

Supporting Information

Two-Photon Absorption by Fluorene Derivatives: Systematic Molecular Design

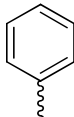
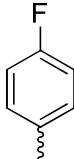
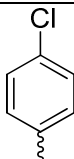
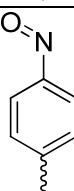
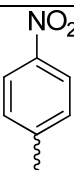
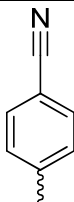
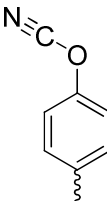
*Gustavo L.C. Moura and Alfredo M. Simas**

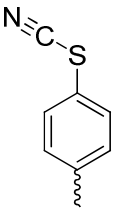
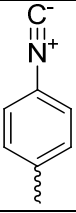
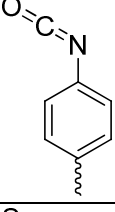
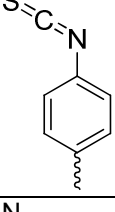
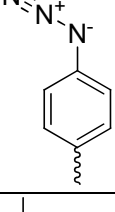
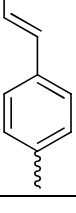
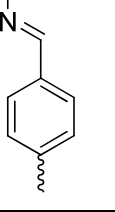
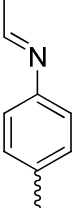
Departamento de Química Fundamental, CCEN, Universidade Federal de Pernambuco.

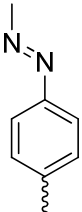
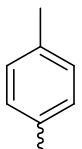
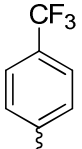
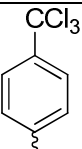
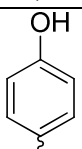
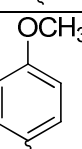
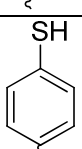
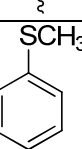
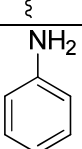
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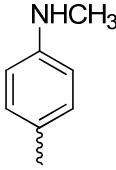
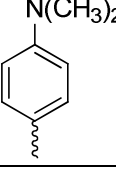
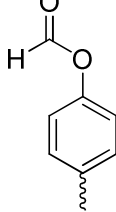
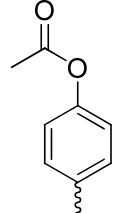
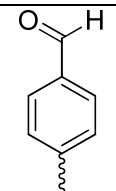
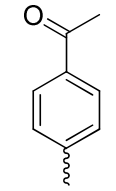
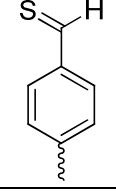
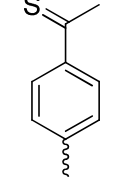
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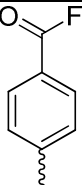
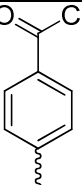
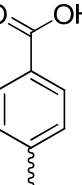
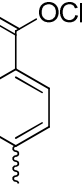
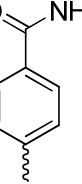
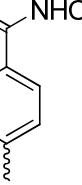
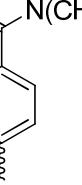
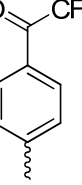
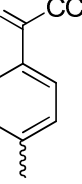
Table S1. Three-level approximation analysis for all molecules studied in the present work. The wavy bond is the position where the group connects to the fluorene unit. The values of the 2PA cross-sections calculated using 100 excited states in the SOS equations are given in Tables S2 through S5. (1GM = 10^{-50} cm⁴/s/photon).

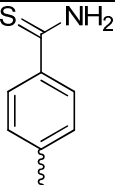
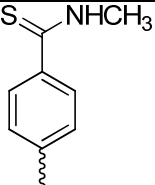
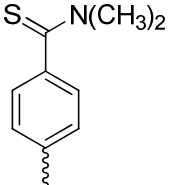
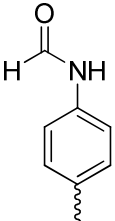
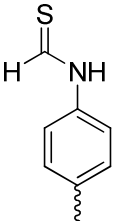
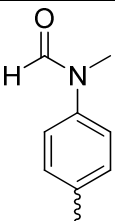
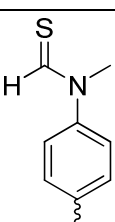
Group	E _{pf} (eV)	E _{det} (eV)	μ _{fo} (D)	μ _{op} (D)	δ ^{3L} (GM)	δ ^{neg} _{approx} (GM)
	5.484	2.192	8.630	11.062	1188	-12
	5.412	2.227	8.872	11.055	1182	-12
	5.442	2.208	8.892	10.738	1152	-12
	5.244	2.257	10.035	9.876	1104	-18
	5.832	1.711	9.487	6.846	1020	-54
	5.316	2.235	9.865	9.686	1074	-18
	5.360	2.235	9.300	11.302	1320	-12

