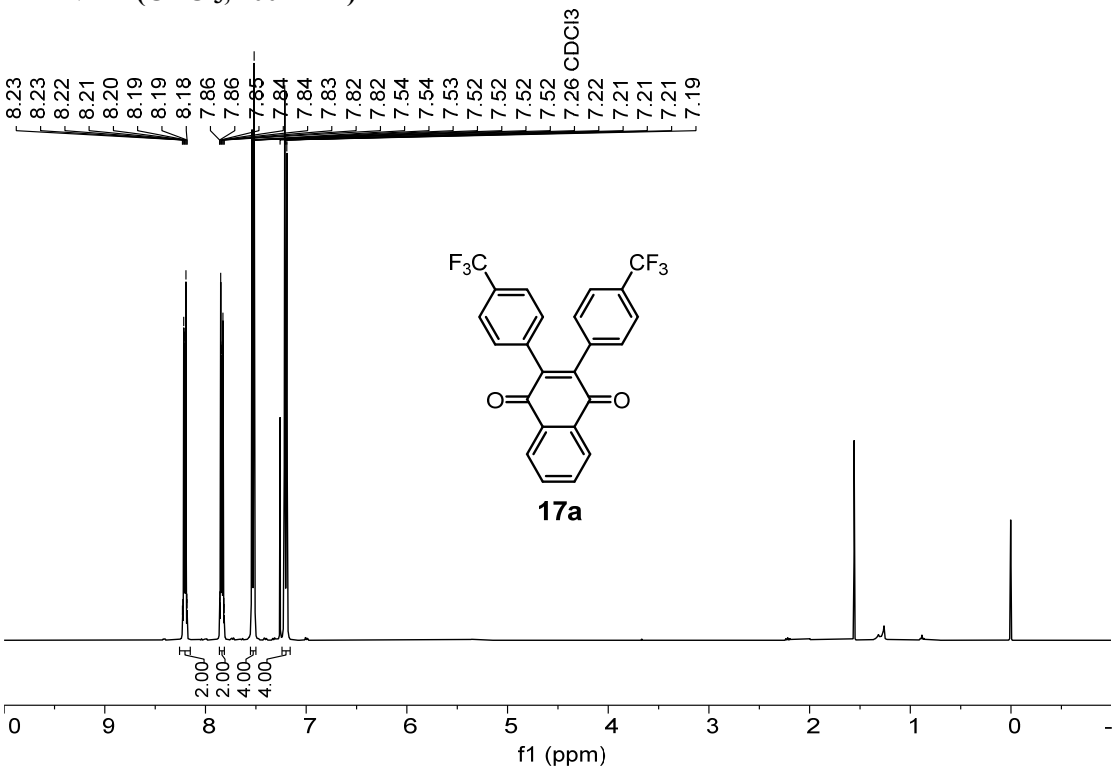
^{13}C NMR ($CDCl_3$, 101 MHz)



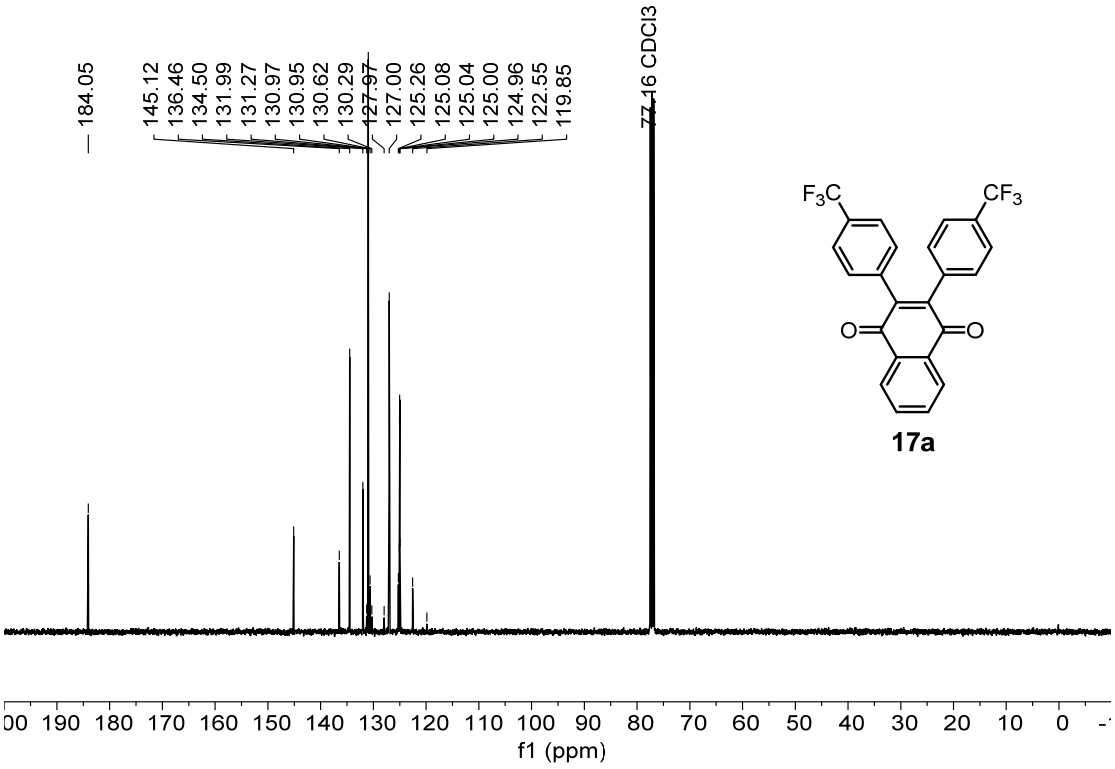
^{19}F NMR ($CDCl_3$, 376 MHz)



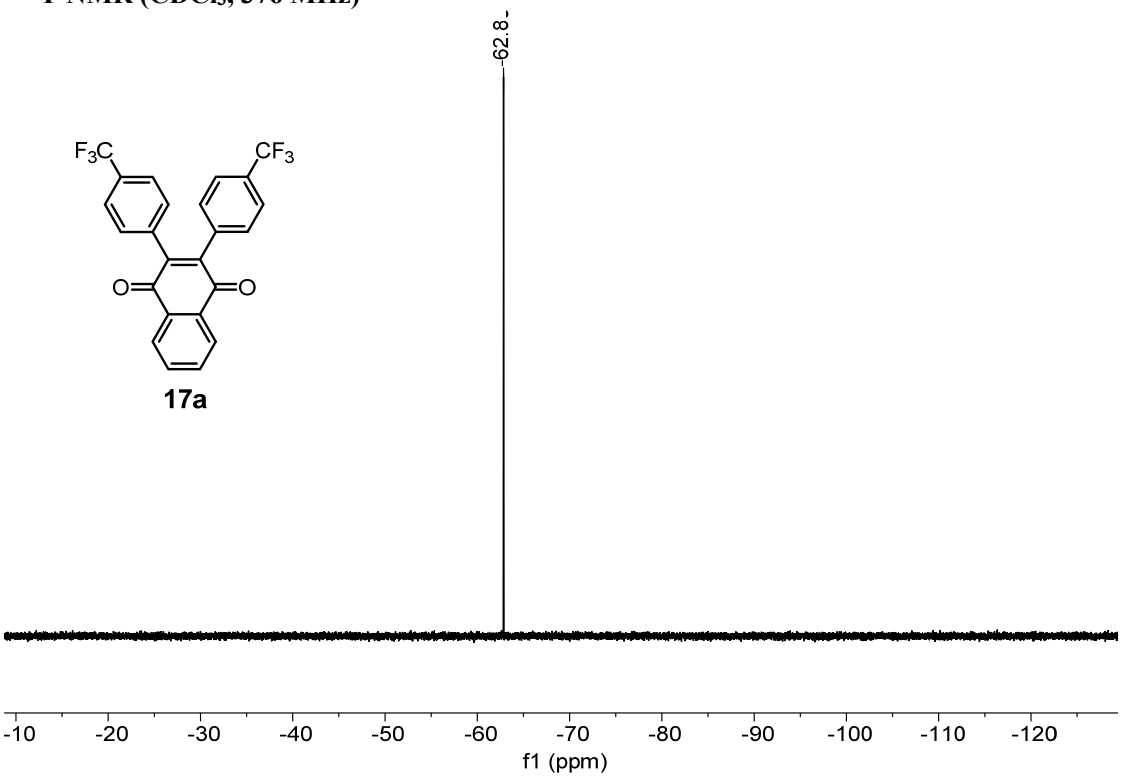
^{1}H NMR ($CDCl_3$, 400 MHz)



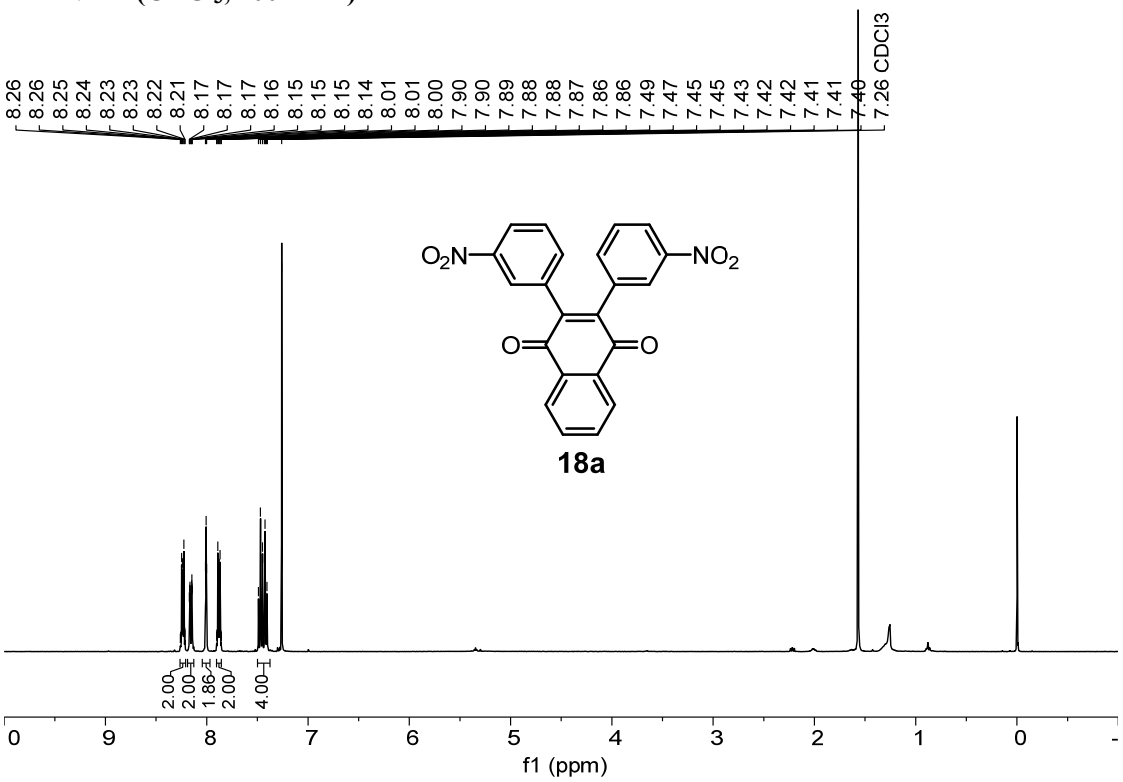
^{13}C NMR ($CDCl_3$, 101 MHz)



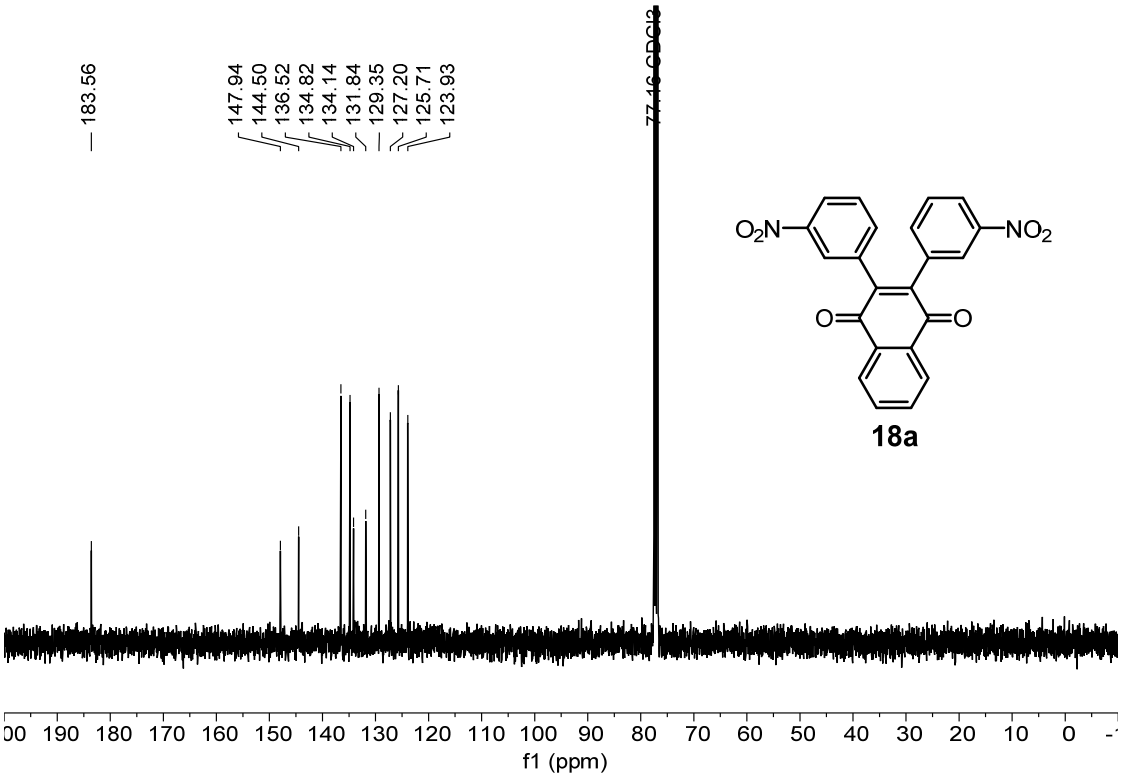
^{19}F NMR ($CDCl_3$, 376 MHz)



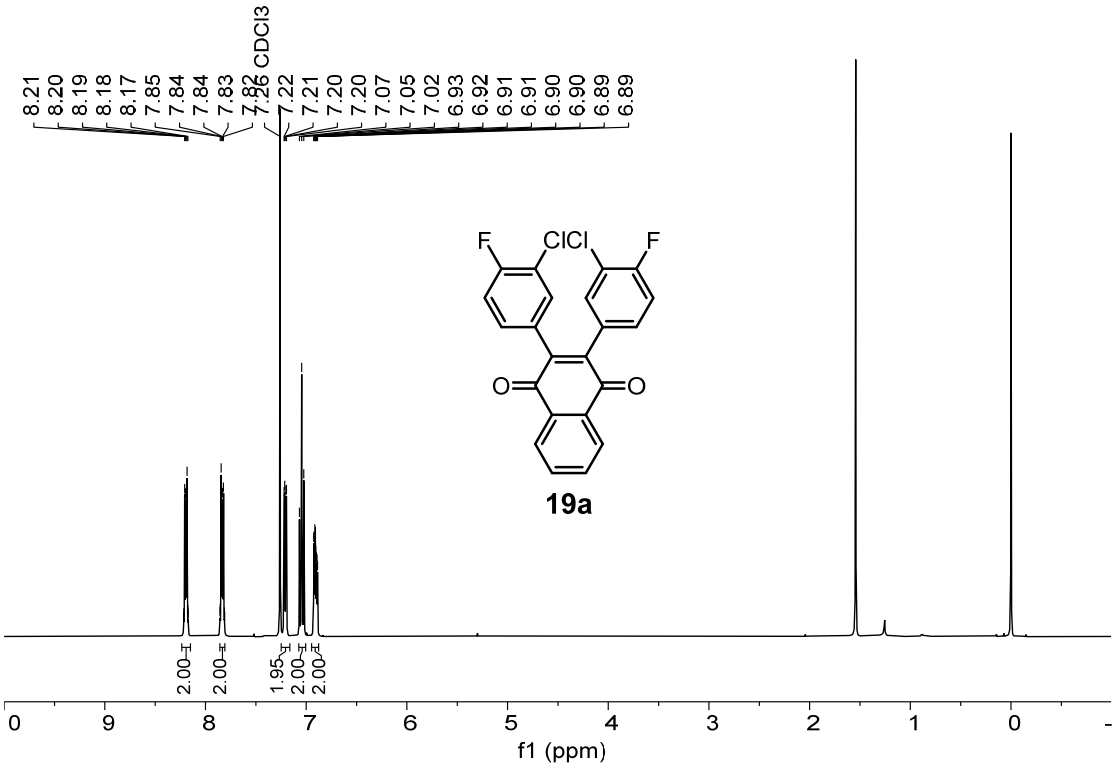
^{1}H NMR ($CDCl_3$, 400 MHz)



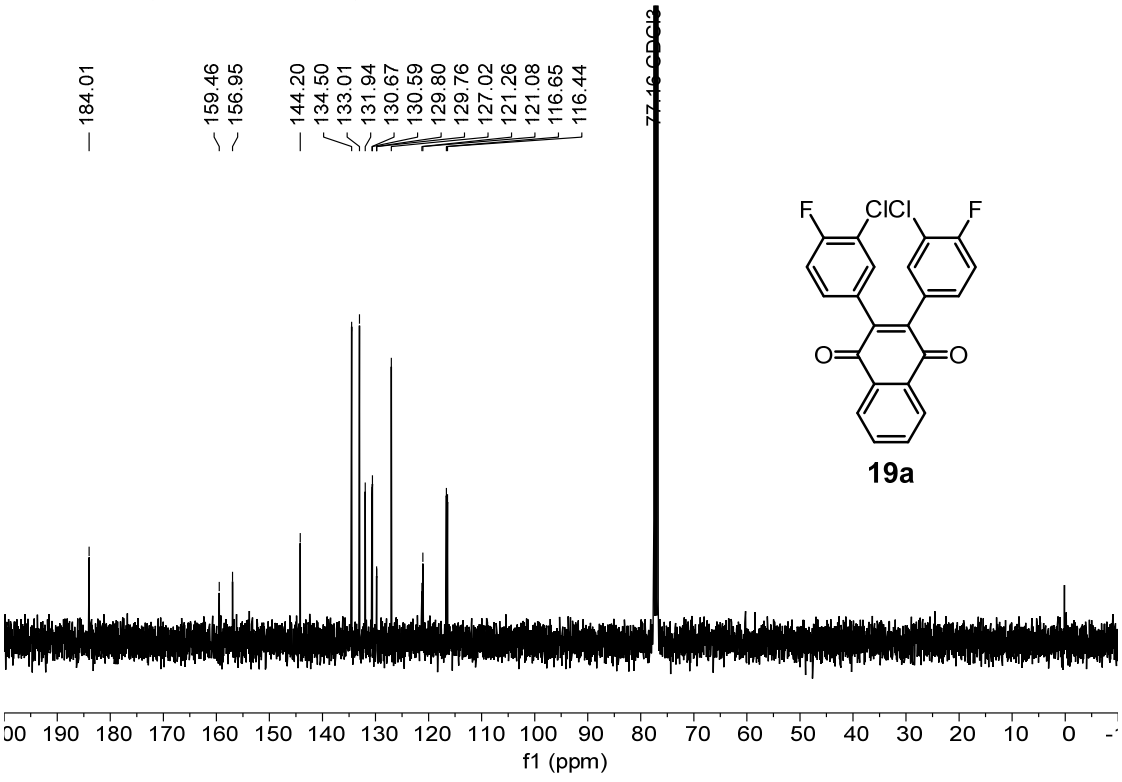
^{13}C NMR ($CDCl_3$, 101 MHz)



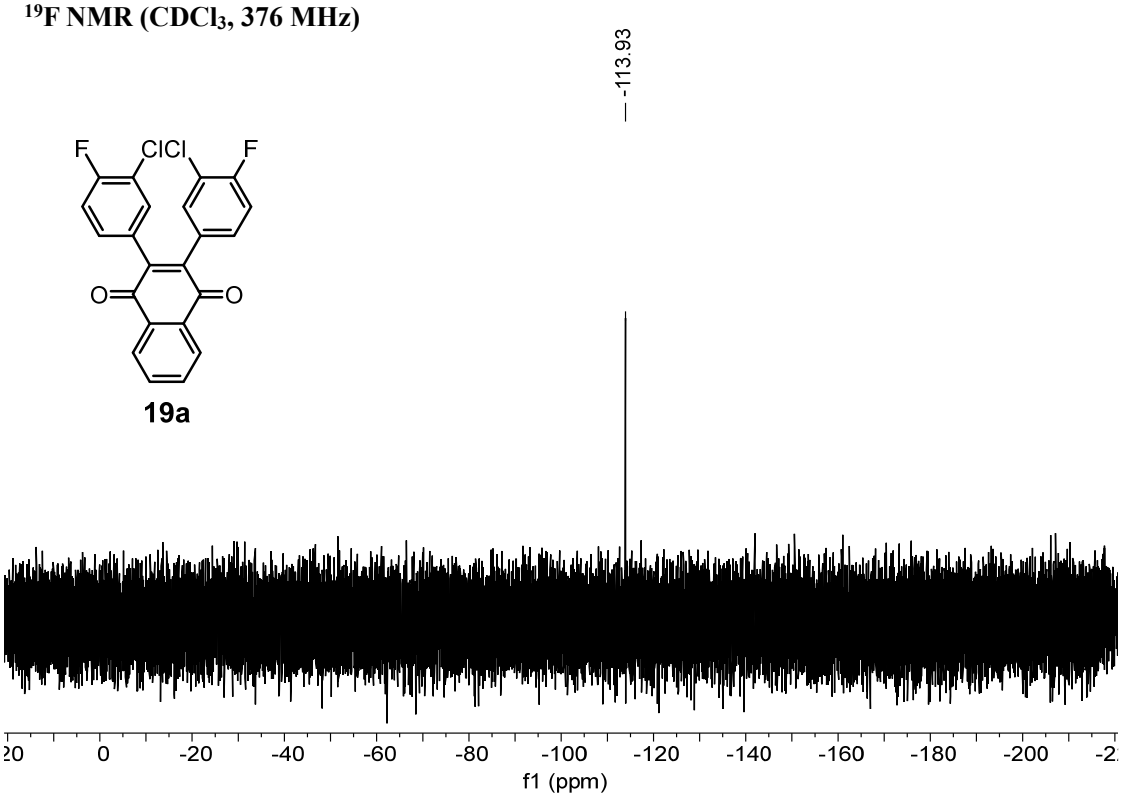
^{1}H NMR ($CDCl_3$, 400 MHz)



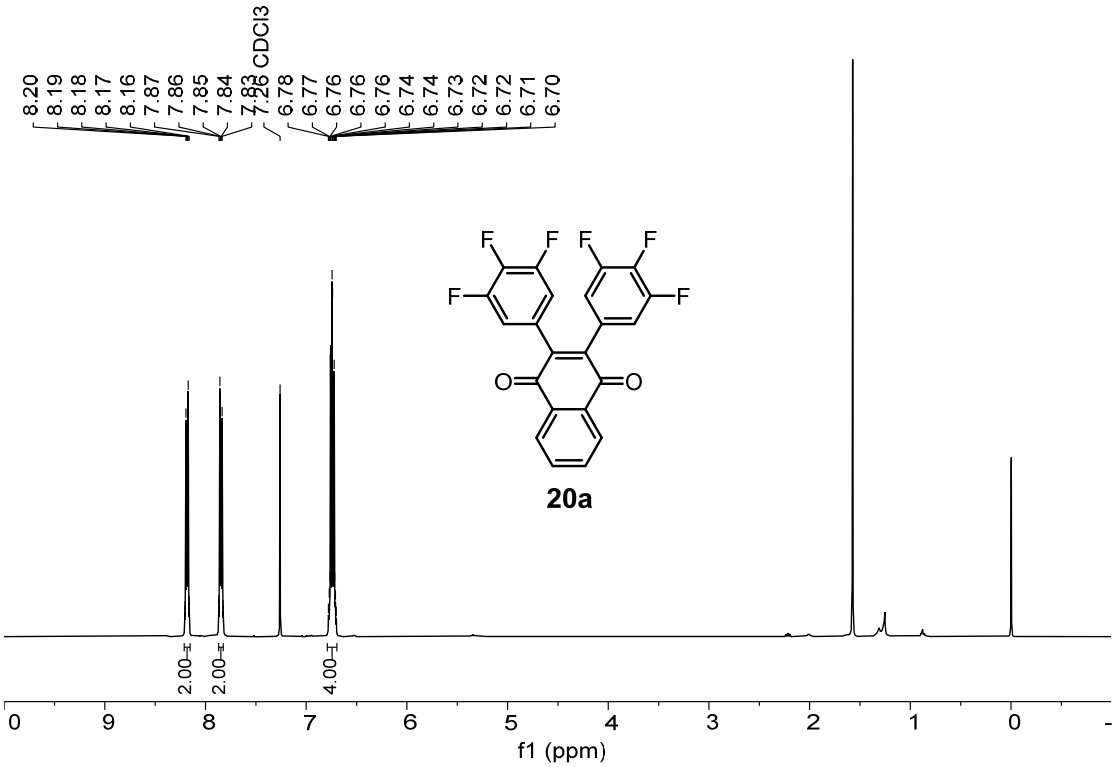
^{13}C NMR ($CDCl_3$, 101 MHz)



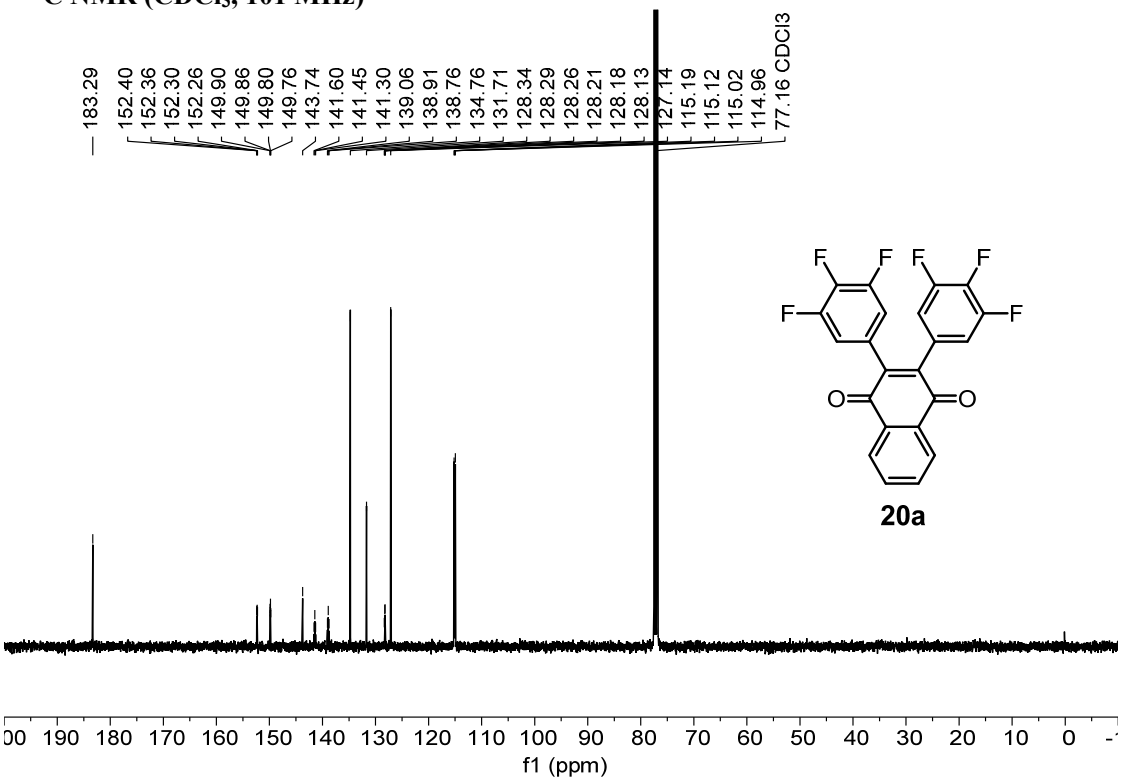
^{19}F NMR ($CDCl_3$, 376 MHz)



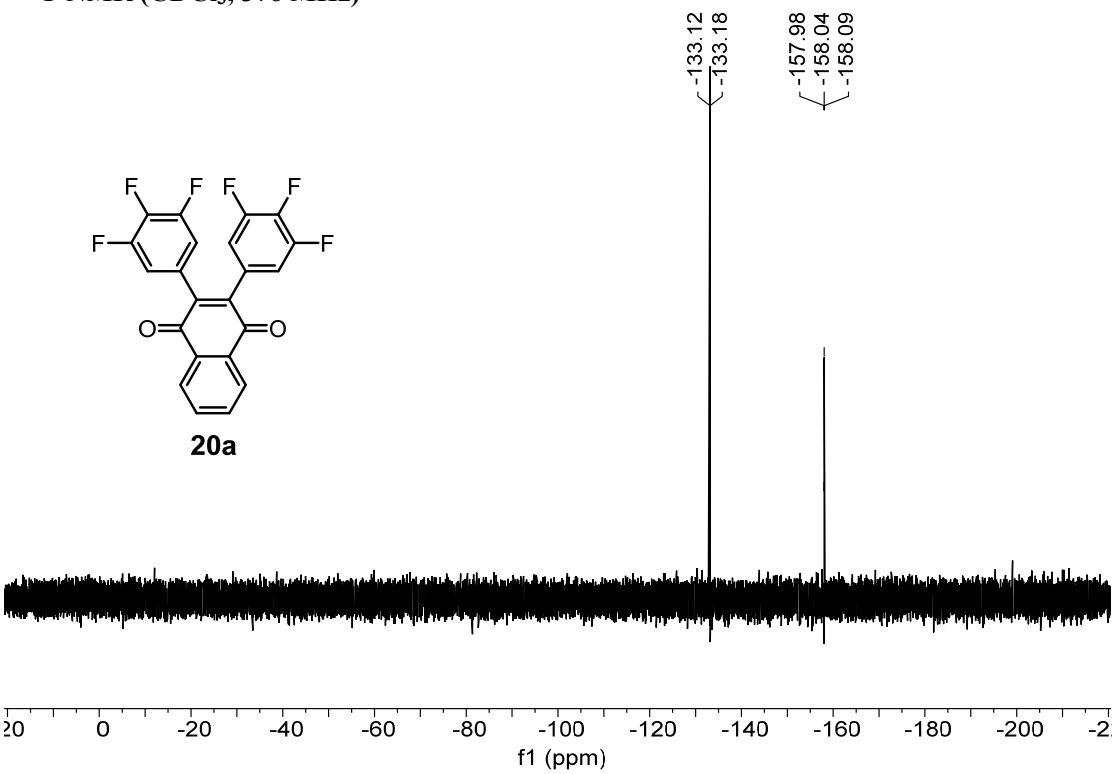
^{1}H NMR ($CDCl_3$, 400 MHz)



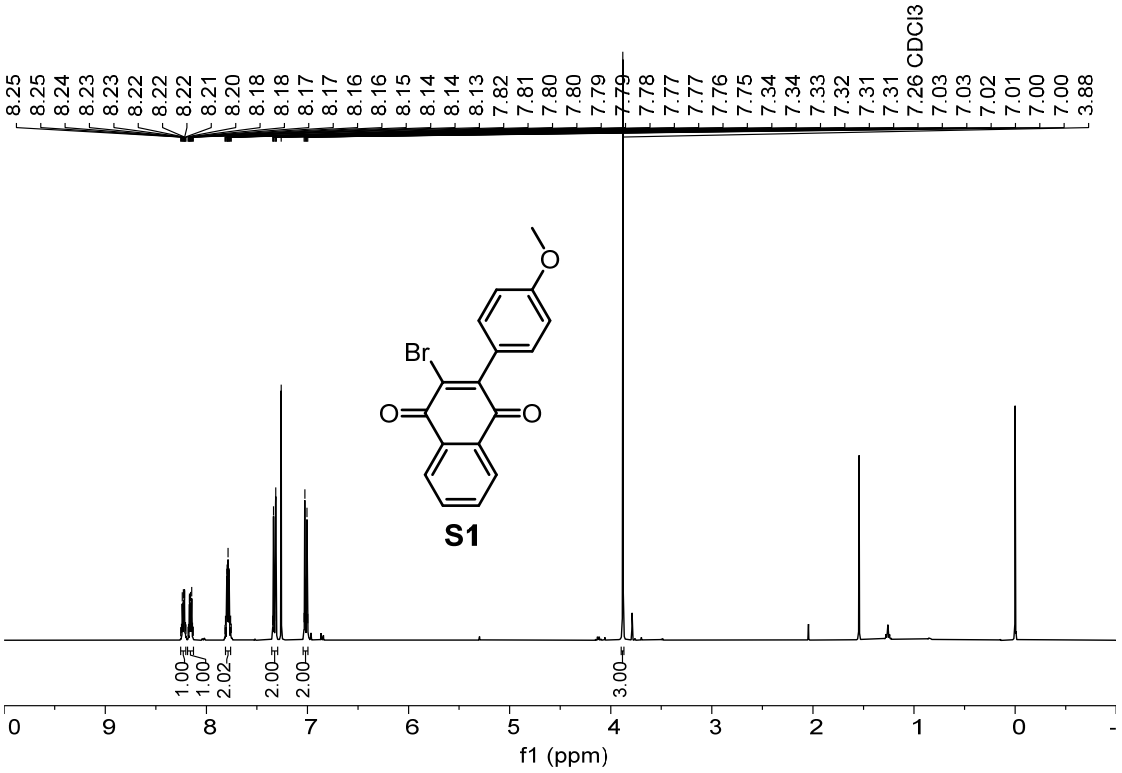
^{13}C NMR ($CDCl_3$, 101 MHz)



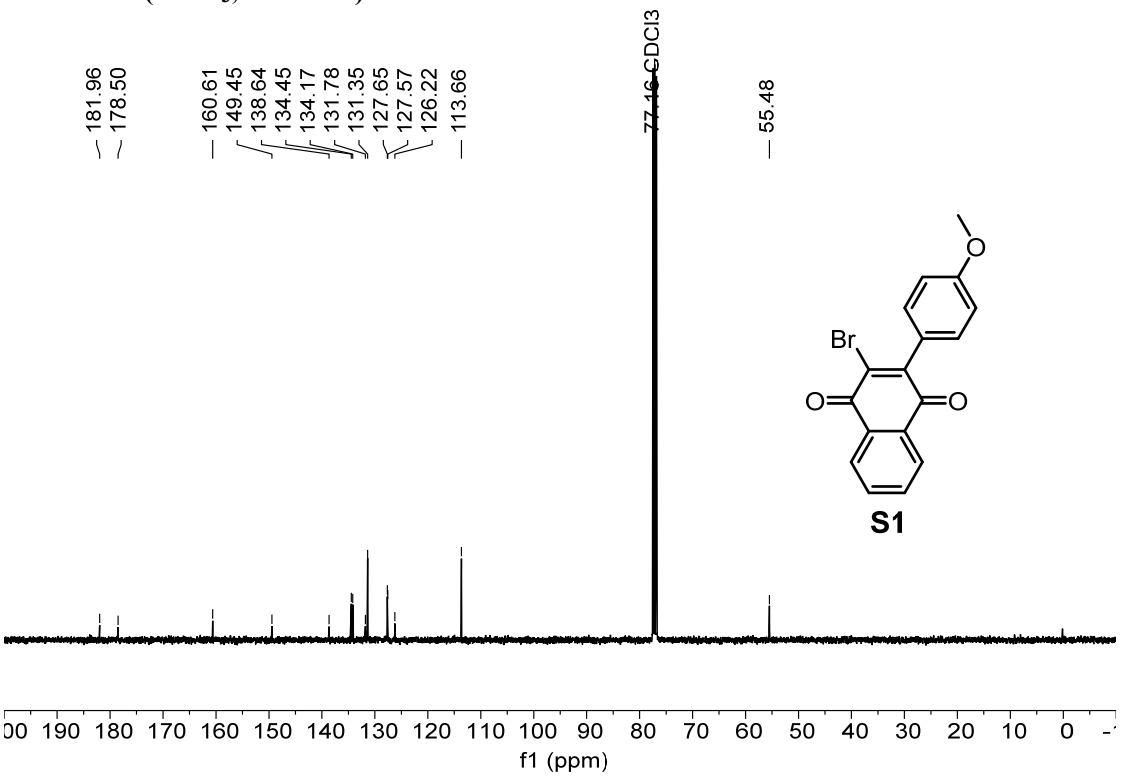
^{19}F NMR ($CDCl_3$, 376 MHz)



