Electronic Supplementary Material (ESI) for Toxicology Research.

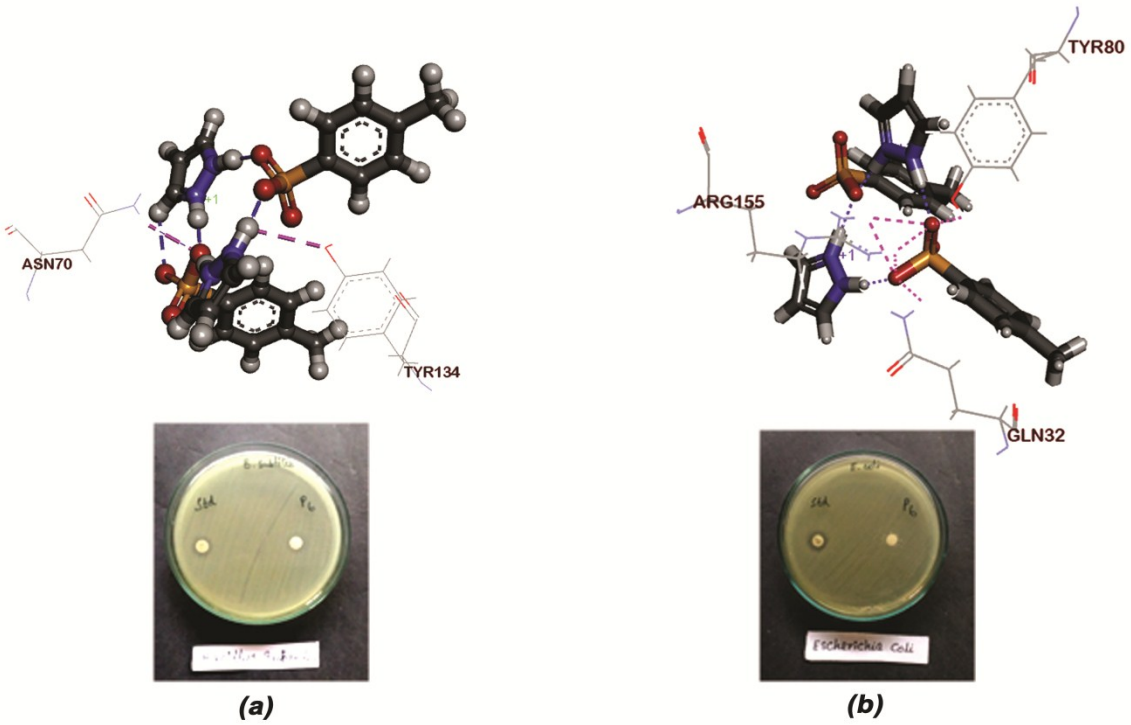

Figure S1. Molecular docking analysis and experimental biological screening of BPPTS against (a) *Bacillus subtilis* and (b) *Escherichia Coli*

