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Article

A Naphthalimide–Sulfonylhydrazine Conjugate as a Fluorescent Chemodosimeter for Hypochlorite

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Supplementary Material

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Table 1. Calculated excitation energy (*E*), wavelength (λ), and oscillator strength (*f*) for low-laying singlet state (S_n) of **1** and **2**.

Compound		Main orbital transition (CIC[a])	*E* (eV) [λ (nm)]	*f*
1	$S_0 \rightarrow S_1$	HOMO → LUMO (0.68894)	3.0808 [402.44]	0.0568
	$S_0 \rightarrow S_2$	HOMO-1 → LUMO (0.61028)	3.6172 [342.76]	0.0555
	$S_0 \rightarrow S_3$	HOMO-3 → LUMO (0.68524)	3.6748 [337.39]	0.0001
	$S_0 \rightarrow S_4$	HOMO → LUMO+1 (0.47616)	4.0263 [307.93]	0.3585
	$S_0 \rightarrow S_5$	HOMO-2 → LUMO (0.42519)	4.0889 [303.22]	0.1647
	$S_0 \rightarrow S_6$	HOMO-6 → LUMO (0.54185)	4.1812 [296.53]	0.0128
2	$S_0 \rightarrow S_1$	HOMO → LUMO (0.69654)	2.9771 [416.46]	0.1315
	$S_0 \rightarrow S_2$	HOMO-1 → LUMO (0.68201)	3.3435 [370.82]	0.0003
	$S_0 \rightarrow S_3$	HOMO-2 → LUMO (0.60894)	3.7187 [333.41]	0.0112
	$S_0 \rightarrow S_4$	HOMO-4 → LUMO (0.44525)	3.8193 [324.62]	0.0093
	$S_0 \rightarrow S_5$	HOMO-2 → LUMO (0.31200)	3.8759 [319.89]	0.0104
	$S_0 \rightarrow S_6$	HOMO-3 → LUMO (0.48423)	4.0390 [306.97]	0.0002

[a] CI expansion coefficients for the main transitions.

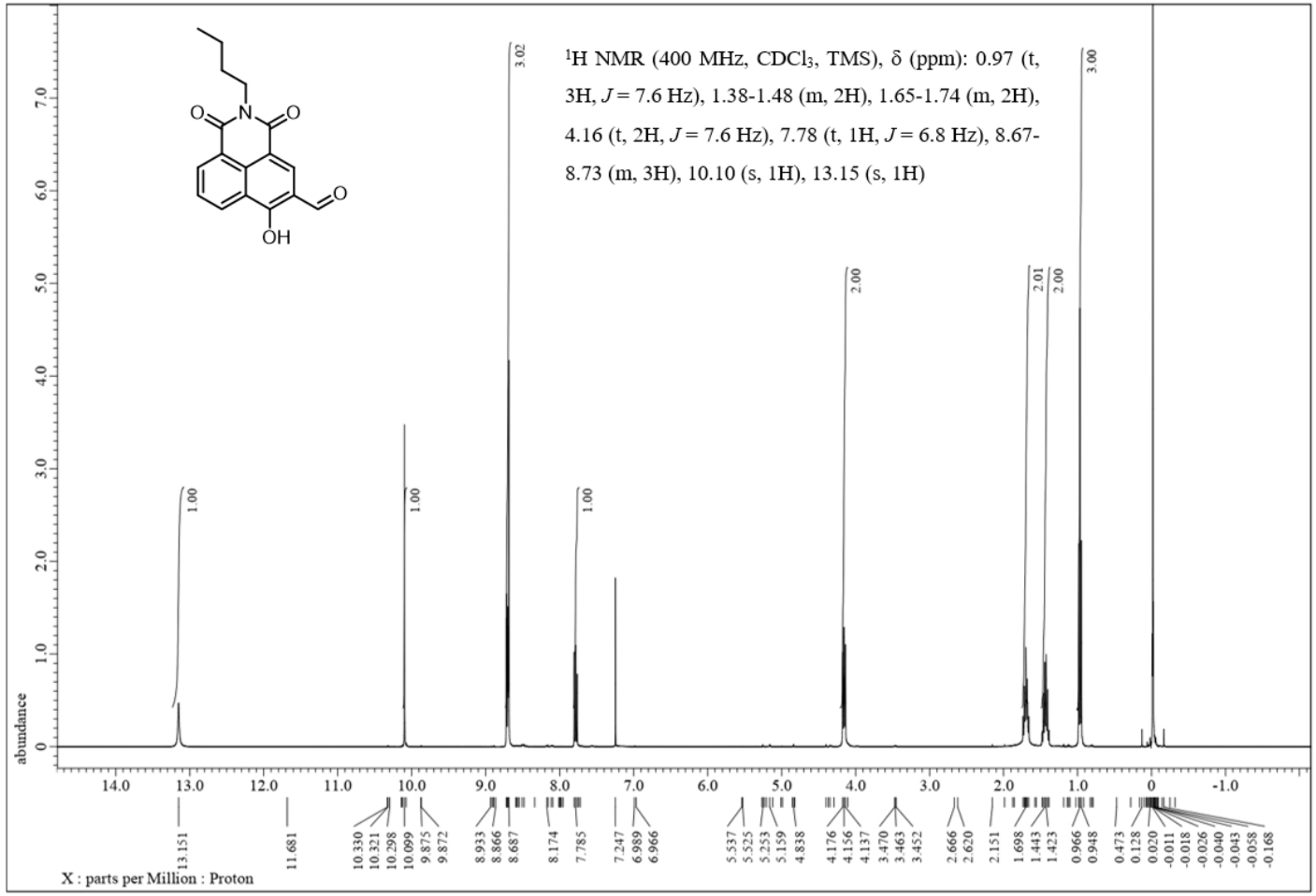


Figure S1. ^{1}H NMR chart of 3-formyl-4-hydroxy-*N*-butyl-1,8-naphthalimide (**3**) (10 mM, $CDCl_3$, 400 MHz).