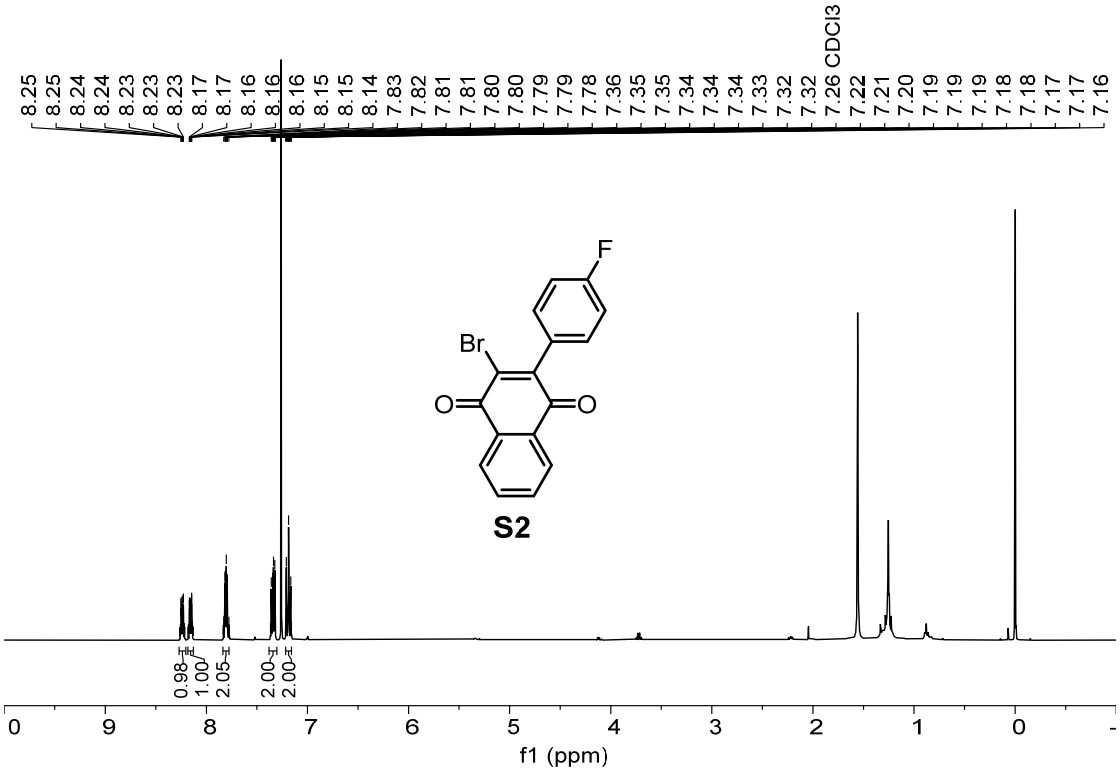
^{1}H NMR ($CDCl_3$, 400 MHz)



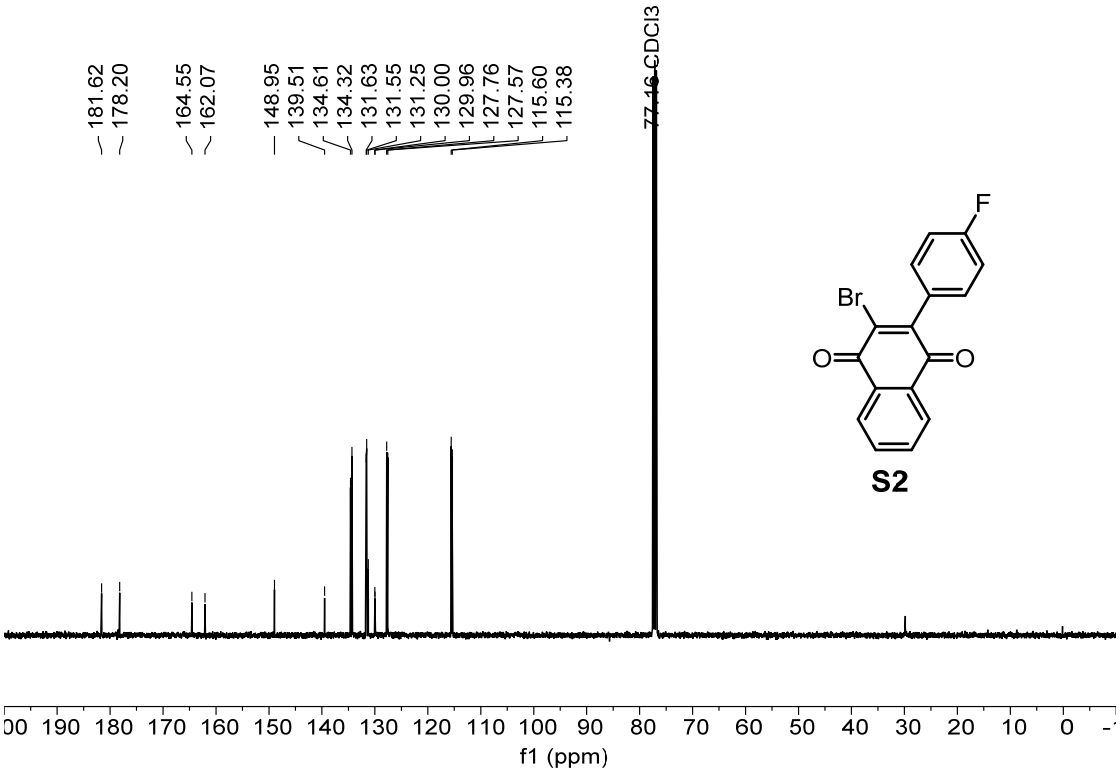
^{13}C NMR ($CDCl_3$, 101 MHz)



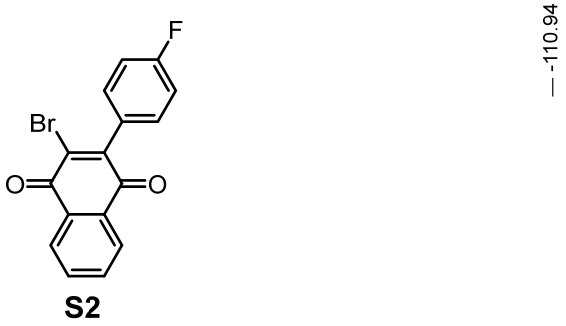
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)

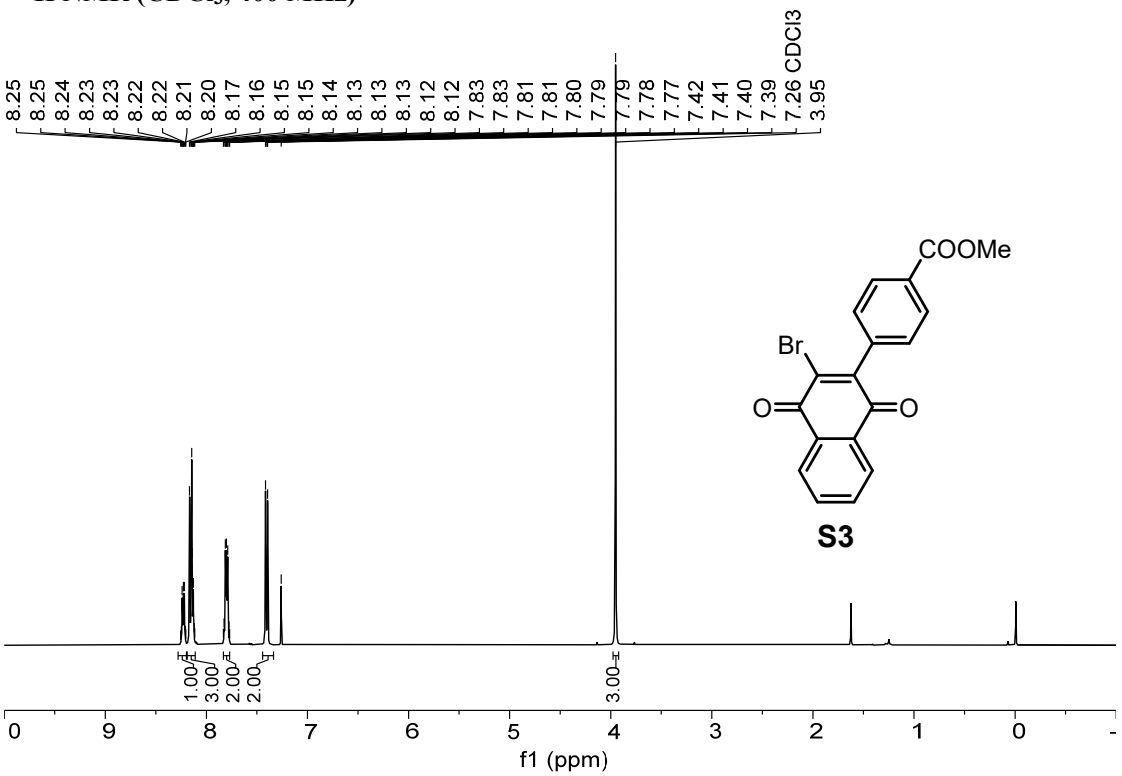


^{19}F NMR ($CDCl_3$, 376 MHz)



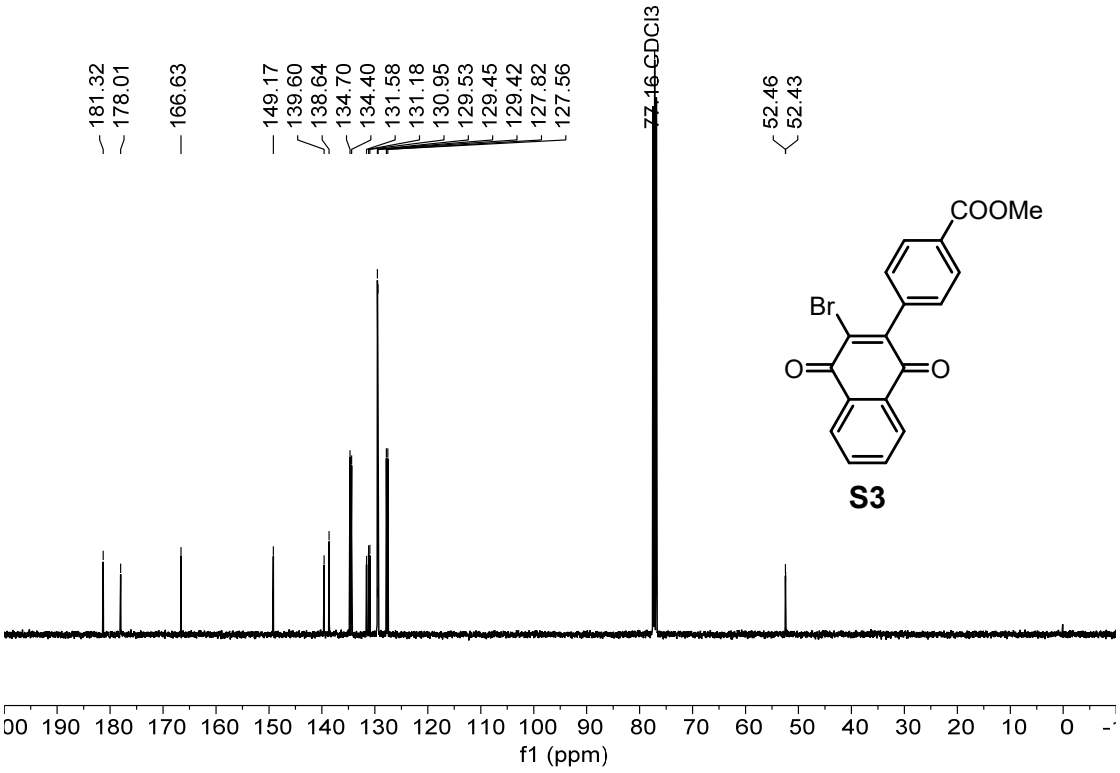
S2

^{1}H NMR ($CDCl_3$, 400 MHz)

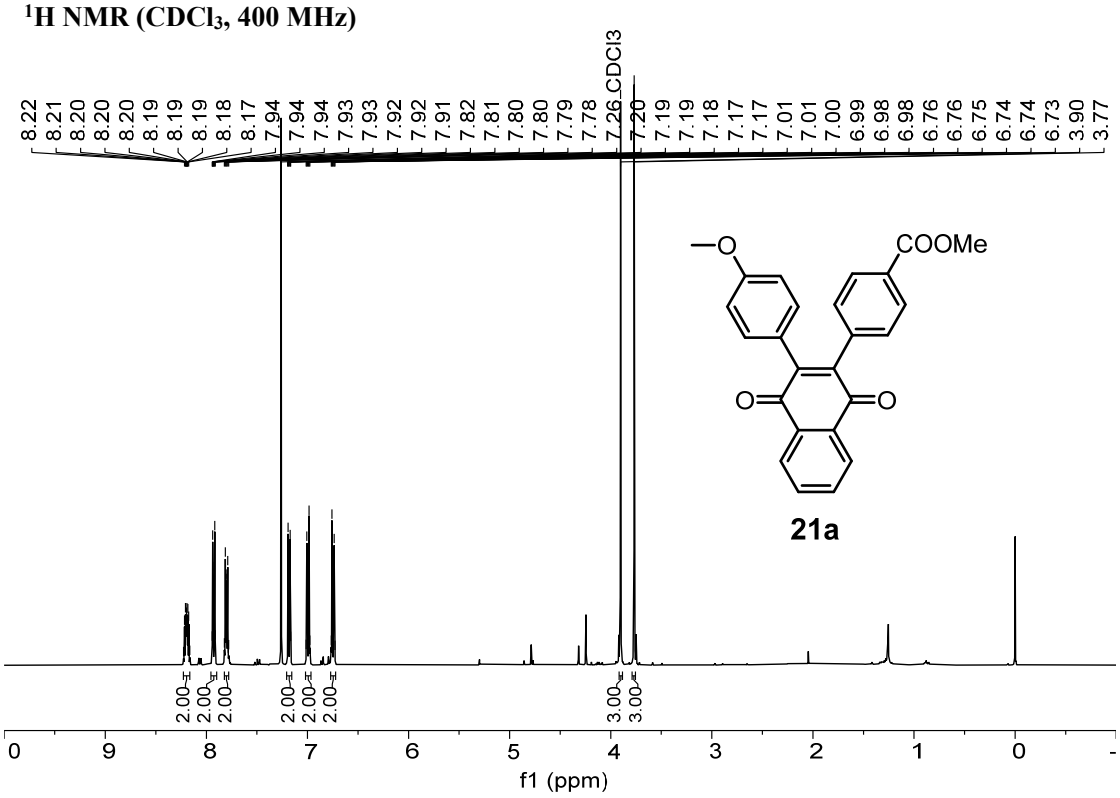


S3

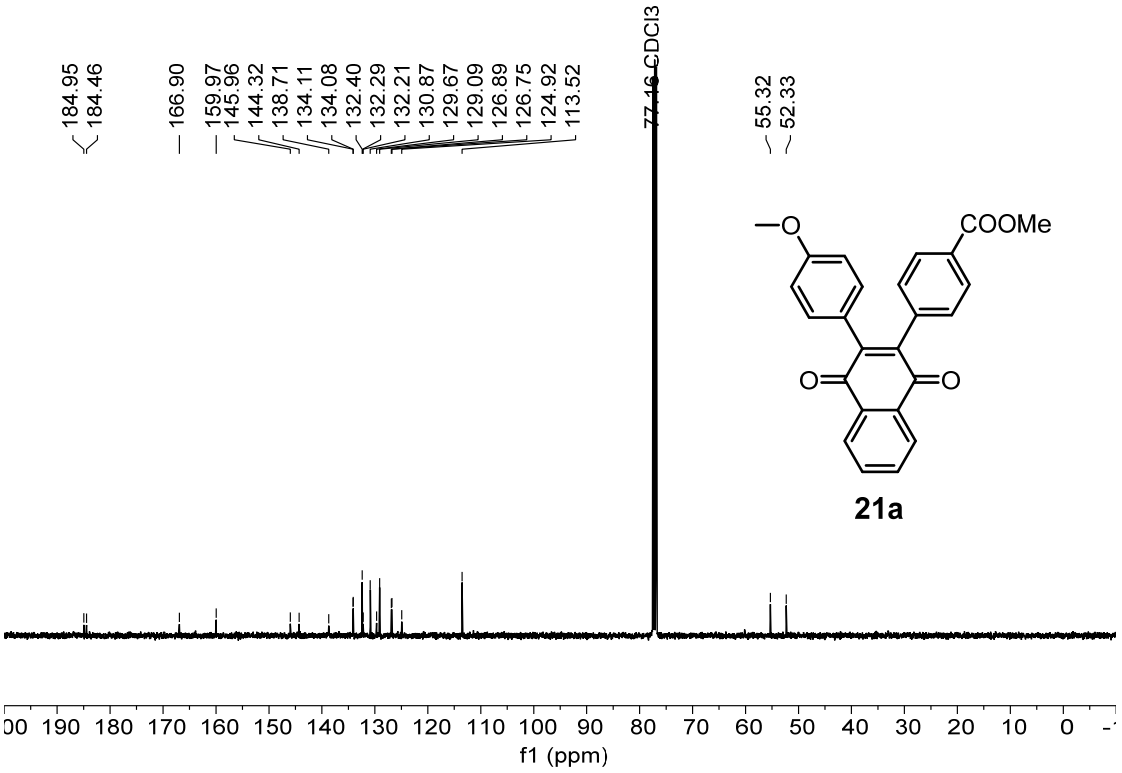
^{13}C NMR ($CDCl_3$, 101 MHz)



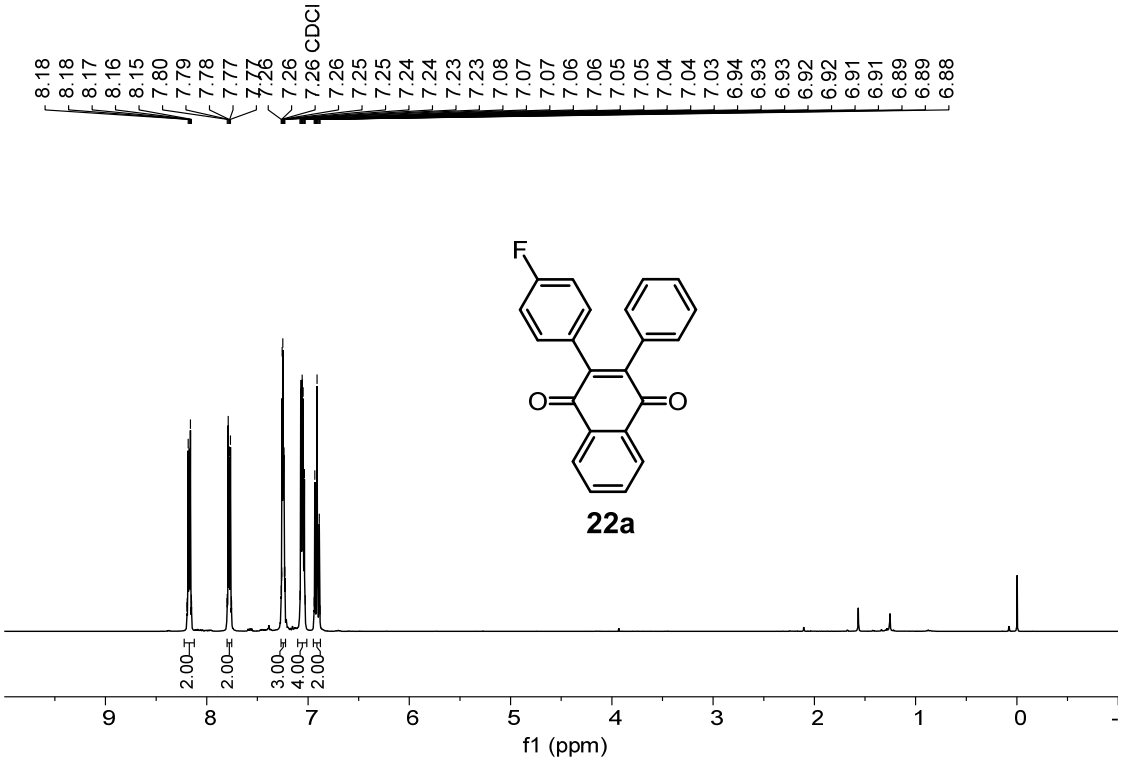
^{1}H NMR ($CDCl_3$, 400 MHz)



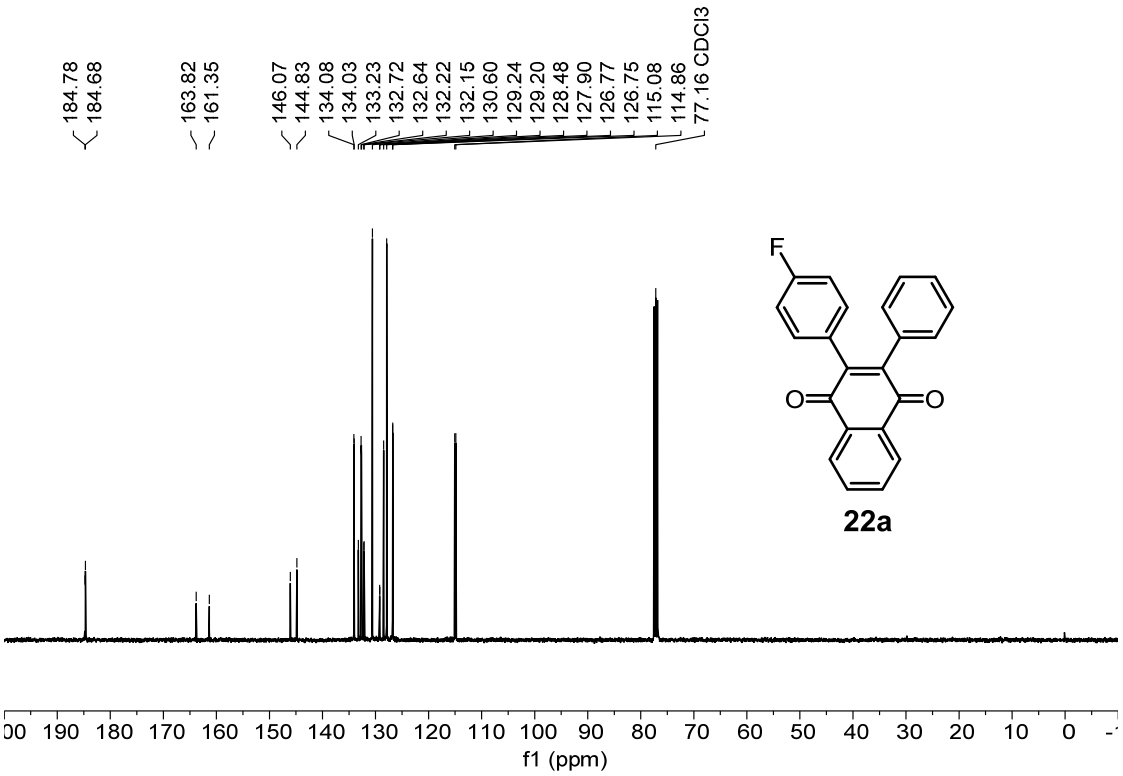
^{13}C NMR ($CDCl_3$, 101 MHz)



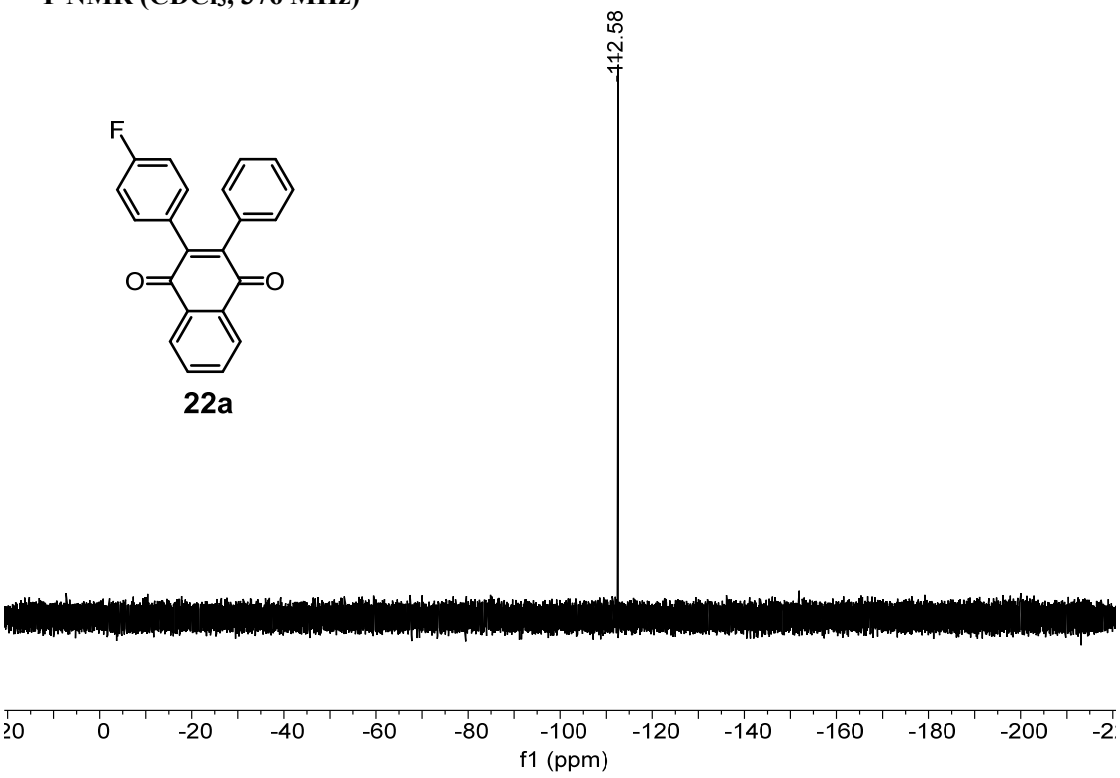
^{1}H NMR ($CDCl_3$, 400 MHz)



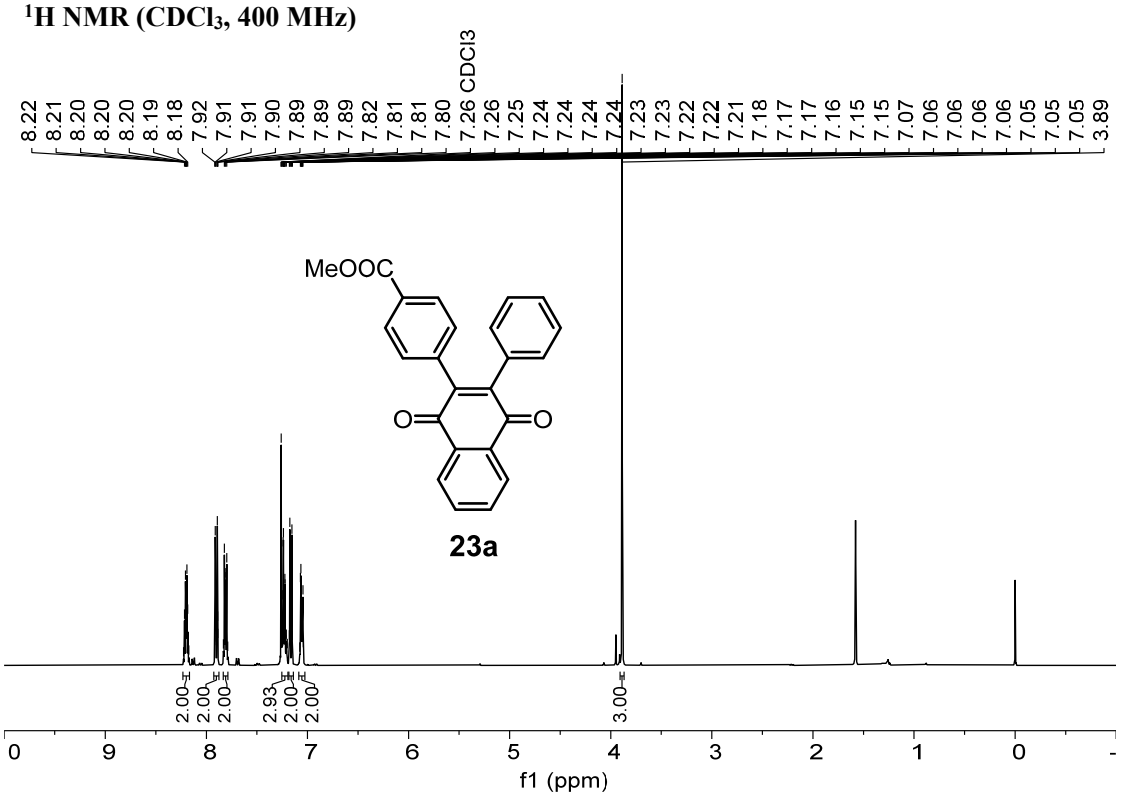
^{13}C NMR ($CDCl_3$, 101 MHz)



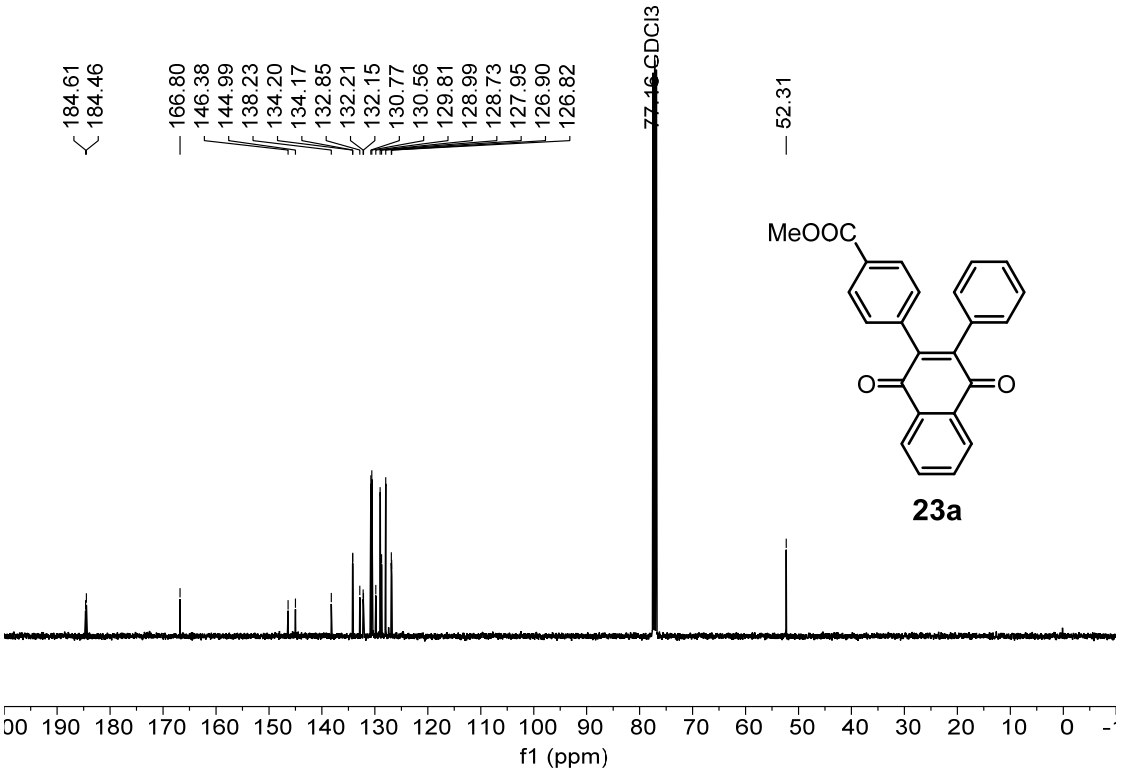
^{19}F NMR ($CDCl_3$, 376 MHz)



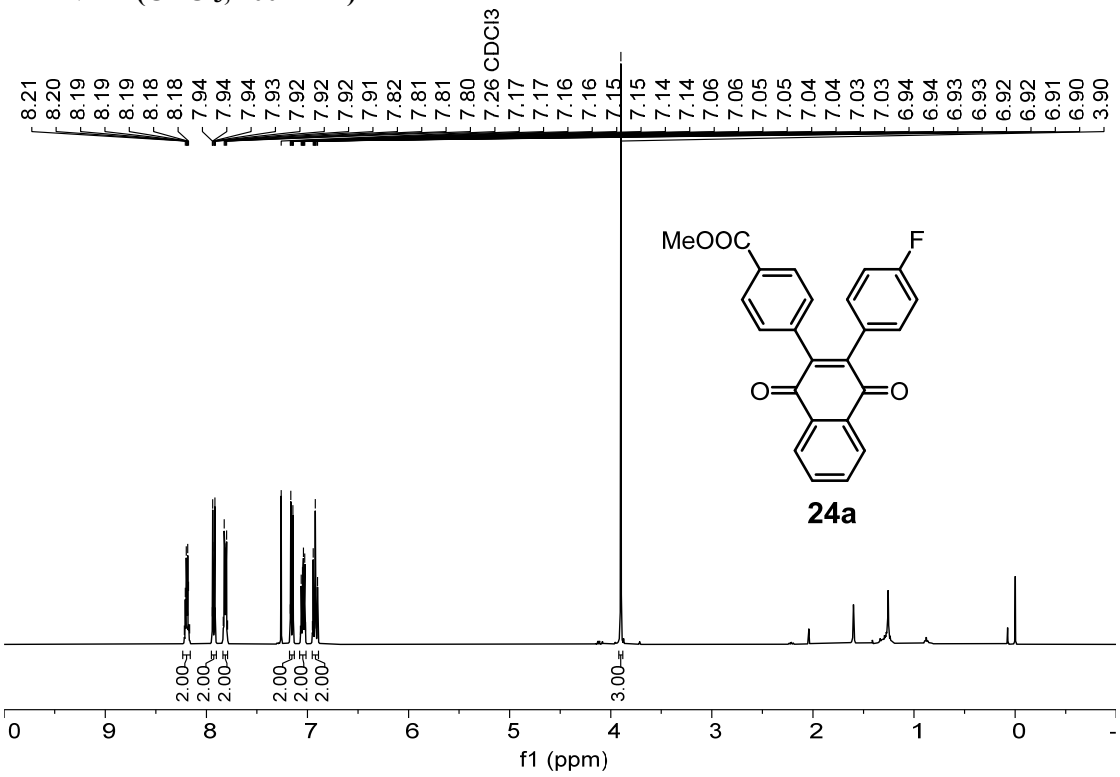
^{1}H NMR ($CDCl_3$, 400 MHz)



