Supplementary Materials

Nonlinear Optical Materials: Predicting the First-Order Molecular Hyperpolarizability of Organic Molecular Structures

Francisco A. Santos [1,*], Carlos E. R. Cardoso [2], José J. Rodrigues, Jr. [1], Leonardo De Boni [3] and Luis M. G. Abegão [2,*]

[1] Department of Physics, Federal University of Sergipe, São Cristovão 49100-000, Brazil; joatan@ufs.br
[2] Photonics Group, Institute of Physics, Federal University of Goiás (UFG), Goiânia 74690-900, Brazil; carlos.ribeiro@discente.ufg.br
[3] Photonics Group, Institute of Physics of São Carlos, University of São Paulo, São Carlos 13560-970, Brazil; deboni@ifsc.usp.br
* Correspondence: fdessian@gmail.com (F.A.S.); luis.abegao@ufg.br (L.M.G.A.)

1 – Optimized Geometries

Table S1. Optimized geometry in solvent for compounds used to perform the calculation of the static (β_0) and dynamic (β_{HRS}) first hyperpolarizability β (in $\mathbf{10^{-30}\ cm^4\ statvolt^{-1}}$). The values below correspond to the functional CAM-B3LYP with the basis set 6-311++G(2d,2p).

Compound: A1

Cartesian coordinates

O	-1.95773	-0.95865	0.74943
C	-0.75457	-1.03800	0.85124
C	0.00000	-2.14640	0.20276
C	-0.72826	-3.12640	-0.46970
C	-0.07937	-4.17720	-1.08579
C	1.30619	-4.25681	-1.04209
C	2.03712	-3.28370	-0.38220
C	1.38865	-2.23099	0.24272
C	0.00000	0.00000	1.67783
C	0.75457	1.03800	0.85124
C	0.00000	2.14640	0.20276
C	-1.38865	2.23099	0.24272
C	-2.03712	3.28370	-0.38220
C	-1.30619	4.25681	-1.04209
C	0.07937	4.17720	-1.08579
C	0.72826	3.12640	-0.46970
O	1.95773	0.95865	0.74943
H	-1.80439	-3.04262	-0.49416
H	-0.64948	-4.93605	-1.60218
H	1.81502	-5.07887	-1.52560
H	3.11558	-3.34099	-0.35368
H	1.97140	-1.46928	0.73811
H	0.73905	-0.48744	2.30690
H	-0.73905	0.48744	2.30690
H	-1.97140	1.46928	0.73811
H	-3.11558	3.34099	-0.35368
H	-1.81502	5.07887	-1.52560
H	0.64948	4.93605	-1.60218
H	1.80439	3.04262	-0.49416

Compound: A2

Cartesian coordinates

O	5.86887	-1.21291	-1.31155
N	5.51530	-0.34114	-0.54046
O	6.27400	0.33348	0.12953
C	4.07785	-0.08786	-0.41132
C	3.18585	-0.84212	-1.14316
C	1.83492	-0.58705	-1.01039
C	3.65402	0.90617	0.43983
C	2.29818	1.12157	0.56478
N	1.91399	2.18083	1.50705
O	0.82836	2.09818	2.05039
O	2.71180	3.07687	1.70384
C	1.34367	0.39036	-0.15144
C	-0.14378	0.64444	-0.02952
C	-0.98093	0.00975	-1.10056
C	-1.07294	0.57009	-2.35928
C	-1.86648	-0.00456	-3.33004
C	-2.58449	-1.15108	-3.03073
C	-2.47531	-1.68393	-1.77605
N	-1.68233	-1.11787	-0.84254
C	-1.63396	-1.76951	0.46147
C	-0.72960	-2.79423	0.66419
C	-0.70980	-3.42647	1.89723
C	-1.58662	-3.03163	2.89527
C	-2.49006	-2.00466	2.66669
C	-2.52192	-1.36300	1.43942
Br	-4.08075	1.88105	0.04504
H	3.54151	-1.61224	-1.80770
H	1.15013	-1.16858	-1.60626
H	4.35771	1.49785	0.99937
H	-0.33692	1.71409	-0.07239
H	-0.47720	0.32861	0.95276
H	-0.51618	1.47116	-2.56372
H	-1.93271	0.44232	-4.31043
H	-3.22516	-1.62748	-3.75447
H	-3.00317	-2.57010	-1.46546
H	-0.05791	-3.10071	-0.12398
H	-0.00967	-4.22947	2.07301
H	-1.56722	-3.52781	3.85454
H	-3.17387	-1.69930	3.44475
H	-3.20767	-0.55036	1.23924

Compound: A3

Cartesian coordinates

N	6.91562	0.43690	-0.19718
C	5.53097	0.34077	-0.15352
C	4.84040	-0.44390	-1.07715
C	3.46010	-0.49736	-1.06219
C	2.71959	0.22162	-0.12765
C	1.24863	0.21551	-0.11599
N	0.50938	1.29839	-0.10664
C	-0.79910	0.88079	-0.09706
C	-1.89620	1.86013	-0.11723
C	-1.69885	3.12116	0.44466
C	-2.70870	4.06771	0.43778
C	-3.93806	3.77514	-0.13369
C	-4.14259	2.52856	-0.70426
C	-3.13167	1.58153	-0.69965
C	-0.84402	-0.49090	-0.09221
C	-1.97754	-1.43212	-0.05248
C	-2.84740	-1.44001	1.03479
C	-3.92601	-2.30812	1.07020
C	-4.14698	-3.18786	0.02187
C	-3.28569	-3.19129	-1.06445
C	-2.21142	-2.31767	-1.10254
N	0.47483	-0.90955	-0.11586
C	0.92666	-2.26952	0.16906
C	0.95826	-2.56823	1.65920
C	3.41335	1.01437	0.78255
C	4.79254	1.07498	0.77493
H	7.39240	-0.33963	-0.62462
H	7.35792	0.73037	0.65802
H	5.39267	-1.00244	-1.82080
H	2.95284	-1.09196	-1.80922
H	-0.74011	3.35171	0.88476
H	-2.53518	5.03840	0.88112
H	-4.72691	4.51391	-0.13988
H	-5.09201	2.29293	-1.16455
H	-3.30229	0.62207	-1.16402
H	-2.67550	-0.75651	1.85402
H	-4.59331	-2.29936	1.92031
H	-4.98754	-3.86646	0.05021
H	-3.45510	-3.86939	-1.88882
H	-1.55550	-2.30984	-1.96212
H	0.26385	-2.95857	-0.34546
H	1.91413	-2.39090	-0.26089
H	1.30405	-3.58746	1.82479
H	-0.03202	-2.46880	2.09936
H	1.63533	-1.88948	2.17509
H	2.85779	1.59195	1.50712
H	5.30816	1.69771	1.49355

Compound: A4

Cartesian coordinates

N	6.96073	0.21714	-0.06334
C	5.57510	0.14278	-0.02168
C	4.83008	1.08419	0.69066
C	3.45156	1.03764	0.68841
C	2.76124	0.05441	-0.01807
C	1.29382	0.07109	-0.02430
N	0.57144	1.16569	-0.08961
C	-0.74202	0.77208	-0.07048
C	-1.82355	1.76475	-0.16045
C	-1.62812	3.04282	0.36133
C	-2.62374	4.00140	0.28286
C	-3.83583	3.70312	-0.32147
C	-4.03794	2.43860	-0.85238
C	-3.04122	1.47985	-0.77604
C	-0.81241	-0.59684	0.01745
C	-1.95581	-1.51832	0.11758
C	-2.87703	-1.38546	1.15387
C	-3.96163	-2.24120	1.24862
C	-4.13800	-3.24936	0.31339
C	-3.22485	-3.39425	-0.71959
C	-2.14389	-2.53394	-0.81783
N	0.49861	-1.03542	0.04353
C	0.92039	-2.40125	0.30413
C	3.50865	-0.87564	-0.73610
C	4.88982	-0.83679	-0.73923
H	7.39344	0.70589	0.70275
H	7.43723	-0.64122	-0.28506
H	5.34194	1.85678	1.24860
H	2.88975	1.77556	1.24194
H	-0.68270	3.27757	0.82737
H	-2.45267	4.98579	0.69589
H	-4.61336	4.45125	-0.38366
H	-4.97362	2.19824	-1.33766
H	-3.20749	0.50523	-1.20988
H	-2.73880	-0.60377	1.88690
H	-4.66801	-2.12309	2.05803
H	-4.98325	-3.91847	0.38870
H	-3.35805	-4.17434	-1.45567
H	-1.44629	-2.64126	-1.63679
H	0.19105	-2.88357	0.94676
H	1.88013	-2.38815	0.80850
H	1.01021	-2.97545	-0.61552
H	3.01105	-1.63255	-1.32498
H	5.44633	-1.56440	-1.31433

Compound: A5

Cartesian coordinates

O	4.05822	-0.59970	0.01745
C	3.28455	0.32861	0.01279
H	3.66570	1.36833	0.01923
C	1.82676	0.21186	-0.00116
C	1.03136	1.35166	-0.00328
C	-0.34376	1.26949	-0.01511
C	-0.98342	0.01654	-0.03031
N	-2.34770	-0.08263	-0.05629
C	-3.16178	1.10991	0.03042
C	-2.98445	-1.37932	0.02991
C	-0.16986	-1.13675	-0.02010
C	1.19913	-1.03280	-0.00817
H	1.50233	2.32663	0.00671
H	-0.92300	2.17767	-0.01207
H	-2.95755	1.79225	-0.79592
H	-3.00158	1.65173	0.96663
H	-4.20856	0.83045	-0.02305
H	-2.68777	-2.02497	-0.79763
H	-4.06026	-1.25008	-0.02157
H	-2.74826	-1.89393	0.96515
H	-0.61886	-2.11614	-0.02122
H	1.81478	-1.92111	-0.00187

Compound: A6

Cartesian coordinates

C	-6.22151	-0.22002	-0.39255
N	-5.04136	-0.97410	-0.02873
C	-5.22551	-2.19638	0.72212
C	-3.81721	-0.34412	-0.00390
C	-2.68790	-0.96218	0.55563
C	-1.45524	-0.34095	0.53461
C	-1.28835	0.92552	-0.01503
C	-0.00322	1.67314	0.00859
C	1.29240	0.94450	-0.01004
C	1.47371	-0.29483	-0.61467
C	2.71436	-0.89762	-0.66784
C	3.84170	-0.28000	-0.10344
N	5.08474	-0.86658	-0.16404
C	5.20509	-2.23364	-0.61997
C	6.17942	-0.29911	0.59237
C	3.65257	0.96921	0.51522
C	2.41223	1.56411	0.53961
O	-0.01233	2.89120	0.04260
C	-2.41619	1.55723	-0.53338
C	-3.64820	0.94477	-0.54130
H	-7.08212	-0.88120	-0.37690
H	-6.13514	0.18068	-1.40178
H	-6.41598	0.61388	0.28996
H	-6.23402	-2.56323	0.55967
H	-5.07978	-2.05662	1.79865
H	-4.53716	-2.97035	0.38448
H	-2.76902	-1.93218	1.01746
H	-0.61476	-0.84545	0.98795
H	0.63642	-0.79447	-1.07900
H	2.80411	-1.85202	-1.15973
H	4.84608	-2.34045	-1.64341
H	4.65054	-2.93688	0.01015
H	6.25183	-2.52002	-0.60974
H	6.37913	0.72694	0.28511
H	7.07803	-0.87735	0.40262
H	5.99121	-0.30108	1.67104
H	4.48247	1.48130	0.97352
H	2.28841	2.53594	0.99492
H	-2.30704	2.55591	-0.93066
H	-4.48721	1.47405	-0.96181

