Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Stimuli-responsive phenothiazine-based donor-acceptor isomers: AIE, mechanochromism and polymorphism

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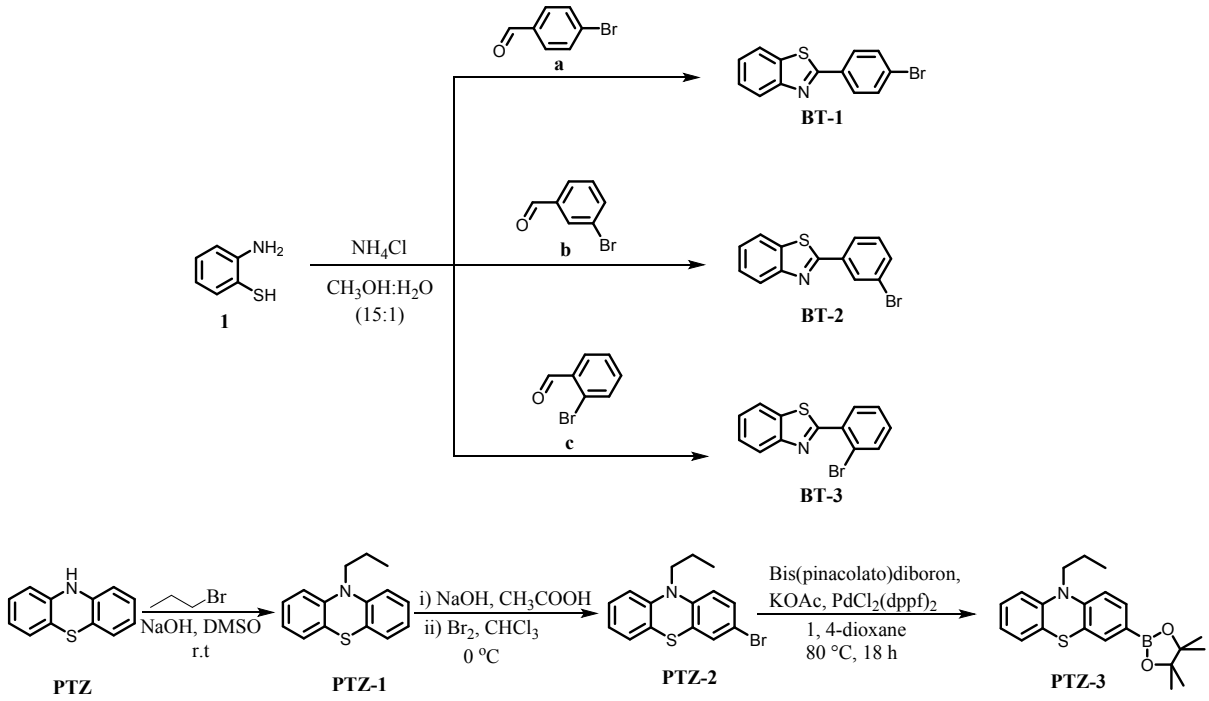
Experimental Section



Scheme S1. Synthetic routes to intermediates.

Solvatochromism

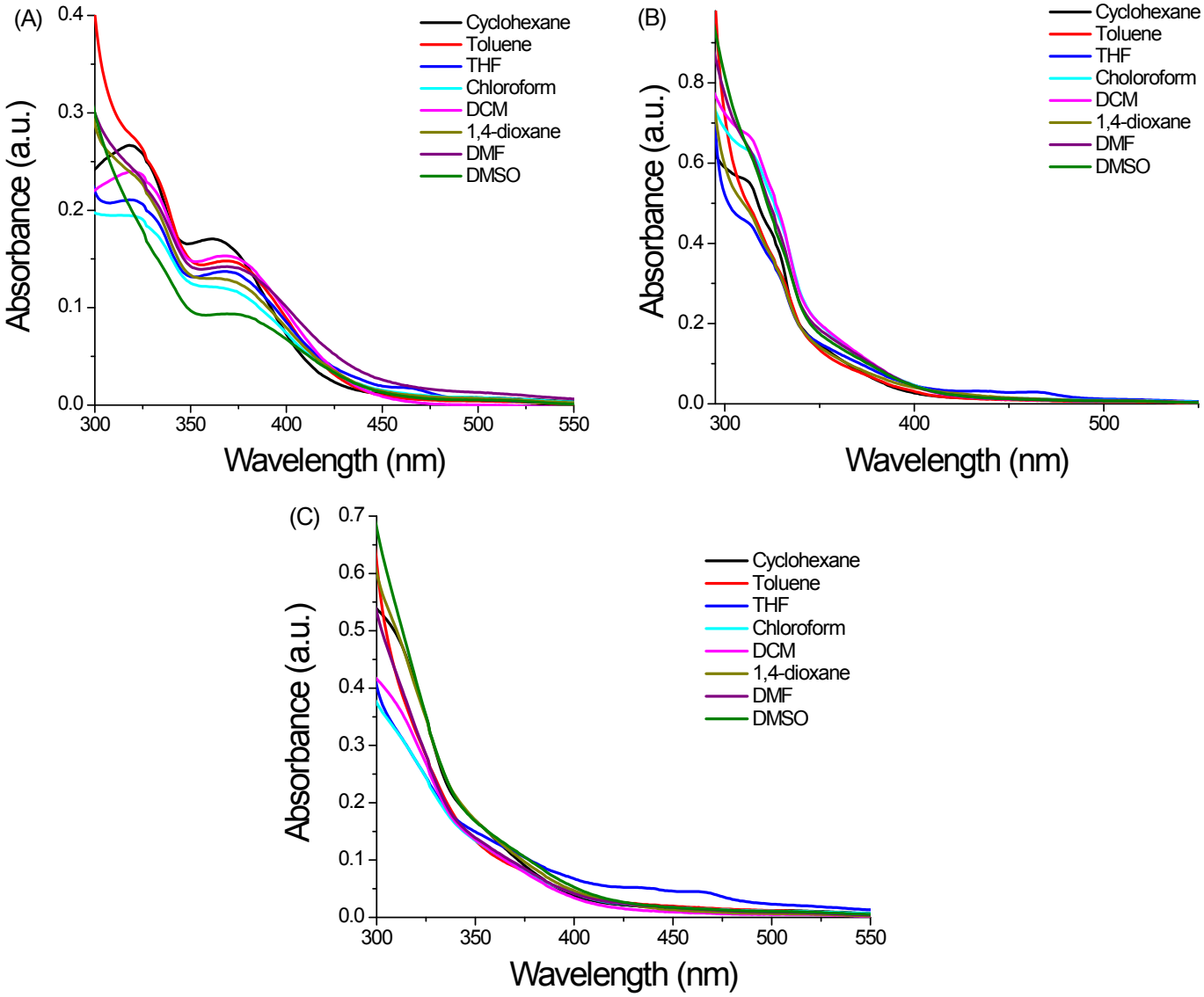


Figure S1. Electronic absorption spectra of (A) ***p*-PTZ**, (B) ***m*-PTZ** and (C) ***o*-PTZ** in solvents of various polarity.

Table S1. Quantum yield of ***p*-PTZ**, ***m*-PTZ** and ***o*-PTZ** in various solvents.

Solvents	ϕ_f[a]		
	***p*-PTZ**	***m*-PTZ**	***o*-PTZ**
Cyclohexane	0.36	0.11	0.09
Toluene	0.50	0.13	0.12
THF	0.43	0.04	0.06
Chloroform	0.68	0.05	0.12
DCM	0.51	0.03	0.12
1,4-dioxane	0.53	0.08	0.14
DMF	0.14	0.004	0.03
DMSO	0.26	0.004	0.02

[a] Fluorescence quantum yields recorded using quinine sulphate as a standard in 0.5 M H_2SO_4 solution.

Aggregation Induced Emission

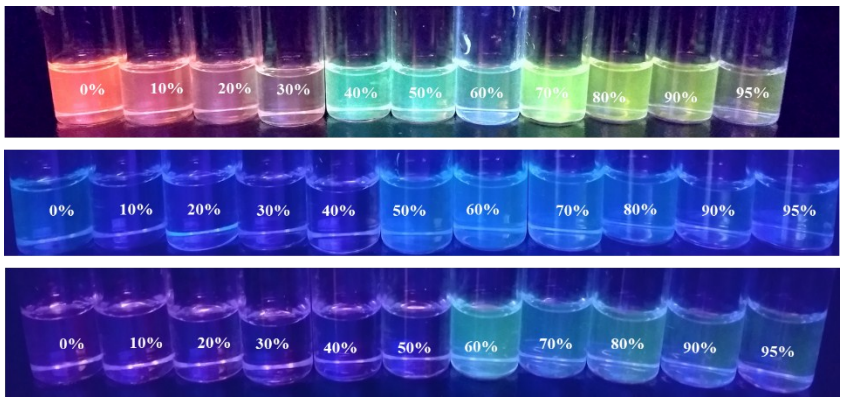


Figure S2. Photographs of ***p*-PTZ**, ***m*-PTZ** and ***o*-PTZ** in THF–water mixtures with different water fractions (10 μM) under 365 nm UV illumination.

Single Crystal X-ray Analysis

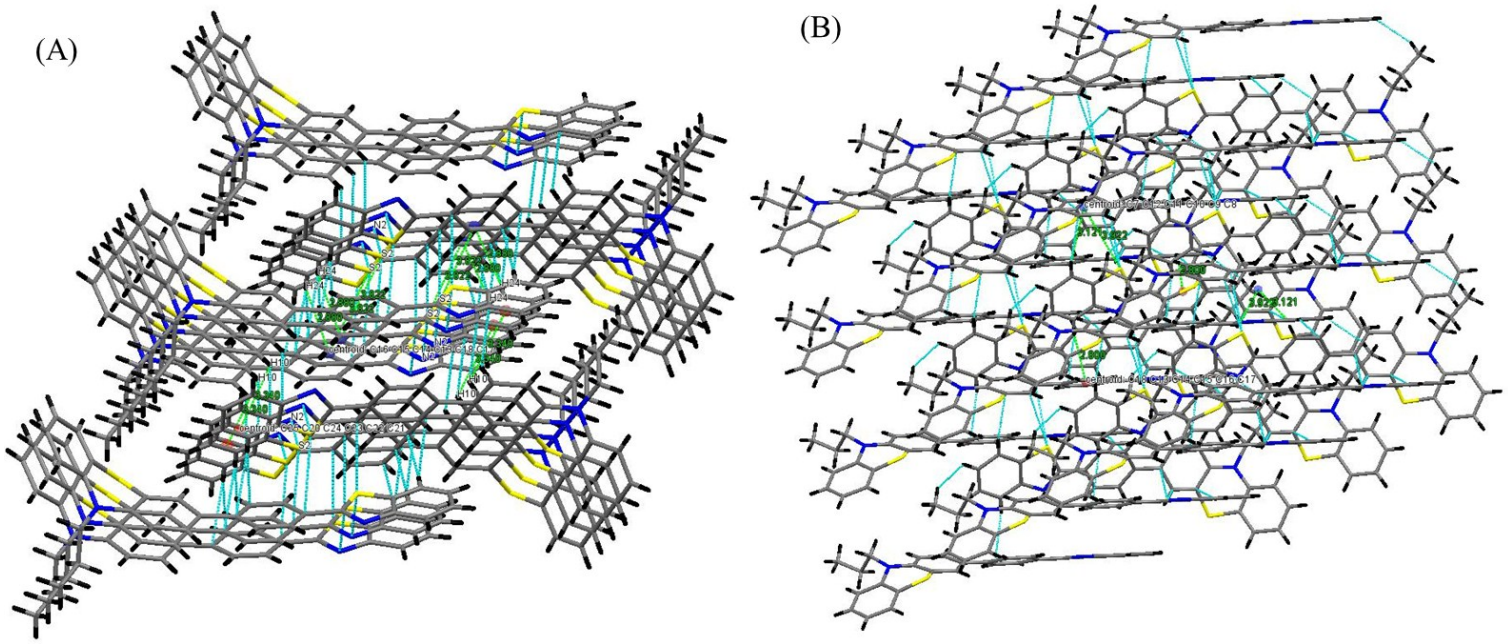


Figure S3. Crystal packing diagram of (A) ***p*-PTZ GC** and (B) ***p*-PTZ YC**.

