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Supporting information for "When motion slows: intrinsic photophysics of thioflavin T and X cations at cryogenic temperatures"

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Computational Data

Table S1: Computational data for thioflavins in this study. Calculations were performed at ωB97XD/def2svp. VEE is the vertical excitation energy, and *f* is the oscillator strength. Angles φ *and* δ refer to twisting and wagging angles, respectively, defined as $\varphi = (\chi_1+\chi_2)/2$ and $\delta = (\chi_1-\chi_2)/2$, where χ_1 is dihedral N11-C7-C21-C23 for ThT^+ and N11-C7-C17-C19 for ThX^+, respectively, and χ_2 is dihedral S12-C7-C21-C22 for ThT^+ and S12-C7-C17-C18 for ThX^+, respectively (numbering consistent with atom coordinates given in Tables S2-5 below)

	S_0 → S_1 (ground-state geometry)				**S_1 → S_0 (S_1 geometry)**			
Ion	**VEE (eV)**	***f***	**φ**	**δ**	**VEE (eV)**	***f***	**φ**	**δ**
ThT^+	3.4996	0.9391	-38.6	-1.7	2.1105	0.0038	-87.2	21.3
ThX^+	3.4411	1.0609	38.5	1.7	2.0823	0.0040	87.4	-21.5

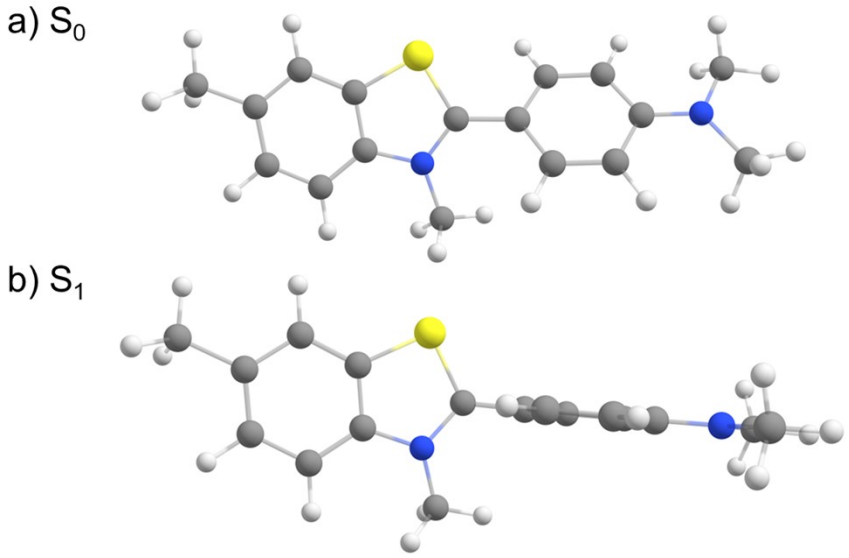

Figure S1: Computed structures of ThT^+ in S_0 (a) and S_1 (b)