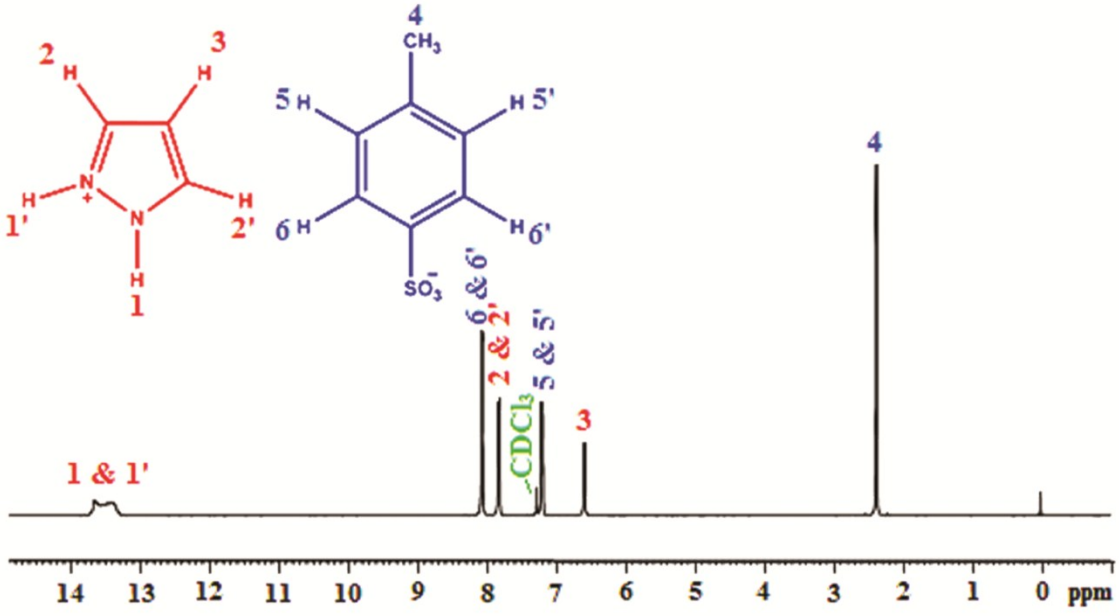

Figure S2a. ^{1}H NMR spectrum of BPPTS

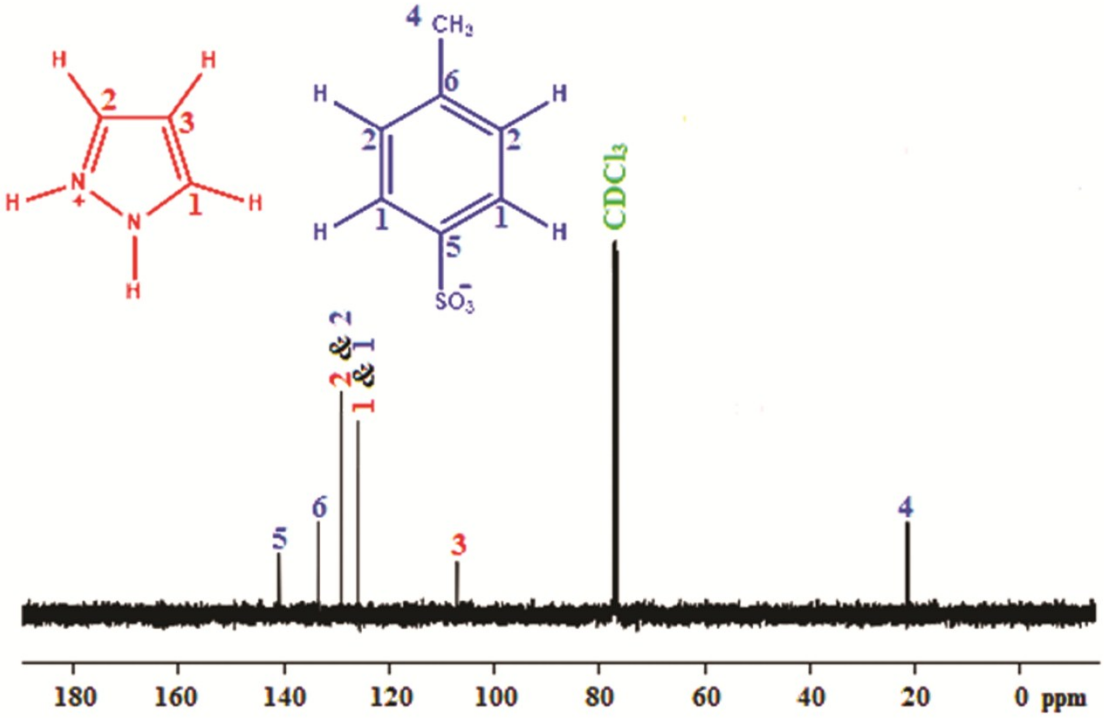

Figure S2b. ^{13}C NMR spectrum of BPPTS

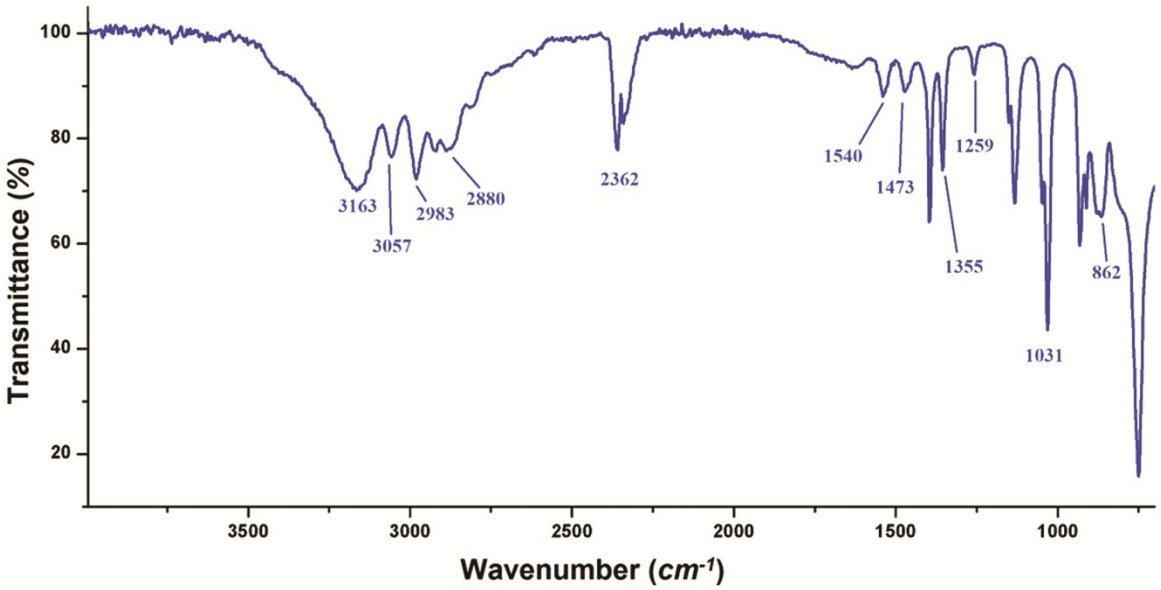

Figure S3a. FT-IR spectrum of BPPTS

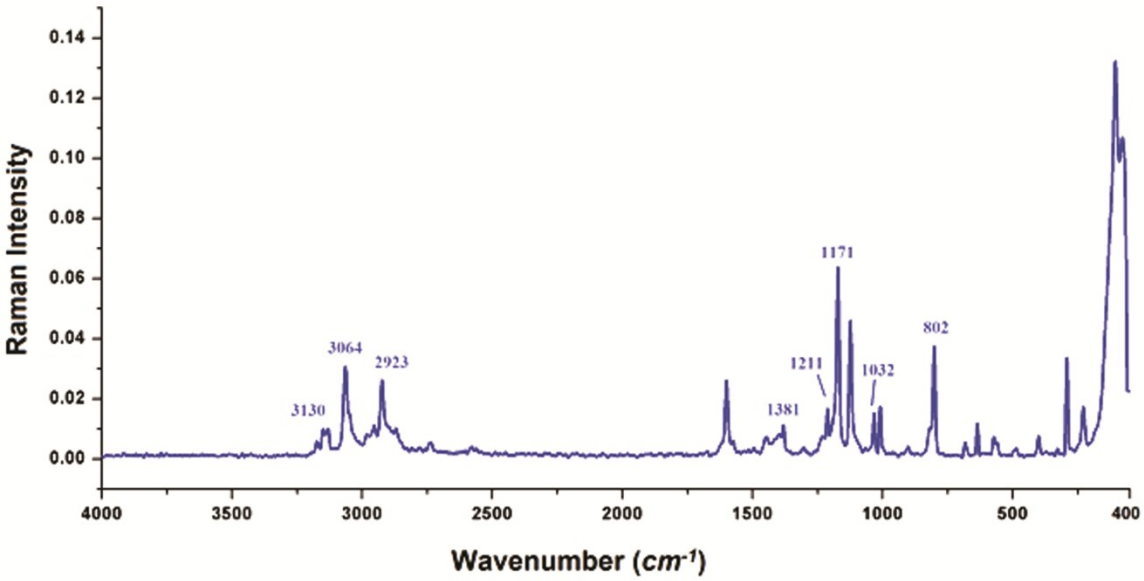

Figure S3b. FT-Raman spectrum of BPPTS

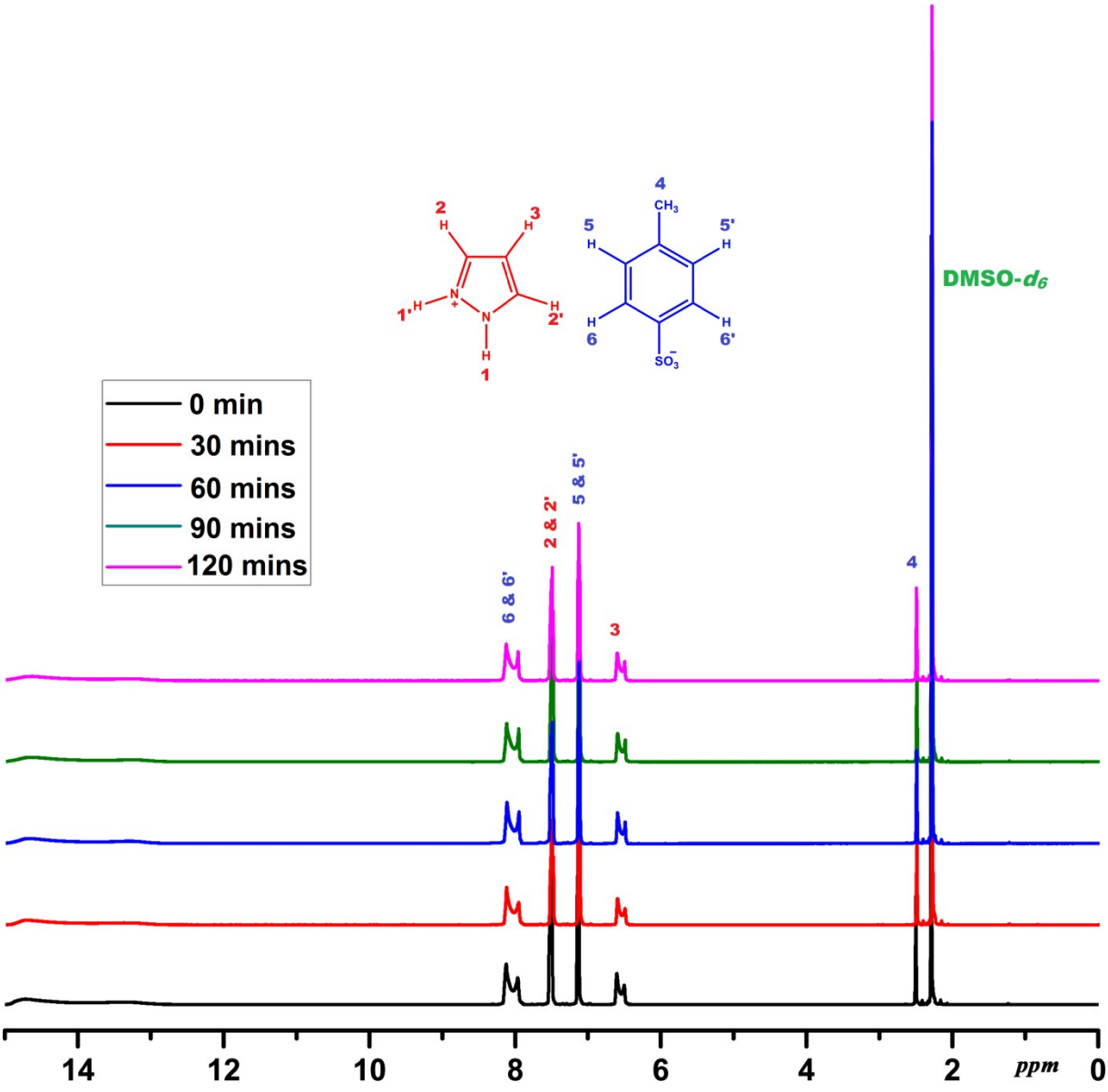

Figure S4. NMR spectra of BPPTS at different time intervals

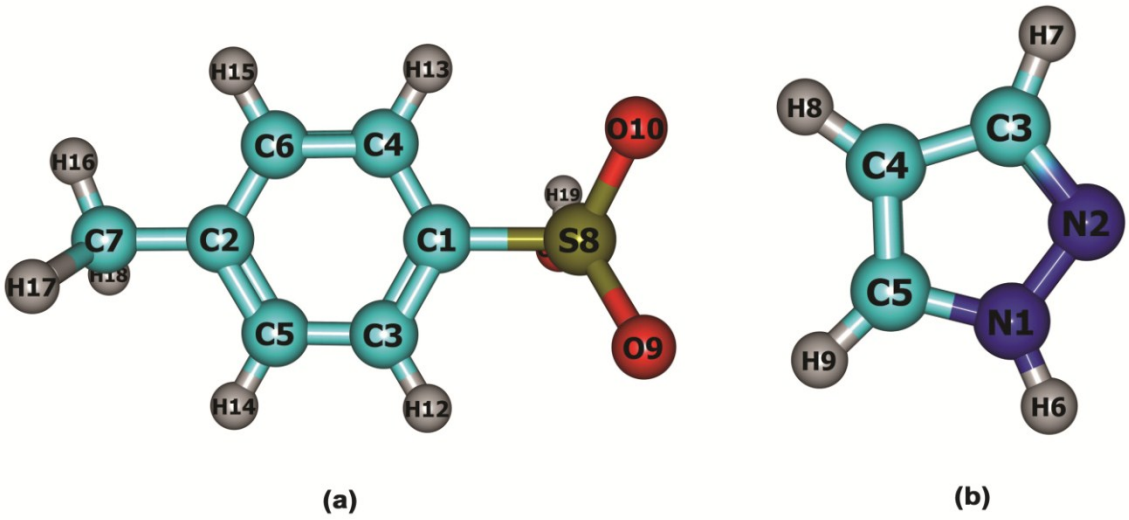

Figure S5. Optimized molecular geometry of (a) *p*-toluenesulphonic acid and (b) Pyrazole

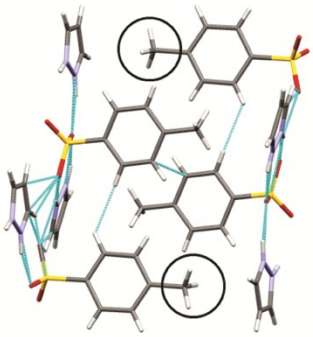

Figure S6. Absence of H…H contacts between CH_3 groups of two neighboring *p*-toluenesulphonate moieties in BPPTS

Table S1

Minimum inhibitory concentration study of BPPTS against pathogens

S.NO	ORGANISMS	1000 µg/ml	500 µg/ml	250 µg/ml	125 µg/ml	62.5 µg/ml	31.25 µg/ml	15.625 µg/ml
1	*Bacillus subtilis*	-	-	-	-	+	+	+
2	*Escherichia Coli*	-	-	-	-	+	+	+
3	*Aspergillus fumigatus*	-	-	-	-	+	+	+

"-" → Absence of growth

"+" → Presence of growth

Table S2: Fukui functions (f_k^+, f_k^- and f_k^0), local softness (s_k^+, s_k^- and s_k^0), local electrophilicity index (ω_k^+, ω_k^- and ω_k^0), and relative electrophilicity and nucleophilicity (f_k^+/ f_k^- and f_k^-/ f_k^+) of BPPTS using Natural atomic charges.