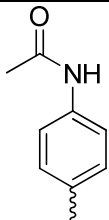
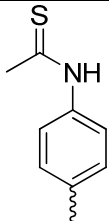
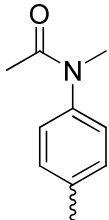
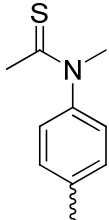
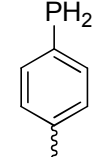
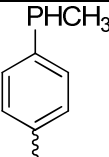
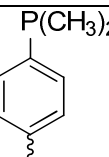
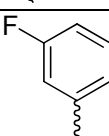
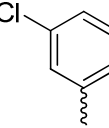
	5.416	2.208	9.115	10.735	1200	-12
	5.324	2.231	9.849	11.234	1452	-18
	5.232	2.240	10.549	12.550	1986	-24
	5.210	2.097	10.679	10.140	1506	-30
	5.024	1.673	9.150	8.884	1242	-36
	5.294	2.218	10.324	12.352	1926	-24
	5.298	2.222	10.279	11.320	1602	-18
	5.266	2.225	10.385	12.055	1824	-24

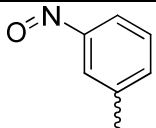
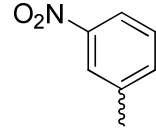
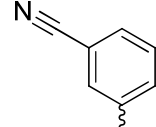
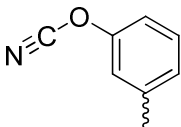
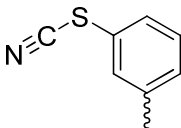
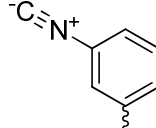
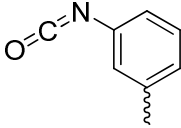
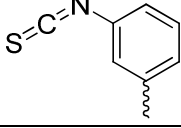
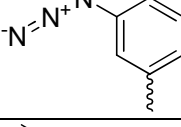
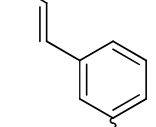
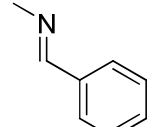
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	5.440	2.206	8.850	10.160	1020	-12
	5.392	2.213	9.232	10.650	1194	-12
	5.260	2.285	9.392	12.039	1410	-12
	5.248	2.284	9.554	12.113	1470	-12
	5.404	2.219	9.108	11.401	1332	-12
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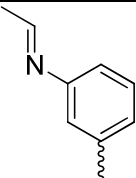
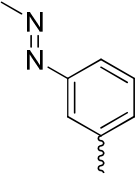
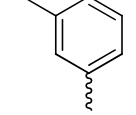
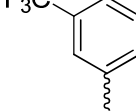
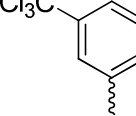
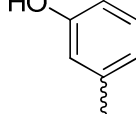
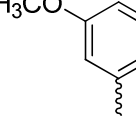
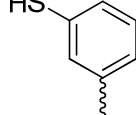
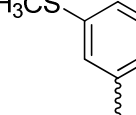
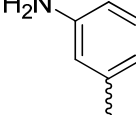
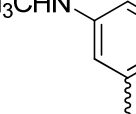
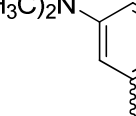
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	5.336	2.252	9.241	11.651	1356	-12
	5.348	2.225	9.574	10.277	1164	-18
	5.380	2.219	9.379	10.493	1182	-18
	5.068	1.942	12.369	7.417	1194	-66
	5.072	2.221	11.055	8.962	1062	-24

