Supporting Information

Donor-Acceptor naphthalimides and peryleneimides for all-solution-processed thin film lasers

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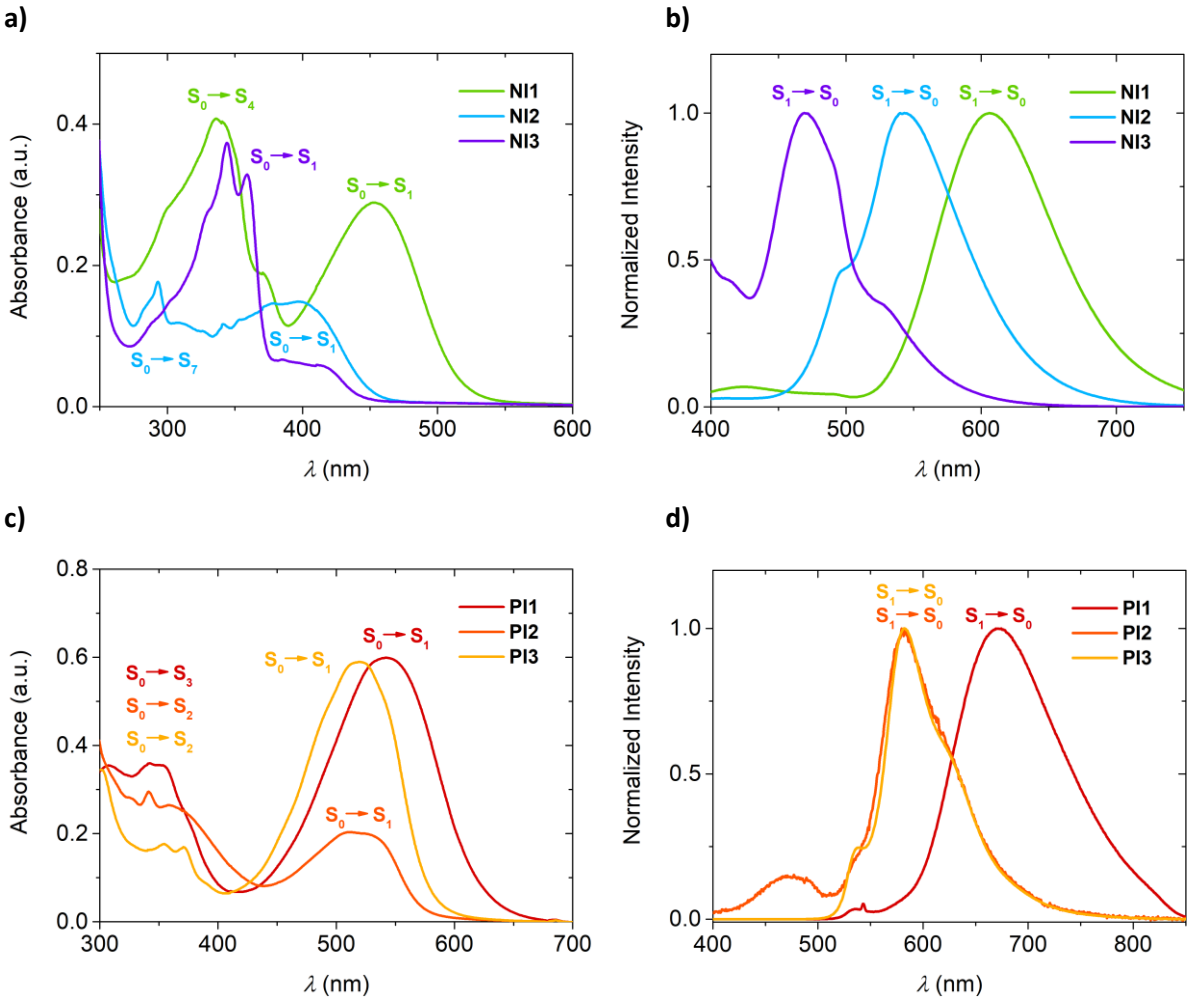

Fig. S1. UV/Visible absorption (left column, a and c) and emission (right column, b and d) spectra of **NI** derivatives (top row, a and b) and **PI** derivatives (bottom row, c and d). The measurements conditions were the same for every derivative (298 K, $CHCl_3$, 1×10^{-5} M).

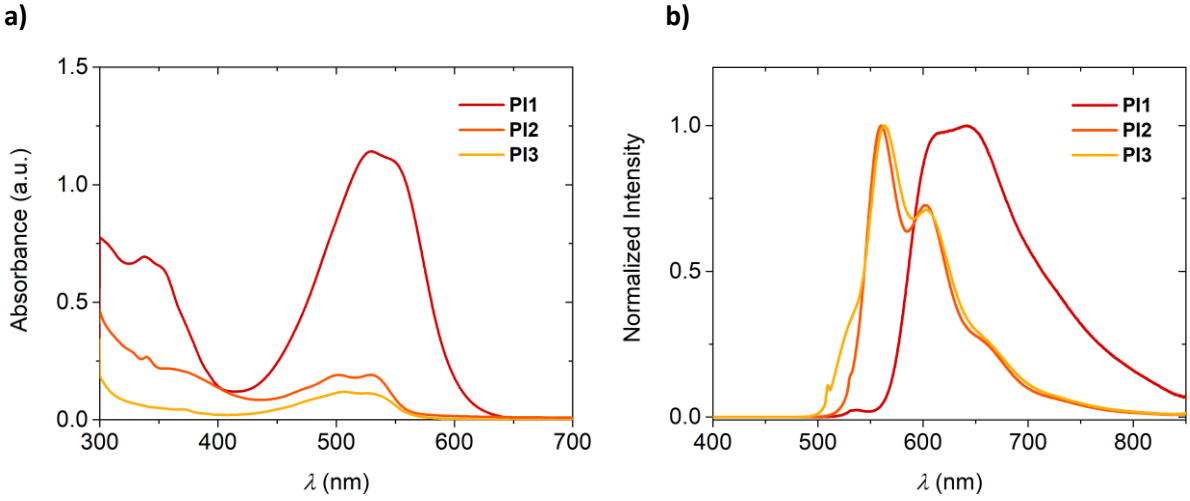

Fig. S2. UV/Visible absorption (a) and emission (b) spectra of **PI** derivatives using toluene as solvent (298 K, 1×10^{-5} M).

Table S1. Cartesian coordinates for optimized geometry of **NI1**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.011826	-1.940847	0.173861
2	6	0	3.545474	-1.948615	-0.057708
3	6	0	2.723100	-0.940297	0.507803
4	6	0	3.298096	0.085083	1.299750
5	6	0	4.757404	0.119233	1.548952
6	6	0	2.989524	-2.949729	-0.834336
7	6	0	1.315681	-0.963870	0.271652
8	6	0	0.781573	-2.004827	-0.526448
9	6	0	1.601021	-2.976226	-1.067130
10	6	0	0.499347	0.070551	0.853864
11	6	0	1.106587	1.063000	1.627645
12	6	0	2.490484	1.069660	1.846344
13	1	0	2.955178	1.843956	2.447031
14	1	0	0.487445	1.839534	2.063230
15	1	0	3.646751	-3.704128	-1.252922
16	1	0	1.174412	-3.766476	-1.676811
17	1	0	-0.288315	-2.023566	-0.705646
18	6	0	-0.903735	0.090941	0.649914
19	6	0	-2.111157	0.124362	0.484975
20	7	0	5.520184	-0.917741	0.987693
21	6	0	6.974393	-0.901778	1.232327
22	6	0	7.741921	-0.102566	0.174150
23	1	0	7.304363	-1.941425	1.237327
24	1	0	7.122513	-0.464851	2.220691
25	6	0	9.251855	-0.096143	0.440213
26	1	0	7.540764	-0.537096	-0.812347
27	1	0	7.362347	0.926155	0.163405
28	6	0	10.046376	0.696758	-0.604872
29	1	0	9.444612	0.324074	1.437468
30	1	0	9.621494	-1.130971	0.467786
31	1	0	9.851314	0.277613	-1.602090
32	1	0	9.675619	1.731121	-0.633027
33	6	0	11.557851	0.706806	-0.346105
34	6	0	12.353793	1.498653	-1.390532
35	1	0	11.927592	-0.328158	-0.316721
36	1	0	11.752208	1.125386	0.651759
37	6	0	13.865615	1.509061	-1.133117
38	1	0	12.159885	1.080686	-2.388882
39	1	0	11.984928	2.534046	-1.420410
40	6	0	14.652961	2.301792	-2.180701
41	1	0	14.059456	1.927140	-0.135888
42	1	0	14.234220	0.474605	-1.103742
43	1	0	15.727217	2.290117	-1.969230
44	1	0	14.507345	1.885854	-3.184213
45	1	0	14.331308	3.349154	-2.209225
46	6	0	-3.517840	0.178951	0.303293