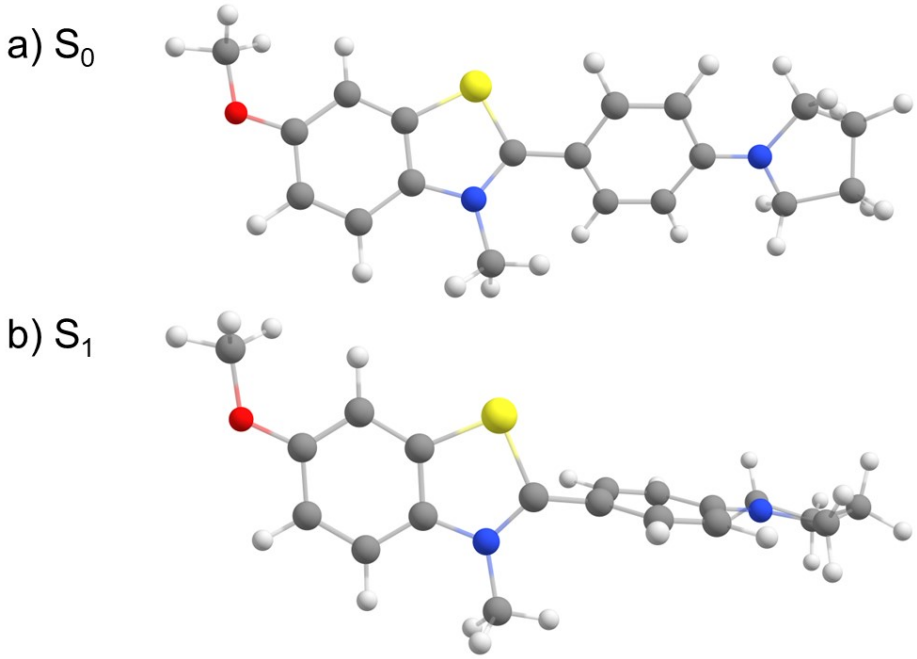

Figure S2: Computed structures of ThX^+ in S_0 (a) and S_1 (b)

Table S2: Coordinates of the ground-state (S_0) geometry of ThT^+

Atom no.	Element	X	Y	Z
1	C	-2.74742	-0.66729	-0.12388
2	C	-2.53479	0.689739	0.127946
3	C	-3.62163	1.560132	0.255718
4	C	-4.89554	1.029672	0.132747
5	C	-5.1266	-0.34155	-0.11373
6	C	-4.03371	-1.19563	-0.24348
7	C	-0.35217	-0.0332	0.03366
8	H	-3.48377	2.626242	0.438014
9	H	-5.75378	1.698616	0.227634
10	H	-4.18147	-2.25931	-0.43971
11	N	-1.17228	1.003456	0.237422
12	S	-1.21829	-1.49034	-0.2806
13	C	-0.74556	2.329058	0.674921
14	H	-0.76704	3.040262	-0.16215
15	H	-1.42704	2.671884	1.463098
16	H	0.267363	2.268514	1.085923
17	C	-6.53497	-0.85405	-0.23745
18	H	-7.05924	-0.35437	-1.06582
19	H	-6.55979	-1.93572	-0.42172
20	H	-7.10493	-0.65068	0.681435
21	C	1.092388	-0.01451	0.039264
22	C	1.811148	-1.11557	0.554594
23	C	1.835787	1.038123	-0.53853
24	C	3.18722	-1.15122	0.534124
25	H	1.274266	-1.95013	1.012709
26	C	3.212206	1.007718	-0.57939
27	H	1.325849	1.878364	-1.01309
28	C	3.942928	-0.08546	-0.03224
29	H	3.689062	-2.01363	0.968348
30	H	3.733278	1.833556	-1.05981
31	N	5.295374	-0.11345	-0.05615
32	C	6.013935	-1.2554	0.481544
33	H	5.750531	-2.18609	-0.04659
34	H	7.090247	-1.09484	0.360379
35	H	5.812683	-1.39239	1.556442
36	C	6.041264	0.990465	-0.63373
37	H	7.113769	0.79554	-0.53037
38	H	5.822617	1.113469	-1.70721
39	H	5.821422	1.939875	-0.11945

