Electronic Supplementary Information

Computational design of two-photon active organic molecules for infrared responsive materials

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Table S1. GFSM-based analysis for $S_0 \rightarrow S_4$ transition for BPCSA molecule.

FINAL STATE = 4, INTERMEDIATE STATE = 1

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	4.7192	4.7192	0.1222	154.4822
40	6.9817	6.9817	-0.1222	-228.5471
10	-2.2645	-0.3039	-0.0700	73.4099
04	6.9817	6.9817	-0.1222	-228.5471
44	18.0020	18.0020	0.1222	589.2942
14	77.5120	69.6318	0.0700	4205.6963
01	-0.3039	-2.2645	-0.0700	73.4099
41	69.6318	77.5120	0.0700	4205.6963
11	1088.0888	1088.0888	0.0401	108618.8408

DELTA-2PA = 117463.74

FINAL STATE = 4, INTERMEDIATE STATE = 2

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	4.7192	4.7192	0.1222	154.4822
40	6.9817	6.9817	-0.1222	-228.5471
20	-0.0670	-0.0283	-0.1080	1.7631
04	6.9817	6.9817	-0.1222	-228.5471
44	18.0020	18.0020	0.1222	589.2942
24	0.9048	0.8407	0.1080	32.3112
02	-0.0283	-0.0670	-0.1080	1.7631
42	0.8407	0.9048	0.1080	32.3112
22	0.1958	0.1958	0.0955	8.1991

DELTA-2PA = 363.03

FINAL STATE = 4, INTERMEDIATE STATE = 3

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	4.7192	4.7192	0.1222	154.4822
40	6.9817	6.9817	-0.1222	-228.5471
30	-0.0213	-0.0112	-0.1104	0.5887
04	6.9817	6.9817	-0.1222	-228.5471
44	18.0020	18.0020	0.1222	589.2942
34	0.0231	0.0078	0.1104	0.5594
03	-0.0112	-0.0213	-0.1104	0.5887
43	0.0078	0.0231	0.1104	0.5594
33	0.0053	0.0053	0.0997	0.2112

DELTA-2PA = 289.19

FINAL STATE = 4, INTERMEDIATE STATE = 5

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	4.7192	4.7192	0.1222	154.4822
40	6.9817	6.9817	-0.1222	-228.5471
50	0.0060	0.0068	-0.1274	-0.2008
04	6.9817	6.9817	-0.1222	-228.5471
44	18.0020	18.0020	0.1222	589.2942
54	0.0114	0.0127	0.1274	0.3785
05	0.0068	0.0060	-0.1274	-0.2008
45	0.0127	0.0114	0.1274	0.3785
55	0.0000	0.0000	0.1328	0.0014

DELTA-2PA = 287.04

Table S2. GFSM-based analysis for $S_0 \rightarrow S_3$ transition for BMCSA molecule.

FINAL STATE = 3, INTERMEDIATE STATE = 1

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0007	0.0007	0.0697	0.0424
30	0.0003	0.0003	-0.0697	-0.0147
10	-0.3426	-0.3339	-0.0360	37.6290
03	0.0003	0.0003	-0.0697	-0.0147
33	0.0001	0.0001	0.0697	0.0051
13	-0.1189	-0.1159	0.0360	-13.0581
01	-0.3339	-0.3426	-0.0360	37.6290
31	-0.1159	-0.1189	0.0360	-13.0581
11	1416.8754	1416.8754	0.0185	305638.2675

DELTA-2PA = 305687.43

FINAL STATE = 3, INTERMEDIATE STATE = 2

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0007	0.0007	0.0697	0.0424
30	0.0003	0.0003	-0.0697	-0.0147
20	-0.2104	-0.2180	-0.0616	13.9184
03	0.0003	0.0003	-0.0697	-0.0147
33	0.0001	0.0001	0.0697	0.0051
23	-0.0730	-0.0757	0.0616	-4.8300
02	-0.2180	-0.2104	-0.0616	13.9184
32	-0.0757	-0.0730	0.0616	-4.8300
22	566.6363	566.6363	0.0544	41702.4484

DELTA-2PA = 41720.64

FINAL STATE = 3, INTERMEDIATE STATE = 4

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0007	0.0007	0.0697	0.0424
30	0.0003	0.0003	-0.0697	-0.0147
40	-0.0000	-0.0000	-0.0876	0.0017
03	0.0003	0.0003	-0.0697	-0.0147
33	0.0001	0.0001	0.0697	0.0051
43	-0.0000	-0.0000	0.0876	-0.0006
04	-0.0000	-0.0000	-0.0876	0.0017
34	-0.0000	-0.0000	0.0876	-0.0006
44	0.0000	0.0000	0.1100	0.0001

DELTA-2PA = 0.02

FINAL STATE = 3, INTERMEDIATE STATE = 5

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0007	0.0007	0.0697	0.0424
30	0.0003	0.0003	-0.0697	-0.0147
50	-0.0030	-0.0029	-0.0996	0.1175
03	0.0003	0.0003	-0.0697	-0.0147
33	0.0001	0.0001	0.0697	0.0051
53	-0.0010	-0.0010	0.0996	-0.0408
05	-0.0029	-0.0030	-0.0996	0.1175
35	-0.0010	-0.0010	0.0996	-0.0408
55	0.1140	0.1140	0.1422	3.2068

DELTA-2PA = 3.38

Table S3. GFSM-based analysis for $S_0 \rightarrow S_4$ transition for BMCSA molecule.

FINAL STATE = 4, INTERMEDIATE STATE = 1

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0006	0.0006	0.0887	0.0286
40	0.0005	0.0005	-0.0887	-0.0238
10	0.2581	0.1979	-0.0305	-29.9058
04	0.0005	0.0005	-0.0887	-0.0238
44	0.0004	0.0004	0.0887	0.0197
14	0.2142	0.1643	0.0305	24.8272
01	0.1979	0.2581	-0.0305	-29.9058
41	0.1643	0.2142	0.0305	24.8272
11	723.8610	723.8610	0.0105	276313.2240

DELTA-2PA = 276303.07

FINAL STATE = 4, INTERMEDIATE STATE = 2

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0006	0.0006	0.0887	0.0286
40	0.0005	0.0005	-0.0887	-0.0238
20	-0.0003	-0.0033	-0.0594	0.1230
04	0.0005	0.0005	-0.0887	-0.0238
44	0.0004	0.0004	0.0887	0.0197
24	-0.0003	-0.0028	0.0594	-0.1021
02	-0.0033	-0.0003	-0.0594	0.1230
42	-0.0028	-0.0003	0.0594	-0.1021
22	0.0407	0.0407	0.0397	4.0971

DELTA-2PA = 4.14

FINAL STATE = 4, INTERMEDIATE STATE = 3

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0006	0.0006	0.0887	0.0286
40	0.0005	0.0005	-0.0887	-0.0238
30	-0.0000	-0.0000	-0.0686	0.0022
04	0.0005	0.0005	-0.0887	-0.0238
44	0.0004	0.0004	0.0887	0.0197
34	-0.0000	-0.0000	0.0686	-0.0018
03	-0.0000	-0.0000	-0.0686	0.0022
43	-0.0000	-0.0000	0.0686	-0.0018
33	0.0000	0.0000	0.0530	0.0002

DELTA-2PA = 0.00

FINAL STATE = 4, INTERMEDIATE STATE = 5

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0006	0.0006	0.0887	0.0286
40	0.0005	0.0005	-0.0887	-0.0238
50	0.0047	0.0036	-0.1023	-0.1625
04	0.0005	0.0005	-0.0887	-0.0238
44	0.0004	0.0004	0.0887	0.0197
54	0.0039	0.0030	0.1023	0.1349
05	0.0036	0.0047	-0.1023	-0.1625
45	0.0030	0.0039	0.1023	0.1349
55	0.3233	0.3233	0.1178	10.9750

DELTA-2PA = 10.92

Table S4. GFSM-based analysis for $S_0 \rightarrow S_2$ transition for BPyMCSA molecule.