47	6	0	-4.283211	1.213047	0.882609
48	6	0	-4.195213	-0.795140	-0.459671
49	6	0	-5.657662	1.268216	0.712764
50	1	0	-3.784772	1.967187	1.482827
51	6	0	-5.568250	-0.736579	-0.640272
52	1	0	-3.626797	-1.594298	-0.924312
53	6	0	-6.328396	0.295492	-0.055054
54	1	0	-6.225624	2.064737	1.179628
55	1	0	-6.064136	-1.489024	-1.242703
56	7	0	-7.724892	0.353307	-0.233242
57	6	0	-8.396627	1.609915	-0.298351
58	6	0	-7.890340	2.648893	-1.094066
59	6	0	-9.581979	1.814389	0.423289
60	6	0	-8.553996	3.872816	-1.152869
61	1	0	-6.979675	2.490764	-1.662234
62	6	0	-10.248309	3.035738	0.344051
63	1	0	-9.974366	1.013311	1.040749
64	6	0	-9.737167	4.072629	-0.438802
65	1	0	-8.150659	4.668171	-1.772815
66	1	0	-11.165146	3.180006	0.908130
67	1	0	-10.255419	5.024921	-0.492985
68	6	0	-8.491119	-0.843787	-0.352387
69	6	0	-8.287536	-1.912053	0.534370
70	6	0	-9.469077	-0.959037	-1.351386
71	6	0	-9.041737	-3.077384	0.411581
72	1	0	-7.539641	-1.822259	1.315228
73	6	0	-10.230743	-2.121395	-1.455097
74	1	0	-9.627006	-0.135284	-2.039461
75	6	0	-10.019163	-3.188050	-0.579447
76	1	0	-8.873555	-3.896220	1.105008
77	1	0	-10.984600	-2.196676	-2.233317
78	1	0	-10.609981	-4.094477	-0.667242
79	8	0	5.292496	0.999196	2.212934
80	8	0	5.757743	-2.782770	-0.311128

Table S2. Cartesian coordinates for optimized geometry of **NI2**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.895344	-1.394409	0.071473
2	6	0	-2.318696	-0.556105	1.058233
3	6	0	-3.136860	0.038224	2.053141
4	6	0	-2.094393	-1.970488	-0.900592
5	6	0	-0.914166	-0.302572	1.055674
6	6	0	-0.712518	-1.735006	-0.918894
7	6	0	-0.377805	0.541992	2.058569
8	6	0	-1.193182	1.109884	3.017325
9	6	0	-2.579307	0.859721	3.016399
10	1	0	-3.232694	1.299675	3.761886

11	1	0	-0.765521	1.754829	3.778412
12	1	0	-2.560952	-2.606482	-1.644873
13	1	0	-0.096999	-2.193248	-1.685189
14	7	0	-5.111143	-1.069910	1.086670
15	6	0	-0.105323	-0.915798	0.034797
16	1	0	0.689813	0.734868	2.058687
17	6	0	-4.600705	-0.211161	2.071659
18	8	0	-5.341987	0.297535	2.902921
19	6	0	-4.353717	-1.661758	0.064418
20	8	0	-4.887865	-2.366255	-0.783323
21	6	0	-6.563058	-1.331225	1.096840
22	1	0	-6.704346	-2.337445	0.700337
23	1	0	-6.881120	-1.299942	2.139679
24	6	0	-7.351305	-0.313207	0.266325
25	1	0	-6.983621	-0.338028	-0.766475
26	1	0	-7.156652	0.691561	0.660030
27	6	0	-8.858096	-0.596061	0.287878
28	1	0	-9.044011	-1.611035	-0.090884
29	1	0	-9.215748	-0.587161	1.327203
30	6	0	-9.673168	0.408430	-0.536034
31	1	0	-9.314407	0.399895	-1.574965
32	1	0	-9.484739	1.423398	-0.158541
33	6	0	-11.181616	0.132890	-0.518218
34	1	0	-11.369270	-0.882818	-0.894703
35	1	0	-11.539418	0.140646	0.521268
36	6	0	-11.997839	1.136607	-1.341755
37	1	0	-11.640003	1.128605	-2.381292
38	1	0	-11.809366	2.152372	-0.965653
39	6	0	-13.506500	0.862712	-1.324116
40	1	0	-13.865350	0.870980	-0.284800
41	1	0	-13.696024	-0.152988	-1.700225
42	6	0	-14.323284	1.866027	-2.147651
43	1	0	-14.134218	2.880789	-1.771676
44	1	0	-13.965285	1.857237	-3.186207
45	6	0	-15.828769	1.585450	-2.124390
46	1	0	-16.223015	1.622434	-1.102415
47	1	0	-16.382943	2.317738	-2.720618
48	1	0	-16.052844	0.591109	-2.527262
49	6	0	1.296682	-0.696209	-0.012461
50	6	0	2.500270	-0.518435	-0.068796
51	6	0	3.906218	-0.321304	-0.150413
52	6	0	4.660789	-0.944719	-1.165348
53	6	0	4.578123	0.499907	0.777711
54	6	0	6.032454	-0.747009	-1.253451
55	1	0	4.155393	-1.571667	-1.892152
56	6	0	5.952348	0.683804	0.699076
57	1	0	4.012841	0.978766	1.570207
58	6	0	6.692830	0.065830	-0.319799
59	1	0	6.599613	-1.207655	-2.054815
60	1	0	6.464156	1.294445	1.434744

61	6	0	8.749523	1.499928	-0.411734
62	6	0	9.058205	-0.752317	-0.496902
63	6	0	8.215483	2.790966	-0.381830
64	6	0	10.145906	1.277585	-0.510174
65	6	0	8.896479	-2.140318	-0.484128
66	6	0	10.342593	-0.156372	-0.561755
67	6	0	9.105564	3.862054	-0.426522
68	1	0	7.145578	2.959384	-0.334264
69	6	0	11.018085	2.371077	-0.553283
70	6	0	10.043452	-2.927490	-0.563335
71	1	0	7.915222	-2.594681	-0.406743
72	6	0	11.478392	-0.970008	-0.640826
73	6	0	10.493280	3.659059	-0.506236
74	1	0	8.713877	4.874607	-0.402731
75	1	0	12.090354	2.214853	-0.628090
76	6	0	11.322608	-2.352834	-0.646172
77	1	0	9.942483	-4.008695	-0.557001
78	1	0	12.468510	-0.526344	-0.691738
79	1	0	11.159481	4.515539	-0.537378
80	1	0	12.195711	-2.994801	-0.708753
81	7	0	8.091501	0.260622	-0.404958

Table S3. Cartesian coordinates for optimized geometry of **NI3**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.707621	-0.588988	1.333733
2	6	0	-1.090383	-1.286108	0.265247
3	6	0	-1.853223	-2.167832	-0.542222
4	6	0	-0.959883	0.270659	2.121861
5	6	0	0.299598	-1.107309	-0.004324
6	6	0	0.406459	0.460555	1.874244
7	6	0	0.877979	-1.823962	-1.080756
8	6	0	0.115732	-2.677658	-1.853441
9	6	0	-1.255967	-2.852322	-1.585548
10	1	0	-1.867264	-3.519299	-2.183609
11	1	0	0.575015	-3.219160	-2.674288
12	1	0	-1.456230	0.791978	2.932936
13	1	0	0.979714	1.136618	2.498991
14	6	0	1.051536	-0.207368	0.830923
15	1	0	1.934531	-1.690586	-1.288434
16	6	0	-3.300339	-2.367425	-0.276937
17	8	0	-3.990164	-3.127351	-0.945014
18	6	0	-3.151728	-0.766177	1.622083
19	8	0	-3.708630	-0.180436	2.542227
20	6	0	2.434964	0.006075	0.604944
21	6	0	3.624864	0.208091	0.432133
22	6	0	4.994872	0.430535	0.220361
23	6	0	5.835691	1.254350	0.927374

24	6	0	7.350448	0.383436	-0.668286
25	6	0	7.182955	1.248554	0.444814
26	1	0	5.496378	1.846740	1.768771
27	6	0	8.590917	0.228935	-1.294376
28	6	0	8.298483	1.964717	0.923475
29	6	0	9.673621	0.948027	-0.800589
30	1	0	8.707378	-0.435343	-2.144746
31	6	0	9.527812	1.810894	0.302052
32	1	0	8.186798	2.630624	1.774152
33	1	0	10.644930	0.841160	-1.273682
34	1	0	10.389411	2.360774	0.667763
35	16	0	5.843546	-0.405521	-1.097694
36	6	0	-5.298705	-1.857843	1.057911
37	1	0	-5.483568	-2.927311	0.943459
38	1	0	-5.458524	-1.569183	2.096703
39	6	0	-6.228611	-1.072383	0.123773
40	1	0	-6.049346	-1.397290	-0.907364
41	1	0	-7.254893	-1.378781	0.368508
42	6	0	-6.115744	0.453349	0.227017
43	1	0	-5.096332	0.766233	-0.034782
44	1	0	-6.266187	0.763932	1.268891
45	6	0	-7.112029	1.185596	-0.680617
46	1	0	-6.960463	0.864554	-1.721228
47	1	0	-8.135317	0.880993	-0.417544
48	6	0	-7.003497	2.713037	-0.600823
49	1	0	-5.981312	3.018975	-0.866268
50	1	0	-7.152927	3.033903	0.440020
51	6	0	-8.000992	3.448184	-1.504401
52	1	0	-7.851017	3.127643	-2.544429
53	1	0	-9.022316	3.142888	-1.238736
54	6	0	-7.885816	4.973046	-1.418663
55	1	0	-8.609981	5.468004	-2.074031
56	1	0	-8.065727	5.327123	-0.397163
57	1	0	-6.885800	5.312012	-1.712488
58	7	0	-3.861670	-1.643227	0.785459

