Electronic Supplementary Material (ESI) for RSC Advances

Supporting information for:

Photoinduced DNA cleavage by atomic oxygen precursors in aqueous solutions

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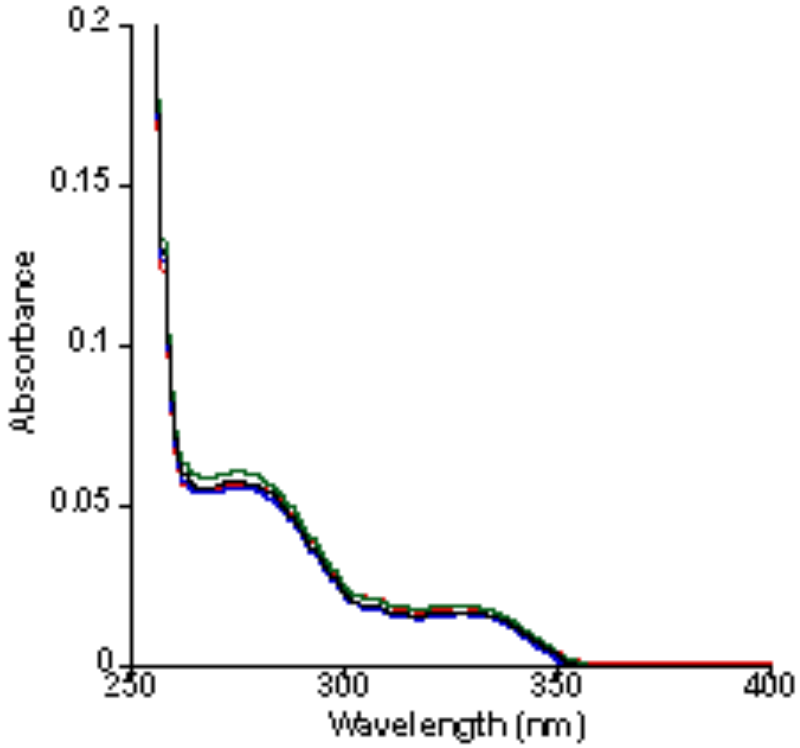
Table of Contents

Absorption titration

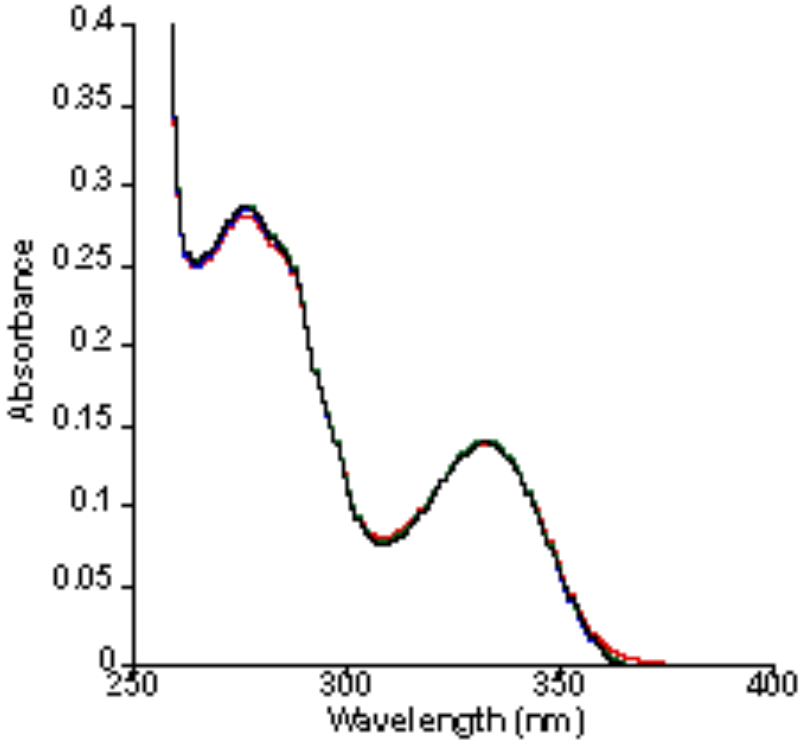
An aqueous solution was used in UV spectrophotometric titrations. The DNA concentration per nucleotide was determined by absorption spectroscopy, using the molar extinction coefficient $6600M^{-1}$ cm^{-1}at 260 nm. In absorption titrations, the concentrations of the sulfoxides were maintained and the different amounts of the DNA were added. All the experiments were performed at room temperature and the absorption spectra are shown in Figure S1.

