First molecular electronic hyperpolarizability of series of π-conjugated oxazole dyes in solution: an experimental and theoretical study

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Supplementary Information

Absorption e emission spectra

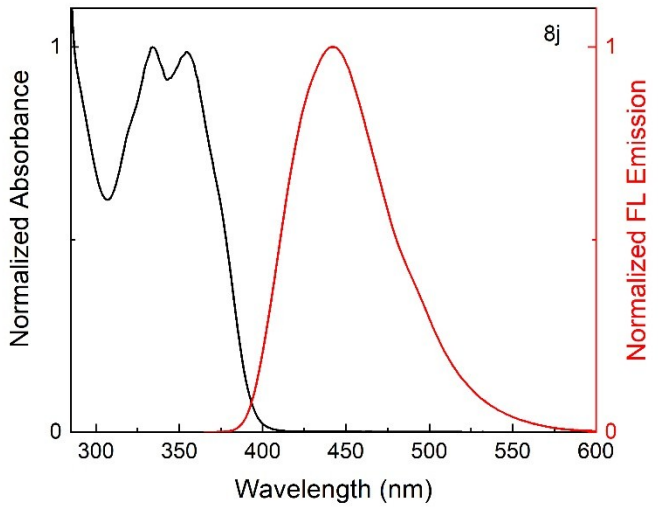


Figure S1: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 8j.

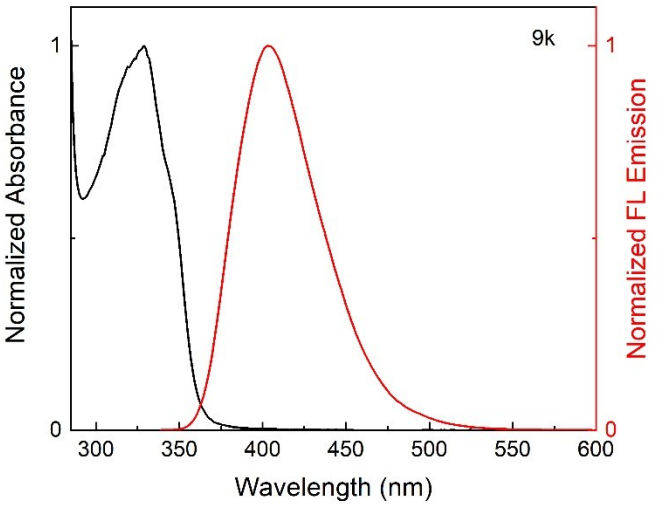


Figure S2: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 9k.

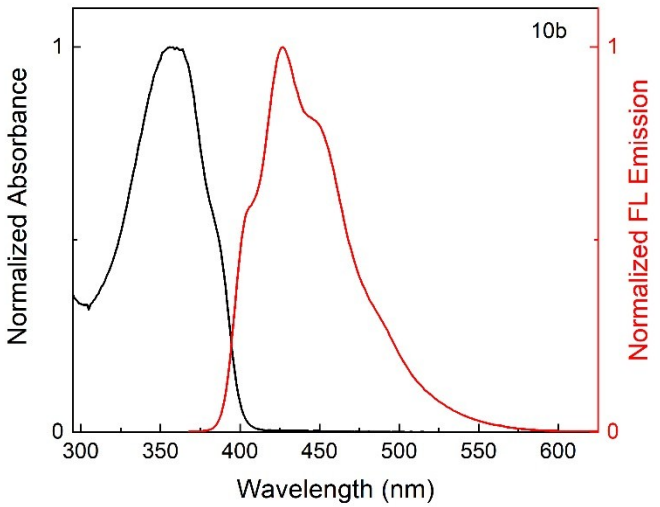


Figure S3: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 10b.

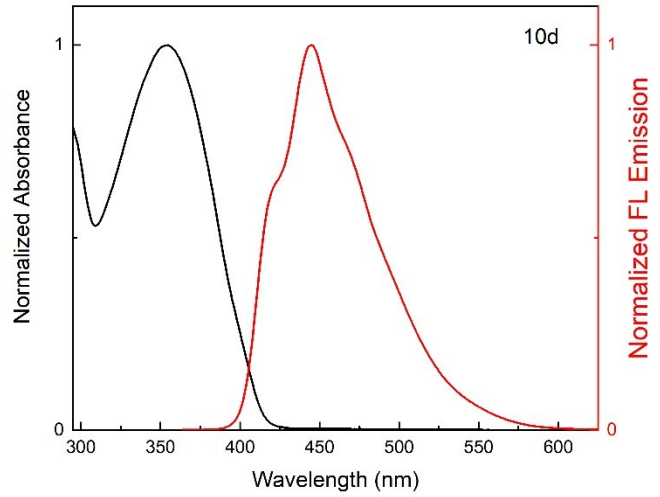


Figure S4: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 10d.

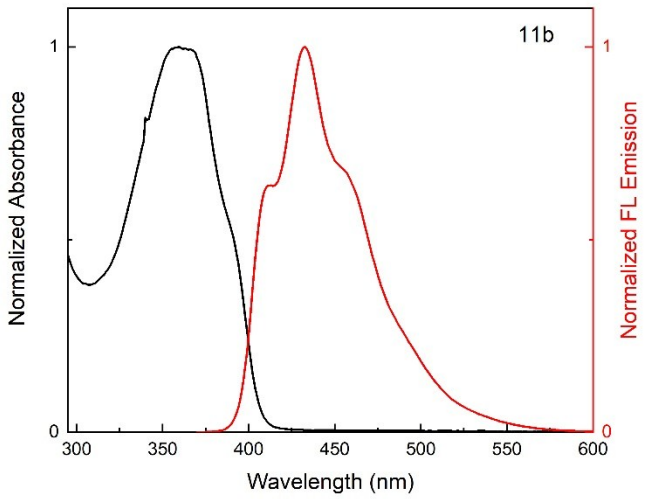


Figure S5: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 11b.

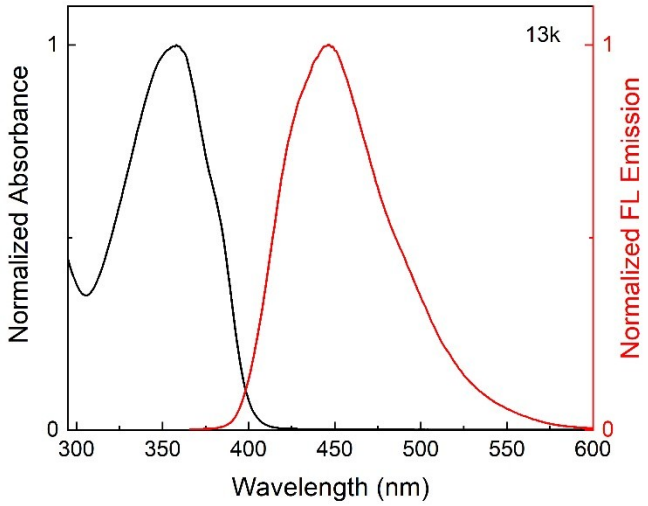


Figure S6: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 13k.