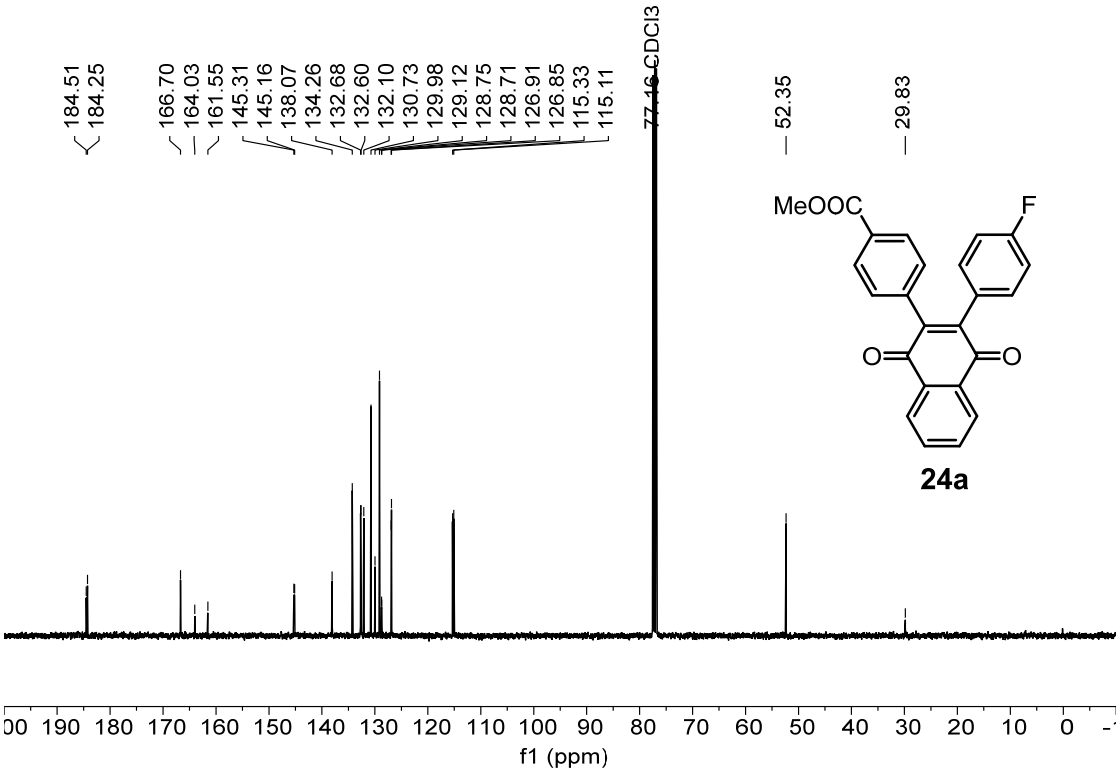
^{13}C NMR ($CDCl_3$, 101 MHz)



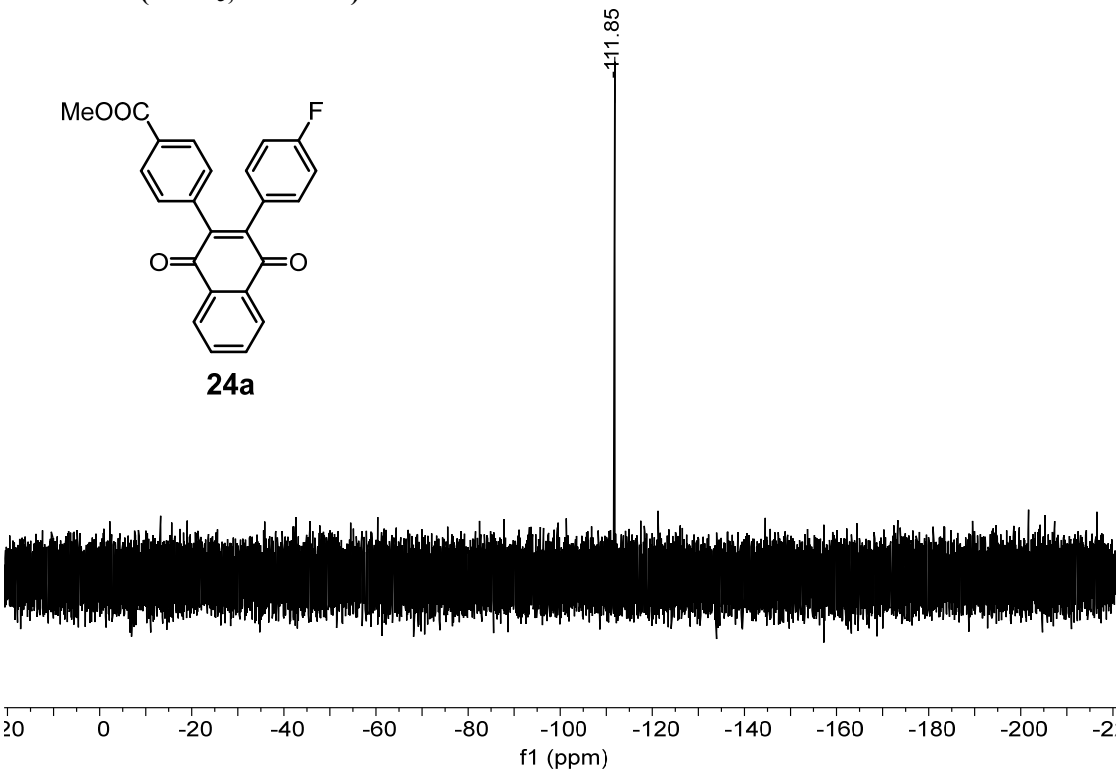
^{1}H NMR ($CDCl_3$, 400 MHz)



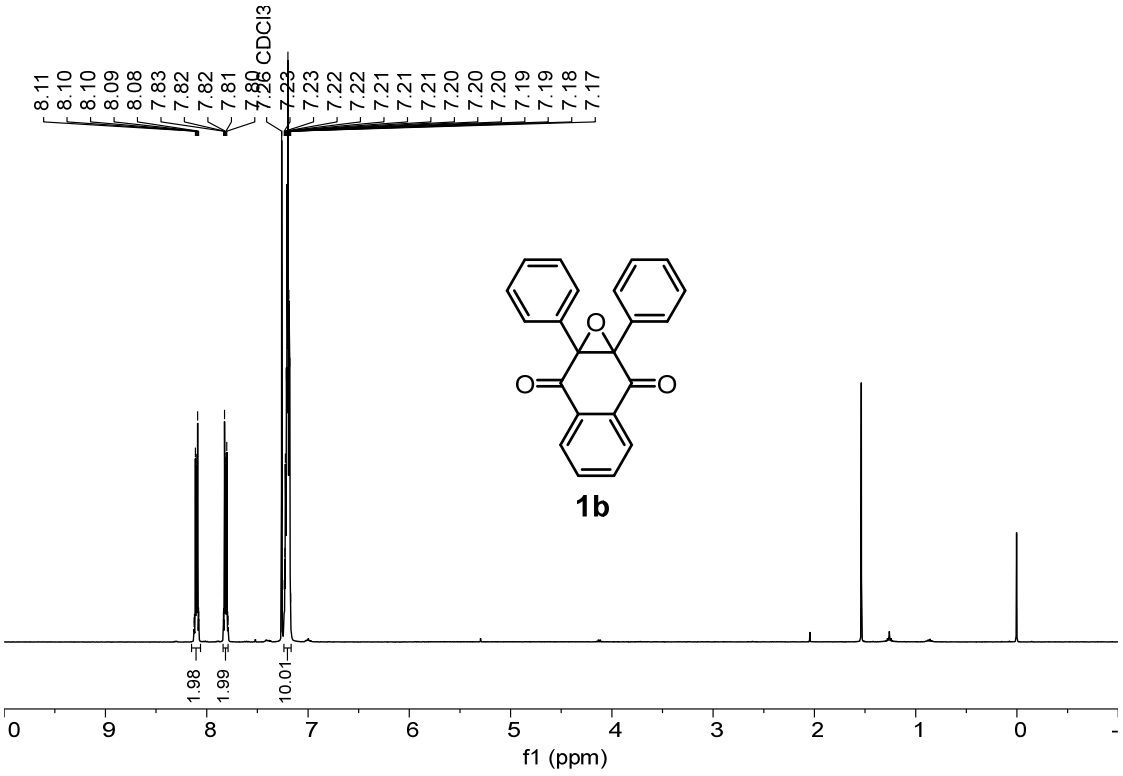
^{13}C NMR ($CDCl_3$, 101 MHz)



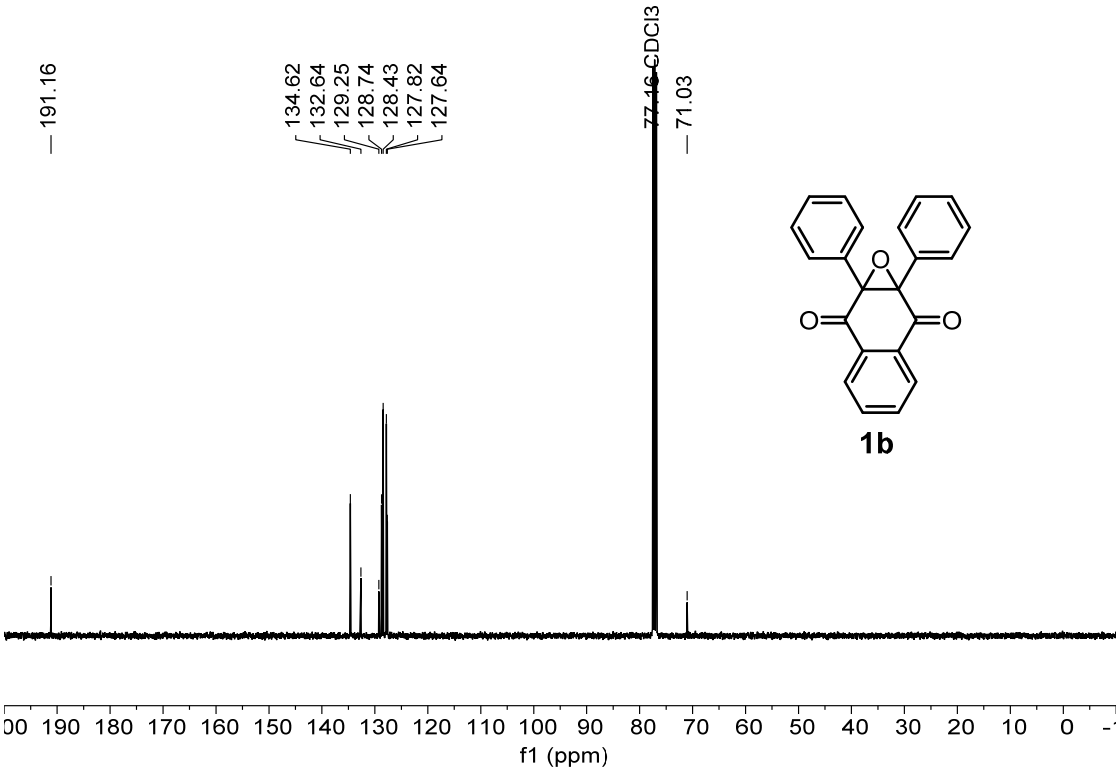
^{19}F NMR ($CDCl_3$, 376 MHz)



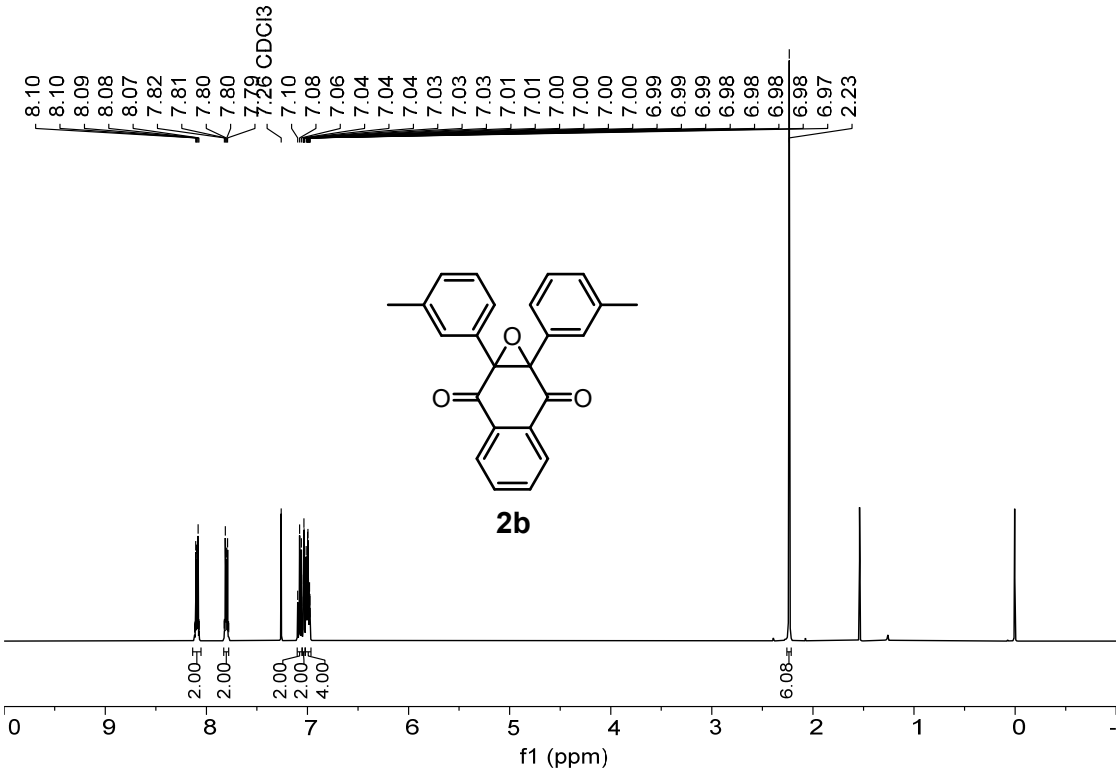
^{1}H NMR ($CDCl_3$, 400 MHz)



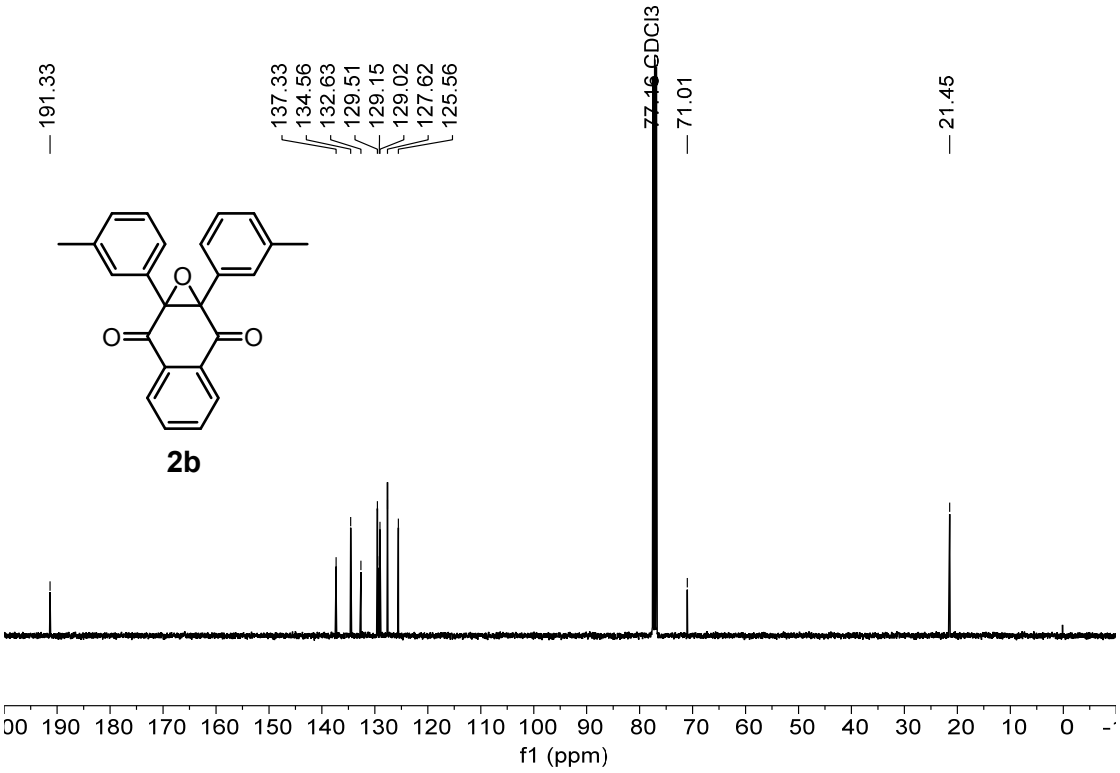
^{13}C NMR ($CDCl_3$, 101 MHz)



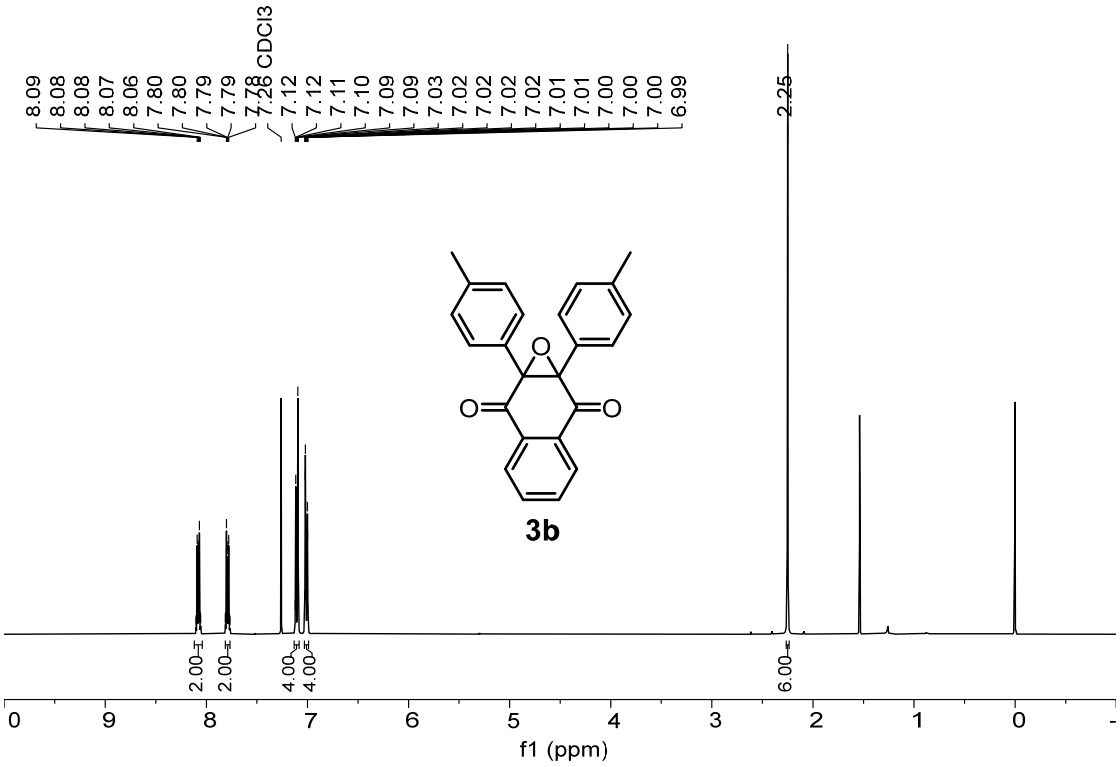
^{1}H NMR ($CDCl_3$, 400 MHz)



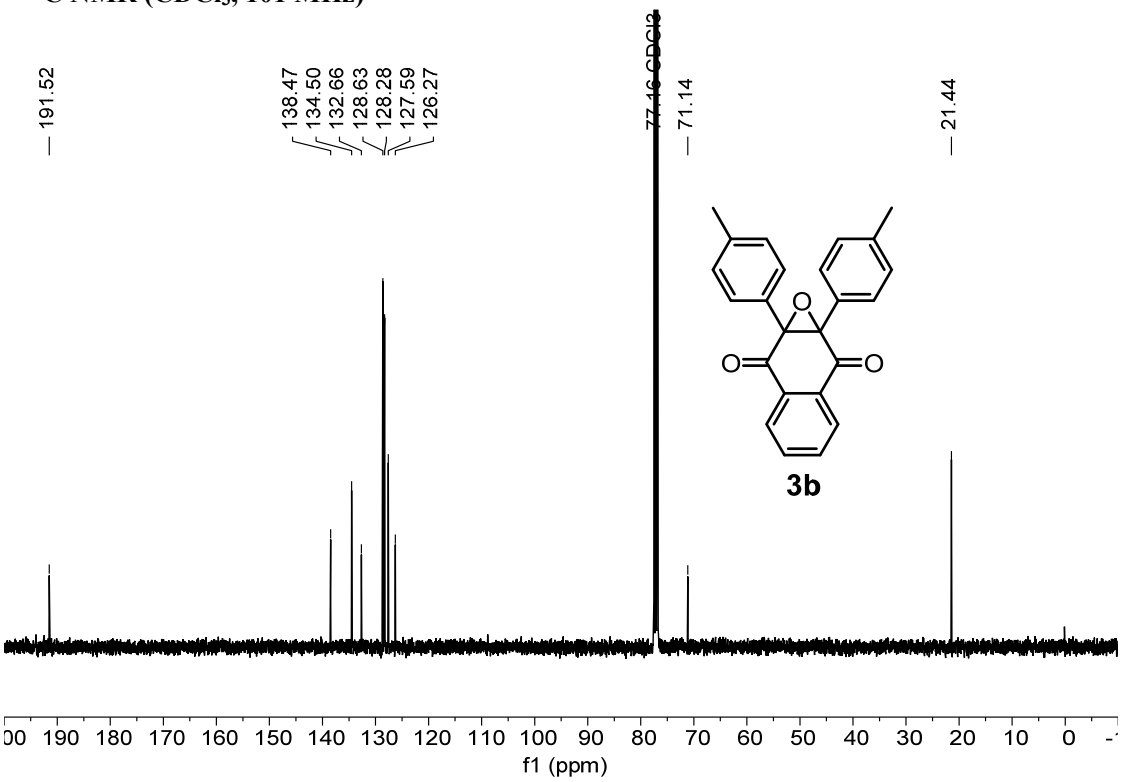
^{13}C NMR ($CDCl_3$, 101 MHz)



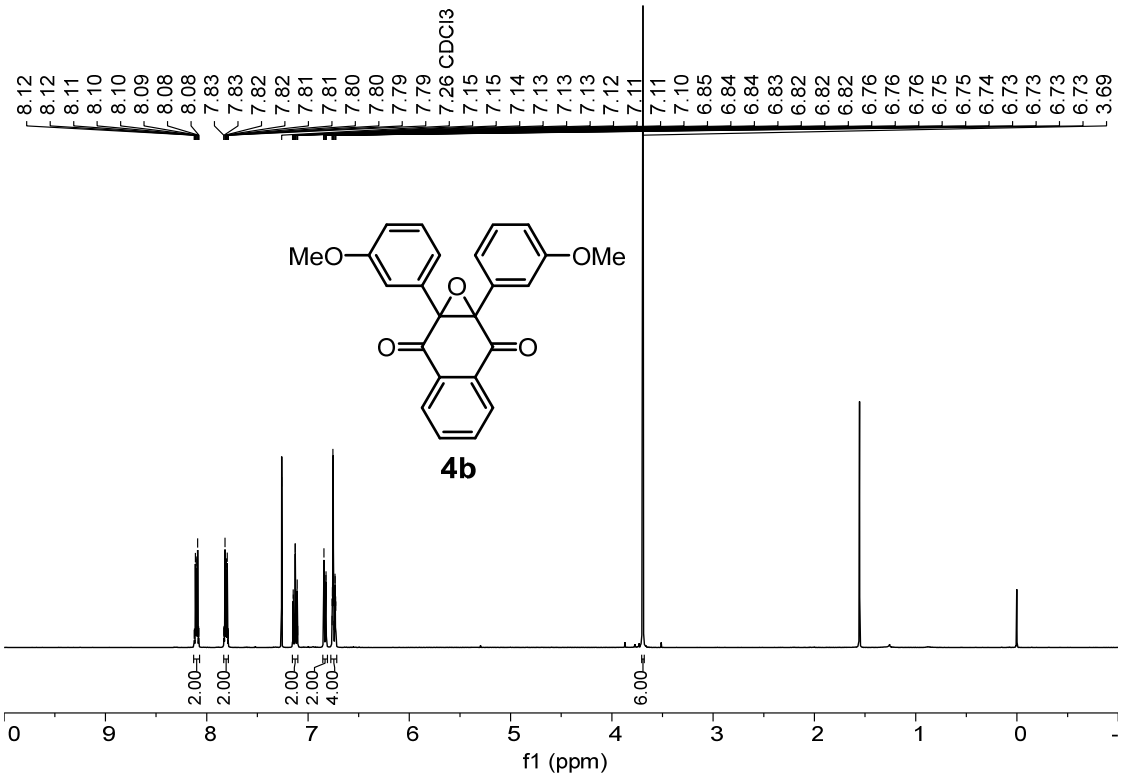
^{1}H NMR ($CDCl_3$, 400 MHz)



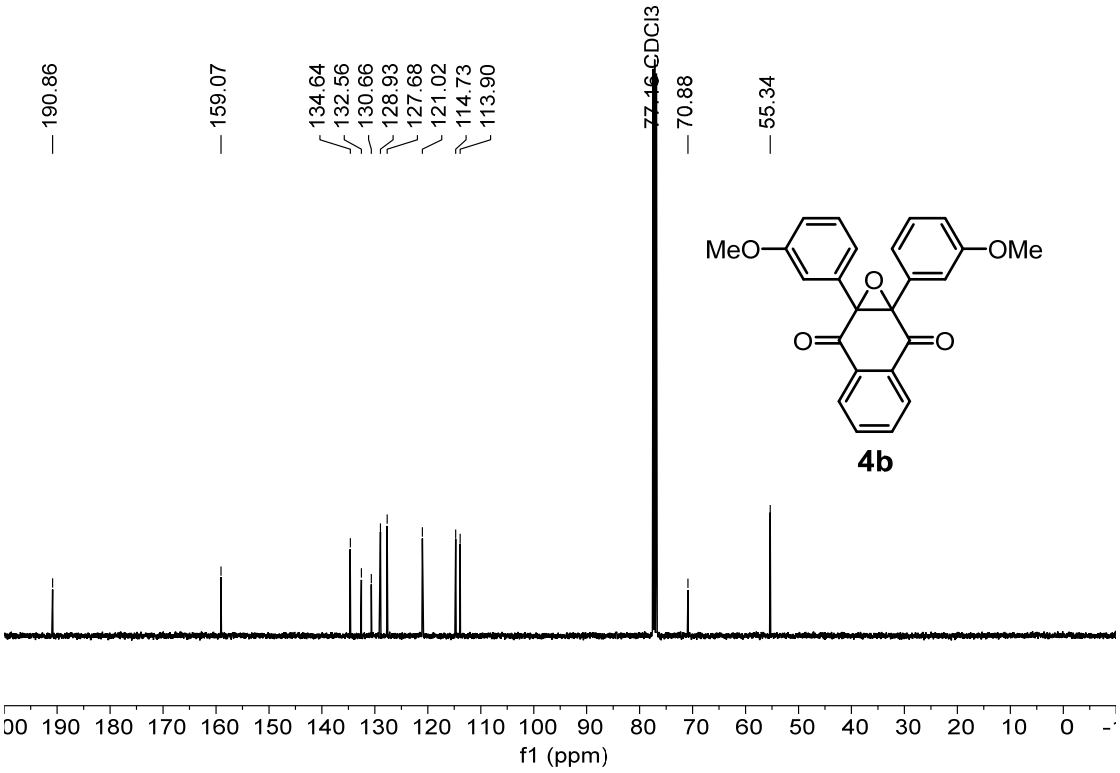
^{13}C NMR ($CDCl_3$, 101 MHz)



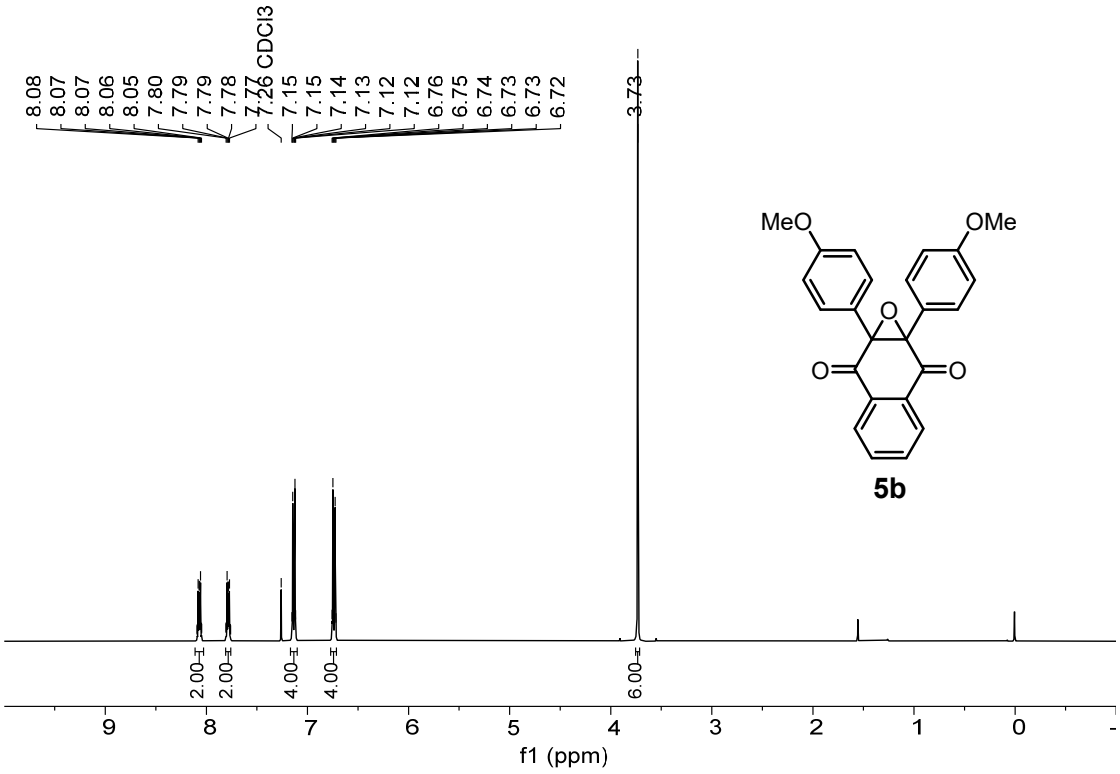
^{1}H NMR ($CDCl_3$, 400 MHz)



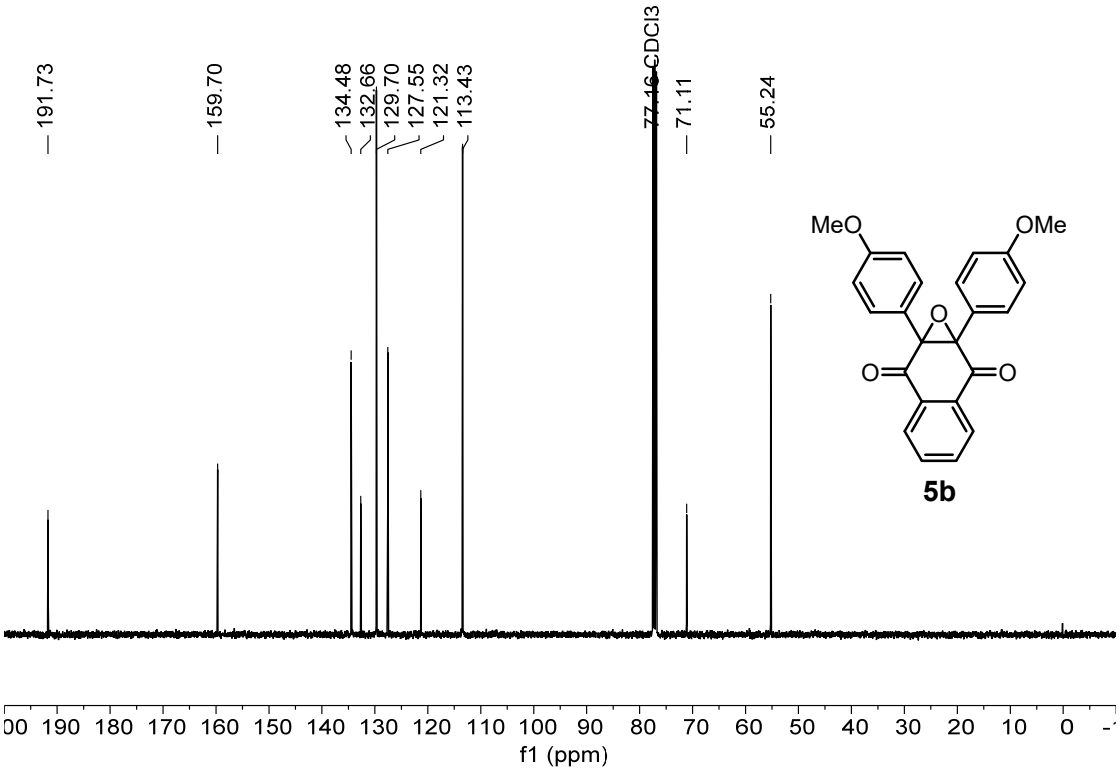
^{13}C NMR ($CDCl_3$, 101 MHz)



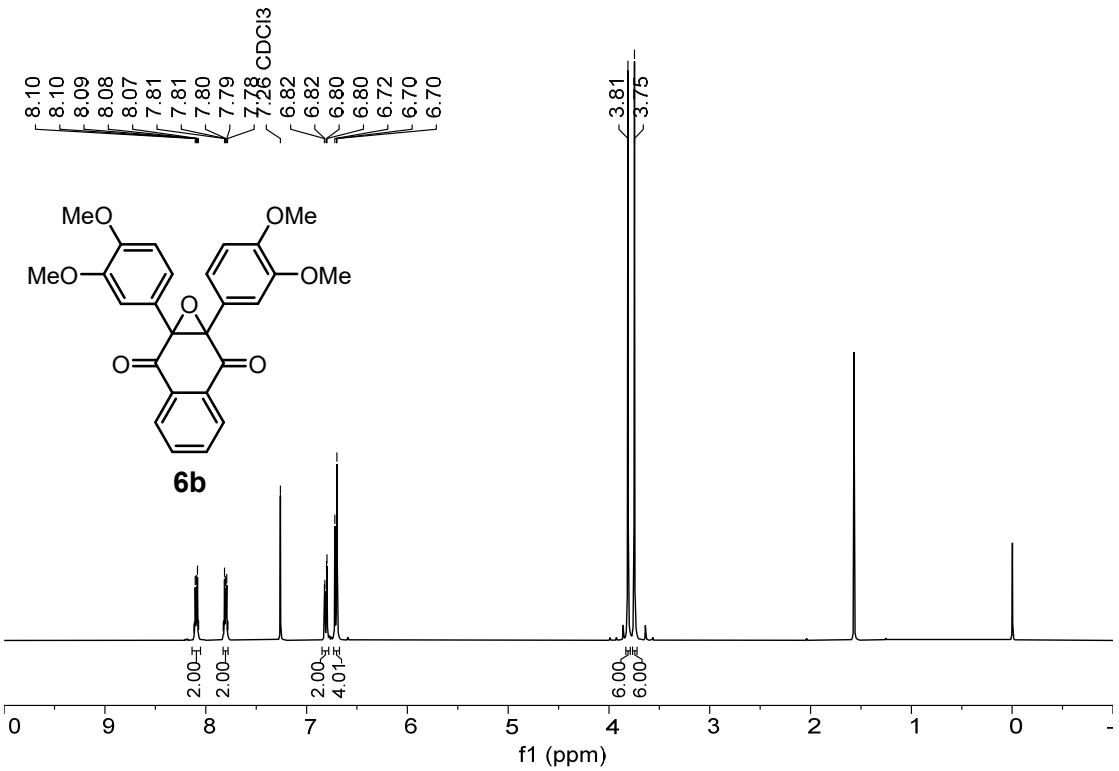
^{1}H NMR ($CDCl_3$, 400 MHz)