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FINAL STATE =  2, INTERMEDIATE STATE =  1
KL          ALPHA          BETA     15xDExDK    DELTA(KL)
00         0.0000        0.0000       0.0452       0.0010
20         0.0000        0.0000      -0.0452      -0.0009
10        -0.0709       -0.0649      -0.0266      10.2047
02         0.0000        0.0000      -0.0452      -0.0009
22         0.0000        0.0000       0.0452       0.0008
12        -0.0643       -0.0588       0.0266      -9.2542
01        -0.0649       -0.0709      -0.0266      10.2047
21        -0.0588       -0.0643       0.0266      -9.2542
11      3862.1792     3862.1792       0.0157  985409.0398
DELTA-2PA =    985410.94

FINAL STATE =  2, INTERMEDIATE STATE =  3
KL          ALPHA          BETA     15xDExDK    DELTA(KL)
00         0.0000        0.0000       0.0452       0.0010
20         0.0000        0.0000      -0.0452      -0.0009
30        -0.0013       -0.0018      -0.0485       0.1268
02         0.0000        0.0000      -0.0452      -0.0009
22         0.0000        0.0000       0.0452       0.0008
32        -0.0011       -0.0016       0.0485      -0.1150
03        -0.0018       -0.0013      -0.0485       0.1268
23        -0.0016       -0.0011       0.0485      -0.1150
33         1.9393        1.9393       0.0520     149.1723
DELTA-2PA =       149.20

FINAL STATE =  2, INTERMEDIATE STATE =  4
KL          ALPHA          BETA     15xDExDK    DELTA(KL)
00         0.0000        0.0000       0.0452       0.0010
20         0.0000        0.0000      -0.0452      -0.0009
40         0.0000        0.0000      -0.0496      -0.0000
02         0.0000        0.0000      -0.0452      -0.0009
22         0.0000        0.0000       0.0452       0.0008
42         0.0000        0.0000       0.0496       0.0000
04         0.0000        0.0000      -0.0496      -0.0000
24         0.0000        0.0000       0.0496       0.0000
44         0.0000        0.0000       0.0544       0.0000
DELTA-2PA =         0.00

FINAL STATE =  2, INTERMEDIATE STATE =  5
KL          ALPHA          BETA     15xDExDK    DELTA(KL)
00         0.0000        0.0000       0.0452       0.0010
20         0.0000        0.0000      -0.0452      -0.0009
50         0.0000        0.0000      -0.0570      -0.0001
02         0.0000        0.0000      -0.0452      -0.0009
22         0.0000        0.0000       0.0452       0.0008
52         0.0000        0.0000       0.0570       0.0001
05         0.0000        0.0000      -0.0570      -0.0001
25         0.0000        0.0000       0.0570       0.0001
55         0.0000        0.0000       0.0718       0.0000
DELTA-2PA =         0.00
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Table S5. GFSM-based analysis for $S_0 \rightarrow S_4$ transition for BPyMCSA molecule.

FINAL STATE = 4, INTERMEDIATE STATE = 1

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0000	0.0000	0.0497	0.0003
40	0.0000	0.0000	-0.0497	-0.0004
10	0.0275	0.0138	-0.0256	-3.2226
04	0.0000	0.0000	-0.0497	-0.0004
44	0.0000	0.0000	0.0497	0.0004
14	0.0297	0.0149	0.0256	3.4828
01	0.0138	0.0275	-0.0256	-3.2226
41	0.0149	0.0297	0.0256	3.4828
11	839.4590	839.4590	0.0132	254167.4534

DELTA-2PA = 254167.97

FINAL STATE = 4, INTERMEDIATE STATE = 2

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0000	0.0000	0.0497	0.0003
40	0.0000	0.0000	-0.0497	-0.0004
20	0.0000	0.0000	-0.0451	-0.0000
04	0.0000	0.0000	-0.0497	-0.0004
44	0.0000	0.0000	0.0497	0.0004
24	0.0000	0.0000	0.0451	0.0000
02	0.0000	0.0000	-0.0451	-0.0000
42	0.0000	0.0000	0.0451	0.0000
22	0.0000	0.0000	0.0409	0.0000

DELTA-2PA = 0.00

FINAL STATE = 4, INTERMEDIATE STATE = 3

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0000	0.0000	0.0497	0.0003
40	0.0000	0.0000	-0.0497	-0.0004
30	-0.0019	-0.0016	-0.0485	0.1444
04	0.0000	0.0000	-0.0497	-0.0004
44	0.0000	0.0000	0.0497	0.0004
34	-0.0021	-0.0017	0.0485	-0.1561
03	-0.0016	-0.0019	-0.0485	0.1444
43	-0.0017	-0.0021	0.0485	-0.1561
33	6.7693	6.7693	0.0474	570.9623

DELTA-2PA = 570.94

FINAL STATE = 4, INTERMEDIATE STATE = 5

KL	ALPHA	BETA	15xDExDK	DELTA(KL)
00	0.0000	0.0000	0.0497	0.0003
40	0.0000	0.0000	-0.0497	-0.0004
50	-0.0000	-0.0000	-0.0574	0.0001
04	0.0000	0.0000	-0.0497	-0.0004
44	0.0000	0.0000	0.0497	0.0004
54	-0.0000	-0.0000	0.0574	-0.0001
05	-0.0000	-0.0000	-0.0574	0.0001
45	-0.0000	-0.0000	0.0574	-0.0001
55	0.0000	0.0000	0.0664	0.0000

DELTA-2PA = 0.00

The 1PA results are listed in Table S6. In addition to the excitation energies and oscillator strengths, the calculated charge-transfer (CT) diagnostic, D_{CT}, of LeBahers, Adamo, and Ciofini,[1] is included for each excited state. For each of the four molecules, the first excited-state has a large oscillator strength, although only for NCSA does it appear to be a CT state. For NCSA, D_{CT} for the transition to S_1 is 5.86 when PBE0 is used and 3.53 with the CAM-B3LYP functional, while D_{CT} is less than 1.0 for the BPSCA molecule and less than 0.1 for BMCSA and BPyMCSA. When the CAM-B3LYP functional is used, the energy of the first excited-state is in good agreement with the CC2 results, significantly better than for PBE0. For the first excited state of each of the four molecules, the average error of the CAM-B3LYP results relative to the CC2 values is only 0.07 eV, while for PBE0 the average error is 0.32 eV. For the higher-energy excited states, the CAM-B3LYP results are also in better agreement with CC2 than with PBE0. When the average errors are calculated, by and large, the CC2 excitation energies listed in Table S6, the CAM-B3LYP error is 0.16 eV, while the PBE0 error is 0.39 eV. Our CAM-B3LYP results for BPyMCSA, are consistent with those in Table 3 in the manuscript.

