Supplementary Information

Supramolecular Assembly between Cationic Pyridinium-Pillararene and Aminosalicylate Drug

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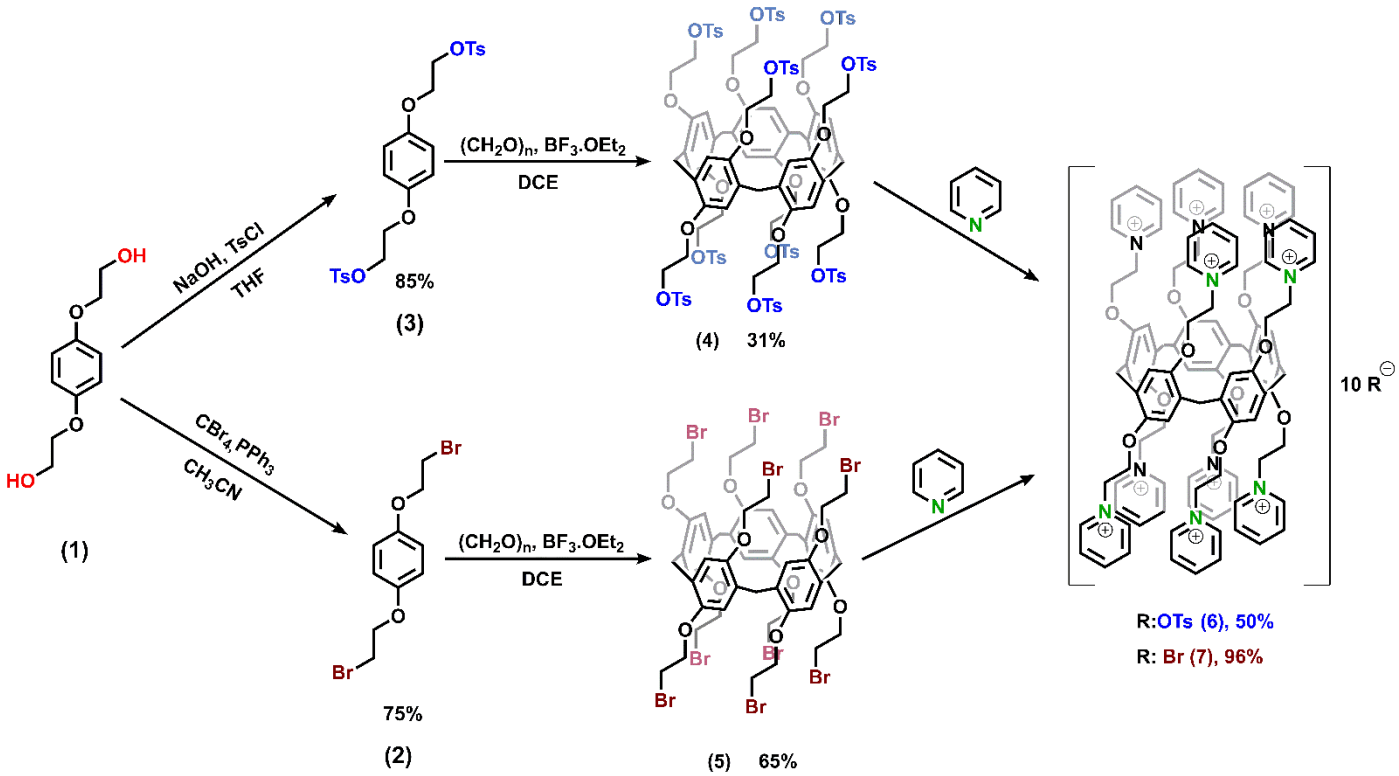

Figure S1. Synthesis of P[5]Py.

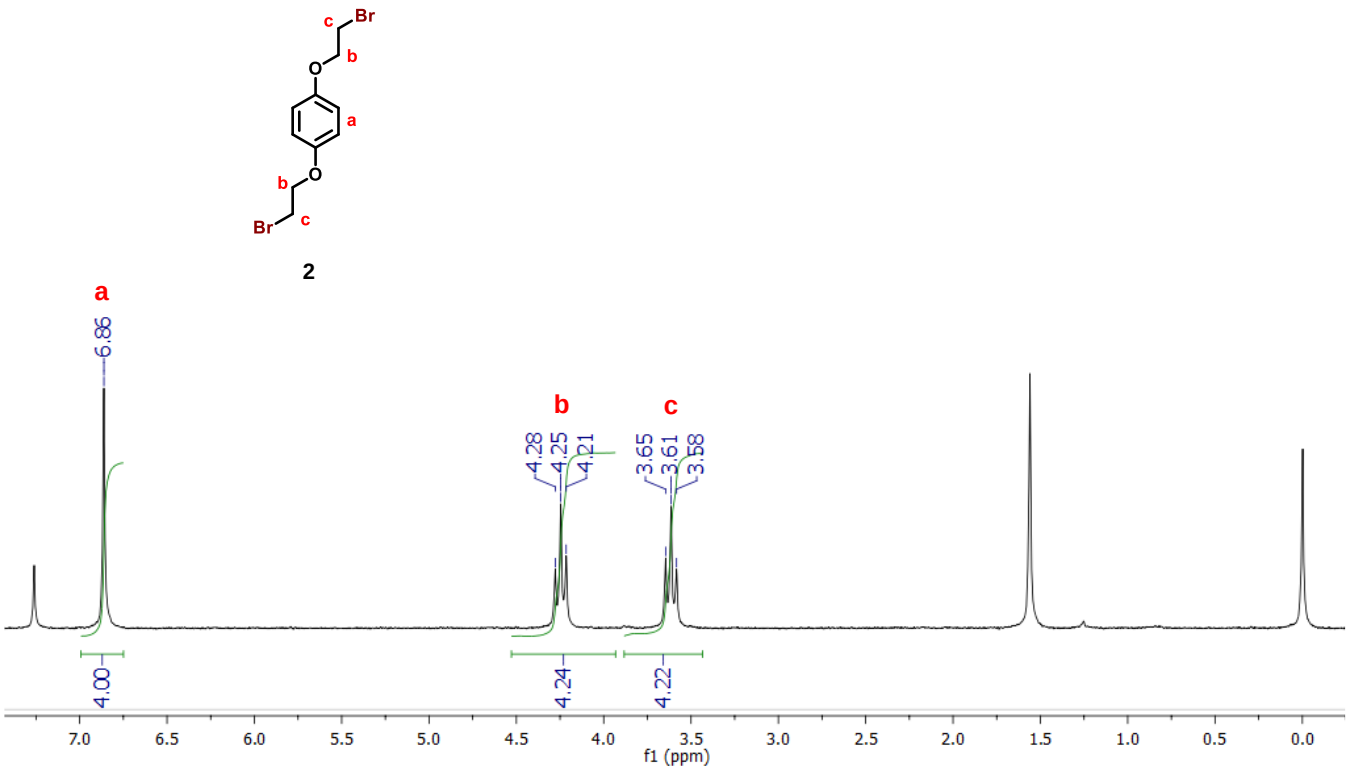

Figure S2. ^{1}H NMR spectra (200 MHz, $CDCl_3$) at 25 ºC for HQBr (compound **2**).

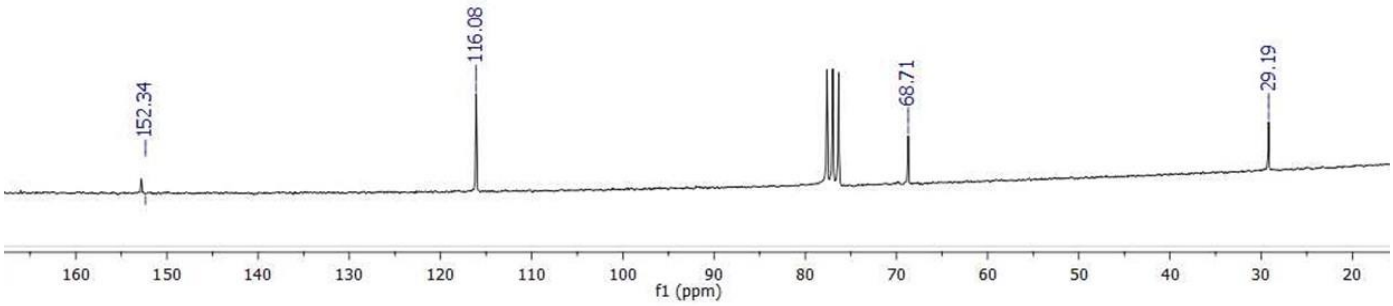

Figure S3. ^{13}C NMR spectra (50 MHz, $CDCl_3$) at 25 ºC for HQBr (compound **2**).

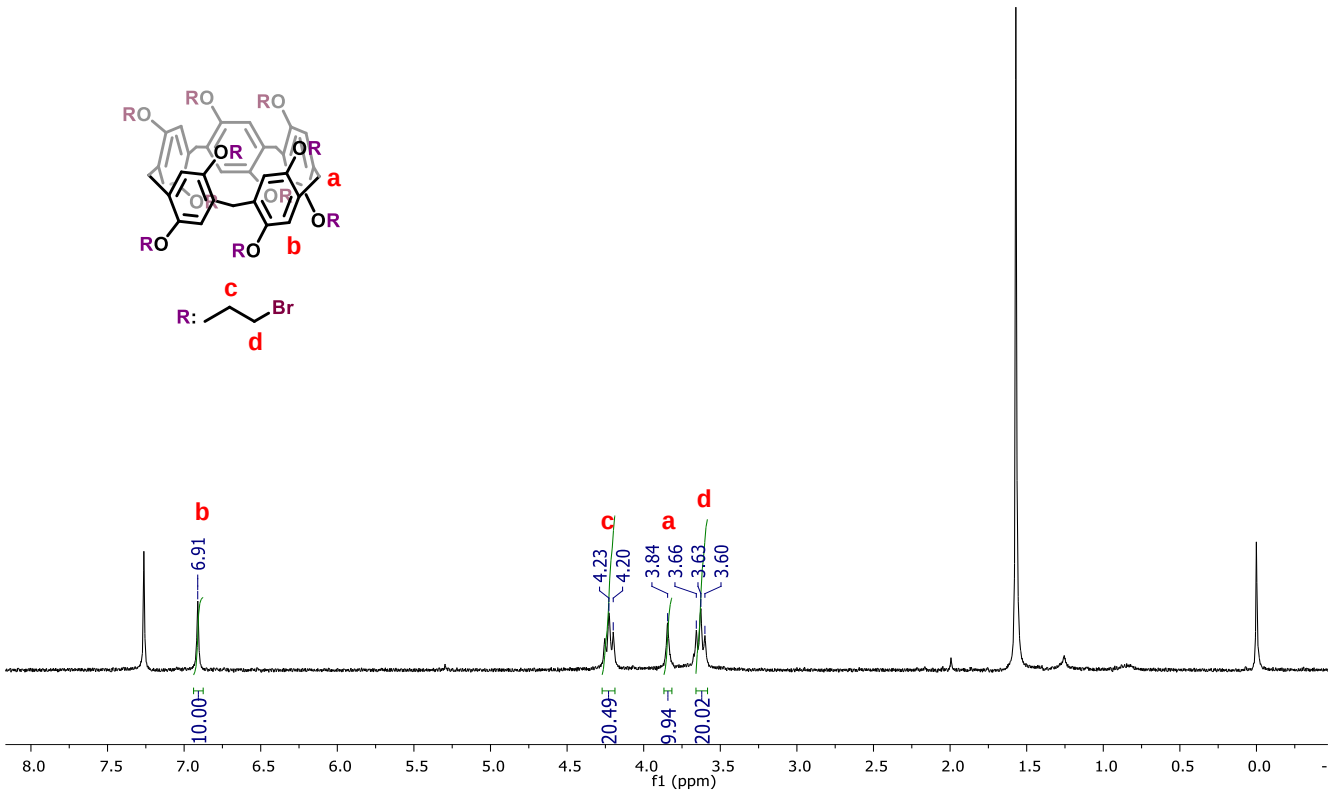

Figure S4. ^{1}H NMR spectra (200 MHz, D_2O) at 25 ºC for P[5]Br (compound **5**).