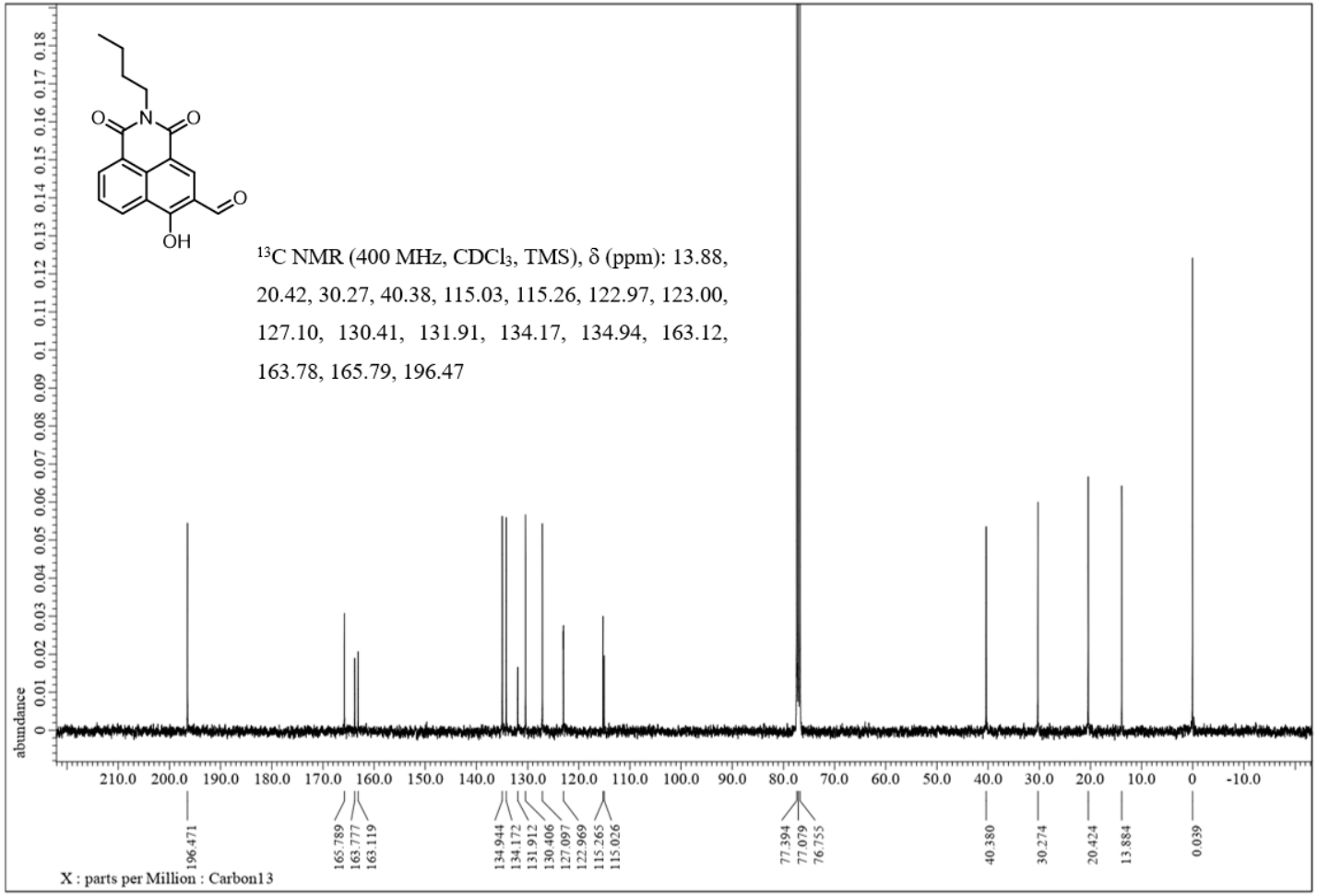


Figure S2. ^{13}C NMR chart of 3-formyl-4-hydroxy-*N*-butyl-1,8-naphthalimide (**3**) (30 mM, CDCl$_3$, 400 MHz).

