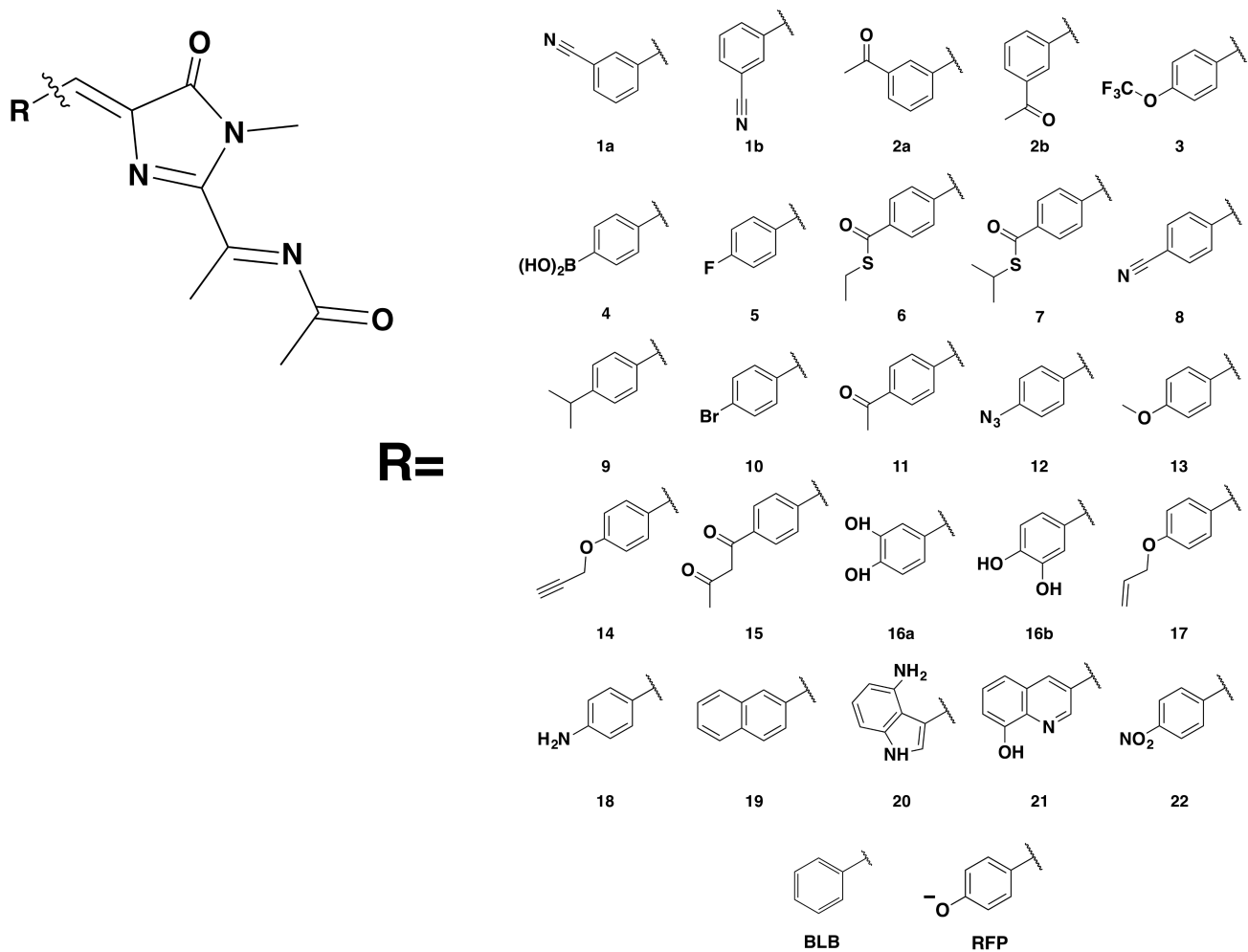


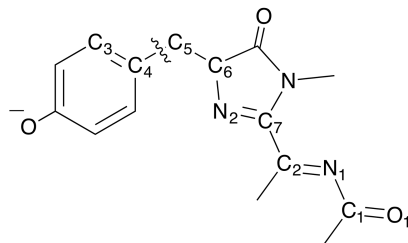
# Electronic Supplementary Information for “Prediction of two-photon absorption enhancement in red fluorescent protein chromophores made from non-canonical amino acids”

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**Fig. S1** Chromophore models built from the RFP-parent structure. RFP and BLB refer to the DsRed and mBlueberry chromophore models, respectively. The rest are built via the replacement of the phenol ring of Tyr-66 with the corresponding moiety in a non-canonical amino acid. The numbering matches the corresponding previously studies models.<sup>1</sup>

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Protein Name (PDB ID)	Tilt Angle (in degree) (C <sub>4</sub> - C <sub>5</sub> - C <sub>6</sub> - N <sub>2</sub> )	Twist Angle (in degree) (C <sub>3</sub> - C <sub>4</sub> - C <sub>5</sub> - C <sub>6</sub> )	$\theta_{\text{acylimine}}$ (in degree) (O <sub>1</sub> - C <sub>1</sub> - N <sub>1</sub> - C <sub>2</sub> )	$\theta_1$ (in degree) (C <sub>1</sub> - N <sub>1</sub> - C <sub>2</sub> - C <sub>7</sub> )	$\theta_2$ (in degree) (N <sub>1</sub> - C <sub>2</sub> - C <sub>7</sub> - N <sub>2</sub> )
FP583 (1GGX)	2	182	145.6	114.5	191.5
DsRED (1G7K)	0.03	181.8	176.4	91.3	183.5
K83M (2H8Q)	-3.4	186.9	181.4	104.6	164.8
Rtms5 H146S (2P4M)	-2	212.6	133.5	111.9	178.0
DsRED.M1(2VAD)	7.4	180	210.7	110.2	175.8
KillerRed (2W1Q)	27.9	168.2	37.5	204.1	229.8
mKeima(pH=8) (2WHU)	-19.4	217.4	121.2	139.1	180.8
mKeima(pH=3.8) (2WHS)	-1.3	179.4	144.4	116.4	180.2
MKEIMA(pH=7)-3IR8	1.3	173.2	168.6	108.2	173.1
KillerRed (3A8S)	28.4	156.4	30.2	181.6	252.5
KillerRed (3GB3)	24.8	164.3	45.2	197.1	222.5
Azami-Green (3ADF)	31	152.6	15.7	228.4	249.5
SuperNova (3WCK)	3.9	172.5	44.6	184.7	224.8
Favina Proteins Ancestor (4DXI)	2.6	178.7	349.6	240.8	253.0
eCGP123 (4TZG)	7.9	167.4	358.9	249.4	235.5
Blue Chromoprotein sgBP (4ZB1)	-10.2	220.6	52.7	199.9	218.4
mPlum (2QLG)	-3.2	185.8	3.5	222.1	256.1
mCHERRY (2H5Q)	26.2	164.3	119.7	140.4	179.1
TagBFP (3M24)	5.2	178.8	168.4	133.8	177.2
Neptune (3IP2)	27.9	168.2	37.5	284.3	229.8
EQFP650 (4EDO)	5.2	178.8	168.4	133.8	177.2
Average	7.7	179.5	129.2	166.5	206.3