Compound: A7

Cartesian coordinates

C	2.20930	-2.35352	0.15997
C	0.84339	-2.03974	0.78929
C	0.95413	-2.11492	2.30917
C	0.29017	-0.68241	0.24715
C	1.29423	0.44570	0.01586
C	1.97044	0.93707	1.25764
C	3.21065	1.40703	1.38563
C	4.27566	1.58030	0.41017
C	5.56291	1.91609	0.72762
C	6.41580	2.04807	-0.39570
C	5.77013	1.82248	-1.56764
S	4.11484	1.44325	-1.31480
N	-0.38373	-1.05198	-0.97825
C	-1.21025	-0.02518	-1.58177
C	-2.05382	0.66710	-0.54432
C	-3.14633	1.44043	-0.88407
C	-3.89552	2.05020	0.10428
N	-5.04234	2.85841	-0.27493
O	-5.69756	3.38187	0.61210
O	-5.29839	2.97818	-1.46288
C	-3.58401	1.90176	1.44814
C	-2.49767	1.13573	1.79476
C	-1.72592	0.52389	0.80622
O	-0.68446	-0.21744	1.23058
C	-0.86578	-2.36308	-0.81994
C	-1.82900	-3.02933	-1.55462
C	-2.10099	-4.35505	-1.22794
C	-1.42921	-4.99188	-0.19836
C	-0.45924	-4.30512	0.52997
C	-0.18596	-2.99358	0.21642
H	2.97807	-1.67283	0.52193
H	2.17336	-2.29679	-0.92639
H	2.50164	-3.36573	0.43243
H	1.68132	-1.39963	2.68710
H	1.29742	-3.10903	2.59220
H	-0.00010	-1.93265	2.79324
H	0.75598	1.28191	-0.43741
H	2.00654	0.10476	-0.72924
H	1.35864	0.93463	2.14900
H	3.50880	1.72012	2.37911
H	5.88376	2.06428	1.74757
H	7.46204	2.30255	-0.33263
H	6.16788	1.85543	-2.56679
H	-1.83901	-0.47765	-2.34250
H	-0.57673	0.69414	-2.10124
H	-3.42695	1.56778	-1.91841
H	-4.18888	2.38415	2.19806
H	-2.22147	0.99744	2.82901
H	-2.36505	-2.55110	-2.36073
H	-2.85443	-4.89033	-1.78832
H	-1.65893	-6.01946	0.04284
H	0.06581	-4.80191	1.33444

Compound: A8

Cartesian coordinates

C	-3.14718	0.67736	0.00860
C	-1.86617	1.28782	0.56500
C	-1.78180	1.02573	2.07560
C	-0.53693	0.83647	-0.14353
C	-0.66548	0.48914	-1.63293
C	-1.30974	-0.71628	-2.27992
C	-1.86598	-1.90125	-2.00965
C	-2.21445	-2.71898	-0.84053
C	-3.02643	-3.80577	-1.02901
S	-3.33665	-4.66559	0.41576
C	-2.35959	-3.57779	1.31779
C	-1.83353	-2.60630	0.53415
N	0.30327	2.01880	0.00059
C	1.65998	1.97862	-0.46896
C	2.24758	0.64244	-0.10301
C	3.60291	0.40327	-0.22846
C	4.12848	-0.81552	0.15202
N	5.55907	-1.04217	0.01450
O	6.00858	-2.11636	0.37882
O	6.24289	-0.14861	-0.45871
C	3.32845	-1.82369	0.66866
C	1.97859	-1.59846	0.78832
C	1.43367	-0.37577	0.39783
O	0.09548	-0.23858	0.55202
C	-0.48891	3.15139	0.02482
C	-0.13185	4.47064	-0.18746
C	-1.12813	5.43859	-0.07447
C	-2.43259	5.09325	0.23191
C	-2.77215	3.75414	0.43829
C	-1.79968	2.78973	0.33037
H	-3.18672	-0.39529	0.17324
H	-3.26810	0.87073	-1.05394
H	-4.00039	1.11642	0.52370
H	-1.81194	-0.03906	2.29463
H	-2.63162	1.49839	2.56463
H	-0.86960	1.43891	2.50038
H	0.34769	0.49896	-2.04115
H	-1.14129	1.36031	-2.09042
H	-1.27740	-0.53496	-3.34994
H	-2.17953	-2.41070	-2.91418
H	-3.45683	-4.13731	-1.95833
H	-2.22478	-3.71794	2.37601
H	-1.18335	-1.84059	0.91043
H	2.22386	2.76600	0.03018
H	1.74890	2.15925	-1.54795
H	4.25932	1.16898	-0.61226
H	3.76568	-2.76381	0.96154
H	1.32211	-2.36248	1.17516
H	0.88148	4.75024	-0.43590
H	-0.87381	6.47642	-0.23791
H	-3.19106	5.85869	0.30638
H	-3.79242	3.48754	0.67829

Compound: A9

Cartesian coordinates

C	-0.06822	3.06445	-1.31231
C	-1.47259	2.49180	-1.16126
C	-2.05028	2.20938	-2.55667
C	-1.57632	1.19970	-0.26945
C	-0.48651	1.16142	0.81823
C	-0.57667	0.02576	1.78922
C	0.33154	-0.92131	2.01154
C	1.66173	-1.08712	1.39324
C	2.56025	-0.03740	1.25746
C	3.80422	-0.26054	0.68129
C	4.93753	0.58939	0.39665
C	5.20081	1.94102	0.58718
C	6.41877	2.45221	0.17981
C	7.37277	1.62445	-0.41839
C	7.13582	0.27710	-0.61882
C	5.91202	-0.23401	-0.20041
N	5.43522	-1.52804	-0.27032
C	6.12574	-2.64537	-0.86691
C	4.15596	-1.55154	0.24600
C	3.27518	-2.61857	0.38654
C	2.04841	-2.36953	0.96680
N	-2.93075	1.29039	0.23910
C	-3.64741	0.17524	0.78643
C	-3.20392	-1.08549	0.09724
C	-3.86027	-2.27954	0.32207
C	-3.46284	-3.42599	-0.33883
N	-4.17013	-4.66888	-0.08629
O	-3.80830	-5.67006	-0.68446
O	-5.09381	-4.65827	0.71284
C	-2.40934	-3.41425	-1.24218
C	-1.74686	-2.23324	-1.46682
C	-2.13070	-1.07127	-0.79563
O	-1.41981	0.03674	-1.08377
C	-3.30584	2.61410	0.33588
C	-4.35764	3.17207	1.04048
C	-4.52302	4.55491	0.97381
C	-3.66232	5.34756	0.23560
C	-2.61002	4.76365	-0.47529
C	-2.43726	3.40263	-0.42242
H	0.60421	2.33697	-1.76548
H	0.35649	3.39042	-0.36654
H	-0.10247	3.92961	-1.97272
H	-1.40253	1.54095	-3.11943
H	-2.13787	3.14753	-3.10157
H	-3.03849	1.75838	-2.49448
H	-0.54881	2.10804	1.35981
H	0.47106	1.14313	0.30946
H	-1.48204	-0.02670	2.37888
H	0.06393	-1.69513	2.72287
H	2.30228	0.94654	1.62211
H	4.46373	2.58490	1.04686
H	6.63717	3.50077	0.32090
H	8.31659	2.04602	-0.73409
H	7.87978	-0.34922	-1.08840
H	7.19376	-2.55547	-0.68732
H	5.95245	-2.70177	-1.94235
H	5.78824	-3.57028	-0.40814
H	3.53318	-3.61471	0.05911

Compound: B1

Cartesian coordinates

C	-0.20619	-3.26698	-0.91160
C	-0.24138	-2.36414	0.31079
N	0.11643	-0.97266	0.03533
C	1.40567	-0.48257	0.00401
C	2.58788	-1.35109	0.18817
C	3.16256	-1.48124	1.44896
C	4.28195	-2.27660	1.63471
C	4.84082	-2.95096	0.56083
C	4.27767	-2.82558	-0.69982
C	3.15861	-2.03046	-0.88453
C	1.28947	0.88204	-0.12881
C	2.32982	1.92068	-0.20125
C	3.64301	1.64282	-0.57803
C	4.59268	2.65003	-0.63198
C	4.25082	3.95505	-0.31552
C	2.94580	4.24443	0.05376
C	1.99667	3.23908	0.10999
N	-0.03451	1.22184	-0.16244
C	-0.71648	0.10535	-0.06566
C	-2.18498	0.08418	-0.03369
C	-2.95242	-0.92643	-0.61066
C	-4.33237	-0.87763	-0.57049
C	-2.83614	1.16046	0.57358
C	-4.21207	1.22289	0.61830
C	-4.94302	0.19556	0.04786
N	-6.40349	0.25001	0.09487
O	-7.02813	-0.66909	-0.40605
O	-6.92384	1.21135	0.63341
H	-0.55845	-4.26009	-0.63756
H	0.80394	-3.36299	-1.29971
H	-0.83859	-2.89067	-1.71311
H	0.45015	-2.73234	1.06456
H	-1.22839	-2.36149	0.76262
H	2.73238	-0.94882	2.28550
H	4.71907	-2.36637	2.61888
H	5.71532	-3.56931	0.70454
H	4.71316	-3.34339	-1.54245
H	2.73213	-1.92106	-1.87174
H	3.92862	0.63663	-0.84140
H	5.60434	2.41224	-0.92962
H	4.99275	4.73961	-0.35961
H	2.66521	5.25882	0.30077
H	0.98074	3.46626	0.39506
H	-2.48114	-1.74750	-1.12416
H	-4.93053	-1.65231	-1.02113
H	-2.24486	1.94879	1.01147
H	-4.71925	2.04813	1.09044

H	1.35321	-3.18866	1.09155
H	-4.71130	0.32721	0.59737
H	-3.53342	0.07785	1.87209
H	-4.69126	-2.32437	1.00922
H	-2.12239	-4.32092	-1.74862
H	-0.91607	-2.18189	-2.15379
H	-5.02645	2.56512	1.63318
H	-5.33540	5.01329	1.52025
H	-3.80304	6.41814	0.20782
H	-1.94585	5.38259	-1.06355

Compound: B2

Cartesian coordinates

C	0.29546	-2.45127	0.33586
N	-0.08855	-1.07440	0.06267
C	-1.38556	-0.60779	0.02532
C	-2.55116	-1.50073	0.13009
C	-2.76706	-2.51036	-0.80521
C	-3.86985	-3.34186	-0.70288
C	-4.77420	-3.17313	0.33411
C	-4.56893	-2.17028	1.26909
C	-3.46390	-1.34186	1.16972
C	-1.28773	0.76209	-0.07239
C	-2.35004	1.77428	-0.17700
C	-3.56393	1.50805	-0.80721
C	-4.54228	2.48426	-0.89796
C	-4.32405	3.74566	-0.36637
C	-3.11513	4.02438	0.25333
C	-2.13759	3.04880	0.34587
N	0.02945	1.12668	-0.07748
C	0.72694	0.01682	-0.00360
C	2.19313	-0.00805	-0.00641
C	2.87484	1.04212	0.61074
C	4.25244	1.08685	0.60988
C	2.92592	-1.00957	-0.64244
C	4.30656	-0.97750	-0.64821
C	4.95022	0.06919	-0.01679
N	6.41212	0.10548	-0.01710
O	6.96187	1.04669	0.52770
O	7.00836	-0.80785	-0.56134
H	-0.46917	-2.91564	0.94909
H	1.23349	-2.46444	0.87934
H	0.40341	-3.02417	-0.58219
H	-2.07514	-2.63582	-1.62643
H	-4.02642	-4.11809	-1.43827
H	-5.63610	-3.82016	0.41268
H	-5.26913	-2.03433	2.08090
H	-3.30377	-0.56283	1.90112
H	-3.74220	0.53540	-1.24071
H	-5.47596	2.25978	-1.39429
H	-5.08752	4.50708	-0.43932
H	-2.93263	5.00612	0.66742
H	-1.19484	3.26797	0.82481
H	2.30840	1.82383	1.09169
H	4.78647	1.89083	1.08901
H	2.42292	-1.80810	-1.16421
H	4.88059	-1.74325	-1.14329