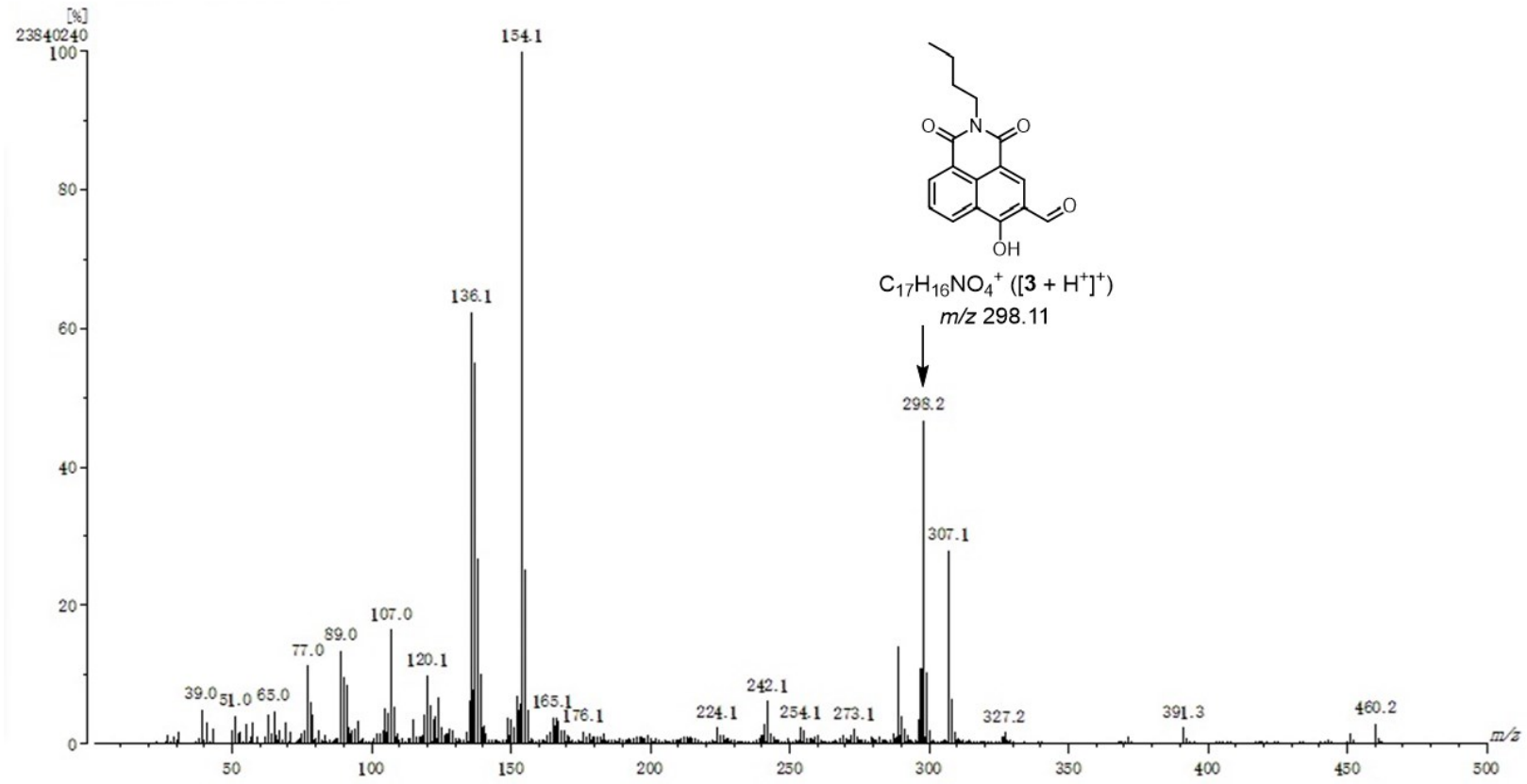


Figure S3. FAB(+)-MS chart of 3-formyl-4-hydroxy-*N*-butyl-1,8-naphthalimide (**3**).

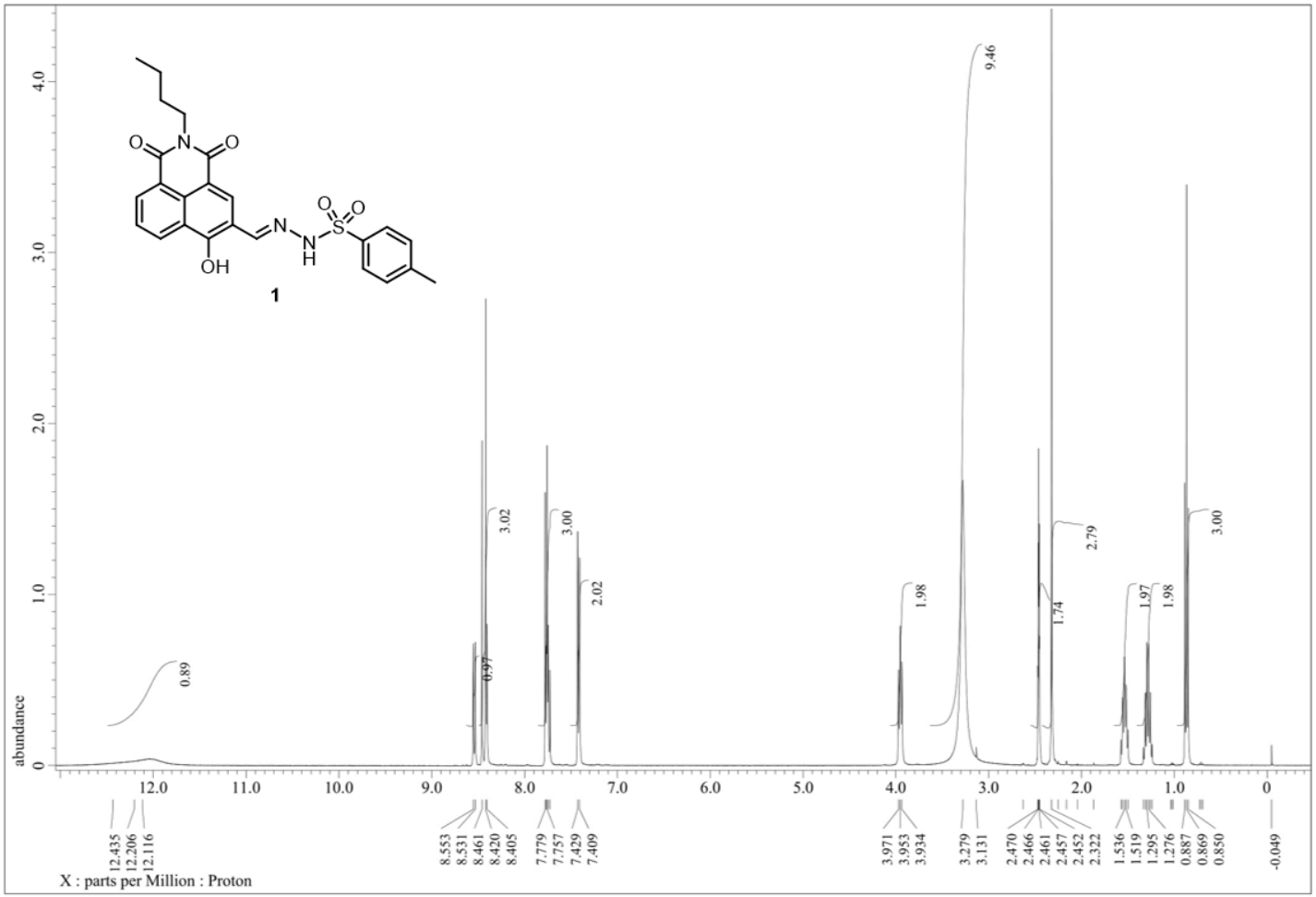


Figure S4. ^{1}H NMR chart of **1** (10 mM, DMSO–d_6, 400 MHz).