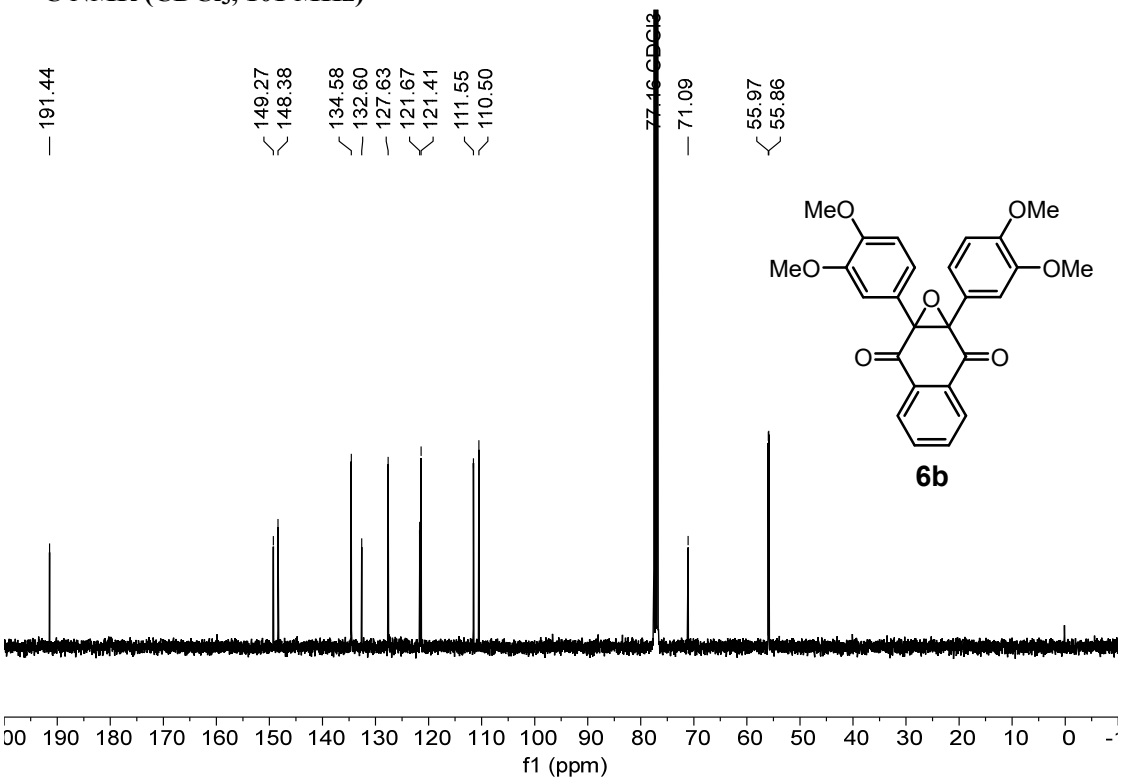
^{13}C NMR ($CDCl_3$, 101 MHz)



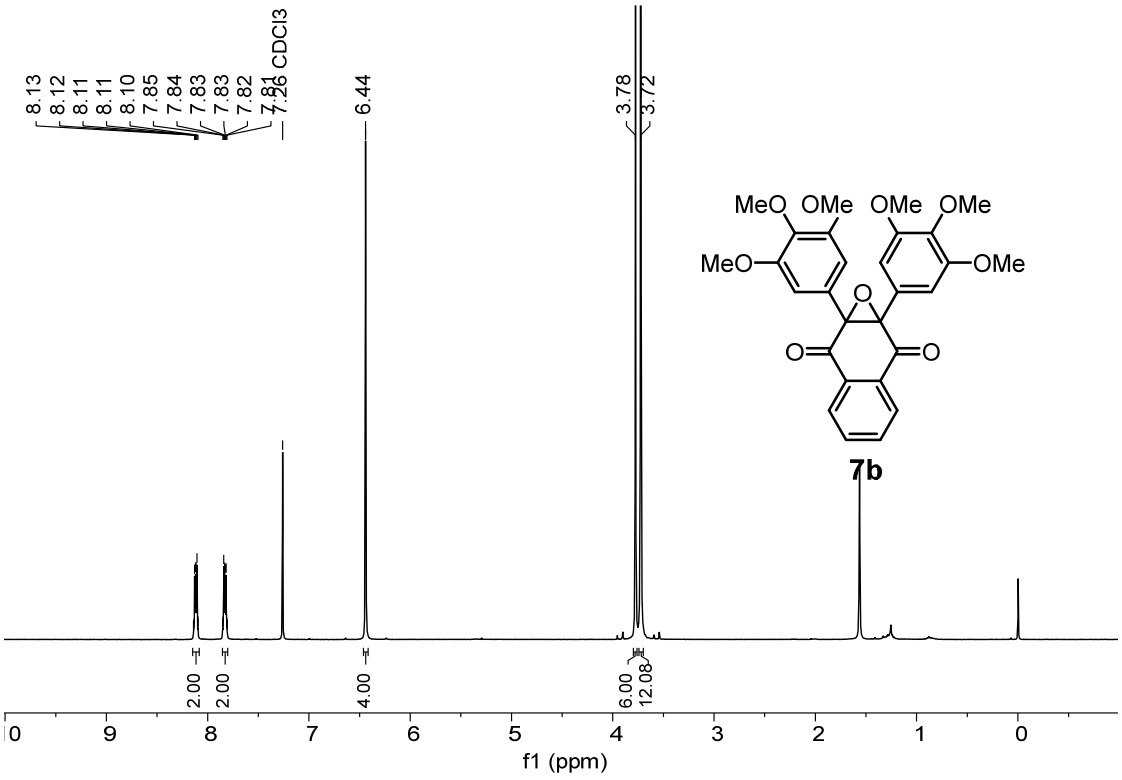
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



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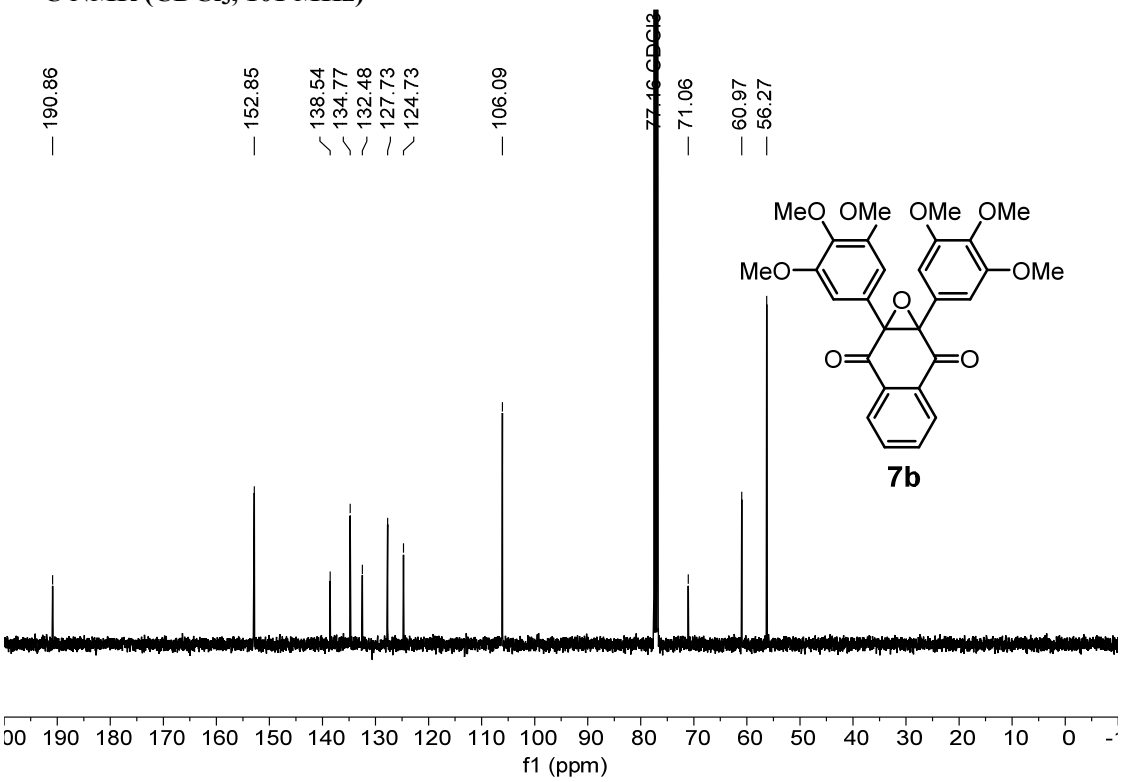
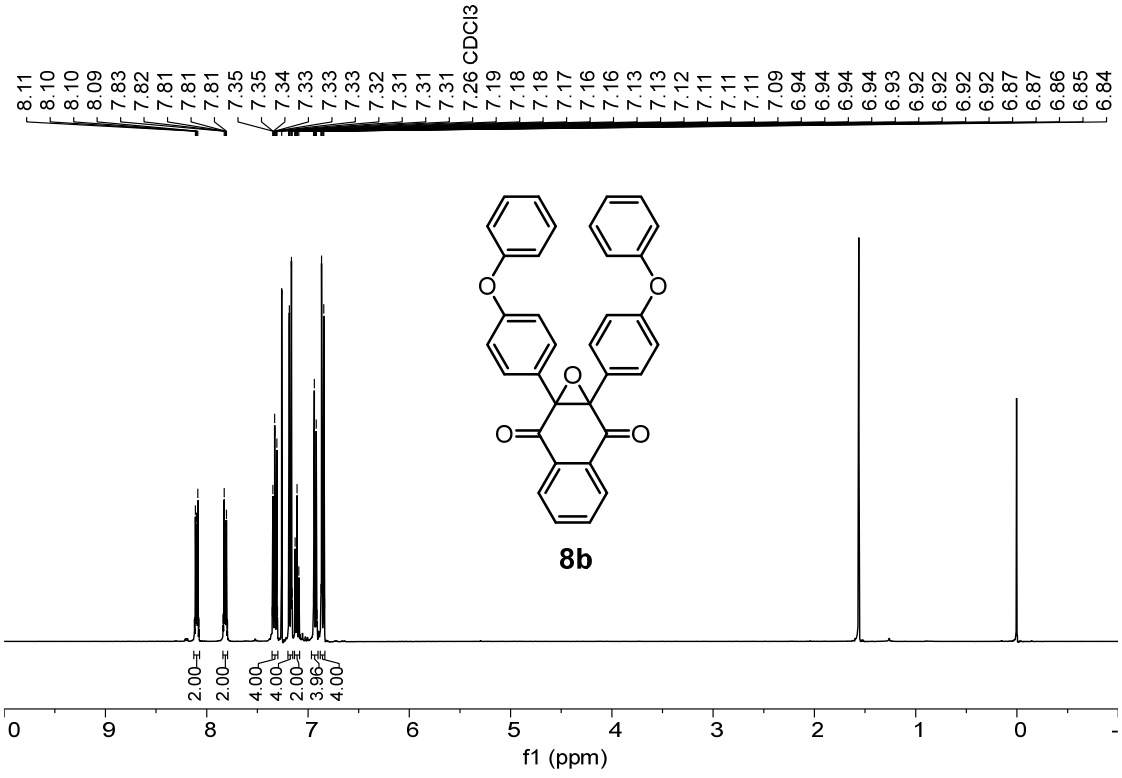


^{1}H NMR ($CDCl_3$, 400 MHz)



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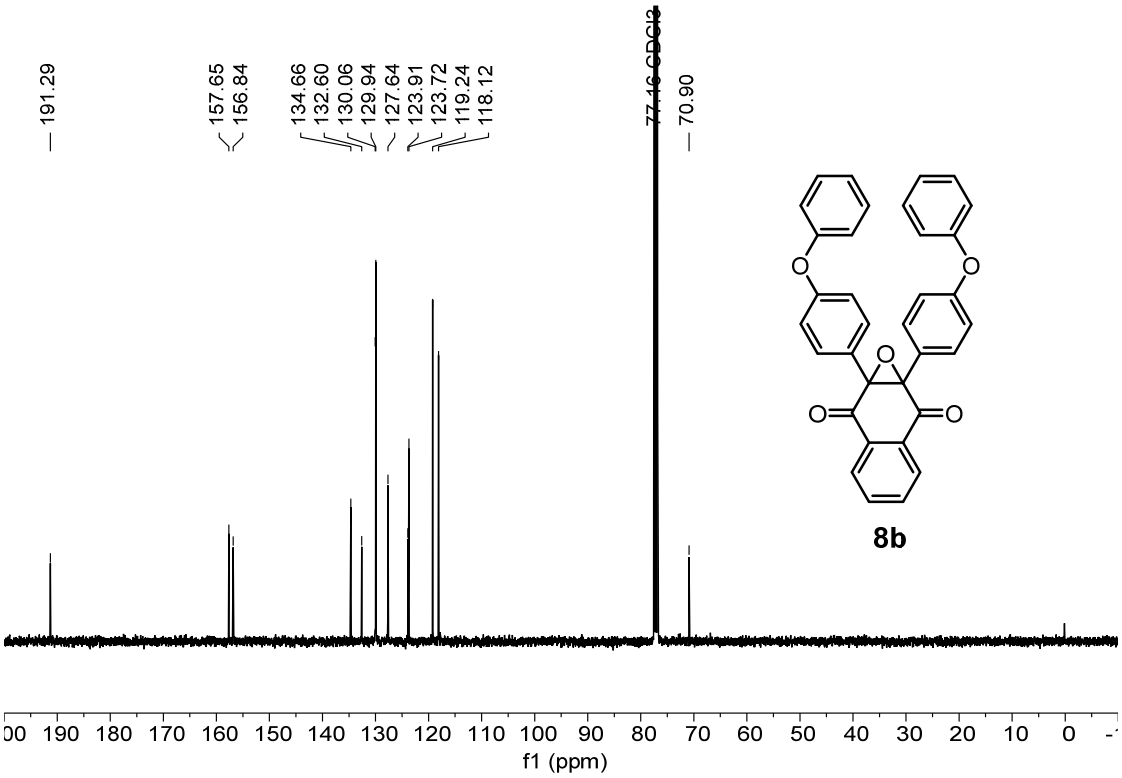

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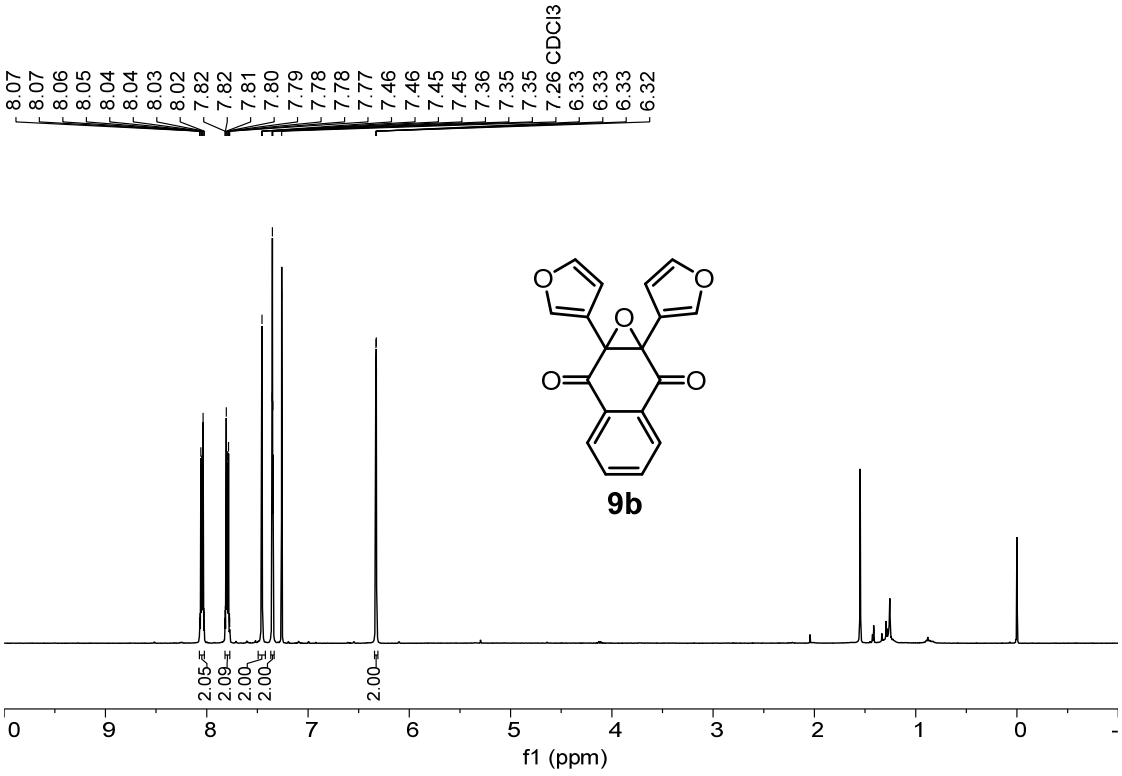
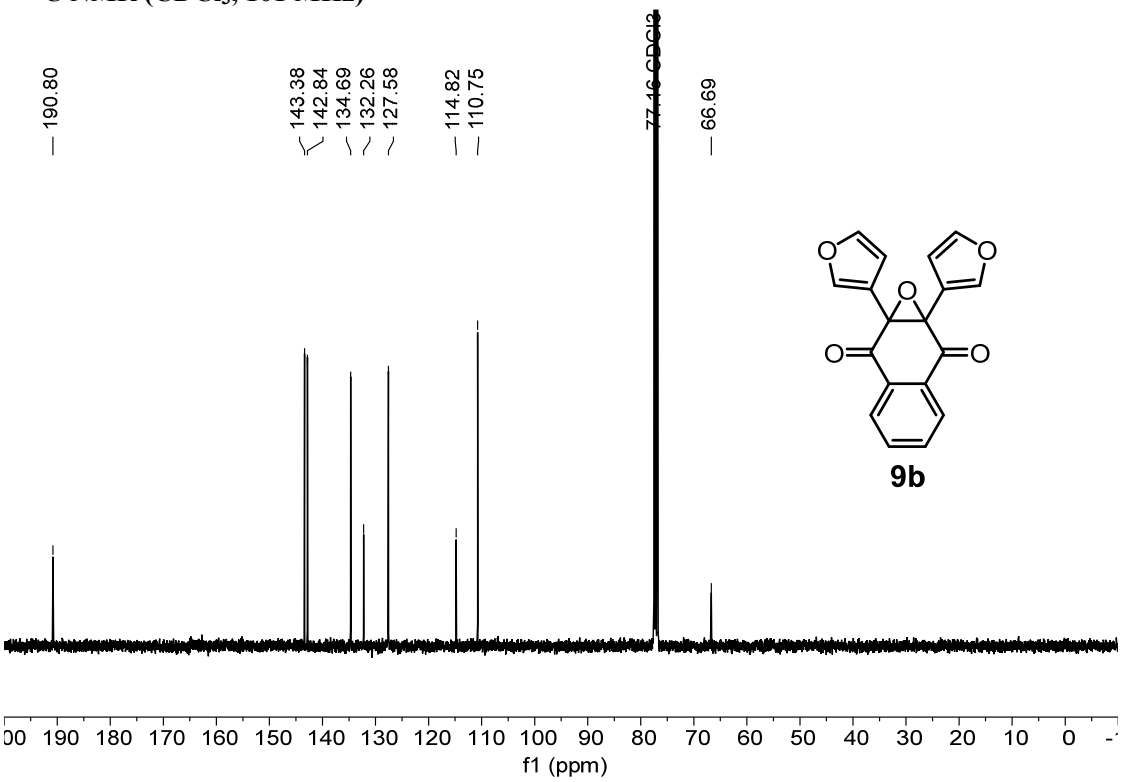
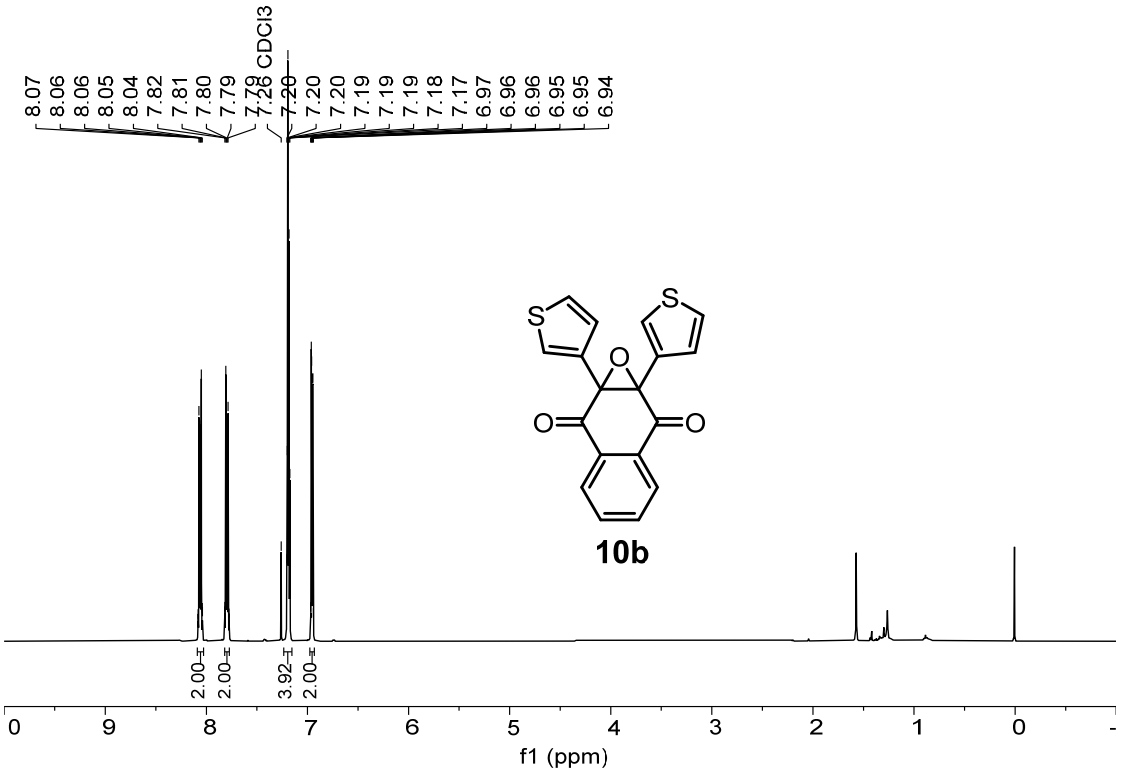


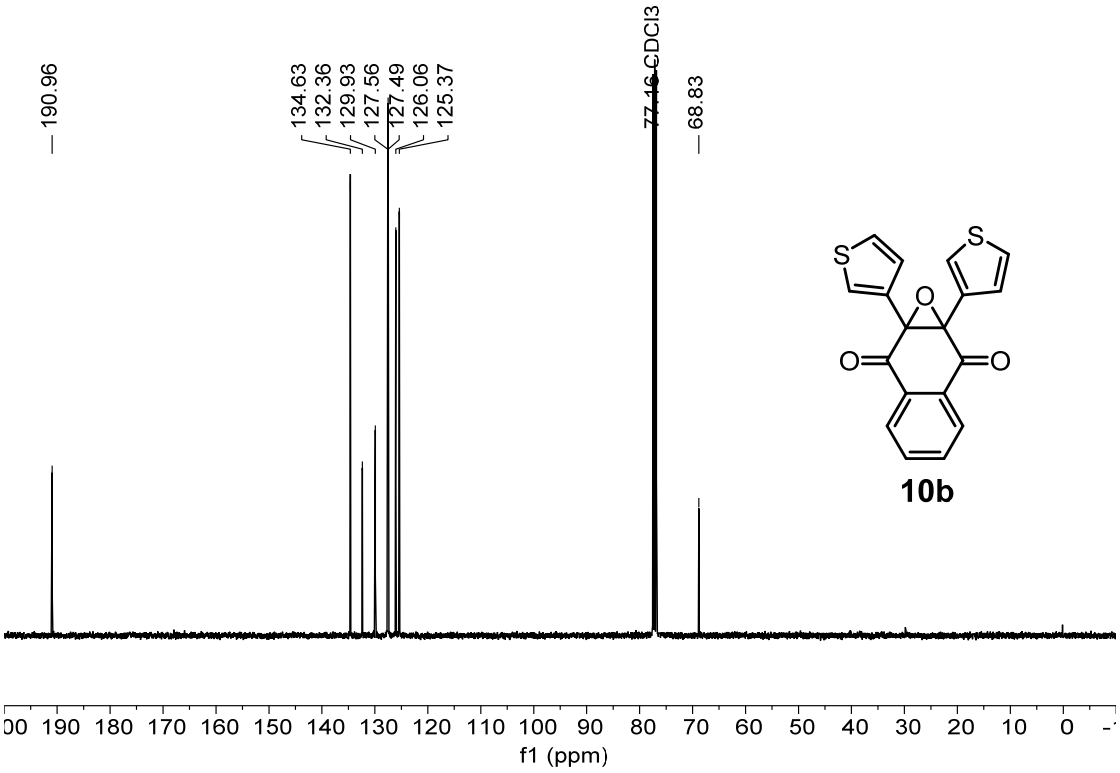
^{13}C NMR ($CDCl_3$, 101 MHz)



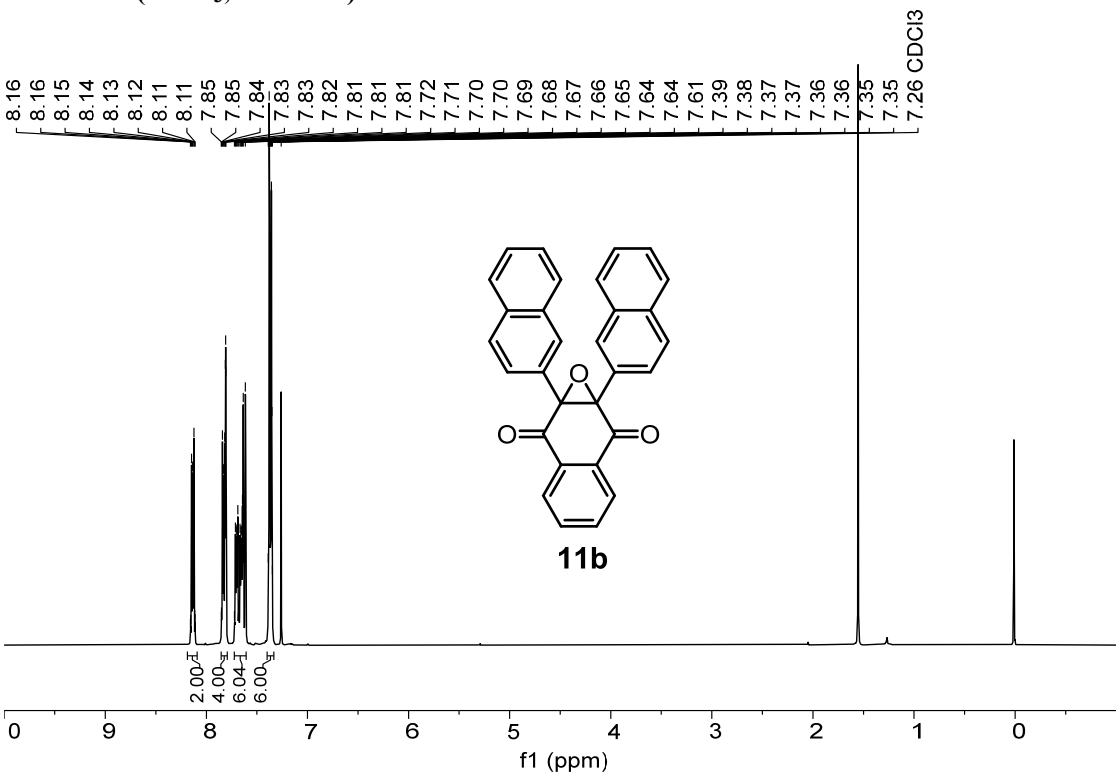
^{1}H NMR ($CDCl_3$, 400 MHz)



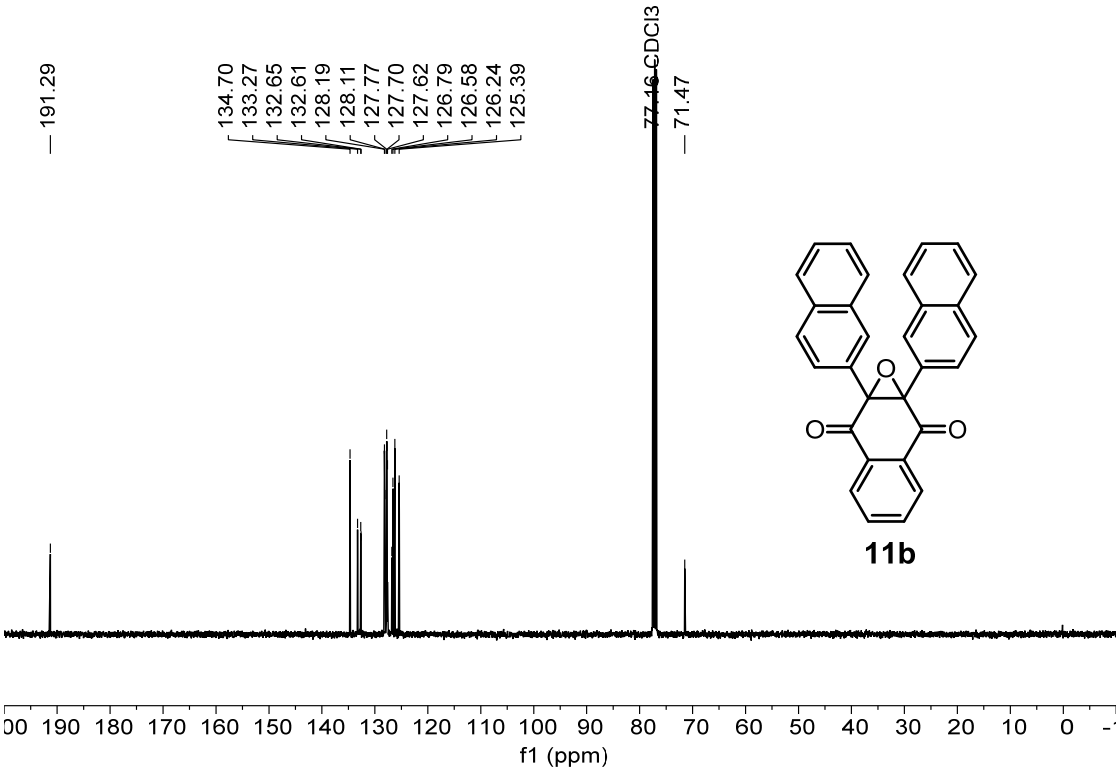
^{13}C NMR ($CDCl_3$, 101 MHz)



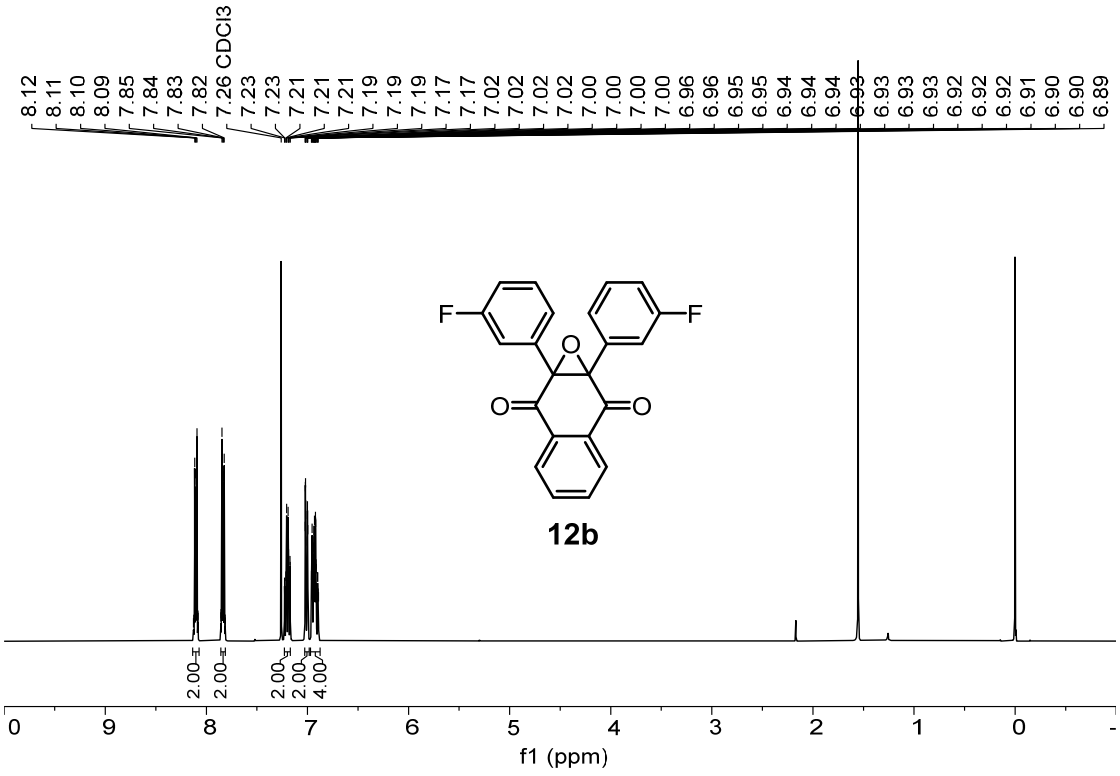
^{1}H NMR ($CDCl_3$, 400 MHz)



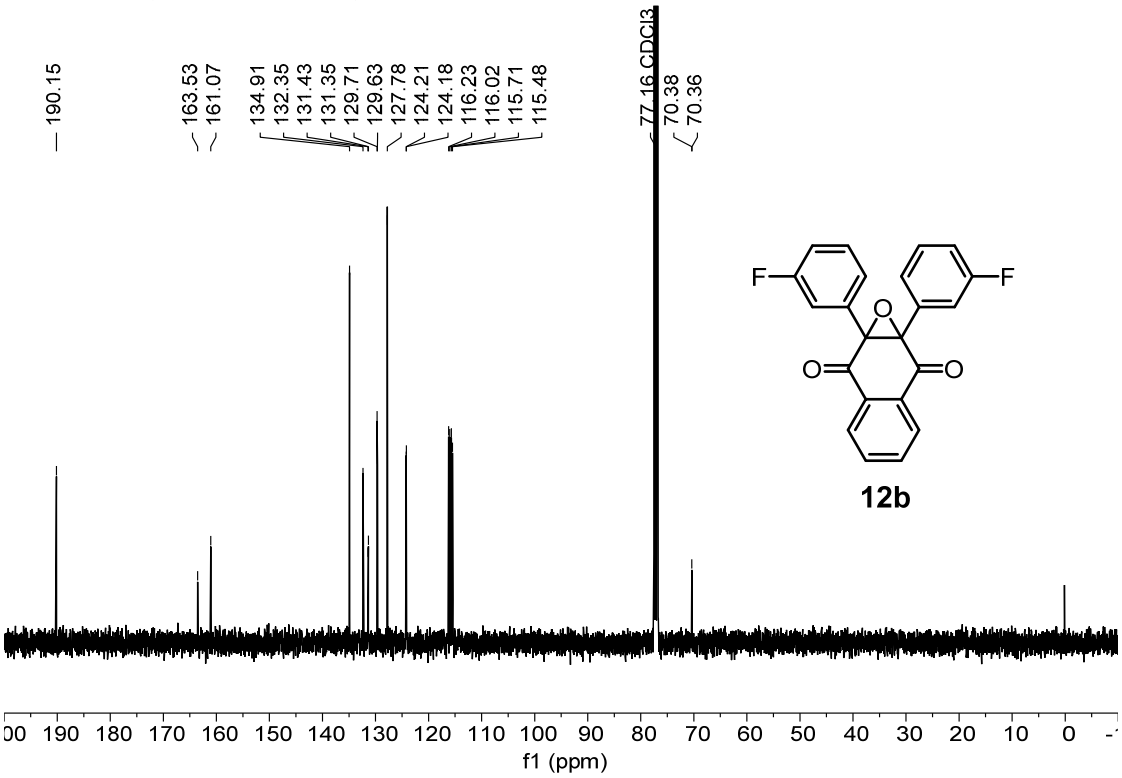
^{13}C NMR ($CDCl_3$, 101 MHz)