Fluorescence titration

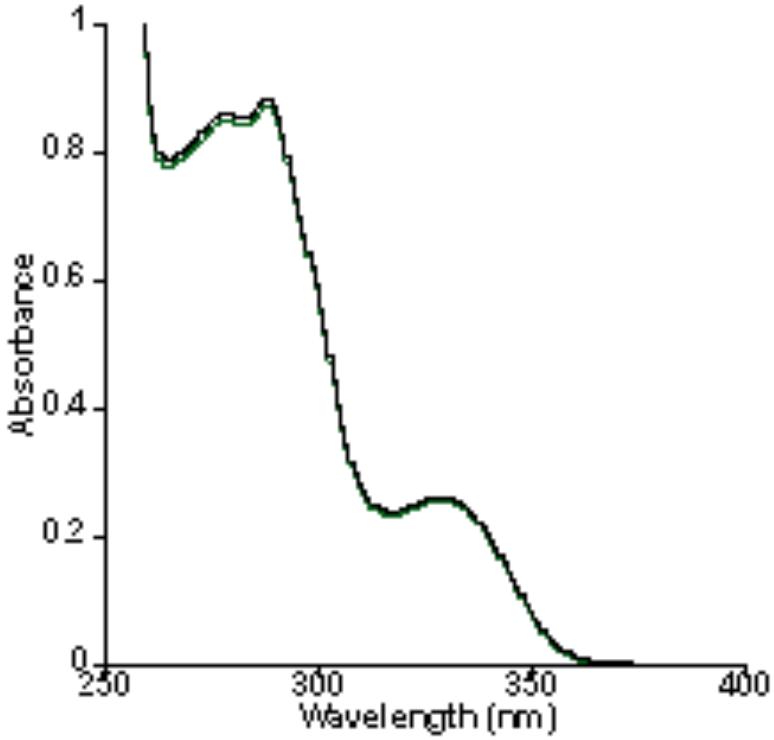
In fluorescence titration experiments, the solutions of the sulfoxide and DNA in water were stored in the dark for 1 h before use. Then different concentration of the DNA were added to a known sulfoxides solution and stirred in the dark for 10 min. The recorded fluorescence data are shown in Figure S2.



(a)

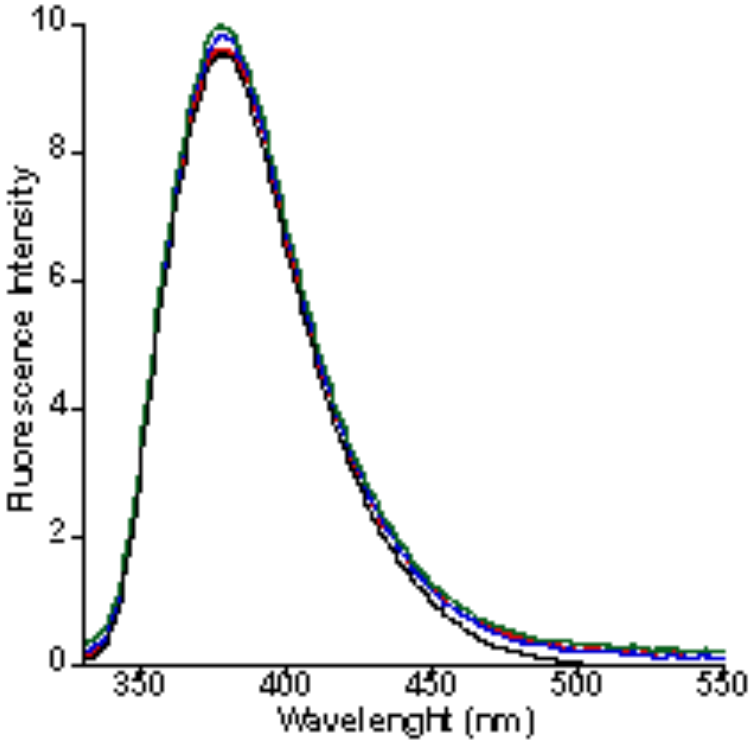


(b)