Compound: B3

Cartesian coordinates

Cl	6.18555	2.69340	1.43880
C	6.20987	1.14933	0.65342
N	7.40148	0.64174	0.41208
C	7.33703	-0.53824	-0.19050
Cl	8.85753	-1.28594	-0.54964
N	6.26618	-1.18975	-0.53830
C	5.10756	-0.56597	-0.23610
N	3.99729	-1.22952	-0.59086
C	2.62986	-0.91912	-0.45503
C	1.73660	-1.83904	-1.00276
C	0.37797	-1.63160	-0.92276
C	-0.13588	-0.49756	-0.29596
C	-1.59375	-0.34098	-0.19818
N	-2.41309	-1.33787	0.03878
C	-3.67903	-0.81288	0.05033
C	-4.84523	-1.67134	0.30915
C	-4.67927	-2.84870	1.03804
C	-5.75385	-3.68221	1.29526
C	-7.01885	-3.35731	0.82883
C	-7.19484	-2.19292	0.09794
C	-6.11957	-1.35919	-0.16224
C	-3.61723	0.53848	-0.18861
C	-4.66588	1.57647	-0.23976
C	-5.28146	2.00524	0.93238
C	-6.27736	2.96772	0.89426
C	-6.66684	3.51819	-0.31661
C	-6.05854	3.09978	-1.49004
C	-5.06663	2.13360	-1.45163
N	-2.27730	0.82811	-0.35439
C	-1.73179	2.14058	-0.65615
C	0.76301	0.40514	0.25850
C	2.13270	0.20920	0.18429
N	5.04413	0.62482	0.36994
H	4.19822	-2.10778	-1.04359
H	2.11413	-2.72331	-1.49836
H	-0.30290	-2.35369	-1.34686
H	-3.69445	-3.10268	1.40014
H	-5.60315	-4.58891	1.86447
H	-7.85845	-4.00756	1.02950
H	-8.17394	-1.93366	-0.28001
H	-6.27337	-0.46506	-0.74674
H	-4.97977	1.57499	1.87675
H	-6.74910	3.28808	1.81227
H	-7.44355	4.26896	-0.34640
H	-6.36142	3.52092	-2.43812

H	-4.60733	1.79671	-2.37081
H	-2.44095	2.69512	-1.25994
H	-0.80981	2.02848	-1.21555
H	-1.53411	2.70312	0.25415
H	0.40281	1.27404	0.78822
H	2.80247	0.92256	0.62804

Compound: B4

Cartesian coordinates

O	-0.00002	2.71399	0.00074
C	-0.00000	1.48245	0.00072
C	-1.25986	0.69765	0.00075
H	-1.17583	-0.38677	0.00093
C	-2.45630	1.31879	0.00041
H	-2.42442	2.40786	0.00006
C	-3.78649	0.71533	0.00034
C	-4.00763	-0.67615	0.00209
H	-3.16439	-1.36005	0.00374
C	-5.29393	-1.20153	0.00188
C	-6.38775	-0.33268	-0.00010
Br	-8.15530	-1.05198	-0.00045
C	-6.20722	1.04870	-0.00180
H	-7.06505	1.71213	-0.00329
H	-5.45246	-2.27441	0.00327
C	-4.91204	1.55988	-0.00153
H	-4.76626	2.63700	-0.00283
C	1.25987	0.69768	0.00061
H	1.17590	-0.38675	0.00069
C	2.45630	1.31882	0.00039
C	3.78650	0.71534	0.00020
C	4.91204	1.55989	0.00013
H	4.76628	2.63701	0.00022
C	6.20723	1.04870	-0.00005
H	7.06506	1.71214	-0.00010
C	6.38776	-0.33267	-0.00018
Br	8.15530	-1.05199	-0.00045
C	5.29393	-1.20152	-0.00012
H	5.45245	-2.27441	-0.00022
C	4.00763	-0.67614	0.00006
H	3.16439	-1.36005	0.00009
H	2.42447	2.40789	0.00034

Compound: B5

Cartesian coordinates

O	-0.00002	2.47123	0.00064
C	-0.00000	1.23969	0.00061
C	-1.25986	0.45489	0.00064
H	-1.17583	-0.62953	0.00082
C	-2.45630	1.07603	0.00030
H	-2.42442	2.16510	-0.00005
C	-3.78649	0.47257	0.00023
C	-4.00763	-0.91891	0.00198
H	-3.16439	-1.60281	0.00364
C	-5.29393	-1.44429	0.00178
C	-6.38775	-0.57544	-0.00020
Cl	-8.15530	-1.29474	-0.00056
C	-6.20722	0.80594	-0.00191
H	-7.06505	1.46937	-0.00340
H	-5.45246	-2.51717	0.00316
C	-4.91204	1.31712	-0.00163
H	-4.76626	2.39424	-0.00294
C	1.25987	0.45492	0.00051
H	1.17590	-0.62952	0.00059
C	2.45630	1.07605	0.00028
C	3.78650	0.47258	0.00010
C	4.91204	1.31713	0.00003
H	4.76628	2.39425	0.00012
C	6.20723	0.80593	-0.00015
H	7.06506	1.46937	-0.00020
C	6.38776	-0.57544	-0.00028
Cl	8.15530	-1.29476	-0.00056
C	5.29393	-1.44429	-0.00022
H	5.45245	-2.51717	-0.00032
C	4.00763	-0.91890	-0.00005
H	3.16439	-1.60282	-0.00002
H	2.42447	2.16513	0.00023

Compound: B6

Cartesian coordinates

O	0.00000	2.39749	-0.00002
C	0.00000	1.17118	-0.00006
C	1.24850	0.38736	-0.00010
H	1.15252	-0.69129	-0.00020
C	2.44222	0.98808	-0.00000
H	2.43533	2.07428	0.00011
C	3.75746	0.36512	-0.00001
C	3.95320	-1.02291	-0.00015
H	3.10223	-1.69153	-0.00027
C	5.21624	-1.56100	-0.00015
C	6.33802	-0.72769	-0.00001
O	7.53661	-1.35223	-0.00002
C	6.16990	0.65043	0.00014
H	7.01856	1.31791	0.00025
H	5.36671	-2.63277	-0.00026

Compound: B7

Cartesian coordinates

O	0.00000	2.34044	0.00033
C	0.00000	1.11684	0.00015
C	-1.25072	0.33187	0.00011
H	-1.15460	-0.74660	-0.00001
C	-2.44116	0.93411	0.00017
H	-2.43577	2.01995	0.00019
C	-3.75926	0.30622	0.00014
C	-3.94343	-1.07916	0.00101
H	-3.08926	-1.74270	0.00185
C	-5.20947	-1.62832	0.00088
C	-6.29615	-0.77678	-0.00013
F	-7.53439	-1.31189	-0.00025
C	-6.16562	0.59303	-0.00096
H	-7.04509	1.22234	-0.00170
H	-5.36381	-2.69880	0.00156

C	4.88767	1.17669	0.00013
H	4.76385	2.25314	0.00024
C	-1.24850	0.38736	-0.00005
H	-1.15252	-0.69129	-0.00005
C	-2.44222	0.98808	-0.00003
C	-3.75746	0.36512	-0.00002
C	-4.88767	1.17669	0.00004
H	-4.76385	2.25314	0.00007
C	-6.16990	0.65043	0.00006
H	-7.01856	1.31791	0.00010
C	-6.33802	-0.72769	0.00001
O	-7.53661	-1.35223	0.00002
C	-5.21624	-1.56100	-0.00006
H	-5.36671	-2.63277	-0.00010
C	-3.95320	-1.02291	-0.00007
H	-3.10223	-1.69153	-0.00013
H	-2.43533	2.07428	-0.00002
C	8.71307	-0.55635	0.00015
H	9.54563	-1.25378	0.00012
H	8.76285	0.06985	0.89290
H	8.76296	0.07006	-0.89246
C	-8.71307	-0.55635	0.00011
H	-9.54563	-1.25379	0.00012
H	-8.76295	0.06999	-0.89254
H	-8.76286	0.06992	0.89282

C	-4.88833	1.12559	-0.00079
H	-4.76293	2.20119	-0.00142
C	1.25072	0.33187	-0.00000
H	1.15460	-0.74660	-0.00019
C	2.44116	0.93412	0.00011
C	3.75926	0.30622	0.00000
C	4.88833	1.12559	0.00029
H	4.76293	2.20119	0.00057
C	6.16562	0.59303	0.00022
H	7.04509	1.22234	0.00044
C	6.29615	-0.77678	-0.00015
F	7.53439	-1.31189	-0.00022
C	5.20946	-1.62832	-0.00045
H	5.36381	-2.69880	-0.00074
C	3.94344	-1.07916	-0.00037
H	2.43577	2.01995	0.00032
H	3.08926	-1.74270	-0.00061

Compound: B8

Cartesian coordinates

C	-6.60377	0.26615	0.0087
C	-6.49331	1.65182	0.00104
C	-5.23637	2.24087	-0.00695
H	-7.38387	2.26832	0.0014
C	-4.09423	1.45428	-0.00745
H	-5.14242	3.32001	-0.01289
C	-4.19941	0.06276	0.00012
H	-3.11603	1.917	-0.01386
C	-5.46709	-0.52435	0.0084
H	-5.56588	-1.60292	0.01499
H	-7.58104	-0.20092	0.0152
C	-3.00772	-0.77431	-0.00075
C	-2.77634	-2.11379	-0.0024
N	-1.42115	-2.34778	-0.00286
H	-3.48822	-2.92225	-0.00363
C	-0.88137	-1.17057	-0.00168
O	-1.78886	-0.16346	-0.00042
C	0.48715	-0.83018	-0.00133
C	1.65405	-0.54474	-0.0009
C	3.03823	-0.21047	-0.00028
C	4.00603	-1.2207	-0.00249
C	5.34911	-0.89767	-0.00185
H	3.69597	-2.25725	-0.0047
C	5.74078	0.44168	0.00102
H	6.09819	-1.67856	-0.00356
C	4.7814	1.4551	0.00323
C	3.43898	1.12984	0.00258
H	5.09202	2.49163	0.00547
H	2.69077	1.91141	0.0043
C	7.13267	0.77769	0.00173
N	8.24953	1.0479	0.00232