Table S3: Coordinates of the excited-state (S_1) geometry of ThT^+

Atom no.	Element	X	Y	Z
1	C	-2.6875	-0.61869	0.274451
2	C	-2.46186	0.717562	-0.0785
3	C	-3.5287	1.49425	-0.53865
4	C	-4.78152	0.902138	-0.66062
5	C	-5.01359	-0.44203	-0.32644
6	C	-3.94384	-1.20377	0.152497
7	C	-0.3577	0.166742	0.758384
8	H	-3.39247	2.544876	-0.79699
9	H	-5.61456	1.508505	-1.02382
10	H	-4.0956	-2.24728	0.436505
11	N	-1.14075	1.115432	0.088504
12	S	-1.21691	-1.36721	0.888675
13	C	-0.74713	2.503065	-0.00254
14	H	-1.11387	2.936502	-0.94288
15	H	-1.14039	3.09492	0.841099
16	H	0.346959	2.580647	-0.00132
17	C	-6.38839	-1.03817	-0.47777
18	H	-6.70538	-1.03409	-1.53179
19	H	-6.42066	-2.07618	-0.12084
20	H	-7.13336	-0.46179	0.090846
21	C	1.084229	0.085403	0.448944
22	C	2.061312	0.392745	1.434861
23	C	1.5399	-0.32995	-0.83752
24	C	3.39945	0.294952	1.171939
25	H	1.71847	0.705534	2.422085
26	C	2.869351	-0.42608	-1.13164
27	H	0.796059	-0.57195	-1.59837
28	C	3.858126	-0.12287	-0.12795
29	H	4.114096	0.531913	1.957537
30	H	3.175295	-0.73631	-2.12898
31	N	5.162811	-0.22804	-0.39486
32	C	6.167776	0.08674	0.619931
33	H	6.076025	-0.59001	1.481392
34	H	7.16437	-0.03681	0.187827
35	H	6.064653	1.126435	0.960228
36	C	5.629696	-0.67123	-1.70797
37	H	6.722422	-0.70544	-1.70712
38	H	5.251594	-1.67758	-1.93576
39	H	5.304868	0.026861	-2.49244

Table S4: Coordinates of the ground-state (S_0) geometry of ThX^+

Atom no.	Element	X	Y	Z
1	C	3.095736	-0.45413	-0.06025
2	C	2.835013	0.903057	0.12803
3	C	3.896845	1.814457	0.219774
4	C	5.184577	1.330146	0.12818
5	C	5.450137	-0.04956	-0.05429
6	C	4.394485	-0.95975	-0.15231
7	C	0.676547	0.108717	0.059795
8	H	3.724935	2.88304	0.351927
9	H	6.039748	2.004032	0.191508
10	H	4.563563	-2.02539	-0.30036
11	N	1.462813	1.177241	0.218459
12	S	1.594939	-1.33289	-0.18487
13	C	0.992434	2.507067	0.592888
14	H	1.658556	2.907315	1.367051
15	H	0.995462	3.179571	-0.27587
16	H	-0.02028	2.433132	1.002321
17	C	-0.7672	0.078	0.059965
18	C	-1.44987	-1.02422	0.622709
19	C	-1.5435	1.079712	-0.5657
20	C	-2.82331	-1.10799	0.600925
21	H	-0.88552	-1.81598	1.122099
22	C	-2.91747	1.001334	-0.60809
23	H	-1.05874	1.912674	-1.07815
24	C	-3.60925	-0.09312	-0.01522
25	H	-3.30621	-1.95856	1.079857
26	H	-3.47224	1.778623	-1.13186
27	C	-5.71536	-1.31507	0.449073
28	C	-5.818	0.884698	-0.57141
29	C	-7.1294	-1.05582	-0.0683
30	H	-5.68477	-1.35458	1.55297
31	H	-5.2965	-2.25848	0.066497
32	C	-7.21363	0.469927	-0.10852
33	H	-5.74899	0.925263	-1.67361
34	H	-5.52186	1.869667	-0.1788
35	H	-7.23893	-1.47047	-1.08241
36	H	-7.89691	-1.51839	0.565513
37	H	-8.00251	0.845811	-0.77272
38	H	-7.40742	0.867921	0.899674
39	N	-4.95219	-0.16842	-0.04266
40	O	6.738225	-0.3803	-0.1259
41	C	7.108212	-1.72879	-0.30802
42	H	6.755741	-2.35653	0.527075
43	H	6.718808	-2.12528	-1.2603