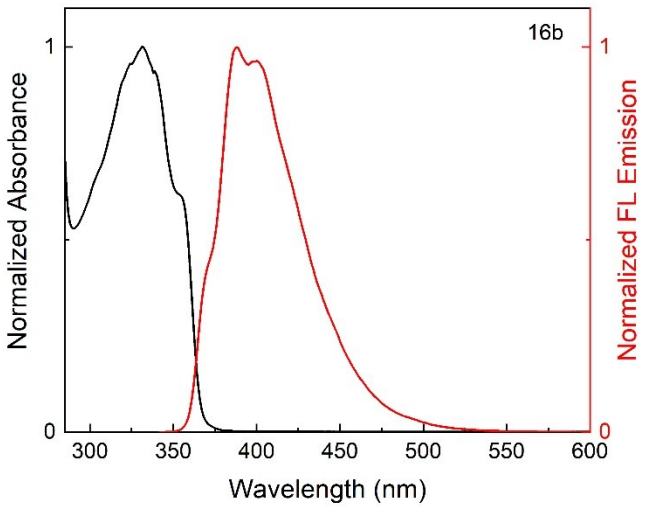


Figure S7: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 16b.

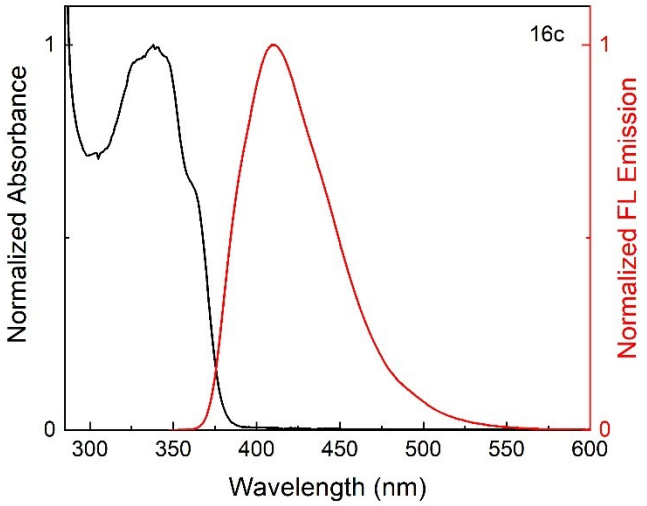


Figure S8: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 16c.

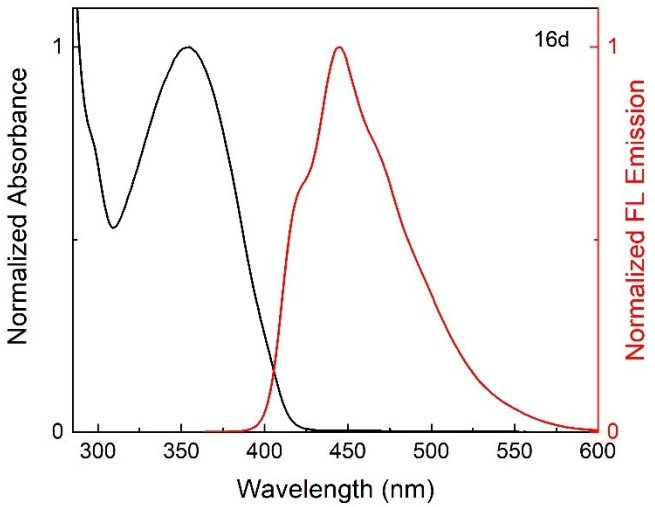


Figure S9: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 16d.

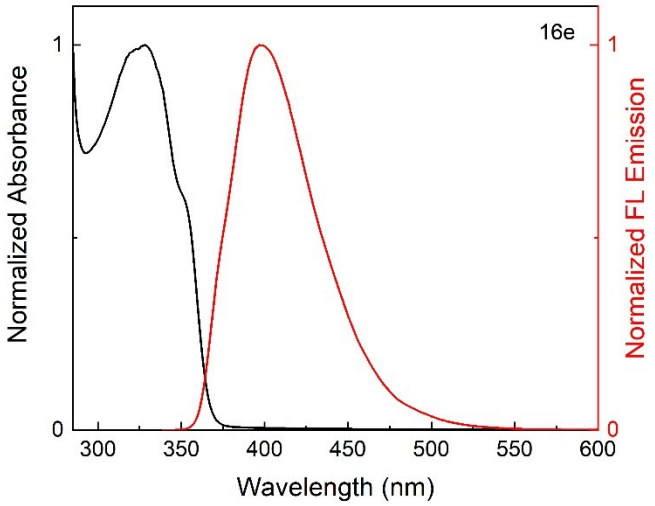


Figure S10: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 16e.

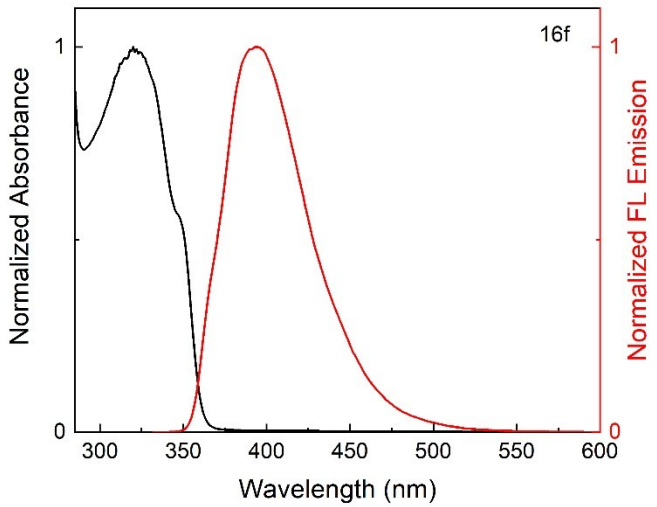
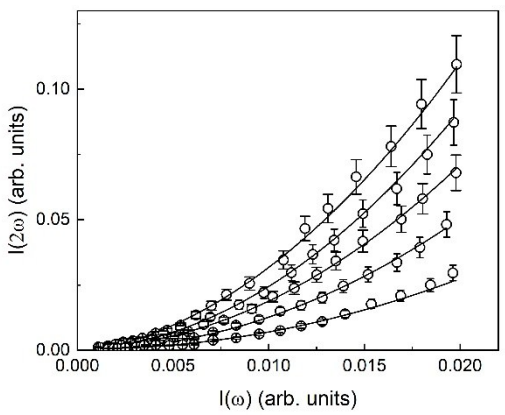
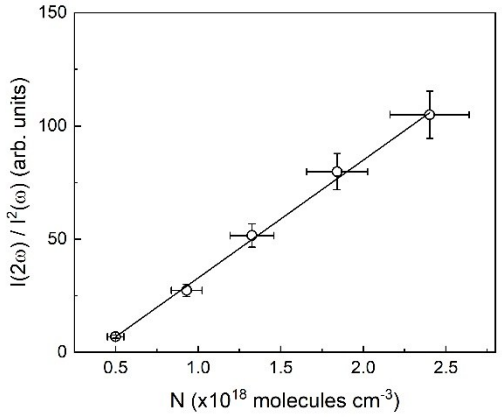


Figure S11: Normalized absorption (black line) and fluorescence (red line) spectra of the compound 16f.