Atoms	Fukui functions(eV)			Local softness(eV)			Local electrophilicity index(eV)			Relative electrophilicity	Relative nucleophilicity
	f_k^+	f_k^-	f_k^0	s_k^+	s_k^-	s_k^0	ω_k^+	ω_k^-	ω_k^0	f_k^+/ f_k^-	f_k^-/ f_k^+
1C	-0.005	-0.089	-0.187	-0.000871	-0.0155038	-0.0325754	-0.014085	-0.250704	-0.52676	0.0561	17.8
2C	-0.015	-0.021	-0.117	-0.002613	-0.0036582	-0.0202943	-0.042254	-0.059155	-0.328169	0.7142	1.4
3C	-0.008	-0.021	-0.119	-0.0013936	-0.0036582	-0.0206427	-0.022535	-0.059155	-0.333803	0.3809	2.625
4C	-0.026	-0.11	-0.091	-0.0045292	-0.019162	-0.0158522	-0.073239	-0.309859	-0.256338	0.2363	4.2307
5C	-0.009	-0.031	-0.123	-0.0015678	-0.0054002	-0.0214266	-0.025352	-0.087324	-0.346479	0.2903	3.4444
6C	0.008	-0.013	-0.098	0.0013936	-0.0022646	-0.0169845	0.0225352	-0.03662	-0.274648	-0.6153	-1.625
7S	-0.001	0.017	1.16	-0.0001742	0.0029614	0.202072	-0.002817	0.047887	3.267604	-0.0588	-17
8O	-0.007	-0.072	-0.524	-0.0012194	-0.0125424	-0.0912808	-0.019718	-0.202817	-1.476056	0.0972	10.2857
9O	0.011	-0.019	-0.532	0.0019162	-0.0033098	-0.0926744	0.0309859	-0.053521	-1.498591	-0.5789	-1.7272
10O	-0.007	-0.07	-0.523	-0.0012194	-0.012194	-0.0911066	-0.019718	-0.197183	-1.473239	0.1	10
11C	0.004	0.02	-0.281	0.0006968	0.003484	-0.0489502	0.0112676	0.056338	-0.791549	0.2	5
12H	0.002	-0.021	0.0915	0.0003484	-0.0036582	0.0159393	0.0056338	-0.059155	0.2577464	-0.0952	-10.5
13H	-0.009	-0.028	0.082	-0.0015678	-0.0048776	0.0142844	-0.025352	-0.078873	0.2309858	0.3214	3.1111
14H	-0.011	-0.032	0.079	-0.0019162	-0.0055744	0.0137618	-0.030986	-0.090141	0.2225351	0.3437	2.9090
15H	-0.007	-0.019	0.0955	-0.0012194	-0.0033098	0.0166361	-0.019718	-0.053521	0.269014	0.3684	2.7142
16H	-0.011	-0.023	0.079	-0.0019162	-0.0040066	0.0137618	-0.030986	-0.064789	0.2225351	0.4782	2.0909
17H	-0.052	0.031	0.0905	-0.0090584	0.0054002	0.0157651	-0.146479	0.087324	0.2549295	-1.6774	-0.5961
18H	0.055	-0.06	0.128	0.009581	-0.010452	0.0222976	0.1549295	-0.169014	0.3605632	-0.9166	-1.0909
19N	-0.039	0.009	-0.186	-0.0067938	0.0015678	-0.0324012	-0.109859	0.025352	-0.523943	-4.3333	-0.2307
20N	-0.039	0.004	-0.188	-0.0067938	0.0006968	-0.0327496	-0.109859	0.011268	-0.529577	-9.75	-0.1025
21C	-0.078	-0.01	-0.067	-0.0135876	-0.001742	-0.0116714	-0.219718	-0.028169	-0.188732	7.8	0.1282
22C	-0.013	-0.011	-0.176	-0.0022646	-0.0019162	-0.0306592	-0.03662	-0.030986	-0.495774	1.1818	0.8461
23C	-0.068	-0.002	-0.047	-0.0118456	-0.0003484	-0.0081874	-0.191549	-0.005634	-0.132394	34	0.0294
24H	-0.008	0.007	0.2325	-0.0013936	0.0012194	0.0405015	-0.022535	0.019718	0.6549293	-1.1428	-0.875
25H	-0.007	0.005	0.2325	-0.0012194	0.000871	0.0405015	-0.019718	0.014085	0.6549293	-1.4	-0.7142