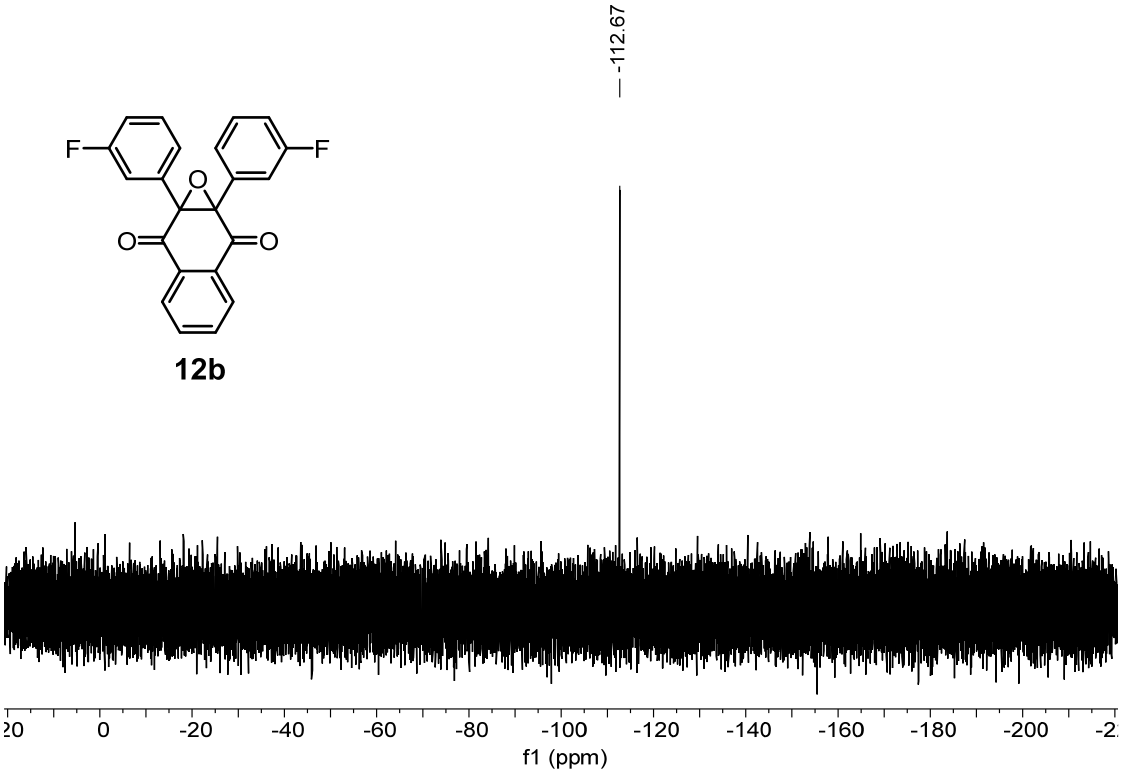
^{1}H NMR ($CDCl_3$, 400 MHz)



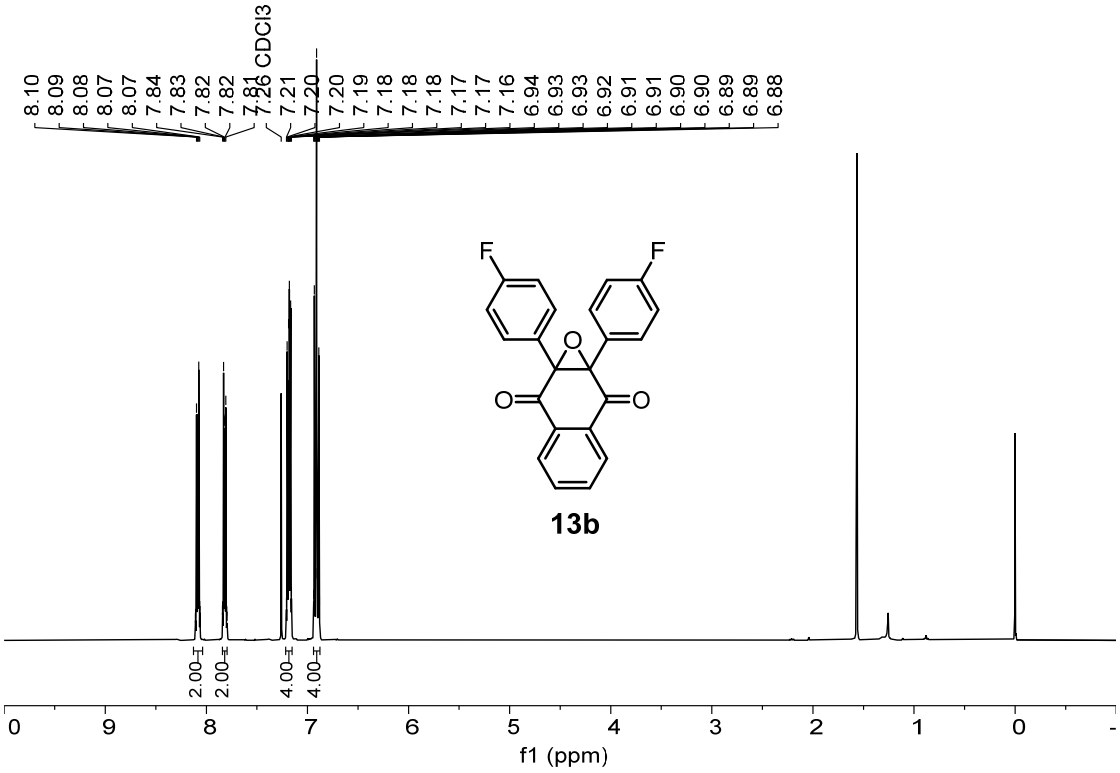
^{13}C NMR ($CDCl_3$, 101 MHz)



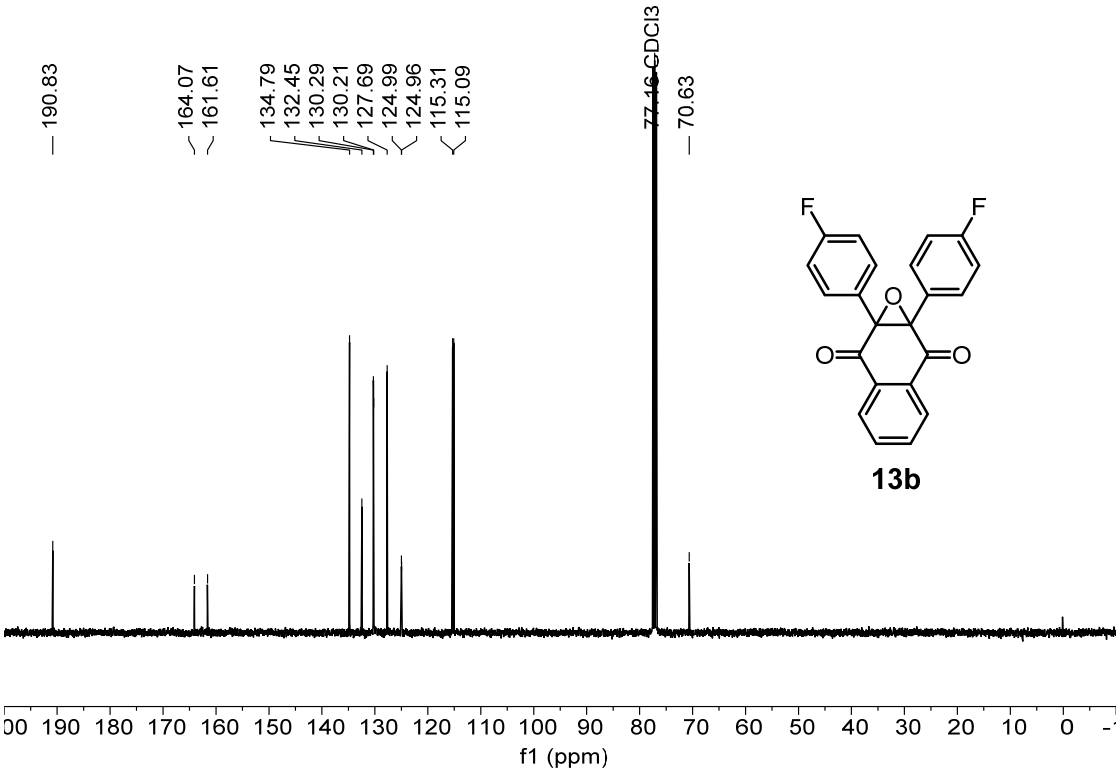
^{19}F NMR ($CDCl_3$, 376 MHz)



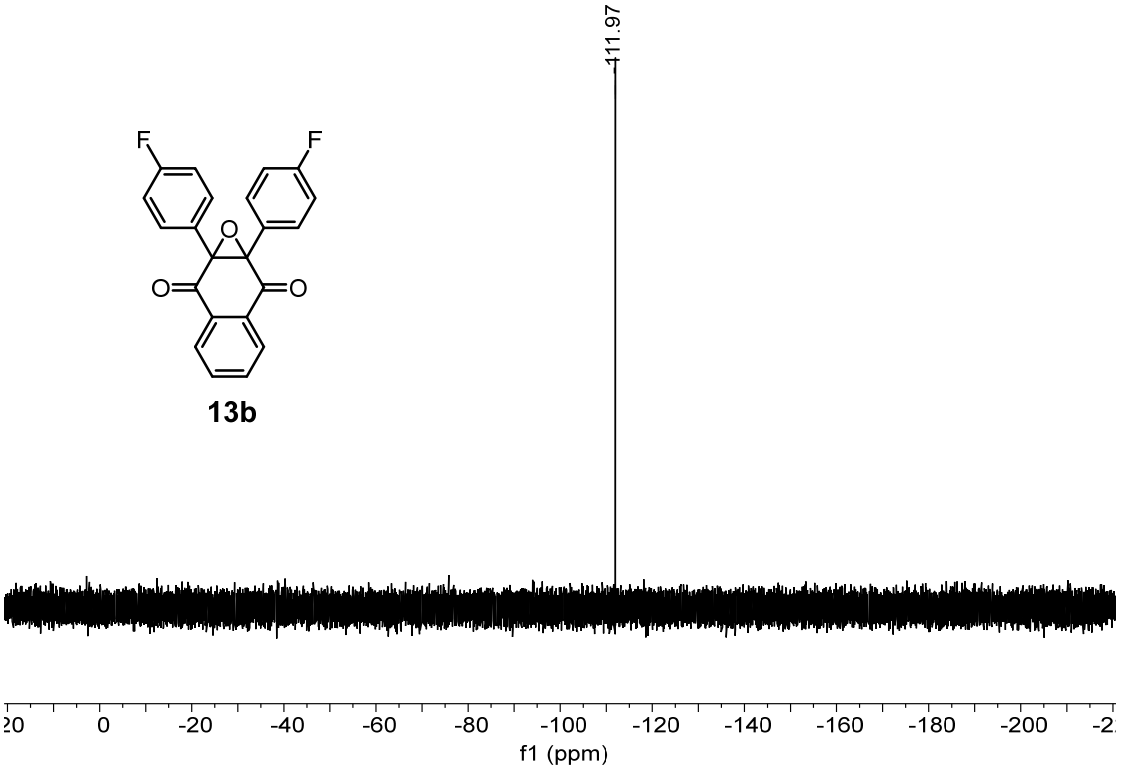
^{1}H NMR ($CDCl_3$, 400 MHz)



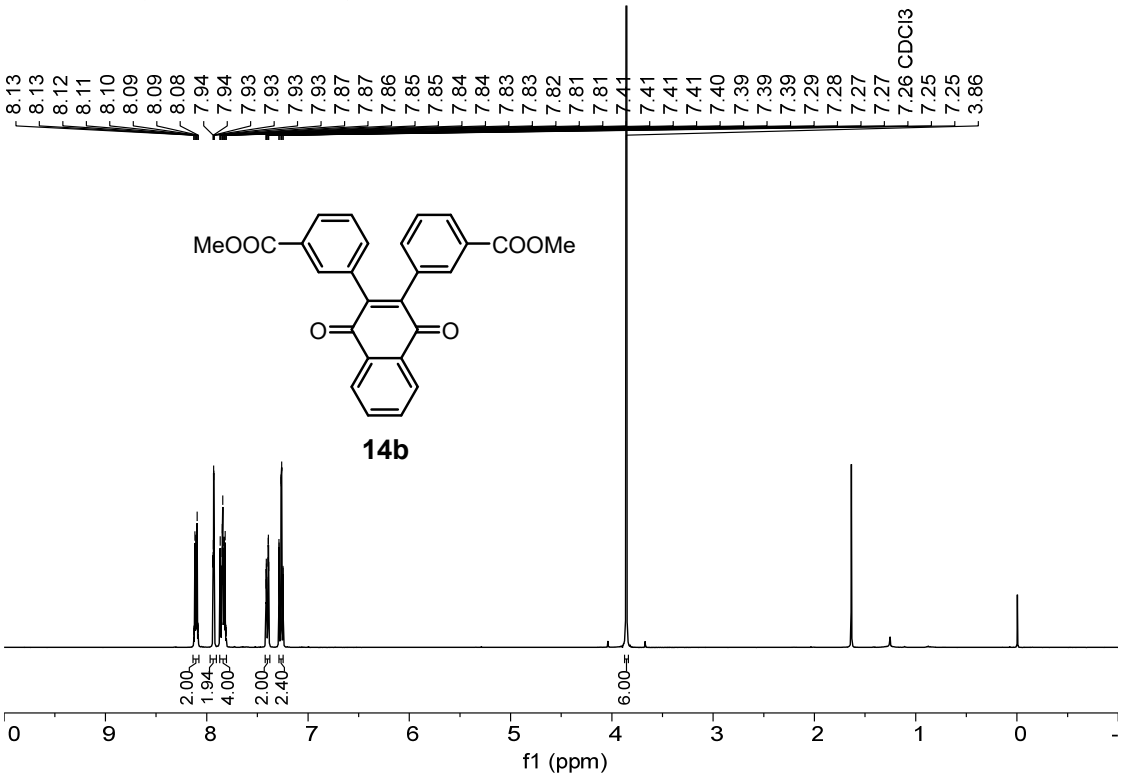
^{13}C NMR ($CDCl_3$, 101 MHz)



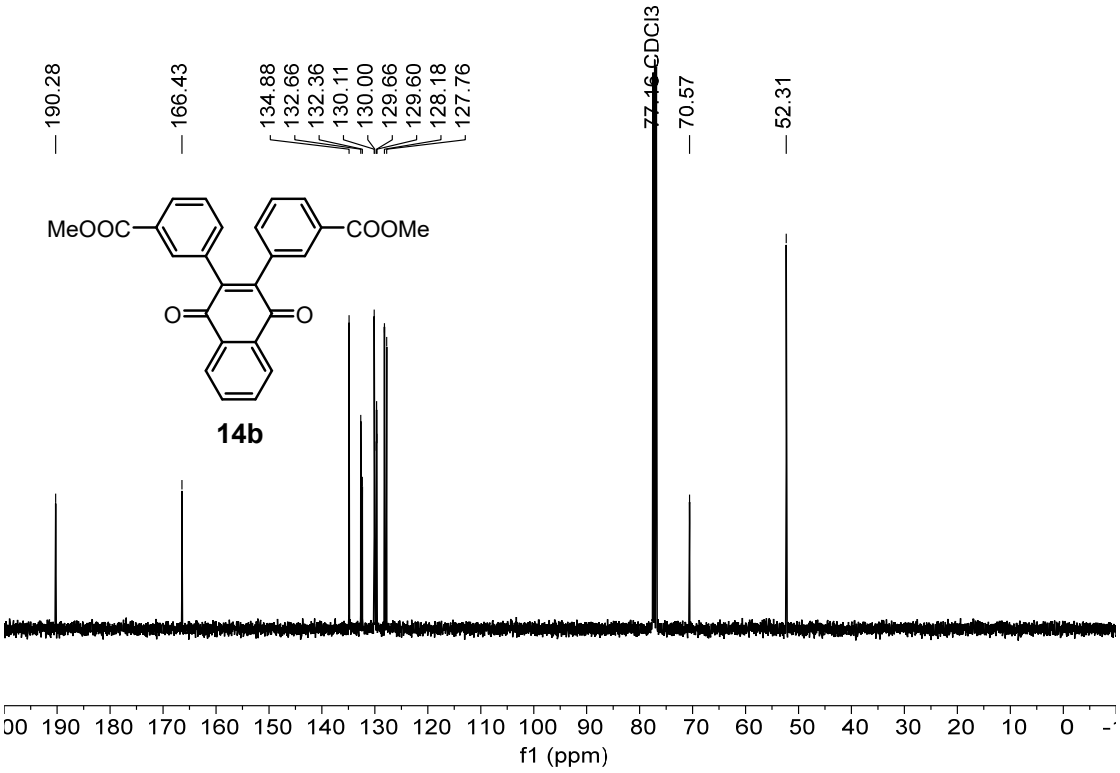
^{19}F NMR ($CDCl_3$, 376 MHz)



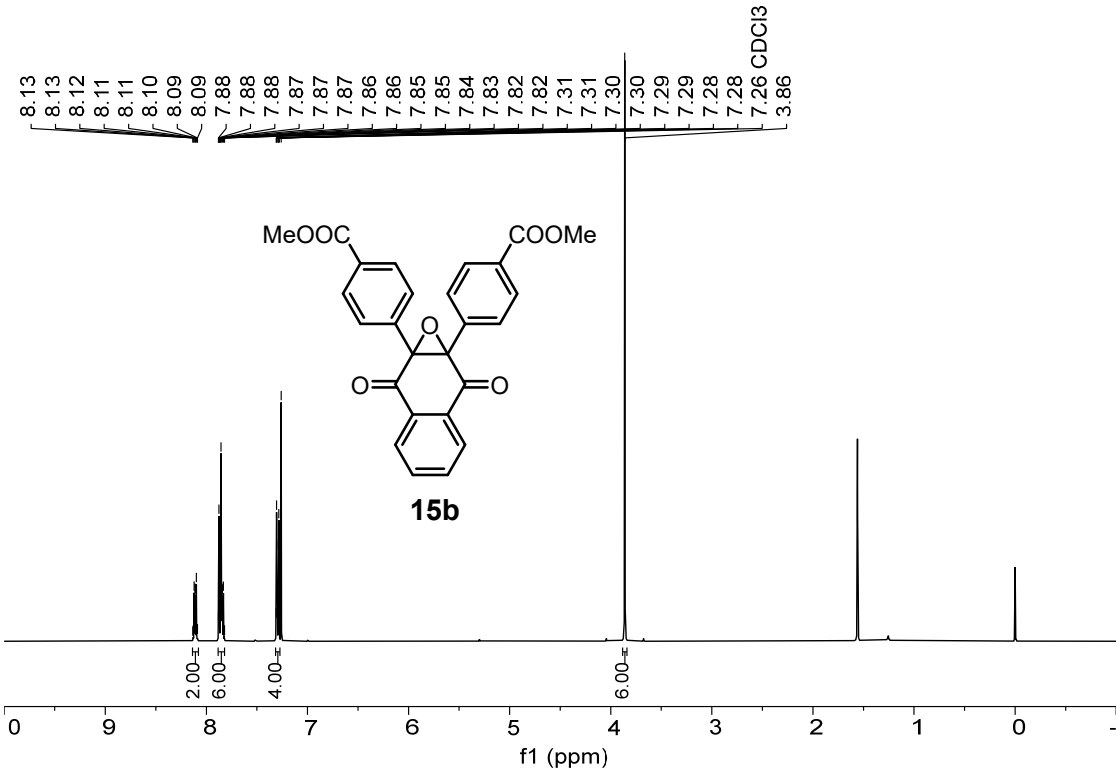
^{1}H NMR ($CDCl_3$, 400 MHz)



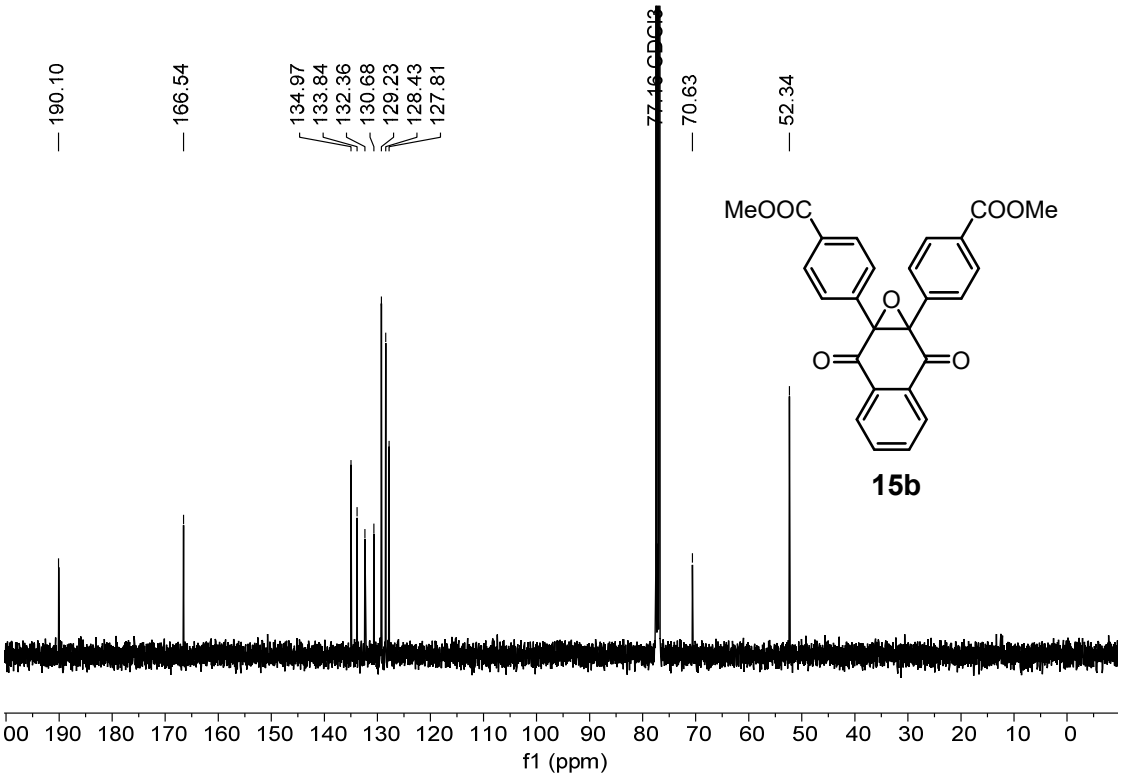
^{13}C NMR ($CDCl_3$, 101 MHz)



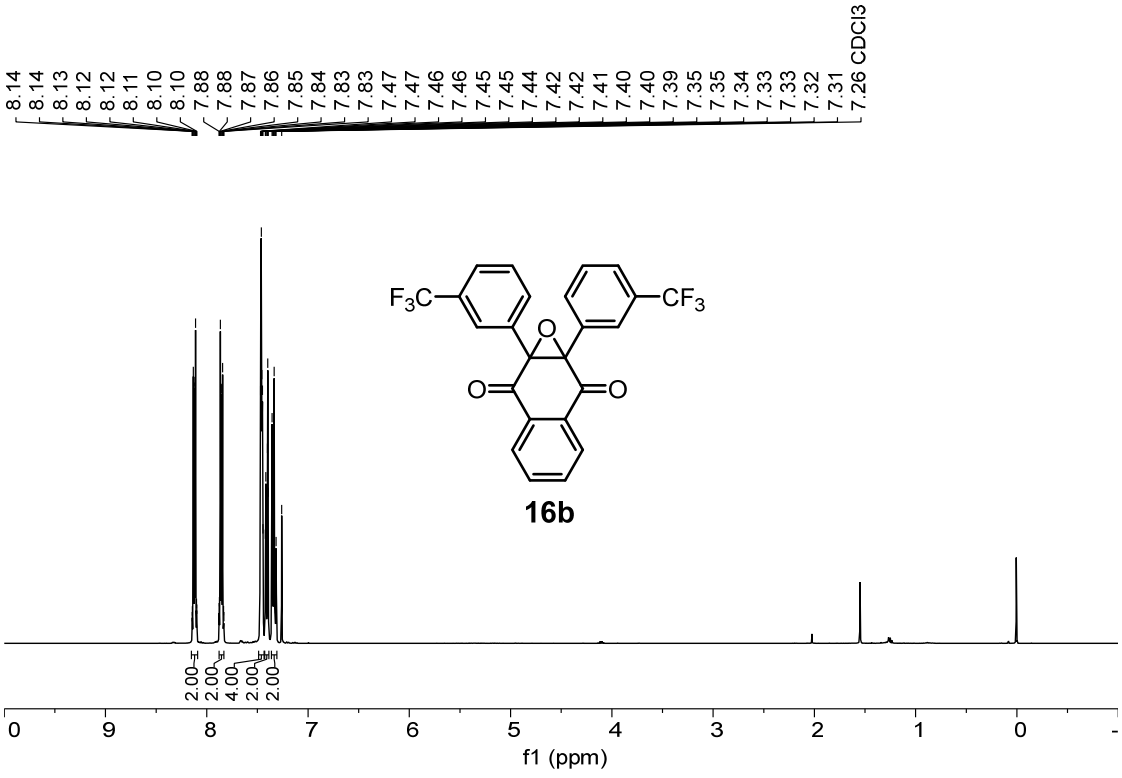
^{1}H NMR ($CDCl_3$, 400 MHz)



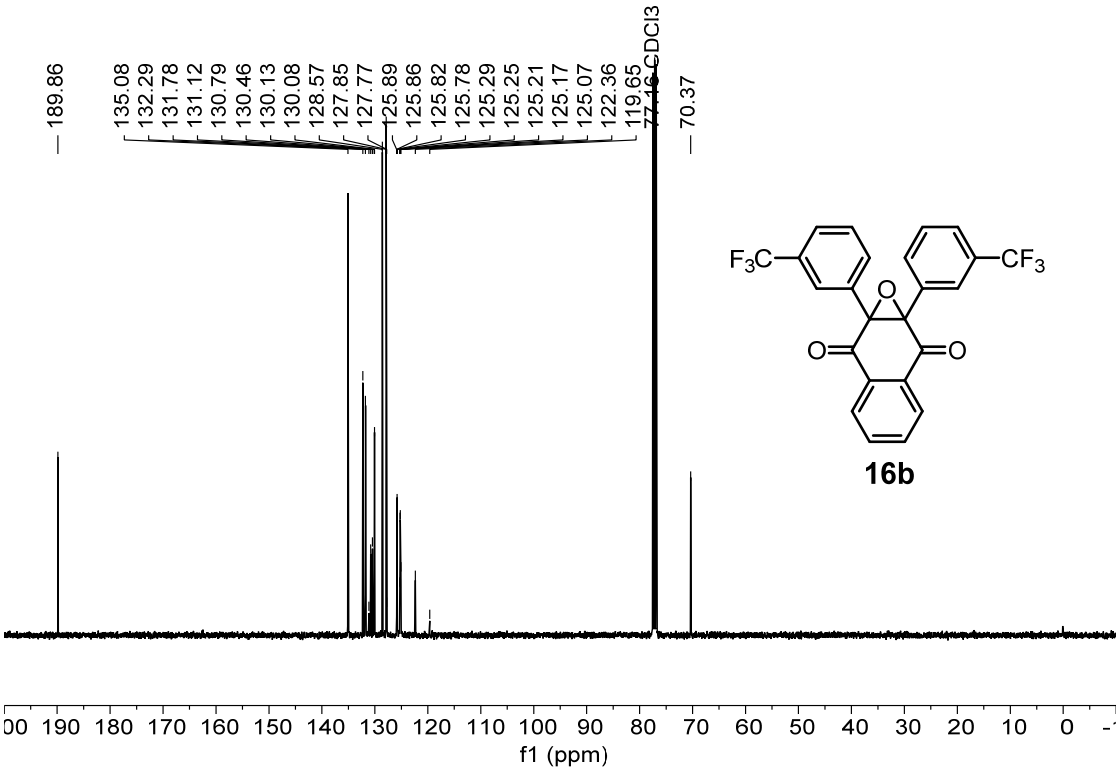
^{13}C NMR ($CDCl_3$, 101 MHz)



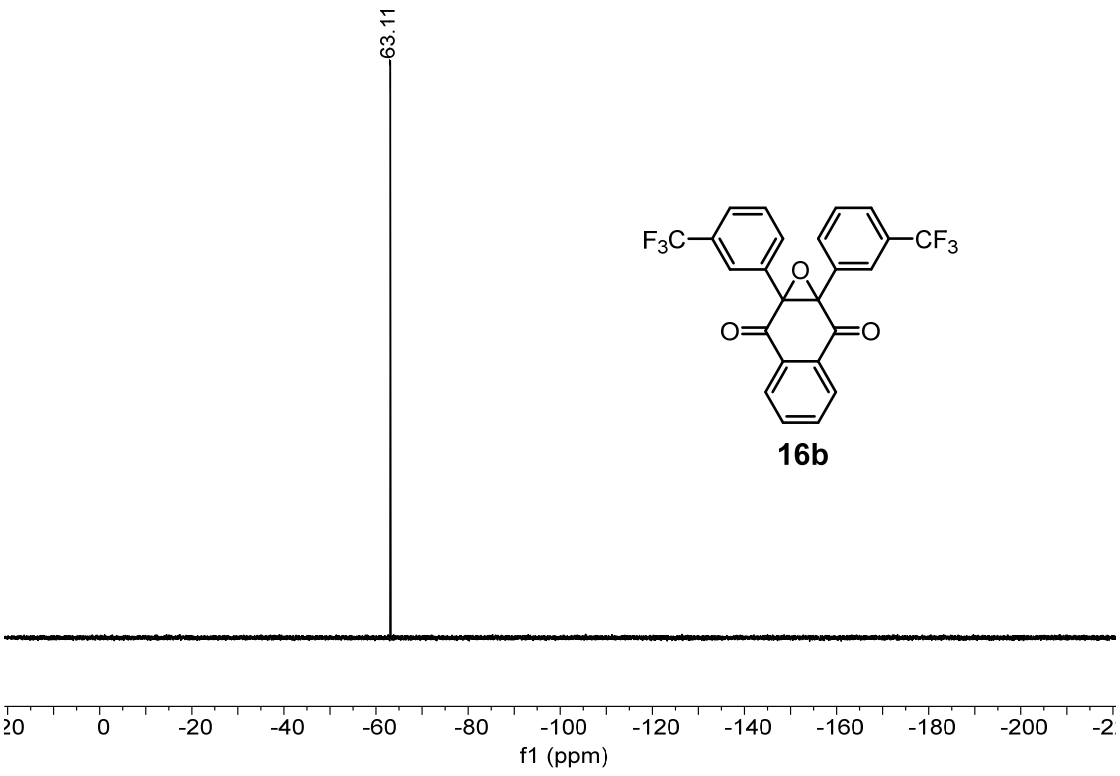
^{1}H NMR ($CDCl_3$, 400 MHz)



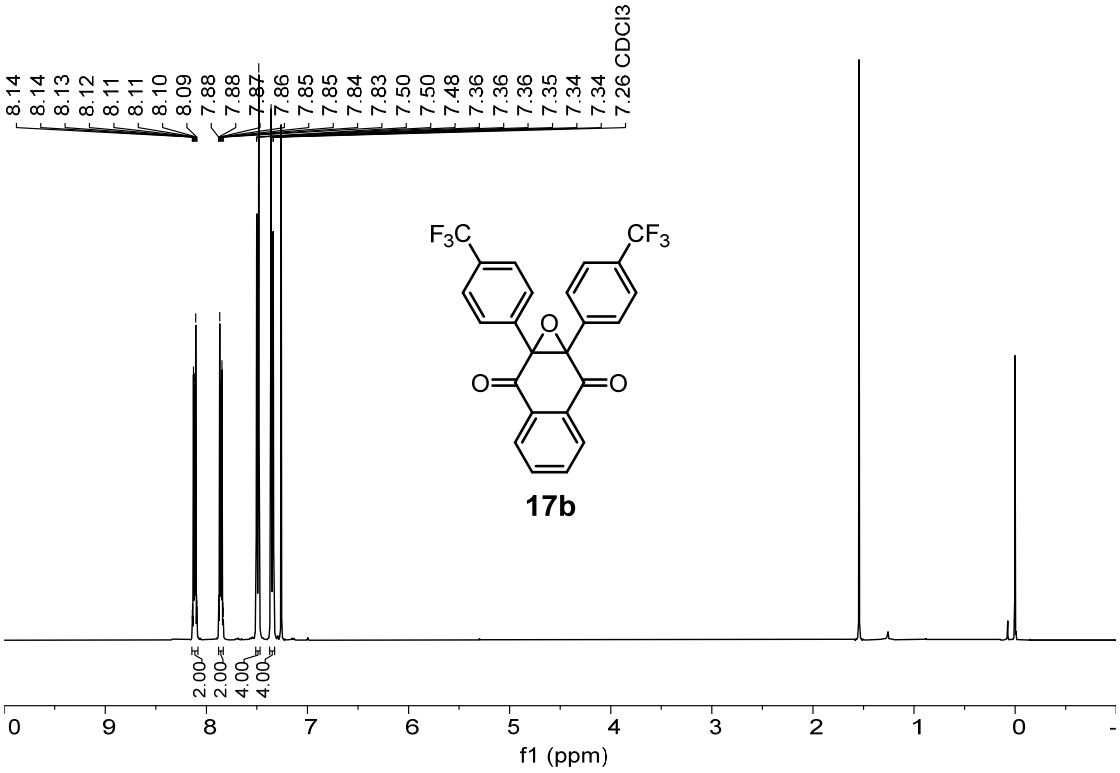
^{13}C NMR ($CDCl_3$, 101 MHz)