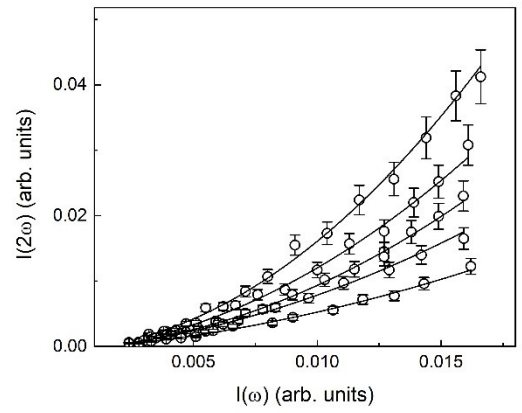


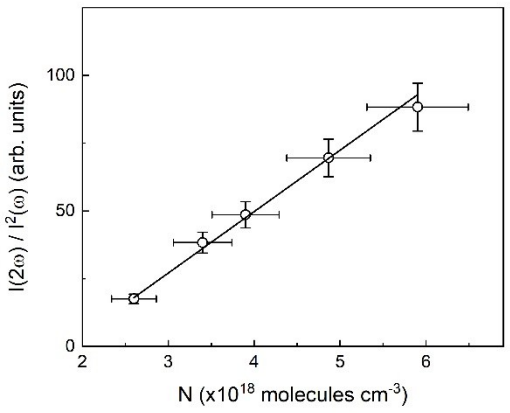
a)



b)

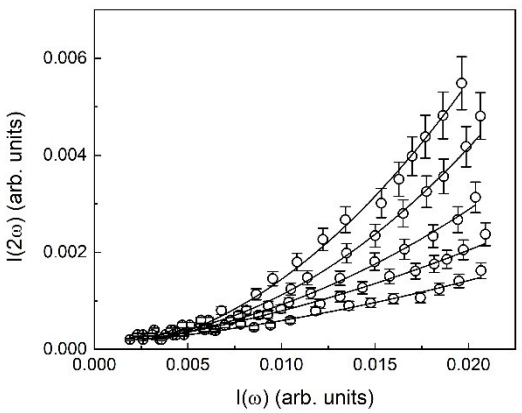
Figure S12: - a) Experimental first hyperpolarizability scattering signals for 9k dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

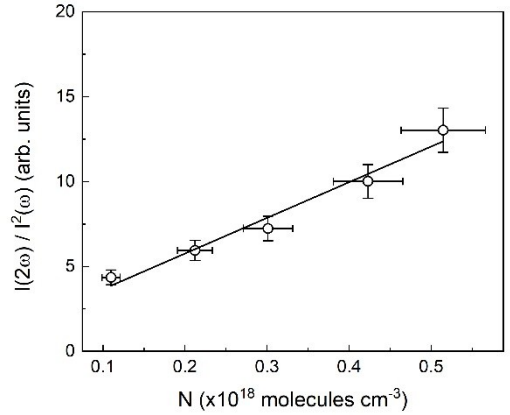




a) b)

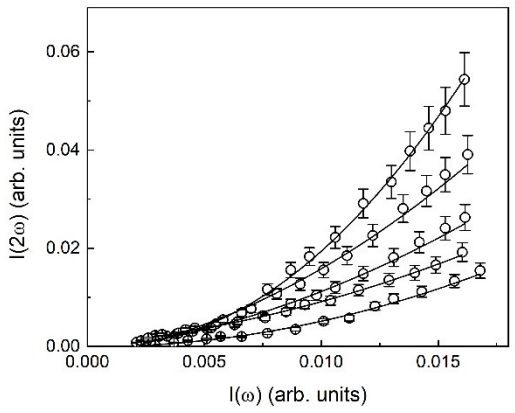
Figure S13: - a) Experimental first hyperpolarizability scattering signals for 10b dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).



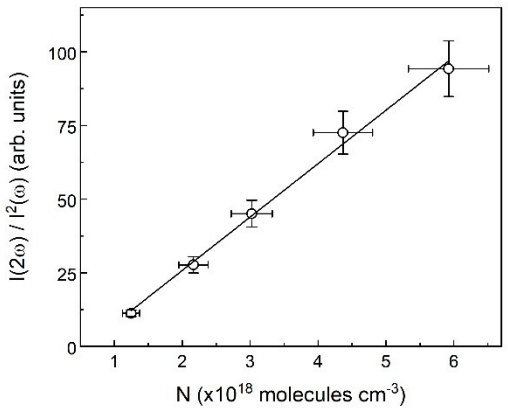


a) b)

Figure S14: - a) Experimental first hyperpolarizability scattering signals for 10d dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

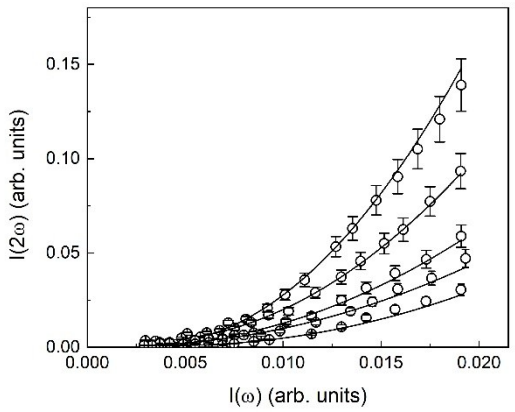


a)

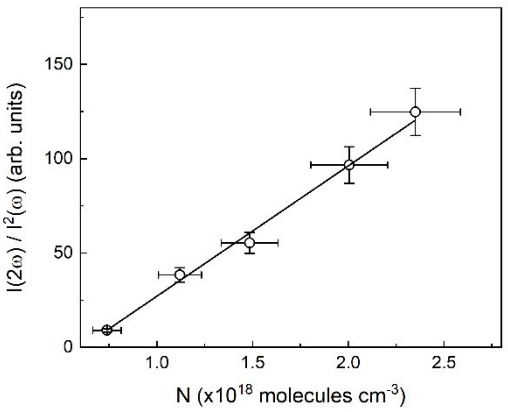


b)

Figure S15: - a) Experimental first hyperpolarizability scattering signals for 11b dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