Table S4. Cartesian coordinates for optimized geometry of **PI1**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.771556	2.585795	-0.538074
2	6	0	4.383197	2.666426	-0.674246
3	6	0	3.536557	1.642037	-0.241687
4	6	0	4.122533	0.480408	0.353246
5	6	0	5.544177	0.407946	0.493101
6	6	0	6.359379	1.473470	0.040835
7	6	0	2.072649	1.719025	-0.377070
8	6	0	3.318426	-0.612037	0.812089
9	6	0	1.860122	-0.537852	0.663763

10	6	0	1.264803	0.625226	0.077322
11	6	0	1.021250	-1.572377	1.079413
12	6	0	3.958944	-1.714200	1.387159
13	6	0	5.348048	-1.775606	1.520065
14	6	0	6.145313	-0.730921	1.081565
15	1	0	5.827531	-2.639447	1.967484
16	1	0	6.412978	3.390180	-0.881367
17	6	0	1.444408	2.828834	-0.936473
18	6	0	0.049643	2.899531	-1.067025
19	6	0	-0.741584	1.856851	-0.638242
20	6	0	-0.160104	0.704458	-0.060950
21	1	0	-0.401609	3.782413	-1.509081
22	1	0	-1.820638	1.900489	-0.735268
23	6	0	-0.366307	-1.505514	0.947090
24	1	0	-0.979428	-2.333573	1.285833
25	6	0	-0.982992	-0.388110	0.388013
26	1	0	3.379034	-2.555153	1.746854
27	1	0	3.971638	3.557225	-1.132350
28	1	0	2.031711	3.669583	-1.285152
29	1	0	1.439803	-2.467462	1.523205
30	6	0	7.614068	-0.824325	1.232800
31	6	0	7.832317	1.414913	0.172592
32	8	0	8.165567	-1.803194	1.724091
33	8	0	8.565887	2.312611	-0.226747
34	7	0	8.367127	0.272614	0.786962
35	6	0	9.832014	0.197065	0.931917
36	6	0	10.510517	-0.456680	-0.276409
37	1	0	10.030031	-0.379571	1.836451
38	1	0	10.189155	1.219416	1.062186
39	6	0	12.033264	-0.529622	-0.113353
40	1	0	10.102713	-1.466095	-0.407276
41	1	0	10.260392	0.117723	-1.176481
42	6	0	12.737696	-1.190049	-1.304685
43	1	0	12.433954	0.484086	0.028516
44	1	0	12.275564	-1.085282	0.803665
45	1	0	12.336779	-2.203775	-1.446346
46	1	0	12.493726	-0.636843	-2.222811
47	6	0	14.261554	-1.266240	-1.150208
48	6	0	14.957552	-1.929633	-2.342354
49	1	0	14.504591	-1.817262	-0.231449
50	1	0	14.661662	-0.252845	-1.009863
51	1	0	16.042865	-1.968327	-2.202827
52	1	0	14.604057	-2.957072	-2.485784
53	1	0	14.761204	-1.381596	-3.270958
54	6	0	-2.394977	-0.342721	0.272561
55	6	0	-3.611270	-0.324333	0.188019
56	6	0	-5.027771	-0.310948	0.097437
57	6	0	-5.791696	-1.425577	0.503498
58	6	0	-5.717311	0.816014	-0.397404
59	6	0	-7.175796	-1.412254	0.425975

60	1	0	-5.283437	-2.299835	0.896970
61	6	0	-7.100630	0.827849	-0.485931
62	1	0	-5.151218	1.681523	-0.726181
63	6	0	-7.858273	-0.285112	-0.071943
64	1	0	-7.741842	-2.275309	0.757706
65	1	0	-7.607476	1.700653	-0.881634
66	7	0	-9.266236	-0.269802	-0.153189
67	6	0	-9.986684	-1.463659	-0.449775
68	6	0	-11.131683	-1.800435	0.287759
69	6	0	-9.568257	-2.308780	-1.489056
70	6	0	-11.845087	-2.958342	-0.015843
71	1	0	-11.456570	-1.150893	1.093673
72	6	0	-10.277852	-3.473887	-1.773243
73	1	0	-8.689365	-2.047051	-2.068901
74	6	0	-11.421192	-3.803831	-1.042803
75	1	0	-12.729753	-3.206037	0.563542
76	1	0	-9.942072	-4.118299	-2.580495
77	1	0	-11.975720	-4.708470	-1.271972
78	6	0	-9.989576	0.938272	0.070242
79	6	0	-9.668473	1.771389	1.152969
80	6	0	-11.041784	1.300755	-0.783987
81	6	0	-10.380187	2.950414	1.365048
82	1	0	-8.863073	1.489387	1.822965
83	6	0	-11.759722	2.472589	-0.553011
84	1	0	-11.291299	0.659781	-1.622917
85	6	0	-11.431292	3.306367	0.517645
86	1	0	-10.120272	3.585179	2.207190
87	1	0	-12.571860	2.740172	-1.222710
88	1	0	-11.988549	4.221813	0.690317

Table S5. Cartesian coordinates for optimized geometry of **PI2**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.809263	-2.299170	-1.415842
2	6	0	4.419612	-2.378787	-1.397157
3	6	0	3.568925	-1.337381	-1.017874
4	6	0	4.151212	-0.087738	-0.635869
5	6	0	5.573585	0.058378	-0.664363
6	6	0	6.393338	-1.026714	-1.057656
7	6	0	2.103969	-1.483367	-0.997151
8	6	0	3.343386	1.020106	-0.224401
9	6	0	1.883502	0.864541	-0.183405
10	6	0	1.291977	-0.380098	-0.574298
11	6	0	1.042269	1.897681	0.229102
12	6	0	3.979832	2.213987	0.127500
13	6	0	5.370295	2.348370	0.094106
14	6	0	6.171183	1.287784	-0.295514
15	1	0	5.847009	3.281799	0.372871

16	1	0	6.453815	-3.050840	-1.710591
17	6	0	1.478830	-2.668394	-1.376022
18	6	0	0.083220	-2.808404	-1.347739
19	6	0	-0.711901	-1.761838	-0.936922
20	6	0	-0.133367	-0.532750	-0.543421
21	1	0	-0.365360	-3.749240	-1.651155
22	1	0	-1.791211	-1.861121	-0.908289
23	6	0	-0.345994	1.756231	0.268149
24	1	0	-0.961987	2.586014	0.597321
25	6	0	-0.957601	0.564011	-0.110506
26	1	0	3.396711	3.072053	0.438183
27	1	0	4.011012	-3.339000	-1.686597
28	1	0	2.068822	-3.515207	-1.704754
29	1	0	1.458092	2.849463	0.536064
30	6	0	7.641919	1.456368	-0.316162
31	6	0	7.867886	-0.897168	-1.085722
32	8	0	8.189056	2.503195	0.011947
33	8	0	8.604166	-1.825405	-1.400136
34	7	0	8.399651	0.352923	-0.735569
35	6	0	9.866111	0.502963	-0.761563
36	6	0	10.517370	0.146350	0.578663
37	1	0	10.072257	1.542477	-1.020355
38	1	0	10.235320	-0.152462	-1.551329
39	6	0	12.042645	0.297450	0.538614
40	1	0	10.100392	0.795597	1.357770
41	1	0	10.253985	-0.886438	0.836712
42	6	0	12.717902	-0.042082	1.872780
43	1	0	12.452543	-0.349050	-0.250244
44	1	0	12.299707	1.327614	0.253952
45	1	0	12.310192	0.606982	2.660780
46	1	0	12.455654	-1.069912	2.161399
47	6	0	14.244644	0.099366	1.840943
48	6	0	14.910886	-0.237297	3.178228
49	1	0	14.506373	1.125565	1.549195
50	1	0	14.651433	-0.551572	1.055083
51	1	0	15.998987	-0.128818	3.122903
52	1	0	14.551354	0.421434	3.976964
53	1	0	14.694672	-1.268488	3.480152
54	6	0	-2.371015	0.449229	-0.059507
55	6	0	-3.585827	0.375177	-0.003252
56	6	0	-5.003685	0.301852	0.072613
57	6	0	-5.749600	1.363775	0.624490
58	6	0	-5.698214	-0.831284	-0.398126
59	6	0	-7.133554	1.290151	0.712084
60	1	0	-5.228492	2.238184	0.999495
61	6	0	-7.083680	-0.896295	-0.327284
62	1	0	-5.140054	-1.652269	-0.835603
63	6	0	-7.815187	0.161272	0.233314
64	1	0	-7.695140	2.099510	1.165663
65	1	0	-7.610146	-1.759687	-0.719102