44	H	8.202919	-1.74849	-0.33328

Table S5: Coordinates of the excited-state (S_1) geometry of ThX^+

Atom no.	Element	X	Y	Z
1	C	3.036562	-0.38956	0.266917
2	C	2.766799	0.92477	-0.12271
3	C	3.807835	1.713736	-0.62462
4	C	5.071433	1.162089	-0.7504
5	C	5.33253	-0.16599	-0.37262
6	C	4.303837	-0.95509	0.148931
7	C	0.69221	0.348069	0.772992
8	H	3.63962	2.75063	-0.9155
9	H	5.902095	1.75026	-1.14151
10	H	4.476416	-1.98183	0.4664
11	N	1.437205	1.294501	0.056593
12	S	1.598471	-1.15793	0.923495
13	C	1.020735	2.674154	-0.04734
14	H	1.413211	3.284879	0.784149
15	H	1.371873	3.103563	-0.99522
16	H	-0.07361	2.736919	-0.03575
17	C	-0.7596	0.223405	0.5137
18	C	-1.70846	0.556322	1.514584
19	C	-1.24883	-0.26452	-0.73061
20	C	-3.05283	0.413779	1.306221
21	H	-1.3393	0.929786	2.470378
22	C	-2.58533	-0.40458	-0.9738
23	H	-0.52658	-0.53529	-1.50203
24	C	-3.54231	-0.0751	0.047129
25	H	-3.75317	0.682764	2.094707
26	H	-2.92519	-0.78384	-1.93591
27	C	-5.89289	0.017831	0.844131
28	C	-5.44201	-0.64643	-1.4475
29	C	-7.15312	-0.57347	0.220965
30	H	-5.9879	1.10389	1.009415
31	H	-5.6154	-0.45133	1.796854
32	C	-6.93137	-0.36672	-1.27531
33	H	-5.24079	-1.72064	-1.59364
34	H	-4.98729	-0.09588	-2.28113
35	H	-7.22259	-1.64615	0.456848
36	H	-8.06241	-0.09003	0.599203
37	H	-7.54641	-1.02323	-1.90324
38	H	-7.15527	0.672658	-1.55944
39	N	-4.84806	-0.22054	-0.16772
40	O	6.598526	-0.58854	-0.54047
41	C	6.946298	-1.89826	-0.16821
42	H	6.784602	-2.07159	0.909356

43	H	6.377931	-2.64932	-0.74299
44	H	8.013466	-2.01535	-0.38998

Experimental data

Table S6: Fluorescence excitation spectrum of thioflavin T (ThT^+), collected with 450-nm longpass filters

Wavelength (nm)	Normalized intensity
420.4131	0.85294
420.6102	0.817069
420.8074	1.000998
421.0045	0.921184
421.2017	1.002368
421.3989	0.892428
421.5962	0.897606
421.7935	0.978726
421.9908	0.838552
422.1882	0.78972
422.3856	1.029072
422.583	0.887289
422.7805	1.055641
422.978	1.045287
423.1755	1.066869
423.3731	0.976939
423.5707	0.993097
423.7683	0.962978
423.966	1.017286
424.1637	0.835052
424.3614	0.941958
424.5592	0.978418
424.7569	1.022872
424.9548	0.934895
425.1526	0.9675
425.3505	0.910095
425.5484	1.051166
425.7463	0.794622
425.9443	0.869481
426.1423	0.824081
426.3403	0.758871
426.5384	0.714511
426.7365	0.728395
426.9346	0.752765
427.1327	0.643364
427.3309	0.697077
427.5291	0.630477
427.7273	0.600674
427.9256	0.693757

428.1238	0.497178
428.3222	0.386104
428.5205	0.459305
428.7189	0.548393
428.9172	0.400173
429.1157	0.300178
429.3141	0.373537
429.5126	0.337152
429.7111	0.24029
429.9096	0.232823
430.1081	0.26667
430.3067	0.234314
430.5053	0.19187
430.7039	0.181134
430.9025	0.197877
431.1012	0.140935
431.2999	0.135263
431.4986	0.144836
431.6973	0.121671
431.8961	0.118691
432.0949	0.143156
432.2937	0.093075
432.4925	0.107117
432.6913	0.063657
432.8902	0.057604
433.0891	0.071561
433.288	0.066302
433.4869	0.052343
433.6859	0.080889
433.8848	0.067178
434.0838	0.050202
434.2828	0.027262
434.4818	0.02626
434.6809	0.038367
434.8799	0.038854
435.079	0.047225
435.2781	0.034616
435.4772	0.03214
435.6763	0.044845
435.8755	0.031659
436.0746	0.026722
436.2738	0.031635
436.473	0.018529
436.6722	0.03125
436.8714	0.011988
437.0707	0.016655