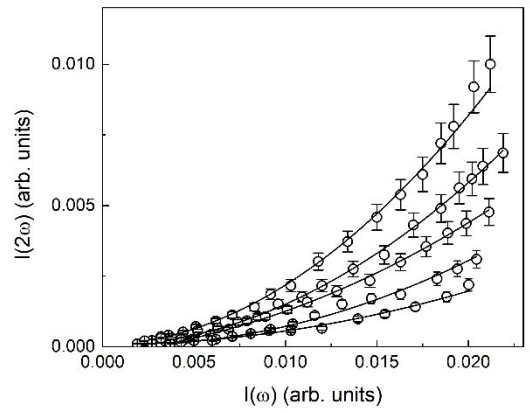


a)

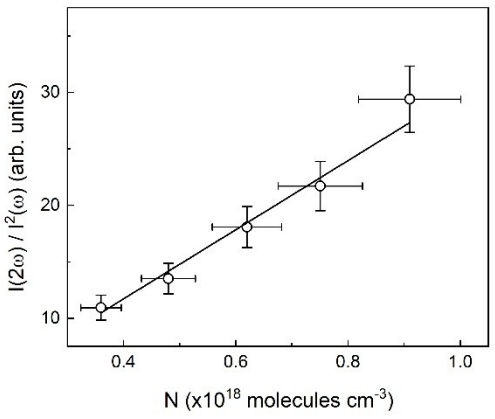


b)

Figure S16: - a) Experimental first hyperpolarizability scattering signals for 13k dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

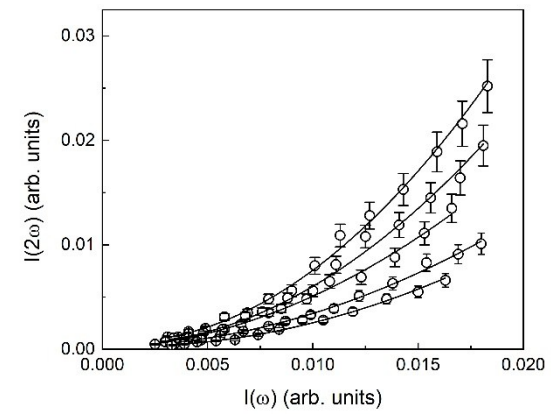


a)

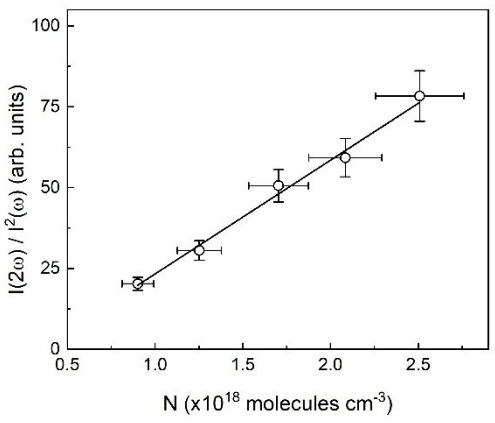


b)

Figure S17: - a) Experimental first hyperpolarizability scattering signals for 16b dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

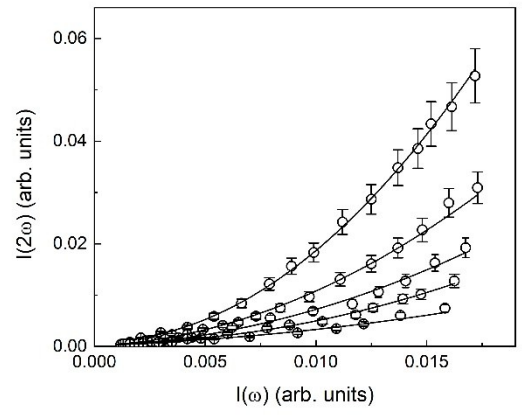


a)

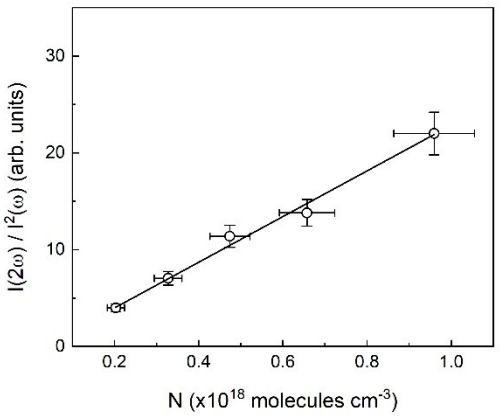


b)

Figure S18: - a) Experimental first hyperpolarizability scattering signals for 16c dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

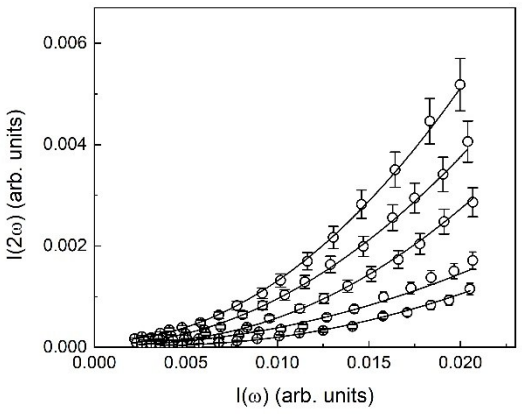


a)

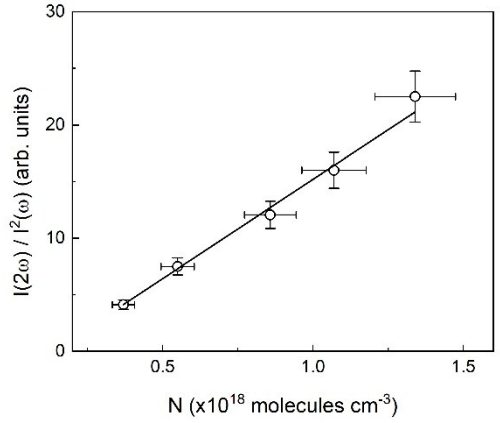


b)

Figure S19: - a) Experimental first hyperpolarizability scattering signals for 16d dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

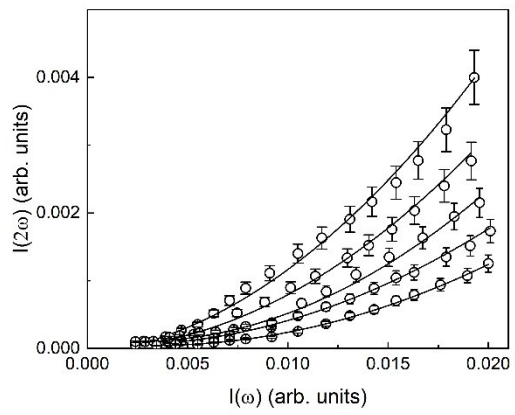


a)

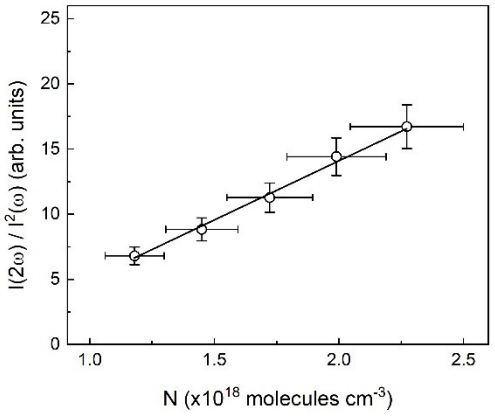


b)

Figure S20: - a) Experimental first hyperpolarizability scattering signals for 16e dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).



a)



b)

Figure S21: - a) Experimental first hyperpolarizability scattering signals for 16f dissolved in toluene; b) linear dependence between the hyperpolarizability signal ($I(2\omega)/I^2(\omega)$) and the sample concentrations with the respectively linear fit (solid line).