Compound: B9

Cartesian coordinates

O	-1.23279	2.53578	0.02798
C	-1.19906	1.31083	0.02589
C	-2.46976	0.53313	0.03290
C	-2.53727	-0.83917	0.30263
C	-3.74776	-1.50064	0.31611
C	-4.92974	-0.80743	0.04754
O	-6.06509	-1.53888	0.07535
C	-7.30466	-0.88990	-0.18053
C	-4.88271	0.55962	-0.22591
C	-3.66045	1.21057	-0.22357
C	0.08351	0.57992	-0.00238
C	1.24456	1.24458	0.06533
C	2.59479	0.69458	0.03374
C	3.68449	1.57081	0.13394
C	4.98423	1.11013	0.11124
C	5.23655	-0.25644	-0.01397
O	6.53841	-0.62335	-0.02696
C	6.85930	-2.00276	-0.15052
C	4.16856	-1.14870	-0.11687
C	2.86930	-0.66886	-0.09238
H	-1.64285	-1.40498	0.52547
H	-3.80350	-2.55953	0.53453
H	-8.06594	-1.66173	-0.10317
H	-7.32296	-0.45977	-1.18458
H	-7.49984	-0.11023	0.55943
H	-5.78317	1.11787	-0.43837
H	-3.61665	2.27237	-0.42856
H	0.06218	-0.49658	-0.09510
H	1.18005	2.32574	0.15413
H	3.50068	2.63481	0.23145
H	5.82232	1.79114	0.18920
H	7.94468	-2.05854	-0.13688

H	6.48597	-2.41065	-1.09293
H	6.45492	-2.57716	0.68637
H	4.33869	-2.21118	-0.21607
H	2.05797	-1.38152	-0.17497

Compound: C1

Cartesian coordinates

C	5.35687	3.29410	-0.10442
N	5.89885	1.96820	0.09910
C	5.06010	0.87944	0.06042
C	3.66314	1.02923	0.03159
C	2.81899	-0.05841	0.02120
C	3.31363	-1.36789	0.03036
C	2.53608	-2.59572	0.01959
C	1.23095	-2.93567	0.00767
C	0.00001	-2.12529	0.00059
C	-1.23092	-2.93567	-0.00710
C	-2.53605	-2.59571	-0.01950
C	-3.31360	-1.36788	-0.03032
C	-2.81898	-0.05840	-0.01991
C	-3.66312	1.02923	-0.03043
C	-5.06006	0.87945	-0.06069
N	-5.89877	1.96824	-0.09952
C	-5.35700	3.29400	0.10536
C	-7.32149	1.77859	0.07786
C	-5.56300	-0.43223	-0.05677
C	-4.70684	-1.50883	-0.04600
O	0.00001	-0.89992	0.00104
C	4.70688	-1.50884	0.04468
C	5.56304	-0.43224	0.05525
C	7.32139	1.77866	-0.07975
H	4.60814	3.53178	0.65033
H	4.89600	3.41291	-1.09039
H	6.15712	4.02148	-0.01206
H	3.22433	2.01344	0.01685
H	1.75322	0.09171	0.00235
H	3.18828	-3.46359	0.02338
H	1.04860	-4.00145	0.00371
H	-1.04858	-4.00145	-0.00341
H	-3.18825	-3.46358	-0.02387
H	-1.75323	0.09172	0.00000
H	-3.22434	2.01344	-0.01466
H	-4.60749	3.53214	-0.64847
H	-4.89715	3.41222	1.09188
H	-6.15715	4.02145	0.01262
H	-7.72963	1.12583	-0.69325
H	-7.82064	2.73839	-0.00899
H	-7.57009	1.34929	1.05410
H	-6.62511	-0.61337	-0.06189
H	-5.13227	-2.50397	-0.04581
H	5.13233	-2.50397	0.04354
H	6.62516	-0.61337	0.05928
H	7.82062	2.73841	0.00711
H	7.56905	1.34987	-1.05646
H	7.73029	1.12550	0.69063

Compound: C2

Cartesian coordinates

C	-0.41366	-1.42348	-1.93783
C	-1.44255	-0.97435	-0.93778
C	-2.63774	-1.67633	-0.82727
Br	-2.93352	-3.24768	-1.88152
C	-3.67167	-1.30440	0.02363
O	-4.82848	-1.99700	0.11337
C	-3.53054	-0.16772	0.81629
C	-4.68218	0.27423	1.69558
C	-5.74790	0.99171	0.85975
C	-4.25341	1.13890	2.87663
C	-2.33532	0.51919	0.72858
C	-1.28725	0.13758	-0.10144
C	-0.00719	0.97320	-0.13402
C	1.32625	0.21712	0.03347
C	1.52026	-0.84029	0.92674
C	0.47419	-1.39765	1.85592
C	2.79792	-1.40328	0.95901
Br	3.16621	-2.89088	2.11144
C	3.85884	-0.95291	0.18909
O	5.08751	-1.51539	0.22964
C	3.66866	0.13495	-0.66328
C	4.82286	0.63196	-1.50920
C	5.00401	-0.25832	-2.74343
C	4.69431	2.09728	-1.91317
C	2.40687	0.68650	-0.71282
O	0.02436	1.58224	-1.46994
S	-0.34910	3.14545	-1.53862
C	-0.17325	3.37713	0.19259
C	-0.17621	4.58549	0.86317
C	-0.00499	4.55733	2.23346
C	0.17269	3.34300	2.88966
C	0.17697	2.14702	2.19389
C	-0.01058	2.16543	0.81975
O	0.68800	3.79966	-2.27922
O	-1.71232	3.30693	-1.94370
H	0.04659	-2.36284	-1.63038
H	0.36842	-0.69301	-2.08238
H	-0.88658	-1.59854	-2.90182
H	-4.79727	-2.75435	-0.48459
H	-5.13651	-0.63317	2.09471
H	-5.34420	1.90923	0.43100
H	-6.60486	1.25534	1.47952
H	-6.10007	0.36237	0.04569
H	-3.87817	2.11017	2.55371
H	-3.47971	0.65586	3.47267
H	-5.10831	1.32544	3.52495
H	-2.21544	1.39311	1.34607
H	-0.42503	-0.80097	1.88679
H	0.87251	-1.47094	2.86624

H	0.18599	-2.40556	1.55713
H	5.08897	-2.24194	0.86491
H	5.72141	0.53016	-0.89996
H	4.13199	-0.19023	-3.39458
H	5.14191	-1.30045	-2.46316
H	5.87625	0.05699	-3.31571
H	3.86606	2.26223	-2.60166
H	5.60328	2.41881	-2.41972
H	4.54498	2.74263	-1.04859
H	2.24282	1.51823	-1.37645
H	-0.29822	5.51643	0.32984
H	0.00260	5.47983	2.79482
H	0.31920	3.33336	3.96009
H	0.33365	1.21724	2.71844

Compound: C3

Cartesian coordinates

C	6.81512	-1.08605	0.04696
N	5.99362	0.09435	-0.10791
C	4.62350	-0.02752	-0.06345
C	3.99646	-1.28197	-0.08182
C	2.62104	-1.38428	-0.06772
C	1.79041	-0.26612	-0.02686
C	0.34486	-0.44910	-0.01608
C	-0.59291	0.50249	-0.01183
C	-2.03861	0.29254	-0.00154
C	-2.63538	-0.97250	0.05626
C	-4.00474	-1.11640	0.06070
C	-4.80120	0.01532	0.00861
N	-6.25553	-0.13422	0.01403
O	-6.71054	-1.26313	0.06394
O	-6.93133	0.87817	-0.03174
C	-4.25247	1.28171	-0.04641
C	-2.87861	1.40900	-0.05048
C	2.41914	0.98008	0.00867
C	3.78913	1.10409	-0.00462
C	6.60259	1.38340	0.13814
H	6.60664	-1.81392	-0.73652
H	6.66965	-1.57613	1.01548
H	7.85968	-0.80459	-0.03905
H	4.58209	-2.18589	-0.10745
H	2.17454	-2.36998	-0.08603
H	0.03116	-1.48628	-0.01666
H	-0.28964	1.54170	-0.02275
H	-2.02274	-1.85966	0.10165
H	-4.46819	-2.08863	0.10544
H	-4.90037	2.14233	-0.08502
H	-2.43985	2.39589	-0.09386
H	1.82714	1.88285	0.05488
H	4.21682	2.09239	0.03207
H	7.67943	1.28999	0.04113
H	6.38032	1.77054	1.13809
H	6.27155	2.12013	-0.59302

Compound: C4

Cartesian coordinates

O	-0.00817	1.85609	2.25320
C	-0.94819	2.42816	1.74505
O	-2.10369	2.56658	2.33931
C	-0.78445	3.04440	0.38135
C	-1.17646	4.35215	0.14610
C	-0.91667	4.95448	-1.07206
C	-0.27996	4.24313	-2.07378
C	0.09738	2.92887	-1.85563
C	-0.15063	2.32235	-0.63019
C	0.18236	0.88995	-0.45141
C	1.51937	0.44820	-0.43706
C	2.64231	1.30218	-0.48545
C	3.91262	0.82255	-0.44239
C	4.17412	-0.57651	-0.34697
N	5.44695	-1.05237	-0.33624
C	5.71120	-2.48066	-0.20852
C	5.65388	-3.01191	1.21920
C	6.59705	-0.15489	-0.38473
C	6.97867	0.46082	0.95600
C	3.06911	-1.43408	-0.26243
C	1.79094	-0.92385	-0.30383
O	0.78815	-1.82153	-0.18885
C	-0.83498	-0.05540	-0.33442
C	-0.50432	-1.42104	-0.17551
C	-1.44673	-2.40113	-0.00513
C	-2.81350	-2.06112	0.04932
C	-3.16382	-0.69141	-0.14962
C	-2.21995	0.25810	-0.33717
N	-3.76377	-2.98989	0.28958
C	-5.17961	-2.62565	0.38084
C	-5.89268	-2.54190	-0.96168
C	-3.41850	-4.39732	0.45776
C	-3.20072	-5.15097	-0.84892
H	-2.87865	2.76267	1.69643
H	-1.69848	4.89185	0.92125
H	-1.22891	5.97412	-1.24366
H	-0.08987	4.70315	-3.03283
H	0.56493	2.36160	-2.64840
H	2.47610	2.36675	-0.53832
H	4.72732	1.52496	-0.46062
H	6.69909	-2.66158	-0.62636
H	5.01382	-3.02556	-0.84345
H	6.41902	-2.55163	1.84073

H	5.82041	-4.08858	1.22306
H	4.68755	-2.81653	1.67946
H	6.40902	0.62528	-1.12009
H	7.43297	-0.73282	-0.77272
H	7.82401	1.13623	0.82877
H	7.26565	-0.30513	1.67343
H	6.15395	1.02716	1.38400
H	3.17408	-2.49766	-0.14080
H	-1.10066	-3.41382	0.10376
H	-4.18961	-0.36551	-0.13425
H	-2.56172	1.27823	-0.45506
H	-5.26855	-1.68445	0.91709
H	-5.65700	-3.37599	1.00694
H	-5.42787	-1.80295	-1.61098
H	-6.93045	-2.24857	-0.81015
H	-5.88397	-3.50119	-1.47610
H	-4.22863	-4.86011	1.01581
H	-2.53609	-4.47226	1.09181
H	-4.10715	-5.16207	-1.45040
H	-2.92043	-6.18308	-0.64115
H	-2.41002	-4.69771	-1.44337
Cl	-4.30174	2.83041	0.45595