**Table S1** Tilt, twist and acylimine ( $\theta_{\text{acylimine}}$ ) dihedral angles for red fluorescent chromophores in their native protein crystal structures. Also included are the two other dihedral angles ( $\theta_1$  and  $\theta_2$ ) defining the geometry of the extended conjugation chain.

**Table S2** Coordinates of the optimized models at the PBE0/6-31+G(d,p) level of theory in the gas phase. All chromophores are capped with methyl groups (see Figure S1) except where noted.

Coordinates for BLB Model			
C	-5.40977	0.15799	0.05968
C	-4.31665	0.97182	0.04862
C	-5.28268	-1.29241	0.04480
C	-3.91326	-1.79368	0.01531
C	-2.97609	0.46139	0.01704
C	-2.82982	-0.96666	0.00656
C	-1.91112	1.36417	0.00275
C	-0.52636	1.17007	-0.02172
C	1.44199	0.28769	-0.03840
C	0.41421	2.28938	-0.02118
C	2.46489	-0.73065	-0.05701
C	4.75710	-1.28481	-0.05084
C	1.98998	-2.15043	-0.21078
C	5.61207	-1.40930	1.19122
C	2.89133	2.40652	-0.06476
N	0.15647	-0.01265	-0.02929
N	1.65951	1.65890	-0.03568
N	3.70984	-0.40288	0.08555
H	-6.27139	-2.05291	0.06118
H	-6.41872	0.56307	0.06585
H	-4.44864	2.05380	0.04444
H	-3.79286	-2.87505	0.00942
H	-1.82169	-1.37362	-0.01024
H	-2.17809	2.42210	0.01818
H	1.05738	-2.29372	0.33679
H	1.78473	-2.36344	-1.26435
H	2.75272	-2.85485	0.12453
H	5.01525	-1.82646	2.01032
H	6.45912	-2.06780	0.98887
H	5.96338	-0.42665	1.51645
H	3.49391	2.23148	0.82853
H	3.48910	2.13282	-0.93934
H	2.60194	3.45933	-0.12559
O	0.24183	3.51189	-0.01863
O	5.03740	-1.85747	-1.09128
Coordinates for RFP model			
C	-5.40977	0.15799	0.05968
C	-4.31665	0.97182	0.04862
C	-5.28268	-1.29241	0.04480
C	-3.91326	-1.79368	0.01531
C	-2.97609	0.46139	0.01704
C	-2.82982	-0.96666	0.00656
C	-1.91112	1.36417	0.00275
C	-0.52636	1.17007	-0.02172
N	0.15647	-0.01265	-0.02929
C	1.44199	0.28769	-0.03840
C	0.41422	2.28938	-0.02118
N	1.65951	1.65890	-0.03568
O	-6.27139	-2.05291	0.06118
O	0.24183	3.51189	-0.01863
H	-6.41872	0.56307	0.06585
H	-4.44864	2.05380	0.04444
H	-3.79286	-2.87505	0.00942
H	-1.82169	-1.37362	-0.01024
H	-2.17809	2.42210	0.01818
C	2.46489	-0.73065	-0.05701
N	3.70984	-0.40288	0.08555
C	4.75710	-1.28481	-0.05084
O	5.03740	-1.85747	-1.09128
C	1.98998	-2.15043	-0.21078

H	1.05738	-2.29372	0.33679
H	1.78473	-2.36344	-1.26435
Coordinates for RFP model with H-capping			
C	4.72554	0.26170	0.06860
C	3.60206	1.03307	0.08040
C	4.65429	-1.19095	-0.00045
C	3.30520	-1.74290	-0.05274
C	2.28205	0.47291	0.03084
C	2.19095	-0.95790	-0.04215
C	1.18311	1.33387	0.05182
C	-0.19303	1.08811	0.01061
C	-2.12492	0.13468	-0.09900
C	-1.17559	2.17051	0.03351
C	-3.10755	-0.91989	-0.17647
C	-5.37470	-1.55642	-0.30392
N	-0.82930	-0.11739	-0.07329
N	-2.39517	1.49501	-0.03583
N	-4.35801	-0.63049	-0.35040
H	5.71755	0.70318	0.12460
H	3.69175	2.11723	0.14864
H	3.22668	-2.82659	-0.11044
H	1.19945	-1.40181	-0.08760
H	1.40926	2.40008	0.10455
H	-2.72537	-1.94774	-0.10702
H	-5.96769	-1.62015	-1.25026
H	-3.27727	1.98448	-0.02137
O	5.67166	-1.91263	-0.01882
O	-1.05076	3.39675	0.10428
O	-5.67160	-2.19616	0.69188
Coordinates for Model Number 1a			
C	-3.39536	-2.24899	0.00832
C	-2.38476	-1.29604	0.00383
C	-2.69784	0.07763	0.01984
C	-1.69458	1.12506	0.01365
C	-4.04789	0.45939	0.03967
C	-5.05922	-0.50410	0.04348
C	-4.73367	-1.86726	0.02798
C	0.54156	2.21786	-0.02553
C	1.67851	0.29258	-0.05799
C	-0.34308	1.02125	-0.00984
C	3.01021	2.49545	-0.12976
C	-6.43229	-0.09646	0.06307
C	2.79654	-0.67344	-0.08351
C	5.12373	-1.02576	-0.02268
C	2.41615	-2.11169	-0.27472
C	5.90687	-1.12135	1.25818
N	1.82478	1.66619	-0.05440
N	0.44018	-0.12246	-0.03291
N	-7.54670	0.23112	0.07907
N	3.98215	-0.22171	0.06579
H	-1.34210	-1.59223	-0.01399
H	-4.31192	1.51275	0.05140
H	-2.06392	2.14989	0.02544
H	-5.52553	-2.60920	0.03069
H	-3.14042	-3.30428	-0.00475
H	2.00870	-2.25115	-1.28109
H	3.27967	-2.76704	-0.15972
H	1.62689	-2.38803	0.42822
H	5.27581	-1.50218	2.06812
H	6.76558	-1.77696	1.11039
H	6.24813	-0.12530	1.55754
H	3.63104	2.37615	0.75953
H	2.65294	3.52534	-0.19963
H	3.60407	2.24485	-1.01029