26H	-0.017	-0.007	0.0925	-0.0029614	-0.0012194	0.0161135	-0.047887	-0.019718	0.2605633	2.4285	0.4117
27H	-0.02	-0.011	0.0915	-0.003484	-0.0019162	0.0159393	-0.056338	-0.030986	0.2577464	1.8181	0.55
28H	-0.016	0.002	0.114	-0.0027872	0.0003484	0.0198588	-0.04507	0.005634	0.3211266	-8	-0.125
29C	-0.03	-0.073	-0.202	-0.005226	-0.0127166	-0.0351884	-0.084507	-0.205634	-0.569014	0.4109	2.4333
30C	-0.017	-0.005	-0.113	-0.0029614	-0.000871	-0.0195975	-0.047887	-0.014085	-0.316901	3.4	0.2941
31C	-0.017	-0.03	-0.133	-0.0029614	-0.005226	-0.0230815	-0.047887	-0.084507	-0.373239	0.5666	1.7647
32C	-0.051	-0.092	-0.106	-0.0088842	-0.0160264	-0.0184652	-0.143662	-0.259155	-0.298591	0.5543	1.8039
33C	-0.031	-0.008	-0.13	-0.0054002	-0.0013936	-0.022646	-0.087324	-0.022535	-0.366197	3.875	0.2580
34C	-0.013	-0.015	-0.108	-0.0022646	-0.002613	-0.0188136	-0.03662	-0.042254	-0.304225	0.8666	1.1538
35S	0	0.012	1.166	0	0.0020904	0.2031172	0	0.033803	3.2845054	0	0
36O	-0.008	-0.014	-0.5	-0.0013936	-0.0024388	-0.0871	-0.022535	-0.039437	-1.40845	0.5714	1.75
37O	-0.005	-0.039	-0.528	-0.000871	-0.0067938	-0.0919776	-0.014085	-0.109859	-1.487323	0.1282	7.8
38O	-0.003	-0.035	-0.526	-0.0005226	-0.006097	-0.0915421	-0.008451	-0.098592	-1.480281	0.0857	11.6667
39C	0	0.017	-0.287	0	0.0029614	-0.0499083	0	0.047887	-0.807042	0	0
40H	-0.017	-0.014	0.0795	-0.0029614	-0.0024388	0.0138489	-0.047887	-0.039437	0.2239436	1.2142	0.82352
41H	-0.078	-0.028	0.015	-0.0135876	-0.0048776	0.002613	-0.219718	-0.078873	0.0422535	2.7857	0.3589
42H	-0.016	-0.022	0.0785	-0.0027872	-0.0038324	0.0136747	-0.04507	-0.061972	0.2211267	0.7272	1.375
43H	-0.006	-0.01	0.1065	-0.0010452	-0.001742	0.0185523	-0.016901	-0.028169	0.2999999	0.6	1.6666
44H	-0.012	-0.017	0.081	-0.0020904	-0.0029614	0.0141102	-0.033803	-0.047887	0.2281689	0.705882	1.4166
45H	-0.013	-0.02	0.0785	-0.0022646	-0.003484	0.0136747	-0.03662	-0.056338	0.2211267	0.65	1.5384
46H	-0.006	-0.016	0.0985	-0.0010452	-0.0027872	0.0171587	-0.016901	-0.04507	0.2774647	0.375	2.6666
47N	-0.036	0.008	-0.184	-0.0062712	0.0013936	-0.0319657	-0.101408	0.022535	-0.516901	-4.5	-0.2222
48N	-0.037	0.005	-0.185	-0.0064454	0.000871	-0.032227	-0.104225	0.014085	-0.521127	-7.4	-0.1351
49C	-0.073	-0.01	-0.063	-0.0127166	-0.001742	-0.0108875	-0.205634	-0.028169	-0.176056	7.3	0.13698
50C	-0.012	-0.012	-0.176	-0.0020904	-0.0020904	-0.0306592	-0.033803	-0.033803	-0.495774	1	1
51C	-0.064	-0.003	-0.044	-0.0111488	-0.0005226	-0.0076648	-0.180282	-0.008451	-0.123944	21.3333	0.0468
52H	-0.008	0.007	0.233	-0.0013936	0.0012194	0.0405886	-0.022535	0.019718	0.6563377	-1.1428	-0.875
53H	-0.005	0.004	0.2335	-0.000871	0.0006968	0.0406757	-0.014084	0.011268	0.6577462	-1.25	-0.8
54H	-0.017	-0.006	0.093	-0.0029614	-0.0010452	0.0162006	-0.047887	-0.016901	0.2619717	2.8333	0.3529
55H	-0.019	-0.01	0.093	-0.0033098	-0.001742	0.0162006	-0.053521	-0.028169	0.2619717	1.9	0.5263
56H	-0.016	0.003	0.115	-0.0027872	0.0005226	0.020033	-0.04507	0.008451	0.3239435	-5.3333	-0.1875

Table S3: Fukui functions (f_k^+, f_k^- and f_k^0), local softness (s_k^+, s_k^- and s_k^0), local electrophilicity index (ω_k^+, ω_k^- and ω_k^0), and relative electrophilicity and nucleophilicity (f_k^+/ f_k^- and f_k^-/ f_k^+) of DPPH using Natural atomic charges.

Atoms	Fukui functions(eV)			Local softness(eV)			Local electrophilicity index(eV)			Relative electrophilicity	Relative nucleophilicity
	f_k^+	f_k^-	f_k^0	s_k^+	s_k^-	s_k^0	ω_k^+	ω_k^-	ω_k^0	f_k^+/ f_k^-	f_k^-/ f_k^+
1 C	-0.026	-0.124	-0.198	-0.0197652	-0.0942648	-0.1501395	-0.001604	-0.007651	-0.012186	0.209677	4.769231
2 C	-0.009	-0.007	-0.102	-0.0068418	-0.0053214	-0.0775404	-0.000555	-0.000432	-0.006293	1.285714	0.777778
3 C	0.007	-0.069	-0.141	0.0053214	-0.0524538	-0.1068081	0.0004319	-0.004257	-0.008669	-0.10145	-9.85714
4 C	0.021	-0.019	0.096	0.0159642	-0.0144438	0.0729792	0.0012957	-0.001172	0.0059232	-1.10526	-0.90476
5 C	-0.01	-0.064	-0.164	-0.007602	-0.0486528	-0.1246728	-0.000617	-0.003949	-0.010119	0.15625	6.4
6 C	-0.012	-0.01	-0.107	-0.0091224	-0.007602	-0.0809613	-0.00074	-0.000617	-0.006571	1.2	0.833333
7 H	-0.014	-0.026	0.0745	-0.0106428	-0.0197652	0.0566349	-0.000864	-0.001604	0.0045967	0.538462	1.857143
8 H	-0.011	-0.028	0.0765	-0.0083622	-0.0212856	0.0581553	-0.000679	-0.001728	0.0047201	0.392857	2.545455
9 H	0.01	-0.021	0.109	0.007602	-0.0159642	0.0828618	0.000617	-0.001296	0.0067253	-0.47619	-2.1
10 H	-0.005	-0.017	0.094	-0.003801	-0.0129234	0.0714588	-0.000309	-0.001049	0.0057998	0.294118	3.4
11 H	-0.013	-0.028	0.074	-0.0098826	-0.0212856	0.0562548	-0.000802	-0.001728	0.0045658	0.464286	2.153846
12 C	0.017	0.025	0.0975	0.0129234	0.019005	0.0741195	0.0010489	0.001543	0.0060158	0.68	1.470588
13 C	-0.001	-0.026	-0.121	-0.0007602	-0.0197652	-0.0916041	-6.17E-05	-0.001604	-0.007435	0.038462	26
14 C	0.01	-0.032	-0.122	0.007602	-0.0243264	-0.0927444	0.000617	-0.001974	-0.007527	-0.3125	-3.2
15 C	-0.013	-0.01	-0.109	-0.0098826	-0.007602	-0.0828618	-0.000802	-0.000617	-0.006725	1.3	0.769231
16 C	-0.007	-0.015	-0.105	-0.0053214	-0.011403	-0.079821	-0.000432	-0.000925	-0.006479	0.466667	2.142857
17 C	-0.019	-0.068	-0.153	-0.0144438	-0.0516936	-0.1163106	-0.001172	-0.004196	-0.00944	0.279412	3.578947
18 H	-0.013	-0.021	0.081	-0.0098826	-0.0159642	0.0615762	-0.000802	-0.001296	0.0049977	0.619048	1.615385
19 H	-0.009	-0.022	0.0835	-0.0068418	-0.0167244	0.0634767	-0.000555	-0.001357	0.005152	0.409091	2.444444
20 N	0.043	0.775	0.6185	0.0326886	0.589155	0.4701837	0.0026531	0.047818	0.0381615	0.055484	18.02326
21 H	0.002	-0.016	0.203	0.0015204	-0.0121632	0.1543206	0.0001234	-0.000987	0.0125251	-0.125	-8
22 C	-0.01	0.009	0.109	-0.007602	0.0068418	0.0828618	-0.000617	0.000555	0.0067253	-1.11111	-0.9
23 C	0.005	-0.011	0.0175	0.003801	-0.0083622	0.0133035	0.0003085	-0.000679	0.0010798	-0.45455	-2.2
24 C	-0.029	-0.001	-0.011	-0.0220458	-0.0007602	-0.0079821	-0.001789	-6.17E-05	-0.000648	29	0.034483
25 C	-0.127	-0.01	-0.182	-0.0965454	-0.007602	-0.1383564	-0.007836	-0.000617	-0.011229	12.7	0.07874