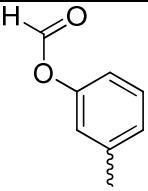
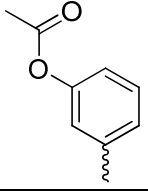
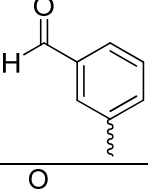
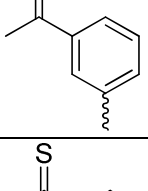
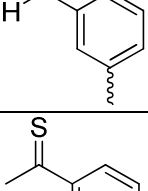
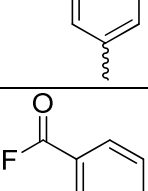
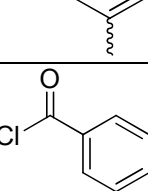
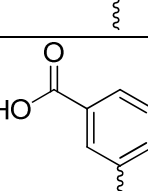
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	5.376	2.217	9.373	10.299	1140	-12
	5.386	2.211	9.393	10.492	1200	-18
	5.406	2.208	9.240	10.741	1230	-12
	5.408	2.206	9.240	10.820	1248	-12
	5.390	2.210	9.315	11.026	1302	-12
	5.320	2.227	9.667	9.636	1032	-18
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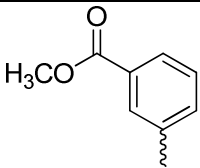
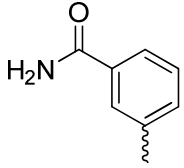
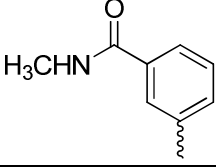
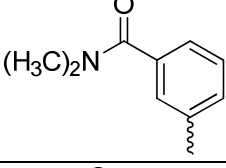
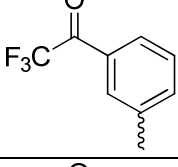
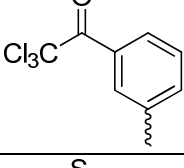
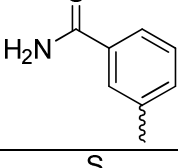
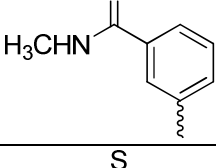
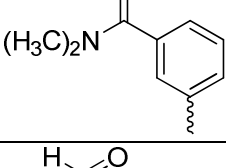
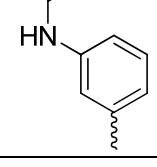
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	5.324	2.226	9.806	9.550	1044	-18
	5.310	2.231	9.880	9.673	1074	-18
	5.270	2.237	10.163	12.151	1758	-18
	5.198	2.133	12.271	10.280	1962	-48
	5.320	2.228	9.810	11.497	1506	-18
	5.262	2.223	11.124	9.137	1206	-30

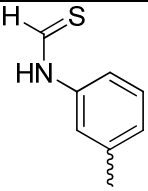
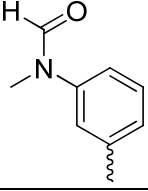
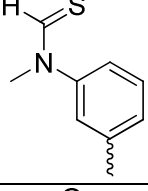
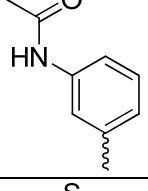
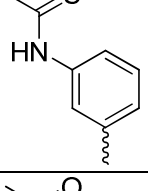
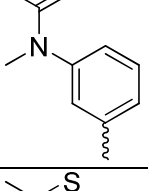
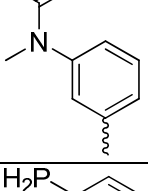
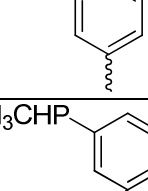
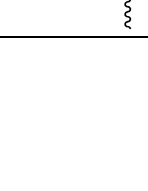
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	5.298	2.223	11.026	10.034	1446	-30
	5.324	2.230	9.770	11.672	1542	-18
	5.310	2.211	10.881	9.752	1350	-24
	5.418	2.212	9.067	11.490	1356	-12
	5.416	2.212	9.110	11.514	1374	-12
	5.434	2.202	9.051	11.458	1362	-12
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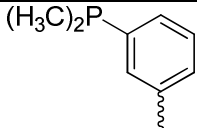
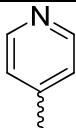
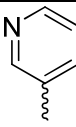
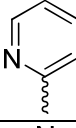
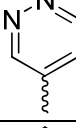
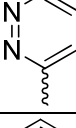
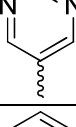
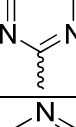
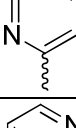
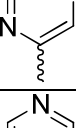
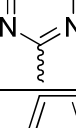
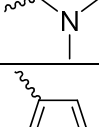
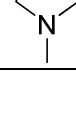
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	5.550	2.116	8.811	9.460	996	-18
	5.560	2.099	8.715	8.549	810	-12
	5.444	2.212	8.664	8.608	702	-12
	5.532	2.145	8.788	9.452	954	-12
	5.540	2.133	9.085	7.891	720	-18
	5.500	2.126	8.269	7.326	510	-12
	5.700	1.983	8.548	5.593	390	-18
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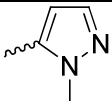
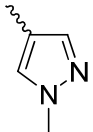
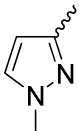
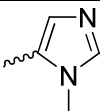
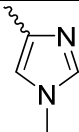
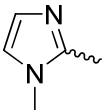
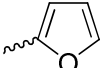
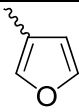
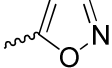
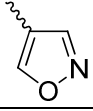
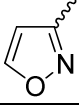
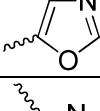
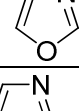
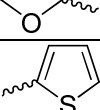
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	5.462	2.210	8.661	9.590	876	-12
	5.440	2.223	8.741	8.549	696	-12
	5.388	2.273	8.794	9.055	738	-12
	5.380	2.297	8.862	8.760	690	-12
	5.460	2.217	8.698	9.407	846	-12
	5.464	2.214	8.685	9.458	852	-12
	5.574	2.115	8.846	6.820	528	-18
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	5.458	2.230	8.770	8.249	654	-12