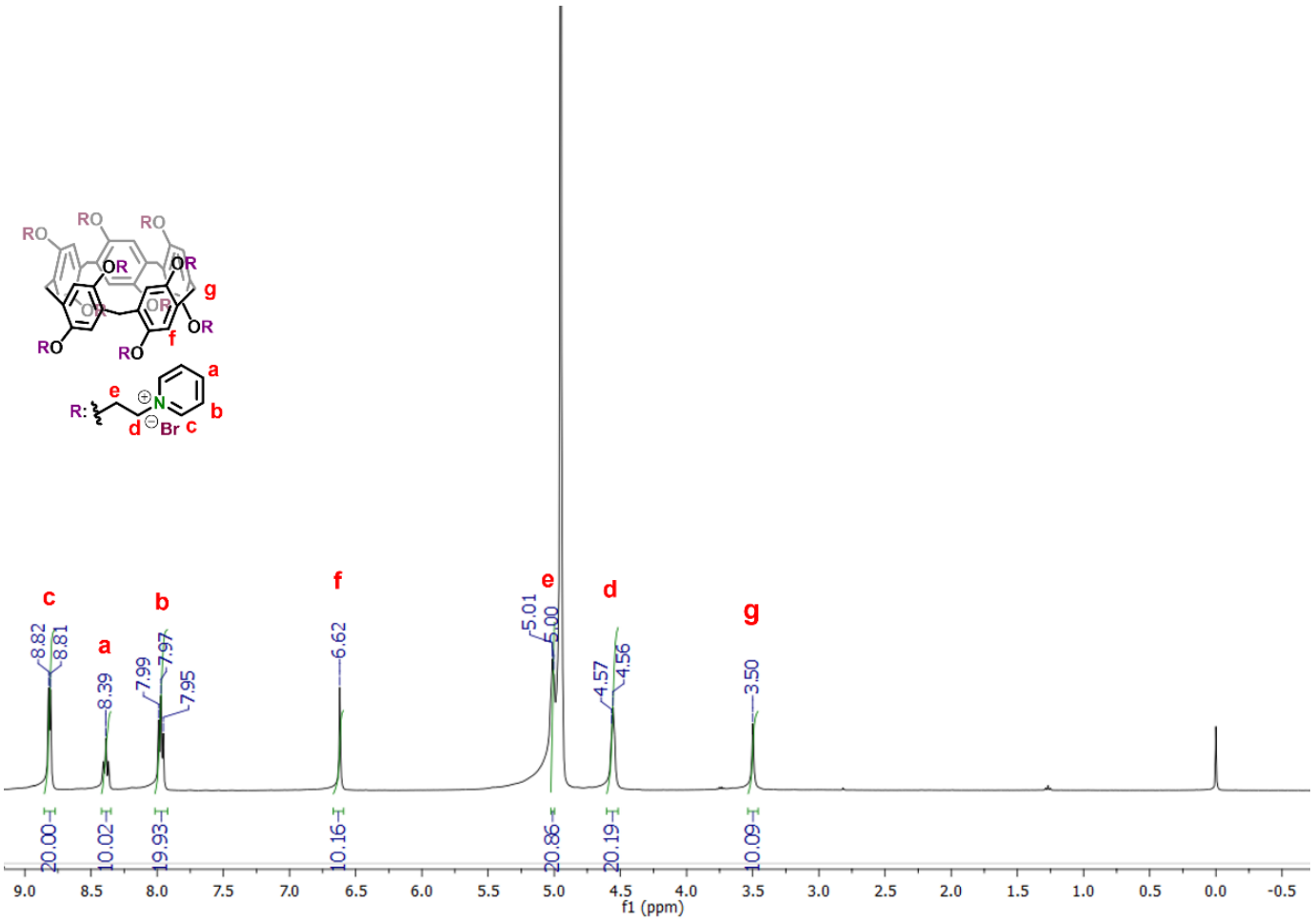

Figure S5. ^{1}H NMR spectra (200 MHz, D_2O) at 25 ºC for P[5]Py (compound **7**).

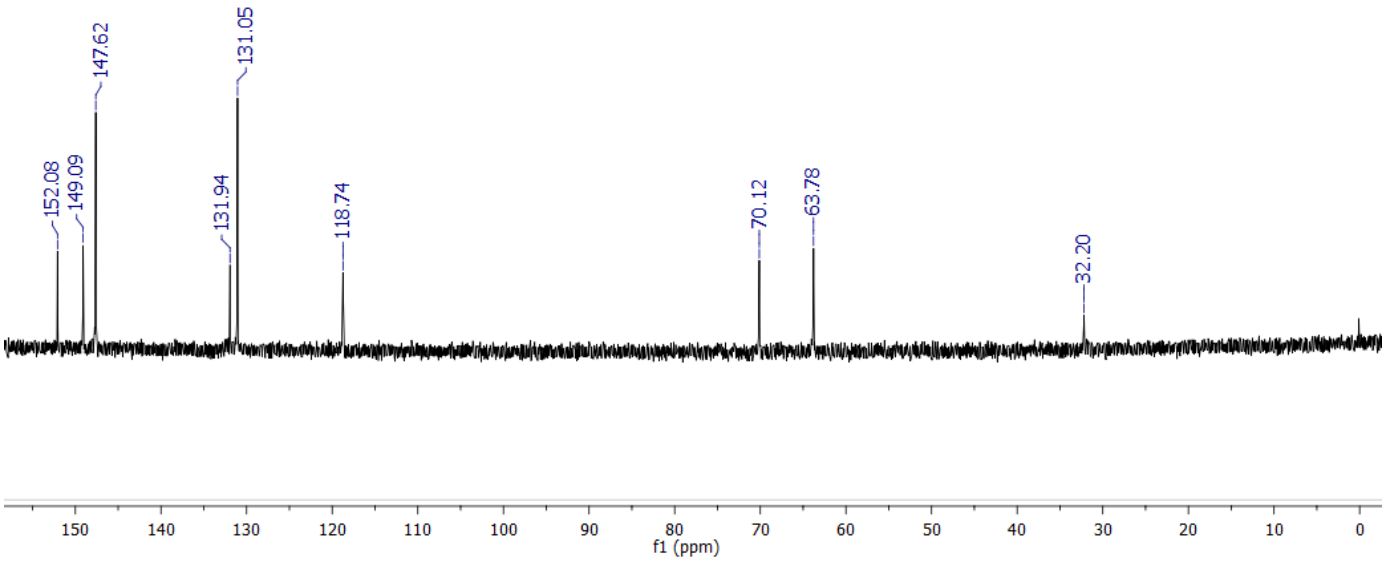

Figure S6. ^{13}C NMR spectra (50 MHz, D_2O) at 25 ºC for P[5]Py (compound **7**).

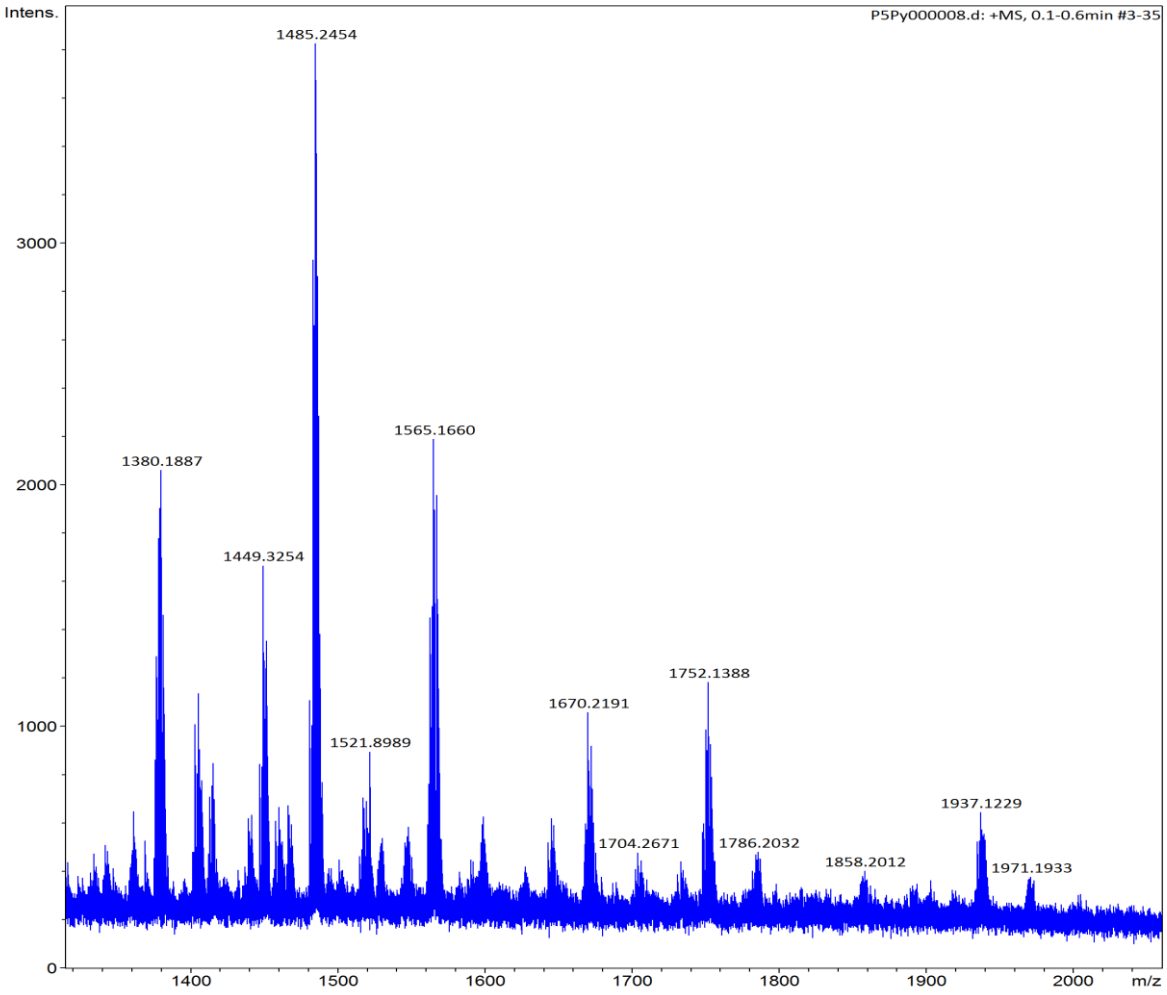

Figure S7. High resolution mass spectrum of P[5]Py (compound **7**).

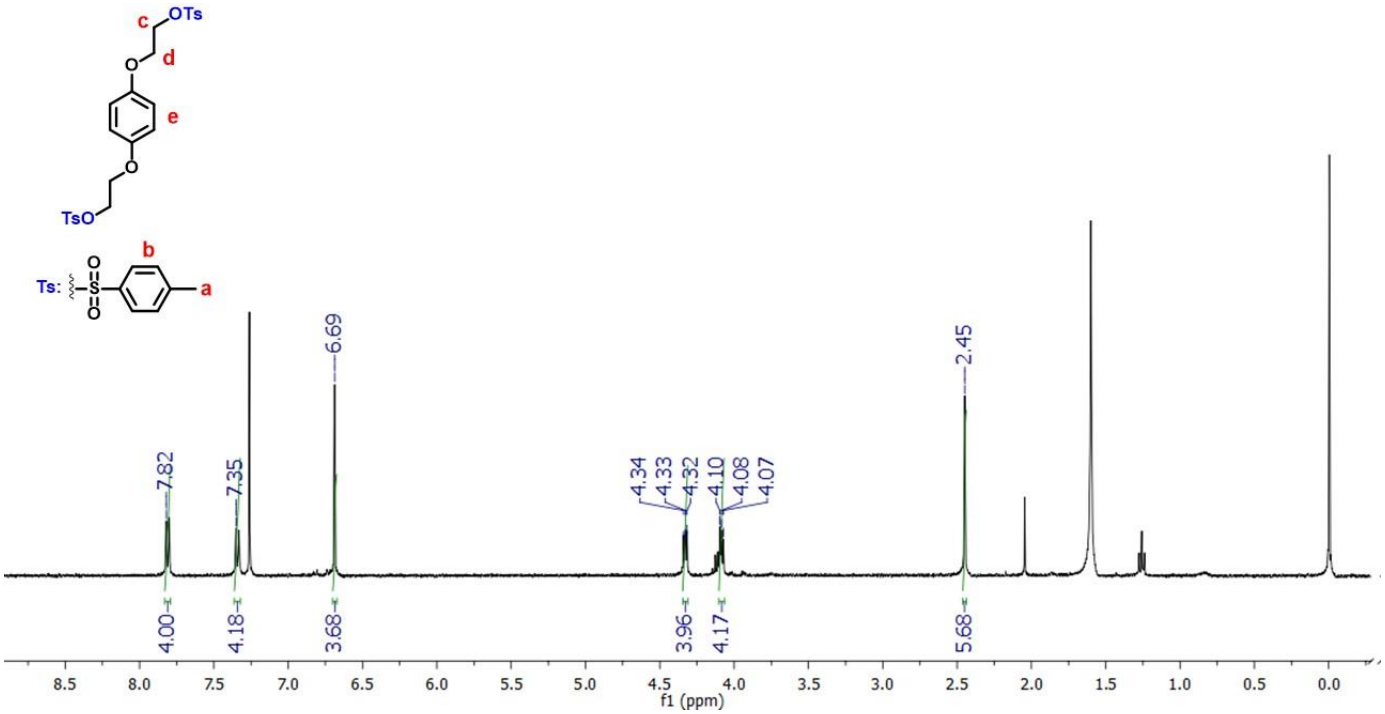

Figure S8. ^{1}H NMR spectra (200 MHz, $CDCl_3$) at 25 ºC, for HQOTs (compound **3**).