O	0.27342	3.40375	-0.02222
O	5.48338	-1.51150	-1.07628
Coordinates for Model Number 1b			
C	3.96281	1.34801	0.01766
C	2.81669	0.55193	-0.00328
C	2.93512	-0.84748	0.03093
C	1.79153	-1.73899	0.01684
C	4.22180	-1.41385	0.08487
C	5.35946	-0.61522	0.10469
C	5.24045	0.76903	0.07156
C	-0.57814	-2.49865	-0.02334
C	-1.42468	-0.42990	-0.08356
C	0.46984	-1.44205	-0.02393
C	-3.06143	-2.41890	-0.09436
C	3.83063	2.77479	-0.01394
C	-2.39191	0.68730	-0.11730
C	-4.65147	1.35995	-0.03735
C	-1.81032	2.05578	-0.31145
C	-5.36869	1.59240	1.26469
N	-1.76769	-1.76813	-0.05878
N	-0.13954	-0.19779	-0.06707
N	3.72564	3.93148	-0.03766
N	-3.62853	0.40934	0.03938
H	1.83237	1.00414	-0.04439
H	4.32153	-2.49577	0.11202
H	6.34326	-1.07210	0.14603
H	2.00822	-2.80599	0.04539
H	6.11964	1.40487	0.08712
H	-1.26766	2.09711	-1.26012
H	-2.59110	2.81608	-0.32045
H	-1.08072	2.26835	0.47459
H	-4.65851	1.85103	2.05717
H	-6.10187	2.38941	1.13817
H	-5.87450	0.67159	1.57330
H	-3.63244	-2.10607	-0.97010
H	-3.63868	-2.18971	0.80265
H	-2.85809	-3.49104	-0.14331
O	-0.48445	-3.71096	-0.00087
O	-4.98176	1.86052	-1.09336
Coordinates for Model Number 2a			
C	-4.64457	-0.44420	0.02937
C	-3.61598	0.49966	0.03303
C	-2.26877	0.11193	0.02470
C	-1.25696	1.15034	0.02193
C	-1.96407	-1.26548	0.01366
C	-2.98353	-2.20649	0.01121
C	-4.31921	-1.80520	0.01841
C	0.99099	2.22340	-0.01475
C	2.10962	0.28583	-0.03569
C	0.09510	1.03721	0.00629
C	3.46230	2.47552	-0.11688
C	-6.05816	0.04979	0.03611
C	-7.18109	-0.95800	0.02106
C	3.21495	-0.69300	-0.05970
C	5.53806	-1.07511	-0.06113
C	2.81287	-2.13221	-0.19433
C	6.36038	-1.14699	1.19684
N	2.26925	1.65844	-0.04135
N	0.86716	-0.11485	-0.00725
N	4.41105	-0.25440	0.04031
H	-3.88768	1.55192	0.04096
H	-0.92408	-1.57139	0.00465
H	-5.10135	-2.55823	0.01491
H	-7.12543	-1.59318	-0.86971

H	-7.13057	-1.61352	0.89732
H	-8.13080	-0.42267	0.02478
H	-2.73916	-3.26471	0.00201
H	2.03590	-2.37512	0.53400
H	2.38211	-2.30006	-1.18634
H	3.67117	-2.79382	-0.07588
H	5.75479	-1.51838	2.03033
H	7.21644	-1.80234	1.03362
H	6.70543	-0.14529	1.47124
H	-1.62089	2.17718	0.02703
H	4.08774	2.34250	0.76740
H	3.11477	3.50953	-0.17549
H	4.04877	2.22701	-1.00306
O	0.73763	3.41323	-0.01649
O	-6.29347	1.24506	0.05287
O	5.86015	-1.59514	-1.11098
Coordinates for Model Number 2b			
C	-4.99835	1.31226	0.09638
C	-3.79492	2.00518	0.08603
C	-2.56456	1.32074	0.05636
C	-1.34359	2.10372	0.04179
C	-2.58097	-0.08329	0.04246
C	-3.78700	-0.78360	0.05338
C	-4.99877	-0.08062	0.07804
C	1.09435	2.62753	-0.01479
C	1.72382	0.48214	-0.09169
C	-0.05550	1.68346	-0.00875
C	3.55570	2.28973	-0.13345
C	-3.72859	-2.28150	0.03625
C	-5.02073	-3.05969	-0.01742
C	2.57136	-0.72728	-0.13952
C	4.74083	-1.63666	-0.00423
C	1.86253	-2.01511	-0.43191
C	5.35363	-2.01689	1.31674
N	2.20259	1.77915	-0.06364
N	0.42339	0.38424	-0.06362
N	3.82262	-0.58640	0.07689
H	-5.93790	1.85611	0.11832
H	-3.79673	3.09237	0.09914
H	-1.65090	-0.63982	0.02044
H	-1.46151	3.18636	0.07275
H	-5.94471	-0.61330	0.08580
H	-5.60042	-2.79182	-0.90735
H	-5.64456	-2.84586	0.85745
H	-4.78748	-4.12438	-0.04229
H	1.51917	-2.01259	-1.47163
H	2.52373	-2.87079	-0.29213
H	0.96943	-2.11120	0.18974
H	4.57465	-2.26711	2.04433
H	6.02586	-2.86369	1.17569
H	5.91062	-1.16579	1.72146
H	4.07998	1.88521	-1.00075
H	4.11860	2.03646	0.76663
H	3.46539	3.37478	-0.22195
O	1.12774	3.84387	0.00971
O	-2.65546	-2.85773	0.06060
O	5.07677	-2.11402	-1.06969
Coordinates for Model Number 3			
C	-2.78881	-0.72597	-0.58073
C	-1.56040	-0.10071	-0.42703
C	-1.48609	1.29319	-0.23526
C	-0.23980	2.01209	-0.07092
C	-2.68321	2.03217	-0.20614
C	-3.91651	1.41345	-0.35689