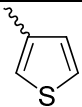
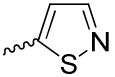
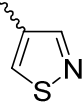
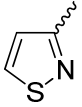
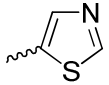
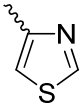
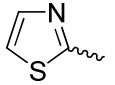
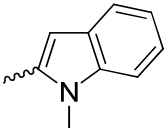
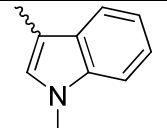
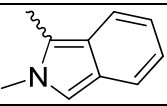
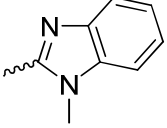
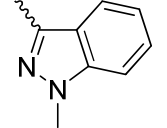
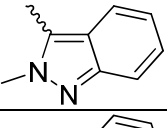
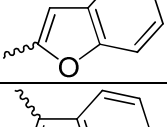
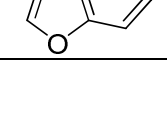
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	5.550	2.123	8.668	9.256	918	-12
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	5.454	2.214	8.792	9.283	840	-12
	5.500	2.143	10.844	8.811	1248	-30
	5.486	2.150	8.738	8.765	792	-12
	5.620	2.049	8.765	7.877	744	-18
	5.590	2.064	8.752	8.797	906	-18
	5.448	2.223	8.746	9.309	828	-12

	5.448	2.220	8.744	9.460	858	-12
	5.458	2.207	8.737	9.952	960	-12
	5.458	2.205	8.747	9.965	966	-12
	5.468	2.188	8.770	9.661	930	-12
	5.584	2.079	8.750	8.590	846	-18
	5.576	2.080	8.685	8.280	774	-18
	5.466	2.182	9.072	8.852	840	-12
	5.472	2.179	8.938	9.833	1014	-12
	5.460	2.189	8.951	9.988	1032	-12
	5.522	2.158	8.830	7.997	678	-12

	5.632	1.993	9.295	5.174	384	-24
	5.524	2.159	8.844	9.280	918	-12
	5.536	2.102	9.587	9.198	1122	-24
	5.430	2.243	8.860	9.697	900	-12
	5.518	2.123	9.075	9.455	1032	-18
	5.484	2.180	8.827	10.910	1218	-12
	5.470	2.167	9.034	9.561	990	-12
	5.466	2.205	8.708	10.208	1008	-12
	5.466	2.201	8.720	10.258	1026	-12

	5.470	2.193	8.717	10.651	1116	-12
	5.820	1.879	8.397	7.540	798	-24
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	5.438	2.163	8.992	9.722	1002	-12
	5.638	1.993	8.560	7.953	774	-18
	5.454	2.083	8.961	10.461	1254	-18
	5.524	2.065	8.769	10.546	1272	-18
	5.508	1.988	9.166	10.535	1488	-24
	5.464	2.135	8.780	8.087	684	-12
	5.612	1.850	7.126	5.036	246	-12
	5.634	1.826	9.000	10.559	1788	-30
	5.074	2.115	9.376	9.244	900	-18
	5.270	2.071	9.054	12.003	1590	-18

	5.236	2.293	8.823	9.542	768	-12
	5.324	2.024	9.184	12.356	1854	-18
	5.302	2.070	9.068	10.806	1308	-18
	5.070	2.184	9.354	9.822	948	-12
	5.158	2.102	9.306	11.407	1410	-18
	5.032	2.306	9.132	10.555	918	-12
	5.014	1.943	10.060	13.469	2544	-30
	5.502	1.935	8.392	7.838	726	-18
	5.228	1.986	9.659	13.725	2532	-24
	5.416	2.041	8.449	11.712	1434	-12
	5.608	1.947	8.339	10.894	1422	-18
	5.078	1.885	10.080	12.849	2532	-36
	5.232	2.049	9.215	12.843	1902	-18
	5.030	1.955	9.997	13.290	2430	-30
	4.958	2.078	9.981	13.045	2004	-24