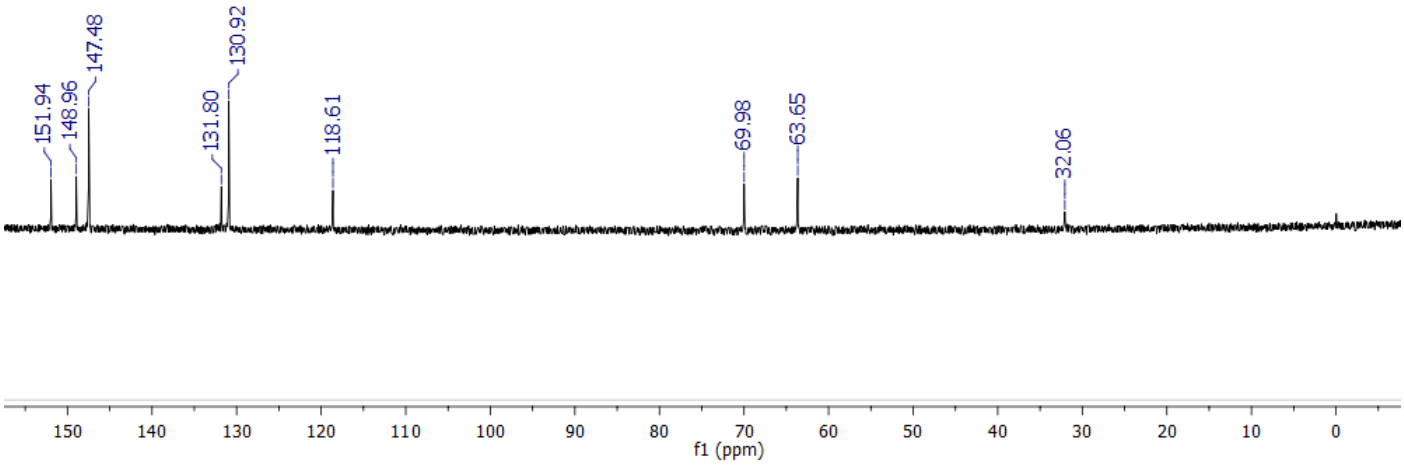

Figure S9. ^{13}C NMR spectra (50 MHz, $CDCl_3$) at 25 ºC, for HQOTs (compound **3**).

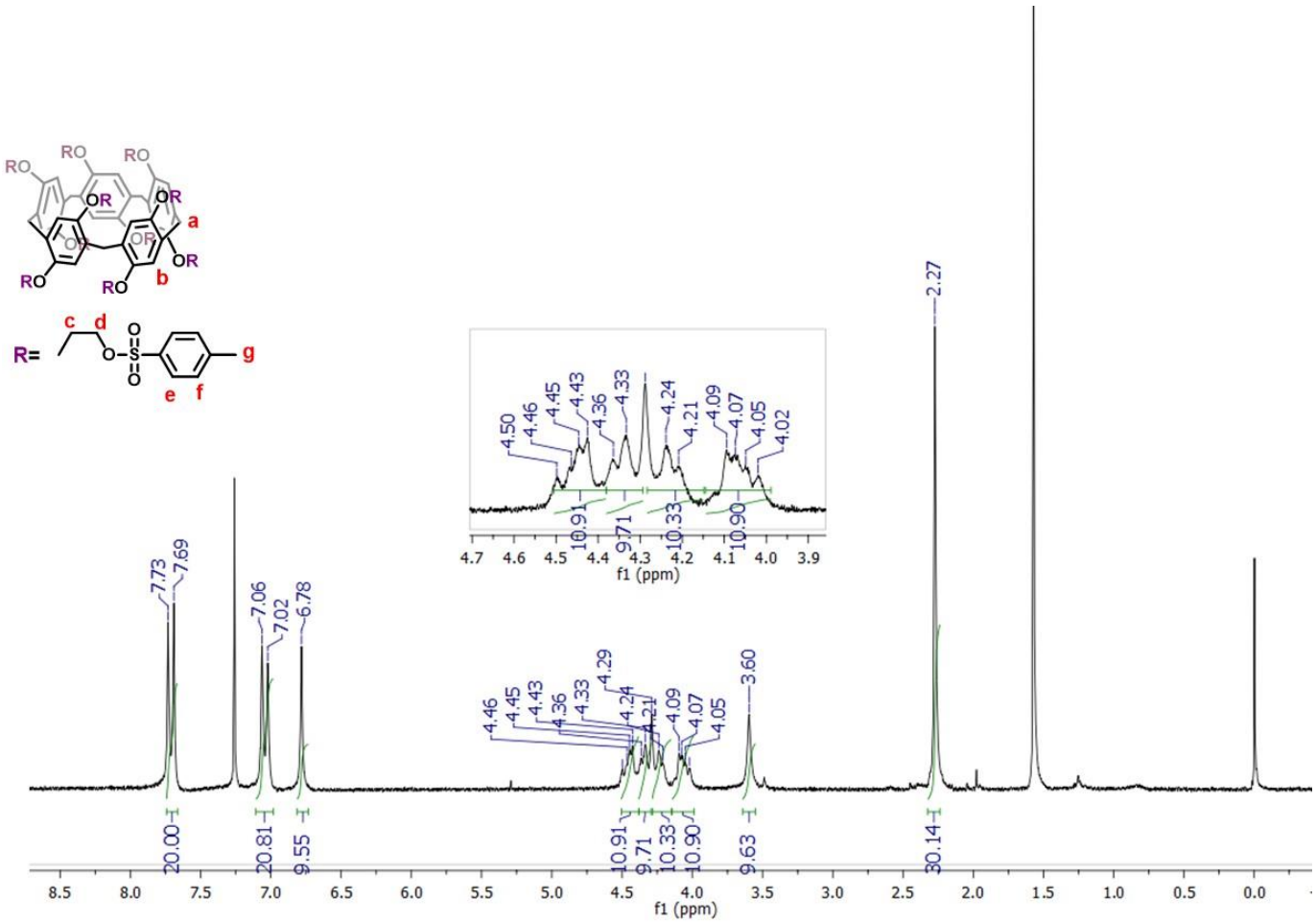

Figure S10. ^{1}H NMR spectra (200 MHz, $CDCl_3$) at 25 ºC, for P[5]OTs (compound **4**).

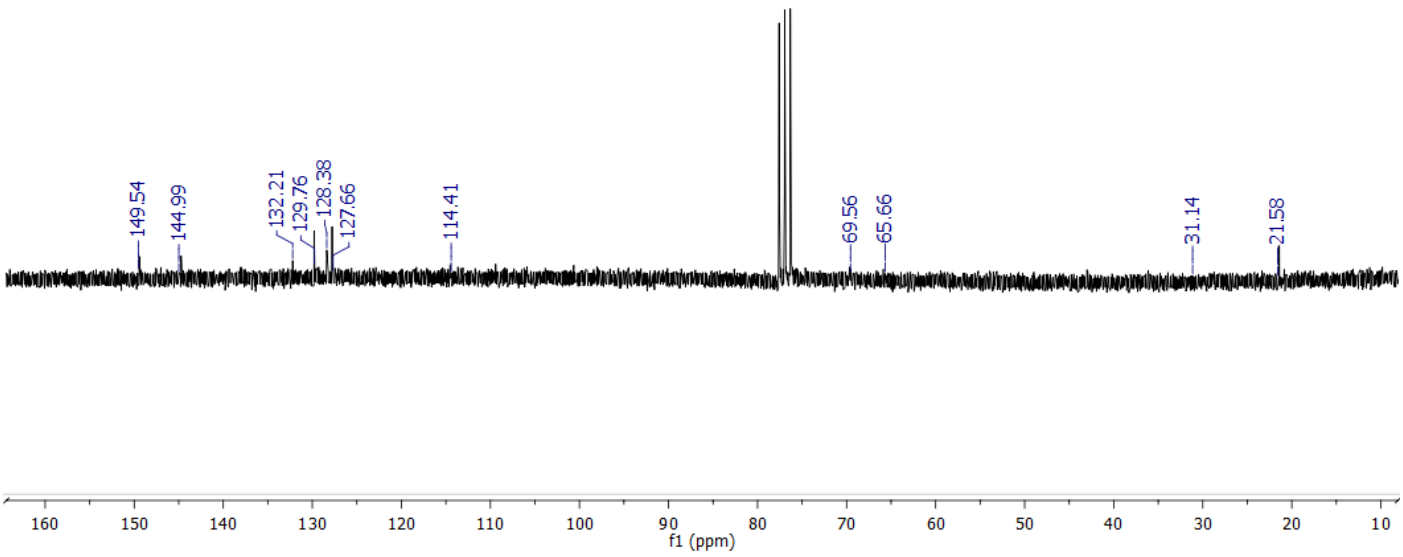

Figure S11. ^{13}C NMR spectra (50 MHz, $CDCl_3$) at 25 ºC, for P[5]OTs (compound **4**) in $CDCl_3$.

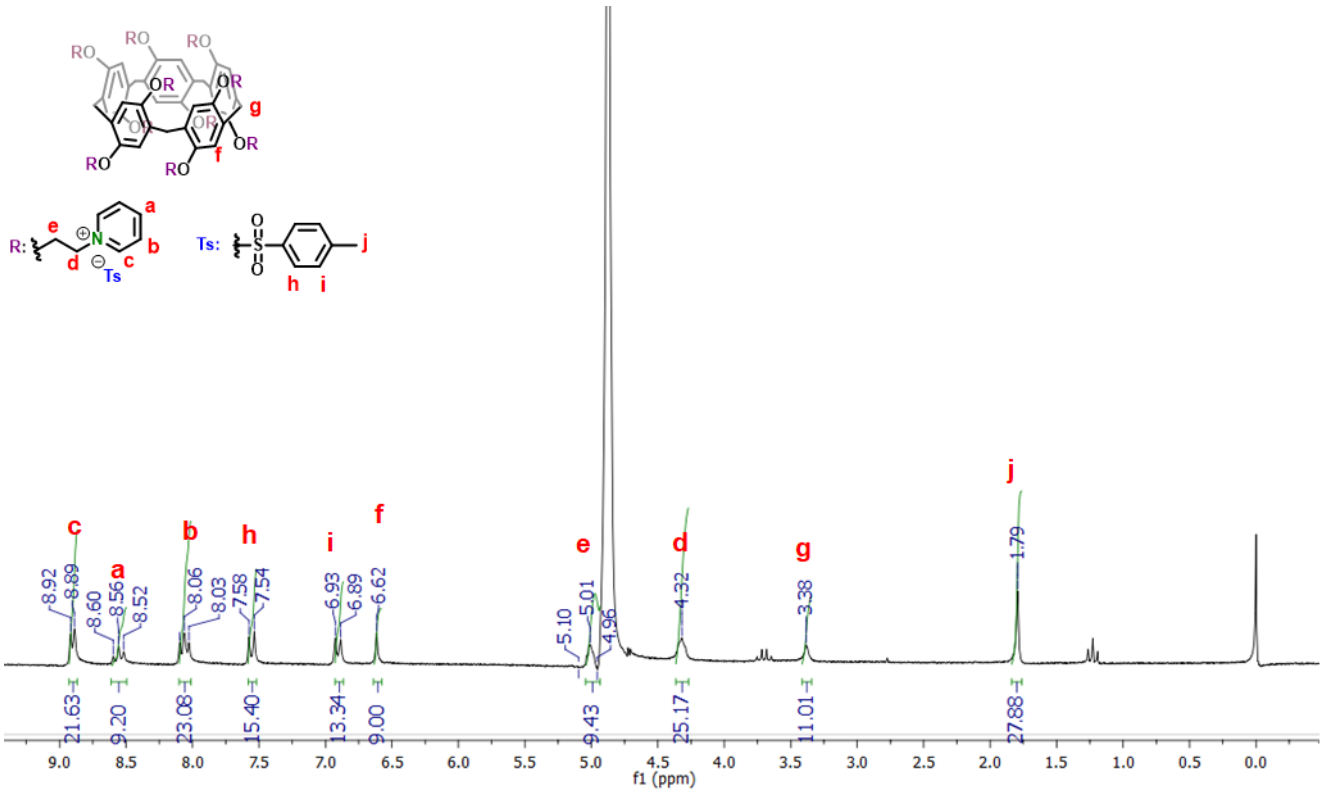

Figure 12. ^{1}H NMR spectra (200 MHz, D_2O) at 25 ºC, for P[5]Py (compound **6**) from tosyl.

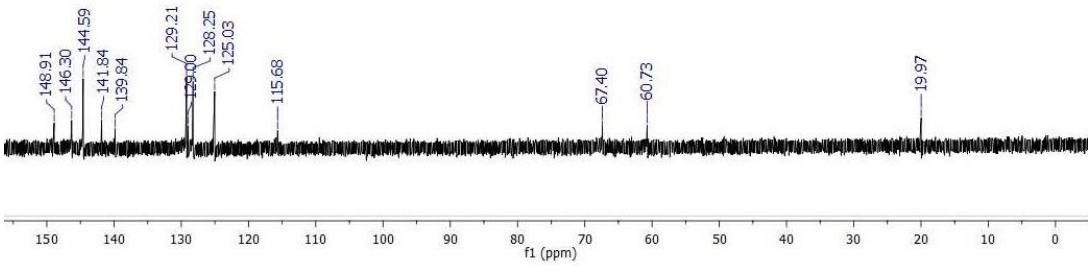

Figure S13. ^{13}C NMR spectra (50 MHz, D_2O) at 25 ºC for P[5]Py (compound **6**) from tosyl.