Table S7 lists the corresponding results with inclusion of the DMSO solvent using PCM, in comparison to the measured absorption for BPCSA that was characterized experimentally. In the gas-phase calculations, the energy of the first excited-state using CAM-B3LYP was in excellent agreement with the CC2 value, while the PBE0 value is fairly close to the value measured in DMSO. When the effects of the DMSO solvent were included, the calculated values were red-shifted such that PBE0 underestimates the excitation energy by 0.25 eV, while CAM-B3LYP overestimates it by 0.14 eV. A modified CAM-B3LYP, denoted mCAM-B3LYP,[2-4] which has been previously tested in cases where less range separation is needed to model charge transfer,

results in slightly better agreement, underestimating the excitation energy by 0.13 eV. The good agreement with the measurement for this functional can be seen in Figure S1.

Table S8 lists measured and calculated emission energies. The first triplet-spin state of BPCSA was optimized to obtain the adiabatic phosphorescence energy, but the calculated values are significantly lower than the measured emission energies of 2.65 eV and 2.76 eV. However, the CAM-B3LYP vertical fluorescence energy is in good agreement with experiment. The CAM-B3LYP adiabatic fluorescence and phosphorescence are in good agreement with the XMC-QDPT2 values. However, the agreement is not as good for the other three molecules. While for BPCSA the CAM-B3LYP functional is in good agreement with QDPT2 for the emission energy from S_1 state, it yields a significantly lower value than QDPT2 for the emission energy from T_1 state. For BPyMCSA and NCSA, the T_1 emission energies calculated with PBE0 and CAM-B3LYP are lower than those reported for QDPT2. For BPyMCSA, the S_1 emission energies calculated with TDDFT are significantly larger than the QDPT2 value. For NCSA, PBE0 is in good agreement with QDPT2 for S_1, but underestimates the T_1 energy. Optimization of the S_1 state with CAM-B3LYP proved to be problematic.

The calculated 2PA spectra are listed in Table S9. The 2PA transition strengths and cross sections are reported for each final state. We note that the 2PA spectra are not consistent across the three levels of theory. The CAM-B3LYP values do show some correlation with the CC2 values; for example, a large 2PA cross-sections for $n = 4$ in BPCSA and for $n = 3$ and 4 in BMSCA. In Figure S2, the 2PA spectra are plotted based on the calculations with the PBE0 and CAM-B3LYP functionals. Not only is the CAMB3LYP spectrum blue-shifted compared to the PBE0 spectrum, but the first peak is the most intense with PBE0, while with CAMB3LYP, the second peak is

dominant. The calculated 2PA cross-section is sensitive to state-energies (Table S9), which can result in quite different 2PA spectra.

Table S6. Calculated 1PA for the four compounds. Both functionals were corrected with the D3 dispersion correction during optimization. The CC2 results are from this work, using the cc-pVDZ basis set. The transition energies are listed under "eV" (in eV), and the O.S. denotes oscillator strengths. D_{CT}[1] is in Å.

CC2		**PBE0**			**CAM-B3LYP**		
eV	O.S.	eV	O.S.	D_{CT}	eV	O.S.	D_{CT}
BPCSA							
3.86	1.63	3.48	1.34	0.92	3.85	1.39	0.58
4.62	0.02	4.28	0.04	2.68	4.85	0.01	0.80
4.67	0.01	4.47	0.01	2.36	4.89	0.01	1.40
4.91	0.07	4.49	0.00	10.22	5.01	0.09	1.54
5.02	0.00	4.52	0.01	2.34	5.25	0.00	1.11
BMCSA							
2.81	1.43	2.49	1.50	0.06	2.96	1.48	0.09
3.49	0.62	3.08	0.00	0.10	3.76	0.24	0.20
3.71	0.00	3.15	0.12	0.12	3.88	0.00	0.10
4.19	0.00	3.71	0.00	0.02	4.44	0.00	0.07
4.50	0.05	4.09	0.13	0.03	4.67	0.06	0.07
NCSA							
3.76	1.33	3.35	1.02	5.86	3.78	1.18	3.53
4.01	0.00	3.94	0.00	1.62	4.06	0.00	0.97
4.58	0.00	3.97	0.00	11.82	4.53	0.00	0.86
4.61	0.01	4.19	0.15	5.31	4.80	0.02	2.15
4.69	0.00	4.39	0.00	4.63	4.82	0.00	2.32
BPyMCSA							
2.37	3.17	2.20	2.47	0.02	2.47	2.73	0.02
2.99	0.00	2.51	0.00	1.30	3.24	0.00	1.12
3.10	0.01	2.55	0.00	0.96	3.27	0.01	0.92
3.13	0.00	2.67	0.00	0.19	3.43	0.00	0.05
3.38	0.00	3.13	0.00	0.01	3.61	0.00	0.01

Table S7. The effect of solvent on 1PA of BPCSA molecule in comparison to experiment. Measured values include absorption spectra in DMSO and excitation spectra dispersed in water and pure powder. Both functionals were corrected with the D3 dispersion correction during optimization. The standard CAM-B3LYP, with $\alpha = 0.19$ and $\beta = 0.46$, is denoted "CAM-B3LYP", while "mCAM-B3LYP" refers to the modified CAM-B3LYP with $\alpha = 0.19$ and $\beta = 0.19$.

CC2 (gas)		**PBE0 (gas)**			**CAM-B3LYP (gas)**		
eV	O.S.	eV	O.S.	D_{CT}	eV	O.S.	D_{CT}
3.86	1.63	3.48	1.34	0.92	3.85	1.39	0.58
4.62	0.02	4.28	0.04	2.68	4.85	0.01	0.80
4.67	0.01	4.47	0.01	2.36	4.89	0.01	1.40
4.91	0.07	4.49	0.00	10.22	5.01	0.09	1.54
5.02	0.00	4.52	0.01	2.34	5.25	0.00	1.11
eV (measured)		**PBE0 (DMSO)**			**CAM-B3LYP (DMSO)**		
		eV	O.S.	D_{CT}	eV	O.S.	D_{CT}
3.56	absorp. (DMSO)	3.32	1.45	0.69	3.70	1.48	0.67
3.28	excit. (water)	4.19	0.02	2.88	4.82	0.04	0.51
2.85	excit. (powder)	4.25	0.01	7.89	4.89	0.00	1.57
		4.45	0.02	2.58	4.91	0.11	0.88
		4.49	0.01	2.53	5.24	0.00	1.59
					mCAM-B3LYP (DMSO)		
					eV	O.S.	D_{CT}
					3.43	1.45	0.50
					4.42	0.03	3.21
					4.56	0.01	0.89
					4.57	0.01	1.36
					4.78	0.20	4.91

Table S8. Emission for molecules in gas-phase. Adiabatic transition energies corrected for zero-point vibrational energy (ΔH) as well as vertical transition energies evaluated at the optimized excited-state geometry. In some cases, the S_0 energy at the T_1 optimized geometry was higher than the T_1 energy, and thus the formal calculation of a vertical emission energy resulted in a negative value (in red, see parentheses). Measured emission energy for BPCSA is 2.76 and 2.65 eV in water and powder, respectively. [a)] DMSO

	QDPT2	**PBE0**	**CAM-B3LYP**
BPCSA			
$\Delta H(S_0 \rightarrow T_1)$	1.60	1.51	1.55 (1.54[a)])
$\Delta H(S_0 \rightarrow S_1)$	3.40	3.11	3.35
vert.$(T_1 \rightarrow S_0)$		(0.42)	(0.70)
vert.$(S_1 \rightarrow S_0)$		2.89	2.74
BMCSA			
$\Delta H(S_0 \rightarrow T_1)$	1.60	1.23	1.38
$\Delta H(S_0 \rightarrow S_1)$	2.70	2.30	2.63
vert.$(T_1 \rightarrow S_0)$		0.96	0.87
vert.$(S_1 \rightarrow S_0)$		2.24	2.46
NCSA			
$\Delta H(S_0 \rightarrow T_1)$	2.60	1.55	1.59
$\Delta H(S_0 \rightarrow S_1)$	3.00	3.11	
vert.$(T_1 \rightarrow S_0)$		(0.29)	(0.59)
vert.$(S_1 \rightarrow S_0)$		3.05	
BPyMCSA			
$\Delta H(S_0 \rightarrow T_1)$	0.86	0.50	0.36
$\Delta H(S_0 \rightarrow S_1)$	1.47	2.00	2.20
vert.$(T_1 \rightarrow S_0)$		0.31	(0.09)
vert.$(S_1 \rightarrow S_0)$		2.03	2.11

Table S9. Calculated two-photon absorption spectra. Both functionals were corrected with the D3 dispersion correction during optimization. The 2PA transition strengths (TPS-TS), and 2PA cross-sections, calculated using a Gaussian line-width function with a width of 0.2 eV, listed under the heading "GM".