66	6	0	-10.125302	1.066671	-0.139119
67	6	0	-9.965783	-0.968476	0.863381
68	6	0	-9.870092	2.274990	-0.793198
69	6	0	-11.448460	0.629309	0.120120
70	6	0	-9.519200	-2.143156	1.474921
71	6	0	-11.346792	-0.665897	0.760039
72	6	0	-10.963277	3.055512	-1.163379
73	1	0	-8.858265	2.595132	-1.014658
74	6	0	-12.528784	1.432876	-0.261583
75	6	0	-10.480239	-3.027105	1.961136
76	1	0	-8.462038	-2.360438	1.577500
77	6	0	-12.291378	-1.571177	1.256566
78	6	0	-12.280350	2.645370	-0.897635
79	1	0	-10.789533	3.999573	-1.671166
80	1	0	-13.547738	1.110207	-0.068131
81	6	0	-11.853145	-2.750787	1.850643
82	1	0	-10.156846	-3.947388	2.438415
83	1	0	-13.352697	-1.352098	1.182921
84	1	0	-13.109767	3.278396	-1.197196
85	1	0	-12.576115	-3.461993	2.237800
86	7	0	-9.226328	0.090184	0.315168

Table S6. Cartesian coordinates for optimized geometry of **PI3**

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.366552	2.621500	0.325150
2	6	0	1.977884	2.719612	0.199885
3	6	0	1.148188	1.597060	0.261371
4	6	0	1.751483	0.314759	0.456546
5	6	0	3.172652	0.223773	0.588686
6	6	0	3.970749	1.391046	0.520272
7	6	0	-0.315594	1.689792	0.132518
8	6	0	0.965968	-0.880252	0.522963
9	6	0	-0.492985	-0.785887	0.384751
10	6	0	-1.105533	0.495020	0.195408
11	6	0	-1.313459	-1.913121	0.433212
12	6	0	1.622663	-2.098932	0.717720
13	6	0	3.011684	-2.177999	0.846803
14	6	0	3.790749	-1.034618	0.785520
15	1	0	3.504399	-3.132398	0.997044
16	1	0	3.994523	3.504179	0.272525
17	6	0	-0.960902	2.910105	-0.049299
18	6	0	-2.355542	2.996593	-0.173375
19	6	0	-3.130140	1.859286	-0.117600
20	6	0	-2.530191	0.591940	0.066124
21	1	0	-2.820437	3.967374	-0.313950
22	1	0	-4.208699	1.917706	-0.212908
23	6	0	-2.700736	-1.829772	0.306915

24	1	0	-3.300397	-2.732375	0.351324
25	6	0	-3.332029	-0.601374	0.125551
26	1	0	1.056949	-3.020609	0.773749
27	1	0	1.553188	3.704448	0.049977
28	1	0	-0.387830	3.827881	-0.098252
29	1	0	-0.881355	-2.896325	0.573041
30	6	0	5.260306	-1.147868	0.925285
31	6	0	5.443727	1.316427	0.649969
32	8	0	5.825185	-2.224218	1.084486
33	8	0	6.161814	2.306972	0.574648
34	7	0	5.995390	0.045454	0.870721
35	6	0	7.459947	-0.050100	1.010301
36	6	0	8.165410	-0.292604	-0.328181
37	1	0	7.658359	-0.873276	1.698203
38	1	0	7.795274	0.888174	1.453629
39	6	0	9.686887	-0.390550	-0.166999
40	1	0	7.778345	-1.219174	-0.768338
41	1	0	7.916082	0.525999	-1.014077
42	6	0	10.419476	-0.655900	-1.487955
43	1	0	10.067380	0.539351	0.278733
44	1	0	9.926296	-1.191859	0.546396
45	1	0	10.038898	-1.586550	-1.932244
46	1	0	10.178526	0.142431	-2.204263
47	6	0	11.942079	-0.754768	-1.334726
48	6	0	12.665599	-1.030689	-2.656232
49	1	0	12.181712	-1.548206	-0.613766
50	1	0	12.322773	0.177644	-0.896164
51	1	0	13.749293	-1.096306	-2.514407
52	1	0	12.330723	-1.974720	-3.100930
53	1	0	12.473550	-0.236587	-3.386806
54	6	0	-4.742673	-0.546286	0.004771
55	6	0	-5.958493	-0.537078	-0.092207
56	6	0	-7.357476	-0.507649	-0.203168
57	6	0	-8.232399	-1.565208	-0.159337
58	6	0	-9.755676	0.221103	-0.458595
59	6	0	-9.603943	-1.181700	-0.301827
60	1	0	-7.900586	-2.588240	-0.027871
61	6	0	-11.014971	0.807780	-0.613837
62	6	0	-10.755550	-1.994054	-0.303535
63	6	0	-12.133518	-0.018384	-0.611607
64	1	0	-11.118726	1.881603	-0.733148
65	6	0	-12.003953	-1.411381	-0.457120
66	1	0	-10.656655	-3.069123	-0.184708
67	1	0	-13.119917	0.419256	-0.730831
68	1	0	-12.893116	-2.034243	-0.458801
69	16	0	-8.203733	1.039126	-0.427250

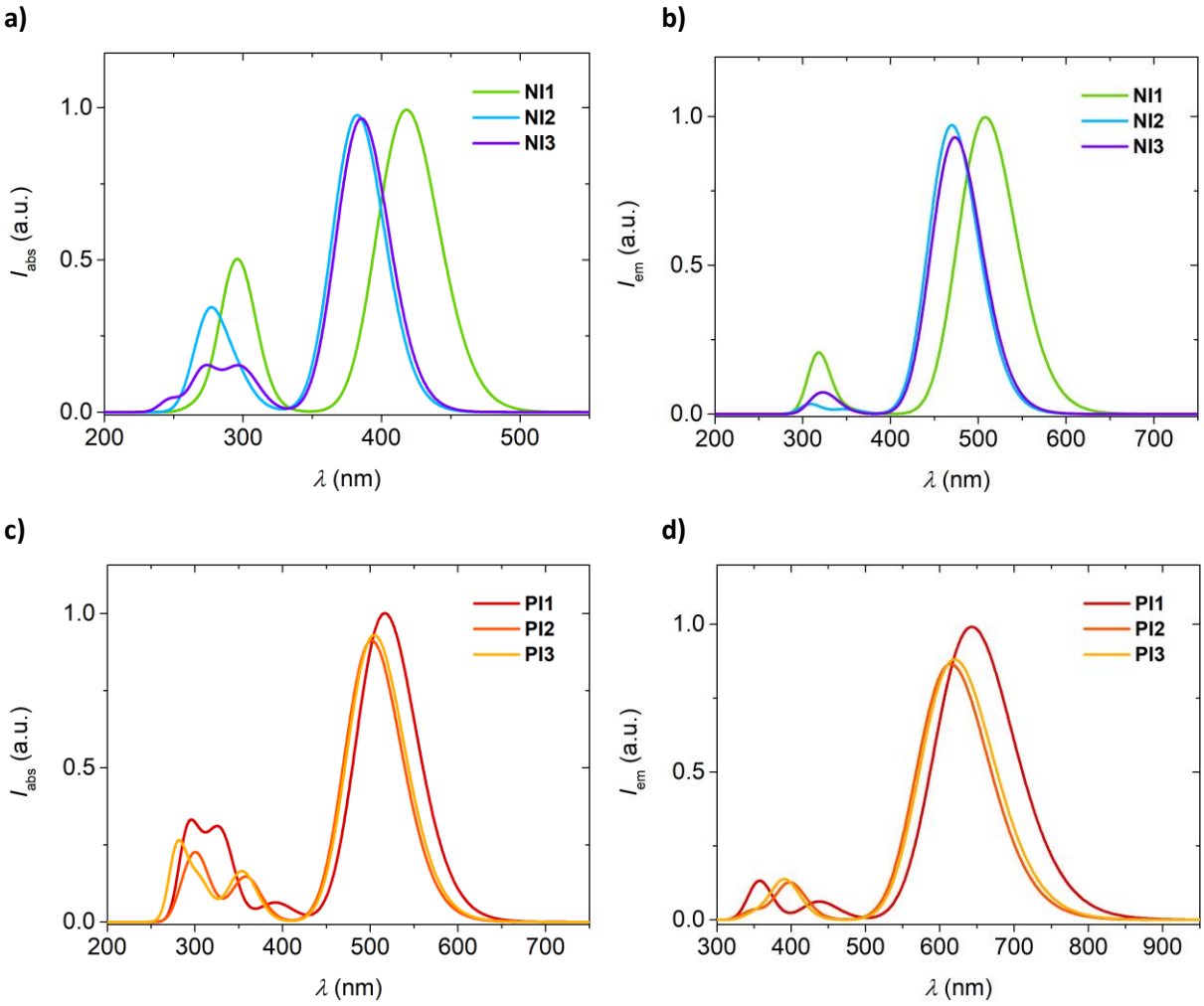

Fig. S3. Theoretical absorption (left column, a and c) and emission (right column, b and d) spectra of NI derivatives (top row, a and b) and PI derivatives (bottom row, c and d) calculated at B3LYP/6-31G(d,p) level .

Table S7. Electronic transitions associated with the absorption spectra of compounds **NI** calculated at M06-2X /6-311+G(2d,p) level.