Compound: C5

Cartesian coordinates

C	2.68984	1.51849	3.70127
C	3.62895	1.39052	2.50875
N	4.87316	0.71143	2.89299
C	5.95031	1.36675	3.30499
C	6.11055	2.77561	3.34832
C	6.40928	3.42354	4.48538
C	6.56027	4.86189	4.53790
C	6.84555	5.52136	5.67174
C	6.99658	6.98065	5.75474
C	6.55681	7.64719	6.89731
C	6.70859	9.03782	7.02176
C	7.32258	9.82059	6.02902
N	7.45332	11.20852	6.15023
C	7.28787	11.82538	7.46482
C	8.32036	11.92697	5.21830
C	7.75884	9.12274	4.88974
C	7.61157	7.73242	4.75484
S	7.17523	0.27364	3.81370
C	6.23371	-1.09500	3.36916
C	6.56599	-2.45643	3.46625
C	5.62776	-3.39772	3.03562
C	4.39910	-2.99571	2.52300
C	4.07284	-1.63679	2.43345
C	5.00694	-0.67173	2.86421
C	6.88688	1.63262	-6.24697
C	6.58765	1.46486	-4.78654
C	6.98524	2.44607	-3.86643
C	6.67955	2.30946	-2.51126
C	5.97132	1.18749	-2.07580
S	5.54705	1.03620	-0.34175
O	6.72132	0.42216	0.26423

Compound: C6

Cartesian coordinates

C	-9.13652	-1.24761	-1.30958
C	-8.37772	-1.86053	-0.13060
C	-6.90643	-1.47839	-0.14303
C	-6.57705	-0.12775	-0.01530
C	-5.35793	0.50812	0.00324
C	-5.26867	1.92888	0.14379
C	-6.41800	2.87309	0.28759
C	-3.94926	2.26058	0.12180
C	-3.12203	1.10444	-0.02950
C	-1.70079	1.17696	-0.08874
C	-0.95477	2.31264	-0.01534
C	0.47323	2.36623	-0.07268
C	1.08283	3.73518	-0.06678
C	2.53041	3.75085	0.41246
C	2.59984	3.50467	1.92310
C	3.15650	5.11058	0.10724
C	3.30625	2.66897	-0.34641
C	1.27142	1.25034	-0.15800
C	2.67252	1.30062	-0.30794
C	3.46573	0.14036	-0.40850
C	4.85465	0.23279	-0.81644
N	5.67573	-0.89602	-0.61667
C	7.09578	-0.71263	-0.96458
C	7.89856	-0.10798	0.17233
C	5.23246	-2.09201	-0.13283
N	3.88313	-2.22953	0.02416
C	3.31422	-3.53105	0.41810
C	3.13897	-3.66010	1.92000
C	2.94484	-1.18294	-0.12125
O	1.76782	-1.46739	0.04430
S	6.29468	-3.34016	0.23307

O	5.29577	2.40351	0.10939
O	4.34935	0.20019	-0.30625
C	5.54627	0.21477	-2.98251
C	5.85432	0.35687	-4.33683
H	1.76631	2.02567	3.40622
H	3.15584	2.09410	4.50720
H	2.42823	0.53453	4.10277
H	3.83147	2.38990	2.11590
H	3.11813	0.84268	1.71468
H	5.96917	3.32010	2.41591
H	6.54794	2.88196	5.41963
H	6.42217	5.40971	3.60656
H	6.96253	4.98664	6.61143
H	6.07515	7.10132	7.70505
H	6.32155	9.49055	7.92930
H	6.27204	11.67798	7.84680
H	7.43565	12.91023	7.41760
H	8.01314	11.42502	8.18182
H	7.97021	11.81817	4.18619
H	9.35601	11.57796	5.29552
H	8.31828	13.00359	5.42289
H	8.23484	9.64230	4.06377
H	7.99485	7.25645	3.85557
H	7.53331	-2.77147	3.84757
H	5.87165	-4.45770	3.08304
H	3.69206	-3.74232	2.16580
H	3.12132	-1.35541	1.99276
H	7.83210	2.16607	-6.39265
H	6.08347	2.19622	-6.73112
H	6.98410	0.65994	-6.74057
H	7.53449	3.32327	-4.19970
H	6.98731	3.06871	-1.79715
H	4.97908	-0.64457	-2.63469
H	5.51752	-0.40225	-5.03867

O	5.36100	1.21696	-1.33102
C	-3.98214	-0.02417	-0.10533
C	-3.65986	-1.38904	-0.24692
C	-2.22177	-1.83448	-0.33318
C	-4.57840	-2.42971	-0.31872
C	-5.96997	-2.48078	-0.27789
C	-9.04760	-1.50801	1.19919
H	-8.68172	-1.52377	-2.25974
H	-9.15584	-0.15935	-1.24968
H	-10.16904	-1.59506	-1.31315
H	-8.42142	-2.94409	-0.24150
H	-7.42130	0.54243	0.08574
H	-7.01538	2.65549	1.17376
H	-7.08724	2.83462	-0.57272
H	-6.05622	3.89485	0.37739
H	-3.57754	3.26939	0.20765
H	-1.16044	0.25677	-0.20428
H	-1.45165	3.26730	0.08798
H	0.46961	4.40739	0.53538
H	1.03481	4.12033	-1.09138
H	2.06887	4.28959	2.46217
H	3.63615	3.51017	2.26103
H	2.16071	2.54911	2.20415
H	2.62044	5.90742	0.62390
H	3.13320	5.32503	-0.96135
H	4.19600	5.14101	0.43415
H	4.32253	2.62385	0.02900
H	3.40420	2.96270	-1.39458
H	0.81817	0.27968	-0.14737
H	7.11500	-0.06251	-1.83077
H	7.48512	-1.68418	-1.23821
H	7.50712	0.86938	0.44718
H	8.93483	0.01761	-0.13882
H	7.88239	-0.75603	1.04600
H	3.97963	-4.29575	0.04035
H	2.35816	-3.61051	-0.08442
H	4.09657	-3.58030	2.42994
H	2.70935	-4.63314	2.15504
H	2.46860	-2.89240	2.30043
H	-1.72203	-1.40326	-1.19869
H	-2.16303	-2.91407	-0.42492
H	-1.66138	-1.54845	0.55477
H	-4.12583	-3.40553	-0.42952
H	-6.37242	-3.48276	-0.36565
H	-9.06277	-0.43080	1.36534
H	-8.52956	-1.97014	2.03822
H	-10.07994	-1.85596	1.20363

Compound: C7

Cartesian coordinates

O	2.63516	3.20890	-0.09342
N	3.40664	2.36786	0.34710
O	4.38000	2.66225	1.03301
C	3.17861	0.96924	0.04590
C	4.30809	0.17721	0.13521
C	4.22089	-1.16828	-0.12095
N	5.40479	-1.98003	-0.04831
O	5.29506	-3.18147	-0.26237
O	6.47187	-1.44400	0.22532
C	2.99495	-1.74245	-0.47417
C	1.88378	-0.95941	-0.53690
C	1.88497	0.44238	-0.26688
C	0.69721	1.20546	-0.34707
C	-0.62295	0.77216	-0.22898
C	-1.67363	1.69597	-0.53404
C	-2.97704	1.36038	-0.43698
C	-1.08809	-0.49390	0.24702
C	-2.40931	-0.77349	0.33702
N	-3.36890	0.12239	-0.01666
C	-4.75953	-0.21812	0.06383
C	-5.58640	0.02719	-1.02091
C	-6.93034	-0.29645	-0.93813
C	-7.44080	-0.87220	0.21482
C	-6.60391	-1.11908	1.29196
C	-5.26123	-0.78718	1.22365
H	5.25124	0.62163	0.40007
H	2.94422	-2.79099	-0.71854
H	0.96747	-1.41186	-0.87304
H	0.81208	2.26114	-0.50366
H	-1.42576	2.69450	-0.85956
H	-3.76975	2.05219	-0.66969
H	-0.40503	-1.25270	0.58473
H	-2.76462	-1.72860	0.68781
H	-5.18126	0.45237	-1.92736
H	-7.57575	-0.10817	-1.78350
H	-8.48860	-1.12773	0.27392
H	-6.99718	-1.56036	2.19599
H	-4.61300	-0.95503	2.07114

Compound: C8

Cartesian coordinates

C	7.51392	1.80789	2.23396
C	8.19179	1.39236	0.94144
N	7.30194	1.32190	-0.22517
C	6.31860	0.29345	-0.12663
C	6.53237	-0.99569	-0.61024
C	5.55362	-1.96474	-0.49538
C	4.32064	-1.68504	0.09356
C	3.32083	-2.75463	0.18790
C	1.98604	-2.67197	0.09246
C	1.22302	-1.49064	-0.24538
C	-0.11634	-1.36060	-0.20706
C	-1.04650	-2.39006	0.18662
C	-2.37187	-2.27102	0.38008
C	-3.16751	-1.06307	0.34998
C	-2.82550	0.24956	0.59991
C	-3.90485	1.12514	0.50148
C	-5.09832	0.50466	0.18079
C	-6.34372	1.18981	0.02525
C	-6.27538	2.61604	0.21127
N	-6.19969	3.74776	0.36342
C	-7.57601	0.67800	-0.27326
C	-7.81320	-0.70966	-0.48507
N	-8.02927	-1.82219	-0.65957
C	-8.72035	1.52108	-0.39214
N	-9.65325	2.17959	-0.49262
S	-4.85096	-1.20630	0.00337
C	4.12211	-0.39996	0.59919
C	5.09966	0.57071	0.48294
C	8.05518	1.31757	-1.48146
C	8.54219	2.70423	-1.87082
H	8.26099	1.90148	3.02142
H	6.77766	1.07794	2.56239
H	7.01632	2.76974	2.11845
H	8.70197	0.42875	1.08491
H	8.96379	2.12140	0.70646
H	7.47372	-1.24809	-1.07619
H	5.74494	-2.95989	-0.87453
H	3.73511	-3.74449	0.34001
H	1.43535	-3.59161	0.23560
H	1.78833	-0.63663	-0.59171
H	-0.53040	-0.41682	-0.53051
H	-0.64693	-3.38822	0.30236
H	-2.92496	-3.18050	0.57425
H	-1.83590	0.55908	0.88807
H	-3.82908	2.18773	0.67065
H	3.20053	-0.15982	1.10793
H	4.92309	1.56654	0.86133
H	8.90821	0.62646	-1.43720
H	7.39258	0.94961	-2.26205
H	9.22951	3.12182	-1.13736
H	7.70084	3.38722	-1.97315
H	9.06894	2.65945	-2.82372