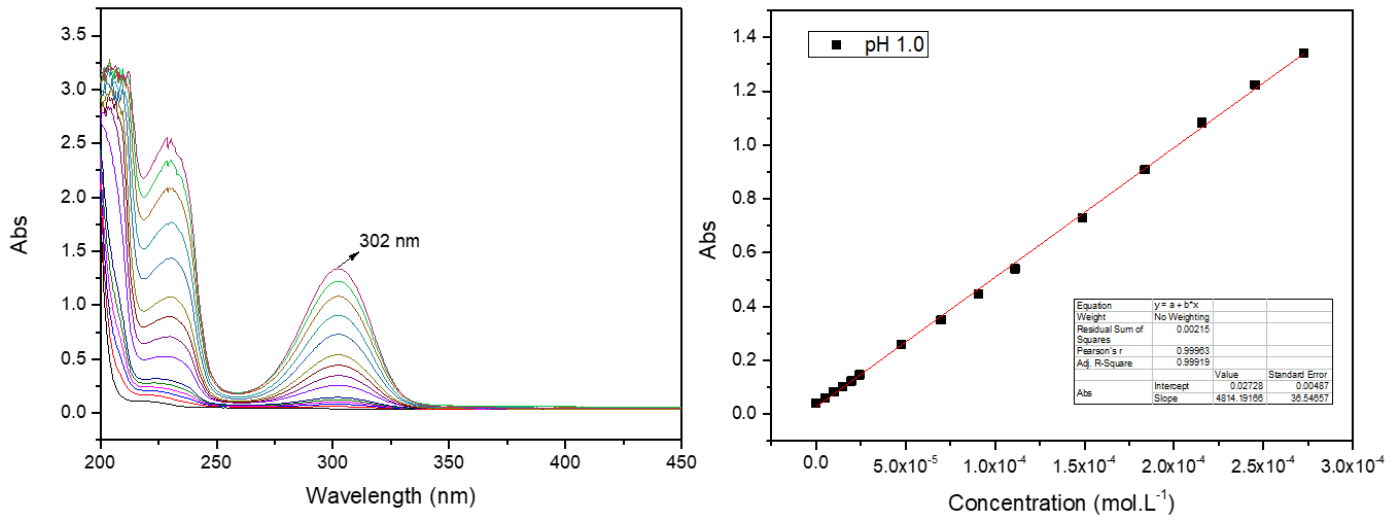

Figure S14. MSZ absorption spectra as a function of an increase of its on concentration, at pH 1.0 and 25 ºC.

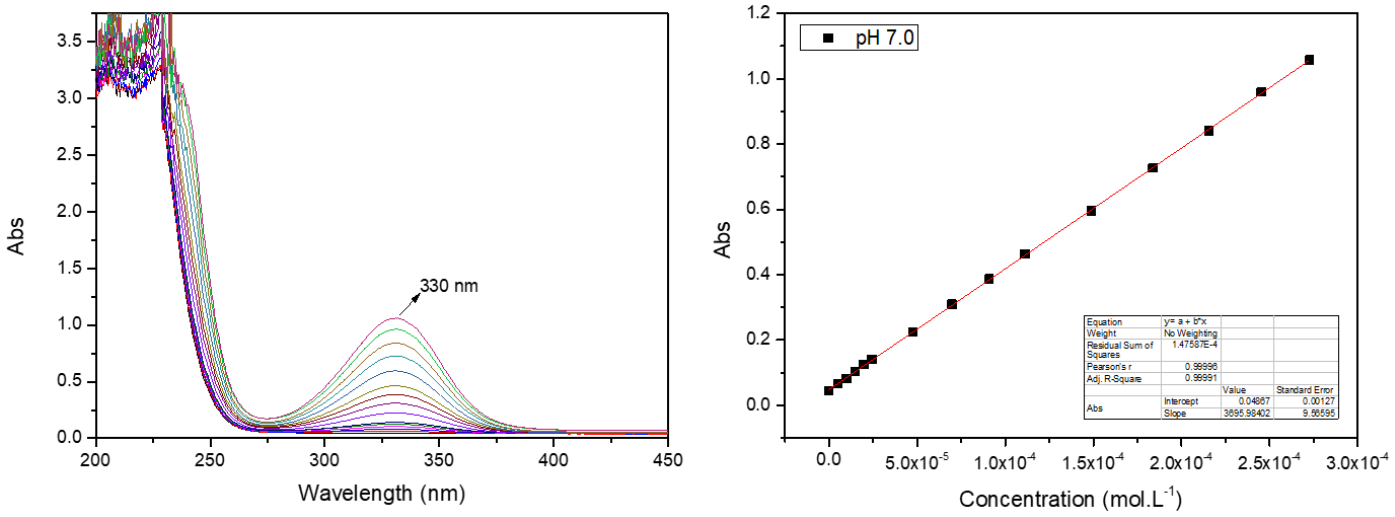

Figure S15. MSZ absorption spectra as a function of an increase of its on concentration, at pH 7.0 and 25 ºC.

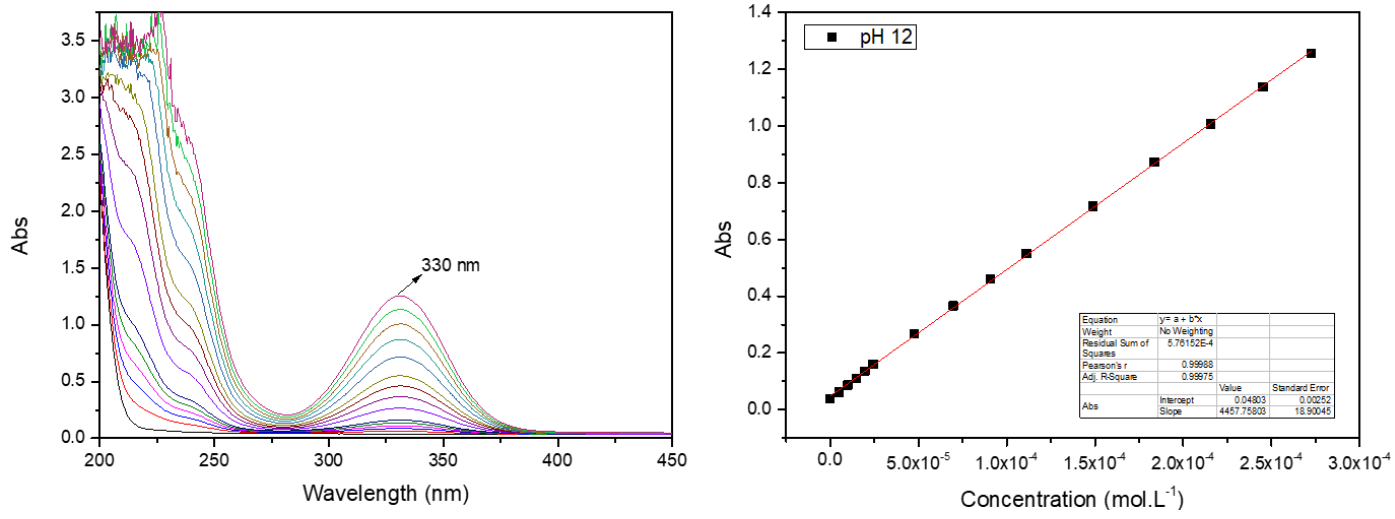

Figure S16. MSZ absorption spectra as a function of an increase of its on concentration, at pH 12.0 and 25 ºC.

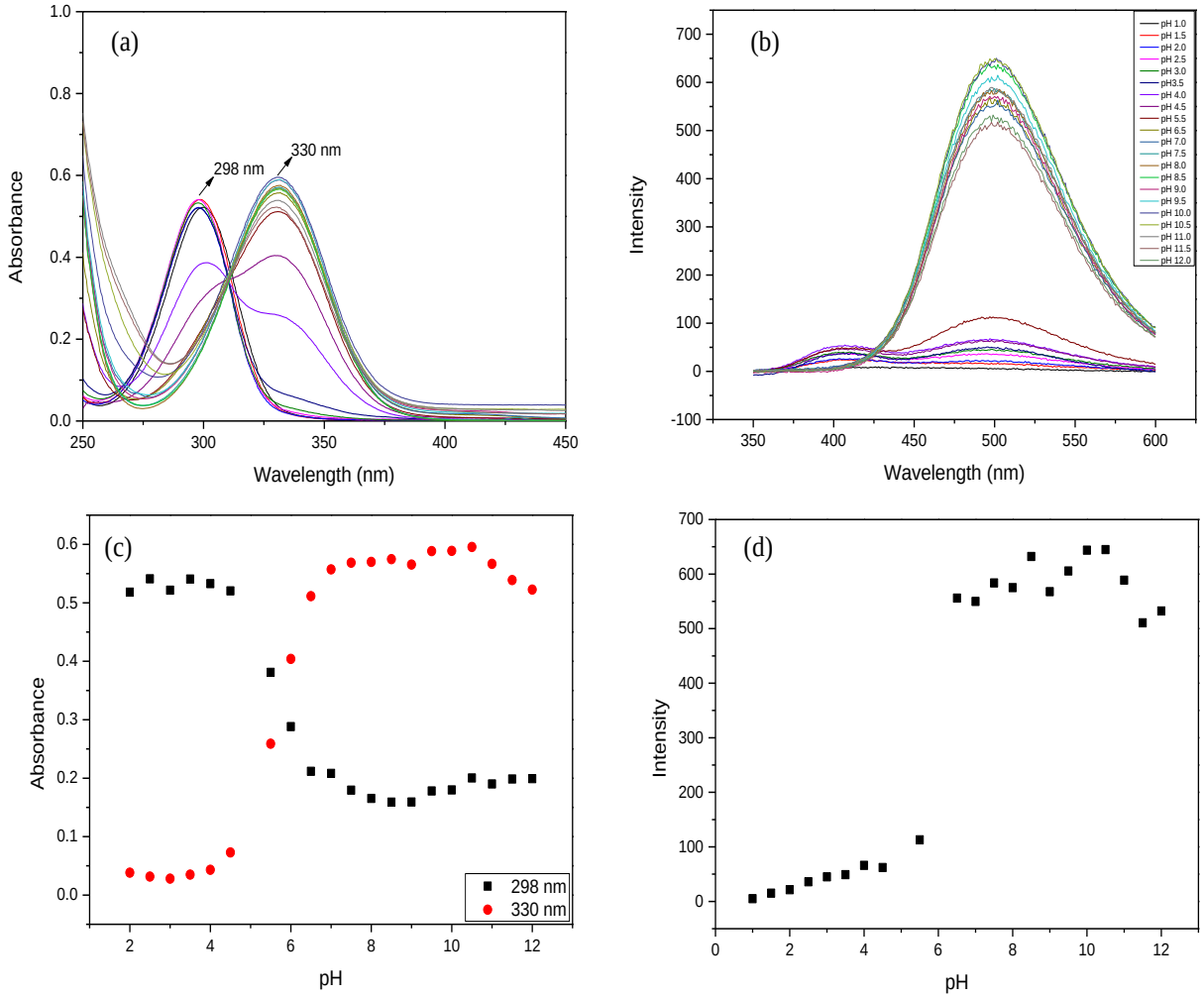

Figure S17. Influence of pH on: UV-Vis absorption, with absorbance in 298 and 330 nm, respectively (a and c); fluorescence intensity with emission in 400 (pH ≤ 5.5) and 500 nm (pH ≥ 6) (b); In (d) the difference in fluorescence intensity at 500 nm is shown.

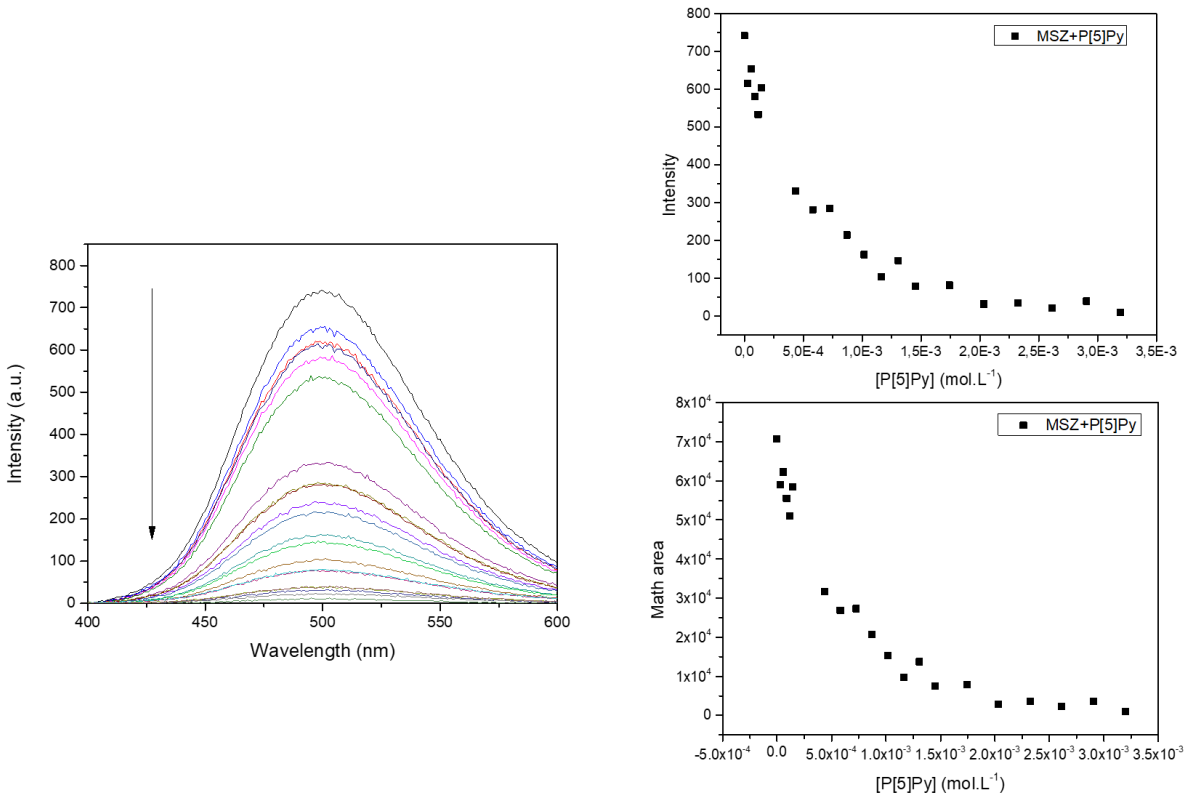

Figure S18. Influence of media pH in MSZ and P[5]Py complexation intensity at 25 ºC. [MSZ] = [P[5]Py] = 1.4×10^{-4} mol L^{-1}, λ_{exc}= 330 nm with a slit of 5 (left). The plot was performed using fluorescence emission intensity (up) and the area under the fluorescence emission spectra (down).