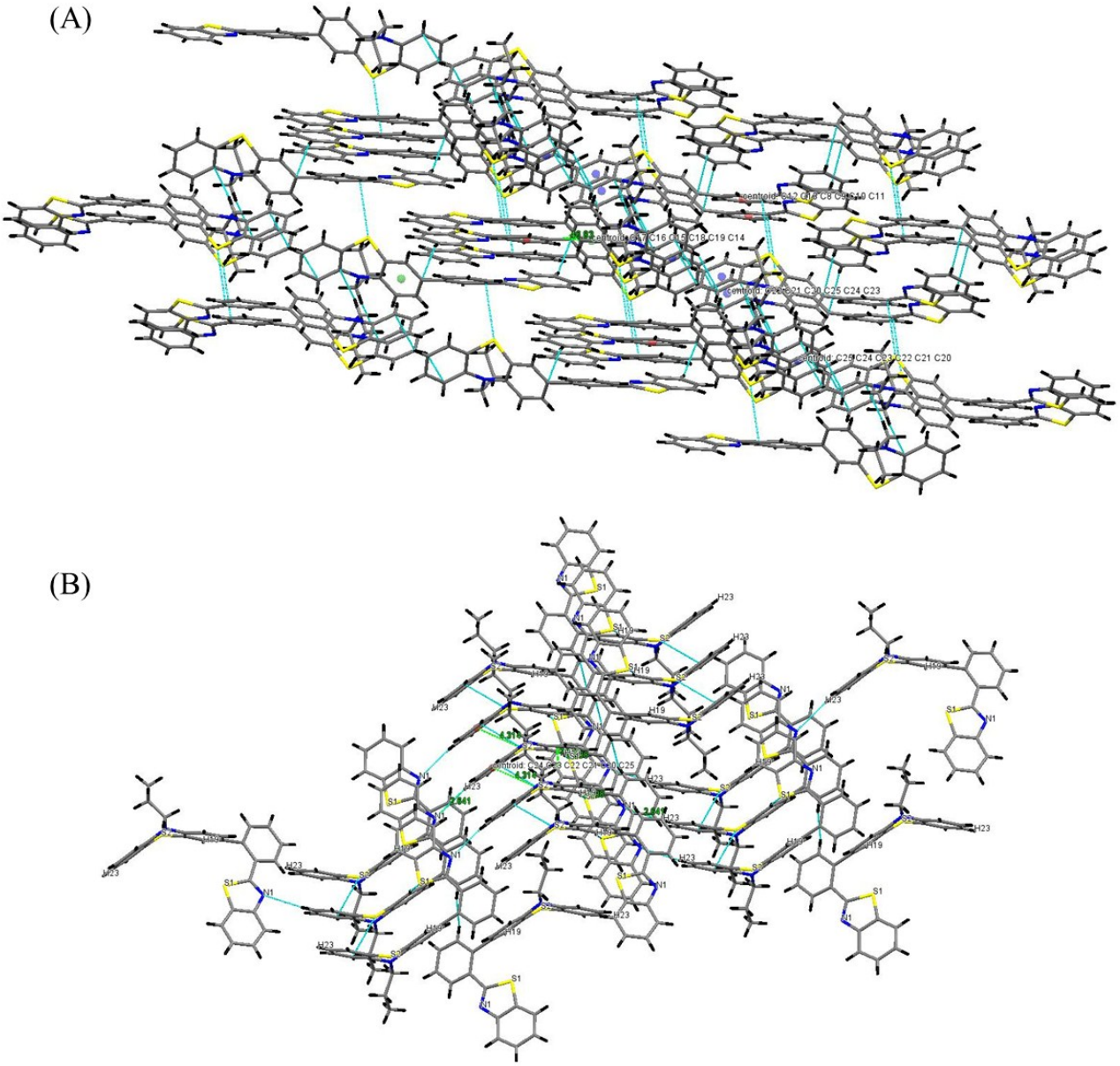


Figure S4. Crystal packing diagram of (A) ***m*-PTZ** and (B) ***o*-PTZ**.

Crystallographic data

Single crystal X-ray structures of ***p*-PTZ GC** and ***p*-PTZ YC** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi omega scan techniques and were scaled and reduced using CrysAlisPro RED software. Diffraction data for ***m*-PTZ** was collected using (BRUKER KAPPA APEX II CCD Duo) with graphite monochromatic Mo Kα radiation (0.71073 Å), on an Xcalibur, Eos, Gemini diffractometer. Single crystal X-ray data for compound ***o*-PTZ** were collected on a Bruker D8 VENTURE diffractometer equipped with CMOS Photon 100 detector and MoKα (λ = 0.71073 Å) radiation was used. The structures were solved by direct methods using SHELXS-97 and refined by full matrix least-squares with SHELXL-97, refining on F2. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2Ueq of their parent atoms. The crystal and refinement data are summarized in Table S1. The CCDC number 1948197, 1948216, 1948223 and 1948310 contains the supplementary crystallographic data for ***p*-PTZ GC**, ***p*-PTZ YC, *m*-PTZ** and ***o*-PTZ**. These data can be obtained free of charge via

www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S2. Crystal data and structure refinement for ***p*-PTZ GC**, ***p*-PTZ YC**, ***m*-PTZ** and ***o*-PTZ**.

Identification code	rm259	rm257	shelx	shelx
Empirical formula	C28 H22 N2 S2	C28 H22 N2 S2	C28 H22 N2 S2	C28 H22 N2 S2
Formula weight	450.59	450.59	450.59	450.59
Temperature	293(2) K	293(2) K	293(2) K	296(2) K
Wavelength	0.71073 A	0.71073 A	0.71073 A	0.71073 A
Crystal system, space group	Monoclinic, P 21	Orthorhombic, P n a 21	Monoclinic P 21/c	Monoclinic, P 21/c
a/(Å)	8.5948(5)	39.769(3)	9.5843(3)	5.7861(2)
b/(Å)	5.5944(3)	7.1785(5)	8.1855(4)	23.6600(7)
c/(Å)	23.1405(11)	7.7524(8)	28.7754(13)	16.4878(5)
Alpha/(°)	90	90	90	90
Beta/(°)	95.751(5)	90	92.432(4)	92.684(2)
Gamma/(°)	90	90	90	90
Volume	1107.06(10) $Å^3$	2213.2(3) $Å^3$	2255.46(17) $Å^3$	2254.69(12) $Å^3$
Z, Calculated density	2, 1.352 mg/m^{-3}	4, 1.352 mg/m^{-3}	4, 1.327 mg/m^{-3}	4, 1.327 mg/m^{-3}

Absorption coefficient	0.260 mm^{-1}	0.260 mm^{-1}	0.255 mm^{-1}	0.255 mm^{-1}
F(000)	472	944	944	944
Crystal size	0.230 x 0.180 x 0.130 mm	0.260 x 0.230 x 0.180 mm	0.250 x 0.100 x 0.060 mm	0.300 x 0.103 x 0.030 mm
Θ range for data collection/(º)	3.384 to 29.083	2.820 to 30.551	3.273 to 29.132	1.506 to 28.433
Reflections collected / unique	9102 / 4635 [R(int) = 0.0708]	23519 / 5412 [R(int) = 0.0968]	25562 / 5521 [R(int) = 0.0674]	24538 / 5645 [R(int) = 0.0691]
Completeness to theta	Θ = 25.242 99.6 %	Θ = 25.242 99.9 %	Θ = 25.242 99.8 %	Θ = 25.242 99.7 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4635 / 3 / 290	5412 / 1 / 289	5521 / 0 / 289	5645 / 2 / 299
Goodness-of-fit on F^2	1.105	1.066	1.029	0.918
Final R indices [I>2sigma(I)]	R1 = 0.1287, wR2 = 0.3277	R1 = 0.0762, wR2 = 0.2056	R1 = 0.0612, wR2 = 0.1138	R1 = 0.0537, wR2 = 0.1199
R indices (all data)	R1 = 0.2379, wR2 = 0.4181	R1 = 0.1058, wR2 = 0.2487	R1 = 0.1204, wR2 = 0.1353	R1 = 0.1379, wR2 = 0.1538
Extinction coefficient	0.050(18)	n/a	n/a	n/a
Largest diff. peak and hole ($e.Å^{-3}$)	0.972 and -0.606	0.658 and -0.623	0.413 and -0.278	0.383 and -0.280