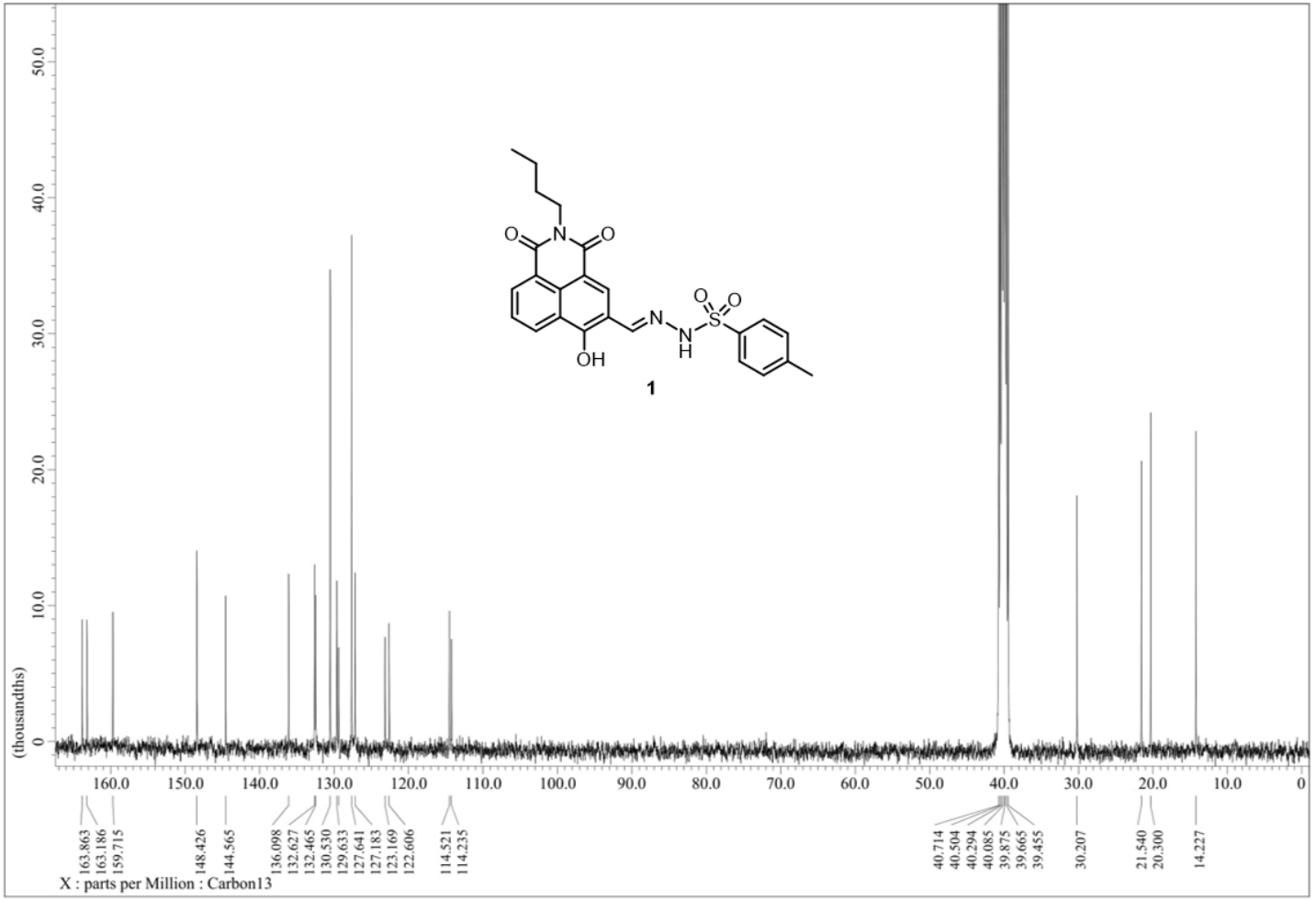


Figure S5. ^{13}C NMR chart of **1** (30 mM, DMSO–d_6, 100 MHz).