Compound: C9

Cartesian coordinates

C	-7.89152	-2.99469	-1.89764
C	-8.66390	-1.87444	-1.22589
N	-8.14207	-1.53374	0.09938
C	-6.78482	-1.06365	0.06646
C	-6.42705	0.12555	-0.56660
C	-5.11471	0.55167	-0.58620
C	-4.10759	-0.19442	0.03153
C	-2.70101	0.21112	0.05126
C	-2.19621	1.37819	-0.35634
C	-0.78456	1.75457	-0.33080
C	0.21374	0.85907	-0.39031
C	1.61726	1.21769	-0.39402
C	1.94692	2.68427	-0.39609
C	0.89444	3.55460	0.30730
C	0.91731	3.28717	1.81551
C	1.21645	5.02687	0.05890
C	-0.48750	3.22969	-0.26754
C	2.53286	0.22501	-0.42070
C	3.97015	0.32316	-0.48165
C	4.80745	1.33947	-0.90119
C	6.15883	1.00178	-0.82615
C	6.39521	-0.27480	-0.35561
C	7.69668	-0.81493	-0.20660
C	8.10366	-2.03542	0.22884
C	7.21207	-3.06663	0.64462
N	6.49562	-3.89765	0.97951
C	9.49806	-2.33575	0.28537
N	10.62031	-2.56964	0.32807
S	4.88729	-1.06273	-0.00208
C	-4.47385	-1.38525	0.65539
C	-5.79110	-1.81210	0.67452
C	-9.04594	-0.63417	0.81876
C	-8.66910	-0.46027	2.27846
H	-8.35548	-3.24713	-2.85026
H	-7.88496	-3.88536	-1.27107
H	-6.85930	-2.71073	-2.09428
H	-9.69839	-2.18650	-1.08423
H	-8.69046	-0.99548	-1.88659
H	-7.18477	0.72254	-1.05499
H	-4.87107	1.47222	-1.09678
H	-2.02427	-0.52439	0.47041
H	-2.87017	2.15175	-0.70638
H	-0.01729	-0.19463	-0.47347
H	2.03774	3.01520	-1.43569
H	2.91504	2.85465	0.07147
H	1.89991	3.51479	2.22913
H	0.68817	2.24903	2.04878
H	0.18694	3.91502	2.32579
H	2.19546	5.28518	0.46357
H	0.47885	5.67079	0.53851
H	1.22049	5.25641	-1.00705
H	-0.57222	3.64526	-1.27717
H	-1.25450	3.72957	0.32682
H	2.14999	-0.78745	-0.38138
H	4.45516	2.27925	-1.28712
H	6.96146	1.66293	-1.11668
H	8.48944	-0.13403	-0.48866
H	-3.71273	-1.98490	1.13652

H	-6.06461	-2.73572	1.16327
H	-10.04110	-1.07368	0.75485
H	-9.10830	0.35036	0.33245
H	-8.63883	-1.42437	2.78396
H	-9.40315	0.16896	2.78019
H	-7.69423	0.01119	2.38910

2 – Hyper-QCC: Post-processing software

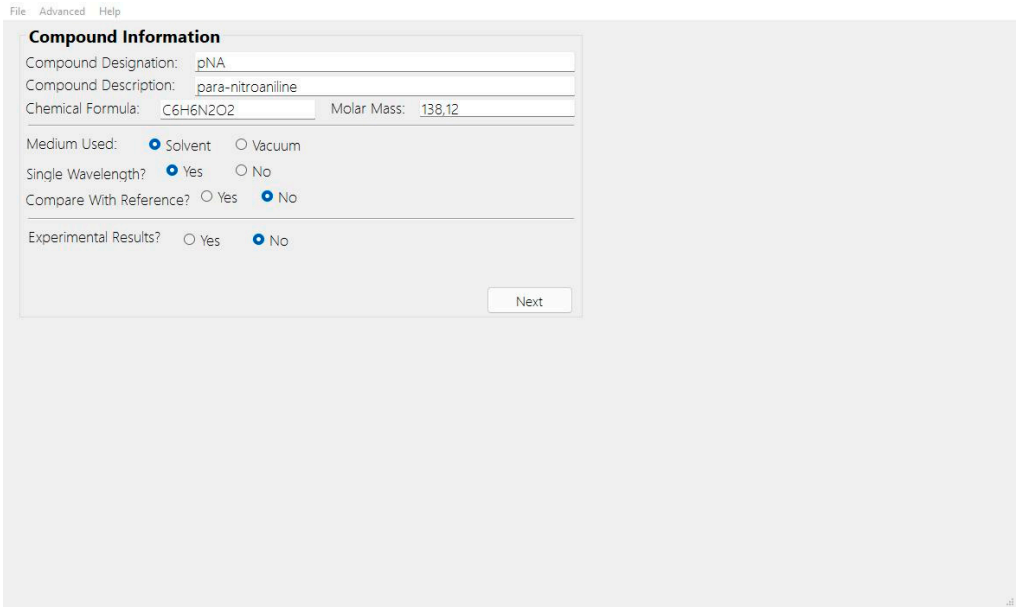

Figure S1. Hyper-QCC first section example. The solvent box is marked since the calculations were carried out using dimethylformamide (DMF) as a medium. Hyper-QCC also offers support to multiple wavelengths calculations, but in this case, the single wavelength is coherent with our logfile.

Once Hyper-QCC is opened, the main window shows some identification information and QCC technical options. Those details are necessary to compare multiple molecules if needed. As an example, we will show how to calculate β_0 and β_{HRS} of the well-known reference molecule used in the HRS experiment - para-nitroaniline (pNA). The pNA geometry optimization was carried out the same as all compounds investigated in this work, and, in this showcase, the tensor components were obtained using the level of theory CAM-B3LYP/6-311++G(2d,2p). The Hyper-QCC first section is shown below in figure S1.

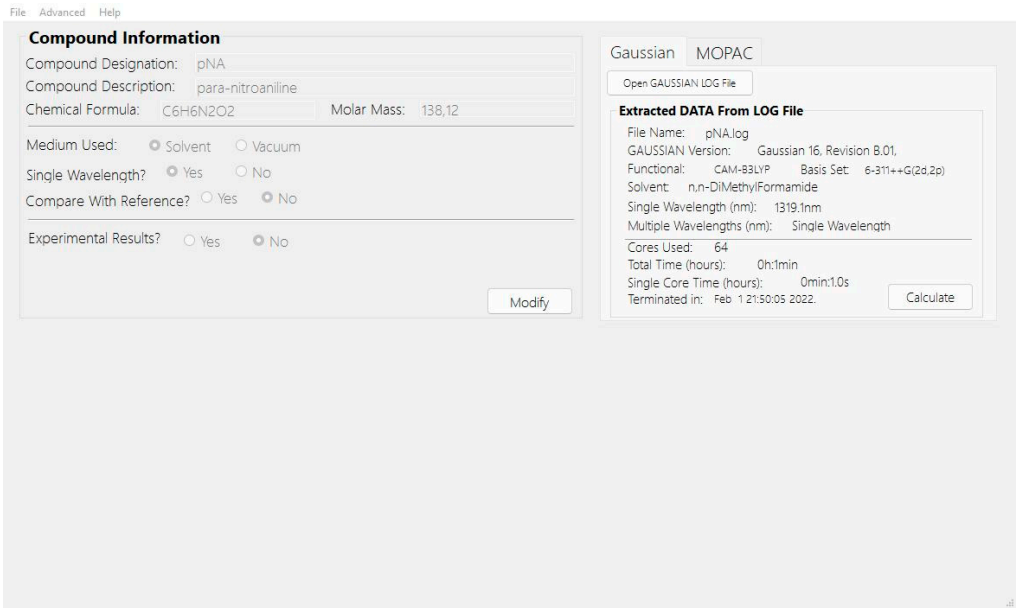

Figure S2. Hyper-QCC second section example. In this section is possible to retrieve the parameters chosen prior to the calculations. It is also possible to visualize the CPU's utilized and its performance.

After the first section is fulfilled, the option to import the tensor calculation logfile will be available. By choosing the logfile, some technical-related details will appear regarding calculation parameters and performance results, as well as the option to calculate β_0 and β_{HRS}. Figure S2 illustrates the described process.

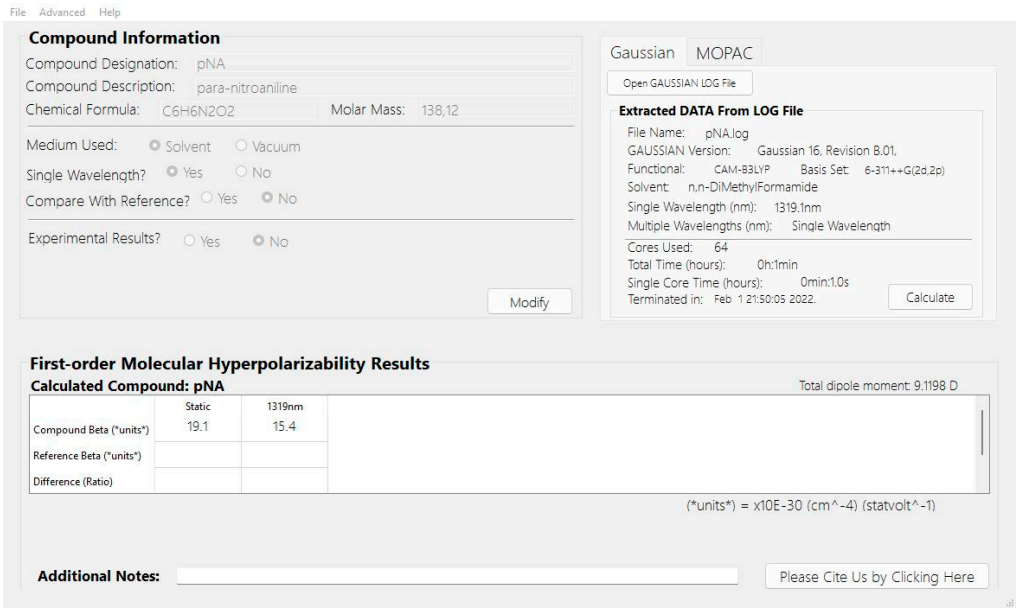

Figure S3. Hyper-QCC results table. The column "Static" for β_0 and the wavelength column displaying β_{HRS}.

Finally, by pressing the "Calculate" button, the β_0 and β_{HRS} will be immediately displayed without further user interaction. As shown in figure S3, the values displayed can be retrieved as text or in a data format. This process could be repeated multiple times, which gives the possibility of one comparing several molecules with the developed software.

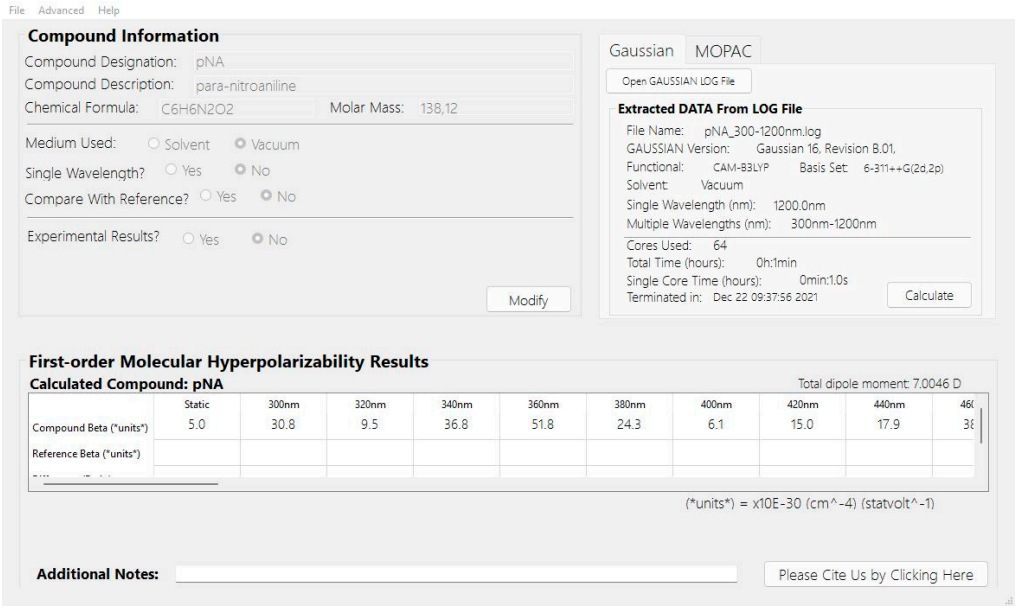

Figure S4. Hyper-QCC results table for multiple tensor logfile. The column "Static" for β_0 and the multiple wavelengths are distributed in the columns displaying β_{HRS}.