CC2			**PBE0 (gas)**			**CAM-B3LYP (gas)**		
eV	2PA-TS	GM	eV	2PA-TS	GM	eV	2PA-TS	GM
BPCSA								
3.86	4600	37.06	3.48	125	0.82	3.85	530	4.25
4.62	1000	11.54	4.28	103367	1025.10	4.85	1561	19.85
4.67	2700	31.84	4.47	144	1.56	4.89	741	9.60
4.91	97900	1276.07	4.49	615	6.71	5.01	28630	388.93
5.02	100	1.36	4.52	2681	29.57	5.25	76	1.14
BMCSA								
2.81	50	0.21	2.49	11	0.04	2.96	13	0.06
3.49	50	0.33	3.08	370000	1895.00	3.76	18	0.14
3.71	491700	3659.12	3.15	28	0.15	3.88	170100	1383.05
4.19	264000	2505.88	3.71	16923	125.70	4.44	353667	3770.54
4.50	50	0.55	4.09	86	0.78	4.67	116	1.37
NCSA								
3.76	25600	195.68	3.35	25563	154.90	3.78	10517	81.06
4.01	50	0.43	3.94	2	0.02	4.06	7	0.07
4.58	50	0.57	3.97	842	7.18	4.53	1	0.01
4.61	300	3.45	4.19	30513	289.90	4.80	1898	23.65
4.69	1100	13.08	4.39	586	6.10	4.82	145	1.82
BPyMCSA								
2.37	0	0.00	2.20	3	0.01	2.47	0	0.00
2.99	858600	4150.13	2.51	37933	129.70	3.24	110567	627.00
3.10	0	0.00	2.55	468	1.64	3.27	1726	9.96
3.13	214200	1134.58	2.67	86533	334.80	3.43	368000	2343.00
3.38	2700	16.68	3.13	4873	25.75	3.61	131267	927.10

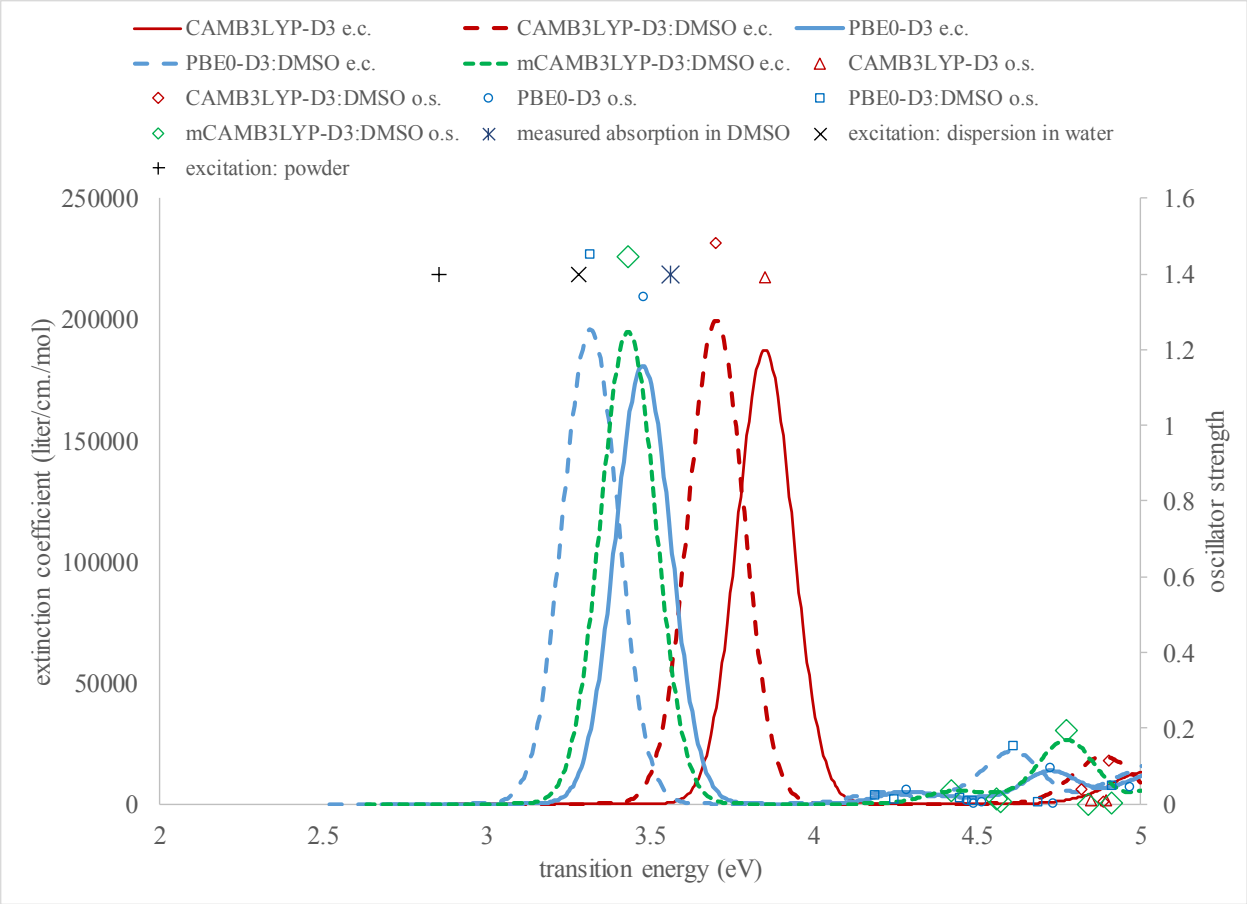

Figure S1. 1PA of BPCSA with several functionals with and without solvent effects, in comparison to experiment.