437.27	0.025025
437.4692	0.026019
437.6685	0.029578
437.8679	-0.00176
438.0672	0.008292
438.2665	0.010012
438.4659	0.011974
438.6653	0.020567
438.8647	0.015605
439.0641	0.008521
439.2636	0.001345
439.4631	0.014222
439.6625	0.019271
439.862	0.040642
440.0616	0.018123
440.2611	-0.00822

Table S7: Fluorescence excitation spectrum of thioflavin X (ThX^+), collected with 450-nm longpass filters

Wavelength (nm)	Normalized intensity
420	0.662461
420.5	0.572034
421	0.403882
421.5	0.559967
422	0.459344
422.2	0.315109
422.4	0.543098
422.5	0.633312
422.6	0.708396
422.8	0.812624
423	0.687684
423.2	0.746394
423.4	0.660386
423.5	0.587194
423.6	0.602976
423.8	0.688062
424	0.667406
424.2	0.553238
424.4	0.633665
424.5	0.622979
424.6	0.658977
424.8	0.656865
425	0.703591
425.2	0.59975
425.4	0.663848

425.5	0.872027
425.6	1.058063
425.8	0.673359
426	0.789839
426.2	0.713303
426.4	0.774463
426.5	0.799712
426.6	0.628515
426.8	0.757514
427	0.746821
427.2	0.660537
427.4	0.726088
427.5	0.720605
427.6	0.716296
427.8	0.763193
428	0.830511
428.2	0.715877
428.4	0.66446
428.5	0.80577
428.6	0.683207
428.8	0.838864
429	0.811729
429.1	0.767332
429.2	0.745272
429.3	0.699429
429.4	0.694066
429.5	0.797509
429.6	0.838251
429.7	0.813925
429.8	0.704316
429.9	0.873184
430	0.928611
430.1	0.844813
430.2	0.833849
430.3	0.904799
430.4	0.893884
430.5	0.854054
430.6	0.796821
430.7	0.775152
430.8	0.83708
430.9	0.732877
431	0.882724
431.1	0.902197
431.2	0.781387
431.3	0.885695
431.4	0.807474

431.5	0.805199
431.6	0.776608
431.7	0.839174
431.8	0.806129
431.9	0.736333
432	0.775208
432.1	0.68967
432.2	0.795427
432.3	0.816996
432.4	0.815236
432.5	0.823272
432.6	0.881919
432.7	0.863918
432.8	0.801921
432.9	0.904801
433	0.833785
433.1	0.936837
433.2	1.149756
433.3	0.99256
433.4	0.95714
433.5	1.012361
433.6	0.993369
433.7	0.987406
433.8	0.937922
433.9	0.915162
434	0.964939
434.1	0.964445
434.2	0.963275
434.3	0.887925
434.4	0.894174
434.5	0.901113
434.6	0.781769
434.7	0.857979
434.8	0.850269
434.9	0.678131
435	0.695974
435.1	0.622741
435.2	0.61517
435.3	0.645156
435.4	0.664284
435.5	0.637607
435.6	0.635153
435.7	0.555756
435.8	0.594283
435.9	0.664301
436	0.592022