	5.472	2.062	7.826	8.667	672	-12
	5.204	2.022	9.660	11.268	1632	-24
	5.268	2.243	8.449	9.874	798	-12
	5.518	2.079	8.124	10.416	1050	-12
	5.002	1.978	9.925	12.011	1890	-24
	5.134	2.294	8.420	11.267	936	-6
	4.892	2.018	9.868	11.665	1620	-24
	5.024	2.068	11.147	7.312	816	-36
	4.990	2.261	9.499	9.090	756	-12
	4.572	1.406	10.351	5.573	732	-96
	4.986	2.277	10.511	10.062	1116	-18
	4.872	2.266	9.903	10.465	1032	-12
	4.684	1.919	10.498	7.944	864	-30
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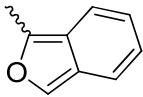
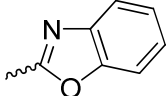
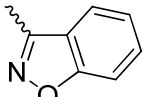
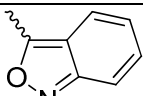
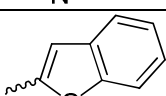
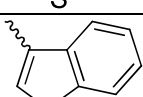
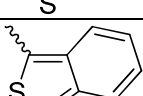
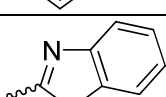
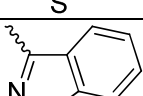
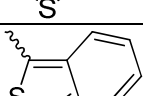
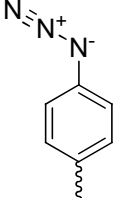
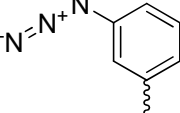
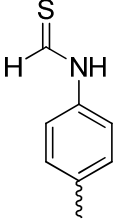
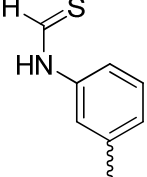
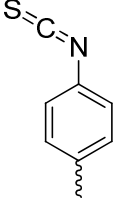
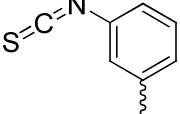
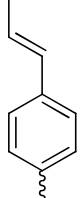
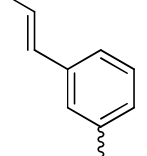
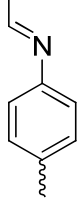
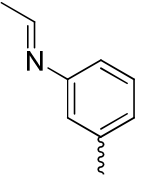
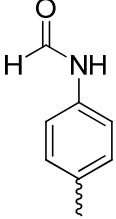
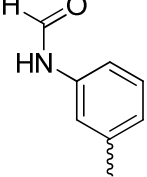
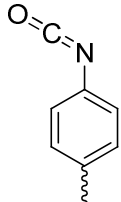
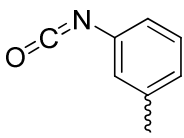
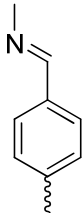
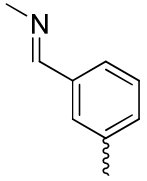
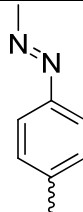
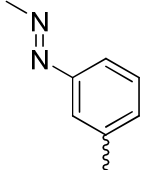
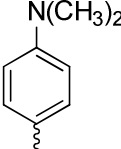
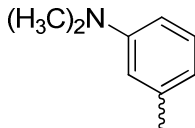
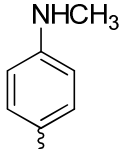
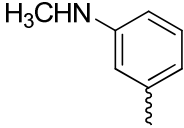
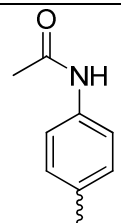
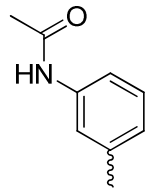
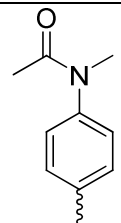
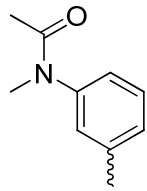
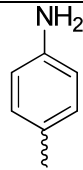
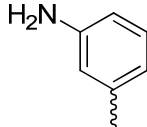
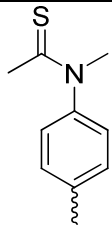
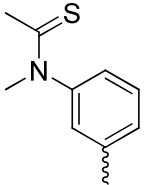
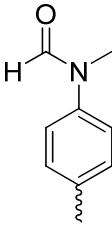
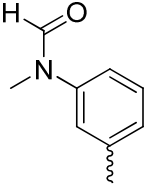
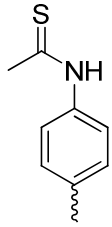
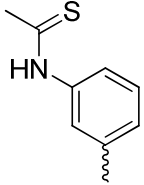
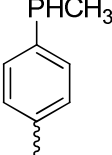
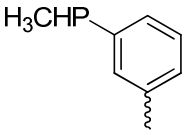
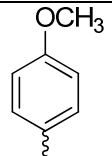
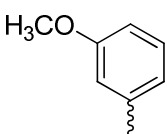
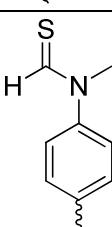
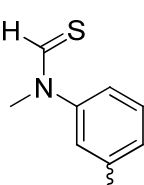
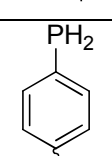
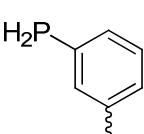
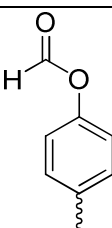
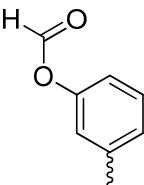
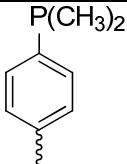
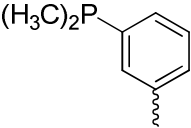
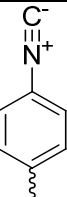
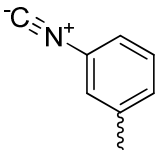
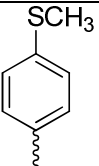
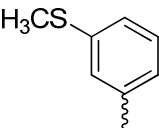
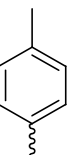
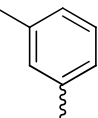
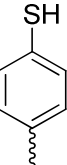
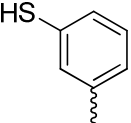
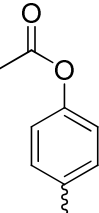
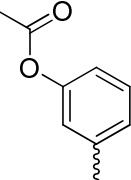
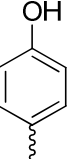
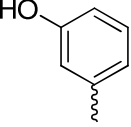
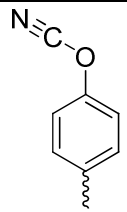
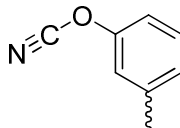
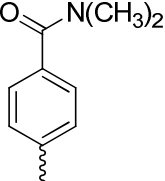
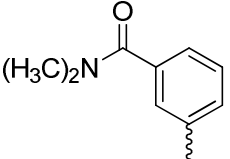
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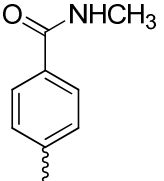
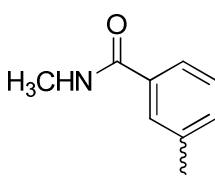
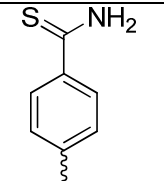
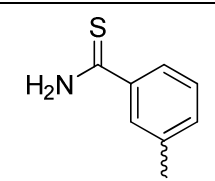
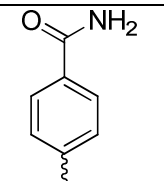
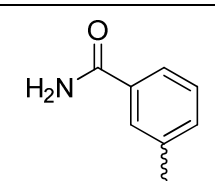
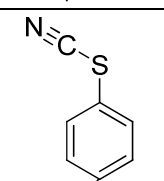
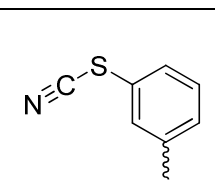
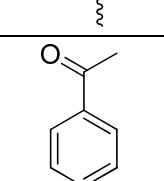
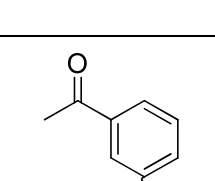
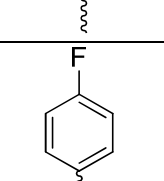
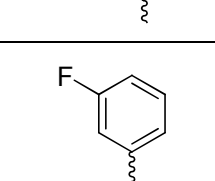
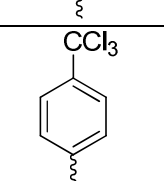
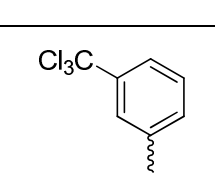
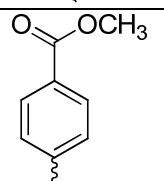
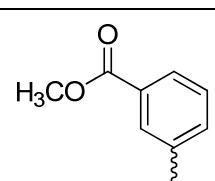
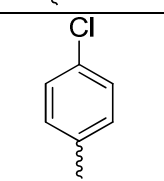
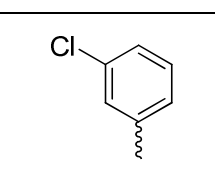
Table S2. Calculated values of λ_{1pa} , λ_{2pa} and $\delta_{\max}$ for the molecules containing *meta*- and *para*-substituted phenyl groups. The wavy bond is the position where the group connects to the fluorene unit. The pairs of molecules are arranged as a function of decreasing values of $\delta_{\max}$ for the molecules with *para*-substituted phenyl groups. (1GM = 10^{-50} cm⁴s/photon)