Compound	Spectrum	Electronic transition	*E* [eV]	*λ* [nm]	*f*	MO [coefficient %]
NI1	**Absorption**	**$S_0 \rightarrow S_1$**	**2.97**	**418.05**	**1.45**	**H→L (77), H-1→L (14)**
		$S_0 \rightarrow S_2$	3.79	326.35	0.01	H-1→L (59), H→L+1 (25)
		$S_0 \rightarrow S_3$	4.05	306.21	0.04	H→L+2 (84)
		$S_0 \rightarrow S_4$	**4.14**	**299.79**	**0.42**	**H-1→L (16), H→L (16), H→L+1 (49)**
		$S_0 \text{->} S_6$	4.29	288.71	0.31	H→L+4 (87)
	Emission	**$S_1 \rightarrow S_0$**	**2.44**	**508.05**	**1.67**	**L→H (87)**
		$S_3 \rightarrow S_0$	3.89	318.19	0.34	L+1→H (64), L→H-1 (17)
NI2	**Absorption**	**$S_0 \rightarrow S_1$**	**3.24**	**382.51**	**1.43**	**H→L (56), H-2→L (38)**
		$S_0 \rightarrow S_2$	3.89	318.45	0.01	H-2→L (49), H→L (21), H→L+1 (17)
		$S_0 \rightarrow S_3$	4.17	297.36	0.1	H-5→L (78), H-2→L+3(11)
		$S_0 \rightarrow S_4$	4.24	292.5	0.1	H→L+2 (83)
		$S_0 \rightarrow S_7$	**4.46**	**277.9**	**0.36**	**H-2→L+1(14), H→L (18), H→L+1 (53)**
	Emission	**$S_1 \rightarrow S_0$**	**2.64**	**469.9**	**1.62**	**L→H (81), L→H-1 (14)**
NI3	**Absorption**	**$S_0 \rightarrow S_1$**	**3.22**	**385.53**	**1.41**	**H→L (88)**
		$S_0 \rightarrow S_2$	4.06	305.15	0.07	H-2→L (16), H-1→L (56), H-L+1 (14)
		$S_0 \rightarrow S_3$	4.16	298.07	0.09	H-3→L (77)
		$S_0 \rightarrow S_4$	4.22	293.21	0.08	H-2→L (43), H-1→L (14), H-1→L+1(17), H→L+1 (13)
		$S_0 \rightarrow S_6$	**4.55**	**272.48**	**0.19**	H-2→L (18), H→L+1 (59)
	Emission	**$S_1 \rightarrow S_0$**	**2.62**	**473.47**	**1.55**	**L→H (95)**

E: Transition energy*, λ:* Transition wavelength*, f:* Transition Oscillator Force*, MO:* Molecular Orbitals (H: HOMO. L: LUMO).

Table S8. Electronic transitions associated with the absorption spectra of compounds **PI** calculated at M06-2X/6-311+G(2d,p) level.

Compound	Spectrum	Electronic transition	*E* [eV]	*λ* [nm]	*f*	MO [coefficient %]
PI1	**Absorption**	**$S_0 \rightarrow S_1$**	**2.40**	**516.64**	**1.67**	**H→L (70), H-1→L (27)**
		$S_0 \rightarrow S_2$	3.16	392.14	0.10	H-1→L (59), H→L (18), H→L+1 (11)
		$S_0 \rightarrow S_3$	**3.74**	**331.95**	**0.39**	**H->L+1 (63)**
		$S_0 \rightarrow S_5$	3.95	313.73	0.12	H-2->L (22), H-1->L+1 (23), H->L+5 (15)
		$S_0 \rightarrow S_7$	4.09	302.87	0.12	H-6->L (64)
		$S_0 \rightarrow S_9$	4.23	292.52	0.1	H-2->L (24), H-1->L+1 (30), H->L+5 (13)
		$S_0 \rightarrow S_{10}$	4.27	290.54	0.32	H-1->L+6 (24), H->L+6 (67)
	Emission	**$S_1 \rightarrow S_0$**	**1.93**	**643.15**	**1.78**	**L→H (98)**
		$S_2 \rightarrow S_0$	2.83	437.79	0.11	L→H-1 (78)
		$S_3 \rightarrow S_0$	3.47	357.68	0.24	L+1→H (77)
PI2	**Absorption**	**$S_0 \rightarrow S_1$**	**2.47**	**501.60**	**1.52**	**H→L (87)**
		$S_0 \rightarrow S_2$	**3.46**	**358.47**	**0.24**	**H-3->L (19), H-1->L (53), H->L+1 (16)**
		$S_0 \rightarrow S_5$	4.05	306.45	0.13	H-6->L (22), H-3->L (25), H->L+1 (18)
		$S_0 \rightarrow S_6$	**4.10**	**302.40**	**0.13**	**H-6->L (47), H-3->L (16)**
		$S_0 \rightarrow S_8$	4.23	293.19	0.10	H-1->L+4 (62), H->L+4 (26)
	Emission	**$S_1 \rightarrow S_0$**	**2.02**	**614.60**	**1.5**	**L→H (96)**
		$S_2 \rightarrow S_0$	3.11	398.40	0.23	H-3->L (21), H-1->L (65)
PI3	**Absorption**	**$S_0 \rightarrow S_1$**	**2.46**	**584.63**	**1.55**	**H→L (96)**
		$S_0 \rightarrow S_2$	**3.50**	**354.05**	**0.27**	**H-2->L (12), H-1->L (51), H->L+1 (26)**
		$S_0 \rightarrow S_5$	4.06	305.20	0.14	H-4->L (49)
		$S_0 \rightarrow S_{10}$	**4.43**	**280.08**	**0.38**	**H-5->L (19), H-2->L+1 (11), H-1->L+1 (17), H->L+3 (11), H->L+4 (17)**
	Emission	**$S_1 \rightarrow S_0$**	**1.99**	**620.16**	**1.58**	**L→H (98)**
		$S_2 \rightarrow S_0$	3.17	391.63	0.24	H-2->L (10), H-1->L (68), H->L+1 (12)

E: Transition energy, *λ:* Transition wavelength, *f:* Transition Oscillator Force, *MO:* Molecular Orbitals (H: HOMO. L: LUMO).

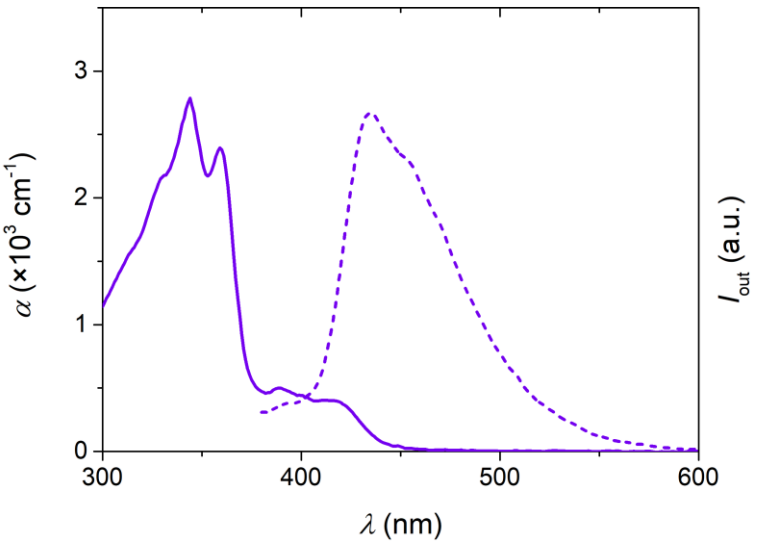

Fig. S4. Optical properties at room temperature of PS films doped with 1wt% of **NI3**. Absorption coefficient, α (solid line, left axis) and photoluminescence intensity (dashed line, right axis) versus wavelength, λ. PL excitation wavelength was 364 nm