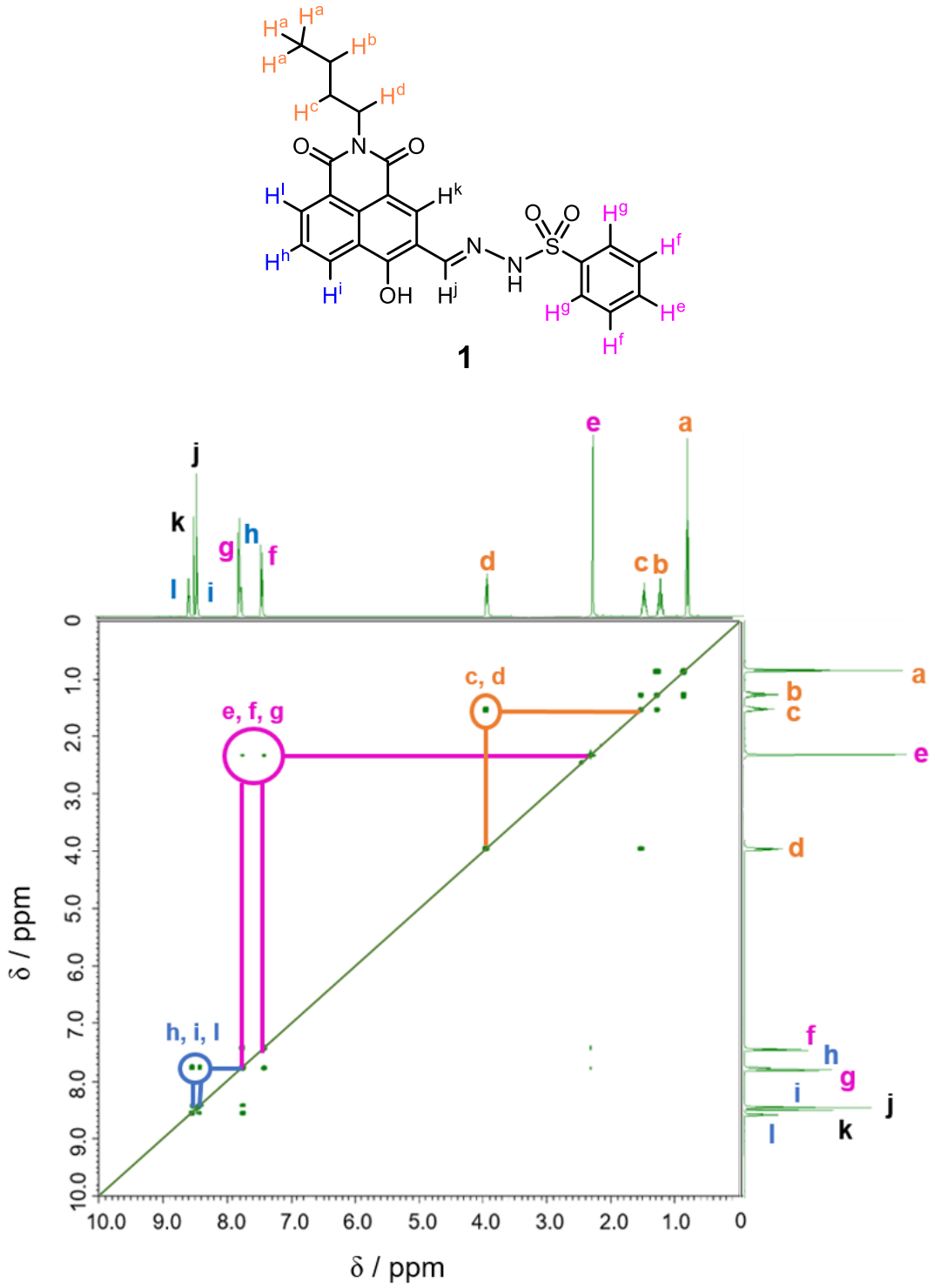


Figure S6. ^{1}H–^{1}H COSY chart of **1** (30 mM, DMSO–d_6, 400 MHz). Colored circles indicate the observed cross peaks. The texts next to the circle mean the coupling protons.

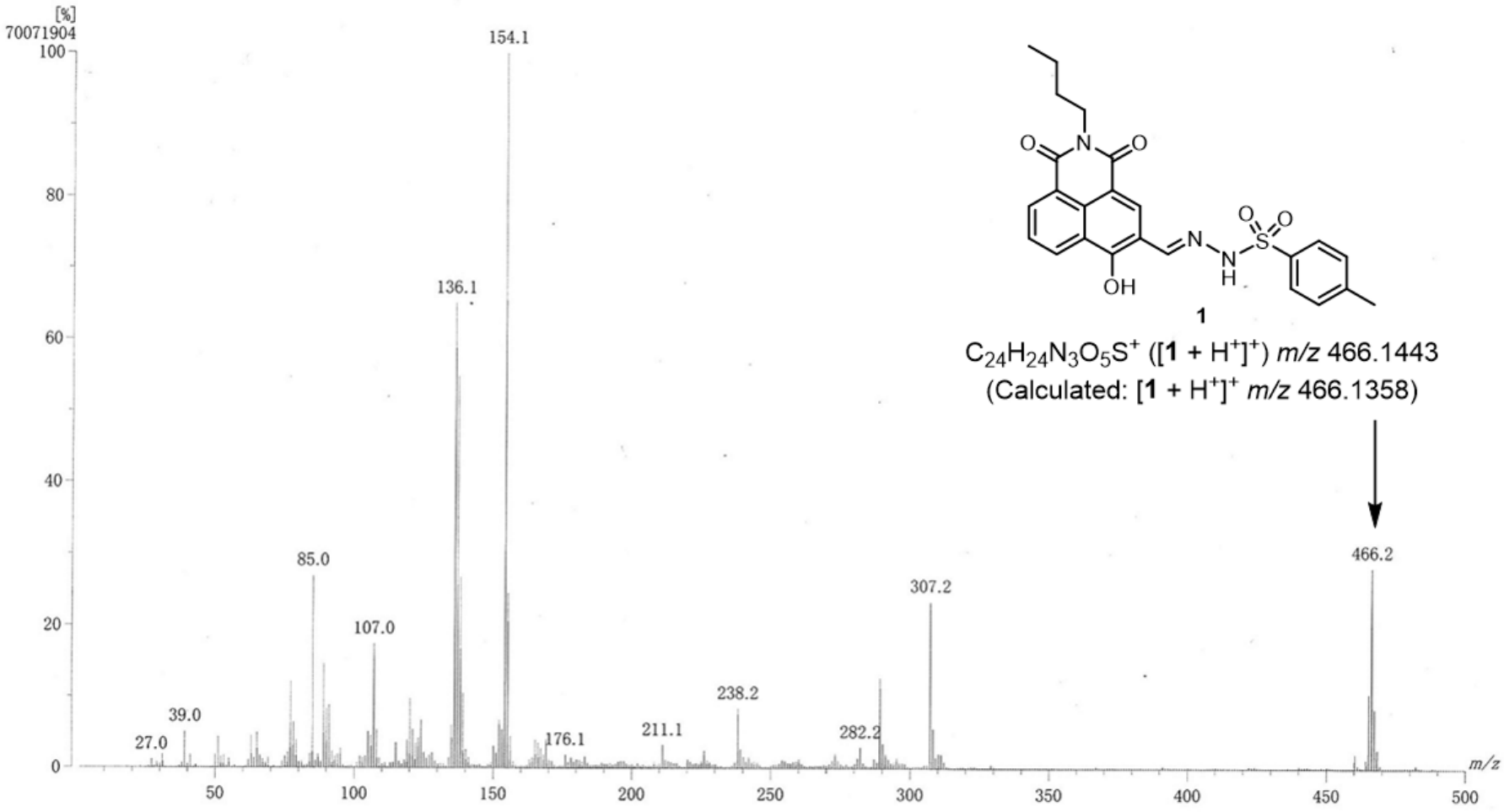


Figure S7. FAB(+)-MS chart of **1**.