26 C	-0.118	-0.013	-0.176	-0.0897036	-0.0098826	-0.1337952	-0.007281	-0.000802	-0.010859	9.076923	0.110169
27 C	0.016	-0.028	0.015	0.0121632	-0.0212856	0.011403	0.0009872	-0.001728	0.0009255	-0.57143	-1.75
28 H	-0.017	-0.011	0.1165	-0.0129234	-0.0083622	0.0885633	-0.001049	-0.000679	0.0071881	1.545455	0.647059
29 H	-0.024	-0.011	0.109	-0.0182448	-0.0083622	0.0828618	-0.001481	-0.000679	0.0067253	2.181818	0.458333
30 N	-0.567	0.397	-0.226	-0.4310334	0.3017994	-0.1718052	-0.034984	0.024495	-0.013944	-1.42821	-0.70018
31 N	-0.067	-0.002	0.169	-0.0509334	-0.0015204	0.1284738	-0.004134	-0.000123	0.0104273	33.5	0.029851
32 O	-0.14	-0.052	-0.341	-0.106428	-0.0395304	-0.2592282	-0.008638	-0.003208	-0.02104	2.692308	0.371429
33 O	-0.145	-0.011	-0.371	-0.110229	-0.0083622	-0.2816541	-0.008947	-0.000679	-0.02286	13.18182	0.075862
34 N	-0.006	0.003	0.2465	-0.0045612	0.0022806	0.1873893	-0.00037	0.000185	0.0152091	-2	-0.5
35 O	-0.061	-0.041	-0.272	-0.0463722	-0.0311682	-0.2067744	-0.003764	-0.00253	-0.016782	1.487805	0.672131
36 O	-0.067	0.019	-0.237	-0.0509334	0.0144438	-0.1801674	-0.004134	0.001172	-0.014623	-3.52632	-0.28358
37 N	0.006	0.006	0.264	0.0045612	0.0045612	0.2006928	0.0003702	0.00037	0.0162888	1	1
38 O	-0.036	-0.029	-0.237	-0.0273672	-0.0220458	-0.1801674	-0.002221	-0.001789	-0.014623	1.241379	0.805556
39 O	0.228	-0.027	0.0275	0.1733256	-0.0205254	0.0209055	0.0140676	-0.001666	0.0016968	-8.44444	-0.11842
40 H	-0.014	-0.021	0.079	-0.0106428	-0.0159642	0.0600558	-0.000864	-0.001296	0.0048743	0.666667	1.5
41 H	-0.004	-0.01	0.1035	-0.0030408	-0.007602	0.0786807	-0.000247	-0.000617	0.006386	0.4	2.5
42 H	0.015	-0.012	0.115	0.011403	-0.0091224	0.087423	0.0009255	-0.00074	0.0070955	-1.25	-0.8

Table S4

Vibrational frequency assignments of BPPTS based on Potential energy distribution (PED) calculation

Calculated wavenumbers (cm^{-1})		Mode of assignments with (PED %)
Unscaled	Scaled	
2812	2750	ν (N19-H24) (29)
2701	2642	ν (N19-H24) (26)
2732	2672	ν (N20-H25) (59)
2812	2750	ν (N47-H52) (62)
2732	2672	ν (N47-H52) (20)
2701	2642	ν (N48-H53) (53)
2617	2559	ν (N48-H53) (39)
3191	3121	ν (C2-H15) (93)
3159	3090	ν (C3-H16) (93)
3167	3097	ν (C5-H17) (94)
3194	3124	ν (C6-H18) (94)
3283	3211	ν (C21-H26) (94)
3267	3195	ν (C21-H26) (52)
3283	3211	ν (C22-H27) (69)
3261	3189	ν (C23-H28) (57)
3267	3195	ν (C49-H54) (49)
3282	3210	ν (C50-H55) (66)
3261	3189	ν (C51-H56) (53)
3103	3035	ν (C11-H12) (79)
3203	3133	ν (C30-H43) (96)
3196	3126	ν (C34-H46) (94)
3072	3004	ν (C11-H13) (53)
3023	2956	ν (C11-H14) (51)
3164	3094	ν (C31-H44) (95)
3160	3090	ν (C33-H45) (94)
3104	3036	ν (C39-H40) (76)
3075	3007	ν (C39-H41) (55)
3075	3007	ν (C39-H42) (52)
201	197	ν (O9-H24) (17)
1639	1603	ν (C3-C2) (29)
1612	1577	ν (C6-C1) (31)
1538	1504	ν (N19-C23) (20)
1200	1174	ν (N47-N48) (26)
1229	1202	ν (C11-C4) (39)
1226	1199	ν (S7-O8) (44)
1226	1199	ν (S7-O10) (44)
1185	1159	ν (S35-O36) (54)
297	290	ν (S35-C29) (40)
278	272	ν (S7-C1) (50)