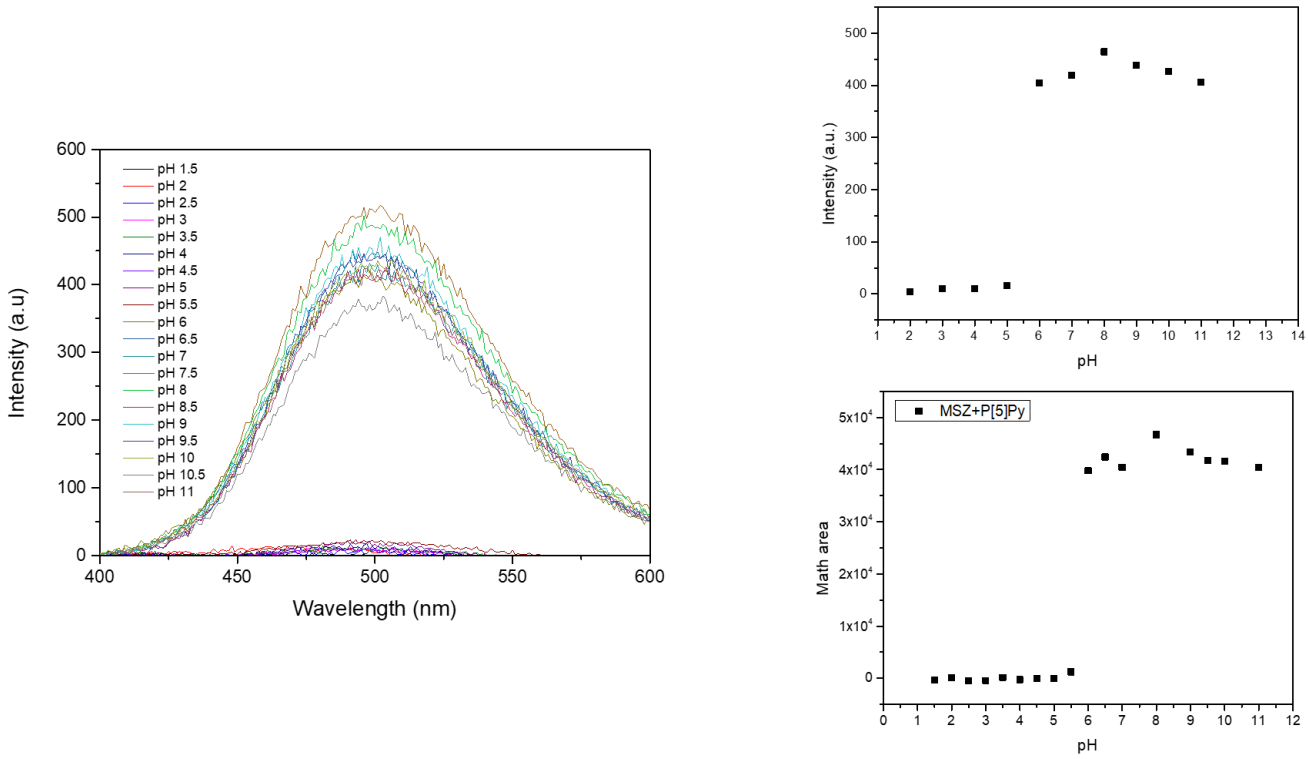

Figure S19. Fluorescence intensity of MSZ (1.4×10^{-4} mol L^{-1}) in the absence of P[5]Py, with increasing pH of the medium, at 25 ºC. The plot was performed using fluorescence emission intensity (up) and the area under the fluorescence emission spectra (down).

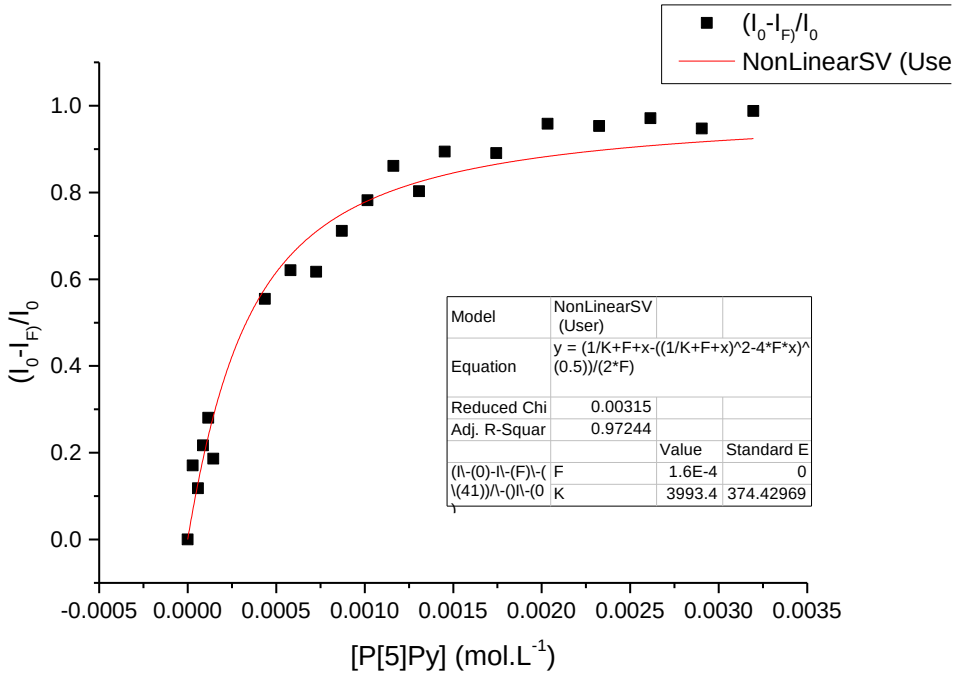

Figure S20. Stern-Volmer plot for MSZ (1.4×10^{-4} mol L^{-1}) in the presence of P[5]Py, at pH = 7.5 and 25 ºC.

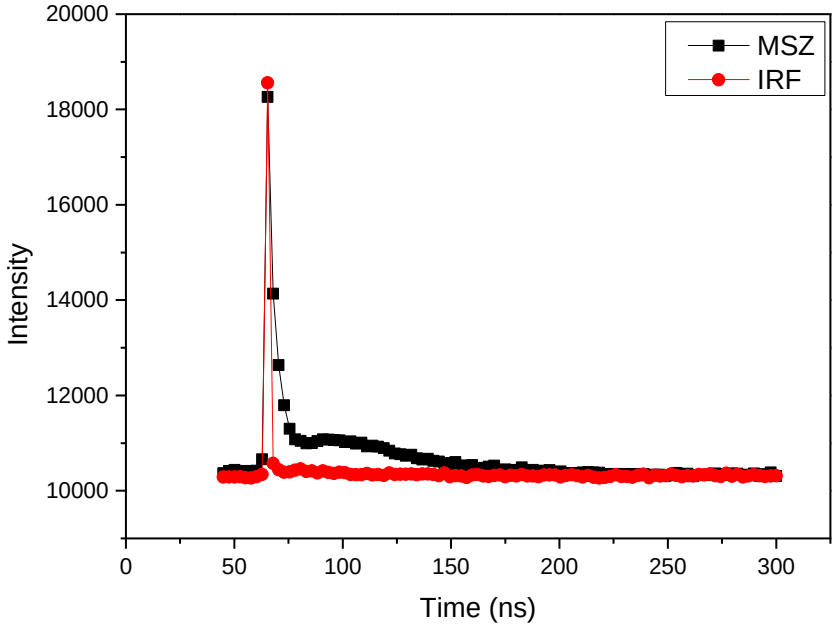

Figure S21. Lifetime fluorescence MSZ (1.4×10^{-4} mol L^{-1}), at pH = 7.5 and 25 ºC.

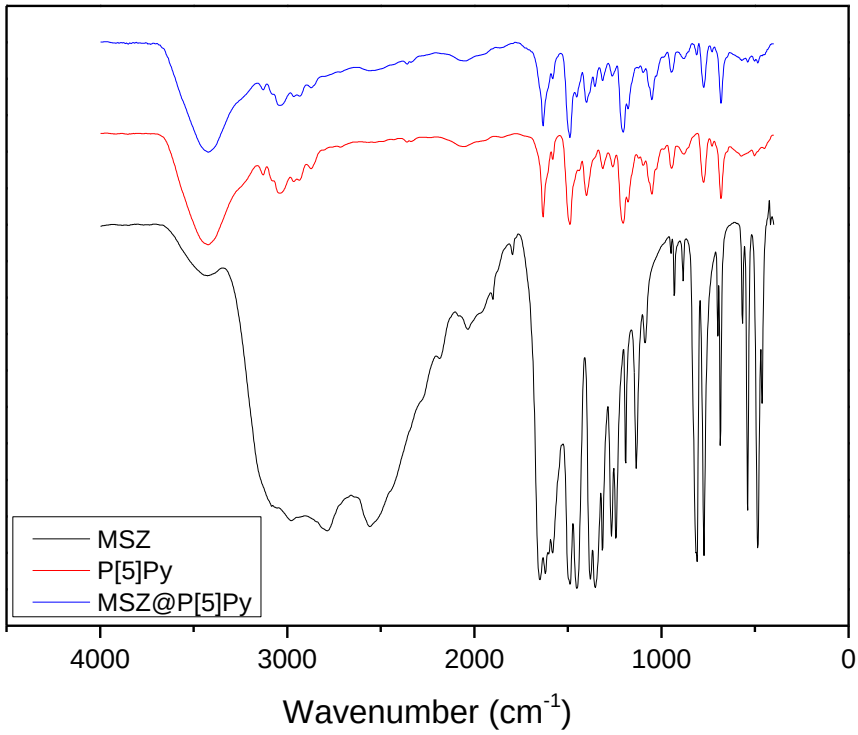

Figure S22. IR (KBr) spectra of MSZ, P[5]Py and MSZ@P[5]Py.