SEM studies

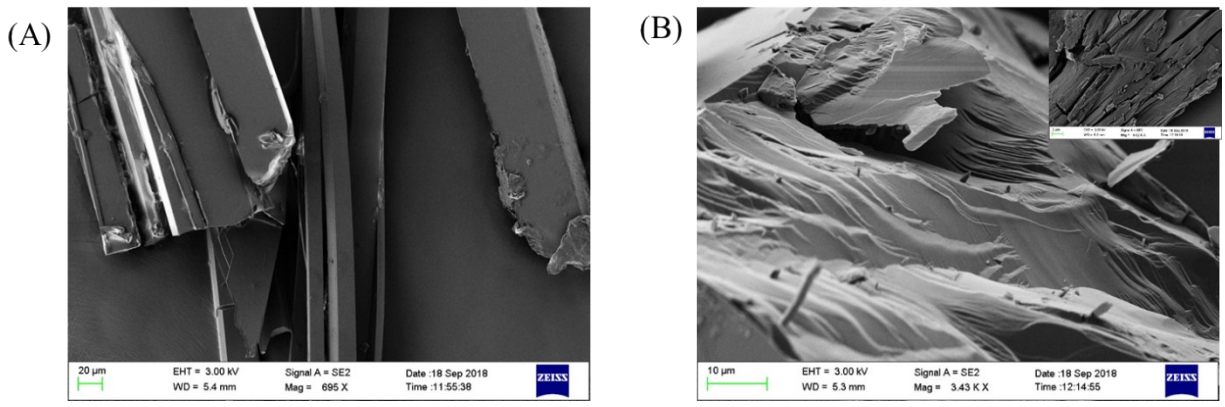
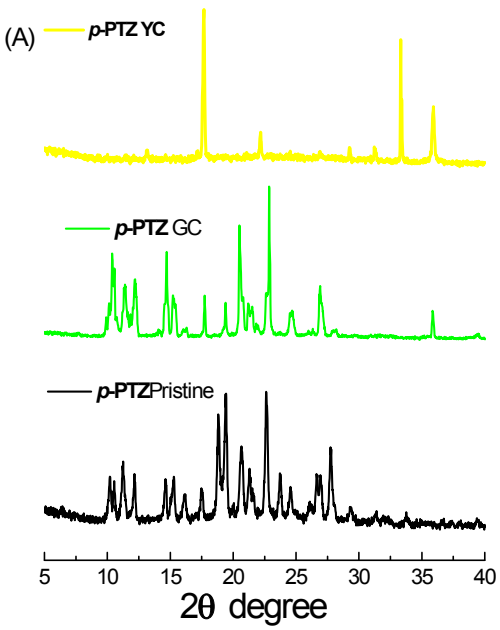
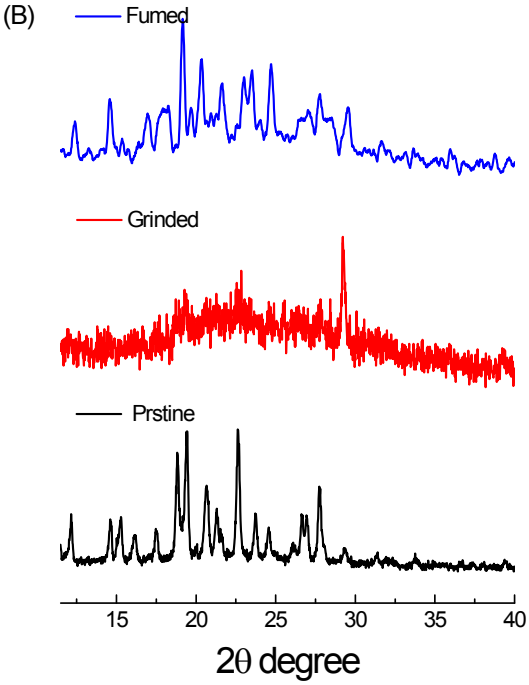
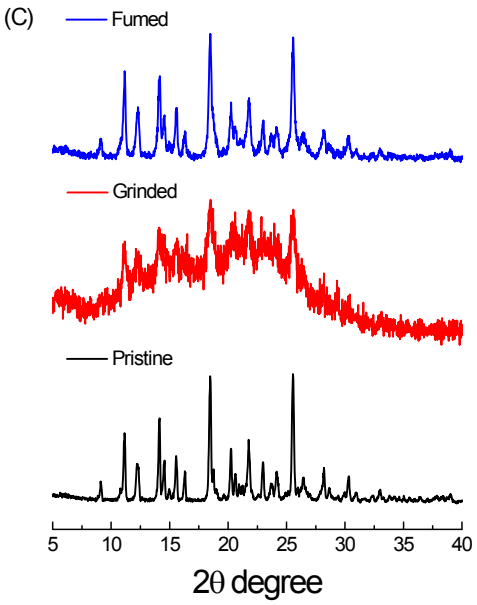


Figure S5. SEM images of the polymorphs (A) ***p*-PTZ GC** and (B) ***p*-PTZ YC**.

PXRD studies


(A)
p-PTZ YC
p-PTZ GC
p-PTZPristine
5 10 15 20 25 30 35 40
2θ degree


(B)
Fumed
Grinded
Prstine
15 20 25 30 35 40
2θ degree


(C)
Fumed
Grinded
Pristine
5 10 15 20 25 30 35 40
2θ degree

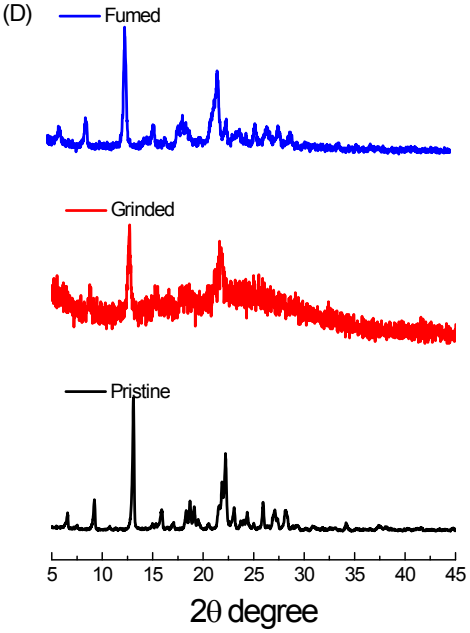

(D)
Fumed
Grinded
Pristine
5 10 15 20 25 30 35 40 45
2θ degree

Figure S6. PXRD patterns of (A) ***p*-PTZ** pristine and its polymorphs ***p*-PTZ GC** and ***p*-PTZ YC** and (B) ***p*-PTZ**, (C) ***m*-PTZ** and (D) ***o*-PTZ** in its pristine, grinded and fumed forms.

DFT calculations

DFT calculation data of *p*-PTZ, ***m*-PTZ** and ***o*-PTZ**

Calculation method: B3LYP/6-31G +(d,p) with Gaussian 09.

***p*-PTZ:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-5.951992	-1.557822	-0.132935
2	7	0	-5.880428	1.052001	0.021709
3	6	0	-7.473224	-0.694649	-0.066458
4	6	0	-8.778051	-1.195737	-0.083327
5	1	0	-8.969946	-2.262207	-0.145443
6	6	0	-9.832012	-0.285022	-0.017621
7	1	0	-10.853952	-0.651892	-0.028903
8	6	0	-9.589798	1.099273	0.062985
9	1	0	-10.429472	1.785902	0.112784
10	6	0	-8.291444	1.597685	0.079652
11	1	0	-8.090484	2.662249	0.141199
12	6	0	-7.215715	0.697277	0.014713
13	6	0	-5.099829	0.014021	-0.049267
14	6	0	-3.634071	0.087786	-0.059915
15	6	0	-3.004148	1.341734	0.045648
16	1	0	-3.619962	2.228770	0.143961
17	6	0	-1.617976	1.440653	0.039074
18	1	0	-1.157968	2.417705	0.151941
19	6	0	-0.800852	0.298920	-0.075853
20	6	0	-1.438032	-0.950832	-0.182006
21	1	0	-0.841475	-1.849990	-0.301102
22	6	0	-2.825720	-1.055560	-0.173059
23	1	0	-3.278176	-2.038512	-0.269055
24	6	0	0.676760	0.413234	-0.087248
25	6	0	1.486421	-0.559047	0.525764
26	6	0	1.322759	1.485893	-0.722197
27	6	0	2.874273	-0.440956	0.541708
28	1	0	1.029849	-1.400791	1.037390
29	6	0	2.712956	1.588895	-0.743619
30	1	0	0.735982	2.231464	-1.249883
31	6	0	3.519511	0.641451	-0.091240
32	16	0	3.863769	-1.618149	1.444804
33	1	0	3.167181	2.407231	-1.290519
34	7	0	4.930061	0.729618	-0.052618
35	6	0	5.260771	-1.657716	0.336729
36	6	0	5.673580	-0.457491	-0.275577
37	6	0	5.578114	2.029979	-0.248556
38	6	0	5.960124	-2.847043	0.121821
39	6	0	6.810327	-0.488050	-1.099542
40	1	0	5.909625	2.168232	-1.290399
41	1	0	4.822199	2.794255	-0.060141
42	6	0	6.743886	2.272874	0.721805
43	6	0	7.108484	-2.856175	-0.673649
44	1	0	5.608347	-3.760871	0.591349
45	6	0	7.528147	-1.672489	-1.282143
46	1	0	7.142982	0.414541	-1.599126
47	1	0	7.498534	1.487093	0.616150

48	1	0	6.358097	2.198294	1.745236
49	6	0	7.391065	3.644167	0.497038
50	1	0	7.660485	-3.779194	-0.820384
51	1	0	8.411603	-1.665563	-1.913695
52	1	0	6.667492	4.457236	0.630190
53	1	0	8.208953	3.810489	1.205036
54	1	0	7.806422	3.731315	-0.514085

Total Energy (HF) = -1986.2178289Hartree

***m*-PTZ**:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.490159	-2.795369	0.240697
2	6	0	3.414093	-1.396203	0.148019
3	6	0	2.152313	-0.778950	0.118824
4	6	0	0.970342	-1.529176	0.187743
5	6	0	1.073163	-2.930048	0.283223
6	1	0	0.173073	-3.531405	0.365883
7	6	0	2.321187	-3.552249	0.305737
8	1	0	2.383793	-4.633299	0.387597
9	1	0	4.453616	-3.295578	0.267168
10	6	0	4.619408	-0.555606	0.074434
11	16	0	6.253929	-1.281370	0.027392
12	7	0	4.600537	0.743708	0.038664
13	6	0	6.928189	0.331928	-0.041615
14	6	0	5.873147	1.278749	-0.026916
15	6	0	8.266443	0.731174	-0.103153
16	6	0	6.172418	2.649954	-0.075167
17	1	0	9.070665	0.002408	-0.114223
18	6	0	8.542267	2.097137	-0.150028
19	6	0	7.503826	3.047430	-0.136207
20	1	0	5.362223	3.371716	-0.064009
21	1	0	9.574659	2.430216	-0.198009
22	1	0	7.747666	4.104820	-0.173887
23	1	0	2.111874	0.299667	0.019525
24	6	0	-0.355187	-0.859240	0.165102
25	6	0	-1.449266	-1.439497	-0.498907
26	6	0	-0.568406	0.363444	0.819784
27	6	0	-2.689834	-0.806609	-0.539885
28	1	0	-1.327261	-2.380188	-1.027277
29	6	0	-1.817551	0.983432	0.813754
30	1	0	0.240090	0.821181	1.381389
31	6	0	-2.899917	0.423813	0.115109
32	16	0	-4.024001	-1.505017	-1.495999
33	1	0	-1.947829	1.901245	1.375669
34	7	0	-4.174473	1.034892	0.053679
35	6	0	-5.361249	-1.047160	-0.408165
36	6	0	-5.311031	0.206316	0.234121
37	6	0	-4.294998	2.478097	0.281364
38	6	0	-6.456846	-1.895498	-0.235321
39	6	0	-6.394499	0.581910	1.044652
40	1	0	-4.576551	2.705499	1.322385
41	1	0	-3.304113	2.909173	0.127673

42	6	0	-5.262581	3.160112	-0.697284
43	6	0	-7.542524	-1.495043	0.547442
44	1	0	-6.459974	-2.863668	-0.727195
45	6	0	-7.504536	-0.254440	1.185549
46	1	0	-6.377313	1.531315	1.567360
47	1	0	-6.255355	2.703539	-0.632036
48	1	0	-4.902664	2.977701	-1.716576
49	6	0	-5.368413	4.666312	-0.433176
50	1	0	-8.400873	-2.149560	0.661807
51	1	0	-8.334704	0.065870	1.808197
52	1	0	-4.393290	5.159920	-0.522231
53	1	0	-6.046074	5.141816	-1.149142
54	1	0	-5.753645	4.871283	0.572865