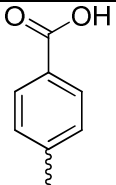
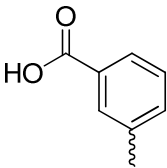
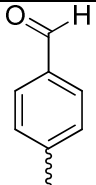
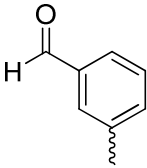
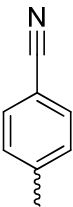
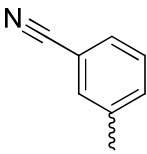
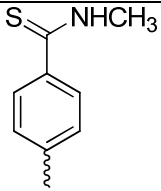
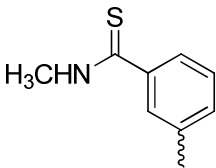
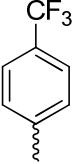
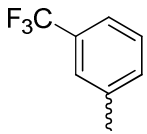
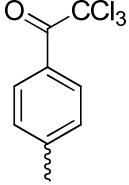
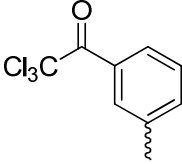
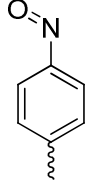
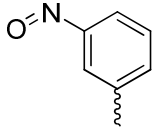
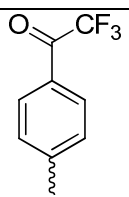
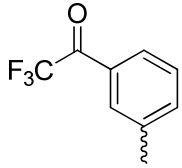
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	338	477	2070		325	440	1212
	339	476	1914		325	451	1110
	330	468	1866		324	455	1146
	331	471	1764		323	455	1188
	330	471	1674		323	449	906