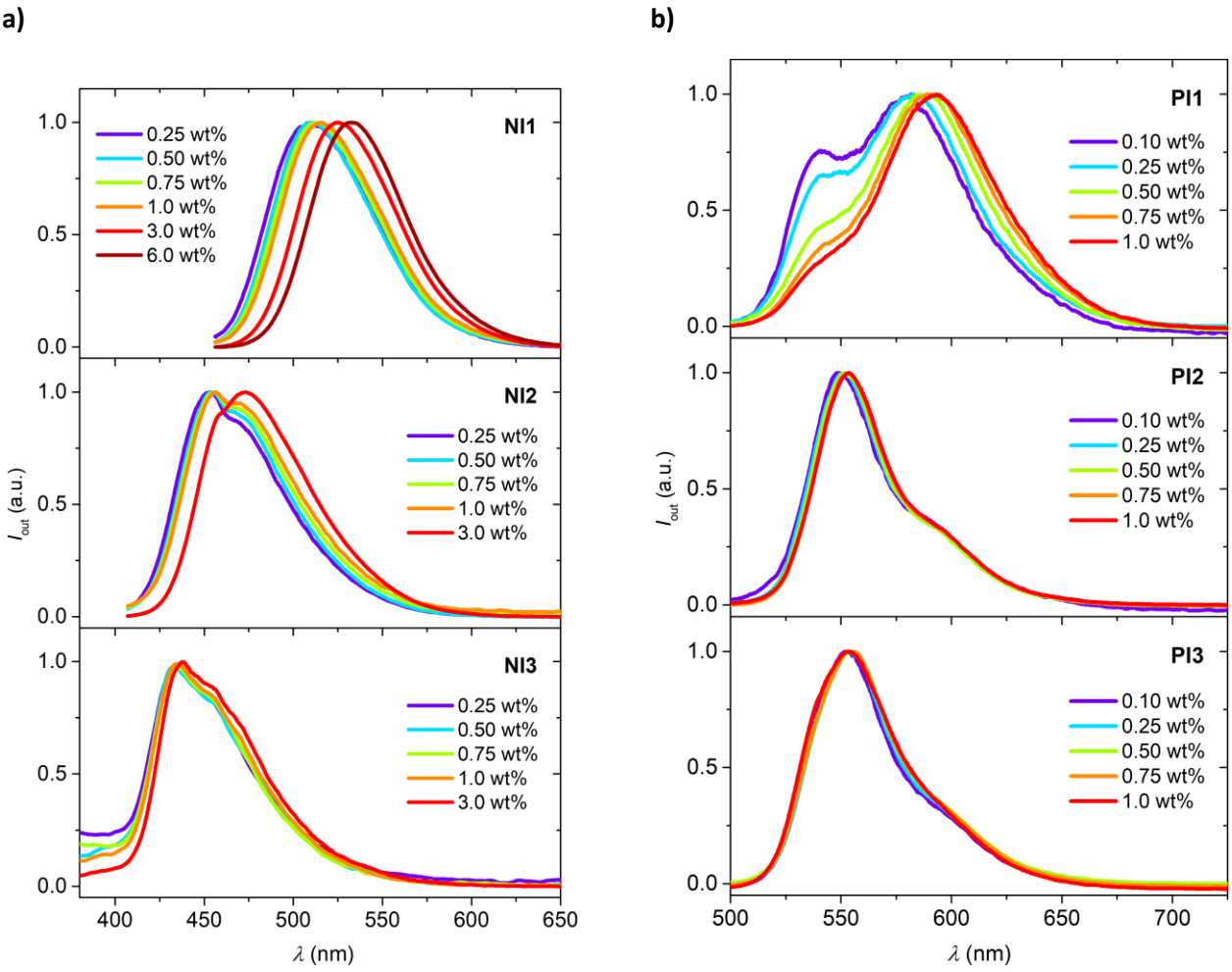

Fig. S5. Evolution of the photoluminescence intensity for different concentrations: a) From 0.25 wt% to 6 wt% of the naphthalendiimide derivatives **NI1**, **NI2**, and **NI3**, from top to down; b) From 0.10 wt% to 1 wt% of the perylenimide derivatives **PI1**, **PI2**, and **PI3**, from top to down.

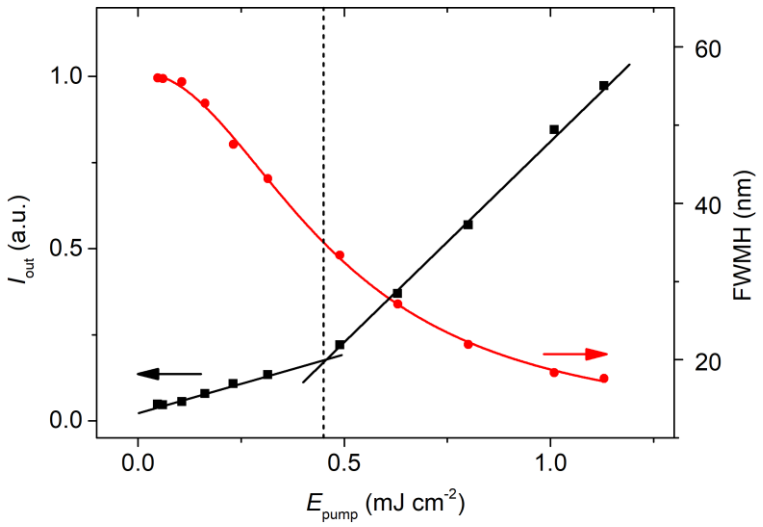

Fig. S6. Amplified spontaneous emission (ASE) threshold determination. Output intensity, I_{out}, (red circles, left axis) and emission linewidth, FWHM, (black squares, right axis) as a function of the pump energy density, E_{pump}, for a PS film doped with 0.5 wt% of **PI2**. ASE threshold was determined as the E_{pump} value at which FWHM reaches the average value between the highest value at low E_{pump} and the lowest value at high E_{pump}. In this case, the ASE threshold is 0.45 mJ cm^{-2} and it is indicated by the dotted line.

Table S9. Optical and ASE properties of PS films doped with a) 1,8-Naphthalimides derivatives and b) peryleneimide derivatives.

a)

Derivative	Conc. [wt. %] in PS[b]	$\lambda_{ABS\text{-}max}$[c] [nm]	$\lambda_{PL\text{-}max}$[d] [nm]	h[e] [nm]	λ_p[f] [nm]	α (λ_p)[g] [$\times 10^3$ cm^{-1}]	t_p (λ_p)[i] [ns]	λ_{ASE}[j] [nm]	FWHM[k] [nm]	$E_{th\text{-}ASE}$[m] [mJ/cm^2]	$I_{th\text{-}ASE}$[m] [kW/cm^2]	$\tau_{1/2}^{ASE}$[n] [pump pulses]
NI1	0.25	338, 450	488, 517, 558	540	450	0.24	3.9	544	36	7.2	1800	-
	0.50	338, 450	516, 558	500	450	0.46	3.9	545	27	1.3	330	-
	0.75	338, 455	518, 556	480	450	0.67	3.9	546	16	0.65	170	7.3×10^2
	1	338, 455	518, 556	460	450	0.88	3.9	547	16	1.1	280	-
	3	338, 455	520, 556	610	450	2.40	3.9	548	16	4.0	1000	-
	6	338, 455	522, 556	500	450	4.82	3.9	-	-	-	-	-
NI2	0.25	400	451, 478	440	355	0.23	5.7	475	27	35	6100	-
	0.50	400	451, 478	450	355	0.42	5.7	474	19	7.7	1350	-
	0.75	400	451, 478, 512	440	355	0.56	5.7	476	19	5.3	930	4.2×10^3
	1	400	452, 478, 512	400	355	0.69	5.7	477	14	10	1800	-
	3	400	480, 512	620	355	1.83	5.7	480	14	16	2800	-
NI3	0.25	344, 359	426, 448, 477	310	355	0.12	5.7	-	-	-	-	-
	0.50	344, 359	426, 448, 477	320	355	0.36	5.7	-	-	-	-	-
	0.75	344, 359	426, 448, 477	330	355	0.60	5.7	-	-	-	-	-
	1	344, 359	427, 448, 477	330	355	0.85	5.7	-	-	-	-	-
	3	344, 359	427, 447, 476	330	355	2.22	5.7	-	-	-	-	-

b)

Derivative	Conc. [wt. %] in PS[b]	$\lambda_{ABS\text{-}max}$[c] [nm]	$\lambda_{PL\text{-}max}$[d] [nm]	h[e] [nm]	λ_p[f] [nm]	α (λ_p)[g] [$\times10^3$ cm^{-1}]	t_p (λ_p)[i] [ns]	λ_{ASE}[j] [nm]	FWHM[k] [nm]	$E_{th\text{-}ASE}$[m] [μJ/cm^2]	$I_{th\text{-}ASE}$[m] [kW/cm^2]	$\tau_{1/2}^{ASE}$[n] [pump pulses]
PI1	0.10	535	575, 612	495	532	0.15	5.7	632	22	1700	300	-
	0.25	535	612	500	532	0.34	5.7	638	15	850	150	2.2×10^4
	0.50	535	614	545	532	0.55	5.7	643	15	1000	180	-
	0.75	535	617	525	532	0.87	5.7	641	15	1700	300	-
	1	535	617	505	532	1.11	5.7	640	11	3500	610	-
PI2	0.10	533	559, 603	490	532	0.08	5.7	-	-	-	-	-
	0.25	509, 533	560, 603	480	532	0.14	5.7	598	19	1000	180	-
	0.50	509, 533	560, 604	490	532	0.21	5.7	598	15	450	80	2.2×10^4
	0.75	509, 533	560, 604	480	532	0.30	5.7	599	13	380	70	-
	1	509, 533	560, 604	500	532	0.41	5.7	599	13	1200	210	-
PI3	0.10	512	561, 605	475	532	0.14	5.7	600	17	900	160	-
	0.25	512	561, 607	475	532	0.27	5.7	601	14	700	120	2.2×10^4
	0.50	512	561, 607	480	532	0.34	5.7	601	13	750	130	-
	0.75	512	562, 607	485	532	0.37	5.7	601	10	800	140	-
	1	512	562, 607	510	532	0.45	5.7	601	12	4500	790	-

[b] Error ~0.1%

[c] Peak absorption wavelengths (maximum absorption peak is underlined)

[d] Peak photoluminescence wavelengths (maximum photoluminescence peak is underlined)

[e] Film thickness (error ~2%)

[f] Pump wavelength

[g] Absorption coefficient at λ_p (error ~2%)

[i] Pump pulse width at λ_p

[j] ASE wavelength (error is ± 0.5 nm)

[k] ASE linewidth (error is ± 1 nm), defined as the full width at half maximum, FWHM, well above the threshold

[m] ASE threshold (error ~10%)

[n] ASE operational lifetime, characterized by the photostability half-life $\tau_{1/2}^{ASE}$ (determined from Fig. 4) measured at 10 Hz with a pump intensity of 2500 kW/cm^2 (error 10%).