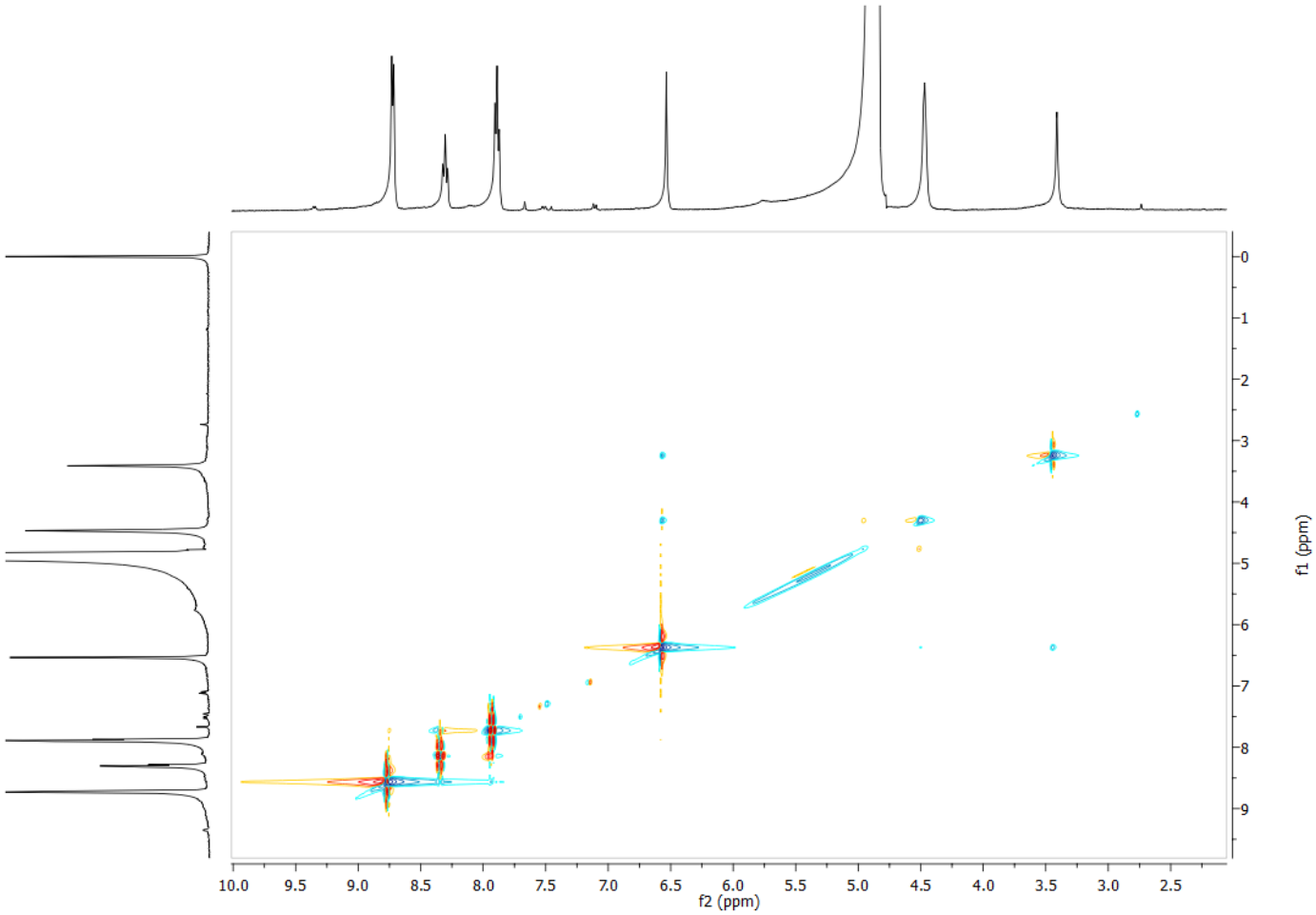

Figure S23. NOESY spectra (400 MHz, D_2O) of MSZ⊂P[5]Py in pH 1.0, at 25 ºC.

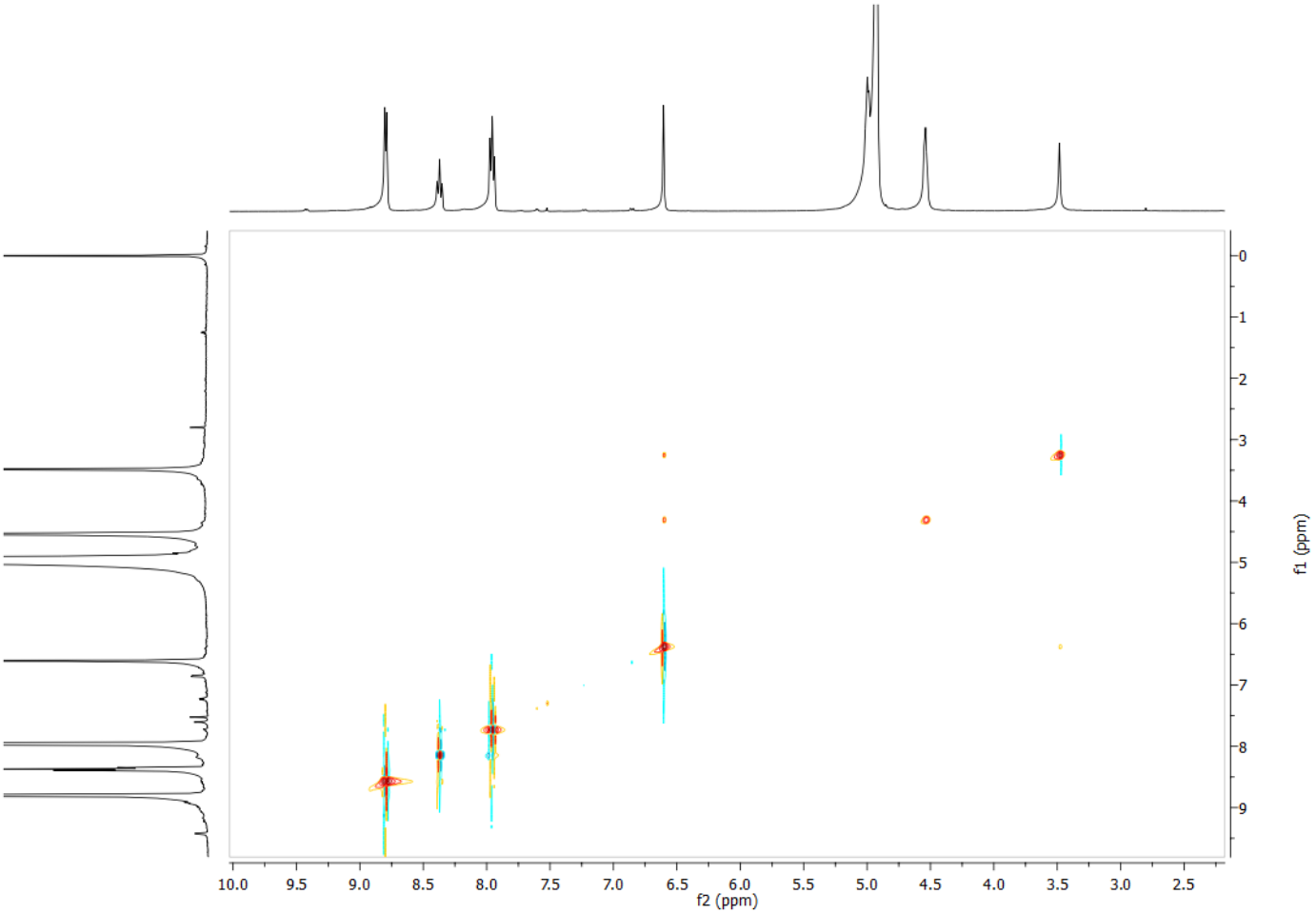

Figure S24. NOESY spectra of (400 MHz, D_2O) MSZ⊂P[5]Py in pH 5.0, at 25 ºC.

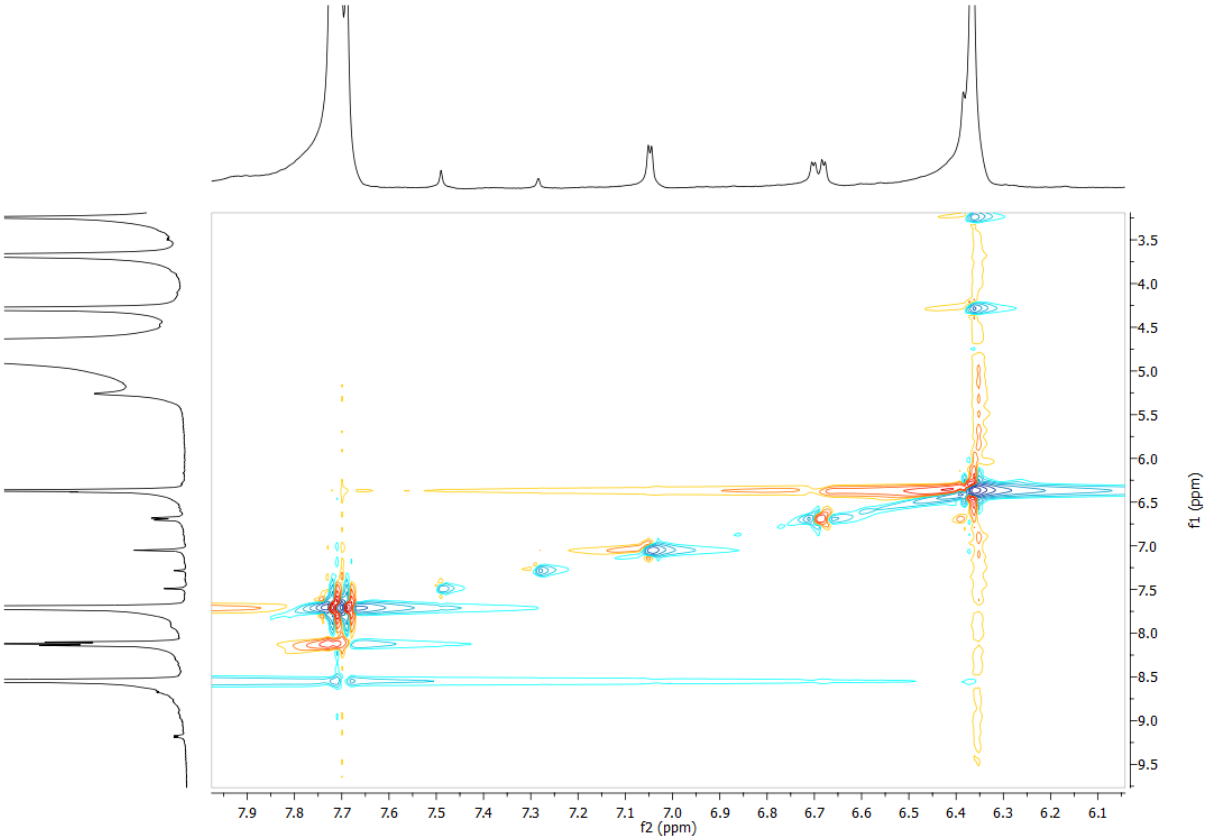

Figure S25. NOESY spectra (400 MHz, D_2O) of MSZ⊂P[5]Py in pH 7.5 at 25 ºC.

DLS

Average size: 455.8 nm

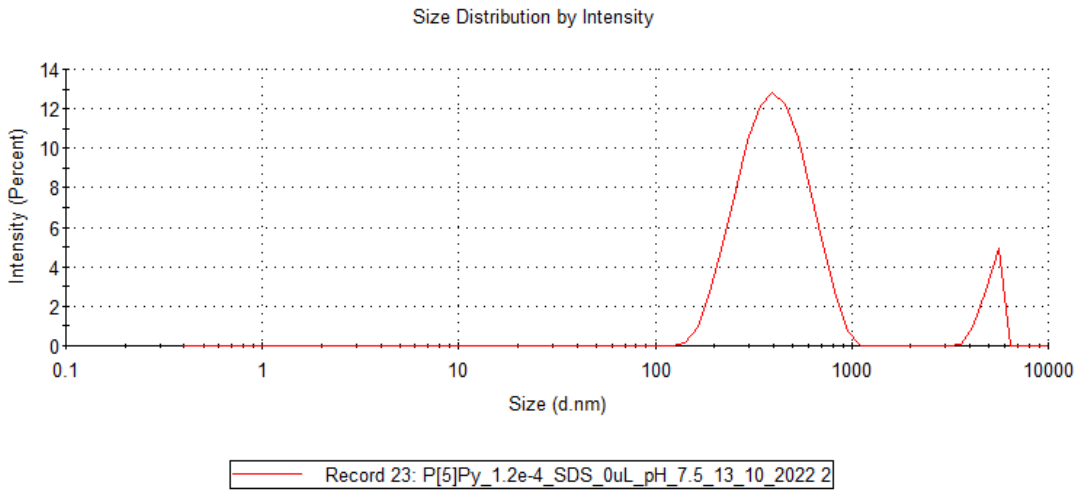

Figure S26. Distribution size for P[5]Py (1.2×10^{-4} mol L^{-1}) aggregates, at pH = 7.5 and 25 ºC.

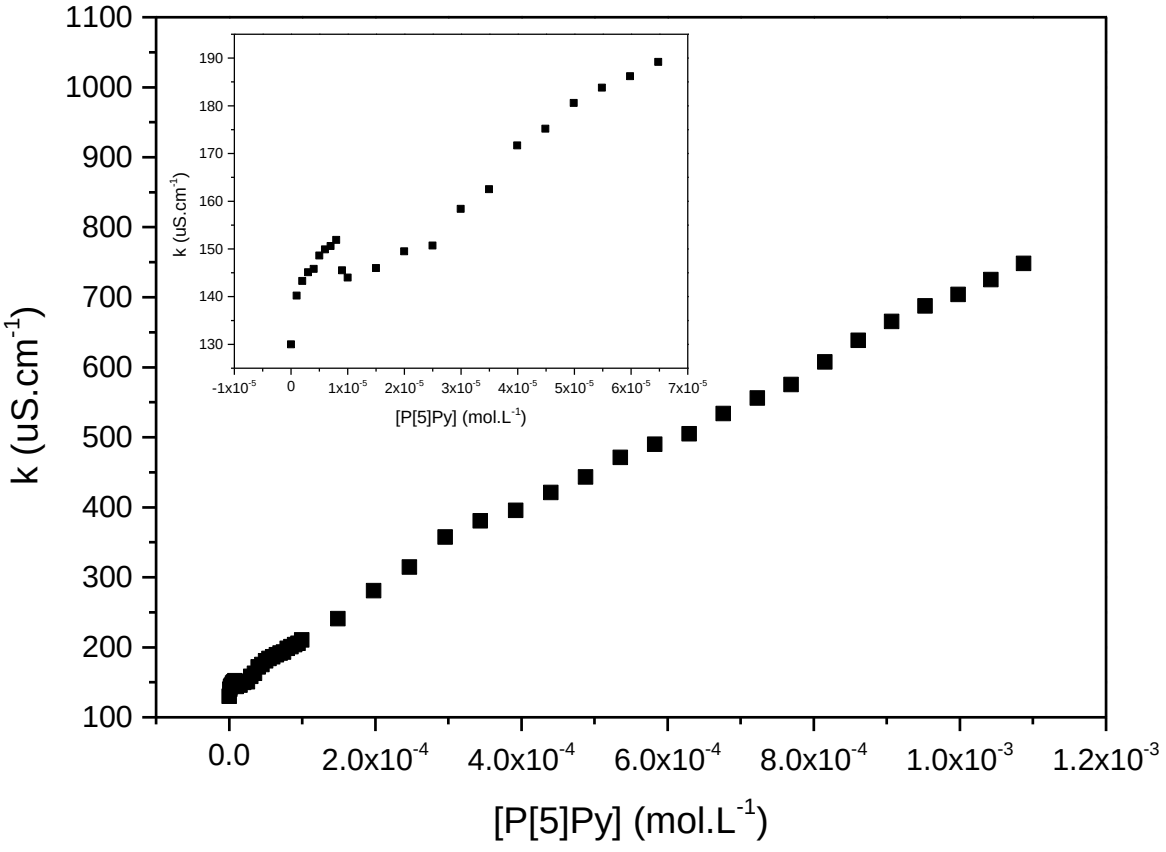

Figure S27. Specific conductance (κ) to P[5]Py at pH = 7.5 and 25 ºC.