436.1	0.574775
436.2	0.624107
436.3	0.59337
436.4	0.610454
436.5	0.555976
436.6	0.569888
436.7	0.603141
436.8	0.62559
436.9	0.604219
437	0.52975
437.1	0.583503
437.2	0.62278
437.3	0.48179
437.4	0.587015
437.5	0.588255
437.6	0.58814
437.7	0.527574
437.8	0.626805
437.9	0.500106
438	0.507103
438.1	0.48768
438.2	0.419464
438.3	0.426429
438.4	0.524802
438.5	0.393365
438.6	0.545506
438.7	0.402074
438.8	0.455181
438.9	0.355323
439	0.401733
439.1	0.45907
439.2	0.420831
439.3	0.361773
439.4	0.406611
439.5	0.302166
439.6	0.421834
439.7	0.309851
439.8	0.375409
439.9	0.261238
440	0.286967
440.1	0.27945
440.2	0.32345
440.3	0.342521
440.4	0.283235
440.5	0.265167
440.6	0.288417

440.7	0.294235
440.8	0.247978
440.9	0.165994
441	0.26438
441.2	0.421327
441.4	0.280659
441.5	0.13554
441.6	0.201288
441.8	0.284815
442	0.15372
442.5	0.116552
443	0.077126
443.5	0.11987
444	0.081895
444.5	0.131399
445	0.070396
445.5	0.061897
446	0.063168
446.5	0.07023
447	0.060996
447.5	0.05998
448	0.019206

Table S8: Dispersed fluorescence of thioflavin T (ThT^+), collected with 450-nm longpass filters

Wavelength (nm)	Normalized intensity
457	0.438515882
458.5	0.617912745
460	0.498637693
461.5	0.411360688
463	0.617137889
464.5	0.635769663
466	0.568797417
467.5	0.671307394
469	0.699343107
470.5	0.67299799
472	0.678157829
473.5	0.705436296
475	0.779523132
476.5	0.801448046
478	0.954675896
479.5	1.048856167
481	1.073686792
482.5	0.953249456
484	0.829395707
485.5	1.020573909

487	0.790635277
488.5	0.90378192
490	1.052254969
491.5	0.93359628
493	1.01823173
494.5	0.841564474
496	0.841670137
497.5	1.027283461
499	0.973941643
500.5	0.96006467
502	0.987695344
503.5	0.927960961
505	0.837549309
506.5	1.012772514
508	1.111126444
509.5	0.891172893
511	0.945483282
512.5	1.071432665
514	1.133016137
515.5	0.853715631
517	0.794844156
518.5	0.937206407
520	1.119737916
521.5	0.959747683
523	0.993718091
524.5	1.084534782
526	1.169328725
527.5	0.980228546
529	0.937699497
530.5	0.988170824
532	0.958426905
533.5	0.927943351
535	0.814374059
536.5	0.83994432
538	0.843131797
539.5	0.962706226
541	0.909100252
542.5	0.780386041
544	0.769432389
545.5	0.839803437
547	0.788610085
548.5	0.782323182
550	0.736342499
551.5	0.882579032
553	0.788786188
554.5	0.753089964

556	0.690714025
557.5	0.838782035
559	0.640225087
560.5	0.712762211
562	0.828937837
563.5	0.640471632
565	0.743862128
566.5	0.651442894
568	0.56516968
569.5	0.563021215
571	0.634765872
572.5	0.599967776
574	0.602010579
575.5	0.514821626
577	0.632546965
578.5	0.655422838
580	0.674442041
581.5	0.542188144
583	0.50650953
584.5	0.504995038
586	0.472327797
587.5	0.423071586
589	0.482224826
590.5	0.478579479
592	0.51078885
593.5	0.562616176
595	0.612330257
596.5	0.397571766
598	0.266233609
599.5	0.362069256
601	0.480093971
602.5	0.447268237
604	0.423177248
605.5	0.385156454
607	0.418299175
608.5	0.312091019
610	0.395687457
611.5	0.24969747
613	0.251440897
614.5	0.302528587
616	0.207097979
617.5	0.345462675
619	0.249204379
620.5	0.273612355
622	0.270301605

Table S9: Dispersed fluorescence of thioflavin X (ThX^+), collected with 450-nm longpass filters