128	125	ν (O38-N20) (16)
1667	1630	δ (H25-N20-C21) (22)
1593	1558	δ (H25-N20-C21) (22)
1040	1017	δ (C33-C34-C29) (22)
1528	1494	δ (H15-C2-C3) (23)
1488	1455	δ (H12-C11-H14) (35)
1488	1455	δ (H13-C11-H12) (42)
1415	1384	δ (H14-C11-H13) (43)
1487	1454	δ (H40-C39-H42) (45)
1414	1383	δ (H42-C39-H41) (44)
1033	1010	δ (C3-C2-C1) (34)
176	172	δ (C6-C1-S7) (52)
896	876	δ (C21-N20-N19) (16)
1033	1010	δ (C2-C1-C6) (16)
929	909	δ (C22-C21-N20) (19)
1227	1200	δ (C32-C31-C30) (12)
928	908	δ (C50-C49-N48) (24)
383	375	δ (C11-C4-C5) (37)
522	511	δ (O10-S7-O8) (60)
538	526	δ (O38-S35-O37) (52)

ν - Stretching wavenumbers and δ - bending wavenumbers

Structural Confirmation of BPPTS by XRD analysis

BPPTS crystallizes in monoclinic crystal system with space group of $P2_1/c$, having Z = 8. The ORTEP of BPPTS drawn in 50% probability is depicted in Figure S7. The crystallographic data and refinement parameters are shown in Table S5.

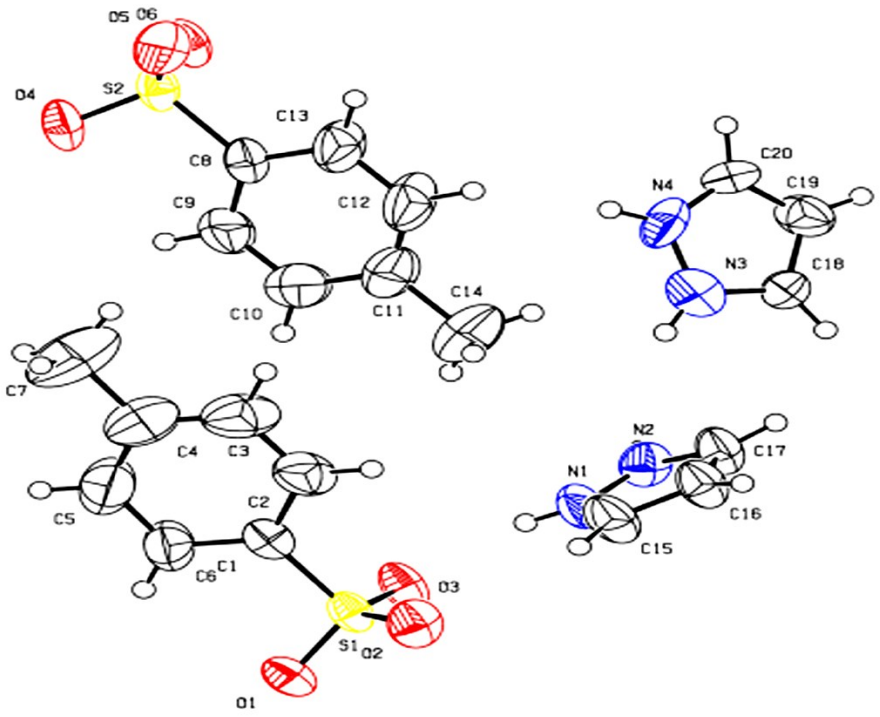

Figure S7. ORTEP of BPPTS with 50% probability

Table S5 Crystallographic data and refinement parameters of BPPTS

Chemical formula	$2(C_7H_7O_3S)\bullet2(C_3H_5N_2)$
Empirical formula weight (M_r)	480.56
Diffractometer	Xcalibur, Eos, Gemini
Radiation Type	Cu $K\alpha$ (λ = 1.541 Å)
Temperature (K)	293
Crystal size (mm)	0.18 × 0.16 × 0.12
Density (D_x)	1.395 Mg/m^3
Crystal system, Space group	Monoclinic, $P2_1/c$
a, b, c (Å)	9.363 (15), 15.757 (3), 15.798 (3)
α, β, γ (°)	90, 100.931 (17) , 90
V (Å^3), Z	2288.76 (7), 8
Refinement method	Least square - Full matrix
No. of reflections- independent, measured and observed	9486, 4398 and 3883
Criterion for observed reflections	$I > 2\sigma(I)$
T_{min}, T_{max}	0.573, 1.000
h, k, l	-11→ h→11, -19→ k → 19, -19 → l → 19

θ_{max} and θ_{min} (˚)	71.8 and 2.8
$wR(F^2)$, $R[F^2 > 2s(F^2)]$	0.159, 0.057
R1, R_{int}	0.06, 0.021
Data completeness	0.979
CCDC No.	1054657

In deprotonated *p*-toluenesulphonate anion, S2-O4 and S1-O3 bond lengths are 1.465 and 1.459 Å, respectively, which are longer by *ca.* 0.010 Å than the normal bond distance of S-O (1.450 Å). The strong intermolecular hydrogen bonding interactions, N2-H18…O4 (2.479 Å) and N4-H23…O3 (2.799 Å)[1] are responsible for this deviation. Similarly, bond distances of C8-S2 (1.765 Å) and C1-S1 (1.761 Å) are increased than the normal C-S bond length (1.752 Å) and the increase in length is due to the presence of resonance involving double bond character of all the S=O groups of *p*-toluenesulphonate anion. The C-H…O intermolecular hydrogen bonding contacts stabilize the whole molecular system (C20-H22…O1 (2.771 Å), C6-H4…O1 (2.886 Å) and C9-H8…O4 (2.916 Å)). Bond angle of O6-S2-O4 is 110.5°, which is smaller than the standard value of O-S-O (112.7°). Similarly, the bond length of C8-S2-O5 is 113.4°, which is greater than the normal value of 106.2°. This contrasting deviation in bond angles of O6-S2-O4 and C8-S2-O5 endorse the formation of intermolecular hydrogen bonding. There is a minor centroid…centroid (π…π) interactions observed on *p*-toluenesulphonate…*p*-toluenesulphonate (C10…C10) and pyrazolium…*p*-toluenesulphonate (C19…C2), which are 3.393 and 3.334 Å, respectively. This creates a direct evidence for the interaction of BPPTS with DNA through a groove mode of binding (C-H…O, N-H…O and O-H…O). A strong intermolecular H…H (H8…H4) contact observed between *p*-toluenesulphonate moieties with a distance of 2.288 Å facilitates a supramolecular bridge.