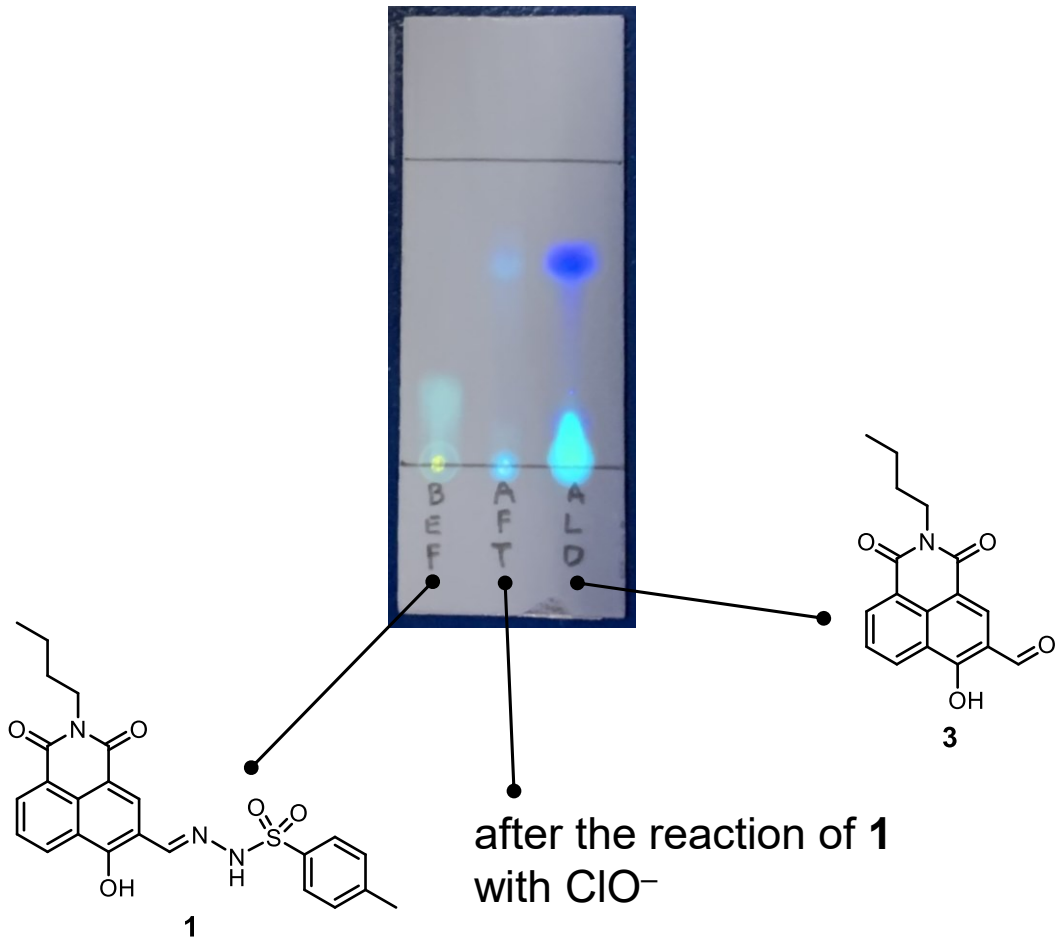


Figure S8. TLC results of (left) **1**, (center) the sample after the reaction of **1** with ClO^-, and (right) **3**, developed in a *n*-hexane/EtOAc (1/1 v/v) mixture under irradiation of 254 nm light.