Wavelength (nm)	Normalized intensity
430	-0.11581
431.5	-0.14863
433	0.11974
434.5	-0.02843
436	-0.05803
437.5	0.079463
439	0.05498
440.5	-0.0077
442	-0.00555
443.5	0.082633
445	-0.0596
446.5	-0.03616
448	0.01771
449.5	0.043963
451	0.051367
452.5	0.21107
454	0.227794
455.5	0.340405
457	0.275934
458.5	0.323746
460	0.336324
461.5	0.444622
463	0.460242
464.5	0.486546
466	0.556961
467.5	0.598558
469	0.620325
470.5	0.609898
472	0.647344
473.5	0.688534
475	0.812061
476.5	0.686843
478	0.758022
479.5	0.743237
481	0.830082
482.5	0.840273
484	0.883777
485.5	0.876774
487	0.905421
488.5	0.964524
490	0.9344

491.5	0.907568
493	1.005099
494.5	0.925391
496	0.99031
497.5	0.964941
499	0.95367
500.5	1.006367
502	0.973224
503.5	1.008588
505	1.044456
506.5	0.962597
508	0.901193
509.5	1.029432
511	1.022914
512.5	1.010736
514	0.97396
515.5	0.904867
517	1.052832
518.5	0.987922
520	0.975751
521.5	1.014554
523	0.981453
524.5	1.00238
526	0.933464
527.5	0.937298
529	0.973711
530.5	0.897403
532	0.843109
533.5	0.85183
535	0.806317
536.5	0.755611
538	0.791253
539.5	0.714864
541	0.774187
542.5	0.959222
544	0.659168
545.5	0.704042
547	0.704062
548.5	0.718287
550	0.701709
551.5	0.669939
553	0.59388
554.5	0.649404
556	0.514786
557.5	0.487872
559	0.58878

560.5	0.575667
562	0.498233
563.5	0.49086
565	0.526662
566.5	0.595598
568	0.352799
569.5	0.429999
571	0.476143
572.5	0.500615
574	0.463733
575.5	0.415967
577	0.441602
578.5	0.358964
580	0.445236
581.5	0.331964
583	0.303057
584.5	0.365997
586	0.404647
587.5	0.391245
589	0.31827
590.5	0.258668
592	0.286518
593.5	0.237336
595	0.3417

Table S10: Dispersed fluorescence of thioflavin X (ThX^+), collected with no longpass filters

Wavelength (nm)	Normalized intensity
437.5	0.093137
439	0.310875
440.5	0.10953
442	0.161252
443.5	0.265538
445	0.222783
446.5	0.356293
448	0.017514
449.5	0.059829
451	0.1944
452.5	0.215837
454	0.076863
455.5	0.51102
457	0.34096
458.5	0.336557
460	0.288097
461.5	0.485059
463	0.524711

464.5	0.360917
466	0.623312
467.5	0.583279
469	0.583199
470.5	0.318001
472	0.346805
473.5	0.66933
475	0.557918
476.5	0.723154
478	0.969577
479.5	0.719111
481	0.749876
482.5	0.675175
484	1.212618
485.5	0.869472
487	1.016529
488.5	0.909877
490	0.98421
491.5	0.955338
493	1.092724
494.5	1.0928
496	0.995805
497.5	1.005985
499	1.048534
500.5	1.068477
502	0.835762
503.5	0.822925
505	1.022005
506.5	1.05624
508	1.03622
509.5	1.013975
511	0.887856
512.5	1.0524
514	1.322638
515.5	1.119146
517	1.106188
518.5	1.249376
520	1.100875
521.5	1.1149
523	1.021683
524.5	0.861113
526	0.842528
527.5	0.908536
529	0.569509
530.5	0.742618
532	1.017207

533.5	0.805024
535	0.466586
536.5	0.541317
538	0.6756
539.5	0.668164
541	0.819907
542.5	0.648031
544	0.500723
545.5	0.685973
547	0.681823
548.5	0.860915
550	0.829121
551.5	0.741917
553	0.817121
554.5	0.83024
556	0.940483
557.5	0.424376
559	0.846869
560.5	0.521646
562	0.531921
563.5	0.536543
565	0.413882