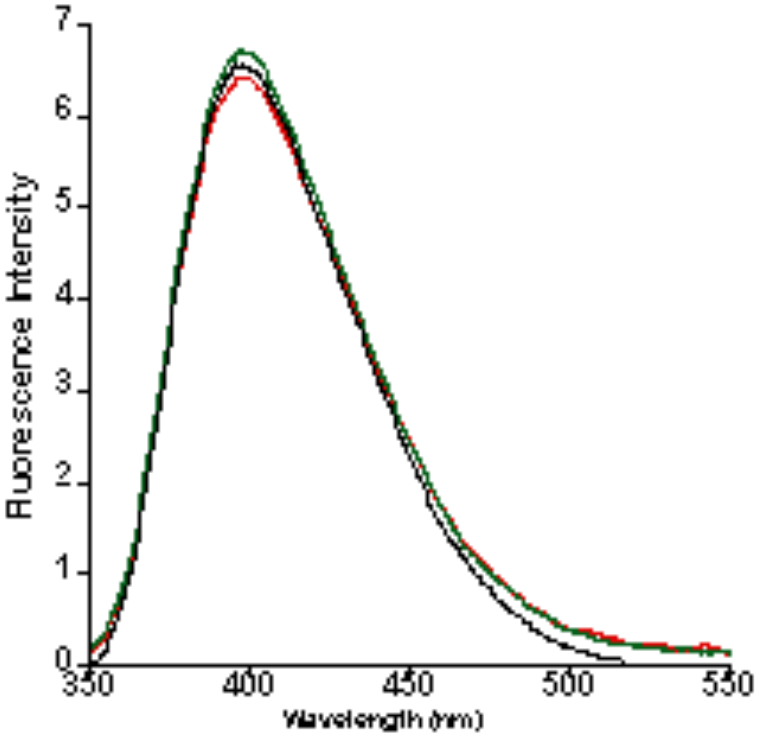


(c)

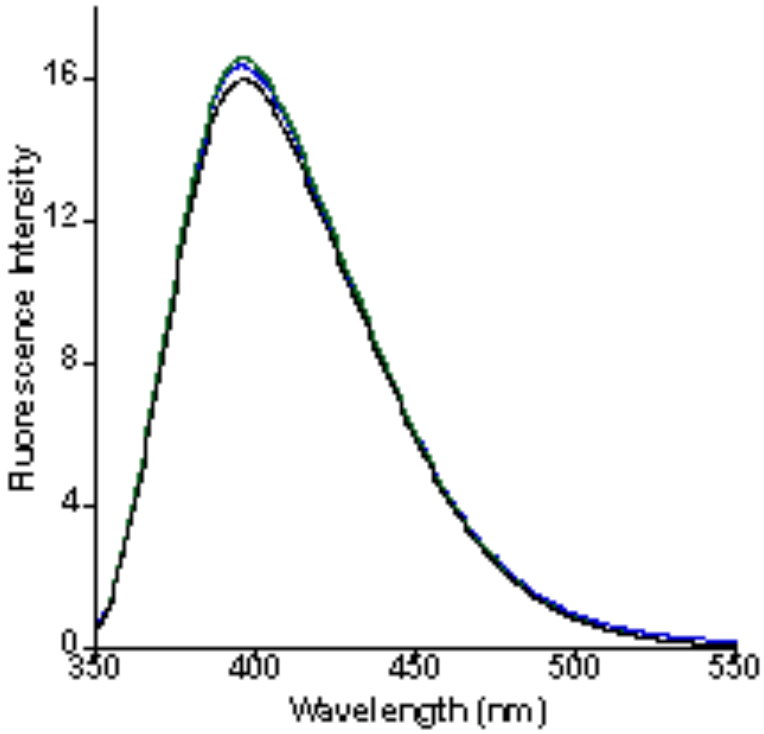
Figure S1 Absorption spectra of sulfoxide (a) **1** (b) **2** and (c) **3** with increasing concentration of DNA of (0 (Red), 30 (Blue), 60 (Green), and100 (Black) μM)



(a)



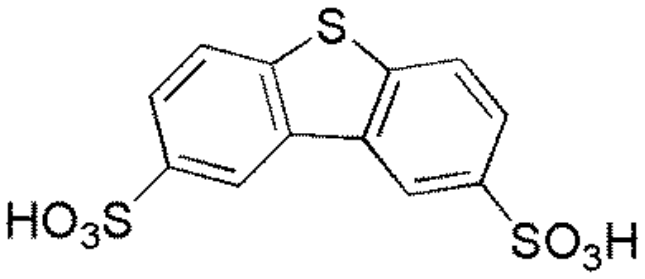
(b)