^{19}F NMR ($CDCl_3$, 376 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



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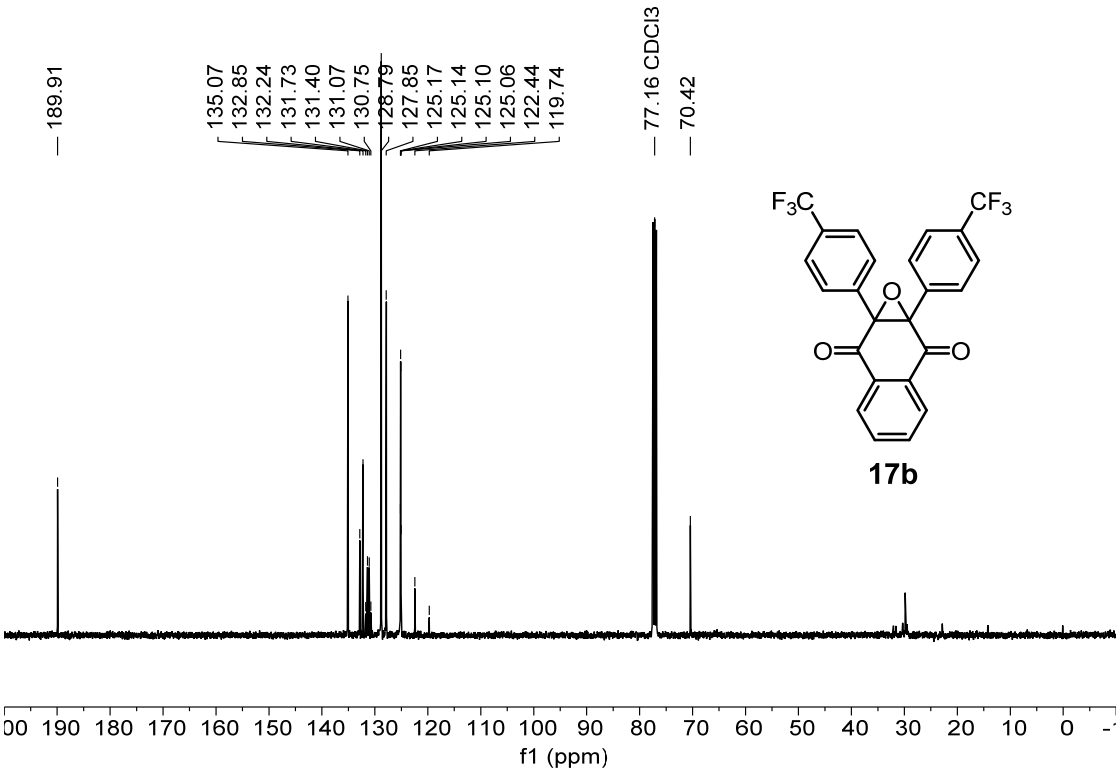
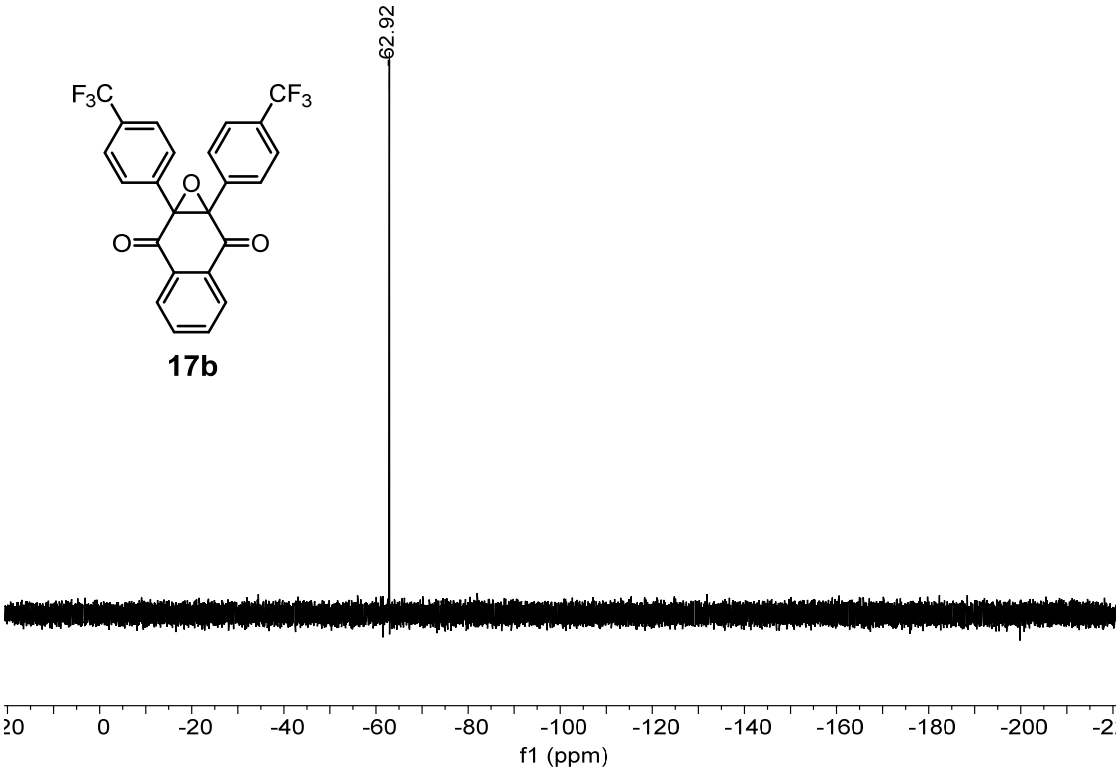
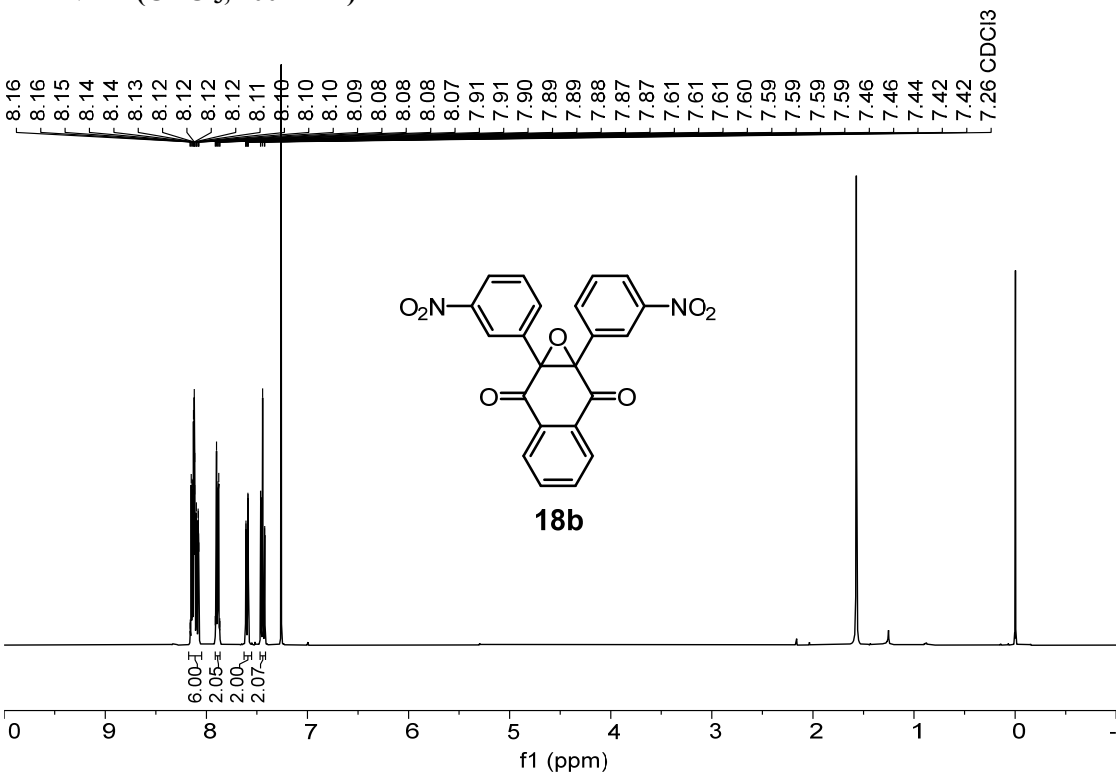


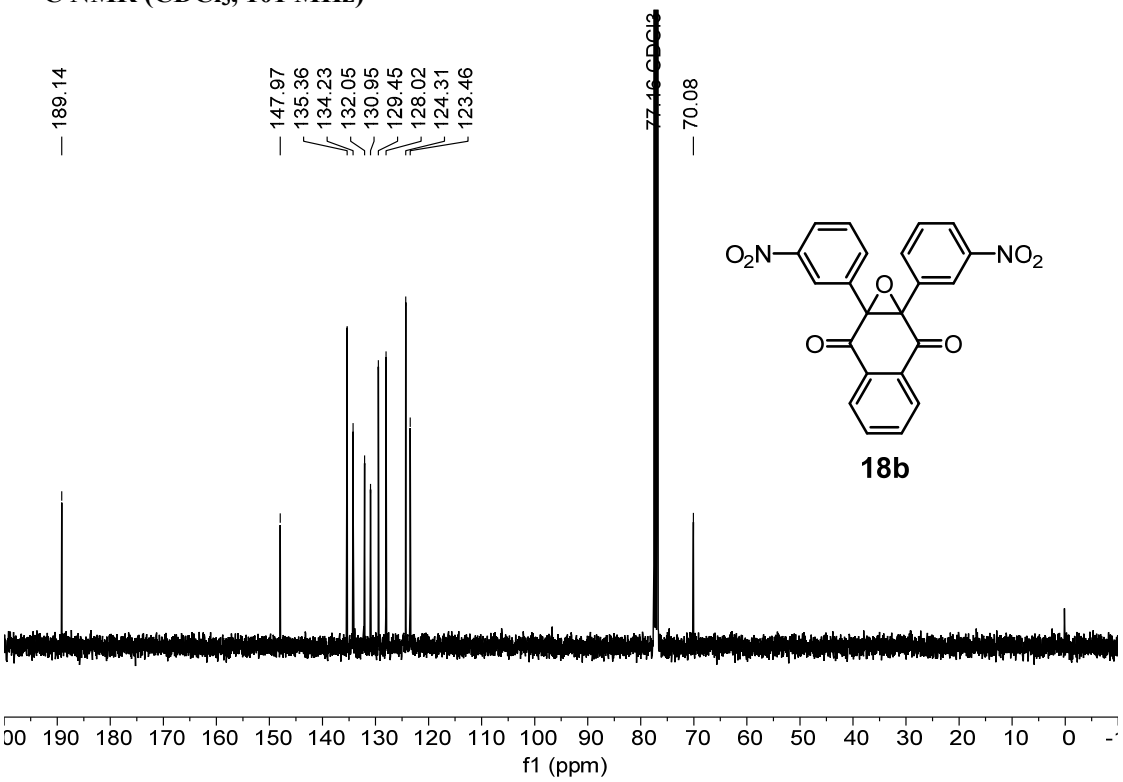
^{19}F NMR ($CDCl_3$, 376 MHz)



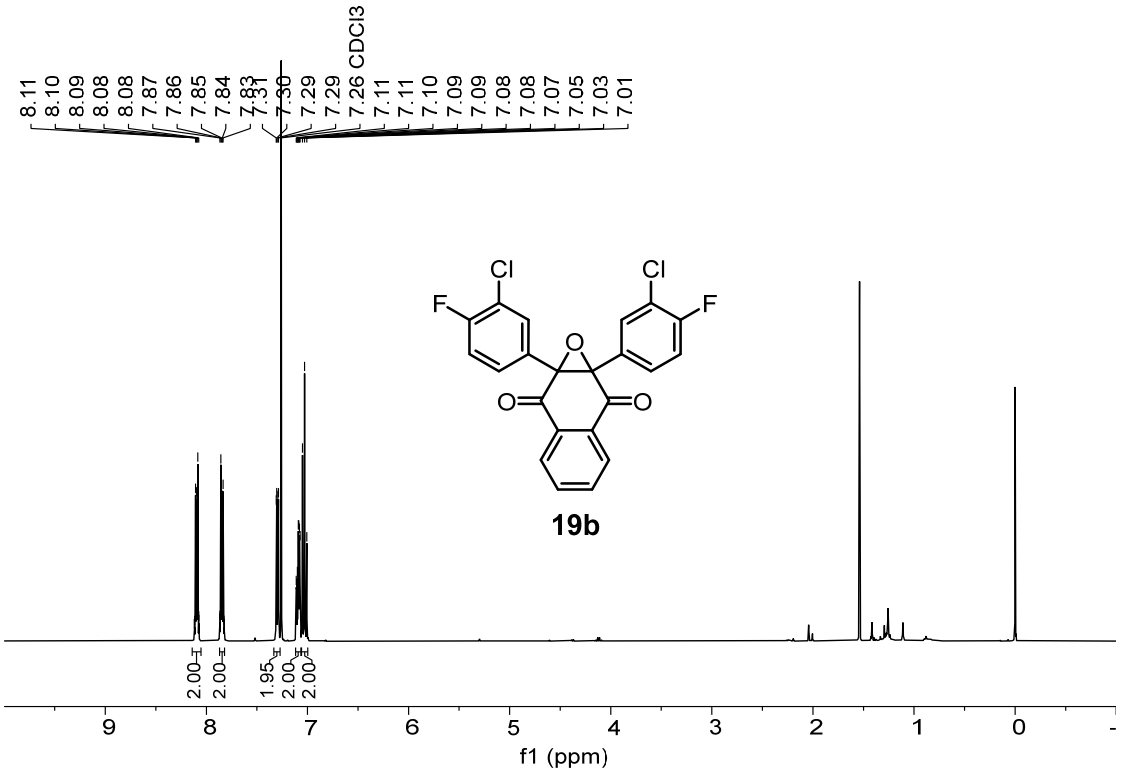
^{1}H NMR ($CDCl_3$, 400 MHz)



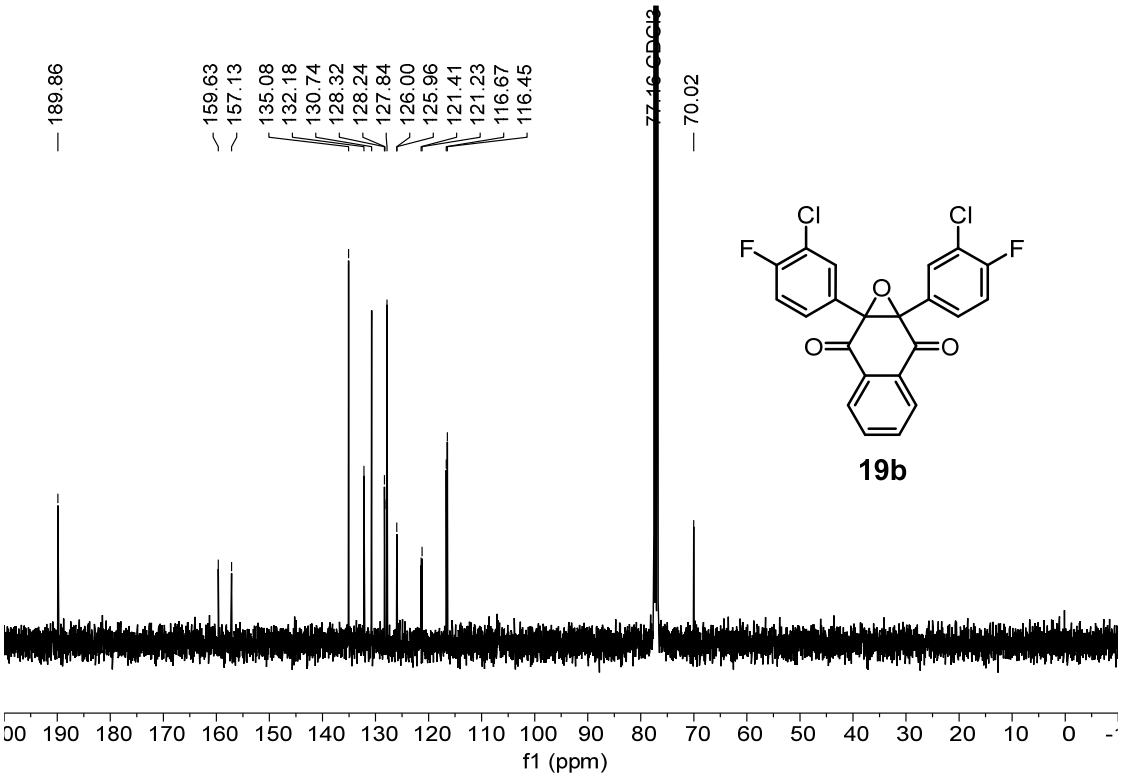
^{13}C NMR ($CDCl_3$, 101 MHz)



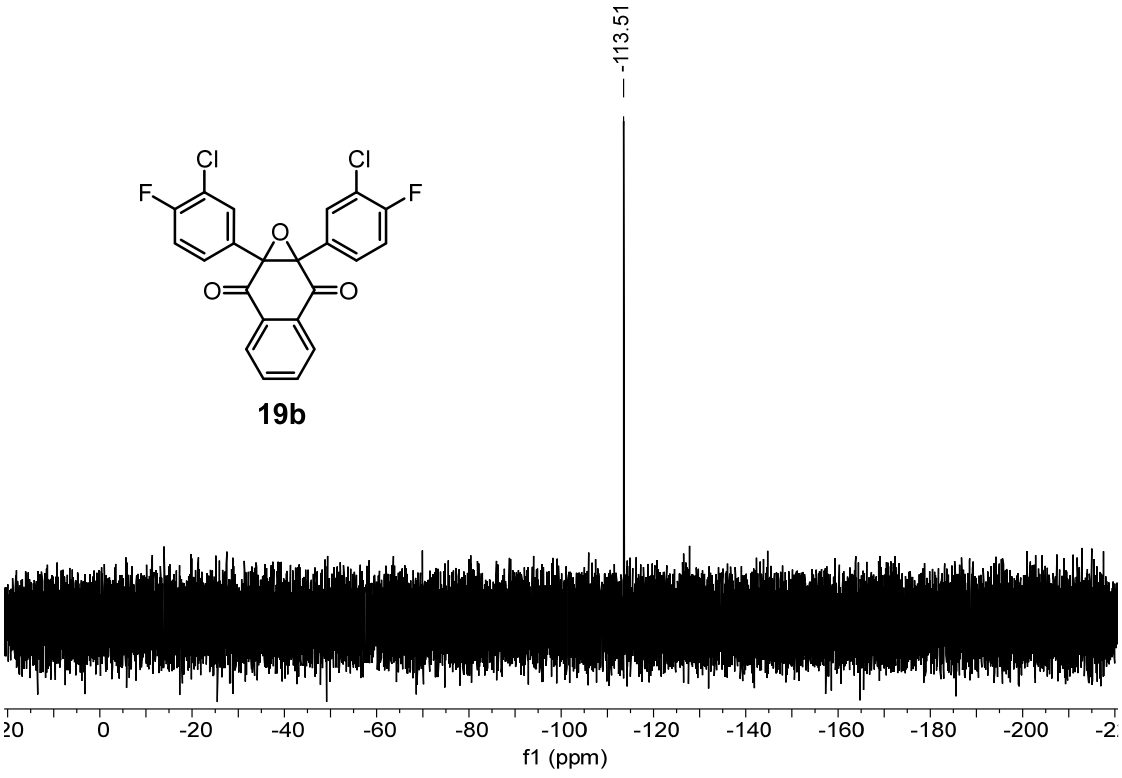
^{1}H NMR ($CDCl_3$, 400 MHz)



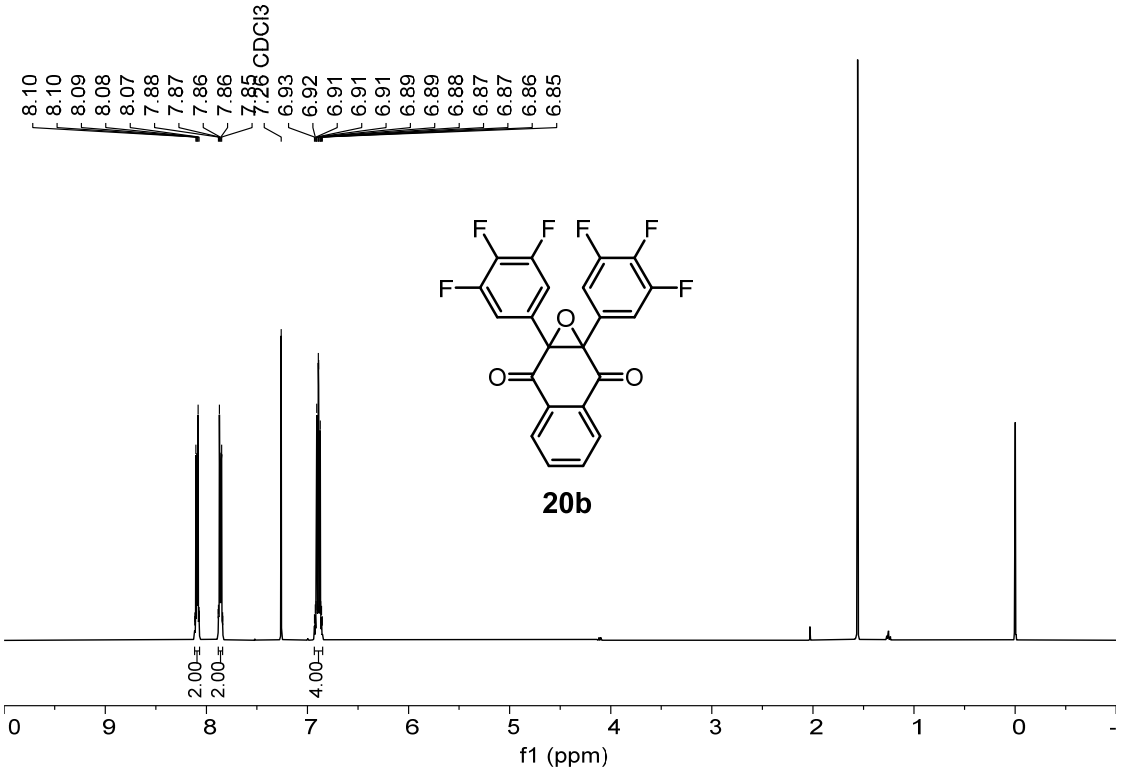
^{13}C NMR ($CDCl_3$, 101 MHz)



^{19}F NMR ($CDCl_3$, 376 MHz)



^{1}H NMR ($CDCl_3$, 400 MHz)



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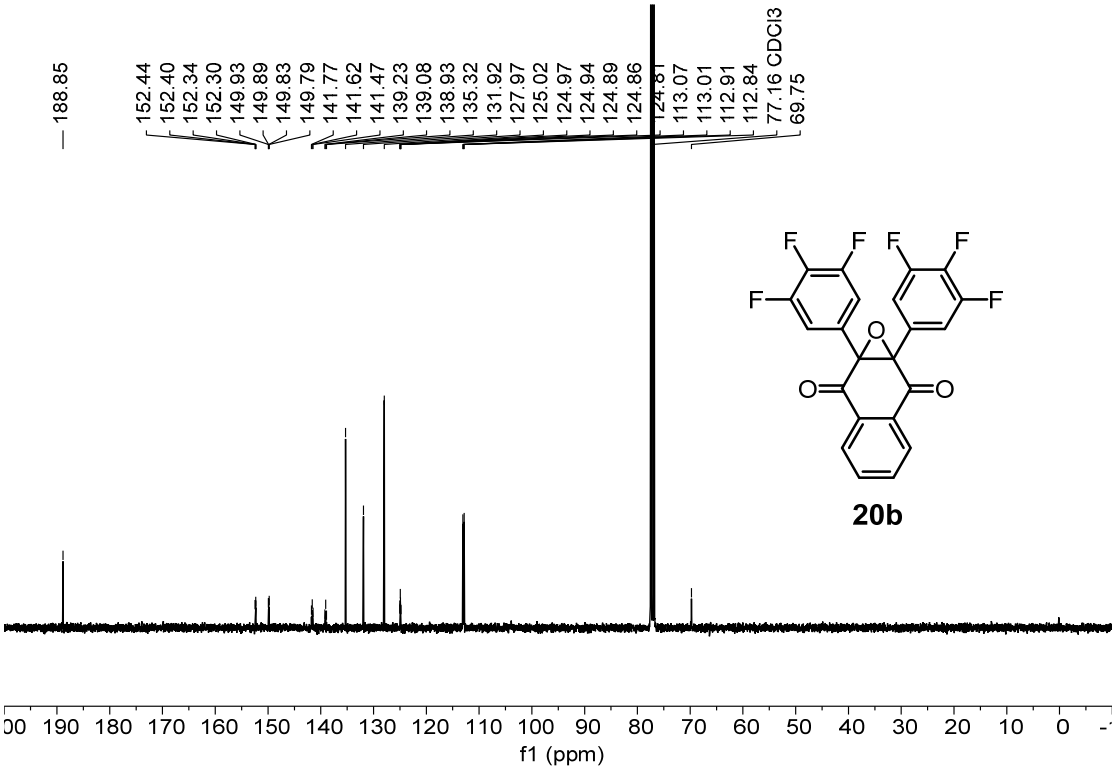

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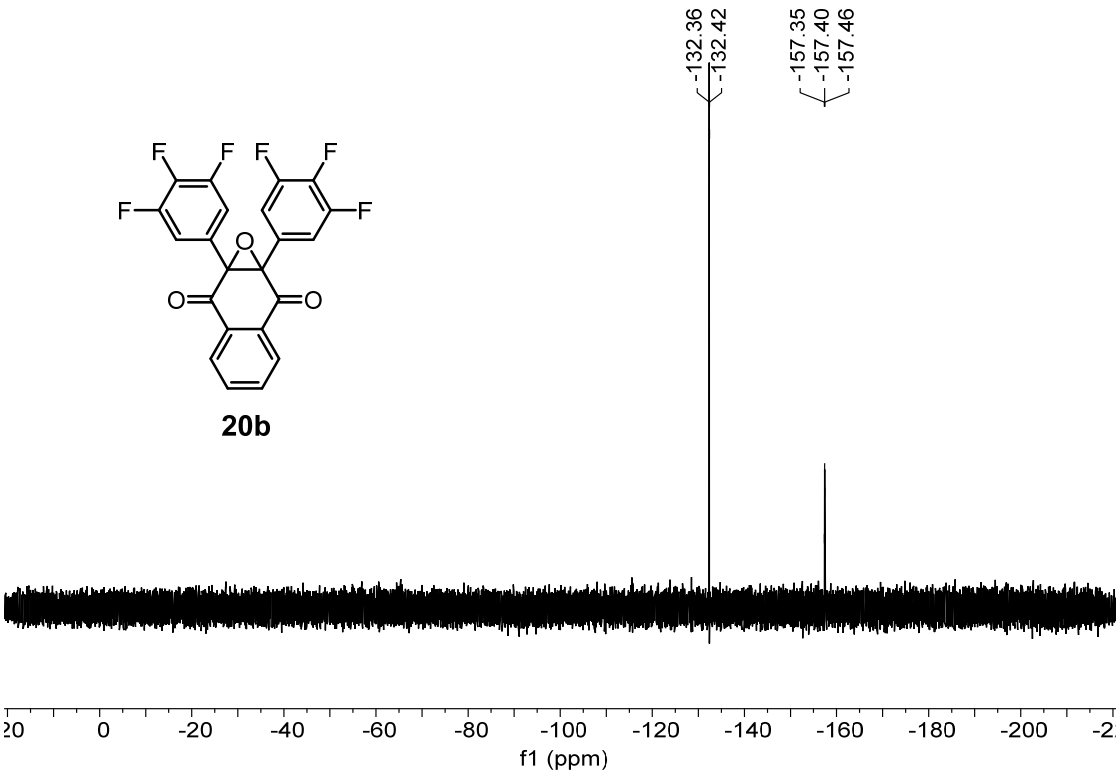

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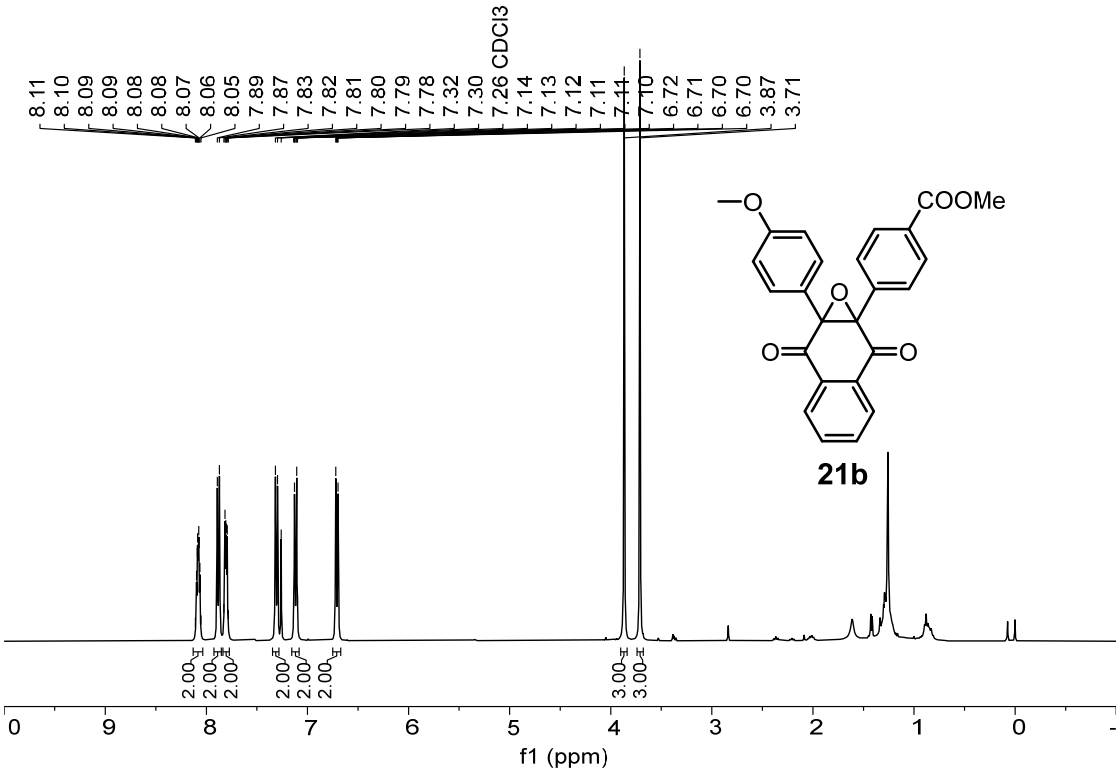

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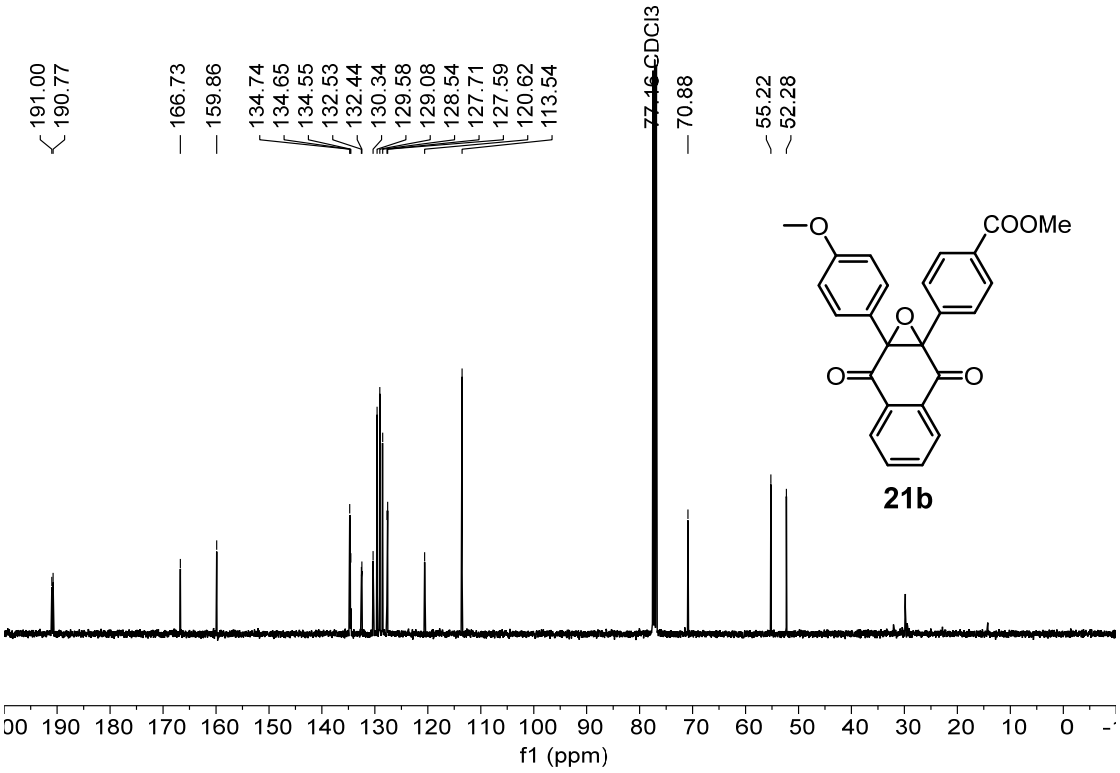

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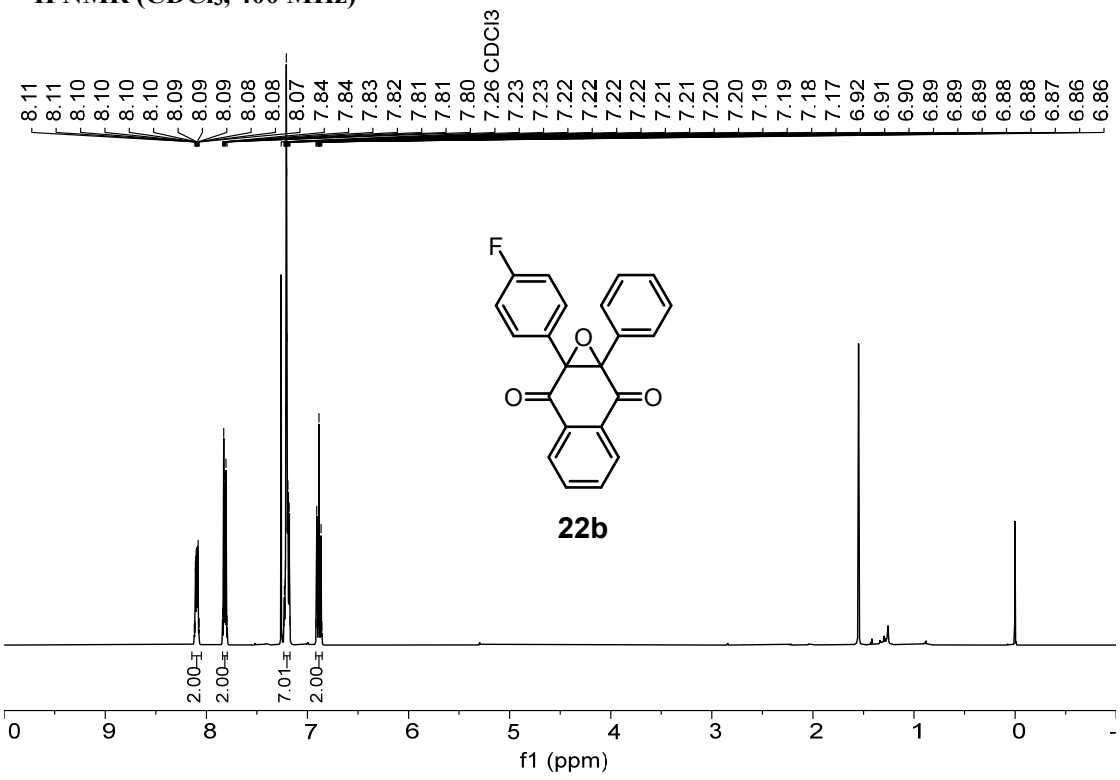

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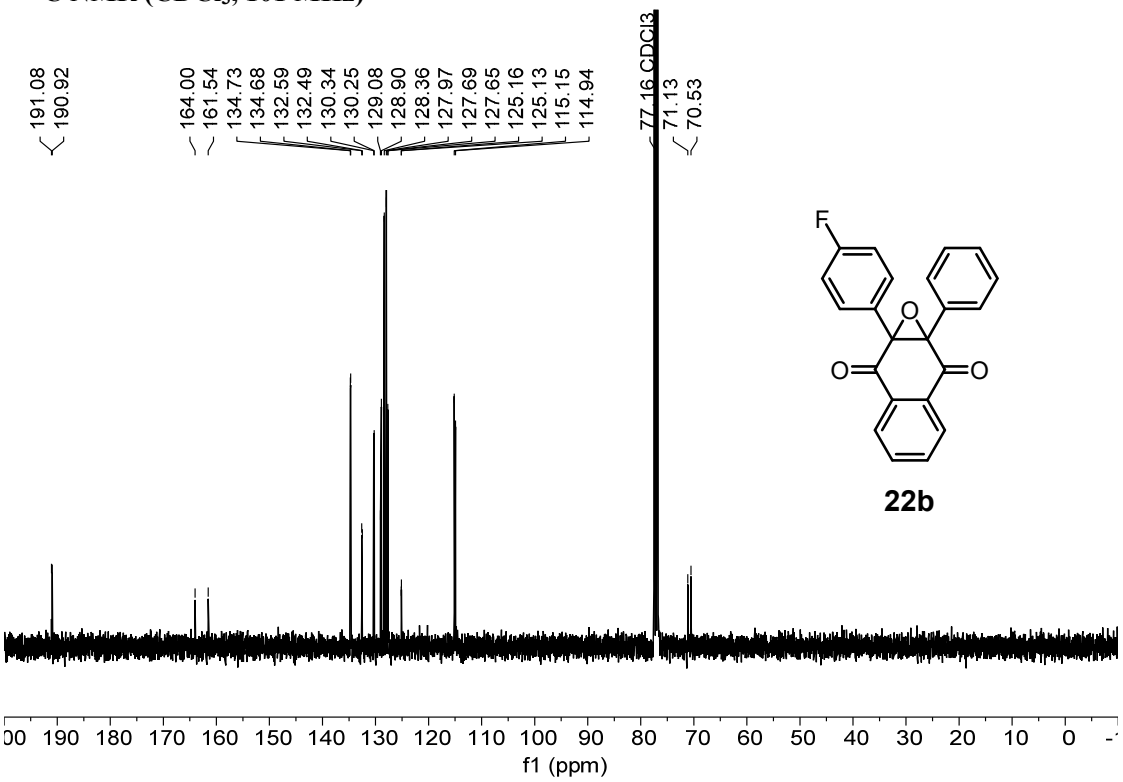