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C	-3.95210	0.03641	-0.53577
C	2.20032	2.45019	0.13579
C	2.78621	0.30255	-0.08088
C	1.03408	1.54668	-0.04853
C	4.65312	2.05038	0.21692
C	-5.83575	-1.09221	0.29766
C	3.60899	-0.92146	-0.16139
C	5.74686	-1.89498	0.02720
C	2.89082	-2.17030	-0.57745
C	6.33898	-2.32785	1.34091
N	3.28921	1.57575	0.10710
N	1.48518	0.24201	-0.17854
N	4.84855	-0.82924	0.13462
H	-2.85798	-1.79700	-0.73839
H	-0.64313	-0.67782	-0.45884
H	-2.64032	3.10889	-0.06537
H	-4.84105	1.98038	-0.34007
H	-0.31840	3.09114	0.05707
H	1.97897	-2.29423	0.01134
H	2.58274	-2.08082	-1.62424
H	3.53285	-3.04617	-0.48265
H	5.54945	-2.56763	2.06041
H	6.98327	-3.19300	1.18244
H	6.92345	-1.50601	1.76695
H	5.13128	1.66144	1.11701
H	4.59052	3.13985	0.26705
H	5.24198	1.75004	-0.65165
O	2.25950	3.65725	0.27739
O	-5.18039	-0.58468	-0.76626
O	6.08337	-2.34564	-1.04972
F	-6.17038	-0.15066	1.19547
F	-5.11830	-2.01848	0.95478
F	-6.94999	-1.66157	-0.14824

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Coordinates for Model Number 4

C	-3.40483	-1.09461	-0.00796
C	-2.20535	-0.39886	-0.01843
C	-2.20298	1.00968	0.01897
C	-0.99879	1.81291	0.01297
C	-3.43981	1.67890	0.06604
C	-4.63131	0.96853	0.07540
C	-4.64466	-0.43357	0.03860
C	1.41230	2.42239	-0.01945
C	2.13256	0.30602	-0.08302
C	0.30354	1.43241	-0.02373
C	3.88553	2.19365	-0.09625
C	3.03190	-0.86445	-0.11972
C	5.24075	-1.67889	-0.02186
C	2.37496	-2.19119	-0.35847
C	5.92978	-1.97551	1.28274
N	2.55605	1.62189	-0.05480
N	0.83581	0.15323	-0.06793
N	4.28116	-0.66644	0.06092
H	-3.39601	-2.18059	-0.03721
H	-1.25784	-0.92453	-0.05625
H	-3.45381	2.76571	0.09599
H	-5.56159	1.53362	0.11448
H	-1.14177	2.89283	0.04250
H	-7.25382	0.23509	0.07351
H	-6.74280	-3.05228	0.03475
H	1.50999	-2.30633	0.29852
H	1.99957	-2.23255	-1.38611
H	3.07853	-3.01191	-0.21712
H	5.19643	-2.22790	2.05595
H	6.63219	-2.79803	1.14537
H	6.46504	-1.08468	1.62657

H	4.44943	1.94282	0.80389
H	3.74518	3.27531	-0.15782
H	4.43809	1.83794	-0.96767
O	1.39343	3.63931	0.00416
O	-7.22999	-0.72445	0.06844
O	-5.87730	-2.63045	0.03046
O	5.54771	-2.18809	-1.08148
B	-5.97283	-1.26971	0.04676
Coordinates for Model Number 5			
C	3.41705	-0.98794	-0.01261
C	2.15538	-0.41733	-0.08848
C	2.00652	0.98162	-0.01604
C	0.72533	1.65212	-0.07920
C	3.16132	1.77311	0.13490
C	4.41863	1.19055	0.20777
C	4.57210	-0.20190	0.13603
C	-1.73119	1.99533	-0.26273
C	-2.19776	-0.18123	-0.49263
C	-0.51964	1.13787	-0.24658
C	-4.14528	1.48583	-0.55626
C	-2.93190	-1.46501	-0.67154
C	-4.58537	-1.10906	0.99740
C	-2.29044	-2.42405	-1.62250
C	-6.08698	-1.03324	0.92449
N	-2.77019	1.07222	-0.41401
N	-0.89678	-0.18694	-0.42684
N	-4.01014	-1.79929	-0.07330
H	3.51869	-2.06844	-0.06565
H	1.27141	-1.03516	-0.19790
H	3.05821	2.85399	0.19503
H	5.29889	1.81656	0.32425
H	0.74288	2.73669	0.02554
H	7.93103	-0.46526	0.42108
H	6.93863	-2.61291	0.21218
H	-1.23120	-2.52880	-1.36987
H	-2.79943	-3.38709	-1.57593
H	-2.33166	-2.03292	-2.64577
H	-6.45774	-0.30663	1.64829
H	-6.42890	-0.78809	-0.08498
H	-6.49364	-2.02026	1.17024
H	-4.65933	0.86637	-1.29511
H	-4.13367	2.52353	-0.89769
H	-4.67265	1.44209	0.40058
O	-1.86697	3.20297	-0.19206
O	7.07292	-0.03751	0.36495
O	6.06020	-2.22860	0.15671
O	-3.94127	-0.73492	1.95918
B	5.98675	-0.86170	0.22446
Coordinates for Model Number 6			
C	-2.53351	-0.16433	0.03024
C	-1.19615	0.19421	0.08198
C	-0.81888	1.54848	-0.00822
C	0.55646	1.99760	0.04050
C	-1.82825	2.51888	-0.15773
C	-3.16440	2.15745	-0.20804
C	-3.53019	0.80996	-0.11170
C	3.03333	1.93407	0.22510
C	3.13715	-0.28428	0.48810
C	1.69647	1.28442	0.21575
C	5.33010	1.04192	0.54399
C	-4.98411	0.48718	-0.16779
C	-7.22062	-1.09423	-0.12343
C	-7.85029	-2.47390	-0.01855
C	3.66471	-1.66344	0.69397