Total Energy (HF) = -1986.2171096Hartree

***o*-PTZ**:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.409365	2.342206	-0.761647
2	6	0	3.221934	1.684477	-0.394889
3	6	0	1.998779	2.402669	-0.387470
4	6	0	2.034313	3.770007	-0.710845
5	6	0	3.221895	4.416821	-1.051801
6	1	0	3.209236	5.473481	-1.302857
7	6	0	4.417071	3.696598	-1.088200
8	1	0	5.348973	4.184252	-1.357549
9	1	0	1.099431	4.322287	-0.723768
10	1	0	5.342718	1.787294	-0.753096
11	6	0	3.307555	0.269796	0.024958
12	16	0	4.287658	-0.883704	-0.934071
13	7	0	2.736833	-0.237473	1.071877
14	6	0	3.870044	-2.134019	0.217023
15	6	0	3.025277	-1.583657	1.214331
16	6	0	4.243317	-3.481657	0.241386
17	6	0	2.552194	-2.402623	2.251895
18	1	0	4.888797	-3.899613	-0.524566
19	6	0	3.761042	-4.278171	1.278719
20	6	0	2.923107	-3.742624	2.275168
21	1	0	1.905654	-1.976153	3.011775
22	1	0	4.036935	-5.327789	1.316027
23	1	0	2.560850	-4.386728	3.070692
24	6	0	0.676575	1.779771	-0.105029
25	6	0	-0.194233	2.333114	0.838442
26	6	0	0.227569	0.656508	-0.815262
27	6	0	-1.464140	1.797248	1.058058
28	1	0	0.120364	3.191888	1.423902
29	6	0	-1.022885	0.092328	-0.573374
30	1	0	0.867928	0.197509	-1.562706
31	6	0	-1.917119	0.665749	0.357105
32	1	0	-2.096136	2.275179	1.793906
33	16	0	-1.415410	-1.453830	-1.358074
34	7	0	-3.197307	0.109173	0.583731
35	6	0	-3.183980	-1.293166	-1.439471

36	6	0	-3.885806	-0.601171	-0.427475
37	6	0	-3.925582	0.490898	1.799199
38	6	0	-3.865376	-1.966101	-2.455584
39	6	0	-5.291683	-0.669330	-0.456868
40	1	0	-3.190805	0.555515	2.608996
41	1	0	-4.585809	-0.344554	2.056152
42	6	0	-4.748407	1.795558	1.751716
43	6	0	-5.260518	-2.026436	-2.464667
44	1	0	-3.289768	-2.467249	-3.228507
45	6	0	-5.966459	-1.383786	-1.450183
46	1	0	-5.878762	-0.164243	0.297710
47	1	0	-4.099466	2.641831	1.505262
48	1	0	-5.487185	1.746917	0.945584
49	6	0	-5.454173	2.054146	3.088167
50	1	0	-7.051696	-1.418109	-1.428522
51	1	0	-6.142092	1.238596	3.341471
52	1	0	-4.734001	2.145422	3.910018
53	1	0	-6.036588	2.980186	3.053767
54	1	0	-5.779275	-2.568196	-3.249037

Total Energy (HF) = -1986.2062057Hartree

TDDFT calculations of *p*-PTZ, *m*-PTZ and *o*-PTZ

***p*-PTZ:**

```
Excitation energies and oscillator strengths:
 Excited State   1:      Singlet-A      2.9903 eV  414.62 nm  f=0.3759
<S**2>=0.000
     118 ->119         0.69915
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1986.10793801
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      3.7131 eV  333.91 nm  f=0.9164
<S**2>=0.000
     117 ->119         0.68505

 Excited State   3:      Singlet-A      3.7871 eV  327.38 nm  f=0.0501
<S**2>=0.000
     118 ->120         0.64512
     118 ->121         0.12625
     118 ->123        -0.15746

 Excited State   4:      Singlet-A      3.9301 eV  315.48 nm  f=0.0546
<S**2>=0.000
     116 ->119         0.19793
     118 ->120        -0.10264
     118 ->121         0.62628
     118 ->122        -0.11499

 Excited State   5:      Singlet-A      4.0373 eV  307.10 nm  f=0.0152
<S**2>=0.000
     115 ->119         0.54719
     116 ->119        -0.25615
     118 ->120        -0.10315
     118 ->122        -0.21531
```

```
     118 ->123        -0.15482
     118 ->124        -0.10477

 Excited State   6:      Singlet-A      4.0613 eV  305.28 nm  f=0.1524
<S**2>=0.000
     115 ->119         0.38066
     116 ->119         0.39216
     118 ->120         0.11986
     118 ->122         0.14050
     118 ->123         0.32602
     118 ->124         0.14833

 Excited State   7:      Singlet-A      4.1694 eV  297.37 nm  f=0.0165
<S**2>=0.000
     116 ->119        -0.40685
     118 ->121         0.20540
     118 ->122         0.42384
     118 ->123         0.25275

 Excited State   8:      Singlet-A      4.2519 eV  291.60 nm  f=0.0079
<S**2>=0.000
     112 ->119        -0.10359
     113 ->119         0.16799
     116 ->119        -0.22964
     118 ->122        -0.35865
     118 ->123         0.28395
     118 ->124         0.40167

 Excited State   9:      Singlet-A      4.4894 eV  276.17 nm  f=0.0299
<S**2>=0.000
     114 ->119         0.23367
     118 ->123        -0.21951
     118 ->124         0.13242
     118 ->125         0.56285
     118 ->127        -0.17476

 Excited State  10:      Singlet-A      4.5261 eV  273.93 nm  f=0.0054
<S**2>=0.000
     112 ->119        -0.18002
     113 ->119         0.38257
     114 ->119        -0.10256
     117 ->121        -0.12510
     117 ->122        -0.17828
     117 ->124         0.16685
     118 ->122         0.30697
     118 ->123        -0.23950
     118 ->124         0.19051
     118 ->125        -0.13464
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   10
LETran=     190.
```

_m_-PTZ

```
Excitation energies and oscillator strengths:
 Excited State   1:      Singlet-A      3.0364 eV  408.33 nm  f=0.0174
<S**2>=0.000
     118 ->119         0.70333
 This state for optimization and/or second-order correction.
```

```
 Total Energy, E(TD-HF/TD-KS) =  -1986.10552408
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      3.5666 eV  347.62 nm  f=0.1550
<S**2>=0.000
     118 ->120         0.66221
     118 ->122        -0.12555
     118 ->123        -0.11533

 Excited State   3:      Singlet-A      3.8851 eV  319.12 nm  f=0.0868
<S**2>=0.000
     116 ->119         0.14229
     117 ->119         0.50296
     118 ->121         0.39290
     118 ->122         0.10191
     118 ->123         0.17535

 Excited State   4:      Singlet-A      3.9327 eV  315.27 nm  f=0.0160
<S**2>=0.000
     115 ->119        -0.10450
     116 ->119        -0.12774
     117 ->119        -0.39875
     117 ->120        -0.10709
     118 ->120         0.10676
     118 ->121         0.51599

 Excited State   5:      Singlet-A      4.0139 eV  308.89 nm  f=0.7229
<S**2>=0.000
     114 ->119         0.13612
     115 ->119        -0.10125
     116 ->119         0.58820
     117 ->119        -0.11341
     118 ->122        -0.15898
     118 ->123        -0.24563

 Excited State   6:      Singlet-A      4.0479 eV  306.29 nm  f=0.0484
<S**2>=0.000
     115 ->119        -0.13881
     116 ->119         0.24945
     117 ->119        -0.13847
     118 ->120         0.12572
     118 ->121        -0.18763
     118 ->122         0.31113
     118 ->123         0.45105
     118 ->124        -0.11044

 Excited State   7:      Singlet-A      4.1435 eV  299.23 nm  f=0.0967
<S**2>=0.000
     115 ->119         0.63155
     116 ->119         0.12411
     117 ->119        -0.18782

 Excited State   8:      Singlet-A      4.2731 eV  290.15 nm  f=0.0176
<S**2>=0.000
     114 ->119         0.36594
     117 ->120         0.24933
     118 ->120         0.10608
```

```
     118 ->122         0.12401
     118 ->124         0.47491

 Excited State   9:      Singlet-A      4.3462 eV  285.27 nm  f=0.0341
<S**2>=0.000
     114 ->119         0.46226
     116 ->119        -0.11942
     116 ->120        -0.17562
     117 ->120         0.10474
     118 ->120        -0.10070
     118 ->122        -0.15410
     118 ->124        -0.37933

 Excited State  10:      Singlet-A      4.4741 eV  277.11 nm  f=0.0078
<S**2>=0.000
     118 ->122         0.54757
     118 ->123        -0.40081
     118 ->124        -0.17136
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   10
LETran=     190.
```

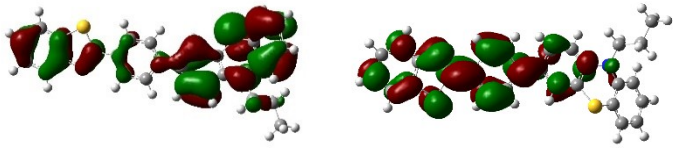
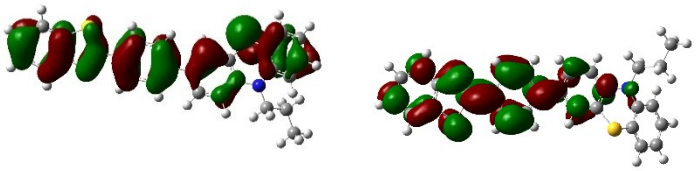
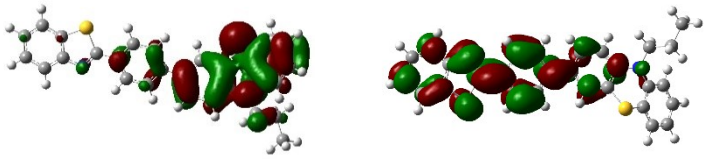
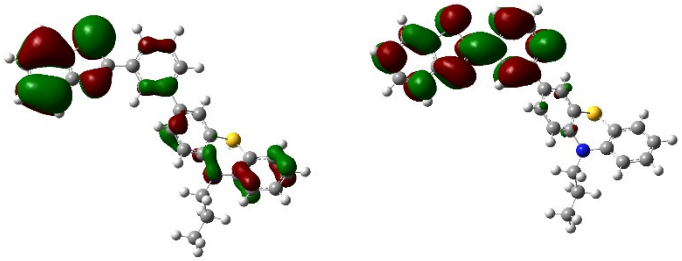
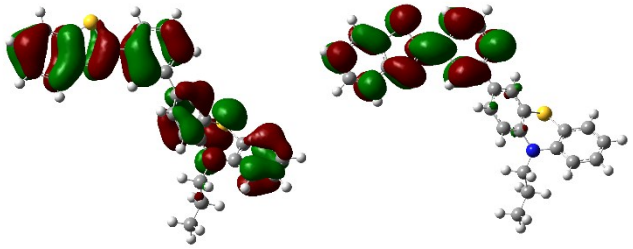
***o*-PTZ**:

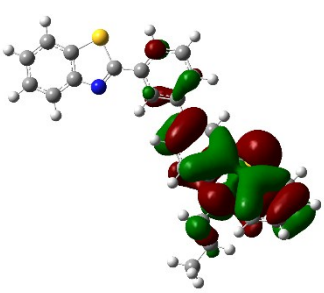
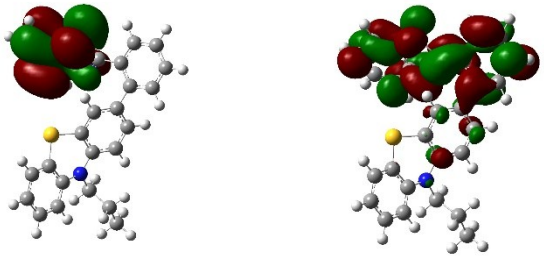
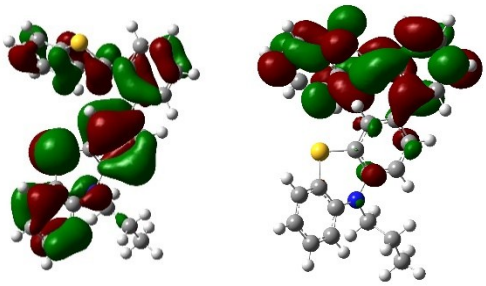
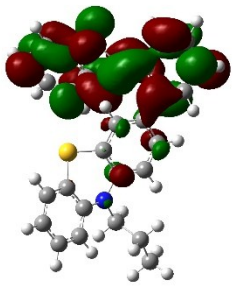
```
Excitation energies and oscillator strengths:
 Excited State   1:      Singlet-A      2.8982 eV  427.80 nm  f=0.0481
<S**2>=0.000
     118 ->119         0.70204
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1986.09969898
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      3.4201 eV  362.52 nm  f=0.0364
<S**2>=0.000
     118 ->120         0.60406
     118 ->121        -0.32763

 Excited State   3:      Singlet-A      3.7094 eV  334.24 nm  f=0.0648
<S**2>=0.000
     118 ->120         0.32159
     118 ->121         0.57807
     118 ->124         0.14325

 Excited State   4:      Singlet-A      3.8680 eV  320.54 nm  f=0.0621
<S**2>=0.000
     118 ->122         0.66474
     118 ->124        -0.15433

 Excited State   5:      Singlet-A      3.9114 eV  316.98 nm  f=0.1159
<S**2>=0.000
     117 ->119         0.68514

 Excited State   6:      Singlet-A      4.0314 eV  307.55 nm  f=0.0385
<S**2>=0.000
     117 ->120         0.11945
     118 ->121        -0.16912
     118 ->122         0.16159
     118 ->123        -0.10117
```

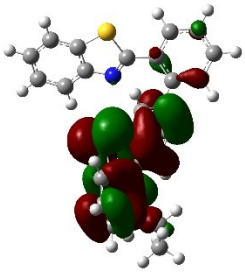
```
     118 ->124         0.57660
     118 ->125        -0.23040

 Excited State   7:      Singlet-A      4.0956 eV  302.73 nm  f=0.0009
<S**2>=0.000
     118 ->123         0.68102
     118 ->124         0.12723

 Excited State   8:      Singlet-A      4.2507 eV  291.68 nm  f=0.0230
<S**2>=0.000
     118 ->124         0.28257
     118 ->125         0.61145

 Excited State   9:      Singlet-A      4.2724 eV  290.20 nm  f=0.0826
<S**2>=0.000
     115 ->119         0.59244
     116 ->119        -0.31054
     116 ->123         0.11317

 Excited State  10:      Singlet-A      4.3276 eV  286.50 nm  f=0.0085
<S**2>=0.000
     118 ->126         0.66817
     118 ->127         0.17303
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   10
LETran=     190.
```

TDDFT data

Table S3. Computed vertical transitions, their oscillator strengths, configurations and corresponding calculated frontier orbitals of ***p*-PTZ**, ***m*-PTZ** and ***o*-PTZ**.

Compound	Wavelength (nm)	f^{a}	Configuration	Assignment
***p*-PTZ**	305.28	0.1524	(HOMO-2)–LUMO (0.39216) 	π-π*
	333.91	0.9164	(HOMO-1)–LUMO (0.68505) 	
	414.62	0.3759	HOMO–LUMO (0.69915) 	ICT
***m*-PTZ**	299.23	0.0967	(HOMO-3)–LUMO (0.63155) 	π-π*
	308.89	0.7229	(HOMO-2)–LUMO (0.58820) 	-

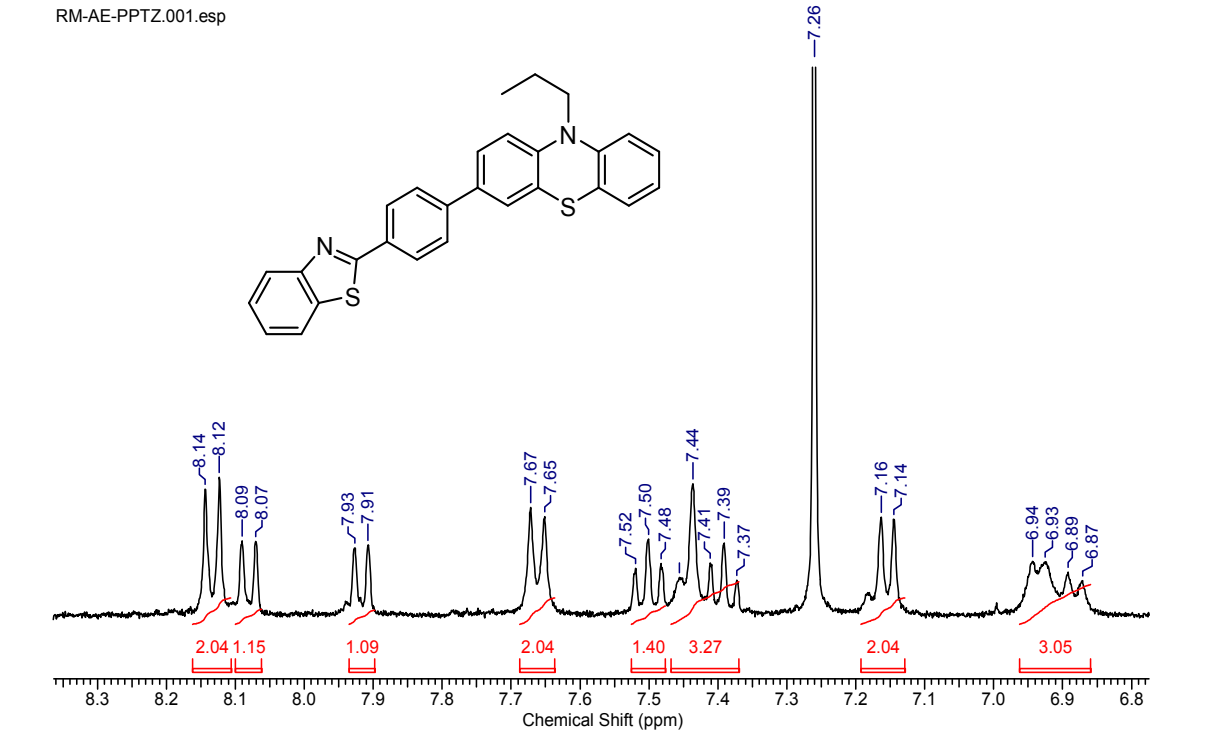
	408.33	0.0174	HOMO–LUMO (0.70333) 	ICT
***o*-PTZ**	290.20	0.0826	(HOMO-3)–LUMO (0.59224) 	π-π*
	316.98	0.1159	(HOMO-1)–LUMO (0.68514) 	-
	427.80	0.0481	HOMO–LUMO (0.70204) 	ICT

[a] Oscillator strength.

Copies of NMR and HRMS of new compounds

^{1}H NMR of ***p*-PTZ**: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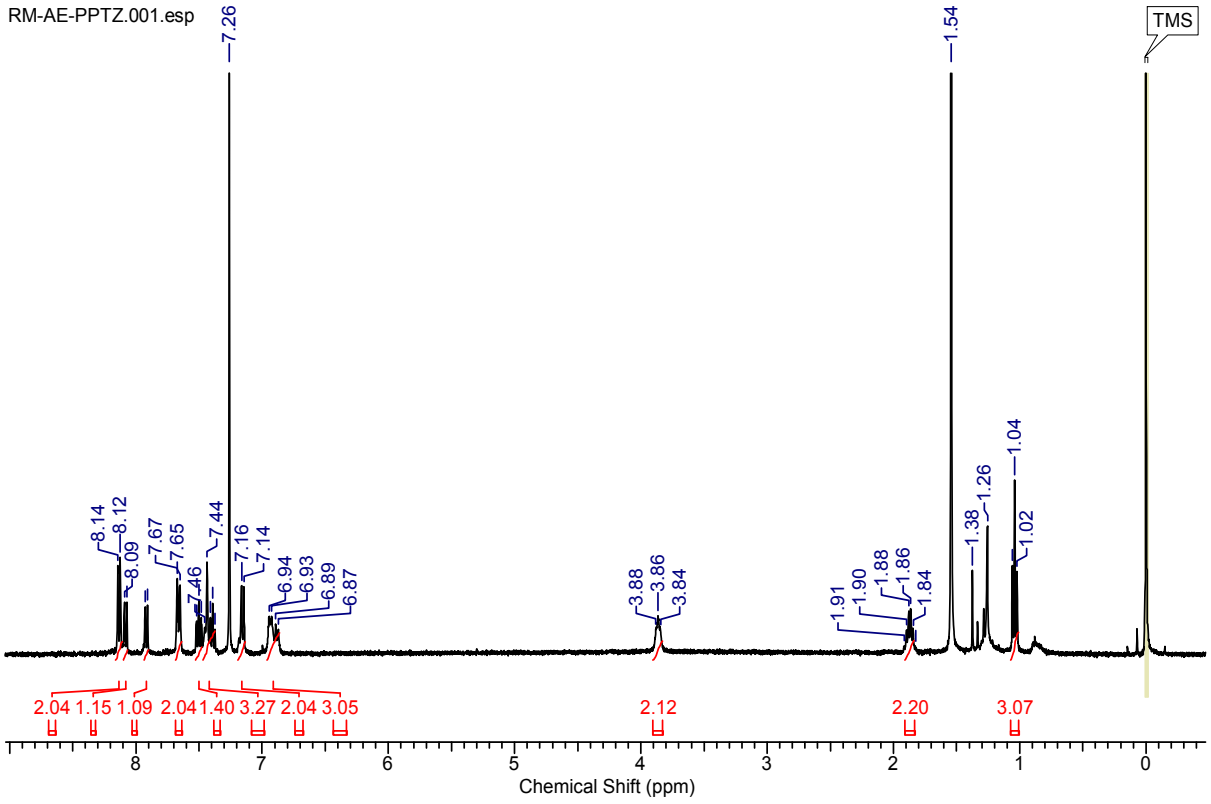
8.12
8.09
8.07
7.93
7.91
7.67
7.65
7.52
7.50
7.48
7.44
7.41
7.39
7.37
7.16
7.14
6.94
6.93
6.89
6.87
2.04 1.15 1.09 2.04 1.40 3.27 2.04 3.05
Chemical Shift (ppm)