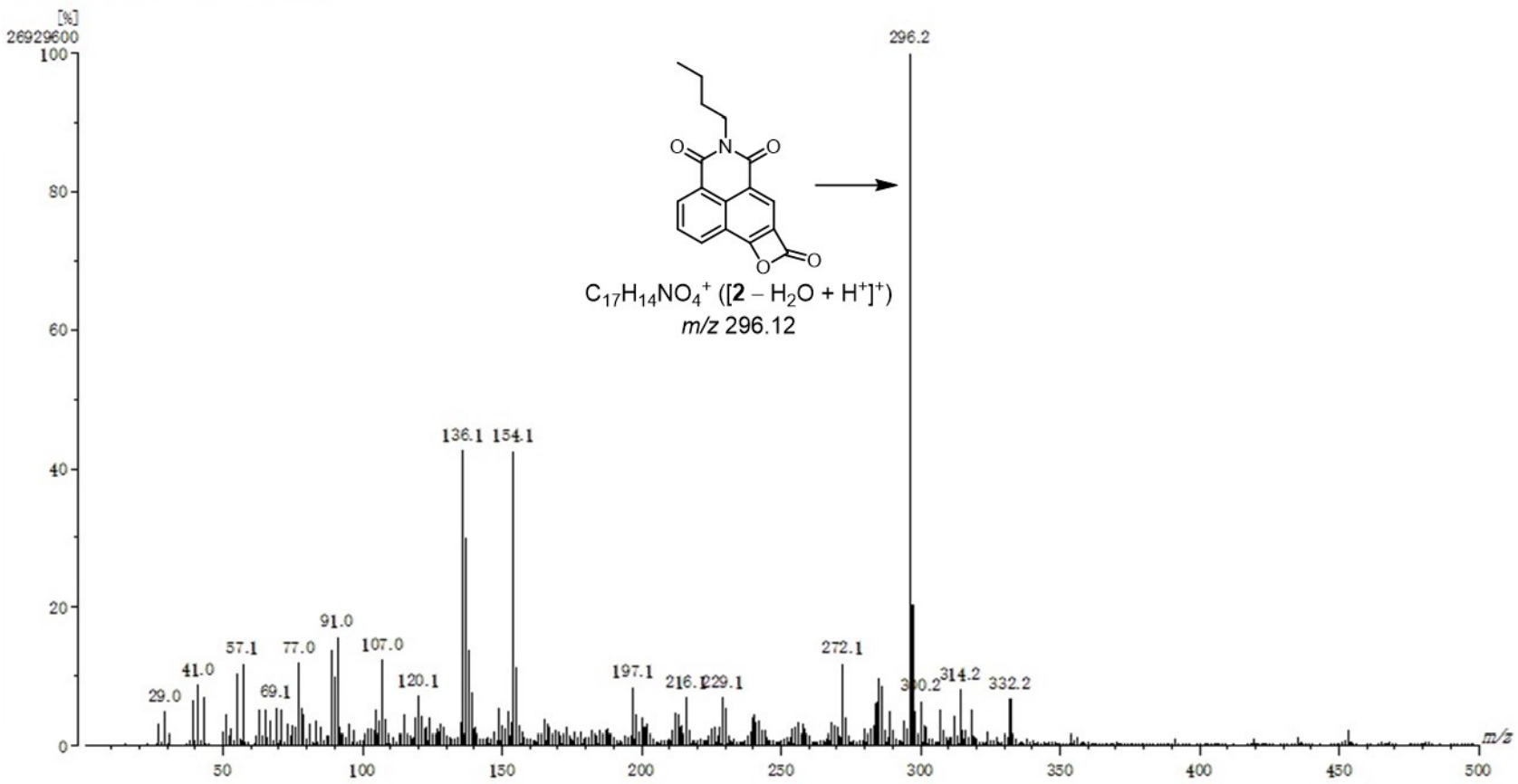


Figure S9. FAB(+)-MS chart of the crude product obtained by the reaction of **1** with ClO^-.

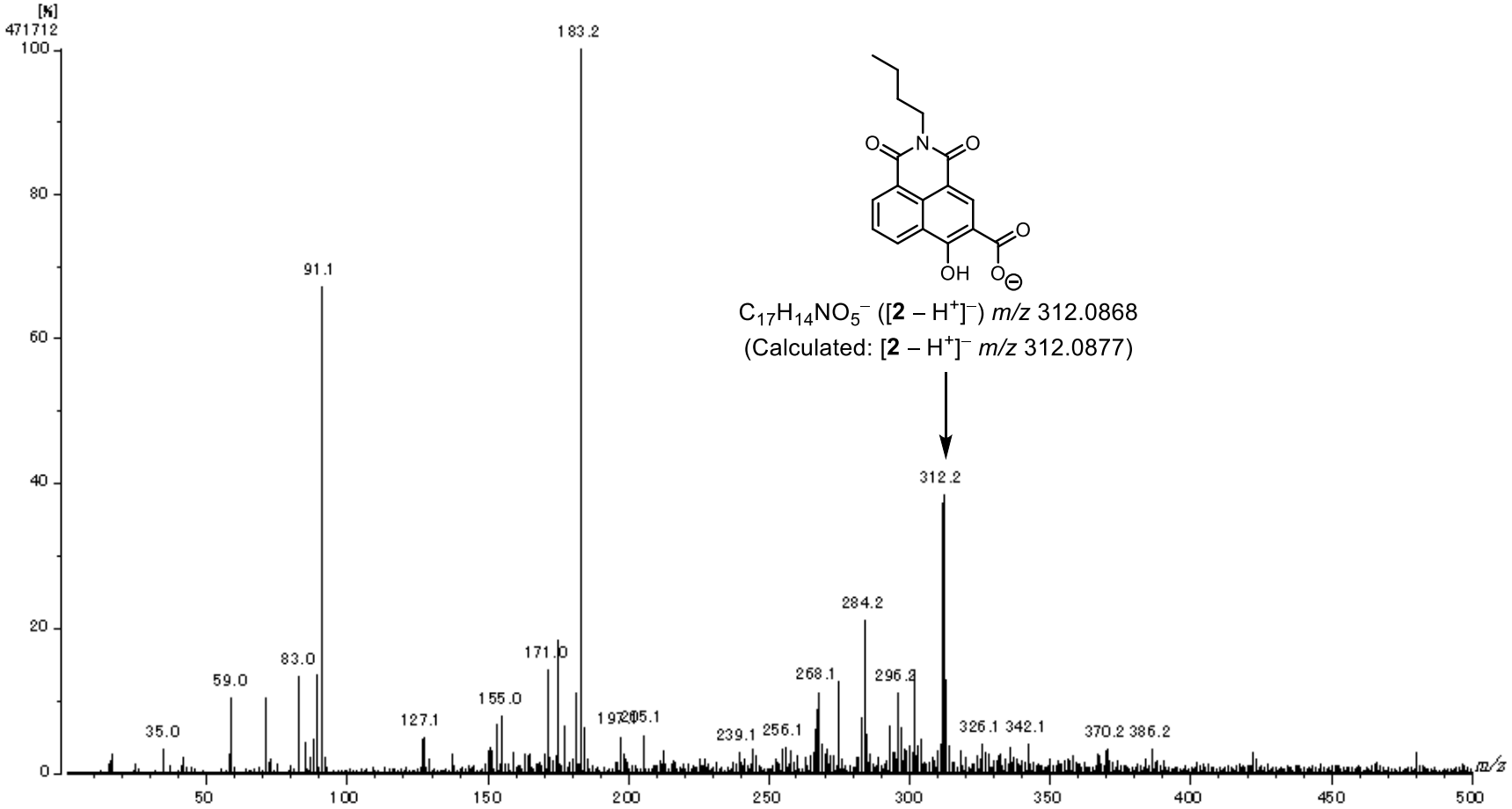
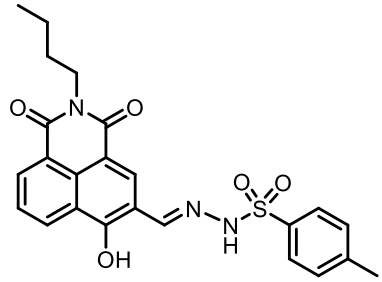
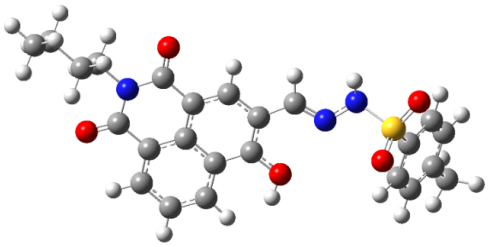


Figure S10. FAB(–)-MS chart of the crude product obtained by the reaction of **1** with ClO^-.