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C	5.31481	-1.59201	-1.01070
C	2.90214	-2.48498	1.68257
C	6.81180	-1.73648	-0.96898
N	3.90642	0.85678	0.39659
N	1.85206	-0.08149	0.41518
N	4.66637	-2.17161	0.08612
H	-2.80121	-1.21486	0.09734
H	-0.42663	-0.56171	0.18811
H	-1.55009	3.56696	-0.23333
H	-3.94553	2.90223	-0.32178
H	0.72044	3.06823	-0.07817
H	-7.57168	-0.42831	0.66910
H	-7.44477	-0.61586	-1.08013
H	-7.49865	-3.13920	-0.81284
H	-7.63041	-2.94519	0.94420
H	-8.93752	-2.38679	-0.10921
H	1.83832	-2.45991	1.42761
H	3.27651	-3.50884	1.67958
H	2.99350	-2.05856	2.68806
H	7.06541	-2.77789	-1.19465
H	7.26759	-1.08916	-1.71891
H	7.20903	-1.51986	0.02679
H	5.73621	0.33020	1.26606
H	5.48723	2.05942	0.90926
H	5.84485	0.93692	-0.41504
O	3.36354	3.10133	0.13717
O	-5.83686	1.33855	-0.32701
O	4.70918	-1.14427	-1.96555
S	-5.41370	-1.23272	0.02012

Coordinates for Model Number 7

C	-2.25135	-0.05028	-0.05208
C	-0.93671	0.38749	-0.04951
C	-0.64571	1.76608	-0.02152
C	0.69835	2.30314	-0.01653
C	-1.71871	2.67778	0.00365
C	-3.03144	2.23747	0.00121
C	-3.31114	0.86611	-0.02787
C	3.18388	2.39836	-0.02692
C	3.44903	0.17858	-0.06615
C	1.89292	1.65963	-0.03388
C	5.55635	1.66024	-0.08711
C	-4.74601	0.45921	-0.03127
C	-6.89080	-1.29366	-0.09431
C	-7.39584	-1.18545	1.33740
C	-7.38043	-2.55459	-0.79589
C	4.08686	-1.15340	-0.08322
C	6.08542	-2.39966	0.01984
C	3.16789	-2.32000	-0.29012
C	6.74434	-2.78834	1.31541
N	4.13658	1.37736	-0.04566
N	2.14813	0.29798	-0.06154
N	5.35127	-1.21242	0.09057
H	-2.45306	-1.11753	-0.07029
H	-0.11864	-0.32347	-0.06880
H	-1.50761	3.74394	0.02498
H	-3.86039	2.93764	0.02106
H	0.78140	3.38928	0.00351
H	-7.19168	-0.40297	-0.65522
H	-7.06133	-2.03805	1.93753
H	-7.04893	-0.26372	1.81069
H	-8.49223	-1.17511	1.33965
H	-7.02930	-2.60564	-1.83035
H	-7.04732	-3.45846	-0.27403
H	-8.47564	-2.56227	-0.80469
H	2.72324	-2.26365	-1.28864

H	3.70511	-3.26462	-0.20374
H	2.34256	-2.27946	0.42496
H	6.00802	-2.84581	2.12362
H	7.24837	-3.74737	1.19340
H	7.47359	-2.02237	1.59855
H	6.05674	1.28701	0.80766
H	5.64435	2.74780	-0.13969
H	6.01924	1.20519	-0.96458
O	3.41749	3.59224	-0.01323
O	-5.64845	1.27117	0.03652
O	6.25111	-2.99107	-1.02853
S	-5.05956	-1.29154	-0.15704
Coordinates for Model Number 8			
C	-3.72742	-1.43414	-0.02592
C	-2.58476	-0.65225	-0.03692
C	-2.67939	0.75271	0.01418
C	-1.52672	1.62953	0.00900
C	-3.95731	1.34027	0.07520
C	-5.10461	0.56393	0.08739
C	-4.99419	-0.83230	0.03708
C	0.84785	2.37110	-0.02036
C	1.68285	0.29867	-0.08382
C	-0.20656	1.32040	-0.02798
C	3.33114	2.27800	-0.08429
C	-6.17154	-1.64452	0.05049
C	2.64323	-0.82395	-0.11602
C	4.89701	-1.51427	-0.03665
C	2.05271	-2.18913	-0.30869
C	5.62715	-1.73639	1.25984
N	2.03375	1.63414	-0.05427
N	0.39580	0.07340	-0.07256
N	-7.12733	-2.30558	0.06219
N	3.88186	-0.55513	0.04054
H	-3.65251	-2.51602	-0.06598
H	-1.60386	-1.11126	-0.08409
H	-4.04247	2.42277	0.11477
H	-6.08534	1.02558	0.13482
H	-1.73101	2.69898	0.04176
H	1.32155	-2.39407	0.47791
H	1.51110	-2.22674	-1.25813
H	2.82879	-2.95428	-0.31650
H	4.92413	-1.97817	2.06394
H	6.35185	-2.54144	1.13543
H	6.14451	-0.81622	1.55048
H	3.90503	2.04275	0.81336
H	3.13361	3.35137	-0.12984
H	3.90250	1.96548	-0.95994
O	0.76082	3.58361	0.00547
O	5.21115	-2.03051	-1.09019
Coordinates for Model Number 9			
C	-3.27777	-1.21481	-0.06882
C	-2.09569	-0.48861	-0.07750
C	-2.12625	0.91757	-0.02110
C	-0.94250	1.74632	-0.02360
C	-3.38330	1.54910	0.04302
C	-4.55787	0.81228	0.05365
C	-4.52863	-0.58745	-0.00255
C	1.45689	2.40532	-0.04345
C	2.22061	0.30246	-0.09612
C	0.36988	1.39534	-0.05486
C	3.93493	2.22385	-0.09815
C	-5.80101	-1.40568	0.01736
C	-6.72511	-1.06077	-1.15467
C	-6.53579	-1.26690	1.35552