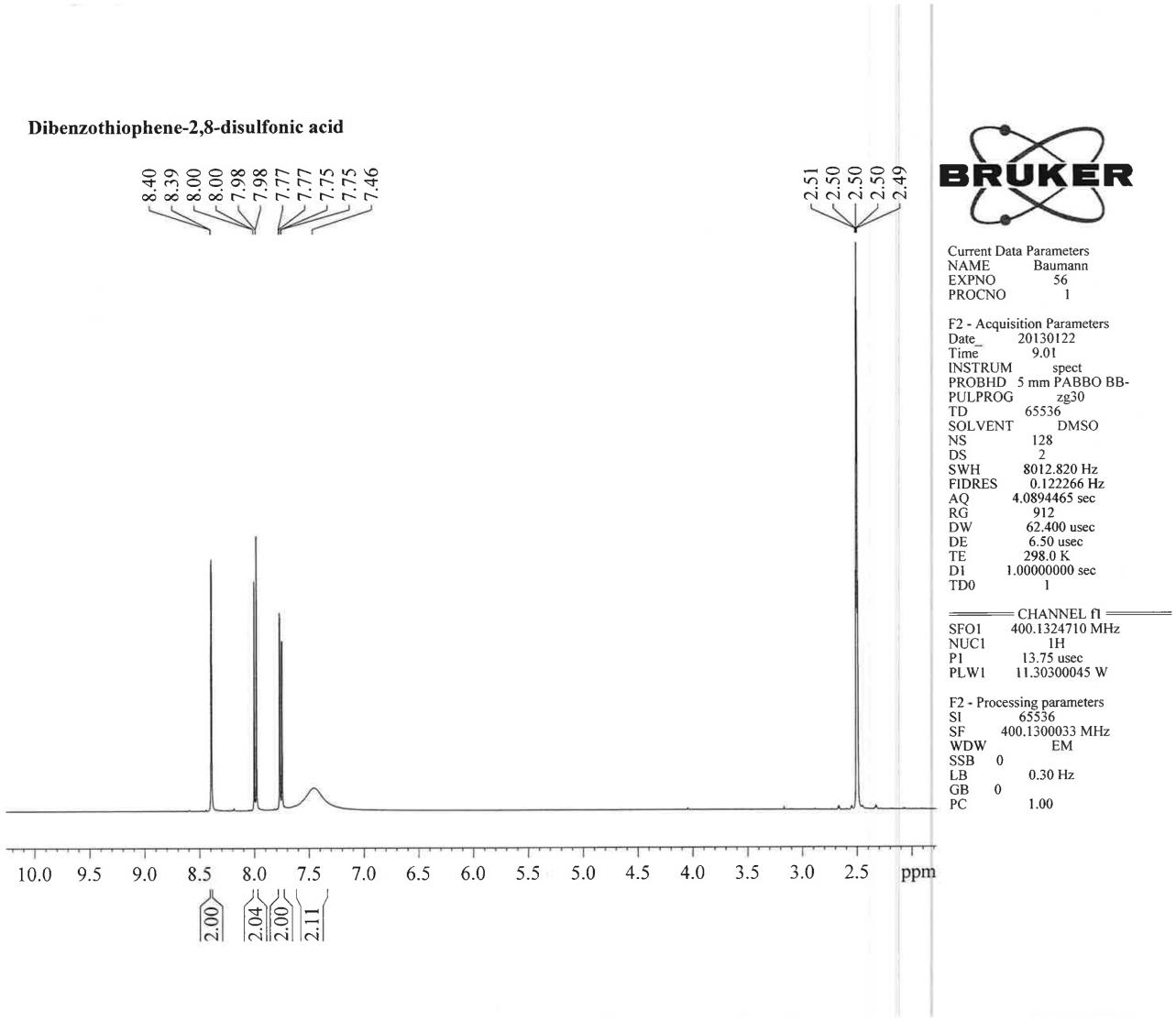
(c)

Figure S2 Fluorescence spectra of sulfoxide (a) 1 (b) 2 and (c) 3 with increasing concentration of DNA (0 (Red), 30 (Blue), 60 (Green), and100 (Black) μM). Excitation wavelength (a) 280 nm, (b) 250 nm, and (c) 320 nm.