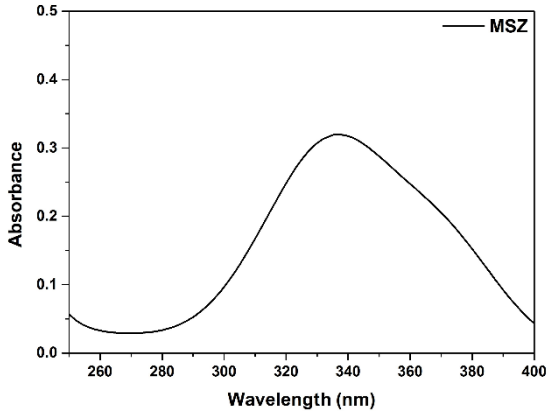

Figure S28. Theoretical UV-Vis spectra for MSZ.

Table S1. Optimized coordinates for MSZ compounds in pH 7

Atom	Coordinates		
	x	y	z
C	1.45042	-6.60643	0.10001
C	2.93937	-6.55761	0.05877
C	3.58855	-5.28984	-0.00684
C	2.8681	-4.07365	-0.01959
C	1.44407	-4.14491	0.01039
C	0.75643	-5.3665	0.07498
H	4.67952	-5.30493	-0.04474
H	3.36331	-3.10981	-0.15184
H	-0.33462	-5.38659	0.12378
O	3.62107	-7.64778	0.08012
H	2.40239	-8.7001	0.16245
N	0.71982	-2.95758	-0.06758
H	1.20314	-2.14215	0.30383
H	-0.24463	-3.02897	0.24736
C	0.69966	-7.84868	0.18184
O	1.43503	-9.01026	0.2103
O	-0.54298	-7.90738	0.22736

Table S2. Optimized coordinates for P[5]Py

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
C	-11.69308	13.19702	-2.90251	O	-19.00463	14.35275	2.27081
C	-10.68049	13.02817	-1.94581	O	-14.57233	17.67989	2.50411
C	-10.3669	11.77448	-1.40256	O	-16.6351	16.22543	-2.54598
C	-11.17418	10.6525	-1.67632	O	-11.20198	16.426	-1.41157
C	-12.14529	10.80783	-2.67839	O	-13.21066	12.1284	-4.42949
C	-12.35091	12.02805	-3.33848	O	-9.2653	11.61107	-0.56208
C	-12.01655	14.573	-3.47937	C	-13.89608	6.45601	-0.6779
C	-10.97403	9.31777	-0.96514	C	-13.27037	5.6569	-1.83669
C	-11.29389	9.59913	1.5535	C	-14.82502	3.87133	-2.52329
C	-12.01668	9.4464	2.74486	C	-12.89857	3.28293	-1.28788
C	-13.34164	8.96724	2.72277	C	-15.2042	2.54245	-2.61109
C	-13.80176	8.44982	1.50166	H	-15.39156	4.67873	-2.98388
C	-13.01398	8.45813	0.34139	C	-13.23695	1.9415	-1.35152
C	-11.77903	9.13909	0.31958	H	-11.99248	3.64003	-0.80188
C	-15.04451	10.22129	4.19401	C	-14.40172	1.55724	-2.02464
C	-14.50711	11.33094	4.86265	H	-16.11207	2.28161	-3.15448
C	-15.24466	12.50308	5.0799	H	-12.5792	1.20335	-0.89297
C	-16.51039	12.67317	4.48613	H	-14.67296	0.50313	-2.10328
C	-17.07343	11.54242	3.87179	N	-13.68474	4.23005	-1.87064
C	-16.39412	10.31816	3.79387	H	-13.58462	6.04154	0.29359
C	-14.21898	8.95681	3.97065	H	-14.9965	6.42547	-0.73751
C	-16.9602	14.95633	3.38463	H	-12.17709	5.68159	-1.75972
C	-15.86349	15.83139	3.42687	H	-13.55349	6.10676	-2.79615
C	-15.57268	16.71599	2.37921	C	-18.32801	8.87491	3.82254
C	-16.28064	16.64443	1.16271	C	-18.3794	7.34728	4.01089
C	-17.41347	15.81593	1.14457	H	-18.49151	9.3909	4.78195
C	-17.7976	15.04844	2.25381	N	-19.6867	6.85046	4.51327
C	-17.25797	14.00187	4.53827	H	-17.61066	7.03434	4.72695
C	-15.88077	17.46812	-0.05755	H	-18.17825	6.84558	3.05636
C	-14.88634	16.7946	-0.99997	C	-20.68591	6.56283	3.63368
C	-15.29591	16.13168	-2.1765	C	-19.86294	6.64048	5.84729
C	-14.37539	15.39387	-2.93508	C	-21.89395	6.04999	4.0752
C	-12.9984	15.40339	-2.65831	H	-20.46601	6.73316	2.58123
C	-12.57249	16.24508	-1.61256	C	-21.05364	6.12779	6.33463
C	-13.50526	16.85473	-0.76243	H	-19.01468	6.87156	6.48908
H	-10.11249	13.90405	-1.62698	C	-22.08667	5.8212	5.44242
H	-12.74478	9.94108	-2.96265	H	-22.66975	5.81135	3.34807
H	-11.07717	15.13406	-3.57561	H	-21.15964	5.95149	7.40491
H	-12.4307	14.4408	-4.48708	H	-23.02396	5.39673	5.80605
H	-11.24397	8.51104	-1.65852	C	-20.17902	15.08667	1.8781
H	-9.9088	9.20744	-0.7217	C	-21.29894	14.6549	2.84297
H	-10.31324	10.07775	1.58349	H	-19.99736	16.17035	1.95331
H	-14.79985	8.00955	1.46429	N	-22.60521	15.31005	2.57303

Table S2. Optimized coordinates for P[5]Py (cont.)

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
H	-13.48268	11.2716	5.23497	H	-21.01541	14.89715	3.87385
H	-18.08018	11.62067	3.45762	H	-21.45182	13.5706	2.77911
H	-14.90266	8.10051	3.90897	C	-22.95045	16.43601	3.25698
H	-13.57539	8.80756	4.84811	C	-23.46932	14.75709	1.67724
H	-15.22799	15.82954	4.31447	C	-24.18337	17.03569	3.0618
H	-18.02613	15.78871	0.24154	H	-22.21965	16.81062	3.97142
H	-18.33568	13.79456	4.54866	C	-24.71229	15.32291	1.44815
H	-17.00697	14.51138	5.47841	H	-23.13547	13.84566	1.18447
H	-16.78828	17.71097	-0.62457	C	-25.08453	16.47476	2.15041
H	-15.4409	18.41323	0.2888	H	-24.44098	17.92452	3.63744
H	-14.73343	14.80375	-3.78051	H	-25.39134	14.84915	0.73963
H	-13.1479	17.4048	0.11017	H	-26.06856	16.92161	1.99904
O	-13.42691	7.8091	-0.8201	C	-16.91089	16.52094	-3.92675
O	-11.45589	9.78557	3.97609	C	-18.13571	17.45407	-3.92501
O	-17.01571	9.1691	3.31187	H	-16.04433	17.01619	-4.39291
O	-14.72345	13.53966	5.8567	N	-18.5761	17.86448	-5.28376
H	-17.90673	18.36741	-3.36364	C	-6.78121	6.74313	7.20812
H	-18.98385	16.95913	-3.43635	H	-6.47482	8.71758	8.06517
C	-18.13454	19.04074	-5.80931	H	-7.42125	4.91543	6.22005
C	-19.45486	17.08806	-5.97651	H	-5.88202	6.30668	7.64615
C	-18.57156	19.47286	-7.05029	C	-7.99334	12.06519	-1.0589
H	-17.45105	19.61946	-5.19067	C	-7.0476	10.84701	-1.07301
C	-19.91814	17.47911	-7.22158	H	-8.09943	12.48614	-2.0702
H	-19.78178	16.1735	-5.4849	N	-5.65461	11.17371	-1.47663
C	-19.47959	18.68933	-7.77067	H	-7.42267	10.08766	-1.76931
H	-18.21691	20.42772	-7.43795	H	-7.00606	10.40018	-0.07201
H	-20.63492	16.84778	-7.74618	C	-5.25478	10.96853	-2.76199
H	-19.85135	19.02405	-8.74056	C	-4.77332	11.63922	-0.54832
C	-13.07276	11.13474	-5.46134	C	-3.94888	11.22031	-3.14854
C	-13.16438	11.88909	-6.8013	H	-6.00683	10.57677	-3.44435
H	-12.10439	10.6183	-5.37063	C	-3.4582	11.90696	-0.88928
N	-13.08423	11.00466	-7.99305	H	-5.15677	11.75957	0.46334
H	-12.34824	12.61708	-6.87617	C	-3.03048	11.69132	-2.20421
H	-14.11354	12.436	-6.85789	H	-3.65121	11.0278	-4.1791

Table S2. Optimized coordinates for P[5]Py (cont.)

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
C	-11.88953	10.82167	-8.62068	H	-2.77004	12.26224	-0.12259
C	-14.21368	10.41945	-8.4797	H	-1.99247	11.87592	-2.48593
C	-11.79933	10.04557	-9.76414	C	-10.71388	17.77792	-1.4295
H	-11.0333	11.33691	-8.18917	C	-9.99836	18.02568	-2.77498
C	-14.1714	9.63389	-9.61921	H	-11.5371	18.49527	-1.29179
H	-15.13608	10.62835	-7.94062	N	-9.33497	19.35349	-2.86001
C	-12.9523	9.44392	-10.27976	H	-10.71367	17.96074	-3.60372
H	-10.83378	9.93249	-10.25681	H	-9.22673	17.26129	-2.92862
H	-15.09324	9.19241	-9.99716	C	-9.95885	20.38845	-3.48704
H	-12.90393	8.84669	-11.19185	C	-8.08814	19.51835	-2.33683
H	-13.87946	10.38742	-5.38241	C	-9.33934	21.62083	-3.61258
H	-20.45178	14.84686	0.83702	H	-10.94513	20.17933	-3.89697
H	-17.13008	15.59583	-4.48553	C	-7.43071	20.73284	-2.43618
C	-14.33676	13.21406	7.20306	H	-7.64232	18.64322	-1.86747
C	-15.34915	13.86864	8.16683	C	-8.05573	21.80261	-3.08678
H	-14.31008	12.12385	7.35025	H	-9.85396	22.42574	-4.13685
N	-14.99174	13.71493	9.60171	H	-6.42732	20.83176	-2.02261
H	-16.34524	13.43238	8.02506	H	-7.54419	22.76068	-3.19324
H	-15.41498	14.94322	7.95636	C	-14.62272	18.52294	3.6695
C	-15.56728	12.73115	10.34641	C	-14.55436	19.97888	3.16793
C	-14.11219	14.58382	10.17327	H	-15.55288	18.34894	4.23173
C	-15.27806	12.599	11.69448	N	-14.51842	20.98792	4.25912
H	-16.27474	12.08594	9.82897	H	-15.42695	20.20181	2.54294
C	-13.79112	14.48921	11.51679	H	-13.65362	20.11959	2.55805
H	-13.70602	15.35675	9.52324	C	-15.66964	21.59687	4.65708
C	-14.38228	13.48896	12.29681	C	-13.32806	21.3302	4.8255
H	-15.76828	11.81465	12.27076	C	-15.65338	22.57716	5.63531
H	-13.09654	15.20771	11.95143	H	-16.58038	21.28776	4.14738
H	-14.1579	13.41249	13.36203	C	-13.26338	22.30334	5.80848
C	-10.17987	9.20271	4.29709	H	-12.44677	20.81785	4.44355
C	-10.35723	8.41226	5.60931	C	-14.43695	22.94503	6.22034
H	-9.84119	8.5397	3.48666	H	-16.58709	23.06204	5.91964
N	-9.09233	7.83763	6.13828	H	-12.29535	22.57022	6.23189
H	-11.05781	7.58254	5.45833	H	-14.40217	23.73033	6.97732
H	-10.77091	9.07036	6.38334	H	-13.76654	18.29958	4.32608
C	-8.26799	8.60802	6.90126	H	-13.32777	13.61746	7.37567
C	-8.78288	6.53458	5.89244	H	-9.43882	10.00677	4.42862
C	-7.10722	8.08356	7.44415	H	-7.60368	12.84816	-0.38965
H	-8.58897	9.63383	7.07378	H	-10.00729	17.88854	-0.59396
C	-7.63351	5.96623	6.4163	H	-19.10292	9.20313	3.10989
H	-9.49679	5.97384	5.29191				