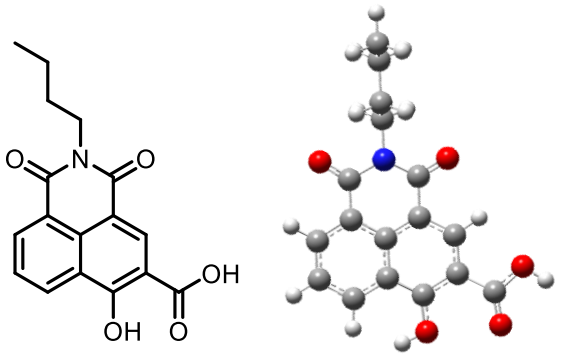
Cartesian Coordinates (in Å) of **1** (DFT/B3LYP/6–31G+(d))





C	-3.25411	2.605044	-0.88675	C	6.90641	1.531296	-0.14101
C	-2.05898	2.943694	-1.51833	C	6.148023	2.233449	0.795648
C	-0.93559	2.127629	-1.37515	C	4.964348	1.683854	1.287869
C	-0.99194	0.962263	-0.59491	C	4.539053	0.431932	0.84343
C	-2.20598	0.618915	0.04204	C	6.604517	3.576983	1.27266
C	-3.33846	1.438922	-0.11468	H	-4.1345	3.255625	-0.99476
C	0.126593	0.131163	-0.4265	H	-2.00076	3.855607	-2.13073
C	0.048192	-1.01681	0.363675	H	0.003396	2.400626	-1.87892
C	-1.14898	-1.35173	0.993463	H	-1.20405	-2.25243	1.622523
C	-2.28271	-0.5453	0.828239	H	-5.52989	-1.95417	-0.29607
C	-3.57422	-0.87807	1.53568	H	-6.35033	-1.63537	1.294715
N	-4.74684	-0.35998	0.826877	H	-7.24499	0.516243	0.401762
C	-4.61714	1.082117	0.604185	H	-6.42454	0.197445	-1.18903
C	-5.87819	-1.16262	0.404575	H	-7.73669	-1.9099	-1.4431
C	-6.89669	-0.27531	-0.29889	H	-8.55714	-1.59111	0.147693
C	-8.08499	-1.11835	-0.74245	H	-9.9719	-0.84714	-1.77006
C	-9.1035	-0.23104	-1.44591	H	-9.45179	0.560505	-0.74526
O	-5.43996	1.893646	0.955844	H	-8.63135	0.241707	-2.33605
O	-3.63387	-1.50092	2.569007	H	1.159207	1.268774	-1.53751
O	1.294353	0.446457	-1.0372	H	1.062825	-2.70131	1.139071
C	1.123547	-1.79643	0.516583	H	3.237638	-3.12207	0.679495
N	2.206526	-1.49463	-0.05235	H	7.07911	-0.27429	-1.32428
N	3.293945	-2.28299	0.102279	H	7.83992	1.96478	-0.52915
S	4.751668	-1.87677	-0.66352	H	4.366251	2.237649	2.02651
C	5.297441	-0.27022	-0.09323	H	3.605581	-0.00158	1.231629
O	4.549681	-1.83693	-2.09883	H	7.561196	3.844176	0.770524
O	5.757615	-2.87135	-0.34512	H	5.831751	4.339459	1.027237
C	6.481085	0.279434	-0.58553	H	6.759922	3.546227	2.374328

Cartesian Coordinates (in Å) of **2** (DFT/B3LYP/6–31G+(d))



C	-0.72245	2.754853	0.405555	O	3.994438	1.395424	-0.72296
C	0.407753	3.470125	0.014469	C	4.110721	-1.32547	-0.41461
C	1.606645	2.801542	-0.23876	O	5.093187	-0.70987	-0.75381
C	1.691863	1.40734	-0.10102	O	4.171562	-2.65389	-0.26677
C	0.543513	0.683505	0.292487	H	-1.66284	3.286518	0.612924
C	-0.66537	1.360978	0.535597	H	0.355036	4.563408	-0.09487
C	2.888404	0.713229	-0.33913	H	2.493647	3.373137	-0.54942
C	2.950522	-0.67263	-0.18453	H	1.873414	-2.47495	0.336062
C	1.817865	-1.384	0.206721	H	-2.54108	-1.75195	-1.23632
C	0.608618	-0.71456	0.43592	H	-3.3172	-2.30332	0.312551
C	-0.6147	-1.47012	0.896178	H	-4.44415	-0.0881	0.536065
N	-1.85982	-0.80206	0.509876	H	-3.66804	0.463271	-1.01281
C	-1.87322	0.58028	0.99465	H	-4.79052	-1.39867	-2.23772
C	-2.92984	-1.42251	-0.24682	H	-5.56664	-1.95003	-0.68885
C	-4.05539	-0.41754	-0.45343	H	-7.12617	-0.5405	-2.03567
C	-5.17928	-1.06923	-1.24823	H	-6.6936	0.265191	-0.46534
C	-6.30484	-0.06425	-1.45483	H	-5.91748	0.816559	-2.01421
O	-2.75109	1.04295	1.683518	H	3.762498	2.337813	-0.77672
O	-0.57165	-2.50786	1.513028	H	5.085356	-2.90728	-0.48021