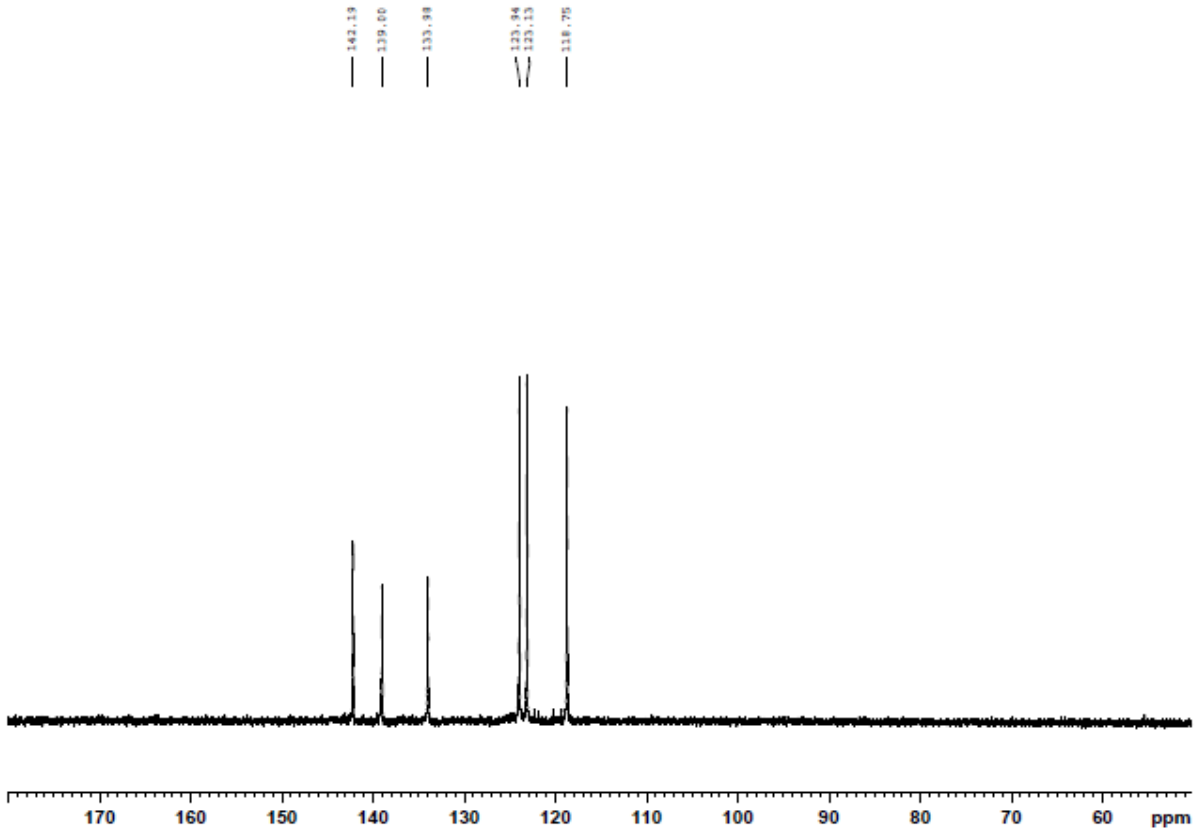
Dibenzothiophene-2,8-disulfonic acid



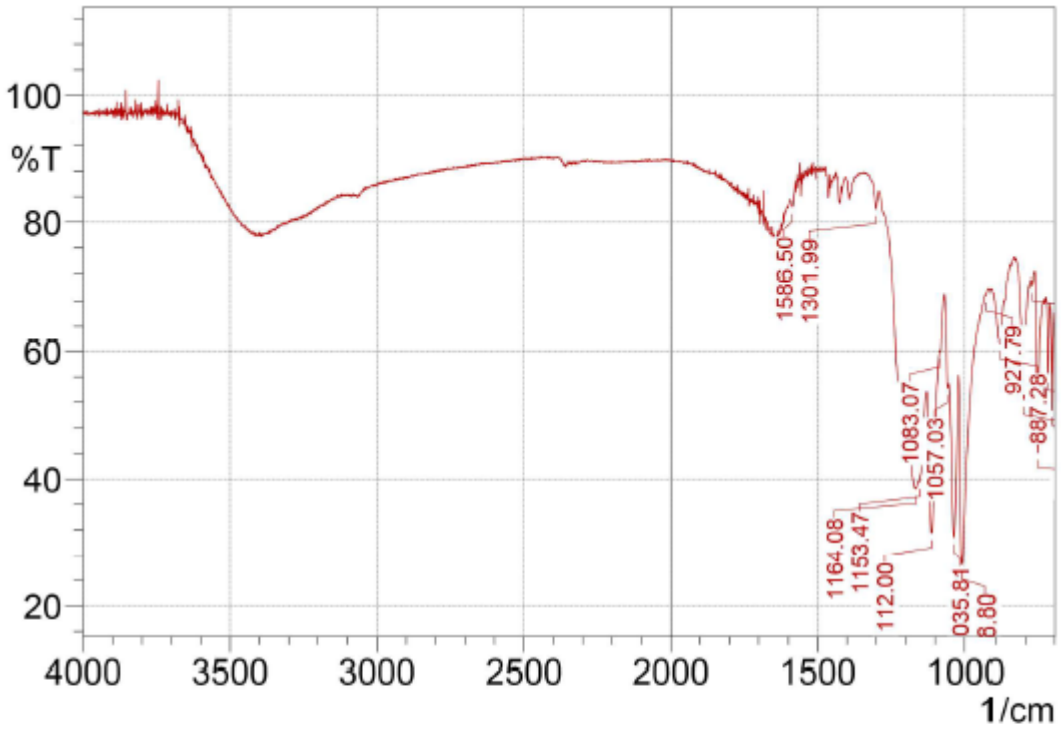
1H-NMR



C13-NMR

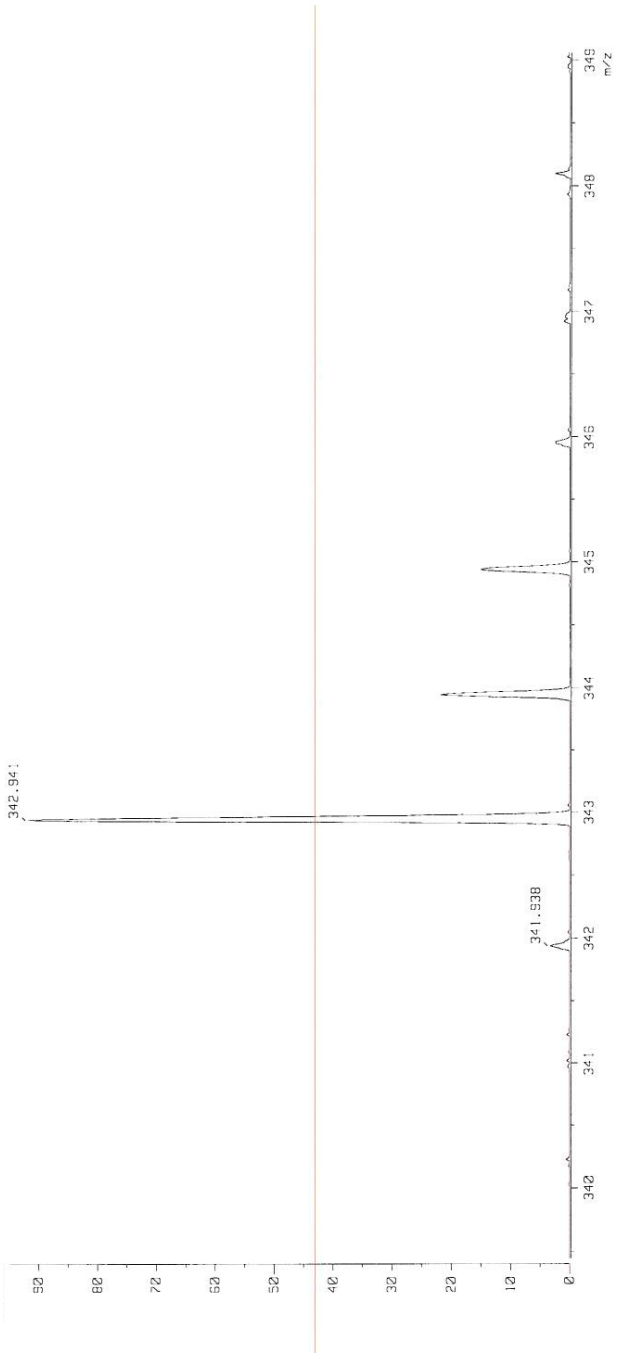


IR SPECTRUM

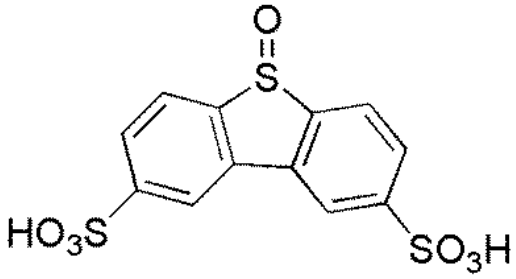


	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	708.86	50.73	16.124	713.69	701.15	2.719	0.511
2	723.33	56.172	11.997	730.08	714.65	3.011	0.434
3	759.01	44.142	26.696	767.69	740.69	5.997	1.806
4	776.37	70.336	1.214	779.27	768.66	1.56	0.037
5	806.27	52.44	19.523	832.31	788.91	8.145	2.028
6	887.28	61.124	9.744	908.5	851.6	9.909	1.582
7	927.79	68.874	0.192	928.76	922	1.074	0.004
8	1008.8	26.541	31.001	1019.41	931.65	25.895	7.752
9	1035.81	30.898	24.706	1053.17	1020.38	12.512	4.148
10	1057.03	54.268	3.611	1067.64	1054.13	3.043	0.169
11	1083.07	59.866	0.723	1084.03	1068.6	2.931	0.046
12	1112	31.511	24.309	1127.43	1084.99	14.942	4.489
13	1153.47	39.604	0.742	1154.43	1130.32	8.185	0.184
14	1164.08	38.565	0.184	1165.04	1154.43	4.312	0.009
15	1301.99	82.098	3.498	1319.35	1292.35	1.973	0.181
16	1586.5	82.398	1.832	1592.29	1577.82	1.145	0.087