Table S3. Optimized coordinates for MSZ⊂P[5]Py

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
C	-13.01107	17.27072	-6.45606	O	-17.64096	18.98232	0.91564
C	-11.77247	17.31662	-5.83514	O	-13.61434	22.37678	-0.77648
C	-11.17078	16.18479	-5.29147	O	-17.42074	20.35139	-4.3616
C	-11.87161	14.97862	-5.26463	O	-12.07859	20.60097	-5.75319
C	-13.05378	14.90737	-5.99046	O	-14.74649	15.92907	-7.39229
C	-13.61541	16.01285	-6.61658	O	-9.89382	16.25102	-4.73649
C	-13.6448	18.53581	-7.0038	C	-15.23311	14.03005	-3.34248
C	-11.37946	13.78623	-4.4832	C	-15.20701	12.56565	-3.83986
C	-10.86138	13.31597	-2.06253	C	-17.48074	11.71154	-4.29813
C	-11.15899	13.2684	-0.70441	C	-16.35336	11.16679	-2.21829
C	-12.35983	13.83276	-0.24474	C	-18.73706	11.33632	-3.58582
C	-13.25343	14.29392	-1.19122	H	-17.58748	12.6304	-4.89273
C	-13.00304	14.23962	-2.55822	C	-17.45953	10.618	-1.67964
C	-11.75508	13.80869	-3.01216	H	-15.39177	11.14004	-1.72515
C	-13.40007	15.14604	1.65858	C	-18.70367	10.76165	-2.37783
C	-12.69638	16.15282	2.30735	H	-19.6546	11.46891	-4.13395
C	-13.28767	17.35816	2.67474	H	-17.4122	10.05448	-0.7634
C	-14.59904	17.63572	2.26188	H	-19.61396	10.42346	-1.90835
C	-15.32932	16.59992	1.69508	N	-16.37481	11.83964	-3.40624
C	-14.77061	15.34917	1.45321	H	-15.59969	14.03967	-2.30862
C	-12.71153	13.87399	1.23083	H	-15.90204	14.63721	-3.95643
C	-15.3897	19.78812	1.19404	H	-14.30965	12.08717	-3.43385
C	-14.39933	20.66289	0.7601	H	-15.14524	12.53856	-4.92951
C	-14.51775	21.39661	-0.41716	C	-16.72374	13.94994	1.62991
C	-15.5962	21.15225	-1.28234	C	-16.73503	12.40598	1.73883
C	-16.61143	20.32867	-0.81765	H	-16.76234	14.41064	2.62367
C	-16.5586	19.71103	0.4296	N	-17.94502	11.85759	2.32483
C	-15.2282	18.99786	2.47488	H	-15.87778	12.09642	2.34044
C	-15.70734	21.8408	-2.62767	H	-16.61181	12.00598	0.7281
C	-15.19743	21.03467	-3.80482	C	-19.00425	11.58817	1.54072
C	-16.05943	20.25853	-4.59355	C	-17.99795	11.58822	3.64128
C	-15.53111	19.43062	-5.58033	C	-20.14945	11.02161	2.05729
C	-14.18658	19.45508	-5.93264	H	-18.90502	11.81075	0.48804
C	-13.37785	20.40523	-5.29788	C	-19.11609	11.02119	4.21403
C	-13.87002	21.11178	-4.20336	H	-17.12076	11.81403	4.22921
H	-11.26854	18.26891	-5.75926	C	-20.21518	10.72137	3.41492
H	-13.55636	13.95578	-6.04129	H	-20.97962	10.80064	1.40481
H	-12.88451	19.07863	-7.56933	H	-19.12415	10.80045	5.27035
H	-14.45271	18.24703	-7.67516	H	-21.09351	10.25686	3.83711
H	-11.7956	12.87737	-4.92741	C	-18.87671	19.64972	1.04802
H	-10.2917	13.73173	-4.54855	C	-19.03689	20.21869	2.48594
H	-9.90917	12.94136	-2.40716	H	-18.97964	20.45685	0.31482
H	-14.19448	14.69761	-0.85893	N	-20.37483	20.70826	2.76952
H	-11.65518	15.98317	2.53649	H	-18.31964	21.03037	2.62929
H	-16.36349	16.77838	1.44002	H	-18.79891	19.41892	3.19145
H	-13.3777	13.0301	1.43359	C	-20.67726	22.00681	2.5872
H	-11.79681	13.7361	1.80582	C	-21.31278	19.86398	3.23858
H	-13.51876	20.78157	1.37355	C	-21.9274	22.50248	2.88675
H	-17.47821	20.17756	-1.44461	H	-19.89182	22.64827	2.21666
H	-16.21624	18.85352	2.91563	C	-22.58029	20.30128	3.55485
H	-14.60098	19.55913	3.16707	H	-21.02296	18.83316	3.37667
H	-16.75912	22.06778	-2.80948	C	-22.90296	21.64501	3.38751
H	-15.13905	22.77047	-2.57468	H	-22.13584	23.55184	2.7465
H	-16.18637	18.75541	-6.11025	H	-23.30647	19.6044	3.94398
H	-13.20373	21.75802	-3.65055	H	-23.8829	22.01494	3.64903
O	-13.96824	14.64667	-3.45589	C	-18.28991	20.34617	-5.48001
O	-10.33341	12.70067	0.2439	C	-19.35042	21.44848	-5.24015

Table S3. Optimized coordinates for MSZ⊂P[5]Py (cont.)

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
O	-15.52819	14.29458	0.95749	H	-17.73756	20.55206	-6.4043
O	-12.62983	18.3048	3.43649	N	-20.32131	21.5789	-6.31363
H	-18.83217	22.40155	-5.11254	C	-6.00794	8.02991	0.69734
H	-19.87544	21.21854	-4.31017	H	-4.62832	9.60764	1.19316
C	-20.14351	22.49822	-7.28017	H	-7.66447	6.73135	0.24054
C	-21.42217	20.80425	-6.32256	H	-5.25467	7.2595	0.62236
C	-21.07534	22.68083	-8.27869	C	-8.8435	16.62777	-5.59212
H	-19.25109	23.10377	-7.2286	C	-8.16347	15.36583	-6.19832
C	-22.38771	20.93989	-7.29578	H	-9.19392	17.28302	-6.39802
H	-21.52625	20.08746	-5.52188	N	-6.9433	15.65626	-6.93058
C	-22.22658	21.89863	-8.29237	H	-8.87308	14.86746	-6.86249
H	-20.91443	23.43854	-9.03005	H	-7.92689	14.69054	-5.37265
H	-23.26806	20.31653	-7.26811	C	-6.95896	15.75253	-8.26966
H	-22.98106	22.0393	-9.05168	C	-5.78811	15.81196	-6.26194
C	-15.1223	14.65223	-7.88275	C	-5.80505	15.99139	-8.98677
C	-16.08747	14.88198	-9.06067	H	-7.9084	15.61301	-8.76507
H	-14.24194	14.09922	-8.23187	C	-4.60229	16.0551	-6.92197
N	-16.58118	13.63328	-9.61125	H	-5.82459	15.7189	-5.18665
H	-15.57164	15.44412	-9.84249	C	-4.59857	16.13956	-8.31075
H	-16.93116	15.47862	-8.70778	H	-5.84491	16.04529	-10.06385
C	-15.9299	13.04514	-10.62484	H	-3.68735	16.16199	-6.35982
C	-17.6889	13.07205	-9.10794	H	-3.67897	16.30664	-8.8516
C	-16.39041	11.87734	-11.19115	C	-11.68952	21.91012	-6.10629
H	-15.04286	13.53627	-10.99676	C	-11.78269	22.09433	-7.64744
C	-18.20069	11.90371	-9.63311	H	-12.30414	22.66366	-5.60249
H	-18.17825	13.58696	-8.29675	N	-11.17786	23.3262	-8.12461
C	-17.54893	11.28854	-10.69309	H	-12.8333	22.07154	-7.94569
H	-15.86062	11.44008	-12.02313	H	-11.2738	21.24792	-8.11526
H	-19.10477	11.48362	-9.22282	C	-11.93431	24.41546	-8.34723
H	-17.94061	10.38485	-11.13345	C	-9.85527	23.37079	-8.3683
H	-15.62701	14.05846	-7.11273	C	-11.38868	25.58161	-8.83921
H	-19.65452	18.90073	0.8673	H	-12.99163	24.33196	-8.14512
H	-18.78087	19.36845	-5.56943	C	-9.25226	24.50842	-8.85891
C	-11.70909	17.85767	4.41599	H	-9.28988	22.46994	-8.18247
C	-11.79327	18.85696	5.59316	C	-10.02498	25.63838	-9.11077
H	-11.96978	16.84884	4.75913	H	-12.02354	26.43423	-9.02466
N	-10.932	18.52029	6.71601	H	-8.19189	24.51008	-9.05898
H	-12.82927	18.8925	5.93746	H	-9.57879	26.53409	-9.51622
H	-11.52423	19.84798	5.22085	C	-13.02618	23.16296	0.24411
C	-11.42196	17.82875	7.75773	C	-12.852	24.58411	-0.34129
C	-9.65399	18.93372	6.72789	H	-13.67313	23.19622	1.1295
C	-10.64407	17.54278	8.86045	N	-12.30799	25.55206	0.59623
H	-12.45677	17.52325	7.70918	H	-13.82887	24.93296	-0.68388
C	-8.82591	18.67751	7.80048	H	-12.19116	24.51618	-1.20843
H	-9.30699	19.49361	5.87206	C	-13.13204	26.35671	1.29303
C	-9.32344	17.97825	8.89569	C	-10.9748	25.67618	0.73784
H	-11.07011	17.00079	9.691	C	-12.64227	27.32461	2.14256
H	-7.80781	19.03556	7.78974	H	-14.19343	26.22887	1.14153
H	-8.70144	17.78621	9.75761	C	-10.42714	26.62462	1.57332
C	-9.33385	11.77966	-0.14394	H	-10.35375	25.01547	0.15173
C	-8.96411	11.00237	1.13888	C	-11.26611	27.47639	2.28705
H	-9.71396	11.0927	-0.91146	H	-13.32712	27.96735	2.67407
N	-7.94042	9.98727	0.94699	H	-9.35471	26.71245	1.65407

Table S3. Optimized coordinates for MSZ⊂P[5]Py (cont.)

Atom	Coordinates			Atom	Coordinates		
	x	y	z		x	y	z
H	-9.8706	10.52784	1.52142	H	-10.85937	28.24358	2.92854
H	-8.61938	11.7231	1.88348	H	-12.04994	22.75092	0.53165
C	-6.64682	10.29268	1.13634	H	-10.69024	17.84272	4.00662
C	-8.29254	8.73331	0.62022	H	-8.45056	12.30191	-0.53712
C	-5.65854	9.33756	1.01823	H	-8.1176	17.17012	-4.9776
H	-6.41196	11.31171	1.40661	H	-10.64752	22.0287	-5.79037
C	-7.35097	7.73419	0.48743	H	-17.59192	14.28672	1.0473
H	-9.34529	8.53244	0.48649	C	-16.84656	9.77203	-7.40744
H	-9.8706	10.52784	1.52142				
H	-8.61938	11.7231	1.88348				
C	-6.64682	10.29268	1.13634				
C	-8.29254	8.73331	0.62022				
C	-5.65854	9.33756	1.01823				
H	-6.41196	11.31171	1.40661				
C	-7.35097	7.73419	0.48743				
H	-9.34529	8.53244	0.48649				
C	-15.95706	9.70259	-8.49506				
C	-15.97008	8.56731	-9.30764				
C	-16.84176	7.53222	-9.07588				
C	-17.74216	7.57831	-7.99093				
C	-17.71565	8.71228	-7.16409				
H	-15.27197	8.49898	-10.13022				
H	-16.8337	6.66759	-9.72068				
H	-18.38411	8.77087	-6.31959				
O	-15.06911	10.71433	-8.72288				
H	-14.41658	10.40267	-9.36608				
N	-18.59554	6.5641	-7.76856				
H	-18.58749	5.7478	-8.35834				
H	-19.2248	6.56834	-6.98417				
C	-16.86461	10.94936	-6.51696				
O	-16.60473	12.09031	-6.86507				
O	-17.22508	10.63679	-5.27834				