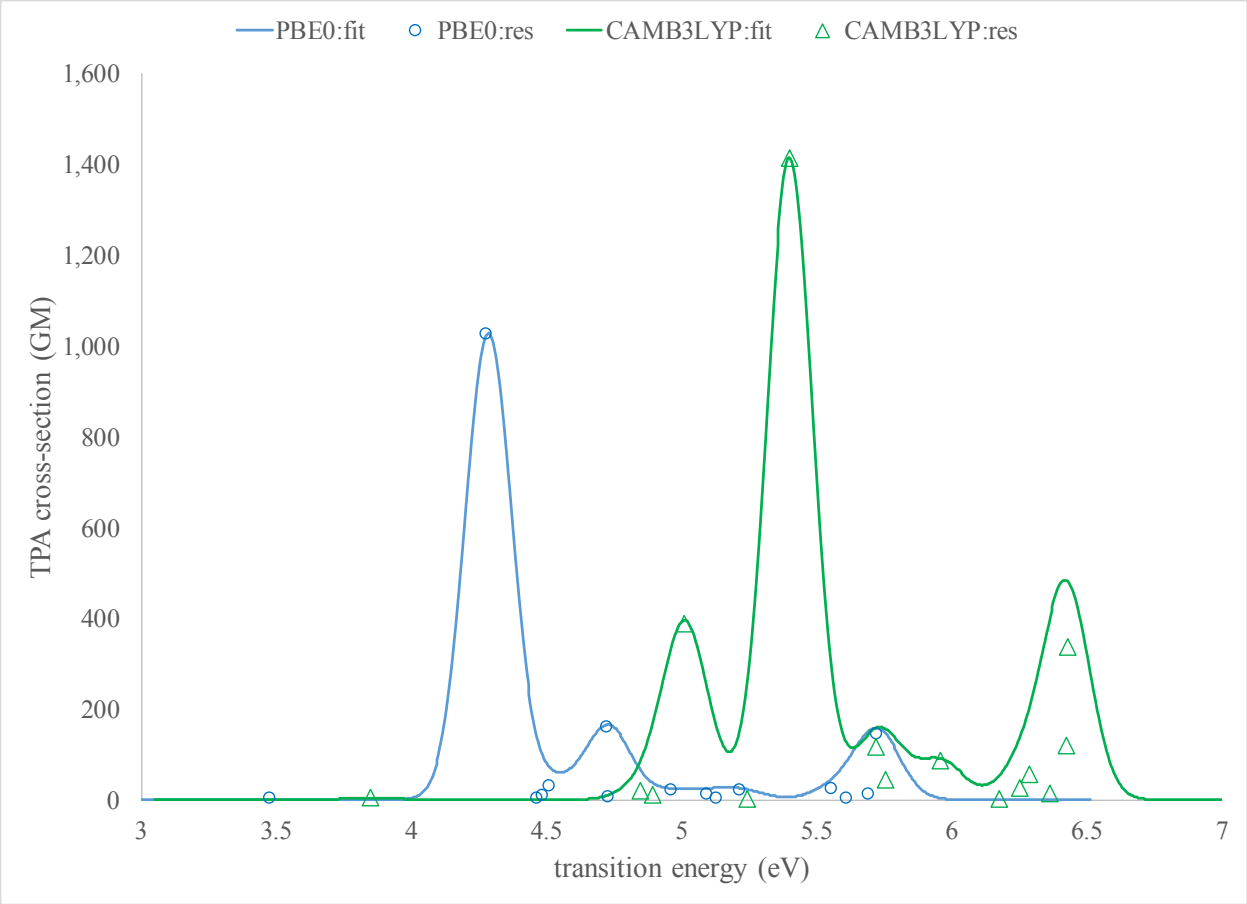

Figure S2. Calculated 2PA cross-section for BPCSA using quadratic response TDDFT and the two functionals indicated. The label "res" indicates the two-photon resonances, while "fit" indicates a fit to a Gaussian form with linewidth 0.2 eV.

BPCSA (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	6.3249585439	-0.4951189009	-0.0605218785
C	7.1629579657	0.0098477757	-1.0729976705
C	8.5116769500	-0.3455409286	-1.1333190200
C	9.0553595961	-1.2140144594	-0.1821240006
C	8.2363296957	-1.7234393899	0.8299354543
C	6.8874406338	-1.3684873516	0.8898107127
H	6.7456898814	0.6687919023	-1.8373448904
H	9.1397373257	0.0526939523	-1.9336883380
H	10.1106982897	-1.4916698418	-0.2289655508
H	8.6519217170	-2.3954986387	1.5844597428
H	6.2662066970	-1.7525735588	1.7016833696
C	4.8898526500	-0.1168283684	0.0014584954
C	4.4610598851	1.1844512919	-0.3164702726
C	3.1154370690	1.5401732196	-0.2573860072
C	2.1297678837	0.6063490867	0.1140921852
C	2.5593047829	-0.6915519200	0.4524333789
C	3.9045966145	-1.0439018670	0.3917491568
H	5.1967899264	1.9426918120	-0.5917925064
H	2.8226387726	2.5628027448	-0.5024458907
C	0.6928764453	0.9916931111	0.1468482133
H	1.8363702730	-1.4376905595	0.7867732897
H	4.1958592386	-2.0658824569	0.6426823411
C	-0.3206345004	0.0824762758	0.0226125426
C	0.4358088884	2.3969670102	0.2912523771
N	0.2686980554	3.5455578252	0.4030537176
C	-1.7707993427	0.2159877612	0.0482545747
C	-2.5280402101	-0.9507219307	-0.1878456800
C	-3.9217339920	-0.9509085397	-0.1899845513
C	-4.6108829448	0.2475435926	0.0534409593
C	-3.8760091916	1.4245655835	0.2956726700
C	-2.4909274882	1.4126847826	0.2938160634
H	-2.0047806504	-1.8916124526	-0.3775685786
H	-4.4556400415	-1.8811834757	-0.3796594933
O	-5.9605120822	0.3778549016	0.0792259688
H	-4.4281579004	2.3465001999	0.4853142362
H	-1.9628557075	2.3444855852	0.4864410365
H	0.0096001378	-0.9464854226	-0.1442638917
C	-6.7764549744	-0.7728010110	-0.1563460425
C	-8.2280751662	-0.3296695668	-0.0752728076
C	-9.2112536678	-1.4847593114	-0.2693791837
N	-10.5870247204	-0.9810438536	-0.2498257127
H	-11.2363699793	-1.7520101226	-0.4186412775
H	-10.8105770618	-0.6451746758	0.6908648575
H	-6.5476677474	-1.1957345618	-1.1525539025
H	-6.5538931468	-1.5486033512	0.6003115610
H	-8.4231258644	0.4432766738	-0.8358485810
H	-8.3948941543	0.1424671710	0.9094843095
H	-9.0390759137	-1.9495335071	-1.2569084158
H	-9.0017873357	-2.2744700638	0.4868847881

NCSA (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	-1.4467442207	1.3701463327	0.2102795192
C	-0.7891401935	0.1250916876	0.0347334958
C	-1.6043129054	-1.0160054331	-0.1285338043
C	-2.9950414587	-0.9468978369	-0.1261109649
C	-3.6222741166	0.2980876295	0.0473205839
C	-2.8283871506	1.4507642265	0.2161718392
C	0.6489728240	-0.0823033629	0.0132449518
C	1.7083594534	0.7821652992	0.0795471323
C	1.5246560345	2.2039364778	0.1432673510
N	1.4176498724	3.3639792221	0.1898054148
O	-4.9602195080	0.4965987339	0.0696196799
C	-5.8383823212	-0.6229803168	-0.0945727620
C	-7.2636901816	-0.0992605555	-0.0360206779
C	-8.3072698696	-1.2106045314	-0.1591834901
N	-9.6537228113	-0.6338175168	-0.1672713971
C	3.1213245094	0.3206190775	0.0550281777
C	4.1490569011	1.1996035510	-0.3460702238
C	5.4760573837	0.7820995384	-0.3982065078
C	5.7864292901	-0.5285953334	-0.0376552595
C	4.7992741329	-1.4214620545	0.3830127008
C	3.4777308273	-0.9917924112	0.4328848060
H	6.2734987590	1.4524942973	-0.7150131821
H	3.9019827331	2.2241425540	-0.6277452348
H	2.7181021007	-1.6834308358	0.7985254318
H	5.0841576845	-2.4302884737	0.6776047667
H	-1.1292049423	-1.9912574527	-0.2630305267
H	-3.5762473888	-1.8585044275	-0.2576143477
H	-3.3338134646	2.4081835245	0.3518259372
H	-0.8718691763	2.2842241862	0.3447473210
H	0.9248378677	-1.1345720852	-0.0956058027
H	-10.3439273244	-1.3762770783	-0.2967547004
H	-9.8578919737	-0.2369763825	0.7538195938
H	-5.6366191159	-1.1144492962	-1.0644565334
H	-5.6507958792	-1.3615394559	0.7070016244
H	-7.4222427337	0.6363760040	-0.8407269598
H	-7.3999135192	0.4381868457	0.9194458006
H	-8.1646778313	-1.7412738632	-1.1177501290
H	-8.1357680336	-1.9641622195	0.6421815331
N	7.1892521463	-0.9794028910	-0.0886938916
O	8.0322458367	-0.1687029146	-0.4563883494
O	7.4240266960	-2.1381282539	0.2382490854