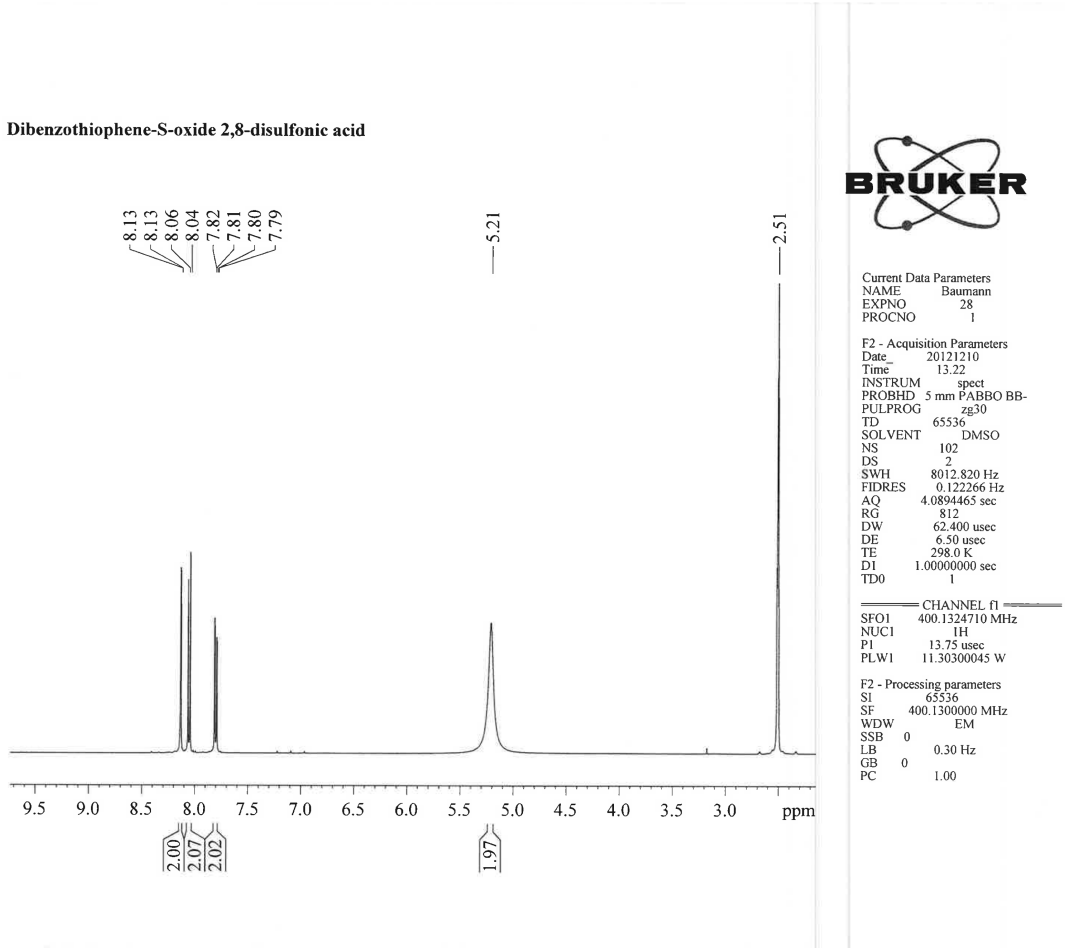
HIGH-RESOLUTION MASS SPEC



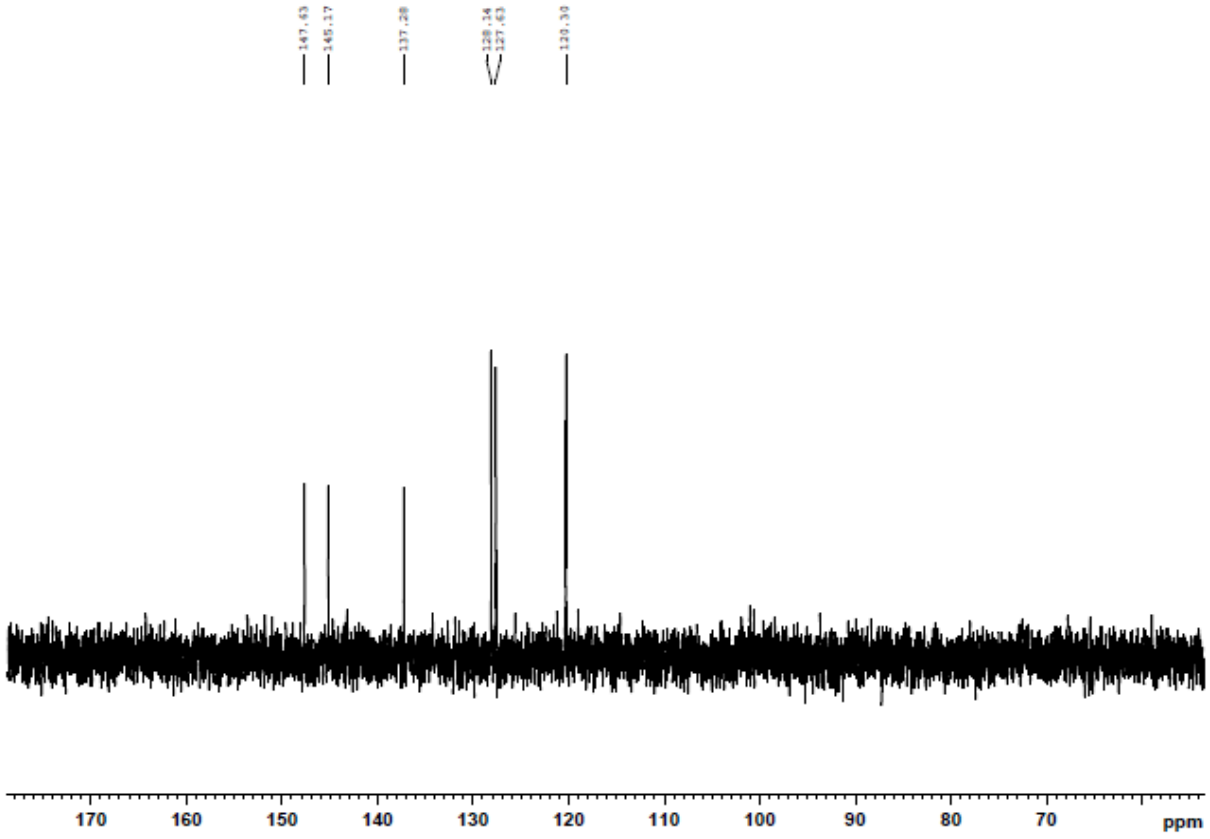
Dibenzothiophene-S-oxide-2,8-disulfonic acid