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C	3.14194	-0.84956	-0.11778
C	5.36025	-1.62808	0.01825
C	2.51616	-2.18866	-0.37292
C	6.04595	-1.90222	1.32981
N	2.61684	1.62688	-0.06662
N	0.92671	0.12604	-0.09299
N	4.38474	-0.63093	0.08645
H	-1.13656	-0.99158	-0.12882
H	-3.42698	2.63481	0.08690
H	-1.10897	2.82294	0.00714
H	-5.51025	1.33339	0.10695
H	-5.50580	-2.45792	-0.09121
H	-6.20829	-1.16465	-2.11369
H	-7.59586	-1.72479	-1.16037
H	-7.09345	-0.03148	-1.08219
H	-5.88644	-1.53262	2.19548
H	-6.88209	-0.23915	1.51170
H	-7.41287	-1.92240	1.37959
H	-3.23498	-2.30078	-0.11540
H	1.61192	-2.30346	0.22820
H	2.21236	-2.25267	-1.42310
H	3.21889	-2.99844	-0.17321
H	5.31143	-2.15075	2.10307
H	6.75648	-2.71992	1.20622
H	6.57162	-1.00220	1.66425
H	4.50208	1.87670	-0.96378
H	4.49598	1.98615	0.80732
H	3.77433	3.30244	-0.16418
O	1.41621	3.62271	-0.02305
O	5.68286	-2.14374	-1.03402

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Coordinates for Model Number 10

C	-3.02655	-0.94193	-0.01198
C	-1.81556	-0.26551	-0.01829
C	-1.77777	1.14227	0.02083
C	-0.55244	1.91084	0.01689
C	-2.99830	1.84054	0.06552
C	-4.21543	1.17356	0.07233
C	-4.21915	-0.21900	0.03352
C	1.87709	2.44398	-0.01818
C	2.52929	0.30526	-0.08040
C	0.73766	1.49059	-0.01883
C	4.34158	2.13470	-0.10732
C	3.39062	-0.89337	-0.11566
C	5.57675	-1.77345	-0.03083
C	2.68848	-2.20122	-0.33067
C	6.26338	-2.08150	1.27237
N	2.99447	1.60641	-0.05616
N	1.22798	0.19451	-0.06172
N	4.64714	-0.73338	0.05039
H	-3.04996	-2.02604	-0.04305
H	-0.88261	-0.81707	-0.05498
H	-2.98886	2.92716	0.09557
H	-5.14862	1.72514	0.10753
H	-0.66368	2.99435	0.04596
H	1.87117	-2.30859	0.38674
H	2.23688	-2.21465	-1.32738
H	3.38162	-3.03890	-0.25180
H	5.52668	-2.33008	2.04386
H	6.95648	-2.91138	1.13206
H	6.80738	-1.19792	1.62095
H	4.90048	1.87570	0.79376
H	4.23639	3.21969	-0.17963
H	4.87883	1.75144	-0.97634
O	1.89915	3.66082	0.00404
O	5.86305	-2.29778	-1.08882

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BR	-5.86775	-1.14565	0.04214
Coordinates for Model Number 11			
C	-3.41353	-1.10410	-0.01126
C	-2.21928	-0.39868	-0.01668
C	-2.22733	1.00925	0.01322
C	-1.02520	1.81597	0.01149
C	-3.46961	1.67371	0.04764
C	-4.65814	0.96450	0.05203
C	-4.64515	-0.43557	0.02291
C	1.38629	2.42634	-0.01432
C	2.10731	0.31104	-0.07956
C	0.27707	1.43549	-0.02136
C	3.85996	2.19898	-0.08705
C	-5.95592	-1.15644	0.02987
C	-5.95995	-2.66511	0.00074
C	3.00554	-0.86069	-0.11643
C	5.21943	-1.67196	-0.04315
C	2.34257	-2.19206	-0.31142
C	5.92575	-1.94831	1.25644
N	2.53065	1.62601	-0.04949
N	0.81021	0.15691	-0.06615
N	4.25764	-0.66088	0.03776
H	-3.38203	-2.18923	-0.03485
H	-1.26834	-0.91843	-0.04443
H	-3.48752	2.76043	0.07102
H	-5.61829	1.47027	0.07808
H	-1.17074	2.89537	0.04025
H	-5.42639	-3.07624	0.86471
H	-6.99326	-3.01280	0.01569
H	-5.46417	-3.04139	-0.90087
H	1.61004	-2.36376	0.48184
H	1.78992	-2.19538	-1.25514
H	3.07847	-2.99599	-0.33173
H	5.20356	-2.19513	2.04184
H	6.63036	-2.76911	1.12030
H	6.46098	-1.05091	1.58252
H	4.42470	1.94035	0.81027
H	3.71877	3.28098	-0.13847
H	4.41173	1.85170	-0.96220
O	1.36630	3.64241	0.01114
O	-7.00168	-0.53083	0.05849
O	5.51396	-2.19432	-1.09968
Coordinates for Model Number 12			
C	-3.55823	-0.91678	0.00984
C	-2.35054	-0.24070	-0.00255
C	-2.31023	1.16826	0.03134
C	-1.08600	1.93244	0.02019
C	-3.53443	1.86432	0.07721
C	-4.74593	1.19641	0.08981
C	-4.76402	-0.20188	0.05627
C	1.34605	2.45793	-0.02623
C	1.99196	0.31635	-0.08001
C	0.20481	1.50919	-0.01804
C	3.80933	2.13941	-0.12416
C	2.84905	-0.88441	-0.11268
C	5.03000	-1.77427	-0.02993
C	2.14459	-2.19072	-0.33036
C	5.72321	-2.08236	1.26991
N	2.46078	1.61620	-0.06391
N	0.68985	0.21145	-0.05599
N	-6.09298	-2.03637	0.04296
N	-6.03319	-0.80581	0.07188
N	-6.28925	-3.15412	0.02023
N	4.10662	-0.72936	0.05366