BMCSA (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	-0.8098831147	-6.3860467612	0.4905229471
C	-0.0060847321	-5.3391825231	-0.0038841157
C	1.2377149678	-5.6968623959	-0.5643468680
C	1.6647433924	-7.0179512389	-0.6061229269
C	0.8609644585	-8.0569230105	-0.0926550492
C	-0.3898692214	-7.7112563600	0.4531240208
C	-0.4602002441	-3.9287797802	0.0687777833
C	-1.8695132344	-3.7527283220	0.2898982068
N	-3.0162452033	-3.6480536882	0.4761805439
N	1.2612736621	-9.3849214261	-0.1907367037
C	0.3898692214	-2.8594949864	-0.0420265060
C	0.1517472914	-1.4264077288	-0.0406694008
C	-1.1229136497	-0.8210103726	-0.0483197340
C	-1.2861284172	0.5609356012	-0.0442843659
C	-0.1517472914	1.4264077288	-0.0406694008
C	1.1229136497	0.8210103726	-0.0483197340
C	1.2861284172	-0.5609356012	-0.0442843659
C	-0.3898692214	2.8594949864	-0.0420265060
C	0.4602002441	3.9287797802	0.0687777833
C	1.8695132344	3.7527283220	0.2898982068
N	3.0162452033	3.6480536882	0.4761805439
O	-2.5108126608	1.1658547399	-0.0424010425
C	-3.6741993235	0.3474990446	-0.0605901911
O	2.5108126608	-1.1658547399	-0.0424010425
C	3.6741993235	-0.3474990446	-0.0605901911
C	0.0060847321	5.3391825231	-0.0038841157
C	-1.2377149678	5.6968623959	-0.5643468680
C	-1.6647433924	7.0179512389	-0.6061229269
C	-0.8609644585	8.0569230105	-0.0926550492
C	0.3898692214	7.7112563600	0.4531240208
C	0.8098831147	6.3860467612	0.4905229471
N	-1.2612736621	9.3849214261	-0.1907367037
H	-1.4453873521	3.1121902916	-0.1338152723
H	-1.8825821281	4.9308977776	-0.9978820132
H	-2.6303146336	7.2587023689	-1.0590327368
H	-2.2632774419	9.5352653285	-0.2518445037
H	-0.8230563040	10.0214866321	0.4673678420
H	1.0402286681	8.4947497353	0.8511043207
H	1.7847421885	6.1559842170	0.9245632988
H	-2.0011301267	-1.4567505860	-0.0581902782
H	2.0011301267	1.4567505860	-0.0581902782
H	1.4453873521	-3.1121902916	-0.1338152723
H	1.8825821281	-4.9308977776	-0.9978820132
H	2.6303146336	-7.2587023689	-1.0590327368
H	2.2632774419	-9.5352653285	-0.2518445037
H	0.8230563040	-10.0214866321	0.4673678420
H	-1.0402286681	-8.4947497353	0.8511043207
H	-1.7847421885	-6.1559842170	0.9245632988
H	4.5260747665	-1.0391973546	-0.0392572903
H	3.7239624075	0.2668687591	-0.9762761892
H	3.7190498809	0.3184642791	0.8178214872
H	-4.5260747665	1.0391973546	-0.0392572903
H	-3.7239624075	-0.2668687591	-0.9762761892
H	-3.7190498809	-0.3184642791	0.8178214872

BPyMCSA (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	-0.0025726741	2.8448615537	-0.3799601977
C	1.0353081191	3.8399431875	-0.3763400239
C	0.7685030655	5.2260787367	-0.3838499015
C	-0.5641255767	5.7899895944	-0.4051713605
C	-0.7727798651	7.1356073357	-0.4079555571
N	0.2604399963	8.0457977476	-0.4016754682
C	1.5509756209	7.5539218679	-0.3794333081
C	1.8183720194	6.2195912649	-0.3763439456
C	2.4225912313	3.4857778981	-0.3631024649
N	3.5678891247	3.2531080820	-0.3523265960
C	0.0025726741	9.4822083809	-0.3025831296
H	-1.0134194446	3.2458642016	-0.3803503812
H	-1.4416081113	5.1473530960	-0.4269434149
H	-1.7759940902	7.5629614318	-0.4255352505
C	-0.0373967590	9.9989214575	1.1396062220
H	2.3418685922	8.3042324454	-0.3730557501
H	2.8605262575	5.9009566797	-0.3715895355
C	-0.3384279793	11.4965881630	1.2205596353
N	-0.2615352307	11.9507481541	2.6102733326
H	-0.4086476229	12.9612172240	2.6508611294
H	-1.0345099822	11.5456152145	3.1448042028
H	0.7859417830	10.0057608613	-0.8745462468
H	-0.9522534754	9.6861575643	-0.8129134162
H	0.9258495434	9.8024214488	1.6390565802
H	-0.8038935589	9.4346029640	1.7018710211
H	0.4232704361	12.0513260619	0.6434029481
H	-1.3131569740	11.6994933327	0.7220111115
C	0.0446380810	1.4591949773	-0.3807732541
C	-1.2125820084	0.7129670550	-0.3813216383
C	-1.2435612806	-0.6528985199	-0.3814844323
C	-0.0446380810	-1.4591949773	-0.3807732541
C	1.2125820084	-0.7129670550	-0.3813216383
C	1.2435612806	0.6528985199	-0.3814844323
O	-2.3381669553	1.4916120716	-0.3816853207
H	-2.1993002716	-1.1645741734	-0.3820971195
C	0.0025726741	-2.8448615537	-0.3799601977
O	2.3381669553	-1.4916120716	-0.3816853207
H	2.1993002716	1.1645741734	-0.3820971195
C	-1.0353081191	-3.8399431875	-0.3763400239
C	-0.7685030655	-5.2260787367	-0.3838499015
C	0.5641255767	-5.7899895944	-0.4051713605
C	0.7727798651	-7.1356073357	-0.4079555571
N	-0.2604399963	-8.0457977476	-0.4016754682
C	-1.5509756209	-7.5539218679	-0.3794333081
C	-1.8183720194	-6.2195912649	-0.3763439456
C	-2.4225912313	-3.4857778981	-0.3631024649
N	-3.5678891247	-3.2531080820	-0.3523265960
C	-0.0025726741	-9.4822083809	-0.3025831296
H	1.0134194446	-3.2458642016	-0.3803503812
H	1.4416081113	-5.1473530960	-0.4269434149
H	1.7759940902	-7.5629614318	-0.4255352505
C	0.0373967590	-9.9989214575	1.1396062220
H	-2.3418685922	-8.3042324454	-0.3730557501
H	-2.8605262575	-5.9009566797	-0.3715895355
C	0.3384279793	-11.4965881630	1.2205596353
N	0.2615352307	-11.9507481541	2.6102733326