Table S1. Optimized geometry in solvent (toluene) for compounds 8j and 9k used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 8j				Sample: 9k			
C	-3.12660	-1.33378	-0.06468	C	5.20078	-0.98391	0.08623
C	-4.34457	-0.65643	-0.10942	C	6.41404	-0.30918	0.10018
O	-5.56075	-1.26561	-0.11135	N	6.52949	1.02562	0.07285
C	-5.61313	-2.69038	-0.09675	H	7.34344	-0.86989	0.13512
H	-6.67087	-2.94545	-0.11692	C	5.39093	1.72641	0.02945
H	-5.15842	-3.09653	0.81239	C	4.12371	1.15316	0.01217
H	-5.12057	-3.11444	-0.97716	H	5.49429	2.80749	0.00729
C	-4.37660	0.74951	-0.15807	C	4.00879	-0.24378	0.04127
O	-5.56429	1.41569	-0.28031	H	3.24323	1.78109	-0.02337
C	-6.28073	1.62484	0.94581	H	5.18913	-2.06668	0.10972
H	-7.19066	2.16088	0.67836	C	2.71824	-0.90460	0.02622
H	-5.68927	2.23150	1.63828	C	2.30037	-2.20443	0.04909
H	-6.54075	0.67070	1.41150	N	0.92518	-2.25351	0.01734
C	-3.16867	1.46612	-0.15676	H	2.89779	-3.10115	0.08659
O	-3.28982	2.81969	-0.19677	C	0.53959	-1.00619	-0.02382
C	-2.10408	3.61011	-0.22737	O	1.58071	-0.12909	-0.02090
H	-2.44183	4.64386	-0.26900	C	-0.81875	-0.48259	-0.06900
H	-1.50201	3.38863	-1.11402	C	-1.88432	-1.39024	-0.07350
H	-1.50202	3.46004	0.67440	C	-3.19275	-0.91217	-0.11868
C	-1.94686	0.78943	-0.11615	H	-1.67007	-2.44801	-0.04735
C	-1.92553	-0.60963	-0.07023	O	-4.29727	-1.70499	-0.13675
H	-1.01510	1.33407	-0.11790	C	-4.11850	-3.12086	-0.14545
H	-3.10499	-2.41321	-0.03003	H	-5.12103	-3.54270	-0.18052
C	-0.65960	-1.32437	-0.02887	H	-3.60962	-3.46239	0.76104
C	-0.29337	-2.64068	0.00958	H	-3.55605	-3.44266	-1.02692
N	1.08133	-2.74372	0.03608	C	-3.44299	0.47285	-0.15296
H	-0.92367	-3.51477	0.01878	O	-4.71708	0.94985	-0.26984
C	1.51484	-1.51543	0.01366	C	-5.48447	0.97293	0.94396
O	0.50853	-0.59571	-0.02611	H	-6.46138	1.37350	0.67640
C	2.88960	-1.04533	0.02549	H	-5.01149	1.62635	1.68331
C	3.95087	-2.00068	0.05820	H	-5.59910	-0.03463	1.35068
N	5.22206	-1.68495	0.07089	C	-2.36269	1.37342	-0.14589
H	3.70005	-3.05667	0.07336	O	-2.69684	2.69019	-0.17895
C	5.56456	-0.36081	0.05196	C	-1.65134	3.65883	-0.21084
C	4.58129	0.67594	0.01914	H	-2.14902	4.62571	-0.25314
C	3.22115	0.29419	0.00613	H	-1.02219	3.53483	-1.09769
H	2.44987	1.05537	-0.01871	H	-1.03238	3.60780	0.69064
C	6.93600	-0.00977	0.06530	C	-1.05070	0.89698	-0.10683
C	7.31543	1.31291	0.04711	H	-0.21425	1.57905	-0.10126
H	7.66601	-0.81000	0.08998				
C	6.34320	2.34122	0.01482				
H	8.36745	1.57424	0.05743				
C	5.00402	2.03089	0.00107				
H	6.66107	3.37738	0.00082				
H	4.25519	2.81553	-0.02375				

Table S2. Optimized geometry in solvent (toluene) for compounds 10b and 10d used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 10b				Sample: 10d			
H	3.22586	1.70926	0.01009	H	7.50645	1.87339	0.86227
C	4.27022	1.42405	0.01744	C	6.60283	1.32200	0.62952
C	5.25907	2.40356	0.03869	C	6.67821	-0.01393	0.23037
H	4.97437	3.44970	0.04808	H	7.64206	-0.50400	0.15267
C	6.60667	2.04692	0.04780	C	5.52183	-0.72416	-0.06787
H	7.37466	2.81150	0.06427	H	5.59601	-1.76100	-0.37445
C	6.95974	0.69595	0.03598	C	4.26156	-0.10836	0.02649
H	8.00482	0.40772	0.04375	C	3.05598	-0.85658	-0.28974
C	5.97802	-0.28701	0.01530	C	2.79173	-2.12577	-0.72349
H	6.26878	-1.33110	0.00808	H	3.48841	-2.91774	-0.94574
C	4.61620	0.06298	0.00490	N	1.43193	-2.30124	-0.85837
C	3.59499	-0.97085	-0.01812	C	0.90366	-1.15600	-0.51211
C	3.60437	-2.33704	-0.04939	C	-0.49618	-0.81870	-0.47938
N	2.31265	-2.81581	-0.05818	H	-1.14242	-1.62984	-0.78729
C	1.55272	-1.75030	-0.03308	C	-0.97495	0.39739	-0.14625
C	0.11587	-1.70616	-0.02867	H	-0.24544	1.17274	0.07278
H	-0.34628	-2.68603	-0.04319	C	-2.36634	0.85827	-0.13726
C	-0.61501	-0.57161	-0.01013	C	-2.57153	2.19524	-0.45630
C	-2.06944	-0.45929	-0.00007	H	-1.70865	2.82591	-0.64202
C	-2.64073	0.83209	-0.02278	C	-3.86002	2.74413	-0.59407
H	-1.98003	1.68865	-0.04780	H	-3.97044	3.78637	-0.87045
C	-4.01521	1.02363	-0.01598	C	-4.96644	1.95550	-0.39317
O	-4.63223	2.23584	-0.03923	H	-5.96480	2.36266	-0.51243
C	-3.82310	3.40761	-0.06897	C	-4.82317	0.59905	-0.00211
H	-3.18870	3.47614	0.82078	C	-3.51297	0.03440	0.15549
H	-3.19917	3.43822	-0.96818	C	-3.42383	-1.29456	0.65046
H	-4.51832	4.24487	-0.08264	H	-2.45355	-1.72351	0.85462
C	-4.87397	-0.10293	0.01838	C	-4.55093	-2.03928	0.91444
O	-6.20412	0.16346	0.02749	H	-4.44953	-3.04724	1.30065
C	-7.11716	-0.93071	0.06595	C	-5.83737	-1.49780	0.70087
H	-7.00763	-1.57044	-0.81537	H	-6.71745	-2.09764	0.90286
H	-6.98271	-1.52785	0.97329	C	-5.96543	-0.20248	0.26286
H	-8.10982	-0.48479	0.06907	H	-6.94803	0.23630	0.12446
C	-4.31463	-1.38035	0.04188	O	1.83886	-0.22899	-0.15301
H	-4.95640	-2.25041	0.06933	C	4.19488	1.23526	0.42929
C	-2.93306	-1.55859	0.03275	H	3.23124	1.72238	0.50700
H	-2.54074	-2.56761	0.05519	C	5.35732	1.94047	0.72712
H	-0.07780	0.37296	-0.00306	H	5.28875	2.97721	1.03677
O	2.27187	-0.58931	-0.00810				
H	4.45297	-3.00158	-0.06694				