H	-3.56536	-2.00345	-0.01759
H	-1.41711	-0.79132	-0.04027
H	-3.52540	2.95091	0.10323
H	-5.68685	1.73558	0.12512
H	-1.19429	3.01645	0.04476
H	1.28664	-2.27065	0.34082
H	1.75375	-2.22857	-1.35223
H	2.82238	-3.03323	-0.19083
H	4.98997	-2.32868	2.04546
H	6.41371	-2.91397	1.12703
H	6.27059	-1.19952	1.61497
H	4.37160	1.88315	0.77557
H	3.70772	3.22435	-0.20205
H	4.34115	1.74931	-0.99351
O	1.37358	3.67537	-0.01043
O	5.30720	-2.30429	-1.08776
Coordinates for Model Number 13			
C	-3.67279	-1.22060	0.01317
C	-2.50219	-0.47529	-0.00455
C	-2.53290	0.93128	0.01928
C	-1.35301	1.75789	0.00546
C	-3.79582	1.56094	0.06101
C	-4.96664	0.83012	0.07830
C	-4.91413	-0.57103	0.05464
C	1.04394	2.42257	-0.03188
C	1.81501	0.32141	-0.08345
C	-0.03787	1.41056	-0.03057
C	3.52171	2.24942	-0.10060
C	-6.12197	-2.61626	0.05318
C	2.73859	-0.82693	-0.11531
C	4.96263	-1.59795	-0.02944
C	2.11181	-2.17070	-0.34485
C	5.69244	-1.85091	1.26269
N	2.20640	1.64738	-0.06206
N	0.52074	0.14265	-0.06735
N	3.98598	-0.60446	0.05751
H	-3.61223	-2.30282	-0.00625
H	-1.54048	-0.97530	-0.03779
H	-3.84405	2.64684	0.08041
H	-5.93757	1.31375	0.10987
H	-1.52054	2.83463	0.02787
H	-7.17365	-2.90323	0.07315
H	-5.65721	-3.00730	-0.86001
H	-5.61587	-3.03432	0.93184
H	1.22084	-2.28250	0.27634
H	1.78660	-2.24593	-1.38780
H	2.82119	-2.97614	-0.15201
H	4.98486	-2.09264	2.06289
H	6.40313	-2.66658	1.12725
H	6.22350	-0.94360	1.56762
H	4.09119	2.00694	0.79832
H	3.35601	3.32781	-0.15709
H	4.08331	1.91129	-0.97343
O	1.00068	3.64076	-0.01484
O	-6.10632	-1.20312	0.07440
O	5.25470	-2.12703	-1.08441
Coordinates for Model Number 14			
C	-3.18833	-0.58267	-0.01951
C	-1.93308	0.01112	-0.01825
C	-1.78810	1.40886	0.03659
C	-0.51267	2.08070	0.03291
C	-2.96228	2.19060	0.09099
C	-4.21565	1.61159	0.09206
C	-4.33757	0.21682	0.03589

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C	1.95070	2.43085	-0.01602
C	2.44302	0.24749	-0.05626
C	0.74633	1.56707	0.00049
C	4.38414	1.93683	-0.12598
C	-5.78887	-1.66339	-0.01573
C	-7.21374	-1.95476	0.00026
C	-8.38812	-2.23388	0.01139
C	3.20700	-1.01322	-0.07882
C	5.31573	-2.06529	-0.04673
C	2.39827	-2.26821	-0.22924
C	6.09246	-2.34617	1.21173
N	3.00269	1.51133	-0.05329
N	1.13691	0.23747	-0.02747
N	4.47879	-0.95140	0.04215
H	-3.25732	-1.66365	-0.06570
H	-1.04230	-0.60592	-0.06275
H	-2.87653	3.27347	0.13279
H	-5.11875	2.21167	0.13420
H	-0.54022	3.16992	0.05597
H	-5.33711	-2.06942	-0.93201
H	-5.30171	-2.14184	0.84576
H	-9.42890	-2.47072	0.02138
H	1.93903	-2.28868	-1.22255
H	3.02221	-3.15515	-0.11932
H	1.58185	-2.27698	0.49664
H	5.41818	-2.44933	2.06833
H	6.68087	-3.25491	1.08142
H	6.75791	-1.50352	1.42604
H	4.93574	1.64348	0.76920
H	4.36005	3.02612	-0.20604
H	4.87881	1.50757	-0.99875
O	2.06745	3.64395	-0.00760
O	-5.60522	-0.25645	0.03860
O	5.47029	-2.67777	-1.08560