Table S10. ASE properties comparison between the **NI** derivatives and **PI** derivatives studied in this work and other small molecules emitting in the same spectral range.

Derivative	Concentration [wt. %] in PS	$\lambda_{ABS\text{-}max}$[b] [nm]	$\lambda_{PL\text{-}max}$[c] [nm]	PLQY[d] [%]	h[e] [nm]	λ_p[f] [nm]	α (λ_p)[g] [$\times10^3$ cm^{-1}]	λ_{ASE}[j] [nm]	FWHM[k] [nm]	$E_{th\text{-}ASE}$[m] [μJ/cm^2]	$\tau_{1/2}^{ASE}$[n] [pump pulses]	Reference
NI1	0.75	338, 455	518, 556	94*	480	450	0.67	546	16	650	7.3×10^2	This work
NI2	0.75	400	451, 478, 512	91*	440	355	0.56	476	19	5300	4.2×10^3	This work
PI1	0.25	535	612	94*	500	532	0.34	638	15	850	2.2×10^4	This work
PI2	0.50	509, 533	560, 604	91*	490	532	0.21	598	15	450	2.2×10^4	This work
PI3	0.25	512	561, 607	63*	475	532	0.27	601	14	700	2.2×10^4	This work
PDI-C6	0.50	-	535, 574	-	610	532	-	579	7	120	1.0×10^4	27
PDI-O	0.50	492, 528	537, 576	-	630	532	-	578	8	40	3.8×10^4	27
***b*-PDI-O**	5.0	487, 520, 560	579, 619	42 ± 3	550	532	2.9	624	7	500	4.8×10^3	29
***b*-PDI-Tp**	1.0	487, 519, 559	570, 616	61 ± 5	550	532	0.6	618	6	230	1.6×10^4	29
***b*-PDI-A**	10.0	485, 518, 558	577, 619	78 ± 3	550	532	5.0	623	6	75	1.8×10^3	29
COPV2	3.0	379, 398, 423	436, 461	85 ± 7	570	423	2.5	463	7	55	1.2×10^3	30, 32
COPV2-Tip	3.8	385, 406, 430	445, 471	90 ± 7	580	430	3.1	474	8	40	~5×10^3 **	32
COPV3	2.0	414, 438, 467	480, 513	100	650	436	1.91	515	8	40	6.0×10^3	30
COPV4	5.0	435, 462, 495	509, 547	100	600	436	2.4	550	8	27	1.0×10^4	30
COPV5	1.0	450, 479, 513	526, 566	100	620	532	0.10	571	8	550	2.2×10^4	30
COPV6	4.0	460, 489, 525	534, 581	94	770	532	2.89	584	8	17	2.4×10^4	30
FZ2	1.0	474, 509, 545	547, 588	73	480	545	4.40	591	4	30	7.5×10^3	33

*Measured in solution (Table 1 from the main text)

[b] Peak absorption wavelengths (maximum absorption peak is underlined); [c] Peak photoluminescence wavelengths (maximum photoluminescence peak is underlined); [d] Photoluminescence quantum yield; [e] Film thickness; [f] Pump wavelength; [g] Absorption coefficient at λ_p; [j] ASE wavelength; [k] ASE linewidth, defined as the full width at half maximum, FWHM, well above the threshold; [m] ASE threshold; [n] ASE operational lifetime, characterized by the photostability half-life $\tau_{1/2}^{ASE}$ measured at 10 Hz with a pump intensity of 2500 kW/cm^2 (** Estimated by comparison with COPV2, as it is only measured at 40 kW/cm^2)

Table S11. Optical and ASE properties (left) and geometrical and performance parameters of top-layer resonator distributed feedback (DFB) lasers (right) based on naphthalendiimide and perylenimide derivatives as active media.

Derivative	Conc. [wt. %] in PS[a]	λ_p[b] [nm]	α [λ_p][c] [$\times 10^3$ cm^{-1}]	t_p (λ_p)[d] [ns]	λ_{ASE}[e] [nm]	FWHM[f] [nm]	$E_{th\text{-}ASE}$[g] [mJ/cm^2]	$I_{th\text{-}ASE}$[g] [kW/cm^2]	$\tau_{1/2}^{ASE}$[i] [pump pulses]	Λ[j] [nm]	λ_{DFB}[k] [nm]	$E_{th\text{-}ASE}$[l] [mJ/cm^2]	$I_{th\text{-}ASE}$[l] [kW/cm^2]
NI1	0.75	450	0.67	3.9	546	16	0.65	170	7.3×10^2	349.5	544.3	0.15	39
										350.3	**546.9**	**0.14**	**35**
										352.0	548.3	0.15	39
										353.7	550.7	0.15	39
NI2	0.75	355	0.56	5.7	476	19	5.3	930	4.2×10^3	300.6	471.4	20	3500
										301.8	473.2	20	3500
										304.9	**477.0**	**17**	**3000**
										306.7	479.1	29	5100
PI1	0.25	532	0.34	5.7	638	15	0.85	150	2.2×10^4	411.5	634.2	0.39	69
										415.2	**638.0**	**0.35**	**62**
										415.7	639.9	0.38	67
										417.7	642.7	0.38	67
PI2	0.50	532	0.21	5.7	598	15	0.45	80	2.2×10^4	384.9	596.2	0.31	54
										385.4	**597.5**	**0.28**	**49**
										388.5	601.5	0.28	49
										390.7	604.3	0.30	53
PI3	0.25	532	0.27	5.7	601	14	0.70	120	2.2×10^4	383.5	593.5	0.49	87
										387.7	599.4	0.32	56
										389.8	**602.8**	**0.34**	**61**
										391.5	605.4	0.31	55

[a] Error ~0.1%; [b] Pump wavelength; [c] Absorption coefficient at λ_p (error ~2%); [d] Pump pulse width at λ_p; [e] ASE wavelength (error is ± 0.5 nm); [f] ASE linewidth (error is ± 2 nm), defined as the full width at half maximum, FWHM, well above the threshold; [g] ASE threshold (error ~20%); [i] ASE operational lifetime, characterized by the photostability half-life $\tau_{1/2}^{ASE}$ (determined from Fig. 4c) measured at 10 Hz with a pump intensity of 2500 kW/cm^2 (error 10%); [j] Grating period (error ~0.5%); [k] DFB wavelength (error is ± 0.5 nm); [l] DFB threshold (error ~10%)

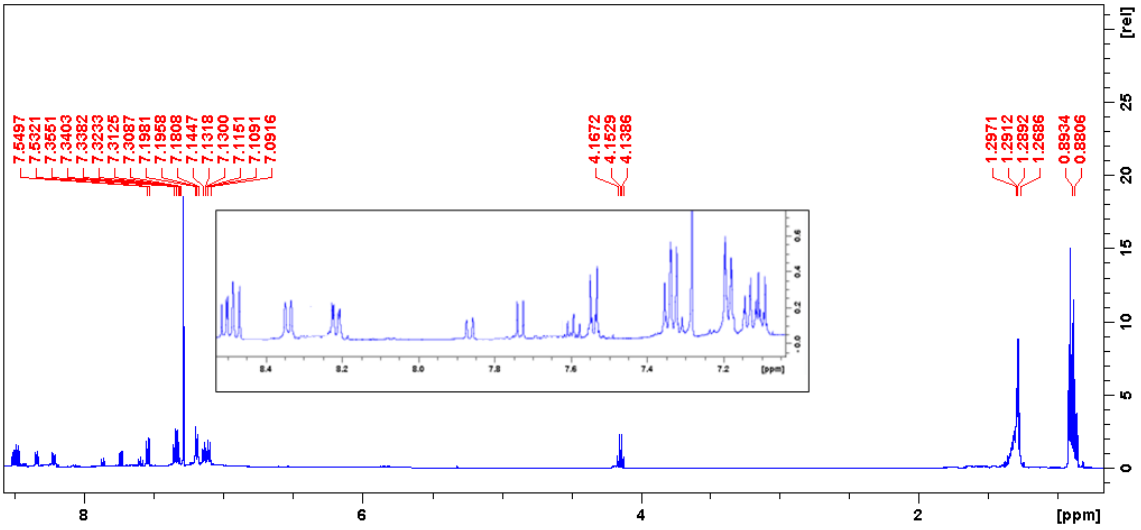

Fig. S7. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of derivative **PI1**