H	0.4086476229	-12.9612172240	2.6508611294
H	1.0345099822	-11.5456152145	3.1448042028
H	-0.7859417830	-10.0057608613	-0.8745462468
H	0.9522534754	-9.6861575643	-0.8129134162
H	-0.9258495434	-9.8024214488	1.6390565802
H	0.8038935589	-9.4346029640	1.7018710211
H	-0.4232704361	-12.0513260619	0.6434029481
H	1.3131569740	-11.6994933327	0.7220111115
C	3.6005437296	-0.8434075493	-0.3828191151
H	4.3521468382	-1.6442816178	-0.3818976488
H	3.7348851332	-0.2135768362	-1.2794859837
H	3.7353599268	-0.2108631726	0.5118262436
C	-3.6005437296	0.8434075493	-0.3828191151
H	-4.3521468382	1.6442816178	-0.3818976488
H	-3.7348851332	0.2135768362	-1.2794859837
H	-3.7353599268	0.2108631726	0.5118262436

BPCSA+ (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	2.4246535937	1.3476316098	-0.3531165465
C	1.7108216144	0.1548962313	-0.0800943264
C	2.4712014817	-1.0041055658	0.1752302525
C	3.8676973522	-0.9966357162	0.1747897633
C	4.5398613781	0.1994870262	-0.0924222858
C	3.8121618444	1.3672729163	-0.3584875385
C	0.2554112390	0.0191367001	-0.0452809545
C	-0.7491225481	0.9376014474	-0.1505741378
C	-0.4694276214	2.3421138658	-0.2790186139
N	-0.2686695581	3.4857217418	-0.3789929295
O	5.9136909059	0.3372930371	-0.1212615384
C	6.7110534867	-0.7892042663	0.1534460106
C	8.1546937920	-0.2868825651	0.0587339570
C	9.1663621892	-1.3886684082	0.3319851299
N	10.5819698609	-0.8379375715	0.2277570518
C	-2.1897406112	0.5741262533	-0.1155048523
C	-3.1573669491	1.5218707790	0.2676409784
C	-4.5073906517	1.1857722663	0.3312010120
C	-4.9567620917	-0.1069780755	0.0051907278
C	-3.9875739613	-1.0469642102	-0.3973874050
C	-2.6378646959	-0.7155368030	-0.4610895132
C	-6.3966187693	-0.4637964779	0.0708503974
C	-7.2221079655	0.0518491676	1.0880674627
C	-8.5754049678	-0.2841261085	1.1521484575
C	-9.1346189121	-1.1405579420	0.1990492993
C	-8.3278243825	-1.6590673265	-0.8182060932
C	-6.9737577449	-1.3257810573	-0.8809375115
H	-6.7931765509	0.7019780340	1.8534864093
H	-9.1950020536	0.1202440915	1.9556855732
H	-10.1938289603	-1.4018523134	0.2482914306
H	-8.7569968373	-2.3209797081	-1.5737413272
H	-6.3620811720	-1.7163903526	-1.6969441485
H	-5.2304146031	1.9523494655	0.6155245644
H	-2.8489583114	2.5383050785	0.5193461296
H	-1.9281811061	-1.4700749718	-0.8051536516
H	-4.2968036228	-2.0615027799	-0.6555631441
H	1.9541596907	-1.9435972448	0.3838682084
H	4.4018373245	-1.9243986374	0.3815963427
H	4.3558751457	2.2894567063	-0.5696690149
H	1.8939594329	2.2732001866	-0.5648727114
H	-0.0768753372	-1.0098126415	0.1134373458
H	11.2965697080	-1.5573183495	0.4072421722
H	10.7633291571	-0.4481975127	-0.7090036817
H	6.5042439946	-1.1933256519	1.1635444898
H	6.5313934314	-1.5999247457	-0.5793352145
H	8.2784403481	0.5374449697	0.7824002222
H	8.3060001089	0.1331044397	-0.9508438954
H	9.0792743314	-1.8068892814	1.3453358486
H	9.1085785778	-2.2118805179	-0.3948884810
H	10.7360113361	-0.0734942451	0.9017179672

NCSA+ (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	-3.5647694927	-0.9708109687	-0.4946522021
C	-3.1839635016	0.3152660537	-0.0600240244
C	-4.1837441762	1.1914332877	0.4070860517
C	-5.5163137992	0.7906573922	0.4702788993
C	-5.8522023132	-0.4955148128	0.0524914244
C	-4.8924131797	-1.3824142692	-0.4357367129
C	-1.7618383987	0.7532519984	-0.0916542687
C	-1.5525242950	2.1731460796	-0.1521092783
N	-1.4109165475	3.3289621638	-0.1962264865
N	-7.2649921692	-0.9296571534	0.1152606661
O	-7.5202311129	-2.0666726561	-0.2625414527
C	-0.7186048719	-0.1251058330	-0.0356838503
C	0.7282425859	0.0758759664	-0.0666763799
C	1.3859382719	1.3122599975	-0.2797912211
C	2.7706263203	1.3928769387	-0.2887037993
C	3.5501091091	0.2450722297	-0.0852788094
C	2.9325383592	-0.9922818049	0.1223802100
C	1.5382961592	-1.0612211809	0.1266268021
O	4.9133750109	0.4445101303	-0.1114073437
C	5.7653988353	-0.6579161200	0.0991288539
C	7.1835383554	-0.0849470920	0.0226154111
C	8.2469234001	-1.1522170336	0.2314847925
N	9.6353247485	-0.5336199710	0.1481076153
O	-8.0820717341	-0.1245441209	0.5426904123
H	-6.2968929956	1.4551118353	0.8376663523
H	-3.9143017457	2.1973011936	0.7326638880
H	-2.8230861602	-1.6524049378	-0.9129198179
H	-5.2025098717	-2.3700681865	-0.7734956937
H	1.0637727994	-2.0318730472	0.2881607841
H	3.5082551605	-1.9045856605	0.2795101015
H	3.2729455122	2.3472359467	-0.4537309035
H	0.8137879292	2.2231414618	-0.4417713075
H	-1.0046780192	-1.1742335361	0.0739361377
H	10.3822495972	-1.2291919815	0.2855635575
H	9.7925992848	-0.0880912635	-0.7679756610
H	5.5844756340	-1.1223697984	1.0876530376
H	5.6158310771	-1.4353562371	-0.6747834425
H	7.2756049240	0.7050596816	0.7880091249
H	7.3072603047	0.3938765746	-0.9642191405
H	8.1870144543	-1.6265303101	1.2218494519
H	8.2200789810	-1.9381279973	-0.5372746381
H	9.7616795662	0.2004991633	0.8605413073

