Supporting Information

3-Morpholino-7-[*N*-methyl-*N*-(4′-carboxyphenyl)amino]phenothiazinium Chloride

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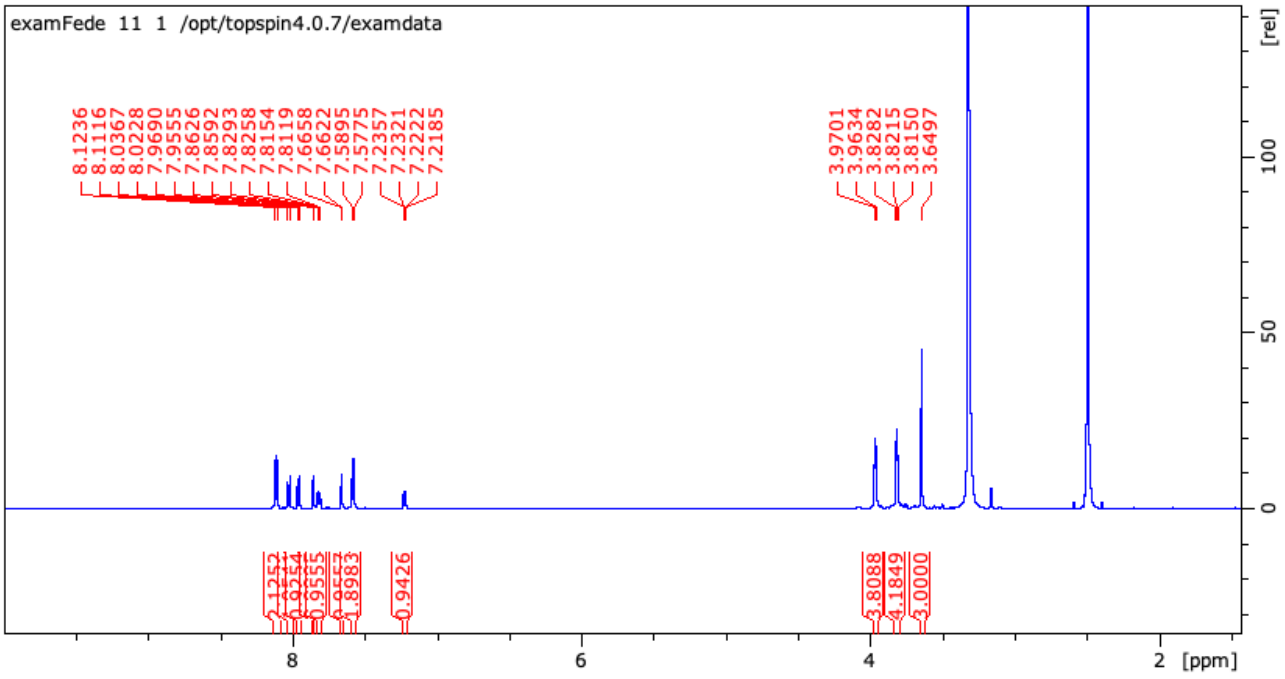