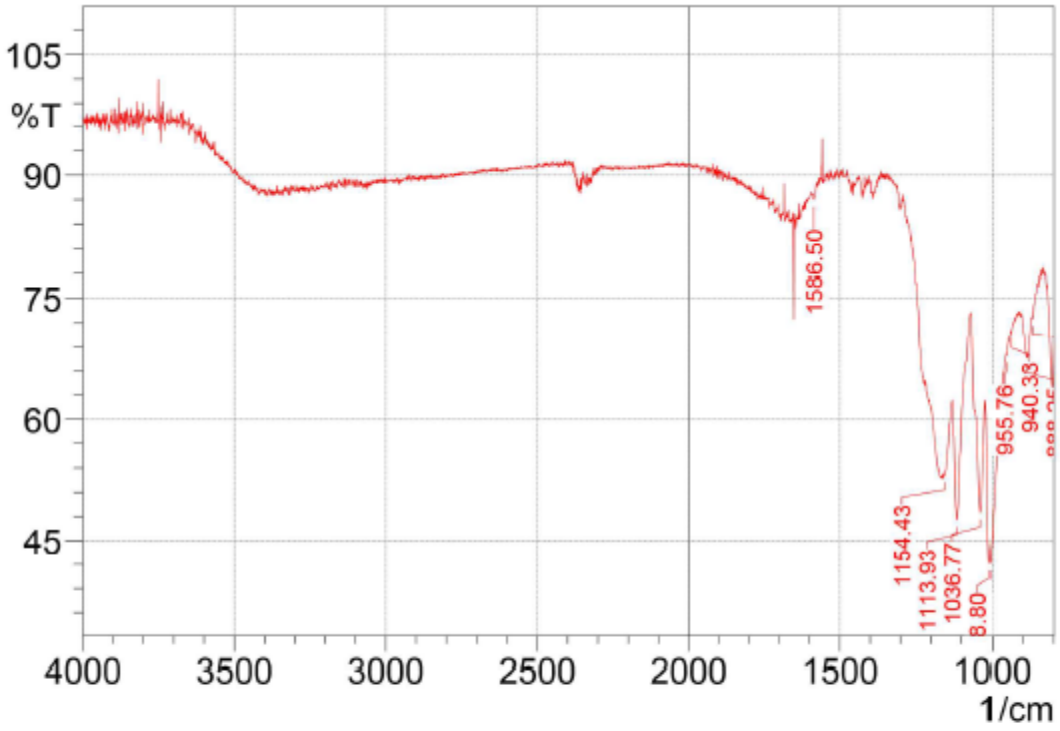
1H-NMR



C13-NMR



IR SPECTRUM



	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area
1	805.31	63.892	7.439	822.67	799.52	3.721	0.527
2	870.89	72.499	0.508	871.85	854.49	2.199	0.021
3	888.25	67.62	1.174	890.18	873.78	2.57	0.083
4	940.33	70.734	0.422	941.29	932.61	1.263	0.006
5	955.76	67.936	0.443	956.72	949.97	1.091	0.005
6	1008.8	42.114	21.215	1020.38	962.51	15.283	4.371
7	1036.77	48.529	12.997	1053.17	1021.34	8.356	1.642
8	1113.93	47.602	17.561	1129.36	1068.6	13.463	3.171
9	1154.43	53.156	1.137	1157.33	1130.32	6.622	0.189
10	1586.5	86.991	1.379	1594.22	1576.86	0.99	0.065

HIGH-RESOLUTION MASS SPEC