	332	474	1602		323	448	978
	330	468	1590		323	451	1188
	334	479	1548		324	452	1092
	330	472	1548		323	454	876
	334	480	1542		323	446	642
	328	467	1518		323	457	996
	328	466	1518		324	452	1248
	332	478	1506		323	445	702

	330	467	1500		325	453	1140
	329	466	1494		323	449	1056
	330	468	1488		325	449	1158
	325	458	1428		323	454	1116
	329	472	1416		323	461	786
	331	471	1416		325	448	1296
	325	458	1416		323	454	1098
	326	462	1410		323	443	870

	325	456	1410		324	453	1182
	328	466	1404		323	448	1068
	325	458	1404		323	454	990
	325	458	1398		323	453	1092
	325	459	1392		323	454	978
	327	465	1386		323	447	1086
	329	471	1380		324	460	816
	326	463	1368		324	446	930
	326	460	1362		324	454	1050

	326	458	1296		324	454	1080
	330	479	1278		324	454	1062
	326	459	1272		323	454	1068
	325	458	1254		324	455	840
	326	461	1254		323	455	1020
	325	458	1242		323	454	948
	326	460	1224		324	456	834
	326	460	1218		323	455	930
	324	456	1206		324	454	1038

	327	461	1164		323	455	876
	327	464	1158		323	455	834
	328	467	1110		323	447	1068
	328	466	1092		324	453	1164
	324	456	1056		323	454	930
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	331	473	1014		323	448	1068
	329	466	1014		324	444	894

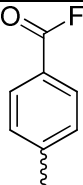
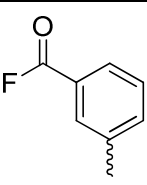
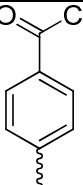
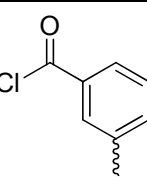
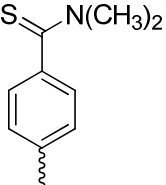
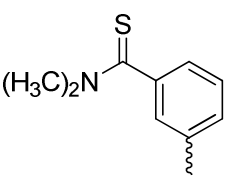
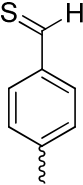
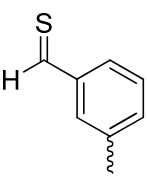
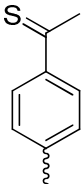
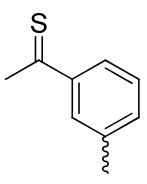
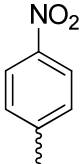
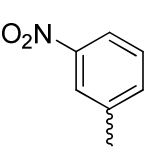
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	329	467	984		324	444	954
	329	467	984		324	454	1194
	354	489	936		324	451	1212
	340	489	912		325	452	942
	329	425	906		324	443	852

Table S3. Calculated values of λ_{1pa} , λ_{2pa} and δ_{max} for the molecules containing six-membered heterocyclic groups. The wavy bond is the position where the group connects to the fluorene unit. (1GM = $10^{-50}\text{cm}^4/\text{s}/\text{photon}$)