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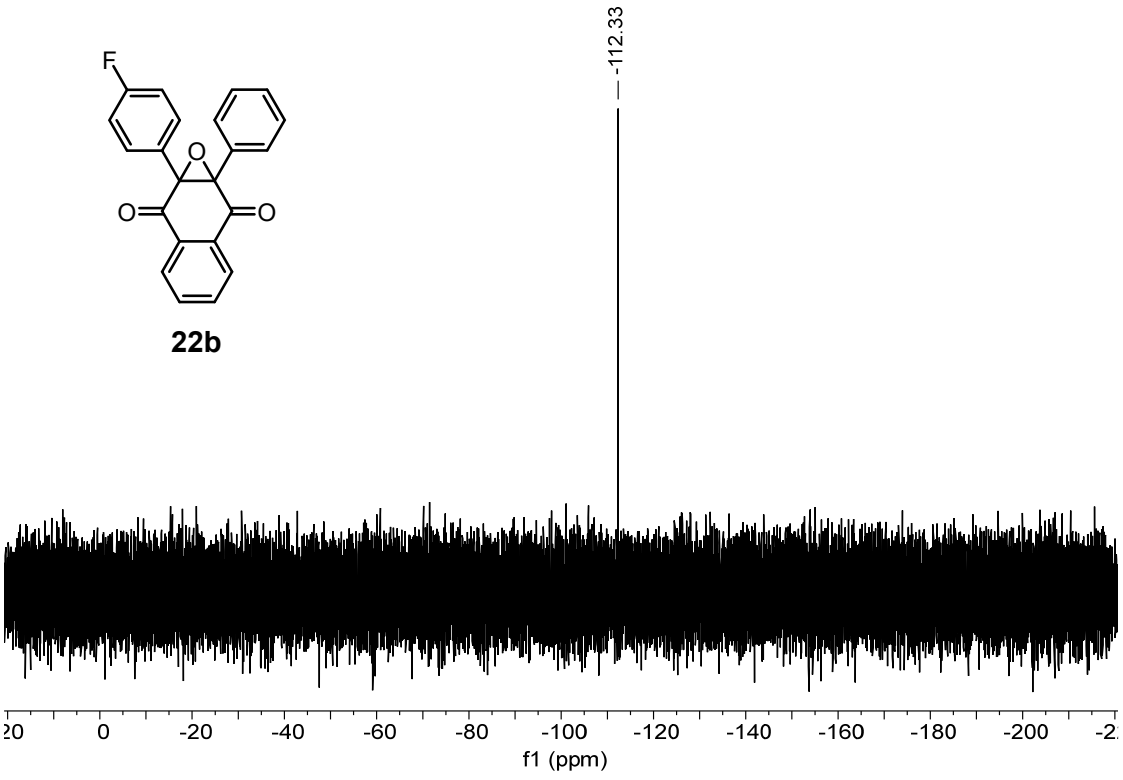

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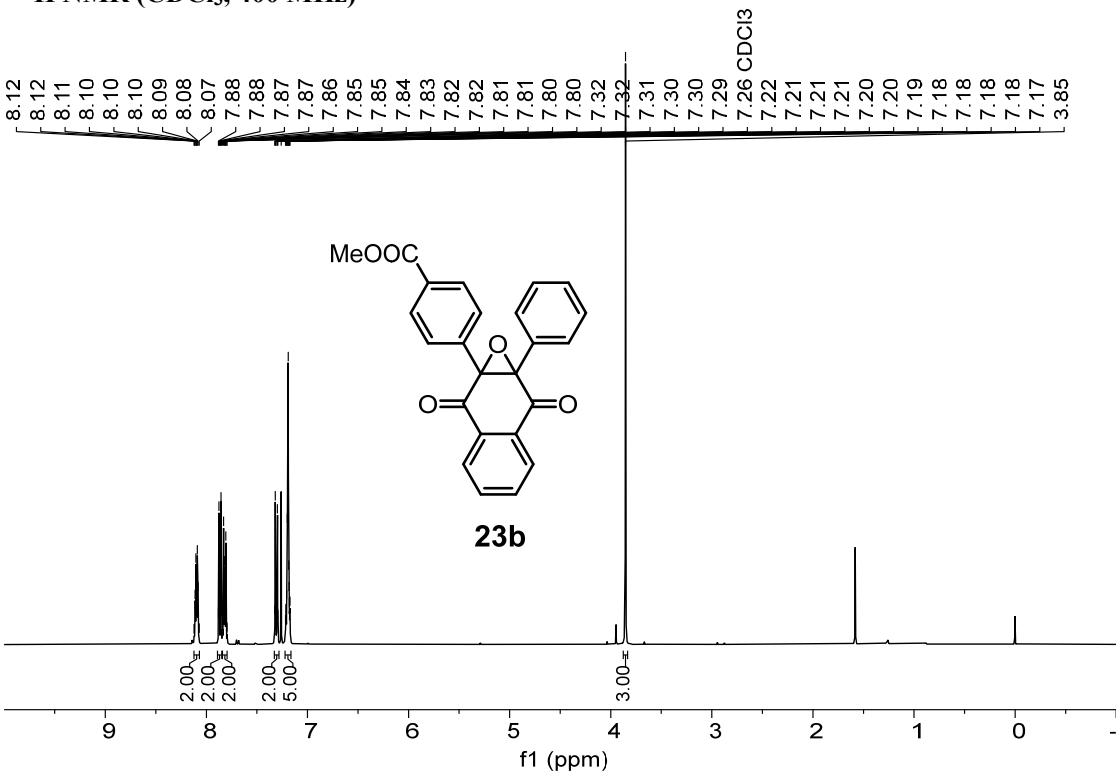

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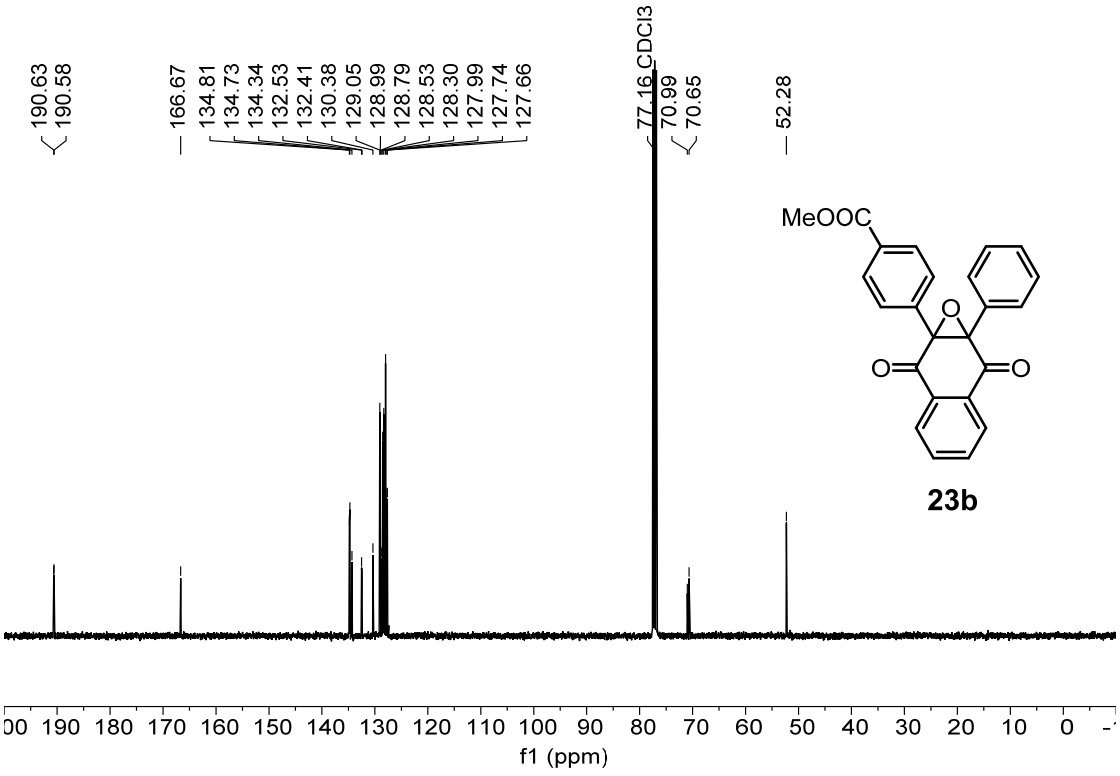

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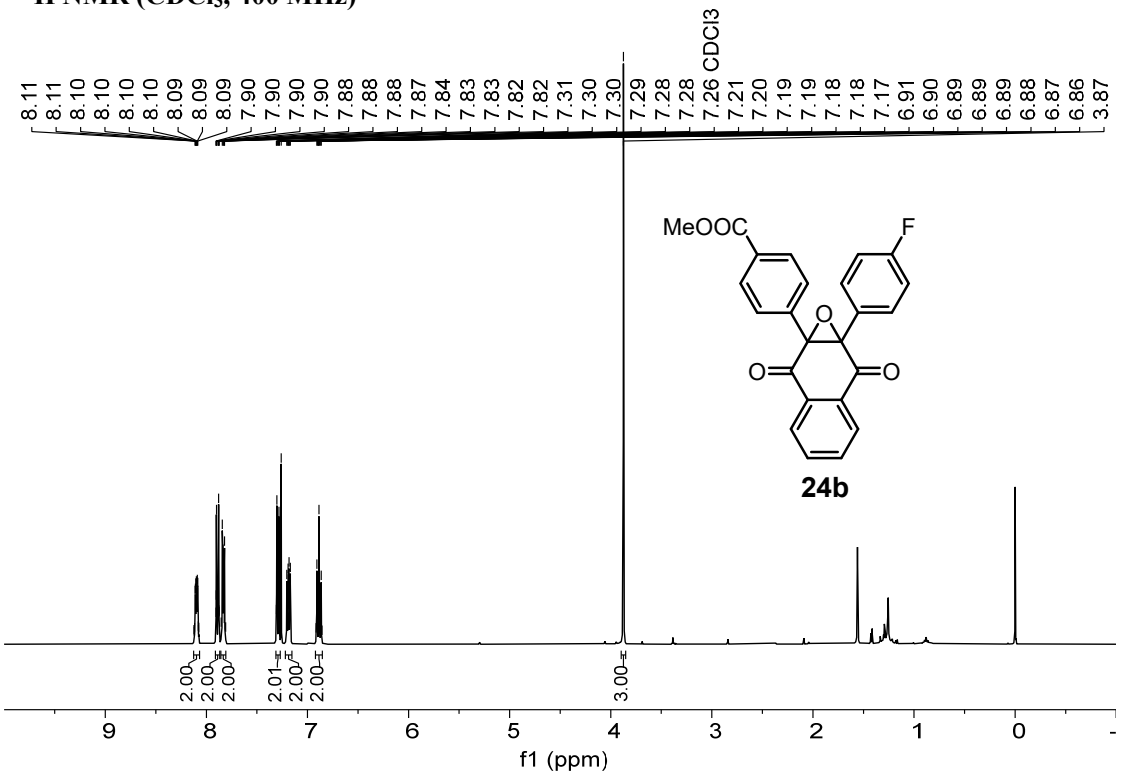

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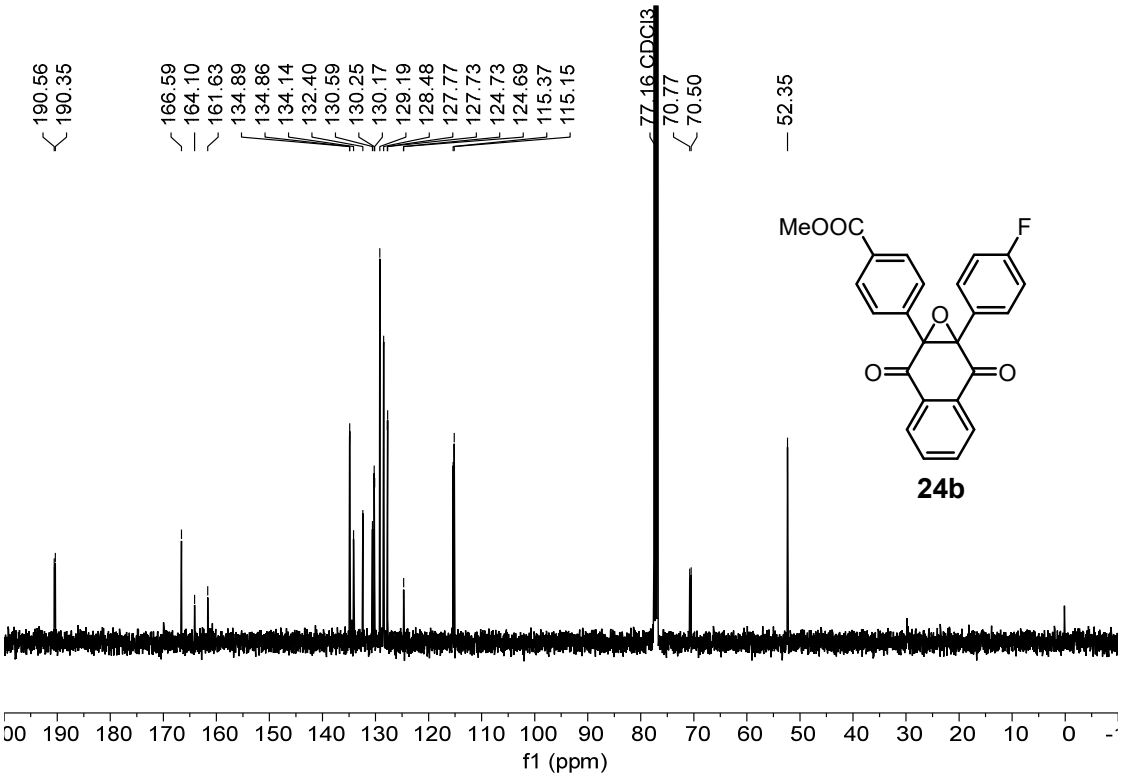

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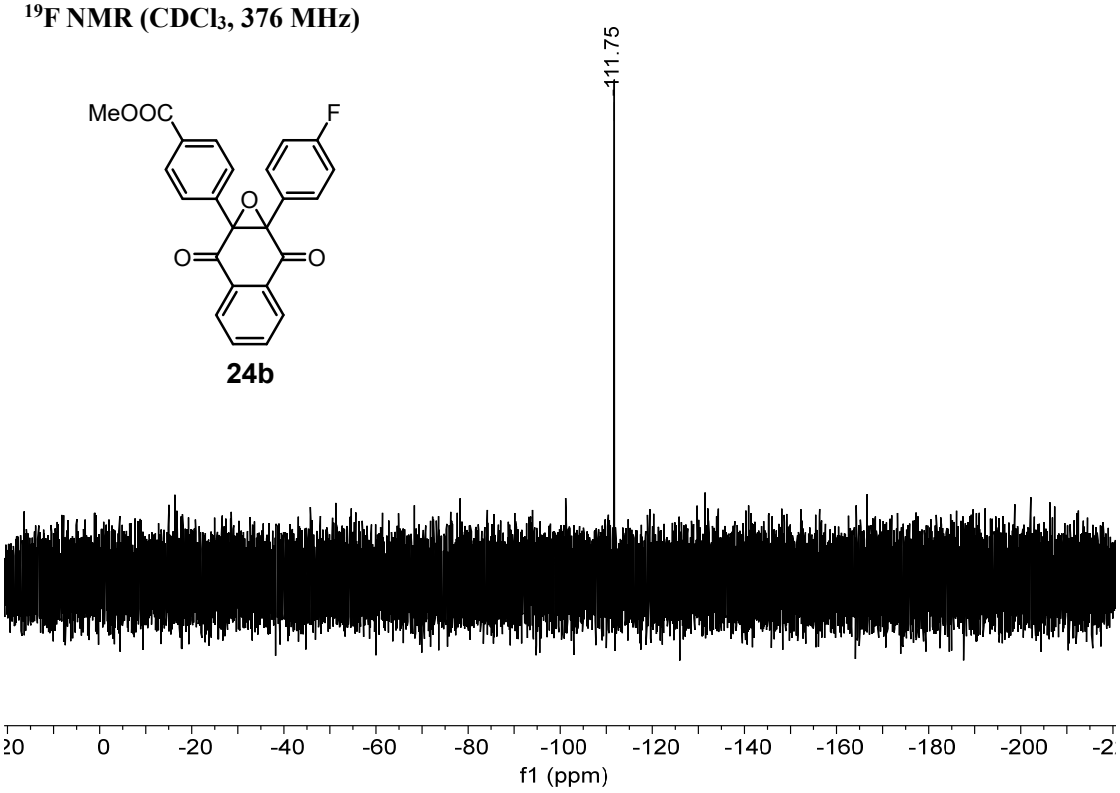
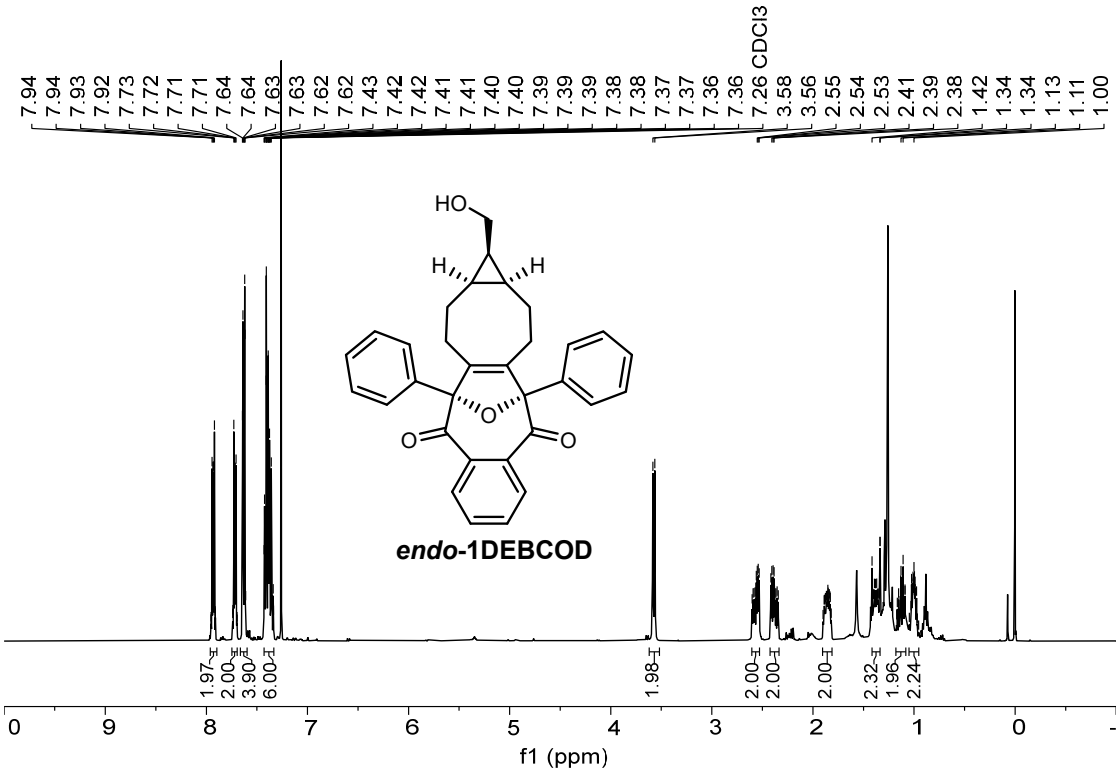
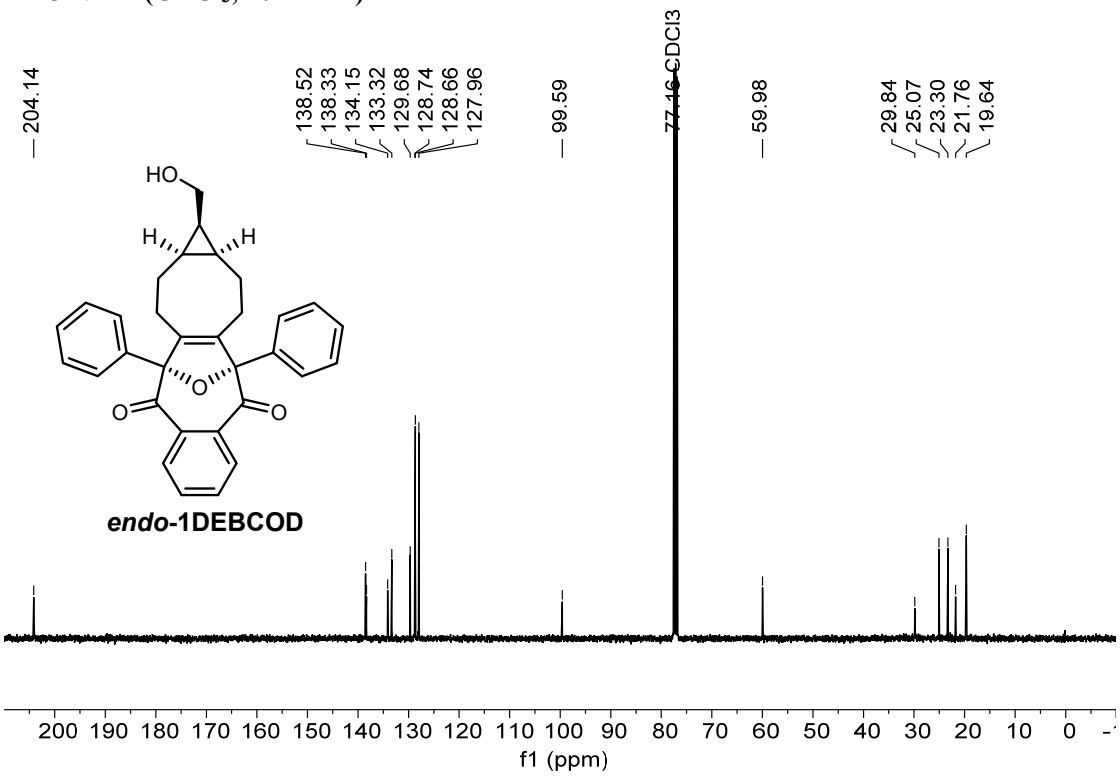


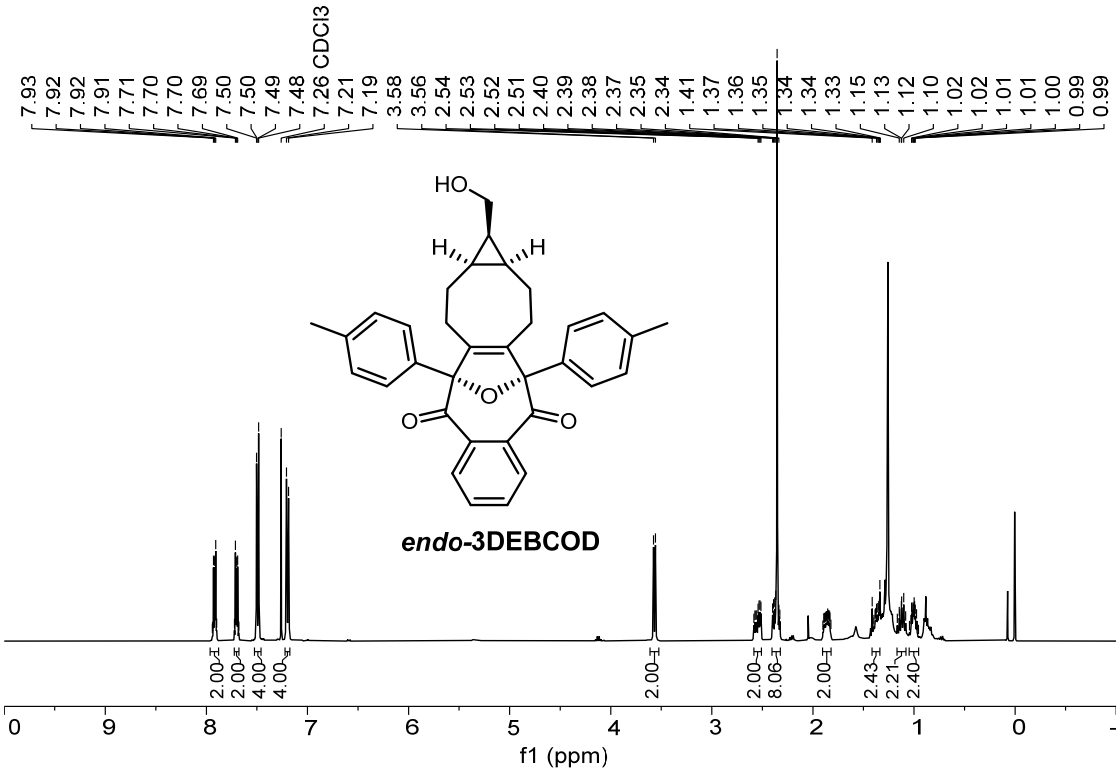
^{1}H NMR ($CDCl_3$, 400 MHz)



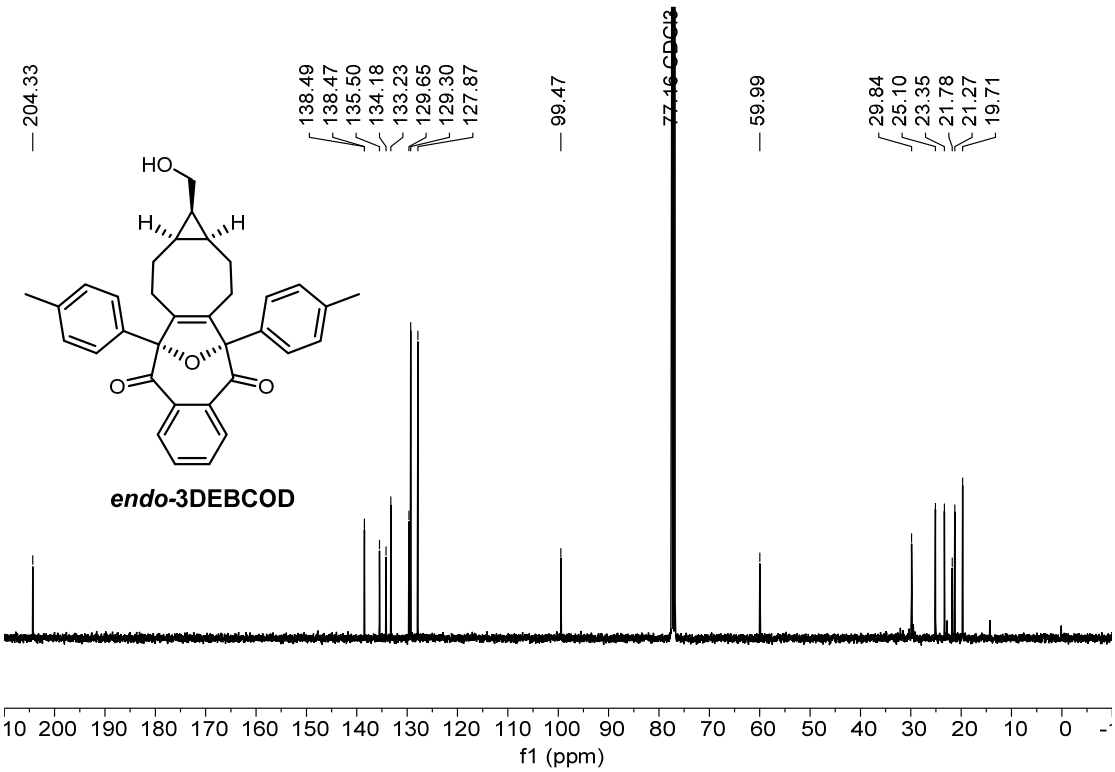
^{13}C NMR ($CDCl_3$, 101 MHz)



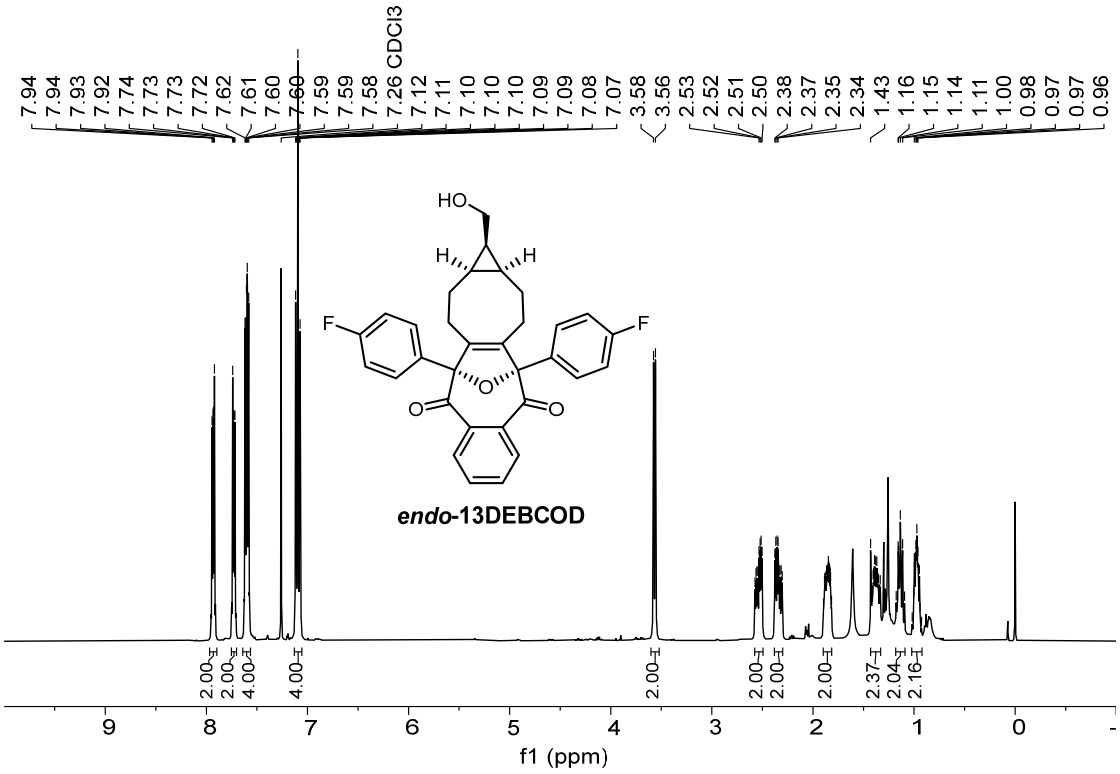
^{1}H NMR ($CDCl_3$, 400 MHz)



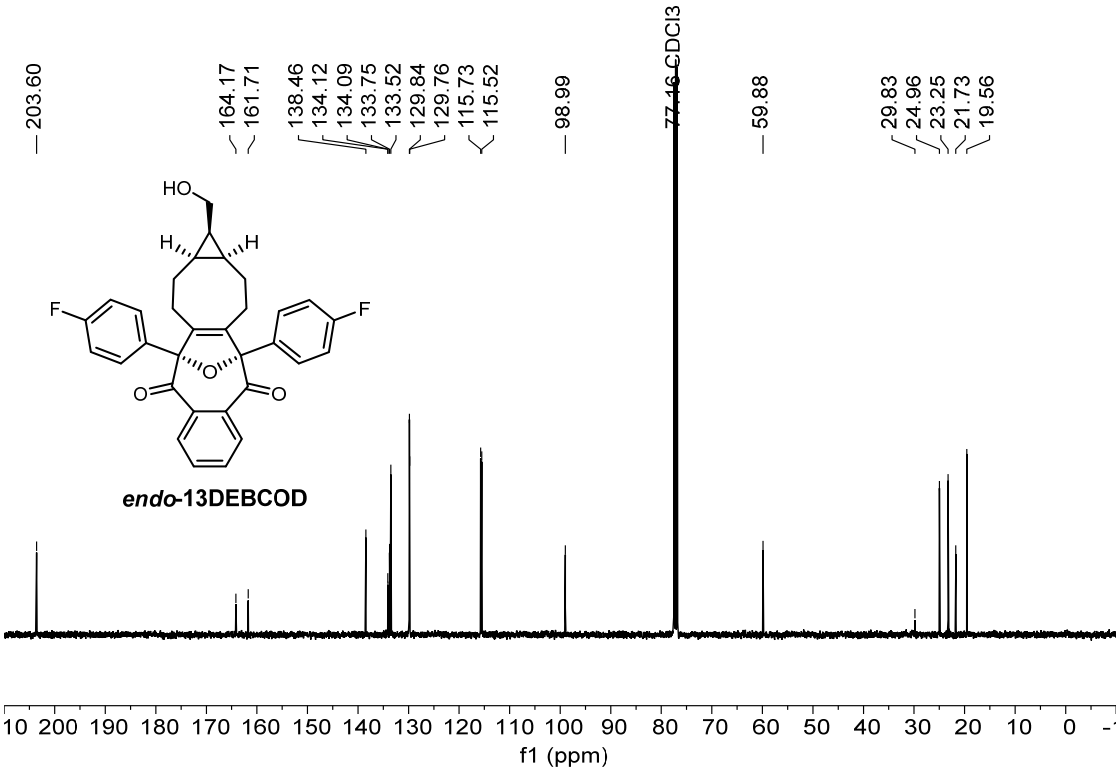
^{13}C NMR ($CDCl_3$, 101 MHz)



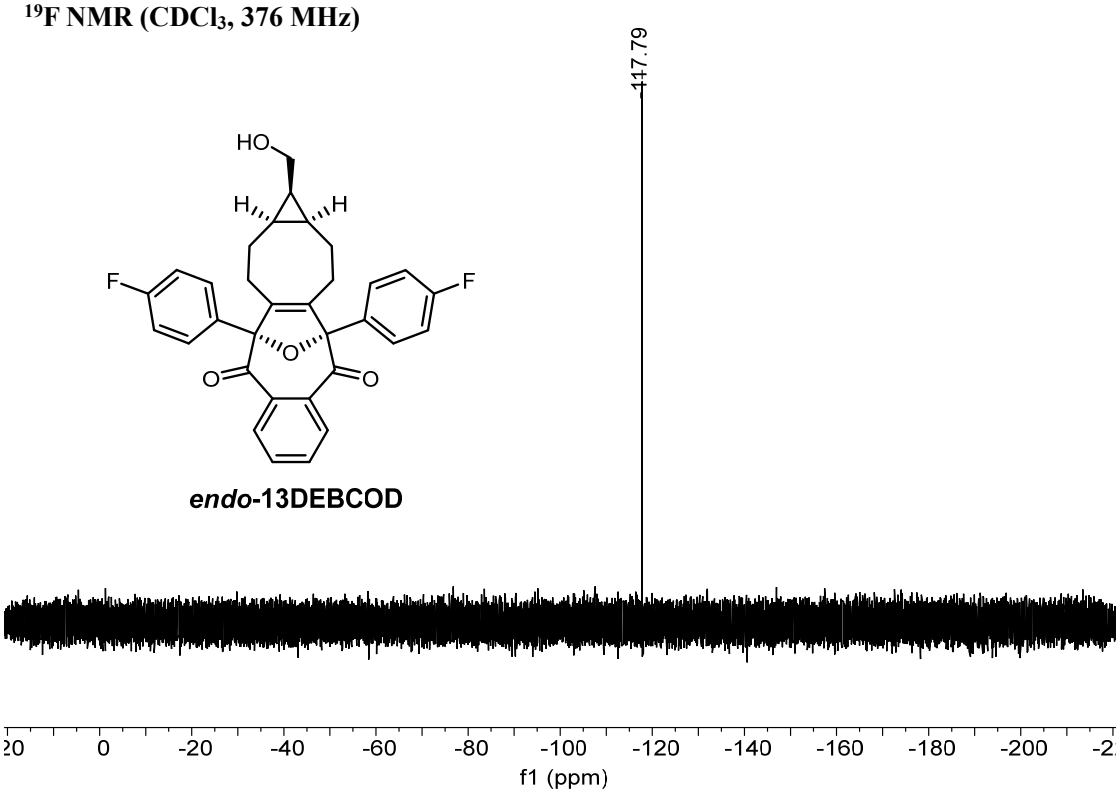
^{1}H NMR ($CDCl_3$, 400 MHz)