In the supramolecular assembly, each and every bis(pyrazolium *p*-toluenesulphonate) asymmetric unit is connected through various N-H…O, C-H…O, O-H…O and N^+-H…O^- inter and intramolecular hydrogen bonding contacts. The molecular structure of BPPTS is found to be a 3D square shaped channels and the pyrazolium moiety acts as a host component for acidic moiety stabilizing the molecular framework. It is interesting to notice that the stability of BPPTS is reinforced by a ring graph set of $R_2^2(6)$, where oxygen atoms acts as a hydrogen acceptor and N-Hs act as a hydrogen donors.[2] Ring graph set is shown in Figure S8. The detailed intra and intermolecular hydrogen bonding parameters are shown in Table S6.

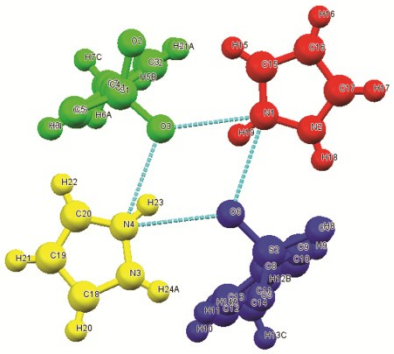

Figure S8. $R_2^2(6)$ **Ring graph set of BPPTS**

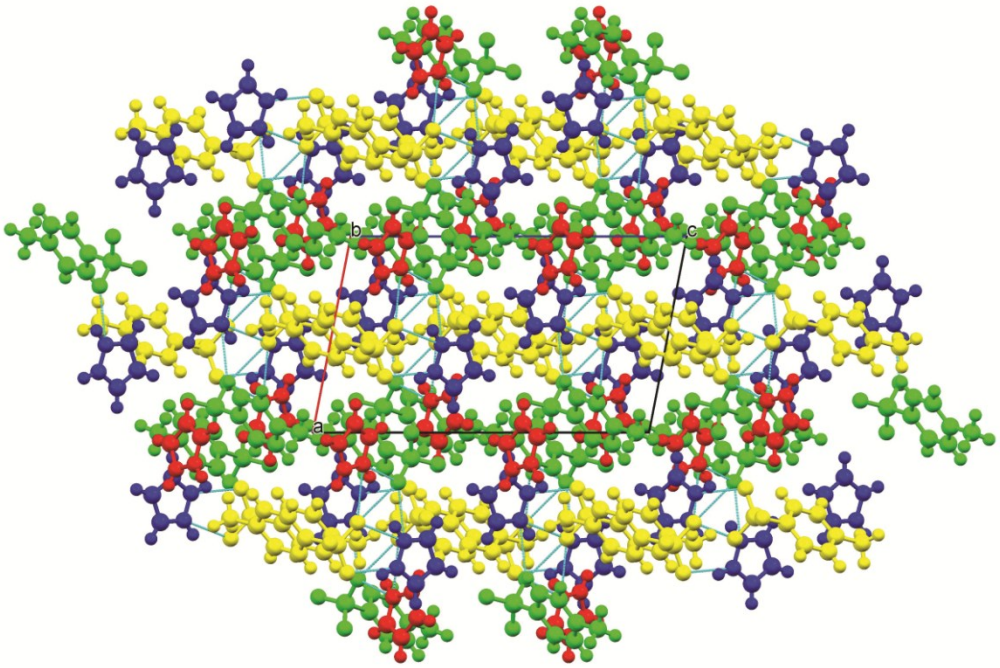

Figure S9. Supramolecular assembly of BPPTS along 'b' axis

Table S6 Inter and intramolecular interactions in BPPTS

D-H…A	D-H (Å)	H…A (Å)	ARU	D…A (Å)	D-H…A (Å)	Symmetry
N(2)-H(18)...O(1)	0.86	2.59	1455.01	3.083 (3)	117	-1+x,y,z
N(2)-H(18)...O(4)	0.86	1.93	3666.02	2.749(3)	158	1-x,1-y,1-z
N(1)-H(19)...O(3)	0.86	2.10	1555.01	2.800(3)	138	
N(1)-H(19)...O(6)	0.86	2.15	3666.02	2.821(3)	134	1-x,1-y,1-z

N(4)-H(23)...O(3)	0.86	2.07	2655.01	2.799(3)	142	-x,1/2+y,1/2-z
N(4)-H(23)...O(6)	0.86	2.26	4564.02	2.900(3)	132	x,3/2-y,-1/2+z
C(6)-H(4)...O(1) (Intra)	0.93	2.51		2.886(4)	105	
C(9)-H(8)...O(4) (Intra)	0.93	2.54		2.916(4)	104	
C(16)-H(16)...O(2)	0.93	2.51	3665.01	3.416(3)	166	1-x,1-y,-z
C(17)-H(17)...O(1)	0.93	2.54	1455.01	3.075(3)	117	-1+x,y,z
C(20)-H(22)...O(1)	0.93	1.94	2655.01	2.771(3)	148	-x,1/2+y,1/2-z
C(20)-H(22)...O(4)	0.93	2.44	4464.02	3.056(3)	124	-1+x,3/2-y,-1/2+z

Atom O6 of the anion forms trifurcated hydrogen bond with hydrogen atoms of N4-H23, N1-H19 and N2-H18 and also the atom O3 forms a trifurcated hydrogen bond with N4-H23, N1-H19 and C15-H15 enabling a strong supramolecular network. Figure S9 depicts the supramolecular 3D network of BPPTS in its asymmetric unit. Twisting of both cation and anion in its asymmetric unit facilitates the supramolecular network through enormous hydrogen bonding interactions. The deviation in angles planar that are observed in the packing diagram along ‘a’ axis are 87.23° between pyrazolium and *p*-toluenesulphonate moieties and 12.16° between two anionic moieties and 17.09° between two cationic moieties.

References

1. S. K. Arora, M. Sundaralingam, *Acta Cryst*. **1971**, *B27*, 1293-1298.
2. P. Muthuraja, T. J. Beaula, T. Shanmugavadivu, V. B. Jothy, M. Dhandapani, *J. Mol. Struct*. **2017**, *1137*, 649-662.