Figure S1. ^{1}H NMR of **3** in DMSO-d$_6$

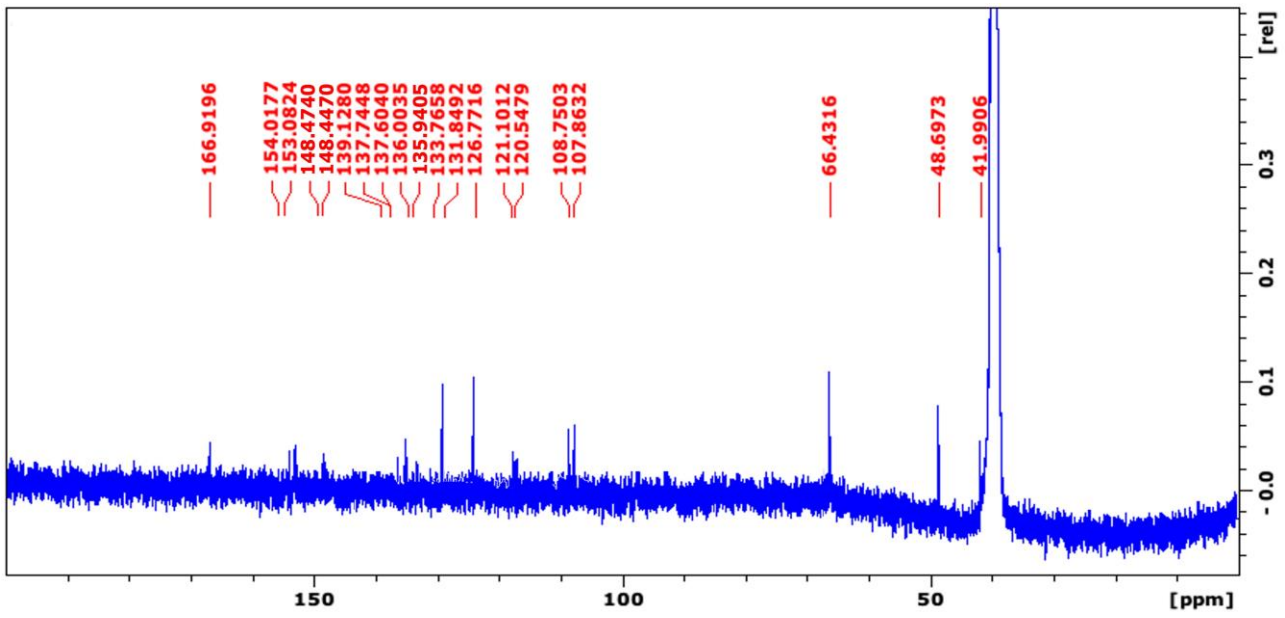

Figure S2. ^{13}C NMR of **3** in DMSO-d$_6$

Optimized cartesian coordinates (in Angstroms) of 3

- **Conformer *a***

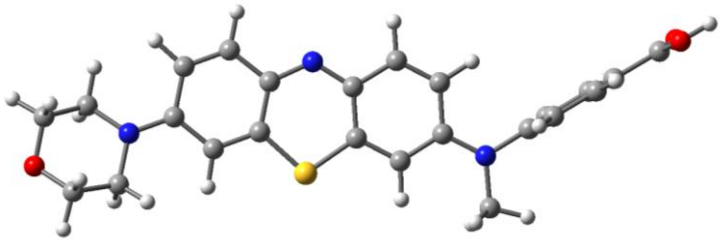

Figure S3. Geometry optimization of conformer *a* of compound **3** (WB97XD functional, 6-31G+(d,p) basis set) in the *vacuum*.

```
Stoichiometry    C24H22N3O3S(1+)
Zero-point correction=                           0.427558 (Hartree/Particle)
 Thermal correction to Energy=                    0.453710
 Thermal correction to Enthalpy=                  0.454654
 Thermal correction to Gibbs Free Energy=         0.367030
 Sum of electronic and zero-point Energies=          -1714.901005
 Sum of electronic and thermal Energies=             -1714.874852
 Sum of electronic and thermal Enthalpies=           -1714.873908
 Sum of electronic and thermal Free Energies=        -1714.961533
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.329434	0.726987	-0.055623
2	6	0	-1.060805	1.350497	-0.105751
3	6	0	0.095324	0.591804	-0.072346
4	6	0	0.043787	-0.839936	0.009450
5	6	0	-1.252835	-1.444624	0.059356
6	6	0	-2.391553	-0.706737	0.029785
7	6	0	2.356980	-1.230364	-0.004278
8	6	0	2.781545	0.135427	-0.073567
9	6	0	4.122894	0.471093	-0.112759
10	1	0	4.389931	1.515076	-0.208984
11	6	0	5.129147	-0.525237	-0.076853
12	6	0	4.702597	-1.898449	-0.023298
13	6	0	3.384262	-2.223165	0.017292
14	1	0	-0.985421	2.429018	-0.169556
15	1	0	-1.287086	-2.526768	0.121784
16	1	0	-3.356993	-1.195058	0.069678
17	1	0	5.428834	-2.697524	0.018046
18	1	0	3.065999	-3.258245	0.076811
19	7	0	1.095614	-1.652332	0.036045
20	16	0	1.617713	1.421905	-0.130982
21	7	0	-3.462812	1.458256	-0.085289
22	6	0	-3.433455	2.917202	-0.168850
23	1	0	-4.459990	3.279223	-0.175851
24	1	0	-2.917907	3.349422	0.695132
25	1	0	-2.942275	3.247644	-1.090128
26	6	0	-4.757522	0.833778	-0.043143
27	6	0	-5.376121	0.455702	-1.233188

28	6	0	-5.387734	0.645489	1.184460
29	6	0	-6.638989	-0.121955	-1.191095
30	1	0	-4.867838	0.611729	-2.179317
31	6	0	-6.652887	0.068483	1.223555
32	1	0	-4.887686	0.946728	2.099363
33	6	0	-7.277427	-0.316014	0.035334
34	1	0	-7.144766	-0.427331	-2.100710
35	1	0	-7.154505	-0.083938	2.172028
36	6	0	-8.634833	-0.940709	0.021087
37	8	0	-9.205237	-1.293011	-0.984331
38	8	0	-9.161053	-1.072908	1.248813
39	1	0	-10.033738	-1.479314	1.149992
40	6	0	7.492938	-1.129470	-0.518714
41	6	0	6.895485	1.193062	-0.050148
42	6	0	8.792373	-0.889030	0.238355
43	1	0	7.659982	-0.970099	-1.592477
44	1	0	7.186796	-2.162506	-0.373401
45	6	0	8.237872	1.311614	0.668408
46	1	0	6.979684	1.571910	-1.078005
47	1	0	6.178109	1.805833	0.495834
48	1	0	9.583445	-1.508766	-0.187242
49	1	0	8.665443	-1.154817	1.299369
50	1	0	8.615088	2.330527	0.565055
51	1	0	8.101701	1.092455	1.738978
52	7	0	6.444202	-0.201235	-0.072699
53	8	0	9.205174	0.452018	0.117780

Rotational constants (GHZ): 0.6179681 0.0364697
0.0351685

- **Conformer *b***

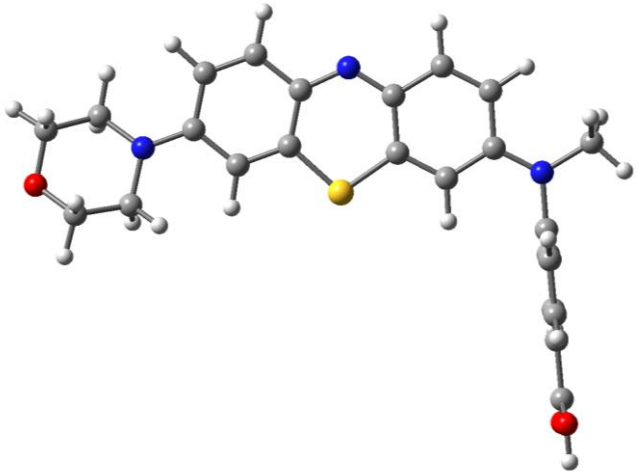

Figure S4. Geometry optimization conformer *b* of compound **3** (WB97XD functional, 6-31G+(d,p) basis set) in the *vacuum*.