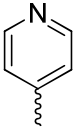
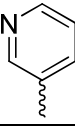
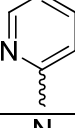
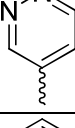
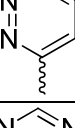
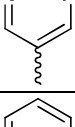
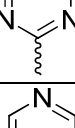
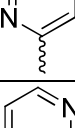
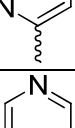
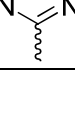
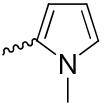
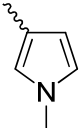
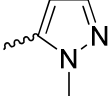
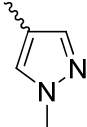
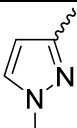
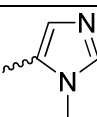
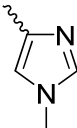
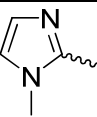
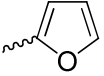
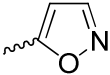
Group	$\lambda^{1pa}(\text{nm})$	$\lambda^{2pa}(\text{nm})$	$\delta_{max}(\text{GM})$
	322	426	822
	326	457	1068
	326	456	1080
	325	440	768
	329	455	1440
	327	449	1392
	331	450	1758
	326	454	744
	332	442	906
	332	440	1734

Table S4. Calculated values of λ_{1pa} , λ_{2pa} and δ_{max} for the molecules containing five-membered heterocyclic groups. The wavy bond is the position where the group connects to the fluorene unit. (1GM = $10^{-50}\text{cm}^4\text{s/photon}$)

Group	$\lambda^{1pa}(\text{nm})$	$\lambda^{2pa}(\text{nm})$	$\delta_{max}(\text{GM})$
	345	489	732
	338	471	1566
	329	474	960
	337	466	1848
	336	468	1446
	342	489	852
	342	481	1470
	338	493	864
	356	495	2412
	333	451	960
	344	474	2448
	333	458	1470

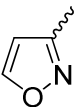
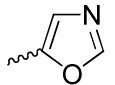
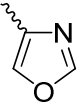
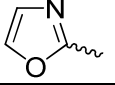
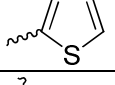
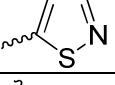
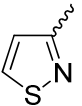
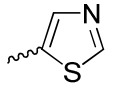
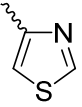
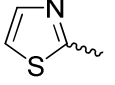
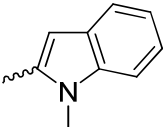
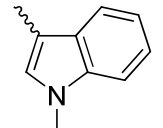
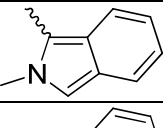
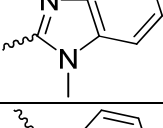
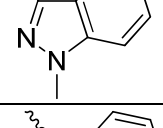
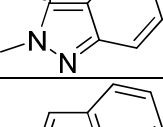
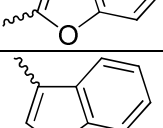
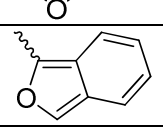
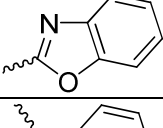
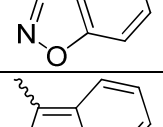
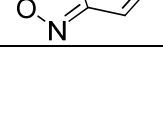
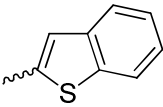
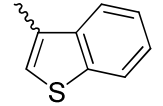
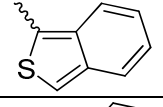
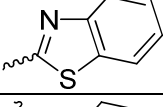
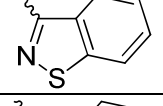
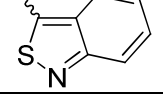
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	356	488	2406
	341	474	1860
	355	493	2280
	352	500	1698
	329	453	900
	343	476	1650
	330	471	816
	326	449	1170
	355	496	1746
	334	483	960
	359	507	1620

Table S5. Calculated values of λ_{1pa} , λ_{2pa} and δ_{max} for the molecules containing benzo derivatives of five-membered heterocyclic groups. The wavy bond is the position where the group connects to the fluorene unit.
(1GM = 10^{-50} cm⁴/s/photon)

Group	λ^{1pa} (nm)	λ^{2pa} (nm)	δ_{max} (GM)
	350	494	966
	342	497	762
	415	542	876
	341	497	1152
	347	509	966
	376	529	900
	366	503	3138
	334	490	774
	404	533	2346
	362	503	3408
	332	469	852
	377	527	1974

	356	503	2784
	323	434	516
	445	571	858
	357	490	1944
	321	423	702
	412	544	696

All geometry optimizations have been carried out using the [RM1 semiempirical molecular orbital model](#).