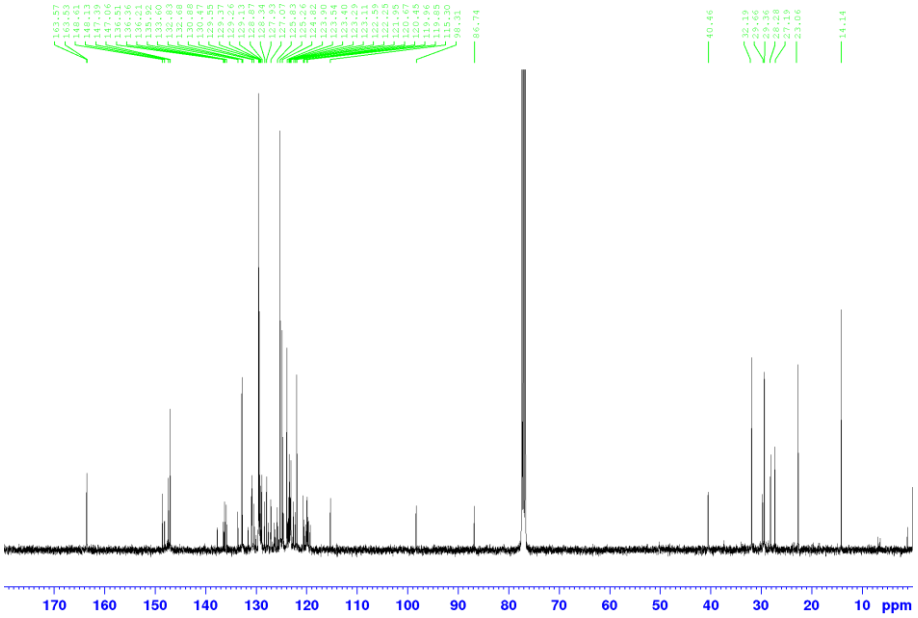

Fig. S8. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of derivative **PI1**

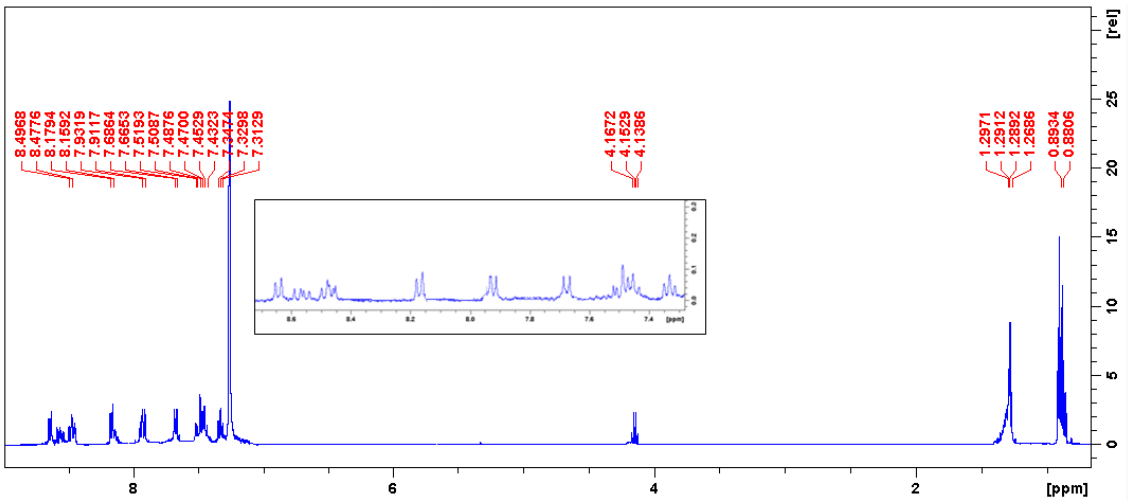

Fig. S9. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of derivative **PI2**

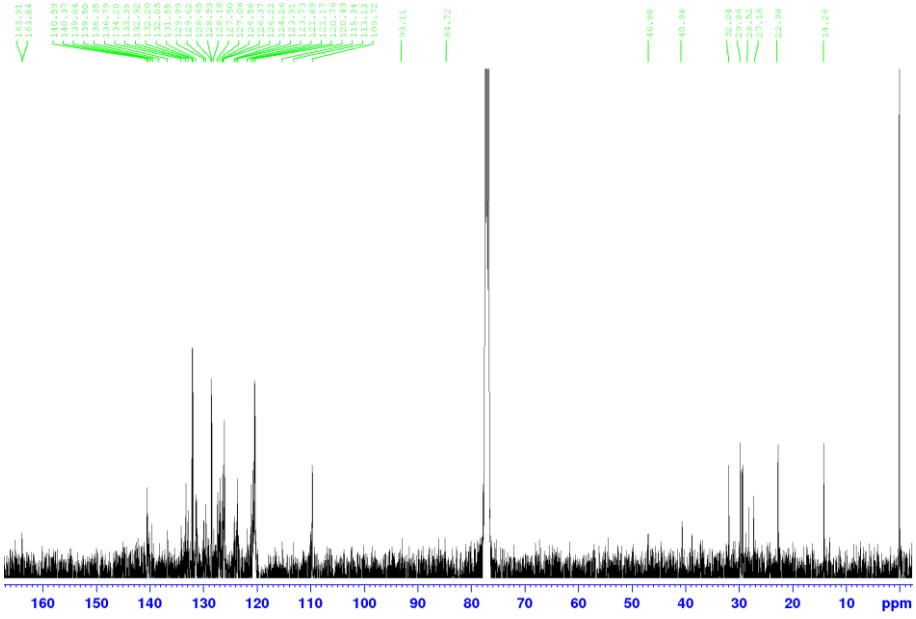

Fig. S10. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of derivative **PI2**

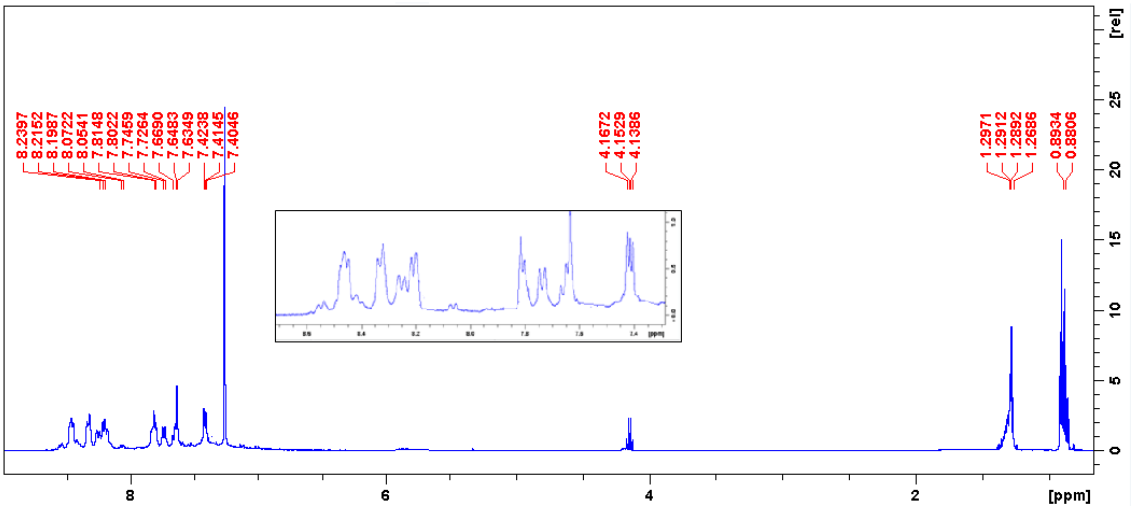

Fig. S11. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of derivative **PI3**

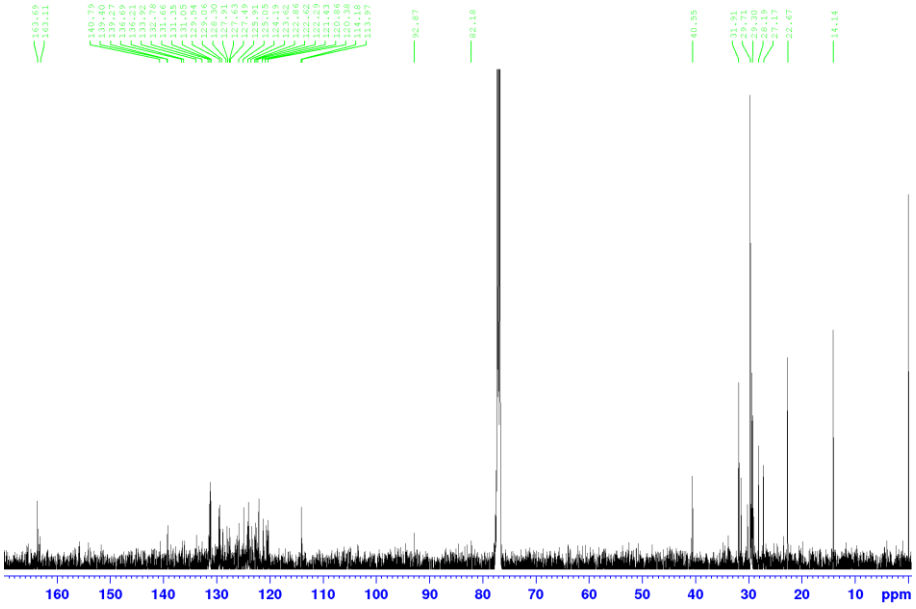

Fig. S12. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of derivative **PI3**