Table S3. Optimized geometry in solvent (toluene) for compounds 11b and 13k used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 11b				Sample: 13k			
C	5.94430	1.31442	0.03679	C	7.46385	0.64023	0.12111
C	4.61483	1.75585	0.03015	N	7.22342	1.95712	0.18463
C	3.57344	0.84332	0.02498	C	5.94017	2.33493	0.17633
H	4.42046	2.82170	0.02922	C	4.86867	1.45106	0.10621
C	3.82360	-0.54159	0.02621	H	5.75501	3.40396	0.22833
H	2.55194	1.20182	0.02019	C	5.12611	0.07425	0.03933
C	5.15824	-0.96874	0.03202	H	3.85365	1.82587	0.10293
C	6.21155	-0.05943	0.03773	C	6.47112	-0.32767	0.04868
H	5.38779	-2.02802	0.03090	H	6.74508	-1.37451	0.00172
H	7.22717	-0.43092	0.04169	H	8.50838	0.34302	0.12918
O	6.89717	2.28722	0.04152	C	4.05364	-0.89802	-0.03682
C	8.27002	1.90156	0.04764	C	3.99062	-2.26013	-0.13017
H	8.51490	1.32191	0.94315	N	2.67720	-2.66573	-0.17093
H	8.83806	2.82975	0.05091	H	4.80327	-2.96754	-0.17125
H	8.52319	1.32317	-0.84637	C	1.97593	-1.56086	-0.10276
C	2.73721	-1.50524	0.02163	O	2.75383	-0.44467	-0.01989
C	2.65199	-2.86996	0.04173	C	0.54300	-1.44091	-0.10654
N	1.32959	-3.25760	0.02257	C	-0.12256	-0.26985	-0.03422
H	3.45205	-3.59187	0.06938	H	0.03104	-2.39308	-0.17439
C	0.64579	-2.14338	-0.00793	C	-1.56898	-0.07423	-0.02985
O	1.44467	-1.03380	-0.00980	H	0.46316	0.64271	0.02812
C	-0.78441	-1.99844	-0.03864	C	-2.48570	-1.14242	-0.07899
C	-1.43408	-0.81670	-0.06694	C	-3.85437	-0.89981	-0.06631
H	-1.31348	-2.94395	-0.03709	H	-2.12356	-2.15909	-0.12844
C	-2.87956	-0.60713	-0.10041	C	-4.34375	0.42633	0.00763
H	-0.83432	0.08919	-0.06440	C	-3.43110	1.48574	0.03801
C	-3.81510	-1.65142	-0.12895	C	-2.05963	1.23531	0.02163
C	-5.17597	-1.37107	-0.15376	H	-1.38224	2.08022	0.06121
H	-3.48988	-2.68421	-0.13054	O	-4.80939	-1.86775	-0.11622
C	-5.64694	-0.06073	-0.15529	C	-4.39807	-3.23101	-0.20187
H	-5.90690	-2.17095	-0.17950	H	-5.31658	-3.81335	-0.23868
C	-4.72018	1.00353	-0.14349	H	-3.81417	-3.52507	0.67585
C	-3.35688	0.71824	-0.10929	H	-3.81574	-3.41172	-1.11042
H	-2.63755	1.52678	-0.10020	O	-5.68576	0.68790	-0.00973
O	-6.99702	0.15727	-0.25224	C	-6.39727	0.38847	1.20465
C	-7.63152	0.75837	0.88792	H	-6.34698	-0.67804	1.43141
H	-8.69010	0.82627	0.64055	H	-5.99040	0.97218	2.03544
H	-7.23268	1.75532	1.08159	H	-7.43163	0.67842	1.02529
H	-7.50299	0.12438	1.77133	O	-3.86212	2.78402	0.15321
O	-5.24389	2.26114	-0.18218	C	-4.50780	3.33393	-1.00730
C	-4.35196	3.37311	-0.21357	H	-4.77836	4.35588	-0.74477
H	-4.98505	4.25713	-0.25974	H	-5.40414	2.76640	-1.26298
H	-3.70876	3.33981	-1.09830	H	-3.81594	3.34608	-1.85588
H	-3.73476	3.41375	0.68954				