BMCSA+ (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	6.3077682223	1.1952117665	-0.4341730435
C	5.3201277513	0.2820455599	-0.0090597975
C	5.7451738410	-0.9847755796	0.4499586695
C	7.0919260853	-1.3352376816	0.4675104955
C	8.0301303450	-0.4020428029	0.0271246825
C	7.6614027337	0.8609959658	-0.4216765617
C	3.8862647094	0.6703265744	-0.0417836102
C	3.6442787073	2.0718026005	-0.2312788923
N	3.4953565136	3.2166721196	-0.3912632599
N	9.4751067698	-0.7673109827	0.0517547131
C	2.8670617601	-0.2398960537	0.0670994931
C	1.4254311852	-0.0745626078	0.0683682023
C	0.6281486054	-1.2627879133	0.0731190251
C	-0.7615781678	-1.1700110353	0.0749858734
C	-1.4254298781	0.0745597514	0.0683680166
C	-0.6281472137	1.2627849975	0.0731271776
C	0.7615795649	1.1700080031	0.0749942043
C	-2.8670603525	0.2398941556	0.0670990523
C	-3.8862651433	-0.6703269978	-0.0417811018
C	-3.6442817924	-2.0718047013	-0.2312689152
N	-3.4953611863	-3.2166754005	-0.3912462421
O	1.2976156902	-2.4414659770	0.0720510709
C	0.5532102648	-3.6641544658	0.0825745561
O	-1.2976142456	2.4414631776	0.0720671230
C	-0.5532090583	3.6641517511	0.0826013764
C	-5.3201279101	-0.2820439290	-0.0090595738
C	-6.3077706036	-1.1952185346	-0.4341501327
C	-7.6614049563	-0.8610020725	-0.4216552179
C	-8.0301304508	0.4020461923	0.0271208229
C	-7.0919240745	1.3352500167	0.4674831423
C	-5.7451719889	0.9847872479	0.4499334188
N	-9.4751066110	0.7673152320	0.0517492449
H	3.1659134469	-1.2847454390	0.1455608876
H	5.0226697480	-1.7105104794	0.8214266657
H	7.3915661192	-2.3202020346	0.8336032821
H	9.6800060379	-1.5875582871	-0.5399629113
H	10.0593679415	0.0066206923	-0.2945056242
H	8.4018312971	1.5896072189	-0.7620559355
H	6.0165077625	2.1860235223	-0.7840346389
H	-1.3488073411	-2.0812962778	0.0829711491
H	1.3488087804	2.0812931239	0.0829867127
H	-3.1659102824	1.2847441478	0.1455588994
H	-5.0226666311	1.7105307469	0.8213820191
H	-7.3915622033	2.3202225402	0.8335555027
H	-9.6800065671	1.5875556676	-0.5399775960
H	-10.0593686824	-0.0066202196	-0.2945010696
H	-8.4018350543	-1.5896203636	-0.7620162260
H	-6.0165119430	-2.1860377625	-0.7839922677
H	-1.3011601509	4.4654674232	0.0656682740
H	0.0583116916	3.7498112326	0.9957451639
H	0.0947063887	3.7451401959	-0.8050801171
H	1.3011612146	-4.4654701379	0.0656362805
H	-0.0583121160	-3.7498210700	0.9957165671
H	-0.0947036471	-3.7451356344	-0.8051086927
H	-9.8045861011	0.9903739146	1.0040106261
H	9.8045879003	-0.9903583727	1.0040181405

BPyMCSA+ (geometry optimized at B3LYP/cc-pVDZ level of theory)

C	-6.2445087380	1.6649578256	-0.3432199155
C	-5.2311322203	0.6304150132	-0.3581215066
C	-5.7598008283	-0.7047238446	-0.5627103187
C	-7.0907675577	-0.9372913178	-0.6968608639
N	-8.0289862638	0.0861811491	-0.6665506305
C	-7.5650082363	1.3871039117	-0.4858195465
C	-3.8612973295	0.9164022168	-0.2080471095
C	-3.5442832966	2.3044522020	-0.0321942007
N	-3.3447499595	3.4448147506	0.1164685184
C	-9.4440487772	-0.1990495909	-0.6366171871
C	-9.9891412043	-0.3597195980	0.8081740681
C	-11.4871528275	-0.6286107941	0.8125603598
N	-12.0179087856	-0.7595827200	2.2354373971
C	-2.8408909148	-0.0933485153	-0.2108051467
C	-1.4559959581	0.0007388878	-0.1827399227
C	-0.6921365232	1.2236138081	-0.1776500867
C	0.6752287663	1.2366177824	-0.1771638020
C	1.4559963233	-0.0007370235	-0.1827392464
C	0.6921368513	-1.2236118819	-0.1776554409
C	-0.6752283482	-1.2366159567	-0.1771698092
C	2.8408910312	0.0933501181	-0.2108035264
C	3.8612966892	-0.9164010420	-0.2080493394
C	3.5442823335	-2.3044512389	-0.0322004269
N	3.3447489593	-3.4448141421	0.1164590880
O	1.4179113018	2.3788831570	-0.1765580285
C	0.7369334750	3.6289059083	-0.1954083907
O	-1.4179110955	-2.3788815271	-0.1765695989
C	-0.7369331098	-3.6289042202	-0.1954252948
C	5.2311314847	-0.6304141612	-0.3581234122
C	5.7598003520	0.7047248447	-0.5627090539
C	7.0907669756	0.9372922809	-0.6968594192
N	8.0289853113	-0.0861804760	-0.6665520539
C	7.5650069663	-1.3871034248	-0.4858241440
C	6.2445075209	-1.6649572117	-0.3432248533
C	9.4440478776	0.1990496623	-0.6366196583
C	9.9891422097	0.3597164034	0.8081712052
C	11.4871539388	0.6286070475	0.8125561475
N	12.0179117490	0.7595759147	2.2354327350
H	3.2096669458	1.1160824059	-0.2433517751
H	5.0930920903	1.5614041479	-0.6378182235
H	7.4888174603	1.9385818514	-0.8677365457
H	8.3258255214	-2.1685348611	-0.4981101354
H	5.9467064308	-2.7074440695	-0.2308993252
H	13.0329002040	0.9415146970	2.2586258578
H	11.5563857700	1.5303415515	2.7409059130
H	9.9820938868	-0.6173976295	-1.1457649399
H	9.6321931307	1.1198288853	-1.2111856579
H	9.7667073847	-0.5632398875	1.3719235903
H	9.4501806711	1.1873180194	1.3015387613
H	12.0635274067	-0.1875806379	0.3525358385
H	11.7504655867	1.5693089283	0.3069356116
H	-1.2312009339	2.1638325977	-0.1819448403
H	1.2312010821	-2.1638306345	-0.1819543750
H	-3.2096665172	-1.1160810723	-0.2433580173
H	-5.0930921908	-1.5614029096	-0.6378217267
H	-7.4888178307	-1.9385806978	-0.8677403346

H	-8.3258271090	2.1685352262	-0.4981034201
H	-5.9467078067	2.7074446304	-0.2308918855
H	-13.0328971348	-0.9415219414	2.2586314882
H	-11.5563818011	-1.5303492193	2.7409084319
H	-9.9820956860	0.6173986402	-1.1457601191
H	-9.6321943478	-1.1198277105	-1.2111849594
H	-9.7667059559	0.5632356435	1.3719281200
H	-9.4501787131	-1.1873221047	1.3015391847
H	-12.0635271950	0.1875776470	0.3525424257
H	-11.7504647929	-1.5693117912	0.3069382517
H	-1.5196668671	-4.3980993489	-0.1867515119
H	-0.1221893225	-3.7388023463	-1.1049491206
H	-0.0894758768	-3.7506126873	0.6893574486
H	1.5196672057	4.3981009418	-0.1867309460
H	0.1221899464	3.7388081408	-1.1049318747
H	0.0894759742	3.7506105230	0.6893746680
H	-11.8473865096	0.0979503869	2.7816324813
H	11.8473898963	-0.0979581917	2.7816263164

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