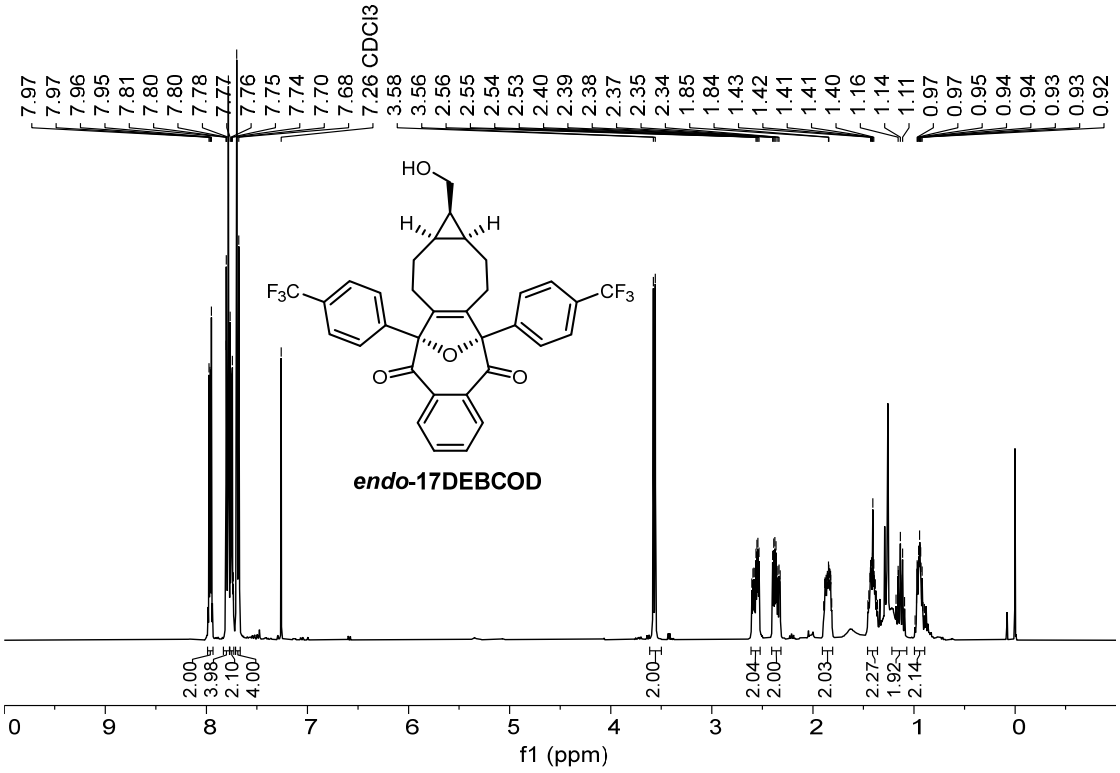
^{13}C NMR ($CDCl_3$, 101 MHz)



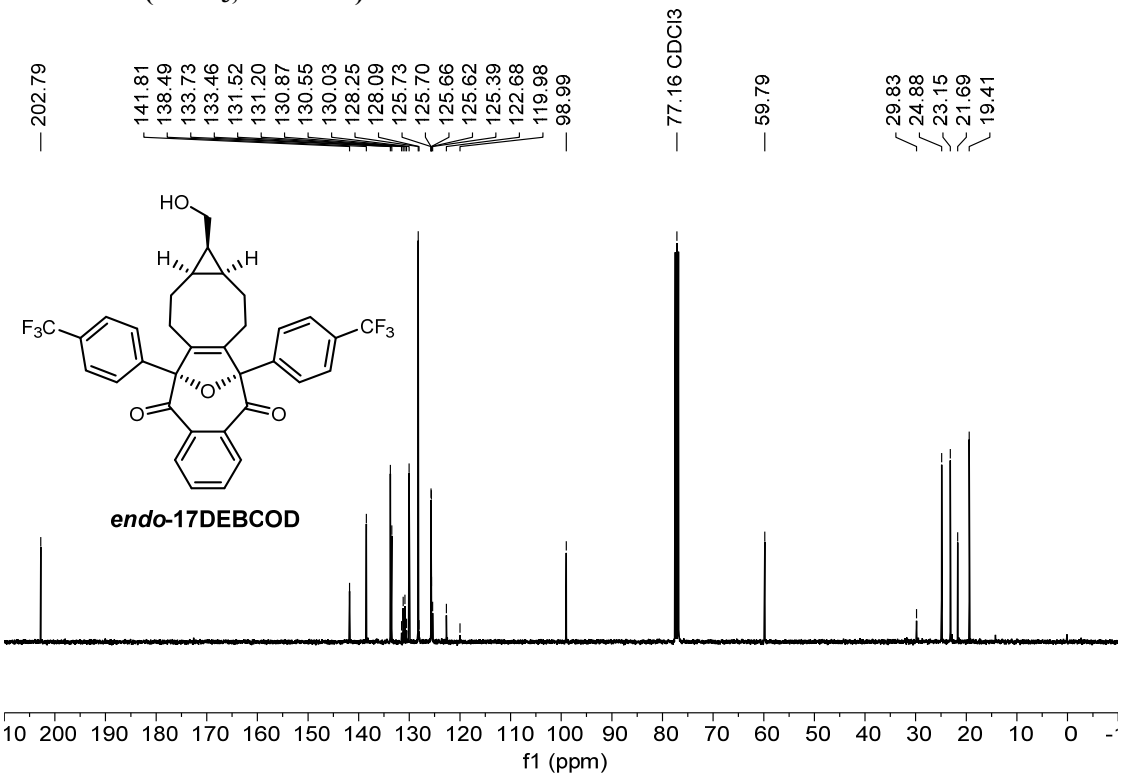
^{19}F NMR ($CDCl_3$, 376 MHz)



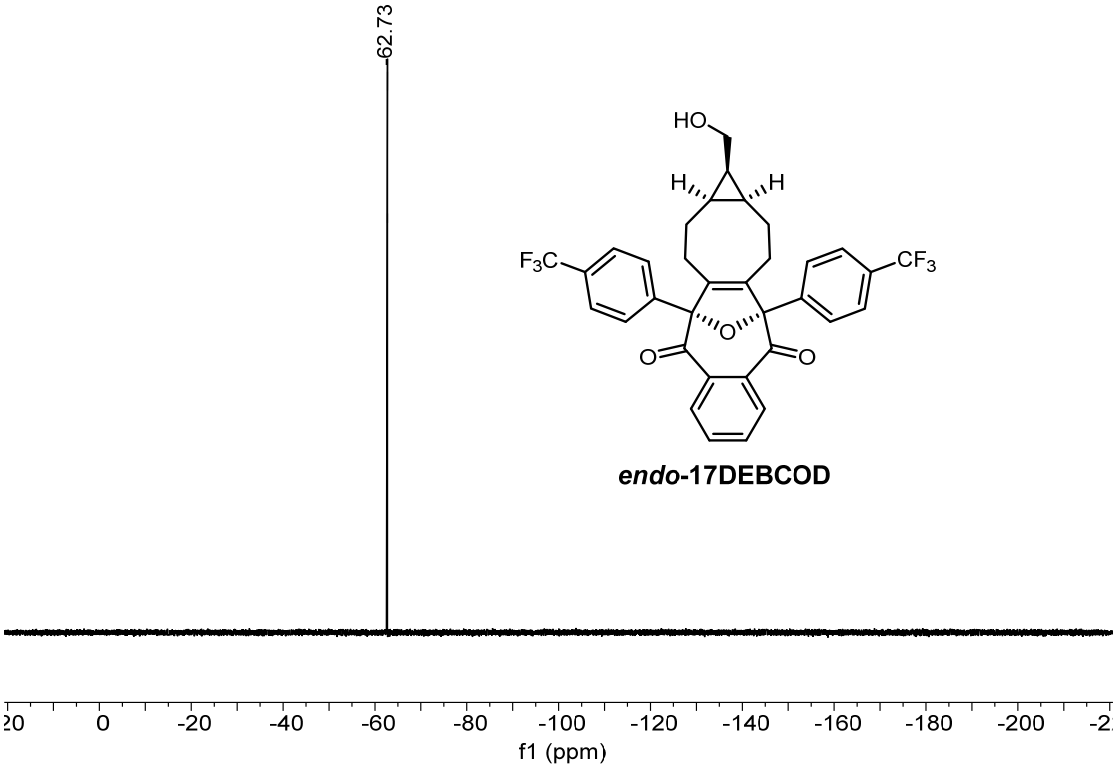
^{1}H NMR ($CDCl_3$, 400 MHz)



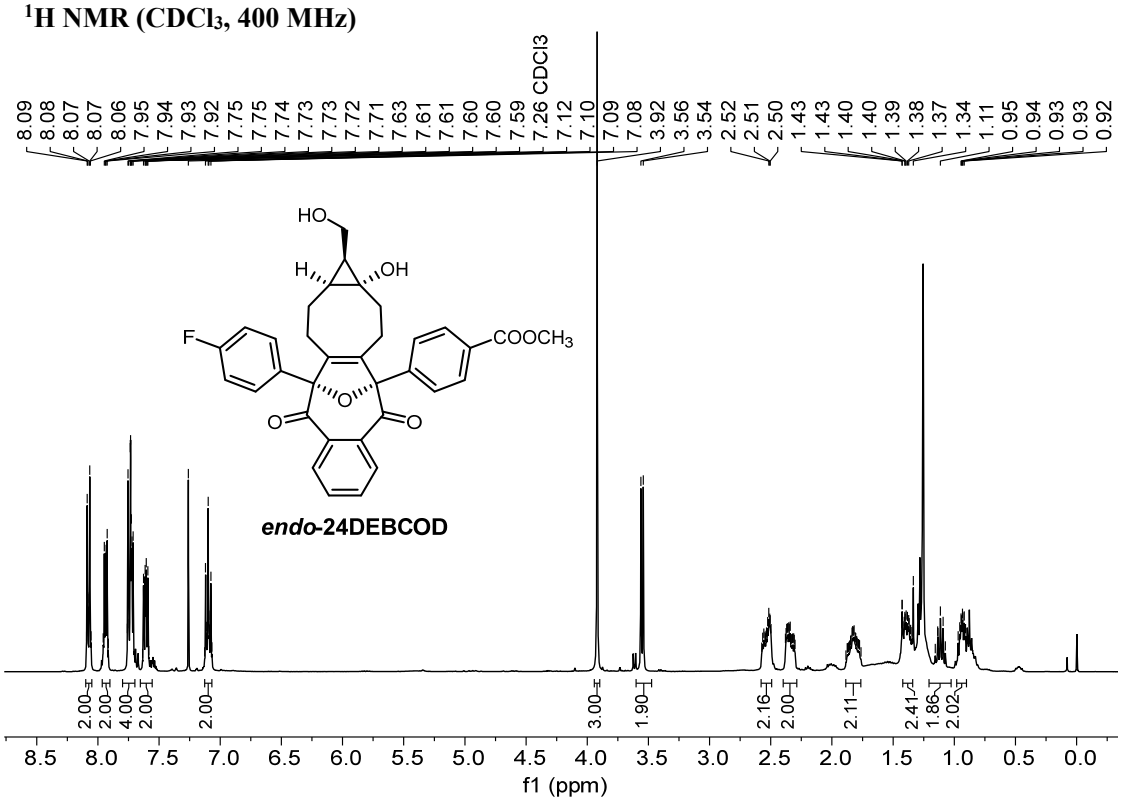
^{13}C NMR ($CDCl_3$, 101 MHz)



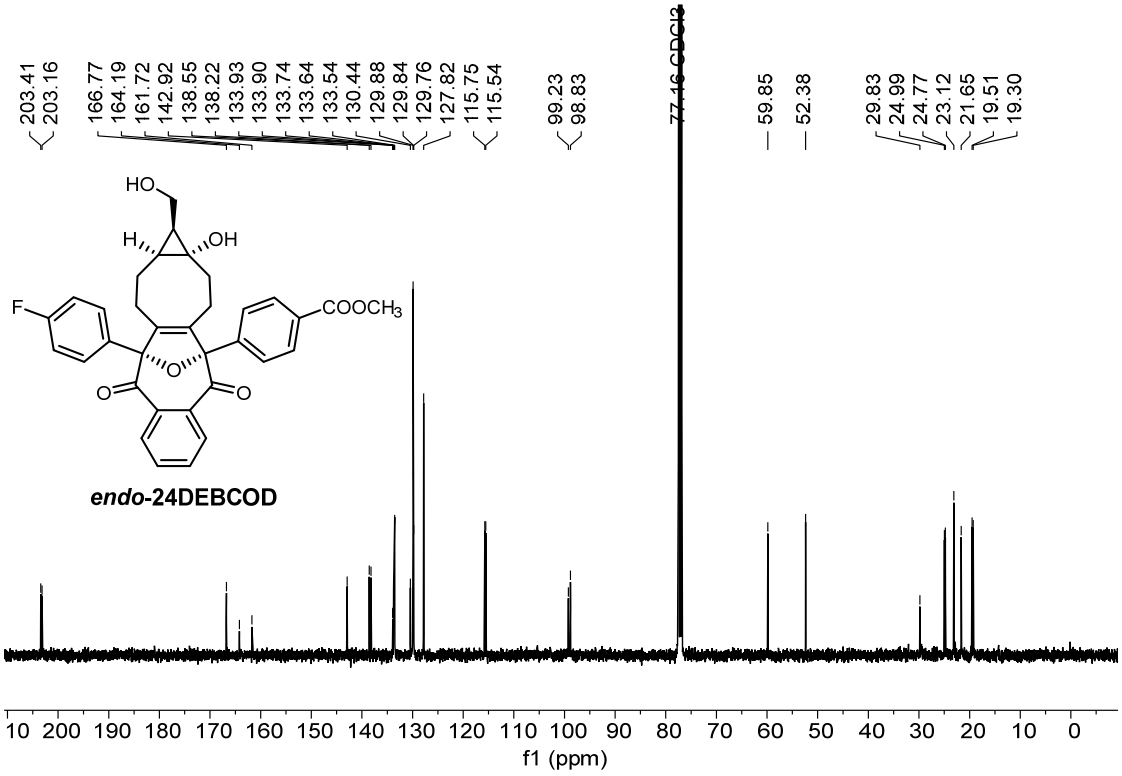
^{19}F NMR ($CDCl_3$, 376 MHz)



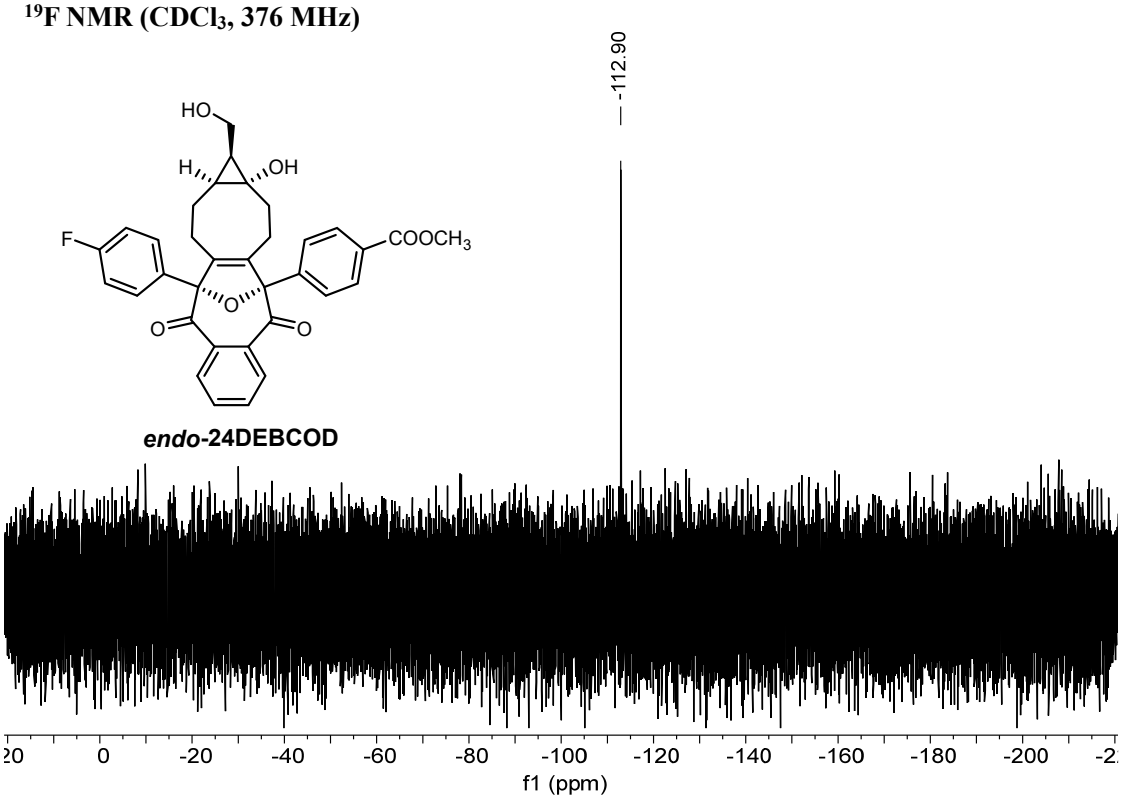
^{1}H NMR ($CDCl_3$, 400 MHz)



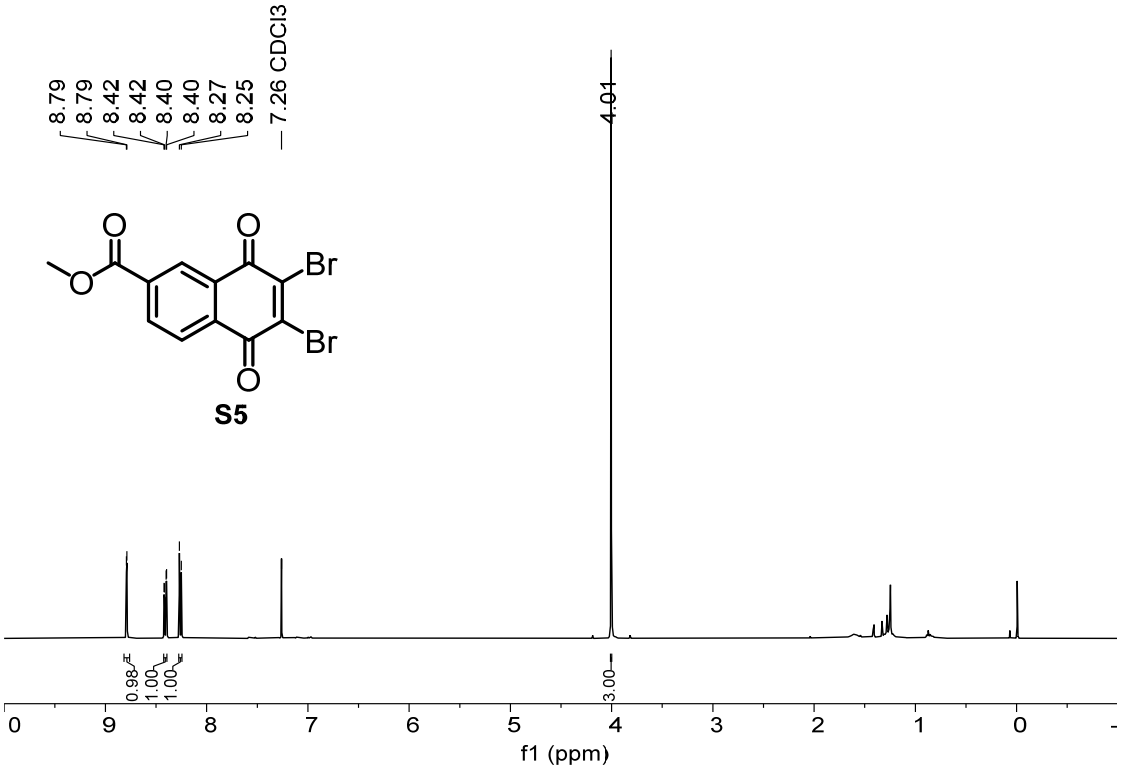
^{13}C NMR ($CDCl_3$, 101 MHz)



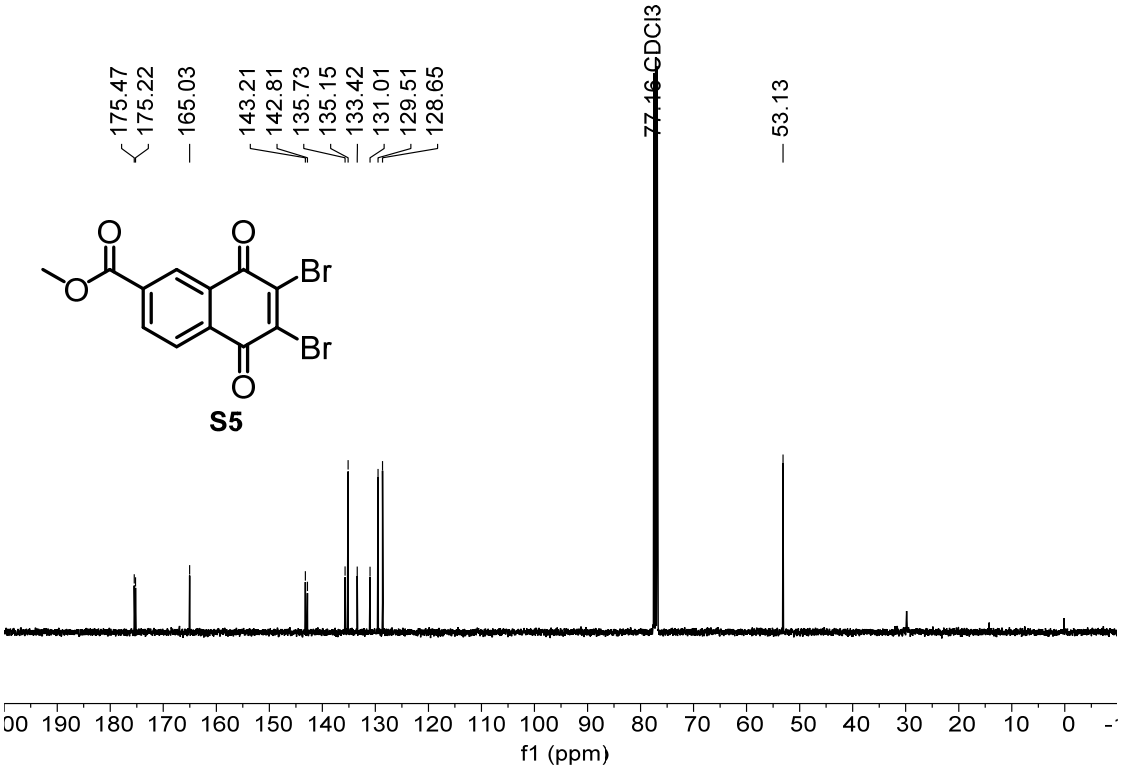
^{19}F NMR ($CDCl_3$, 376 MHz)



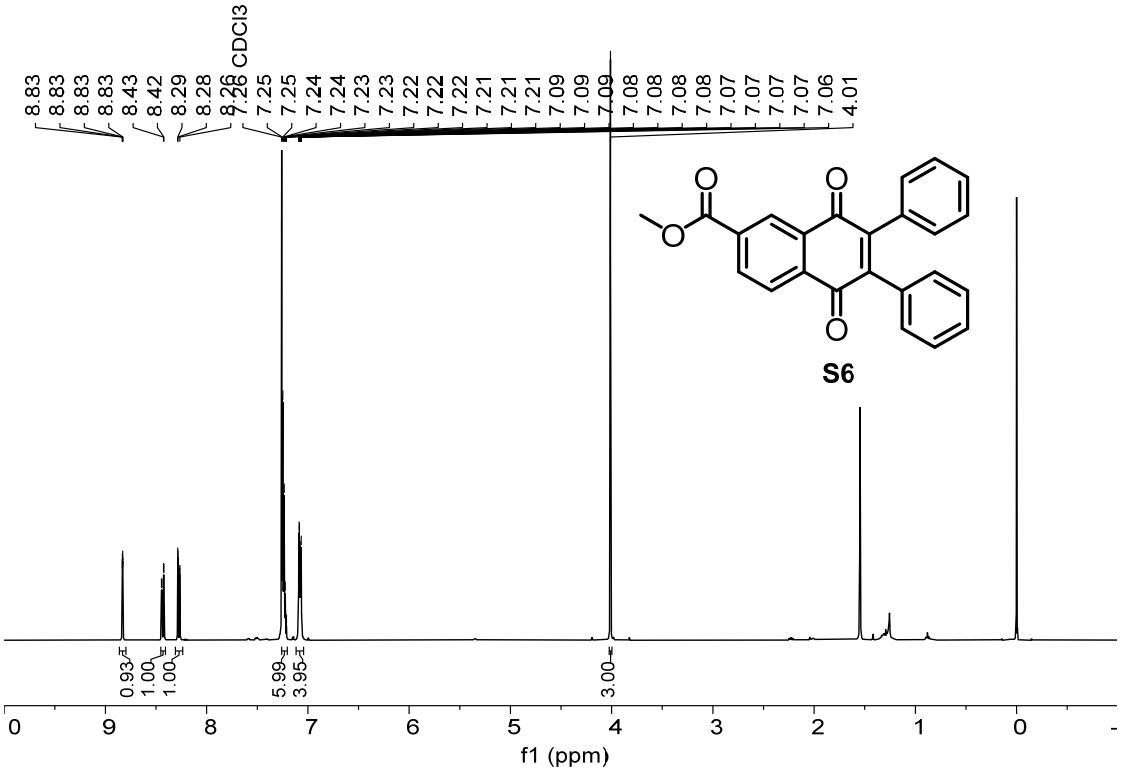
^{1}H NMR ($CDCl_3$, 400 MHz)



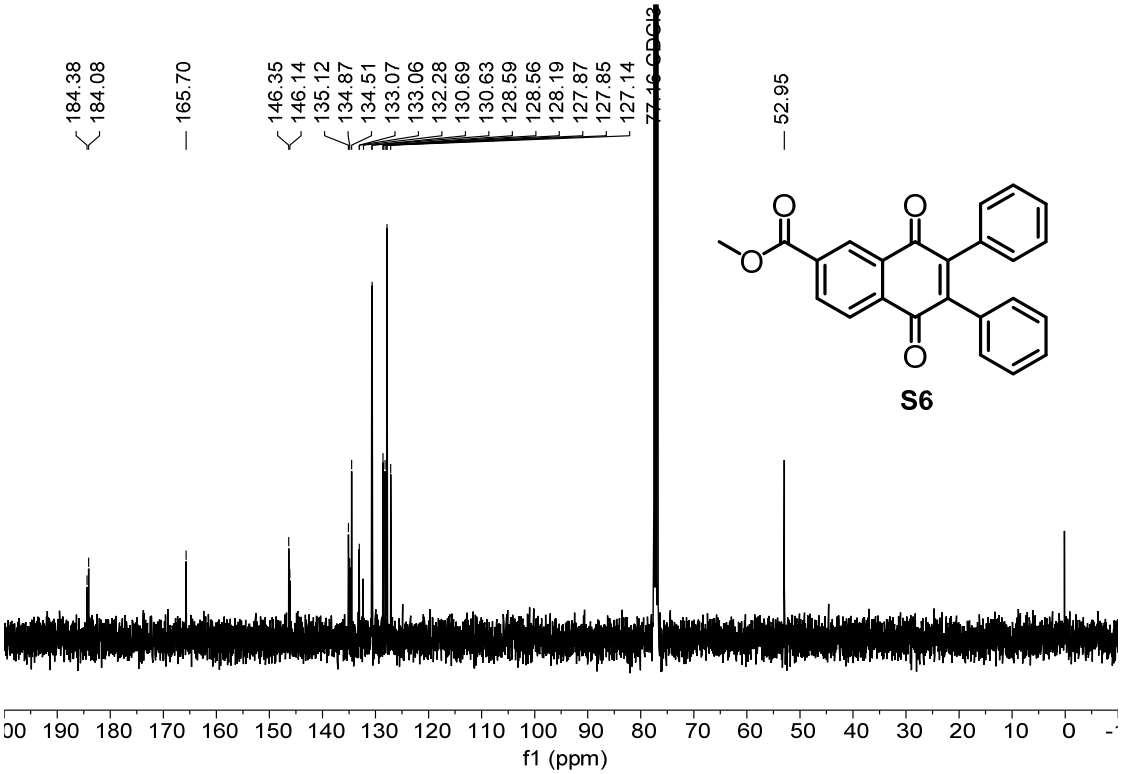
^{13}C NMR ($CDCl_3$, 101 MHz)



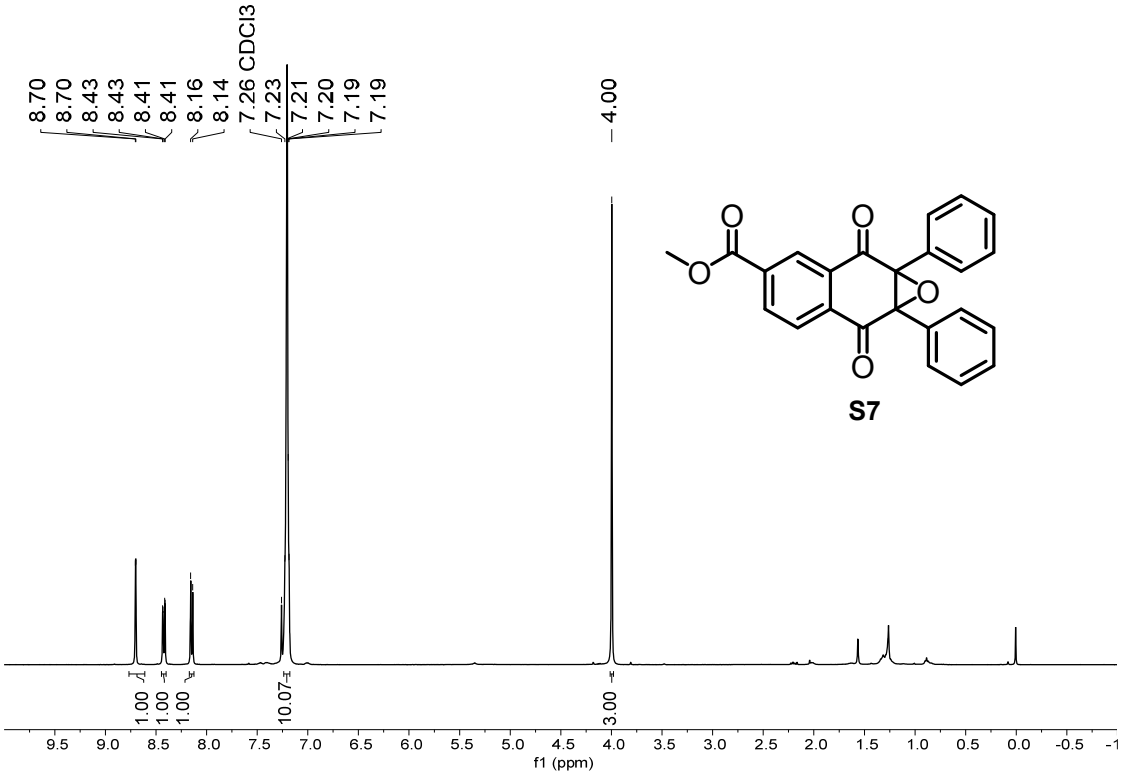
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 101 MHz)

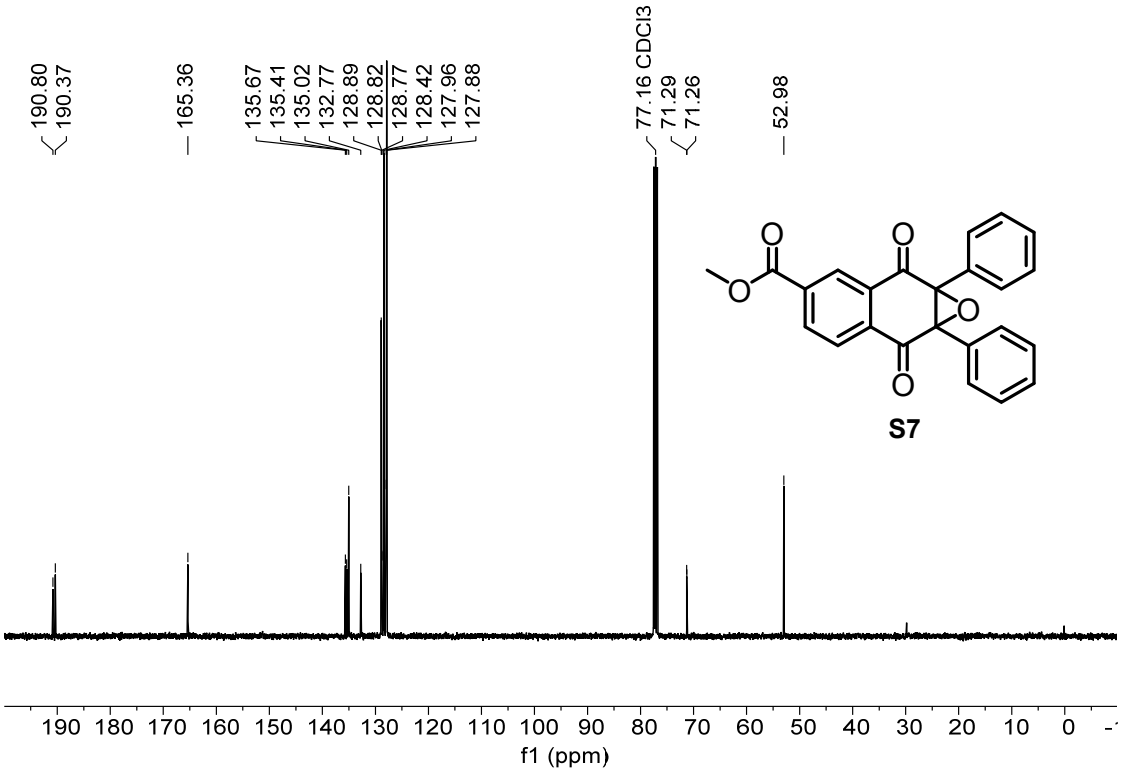


^{1}H NMR ($CDCl_3$, 400 MHz)



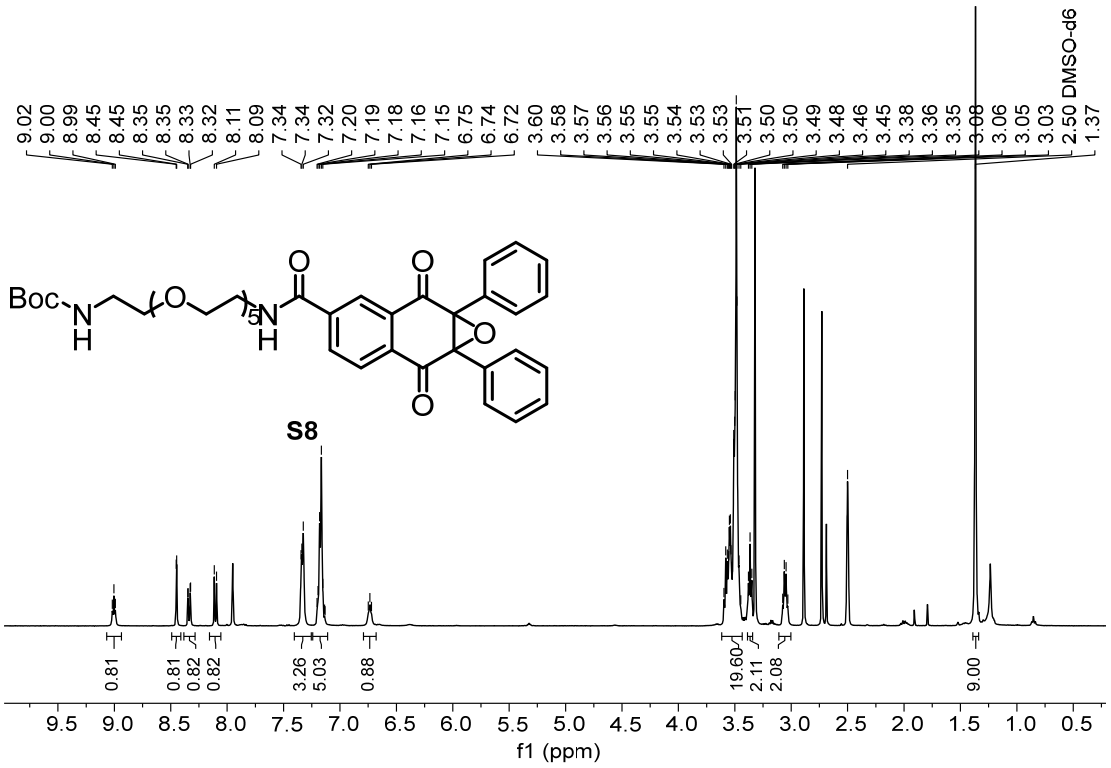
S7

^{13}C NMR ($CDCl_3$, 101 MHz)



S7

^{1}H NMR (DMSO-d_6, 400 MHz)



^{13}C NMR (DMSO-d_6, 101 MHz)