Table S4. Optimized geometry in solvent (toluene) for compounds 16b and 16c used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 16b				Sample: 16c			
C	-7.27109	0.34903	0.01241	C	-6.62859	0.25116	0.00731
C	-7.08988	1.73334	-0.00176	C	-6.52822	1.64352	0.00111
C	-6.17322	-0.50273	0.01347	C	-5.26977	2.24364	-0.00549
H	-8.27177	-0.06774	0.02307	H	-7.42375	2.25398	0.00152
C	-4.86748	0.01731	-0.00017	C	-4.11765	1.46319	-0.00604
H	-6.32933	-1.57511	0.02542	H	-5.18335	3.32417	-0.01028
C	-4.69367	1.41053	-0.01423	C	-4.21048	0.06236	0.00010
C	-5.79811	2.25756	-0.01496	H	-3.14330	1.93500	-0.01137
H	-3.69310	1.82376	-0.02476	C	-5.48265	-0.53466	0.00693
H	-5.64797	3.33119	-0.02592	H	-5.57593	-1.61423	0.01227
H	-7.94802	2.39542	-0.00236	H	-7.60308	-0.22339	0.01268
C	-3.72278	-0.87997	0.00021	C	-3.01556	-0.76677	-0.00072
C	-3.56009	-2.23834	0.00099	C	-2.77597	-2.11633	-0.00233
N	-2.21975	-2.55221	0.00039	N	-1.42204	-2.35130	-0.00293
H	-4.31696	-3.00586	0.00144	H	-3.48731	-2.92612	-0.00354
C	-1.60351	-1.39937	-0.00094	C	-0.87385	-1.16521	-0.00144
O	-2.46332	-0.33343	-0.00114	O	-1.79200	-0.15053	-0.00039
C	-0.22539	-1.13623	-0.00145	C	0.48809	-0.82760	-0.00106
C	0.96534	-0.91329	-0.00152	C	1.66415	-0.54187	-0.00064
C	2.35939	-0.65267	-0.00135	C	3.04325	-0.21097	-0.00016
C	3.28474	-1.70077	-0.00405	C	4.01939	-1.22619	-0.00146
C	4.65205	-1.42868	-0.00367	C	5.36663	-0.90345	-0.00096
H	2.93824	-2.72625	-0.00644	H	3.70933	-2.26337	-0.00286
C	5.11972	-0.11641	-0.00055	C	5.76564	0.44244	0.00087
H	5.35132	-2.25331	-0.00584	H	6.11437	-1.68644	-0.00195
C	4.18712	0.95532	0.00222	C	4.79923	1.46068	0.00218
C	2.82855	0.68080	0.00175	C	3.45241	1.13663	0.00166
H	2.10770	1.48578	0.00379	H	5.11027	2.49771	0.00361
O	6.42605	0.24071	0.00015	H	2.70591	1.92066	0.00268
C	7.41517	-0.78726	-0.00275	C	7.15554	0.77615	0.00143
H	8.37328	-0.27163	-0.00186	N	8.27965	1.04644	0.00189
H	7.33649	-1.41009	-0.89912				
H	7.33721	-1.41446	0.89064				
O	4.72506	2.20234	0.00517				
C	3.84201	3.32140	0.00898				
H	4.48280	4.20089	0.01158				
H	3.21169	3.32643	0.90394				
H	3.21113	3.33212	-0.88553				

Table S5. Optimized geometry in solvent (toluene) for compounds 16d and 16e used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 16d				Sample: 16e			
C	-6.65893	0.45572	0.00061	C	7.56503	0.36203	0.04572
C	-6.42047	1.83140	0.00032	C	7.42493	1.75063	0.01388
C	-5.10832	2.30241	-0.00010	C	6.15001	2.31380	-0.02186
H	-7.25065	2.52820	0.00044	H	8.30246	2.38672	0.01723
C	-4.03981	1.41066	-0.00024	C	5.02080	1.50045	-0.02609
H	-4.91422	3.36897	-0.00033	H	6.03269	3.39116	-0.04653
C	-4.27135	0.02586	0.00004	C	5.15366	0.10322	0.00558
H	-3.02318	1.78270	-0.00058	H	4.03346	1.94357	-0.05437
C	-5.59709	-0.44056	0.00049	C	6.44217	-0.45644	0.04206
H	-5.79689	-1.50572	0.00076	H	6.56599	-1.53265	0.06864
H	-7.67596	0.08060	0.00096	H	8.55252	-0.08402	0.07431
C	-3.16488	-0.91808	-0.00013	C	3.98319	-0.76023	0.00095
C	-3.05991	-2.28296	-0.00052	C	3.78300	-2.11560	0.00427
N	-1.73468	-2.65236	-0.00070	N	2.43591	-2.38997	-0.00376
H	-3.84860	-3.01766	-0.00075	H	4.51768	-2.90422	0.01091
C	-1.07075	-1.52663	-0.00030	C	1.85368	-1.22049	-0.01190
O	-1.88451	-0.42538	0.00008	O	2.74197	-0.17953	-0.01006
C	0.31749	-1.32350	-0.00028	C	0.48218	-0.92188	-0.02018
C	1.51681	-1.15450	-0.00010	C	-0.70131	-0.66997	-0.02509
C	2.92415	-0.97705	0.00007	C	-2.09102	-0.37943	-0.02890
C	3.75335	-2.09232	0.00030	C	-3.03607	-1.42174	-0.02568
C	5.15348	-1.95166	0.00047	C	-4.39413	-1.13593	-0.02762
H	3.30926	-3.08017	0.00036	H	-2.69660	-2.44968	-0.02263
C	5.72707	-0.70129	0.00039	C	-4.82757	0.19131	-0.03682
H	5.77590	-2.83878	0.00064	H	-5.11466	-1.94379	-0.02898
C	4.92270	0.46781	0.00016	C	-3.89949	1.23495	-0.03987
H	6.80637	-0.59265	0.00051	C	-2.54077	0.95388	-0.03762
C	3.49780	0.34221	0.00000	H	-4.23691	2.26361	-0.05061
C	2.70843	1.51946	-0.00024	H	-1.81920	1.76096	-0.04371
C	3.29806	2.76265	-0.00033	C	-6.29761	0.49984	0.01691
H	1.62883	1.42856	-0.00037	F	-7.04990	-0.47400	-0.54337
C	4.70607	2.88926	-0.00017	F	-6.60508	1.65444	-0.61766
H	2.67966	3.65306	-0.00052	F	-6.73933	0.63777	1.29615
C	5.49806	1.76640	0.00007				
H	5.15745	3.87482	-0.00024				
H	6.57919	1.85585	0.00020				

Table S6. Optimized geometry in solvent (toluene) for compound 16f used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 $statvolt^{-1}$). The values below correspond to the functional B3LYP with the basis set 6-311+G(d,p).

Sample: 16f				
C	5.89663	0.05356	0.00005	
C	5.86291	1.44920	0.00019	
C	4.63437	2.10826	0.00024	
H	6.78653	2.01629	0.00025	
C	3.44645	1.38329	0.00015	
H	4.59903	3.19170	0.00034	
C	3.47216	-0.02037	0.00001	
H	2.49562	1.90089	0.00019	
C	4.71463	-0.67701	-0.00004	
H	4.75669	-1.75989	-0.00014	
H	6.84742	-0.46697	0.00001	
C	2.23857	-0.79113	-0.00008	
C	1.93348	-2.12628	-0.00023	
N	0.56856	-2.29533	-0.00026	
H	2.60430	-2.96989	-0.00033	
C	0.07932	-1.08402	-0.00012	
O	1.04545	-0.11543	-0.00002	
C	-1.26563	-0.68105	-0.00009	
C	-2.42775	-0.34385	-0.00006	
C	-3.79089	0.04740	-0.00001	
C	-4.82914	-0.89875	0.00050	
C	-6.14179	-0.44943	0.00053	
H	-4.59808	-1.95697	0.00086	
C	-6.38281	0.92379	0.00006	
H	-6.96877	-1.14893	0.00091	
N	-5.40720	1.84112	-0.00044	
H	-7.39940	1.30471	0.00008	
C	-4.14810	1.41034	-0.00047	
H	-3.37091	2.16820	-0.00088	

Table S7: Theoretical values for static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 statvolt^{-1}) in toluene medium of the investigated compounds. These results were obtained by using the basis set 6-311+G(d,p).