Moreover, Hyper-QCC also supports multiple tensor calculations output files by selecting "No" in the "Single Wavelength?" option in the first section. In figure S4, we displayed an example using the pNA molecule again, varying the incident wavelength from 300 nm to 1200 nm, with a 20 nm step. Hyper-QCC presents ~~are~~ other functionalities, such as comparing the β_{HRS} calculated value to the experimental ones, as well as comparing it to a reference compound.

Complete list of the Hyper-QCC functionalities:

1. Computational Functionalities

- Identify and print the Functional used;
- Identify and print on screen Basis-Set used;
- Identify and print the medium used (solvent or gas-phase). If solvent, it will indicate the solvent;
- Identify and print the wavelength used. If multiple wavelengths were used it would indicate the spectrum.
- Identify and print the number of cores used and the calculation's computational cost;
- Extract βHRS tensor components, calculate and print the final result of multiple calculations;
- Extract β0 tensor components, calculate and print the final result of multiple calculations;
- Compare βHRS and β0 with reference molecules calculations built in.
- Compare the βHRS of multiple files in a single table.
- Compare the βHRS retrieve from the input with experimental results.
- Identify and print the Permanent Dipole Moment;

2. Export Functionalities

- Exports a .txt file to easily read the computational data functionalities described above;
- Exports a .dat file to be imported into graphic analysis software;
- Exports a print screen for general purposes.

3. Future Functionalities

- All the computational functionalities above will be implemented for the MOPAC output files.

3 – Results

Table S2: Theoretical values for static (β_0) and dynamic at 1064 nm (β_{HRS}) first-order molecular hyperpolarizability (in 10^{-30} cm^4 $statvolt^{-1}$) in a solvent medium of the investigated compounds. The computational cost (CC) is represented in terms of one single core, and the units are in hours. However, 64 cores (2.35 GHz) with 128 GB of RAM were used to perform the calculations.

	B3LYP			CAM-B3LYP			EXPERIMENTAL
MOLECULE	**β_0**	**β_{HRS}**	**CC**	**β_0**	**β_{HRS}**	**CC**	**β_{HRS}**
A1	4.7	4.2	20.3	4.0	3.4	19.2	7 ± 1
A2	9.9	109.6	61.9	5.1	6.0	34.1	7 ± 2
A3	9.2	11.7	41.6	6.7	7.6	37.3	8 ± 4
A4	10.0	13.5	34.1	7.0	8.2	30.9	9 ± 4
A5	11.0	18.4	2.1	10.2	15.4	2.1	17 ± 2
A6	17.5	31.1	18.1	13.7	20.6	13.9	18 ± 2
A7	16.4	27.1	81.1	12.4	16.5	56.5	17 ± 3
A8	17.9	65.3	88.5	11.2	15.4	165.3	18 ± 4
A9	28.8	449.0	160.0	14.6	21.6	290.1	17 ± 3
B1	87.5	461.0	53.3	35.9	64.1	45.9	44 ± 9
B2	99.2	590.7	43.7	39.4	73.0	38.4	44 ± 9
B3	33.7	78.3	59.7	14.8	24.2	53.3	48 ± 10
B4	15.3	40.3	11.7	9.1	34.2	8.5	25 ± 5
B5	14.2	39.4	10.7	7.2	26.4	8.5	27 ± 5
B6	48.3	69.8	49.1	33.2	42.5	45.9	52 ± 10
B7	29.2	43.1	39.5	21.1	25.5	34.1	24 ± 5
B8	29.2	63.3	11.7	22.4	48.3	8.5	45 ± 9
B9	30.4	52.3	13.9	26.6	35.0	10.7	38 ± 8
C1	57.8	197.7	27.7	41.4	90.4	20.3	111 ± 11
C2	59.3	1438.6	119.5	59.5	302.9	81.1	546 ± 56
C3	194.6	4759.5	16.0	95.8	282.1	11.7	294 ± 30
C4	38.7	161.9	112.0	38.3	103.5	80.0	252 ± 26
C5	181.2	1684.2	104.5	123.7	1181.7	66.1	1932 ± 200
C6	178.7	590.8	185.6	243.9	1069.3	110.9	695 ± 95
C7	76.0	689.7	32.0	76.0	539.1	24.5	450 ± 50
C8	314.7	5626.2	57.6	146.2	1377.7	39.5	1410 ± 282
C9	193.5	18344.0	75.7	118.2	675.4	53.3	1125 ± 225

Table S3: Theoretical values for static (β_0) and dynamic at 1064 nm (β_{HRS}) first-order molecular hyperpolarizability (in 10^{-30} cm^4 $statvolt^{-1}$) in a solvent medium of the investigated compounds. The computational cost (CC) is represented in terms of one single core, and the units are in hours. However, 64 cores (2.35 GHz) with 128 GB of RAM were used to perform the calculations.

	M06-2X			TPSSh			EXPERIMENTAL
MOLECULE	**β_0**	**β_{HRS}**	**CC**	**β_0**	**β_{HRS}**	**CC**	**β_{HRS}**
A1	3.8	3.2	21.3	4.6	4.1	5.3	7 ± 1
A2	4.8	5.6	37.3	12.5	16.8	337.1	7 ± 2
A3	6.8	7.8	35.2	10.3	734.5	257.1	8 ± 4
A4	7.1	8.3	28.8	11.3	1386.3	215.5	9 ± 4
A5	10.3	15.7	2.1	11.2	19.1	22.4	17 ± 2
A6	13.8	21.0	16.0	18.9	36.1	116.3	18 ± 2
A7	11.1	14.5	62.9	17.7	40.4	94.9	17 ± 3
A8	10.0	13.4	69.3	21.3	50.1	489.6	18 ± 4
A9	13.9	20.2	112.0	37.4	514.1	917.3	17 ± 3
B1	34.9	61.6	42.7	107.7	1805.1	61.9	44 ± 9
B2	38.4	70.3	35.2	122.2	2851.2	51.2	44 ± 9
B3	15.9	26.2	48.0	42.9	119.8	69.3	48 ± 10
B4	10.3	35.9	10.7	44.1	83.3	13.9	25 ± 5
B5	9.8	33.7	9.6	33.9	58.9	12.8	27 ± 5
B6	32.6	42.5	49.1	53.4	97.5	16.0	52 ± 10
B7	19.2	33.1	30.9	29.6	45.7	10.7	24 ± 5
B8	22.5	47.6	9.6	209.4	56.7	13.9	45 ± 9
B9	25.6	37.1	12.8	40.0	68.5	17.1	38 ± 8
C1	43.9	98.7	23.5	64.1	278.5	33.1	111 ± 11
C2	62.6	430.3	86.4	59.3	3506.2	139.7	546 ± 56
C3	97.3	287.4	12.8	227.8	4123.6	18.1	294 ± 30
C4	39.6	119.6	151.5	41.9	203.5	157.9	252 ± 26
C5	135.7	1615.3	70.4	201.4	1293.7	220.8	1932 ± 200
C6	257.7	1502.8	124.8	162.9	97.5	226.1	695 ± 95
C7	73.7	480.9	25.6	72.2	3523.0	41.6	450 ± 50
C8	148.7	1485.5	41.6	436.0	1112.5	62.9	1410 ± 282
C9	120.3	705.8	58.7	219.0	4430.0	87.5	1125 ± 225

Table S4: Theoretical values for static (β_0) and dynamic at 1064 nm (β_{HRS}) first-order molecular hyperpolarizability (in 10^{-30} cm^4 $statvolt^{-1}$) in a solvent medium of the investigated compounds. The computational cost (CC) is represented in terms of one single core, and the units are in hours. However, 64 cores (2.35 GHz) with 128 GB of RAM were used to perform the calculations.

	PBE1PBE			wB97xD			EXPERIMENTAL
MOLECULE	**β_0**	**β_{HRS}**	**CC**	**β_0**	**β_{HRS}**	**CC**	**β_{HRS}**
A1	4.3	3.7	4.3	3.8	3.1	4.3	7 ± 1
A2	8.1	89.5	46.9	4.7	5.3	30.9	7 ± 2
A3	8.6	10.6	38.4	6.4	4123.6	28.8	8 ± 4
A4	9.3	12.0	32.0	6.7	7.7	26.2	9 ± 4
A5	10.8	17.4	2.1	9.9	14.9	1.8	17 ± 2
A6	16.6	28.2	17.1	13.2	19.4	13.9	18 ± 2
A7	14.8	22.2	73.6	11.6	15.3	54.4	17 ± 3
A8	15.3	29.9	80.0	10.3	13.8	57.6	18 ± 4
A9	23.5	73.2	144.0	12.9	18.3	101.3	17 ± 3
B1	70.6	232.4	48.0	30.0	49.5	38.4	44 ± 9
B2	79.6	282.7	39.5	32.4	55.2	32.0	44 ± 9
B3	28.5	59.6	54.4	12.8	20.1	42.7	48 ± 10
B4	35.8	56.3	10.7	22.8	28.9	9.6	25 ± 5
B5	27.9	41.4	9.6	18.7	23.1	8.5	27 ± 5
B6	44.1	66.9	12.8	30.4	37.4	10.7	52 ± 10
B7	25.0	34.1	8.5	18.2	21.2	7.5	24 ± 5
B8	43.2	123.2	10.7	21.3	43.2	9.6	45 ± 9
B9	34.0	51.5	12.8	25.6	37.1	11.7	38 ± 8
C1	55.0	167.7	26.7	38.9	81.2	20.3	111 ± 11
C2	59.3	734.5	112.0	59.6	280.6	80.0	546 ± 56
C3	167.8	1386.3	14.9	80.1	206.1	10.7	294 ± 30
C4	38.1	136.0	126.9	38.5	100.4	74.7	252 ± 26
C5	171.6	2660.5	157.9	113.7	811.4	62.9	1932 ± 200
C6	188.0	41.4	155.7	253.7	1533.2	100.3	695 ± 95
C7	73.3	966.8	30.9	72.8	469.9	21.3	450 ± 50
C8	176.6	2567.1	57.6	127.4	852.8	37.3	1410 ± 282
C9	176.6	6407.2	70.4	104.7	508.2	50.1	1125 ± 225

Table S5: Theoretical values for static (β_0) and dynamic at 1064 nm (β_{HRS}) first-order molecular hyperpolarizability (in 10^{-30} cm^4 $statvolt^{-1}$) in a solvent medium of the investigated compounds. The computational cost (CC) is represented in terms of one single core, and the units are in hours. However, 64 cores (2.35 GHz) with 128 GB of RAM were used to perform the calculations.