```
Stoichiometry    C24H22N3O3S(1+)
Zero-point correction=                           0.427622 (Hartree/Particle)
 Thermal correction to Energy=                    0.453750
 Thermal correction to Enthalpy=                  0.454694
 Thermal correction to Gibbs Free Energy=         0.367503
 Sum of electronic and zero-point Energies=          -1714.900941
 Sum of electronic and thermal Energies=             -1714.874813
 Sum of electronic and thermal Enthalpies=           -1714.873869
 Sum of electronic and thermal Free Energies=        -1714.961060
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.654244	-2.131699	0.078106
2	6	0	-1.777489	-1.020706	0.053268
3	6	0	-0.410226	-1.207115	0.028103
4	6	0	0.162365	-2.523730	0.024862
5	6	0	-0.743931	-3.628372	0.053979
6	6	0	-2.092000	-3.452711	0.080888
7	6	0	2.415933	-1.878536	-0.039786
8	6	0	2.209104	-0.460565	-0.031312
9	6	0	3.274278	0.420606	-0.067849
10	1	0	3.063161	1.481031	-0.104470
11	6	0	4.611811	-0.045279	-0.107468
12	6	0	4.819115	-1.469391	-0.130424
13	6	0	3.770543	-2.331495	-0.091370
14	1	0	-2.187485	-0.017483	0.058092
15	1	0	-0.307640	-4.621264	0.050511
16	1	0	-2.739956	-4.319037	0.098555
17	1	0	5.819102	-1.878491	-0.146948
18	1	0	3.930020	-3.404252	-0.089768
19	7	0	1.462019	-2.804636	-0.009449
20	16	0	0.605147	0.201951	0.004778
21	7	0	-3.993089	-1.959017	0.103181
22	6	0	6.986960	0.450339	-0.618894

23	6	0	5.468982	2.263409	-0.003977
24	6	0	8.084851	1.188936	0.135250
25	1	0	7.028910	0.719704	-1.682797
26	1	0	7.159587	-0.619594	-0.533626
27	6	0	6.656378	2.912543	0.703954
28	1	0	5.345047	2.690814	-1.008397
29	1	0	4.578881	2.481090	0.586239
30	1	0	9.048803	0.991691	-0.336873
31	1	0	8.123812	0.842401	1.179715
32	1	0	6.555794	3.998303	0.657534
33	1	0	6.666938	2.603847	1.760967
34	7	0	5.658633	0.813269	-0.104577
35	8	0	7.877857	2.581177	0.090838
36	6	0	-4.568737	-0.644386	0.042650
37	6	0	-4.738742	-0.025214	-1.194748
38	6	0	-4.972208	-0.017224	1.219021
39	6	0	-5.313072	1.238343	-1.252047
40	1	0	-4.421345	-0.533091	-2.099878
41	6	0	-5.552475	1.245741	1.158293
42	1	0	-4.830245	-0.516395	2.172220
43	6	0	-5.719534	1.874414	-0.077260
44	1	0	-5.458012	1.743960	-2.200661
45	1	0	-5.873282	1.743885	2.065767
46	6	0	-6.331188	3.232189	-0.197212
47	8	0	-6.468187	3.821447	-1.243511
48	8	0	-6.714927	3.737766	0.985617
49	1	0	-7.102308	4.608743	0.818822
50	6	0	-4.922114	-3.088971	0.161037
51	1	0	-4.838854	-3.714820	-0.733187
52	1	0	-4.745964	-3.698131	1.052556
53	1	0	-5.934357	-2.691312	0.209141

Rotational constants (GHZ): 0.2342580 0.0503032
0.0424783