Molecule	B3LYP		CAM-B3LYP		M06-2X		Experimental
	β_0	β_{HRS}	β_0	β_{HRS}	β_0	β_{HRS}	β_{HRS}
8j	29.4	99.8	12.2	24.5	13.0	26.4	42 ± 4
9k	18.9	45.5	11.2	18.8	11.0	18.3	35 ± 4
10b	20.3	68.6	12.4	24.3	11.5	22.6	34 ± 3
10d	8.5	25.6	3.5	6.2	4.3	8.2	15 ± 2
11b	18.5	73.7	7.9	17.7	8.7	20.1	30 ± 3
13k	24.4	82.2	13.6	26.6	12.3	23.6	38 ± 4
16b	20.2	55.5	11.7	20.5	10.9	19.3	29 ± 3
16c	54.0	187.7	23.3	48.7	24.6	51.5	48 ± 5
16d	11.9	40.0	4.6	9.7	5.7	12.1	17 ± 2
16e	32.2	96.7	14.0	28.4	15.1	30.3	31 ± 3
16f	21.8	61.8	9.6	19.1	10.2	20.4	22 ± 2

Table S8: Theoretical values for static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in 10^{-30} cm^4 statvolt^{-1}) in toluene medium of the investigated compounds. These results were obtained by using the basis set 6-311++G(d,p).

Molecule	B3LYP		CAM-B3LYP		M06-2X		Experimental
	β_0	β_{HRS}	β_0	β_{HRS}	β_0	β_{HRS}	β_{HRS}
8j	29.2	99.5	13.8	29.3	14.5	31.3	42 ± 4
9k	18.8	45.2	13.2	21.4	12.0	20.9	35 ± 4
10b	20.1	68.1	13.7	28.6	12.8	26.9	34 ± 3
10d	8.4	25.6	4.1	8.1	5.0	10.4	15 ± 2
11b	18.4	73.7	9.0	22.3	9.7	24.6	30 ± 3
13k	24.4	81.8	15.6	32.7	14.8	31.0	38 ± 4
16b	20.0	51.1	12.7	23.5	11.9	22.0	29 ± 3
16c	54.0	187.7	28.1	62.9	29.7	66.6	48 ± 5
16d	11.9	40.0	5.5	12.6	6.6	15.0	17 ± 2
16e	32.2	96.7	17.2	36.8	18.7	39.8	31 ± 3
16f	21.8	61.8	11.3	23.9	11.9	25.0	22 ± 2

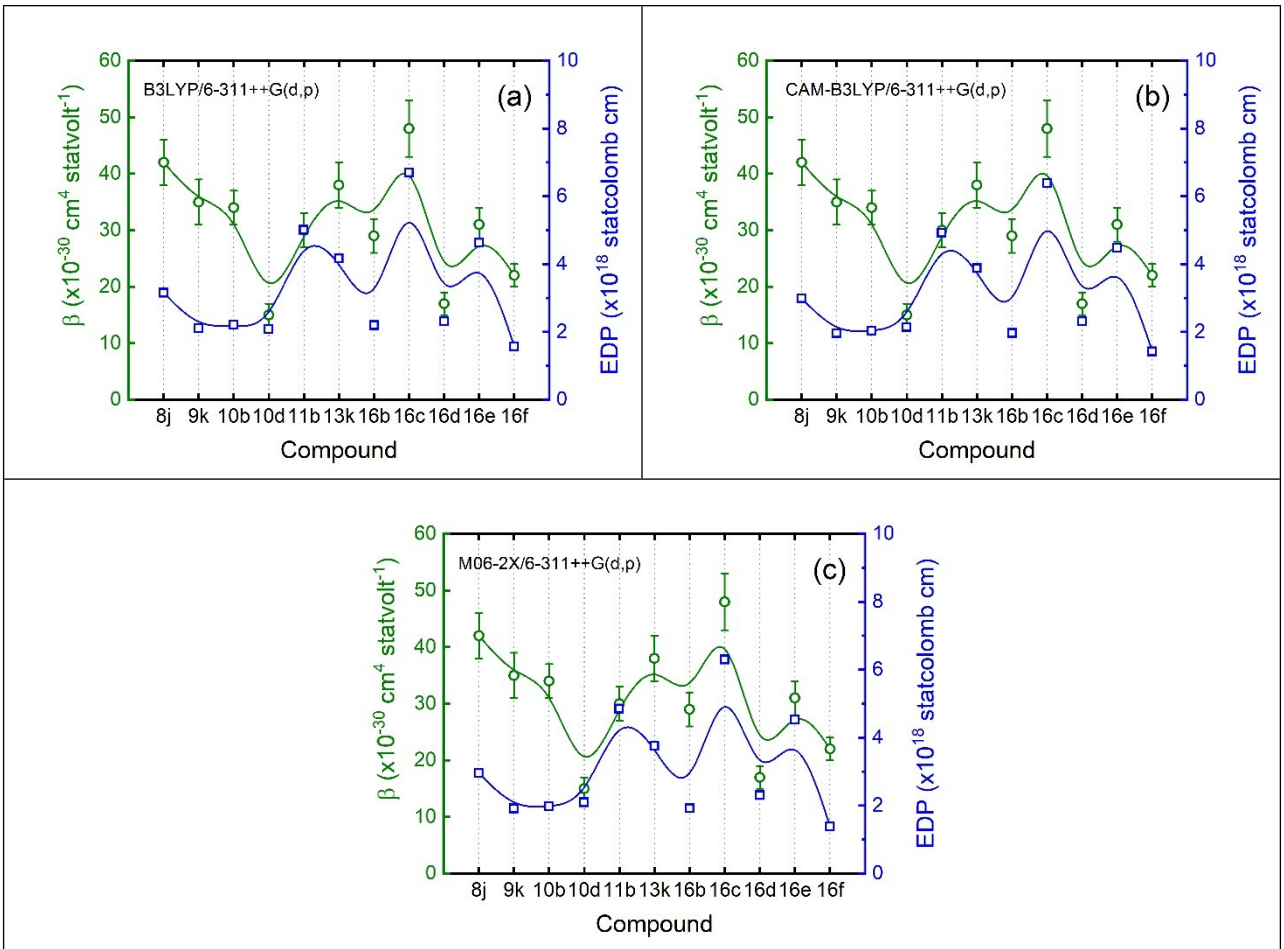


Figure S22: The left axis corresponds to the values for experimental first hyperpolarizability (β) (in 10^{-30} cm^4 $statvolt^{-1}$) (circles), while the right axis corresponds to the theoretical values of the electric dipole moments (EDP) (squares) in toluene medium of the investigated compounds; (a) represents the values obtained by using B3LYP method, (b) the values obtained by using CAM-B3LYP, and (c) the values obtained by using M06-2X. In all the results, the basis set used was the 6-311++G(d,p). The solid lines are just guidelines to the eye.