	HF			EXPERIMENTAL
MOLECULE	**β_0**	**β_{HRS}**	**CC**	**β_{HRS}**
A1	2.9	2.3	2.1	7 ± 1
A2	3.2	3.1	21.3	7 ± 2
A3	4.4	4.8	22.4	8 ± 4
A4	4.5	4.9	18.1	9 ± 4
A5	7.2	9.5	1.1	17 ± 2
A6	8.6	11.1	9.6	18 ± 2
A7	7.1	8.0	38.4	17 ± 3
A8	5.8	6.6	41.6	18 ± 4
A9	7.1	8.3	70.4	17 ± 3
B1	17.2	22.8	25.6	44 ± 9
B2	18.7	25.4	21.3	44 ± 9
B3	7.1	9.3	29.9	48 ± 10
B4	14.1	15.2	6.4	25 ± 5
B5	12.3	13.1	5.3	27 ± 5
B6	19.3	20.1	7.5	52 ± 10
B7	12.0	12.2	4.3	24 ± 5
B8	14.2	24.2	6.4	45 ± 9
B9	15.0	16.5	7.5	38 ± 8
C1	22.5	35.8	13.9	111 ± 11
C2	48.6	98.4	52.3	546 ± 56
C3	45.2	83.3	7.5	294 ± 30
C4	37.6	62.6	49.1	252 ± 26
C5	47.7	130.3	41.6	1932 ± 200
C6	160.9	1324.9	68.3	695 ± 95
C7	48.4	108.5	13.9	450 ± 50
C8	80.1	263.2	25.6	1410 ± 282
C9	68.8	194.7	34.1	1125 ± 225

Table S6: All $\beta_{HRS.}$ values are in 10^{-30} cm^4 statvolt^{-1} units and computational cost per core (CC) in hour. 64 cores were used in the calculations. The relative error was calculated considering the following equation $RE = |\beta_{DZ} - \beta_{TZ}|/\beta_{TZ}$.

MOLECULE	DOUBLE-ZETA (DZ) CAM-B3LYP/6-31++G(2D,2P)			TRIPLE-ZETA (TZ) CAM-B3LYP/6-311++G(2D,2P)			RELATIVE ERROR
	β_0	β_{HRS}	CC	β_0	β_{HRS}	CC	β_{HRS}
A1	4.0	3.3	2.1	4.0	3.4	19.2	0.03
A2	4.9	5.7	21.3	5.1	6.0	34.1	0.05
A3	7.0	8.0	19.2	6.7	7.6	37.3	0.05
A4	7.3	8.5	17.1	7.0	8.2	30.9	0.04
A5	10.3	15.5	2.1	10.2	15.4	2.1	0.01
A6	13.9	20.7	9.6	13.7	20.6	13.9	0.00
A7	12.4	16.6	35.2	12.4	16.5	56.5	0.01
A8	11.2	15.4	37.3	11.2	15.4	165.3	0.00
A9	14.7	21.7	67.2	14.6	21.6	290.1	0.00
B1	35.8	64.0	24.5	35.9	64.1	45.9	0.00
B2	39.4	72.9	20.3	39.4	73.0	38.4	0.00
B3	14.7	24.0	28.8	14.8	24.2	53.3	0.01
B4	24.5	31.9	6.4	9.1	34.2	8.5	0.07
B5	20.3	25.6	5.3	7.2	26.4	8.5	0.03
B6	33.0	41.7	7.5	33.2	42.5	45.9	0.02
B7	19.6	23.2	4.3	21.1	25.5	34.1	0.09
B8	24.0	50.6	5.3	22.4	45.6	8.5	0.11
B9	26.7	35.5	7.5	26.6	35.0	10.7	0.01
C1	41.6	89.6	12.8	41.4	90.4	20.3	0.01
C2	59.8	297.8	54.4	59.5	302.9	81.1	0.02
C3	95.7	278.9	7.5	95.8	282.1	11.7	0.01
C4	38.7	103.1	51.2	38.3	103.5	80.0	0.00
C5	123.8	1169.	42.7	123.7	1181.7	66.1	0.01
C6	244.1	1243.3	69.3	243.9	1069.3	110.9	0.16
C7	75.9	533.9	14.9	76.0	539.1	24.5	0.01
C8	147.7	1392.5	24.5	146.2	1377.7	39.5	0.01
C9	118.2	669.3	33.1	118.2	675.4	53.3	0.01

Table S7: The following data was obtained for compound A7. All β_0 *and* $\beta_{HRS.}$ values are in 10^{-30} cm^4 $statvolt^{-1}$ units and computational cost per core (CC) in hour. 64 cores were used in the calculations. The relative error was calculated considering the following equation $RE = |\beta_{HRS} - \beta_{HRS-EXP}|/\beta_{HRS-EXP}$.

$$\boldsymbol{\beta_{HRS-EXP.} = 17}$$

Functional	Basis-Set	β_0	β_{HRS}	Relative Error to Exp. Value	CC
HF	(2d,2p)	7.1	8.0	0.53	38.4
	(2df, 2pd)	5.8	6.6	0.61	75.7
CAM-B3LYP	(2d,2p)	12.4	16.5	0.03	56.5
	(2df, 2pd)	12.2	16.3	0.04	124.8
B3LYP	(2d,2p)	16.4	27.1	0.59	81.1
	(2df, 2pd)	16.3	26.7	0.57	158.9
M06-2X	(2d,2p)	11.1	14.5	0.15	62.9
	(2df, 2pd)	11.0	14.2	0.16	124.8
TPSSh	(2d,2p)	17.7	40.4	1.38	94.9
	(2df, 2pd)	17.5	38.4	1.26	184.5
PBE1PBE	(2d,2p)	14.8	22.2	0.31	73.6
	(2df, 2pd)	11.9	21.8	0.28	153.6
wB97xD	(2d,2p)	11.6	15.3	0.10	54.4
	(2df, 2pd)	11.9	15.7	0.08	117.3

Table S8: The following data was obtained for compound B6. All β_0 *and* $\beta_{HRS.}$ values are in 10^{-30} cm^4 $statvolt^{-1}$ units and computational cost per core (CC) in hour. 64 cores were used in the calculations. The relative error was calculated considering the following equation $RE = |\beta_{HRS} - \beta_{HRS-EXP}|/\beta_{HRS-EXP}$.

$$\boldsymbol{\beta_{HRS-EXP} = 52}$$

Functional	Basis-Set	β_0	β_{HRS}	Relative Error to Exp. Value	C.C.
HF	(2d,2p)	19.3	20.1	0.61	7.5
	(2df, 2pd)	19.1	19.9	0.62	16.0
CAM-B3LYP	(2d,2p)	33.2	42.5	0.18	45.9
	(2df, 2pd)	32.4	41.0	0.21	293.3
B3LYP	(2d,2p)	48.3	69.8	0.34	49.1
	(2df, 2pd)	47.4	76.9	0.48	315.7
M06-2X	(2d,2p)	32.6	42.5	0.18	49.1
	(2df, 2pd)	31.6	40.8	0.22	280.5
TPSSh	(2d,2p)	53.4	97.5	0.88	16.0
	(2df, 2pd)	52.9	96.1	0.85	32.0
PBE1PBE	(2d,2p)	44.1	66.9	0.29	12.8
	(2df, 2pd)	43.7	66.1	0.27	26.7
wB97xD	(2d,2p)	30.4	37.4	0.28	10.7
	(2df, 2pd)	11.9	37.7	0.28	26.7

Table S9: The following data was obtained for compound C8. All β_0 *and* $\beta_{HRS.}$ values are in 10^{-30} cm^4 $statvolt^{-1}$ units and computational cost per core (CC) in hour. 64 cores were used in the calculations. The relative error was calculated considering the following equation $RE = |\beta_{HRS} - \beta_{HRS-EXP}|/\beta_{HRS-EXP}$.

$$\boldsymbol{\beta_{HRS-EXP} = 1410}$$

Functional	Basis-Set	β_0	β_{HRS}	Relative Error to Exp. Value	C.C.
HF	(2d,2p)	80.1	263.2	0.81	25.6
	(2df, 2pd)	68.8	194.7	0.86	52.3
CAM-B3LYP	(2d,2p)	314.7	1377.7	0.02	39.5
	(2df, 2pd)	145.0	1345.9	0.05	84.3
B3LYP	(2d,2p)	314.7	5626.2	2.99	57.6
	(2df, 2pd)	311.7	4706.8	2.34	118.4
M06-2X	(2d,2p)	148.7	1485.5	0.05	41.6
	(2df, 2pd)	147.5	1455.6	0.03	85.3
TPSSh	(2d,2p)	436.0	1112.5	0.21	62.9
	(2df, 2pd)	430.6	1126.1	0.20	124.8
PBE1PBE	(2d,2p)	176.6	2567.1	0.82	57.6
	(2df, 2pd)	269.2	2578.5	0.83	116.3
wB97xD	(2d,2p)	127.4	852.8	0.40	37.7
	(2df, 2pd)	128.4	841.8	0.40	82.1

4 – Computational Details of C5.

We have calculated C5 in both forms, i.e., the cationic-conjugated molecule with its counterion (C5-Full) and the cationic-conjugated molecule separated from its counterion (C5-Cationic Part, C5-Anionic Part). As verified (table S10), when the parts were computed separately, the calculated dynamic first-order molecular hyperpolarizability from the cationic part achieved a value one order of magnitude lower than the experimental one.

Table S10: *All β_0 and $\beta_{HRS.}$ values are in 10^{-30} cm^4 $statvolt^{-1}$ units.*

MOLECULE	CAM-B3LYP 6-311++G(2D,2P)		EXPERIMENTAL
	β_0	β_{HRS}	β_{HRS}
C5-FULL	123.7	1181.7	1932 ± 200
C5-CATIONIC	17.7	111.7	
C5-ANIONIC	2.8	3.1	

Regarding the Potential Energy Surface (PES), we have decided to start with the geometry depicted in Figure S1. Still, there are countless possibilities for the geometry starting point. However, in this work, we decided to use the same approach for all investigated molecules' geometry starting points:

1. Generating the Simplified Molecular Input Line Entry System (SMILES);
2. Importing SMILES to Avogadro;
3. The "Optimize Geometry" command in Avogadro is executed to create the geometry starting point.
4. Only after defining the starting point the cartesian coordinates were applied to the Gaussian command file for optimization, i.e., to calculate the PES local minimum.

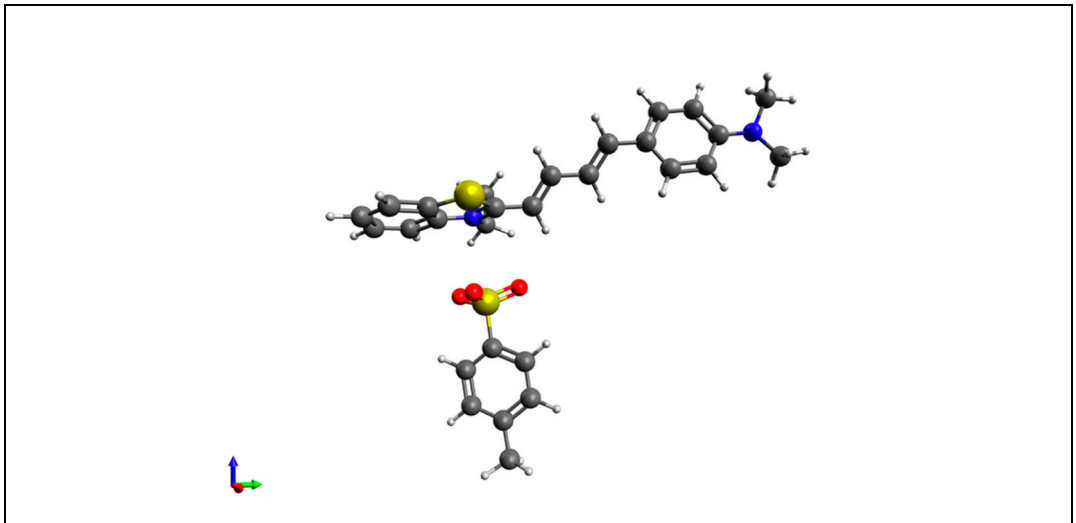

Figure S5 – Optimized Geometry used in the calculations of compound C5.