RM-AE-PPTZ.001.esp
7.26
1.54
TMS
8.14
8.12
8.09
7.67
7.65
7.46
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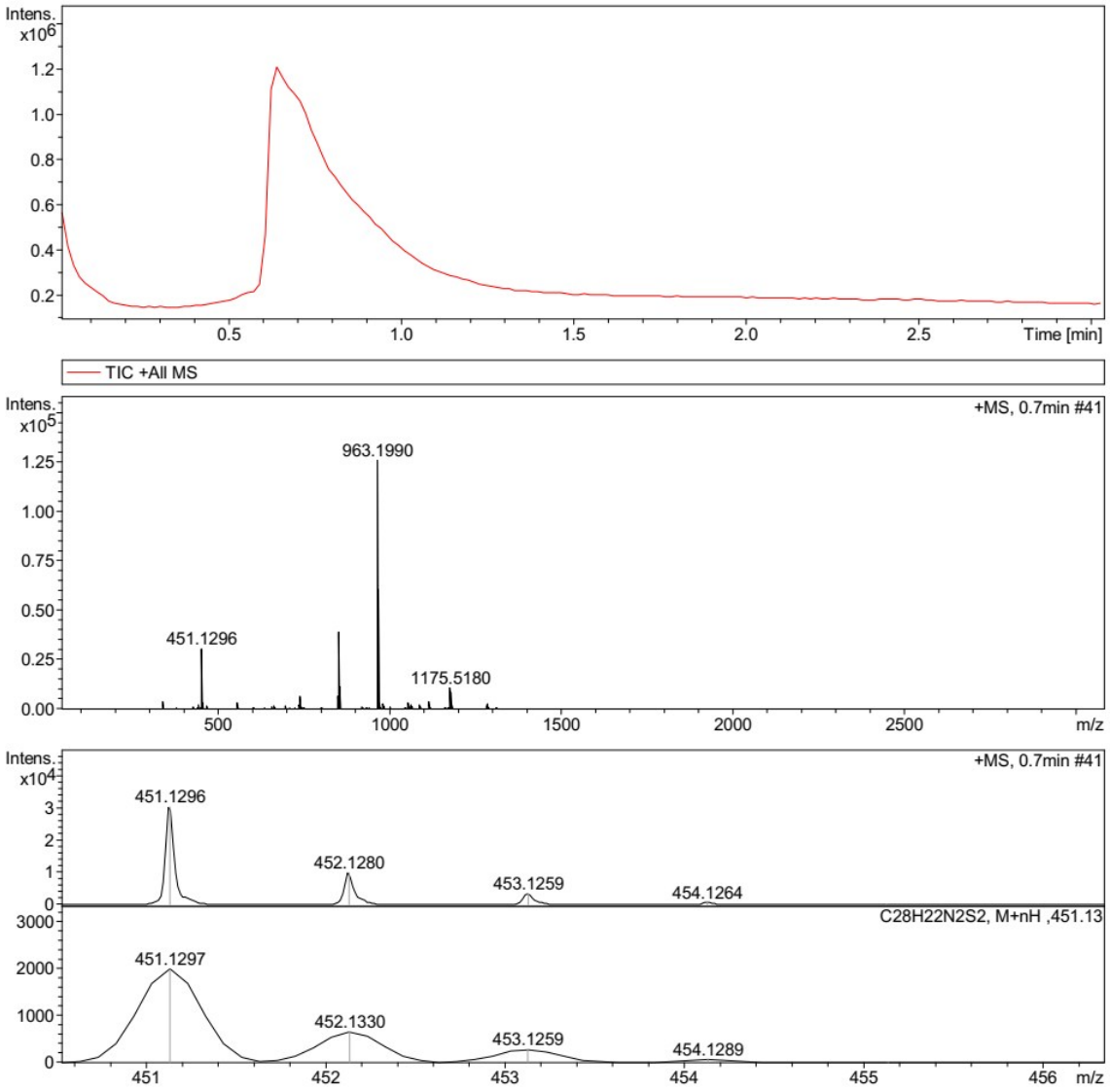
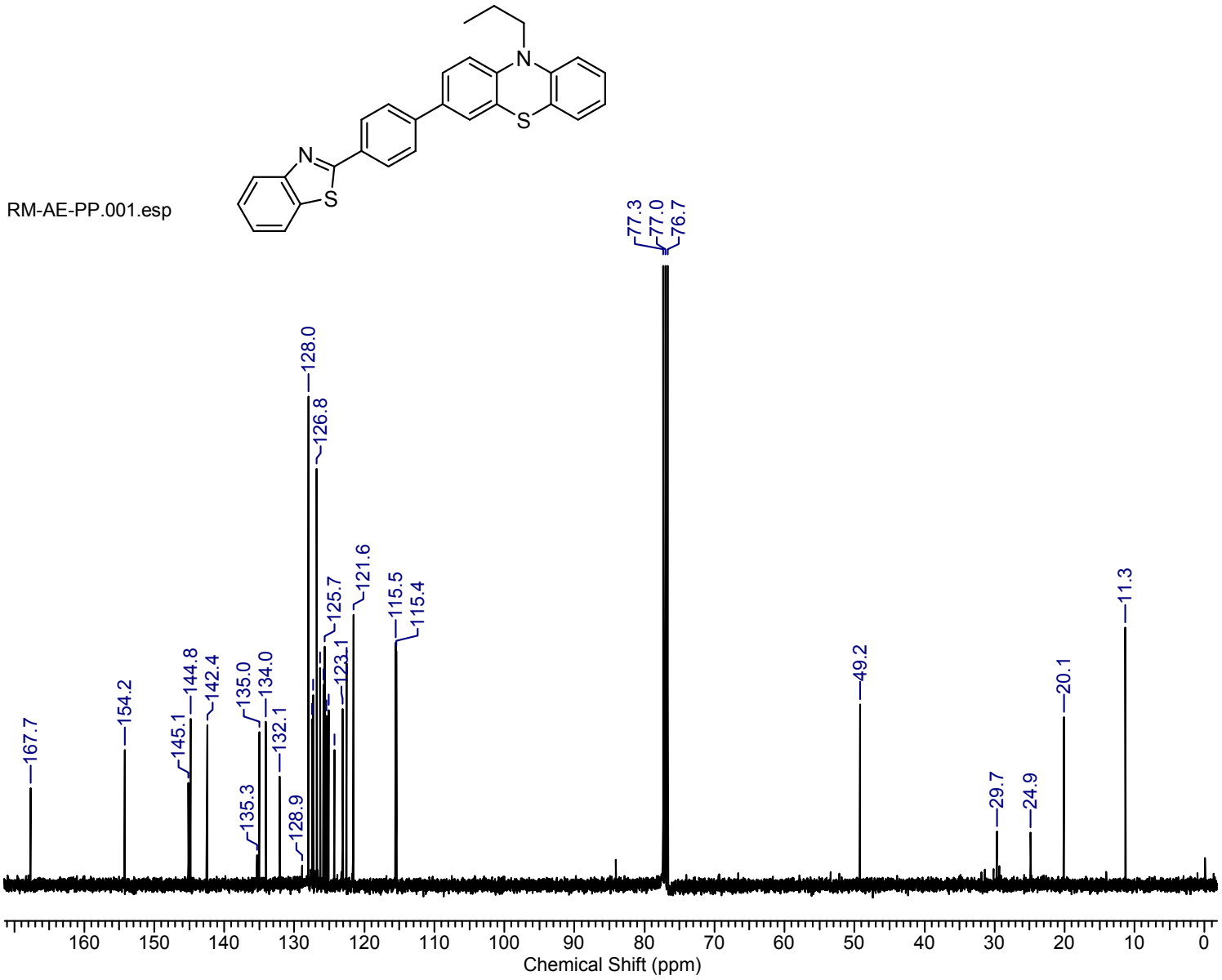
6.93
6.89
6.87
3.88
3.86
3.84
1.91
1.90
1.88
1.86
1.84
1.38
1.26
1.04
1.02
2.04 1.15 1.09 2.04 1.40 3.27 2.04 3.05
2.12
2.20
3.07
Chemical Shift (ppm)

HRMS of ***p*-PTZ**:

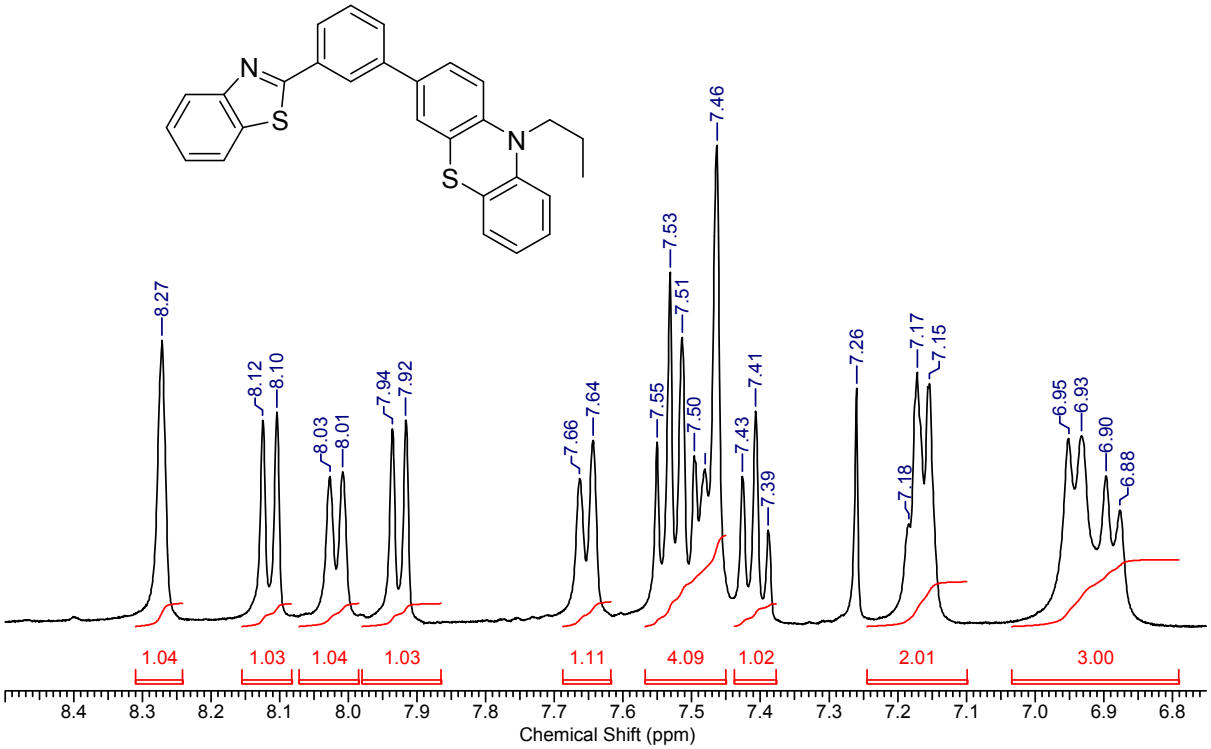


^{13}C NMR of ***p*-PTZ**:

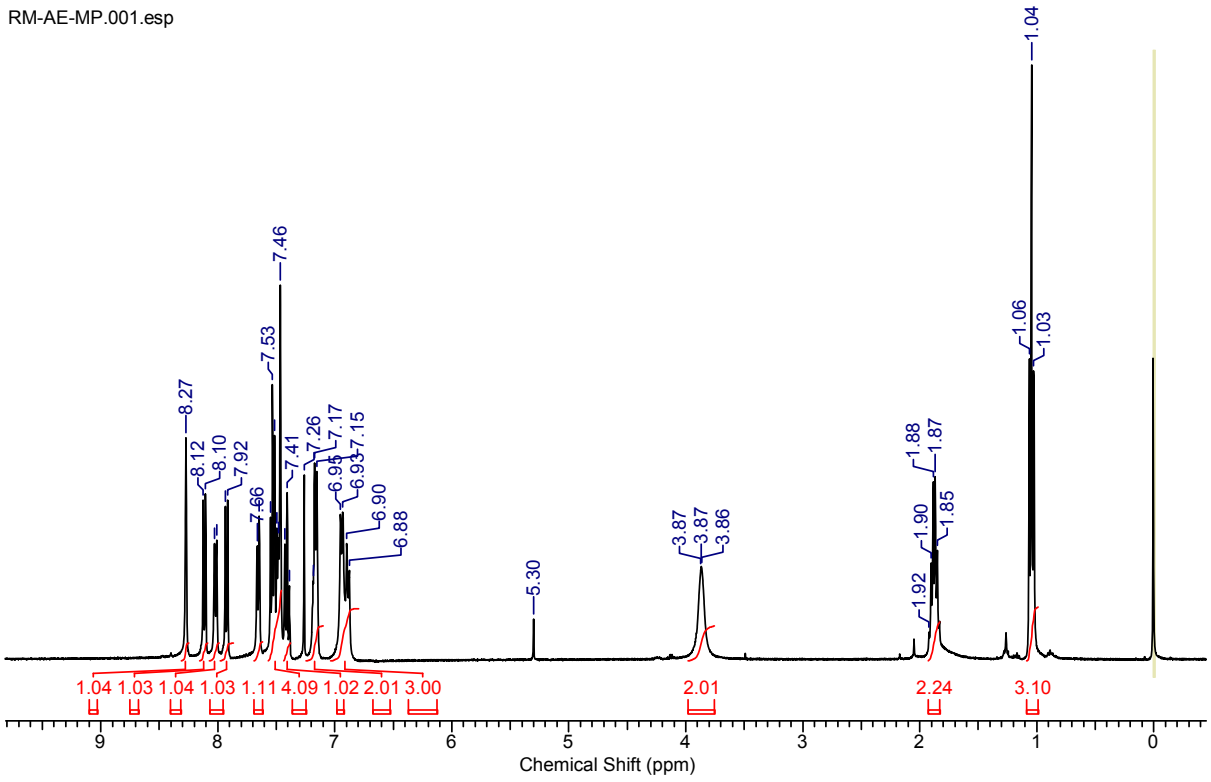


^{1}H NMR of ***m*-PTZ**:

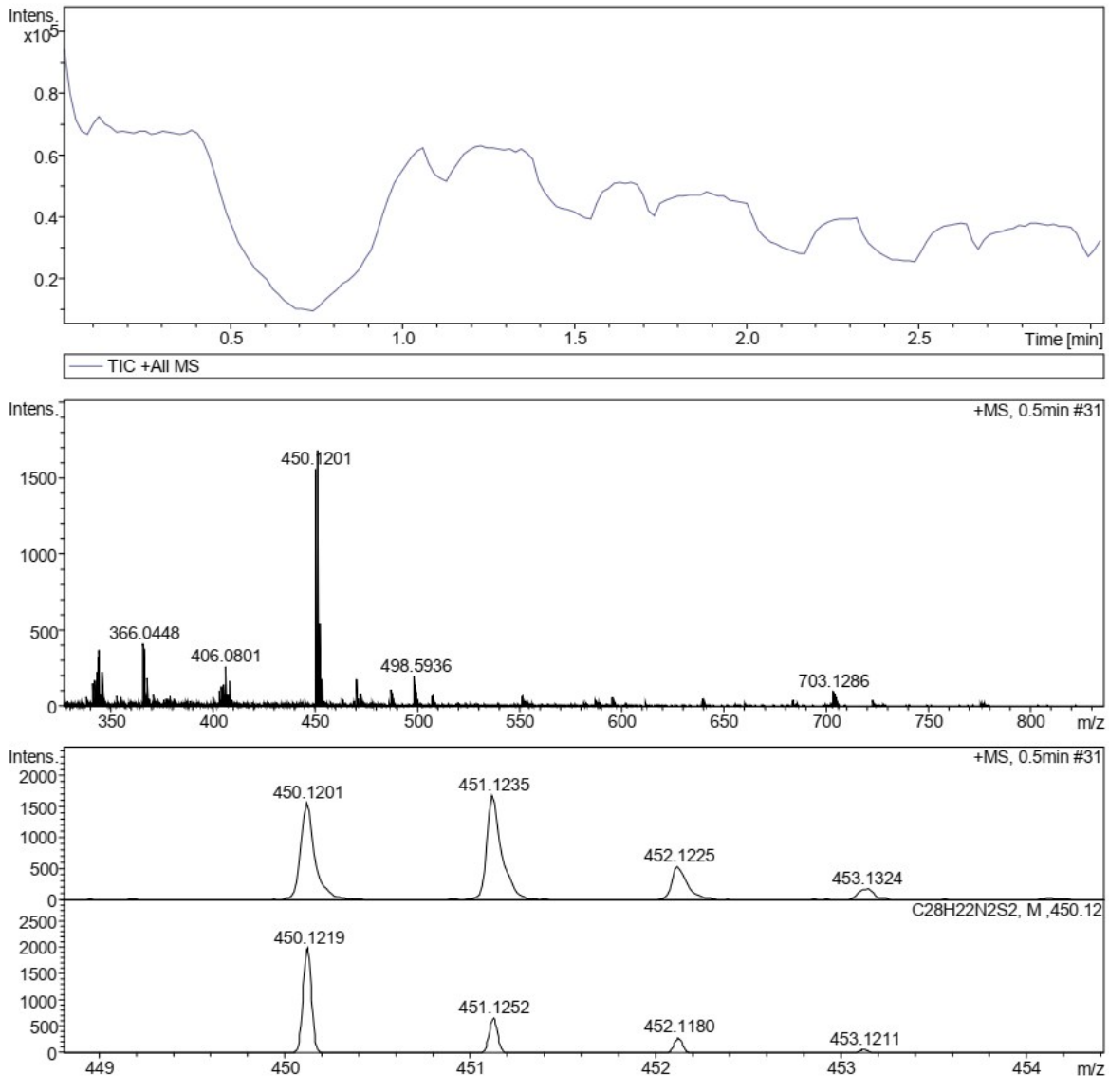
RM-AE-MP.001.esp



RM-AE-MP.001.esp



HRMS of ***m*-PTZ**:


Intens.
x10^5
0.8
0.6
0.4
0.2
0.5
1.0
1.5
2.0
2.5
Time [min]
TIC +All MS
Intens.
+MS, 0.5min #31
450.1201
1500
1000
500
366.0448
406.0801
498.5936
703.1286
0
350
400
450
500
550
600
650
700
750
800
m/z
Intens.
+MS, 0.5min #31
2000
1500
1000
500
450.1201
451.1235
452.1225
453.1324
0
C28H22N2S2, M ,450.12
2500
2000
1500
1000
500
450.1219
451.1252
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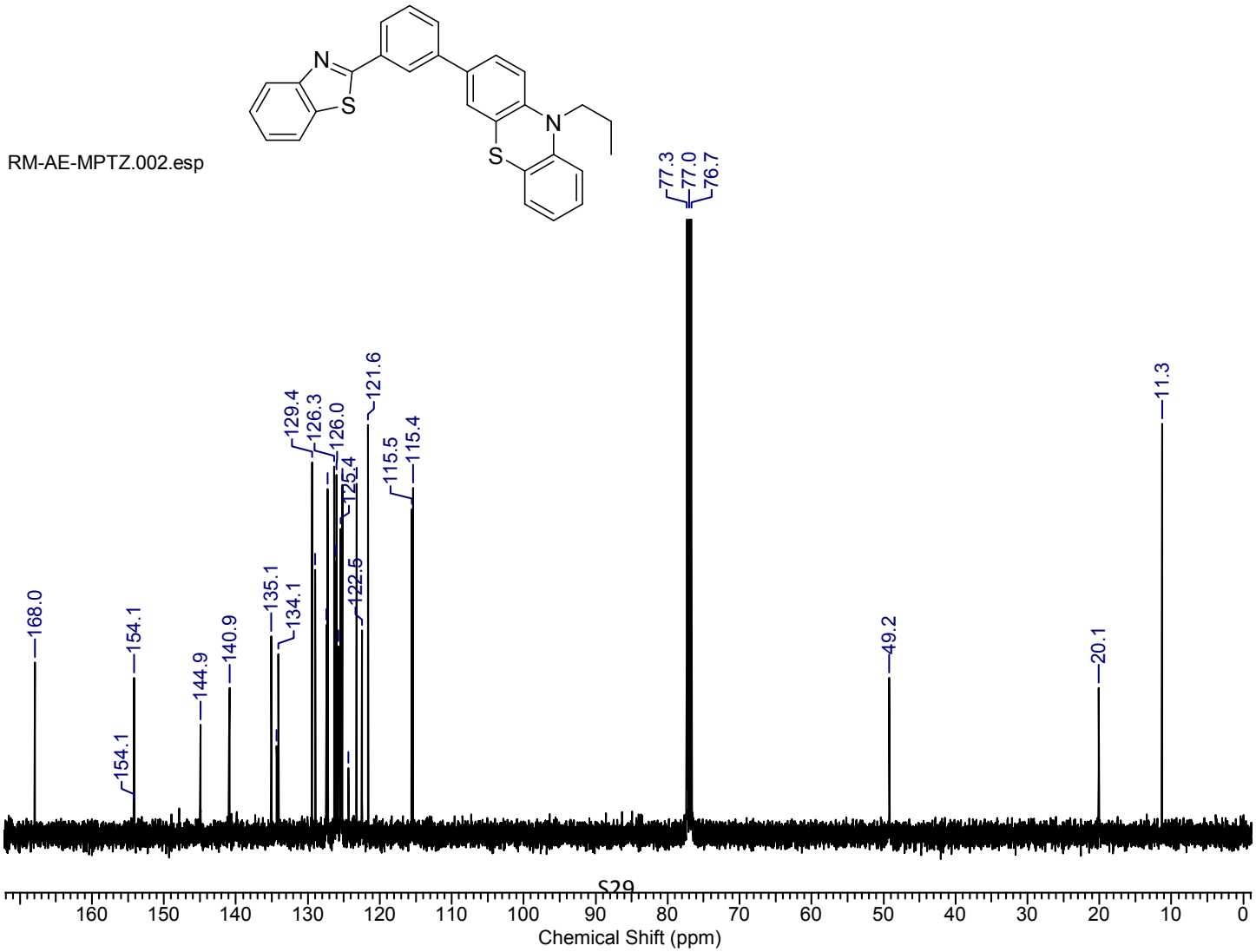
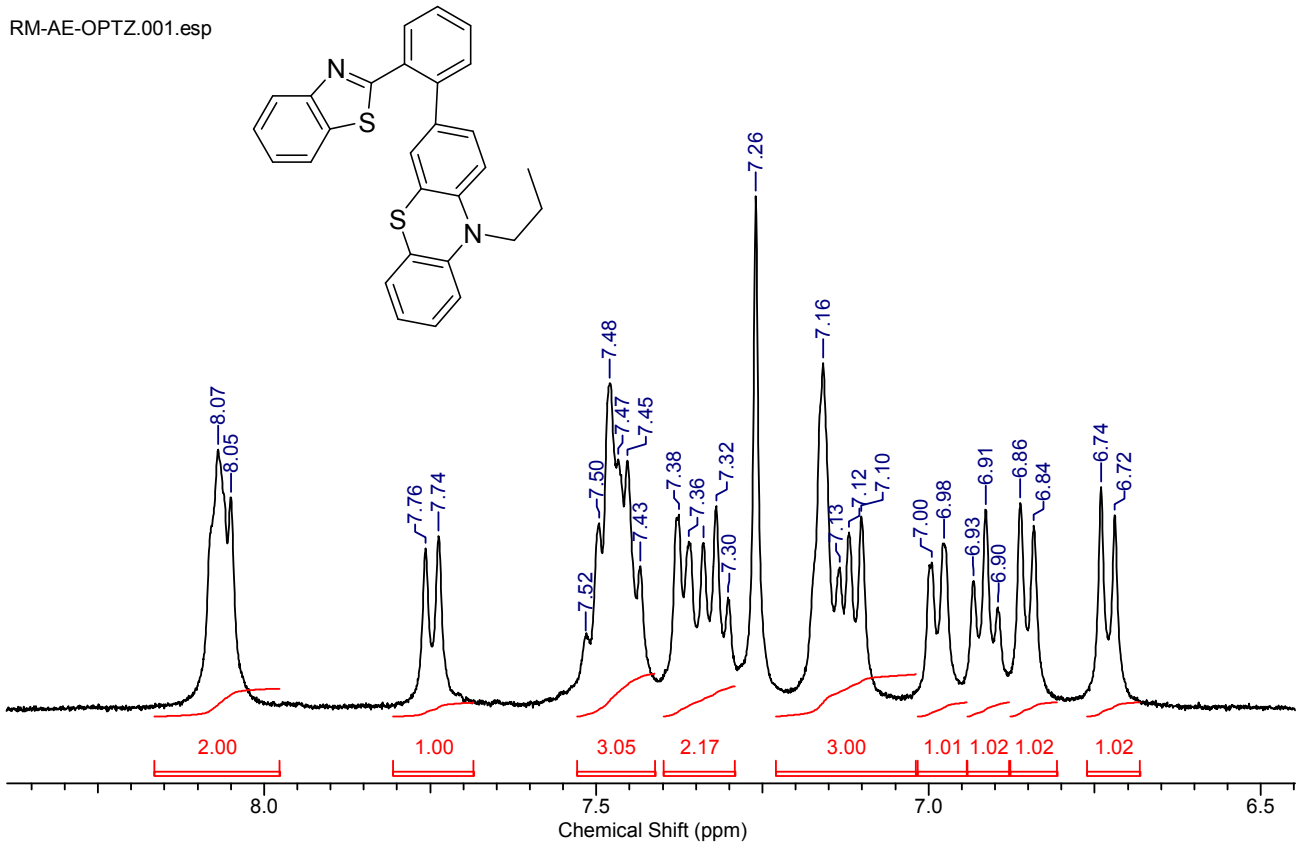
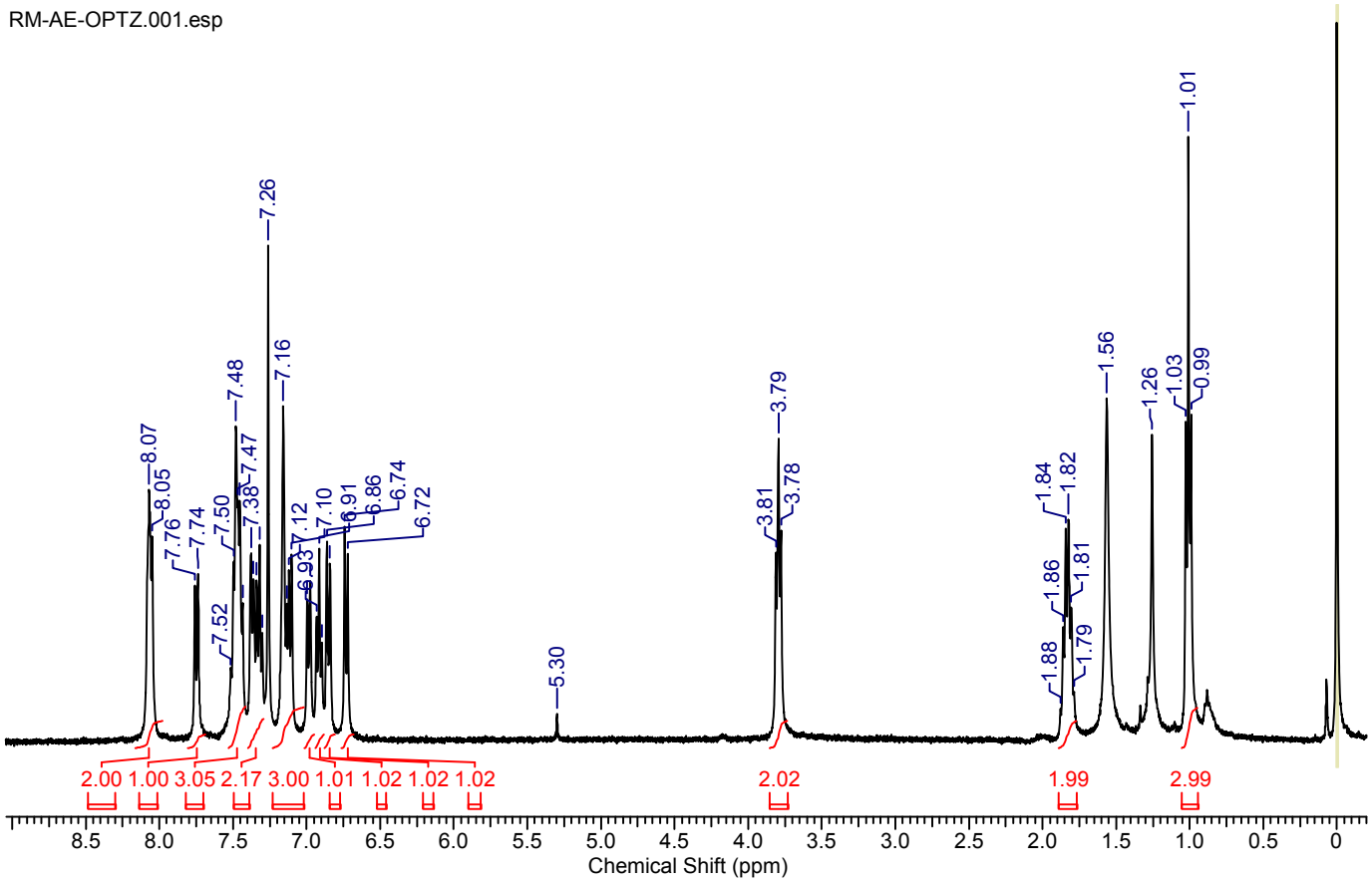
453.1211
0
449
450
451
452
453
454
m/z

^{13}C NMR of ***m*-PTZ**:

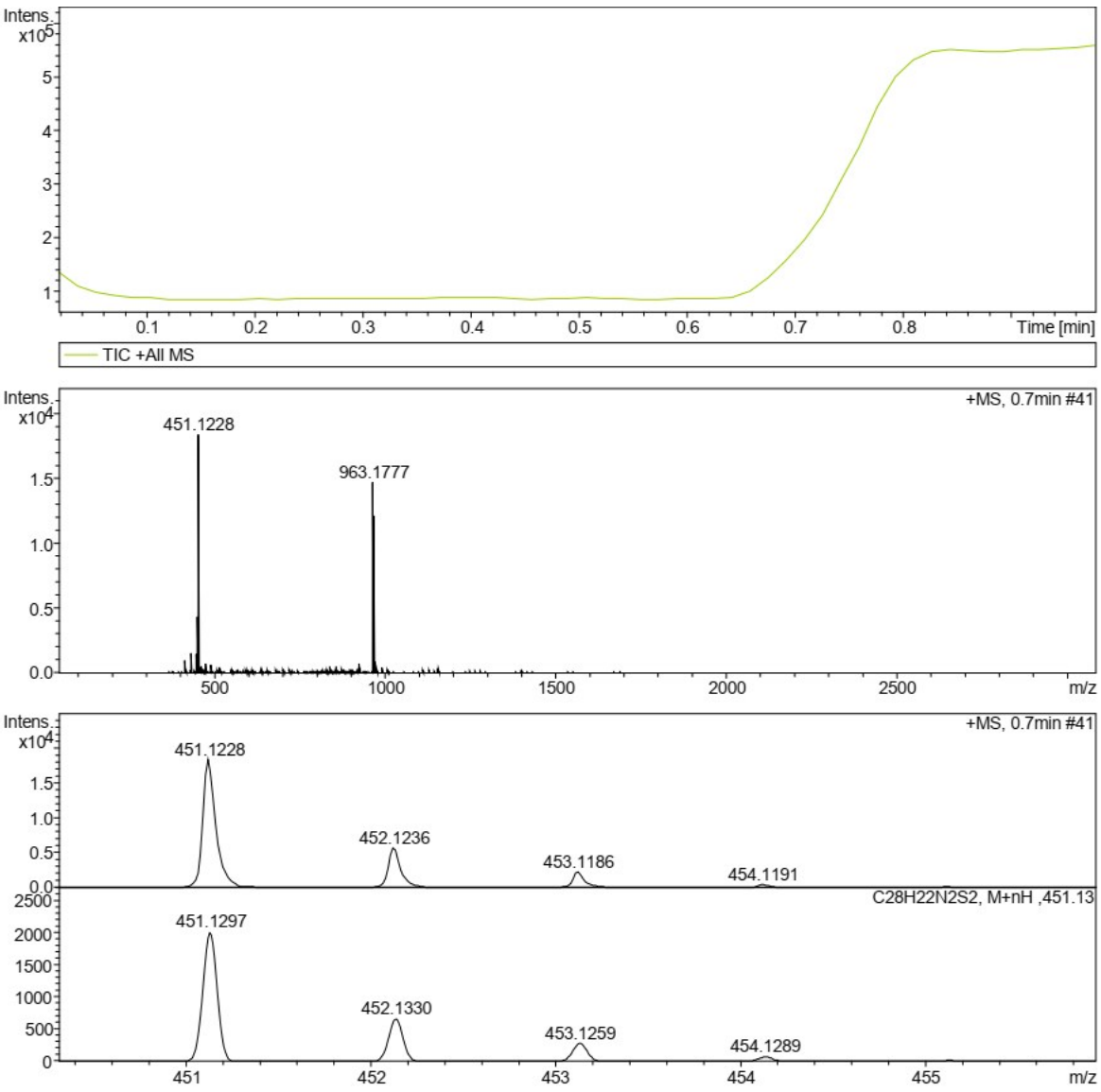


^{1}H NMR of ***o*-PTZ**:





HRMS of ***o*-PTZ**:



^{13}C NMR of ***o*-PTZ**:

RM-AE-OP.001.esp