Coordinates for Model Number 15

C	-2.55953	-0.27567	-0.04361
C	-1.26796	0.22908	-0.04840
C	-1.04850	1.61914	0.00009
C	0.26909	2.22048	-0.00713
C	-2.16711	2.47439	0.05357
C	-3.45428	1.96574	0.06227
C	-3.66714	0.58219	0.01378
C	2.74954	2.42193	-0.04647
C	3.10806	0.21557	-0.07244
C	1.49003	1.62916	-0.03303
C	5.15036	1.78277	-0.13889
C	-5.07678	0.09053	0.03231
C	-5.31425	-1.40943	-0.05522
C	-6.78567	-1.78910	-0.14385
C	-7.63150	-1.58435	1.08134
C	3.79916	-1.09045	-0.08273
C	5.84145	-2.25994	0.02695
C	2.92555	-2.29353	-0.27944
C	6.51130	-2.61799	1.32544
N	3.74434	1.44153	-0.07030
N	1.80318	0.27949	-0.05382
N	5.06489	-1.09837	0.08921
H	-2.70008	-1.35138	-0.08640
H	-0.41375	-0.43681	-0.09261
H	-2.01023	3.54944	0.08830
H	-4.31887	2.62063	0.10458
H	0.30242	3.30917	0.00919
H	-4.85678	-1.88165	0.82529
H	-4.81195	-1.80800	-0.94310
H	-7.65849	-0.51617	1.32125

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H	-8.64187	-1.95304	0.89992
H	-7.19343	-2.10414	1.94141
H	2.10067	-2.27821	0.43698
H	2.47789	-2.26188	-1.27765
H	3.49819	-3.21639	-0.18656
H	5.77943	-2.67960	2.13743
H	7.03531	-3.56776	1.21385
H	7.22622	-1.83364	1.59515
H	5.67788	1.46145	0.76068
H	5.19166	2.87079	-0.22635
H	5.62117	1.31961	-1.00760
O	2.93109	3.62427	-0.04498
O	-6.00617	0.87421	0.11366
O	-7.22671	-2.25705	-1.17265
O	6.02884	-2.85044	-1.01790

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Coordinates for Model Number 16a

C	-3.49974	-1.82217	-0.02308
C	-2.40535	-0.96886	-0.03463
C	-2.59700	0.42512	0.00615
C	-1.51232	1.37754	-0.00468
C	-3.91209	0.92925	0.05731
C	-5.00371	0.07910	0.07060
C	-4.79212	-1.30735	0.03025
C	0.79672	2.29989	-0.04255
C	1.79390	0.29608	-0.05976
C	-0.16833	1.17405	-0.02828
C	3.27917	2.39920	-0.11248
C	2.83880	-0.74400	-0.07123
C	5.14028	-1.25193	-0.03975
C	2.35949	-2.15807	-0.21646
C	5.95488	-1.35125	1.22211
N	2.03743	1.65689	-0.06210
N	0.52765	-0.02472	-0.04182
N	4.05750	-0.37579	0.04985
H	-3.35183	-2.89973	-0.05581
H	-1.39802	-1.36619	-0.07616
H	-4.09297	1.99992	0.08668
H	-1.79474	2.42980	0.00809
H	-5.70933	-3.00181	0.01126
H	-6.88692	-0.15039	0.11894
H	1.54460	-2.35268	0.48440
H	1.95539	-2.30461	-1.22313
H	3.17431	-2.86703	-0.06719
H	5.33340	-1.70487	2.05188
H	6.78970	-2.03416	1.06184
H	6.33003	-0.36155	1.50058
H	3.87834	2.22300	0.78236
H	2.99697	3.45304	-0.17124
H	3.86642	2.11980	-0.98905
O	0.62202	3.50574	-0.04199
O	-5.92483	-2.06436	0.04637
O	-6.25930	0.58399	0.12062
O	5.44271	-1.79930	-1.08249

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Coordinates for Model Number 16b

C	-3.72932	-1.36345	0.00468
C	-2.59078	-0.57926	-0.01054
C	-2.69235	0.82621	0.01866
C	-1.54347	1.69993	0.00885
C	-3.96891	1.41500	0.06247
C	-5.11396	0.62867	0.07721
C	-4.99698	-0.75581	0.04866
C	0.83005	2.44770	-0.02229
C	1.66986	0.37381	-0.07899
C	-0.21854	1.39884	-0.02596

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C	3.31286	2.35657	-0.08533
C	2.62739	-0.74738	-0.10972
C	4.88093	-1.44330	-0.04893
C	2.03255	-2.11416	-0.28082
C	5.62830	-1.65039	1.24164
N	2.01734	1.71227	-0.05361
N	0.38347	0.15103	-0.06577
N	3.87047	-0.48386	0.03047
H	-1.61636	-1.05284	-0.04456
H	-4.05983	2.49693	0.08556
H	-1.75076	2.76921	0.03492
H	-6.88468	-1.14354	0.08893
H	-6.09886	1.08908	0.11063
H	-4.50908	-3.09458	-0.00883
H	1.30903	-2.30916	0.51522
H	1.47880	-2.16126	-1.22259
H	2.80761	-2.88051	-0.28907
H	4.93540	-1.87946	2.05785
H	6.34977	-2.45851	1.11873
H	6.15123	-0.72761	1.51281
H	3.88323	2.04772	-0.96328
H	3.89084	2.11943	0.80960
H	3.11396	3.43006	-0.12690
O	0.74587	3.66338	-0.00049
O	-6.04932	-1.62089	0.06030
O	-3.62166	-2.71306	-0.02206
O	5.18667	-1.97532	-1.09832

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Coordinates for Model Number 17

C	-3.12807	-0.45900	-0.14519
C	-1.86062	0.10567	-0.10763
C	-1.68460	1.49743	-0.00103
C	-0.39532	2.13913	0.03963
C	-2.84199	2.30332	0.06478
C	-4.10747	1.75287	0.02991
C	-4.26165	0.36307	-0.07492
C	2.07584	2.43502	0.05204
C	2.52121	0.24328	-0.04924
C	0.85336	1.59890	0.01376
C	4.49998	1.88986	-0.01301
C	-5.76616	-1.48570	-0.19244
C	-7.24168	-1.70930	-0.20348
C	-7.86395	-2.56701	0.60307
C	3.25610	-1.03350	-0.09602
C	5.33715	-2.13823	-0.06118
C	2.42017	-2.26433	-0.29280
C	6.08676	-2.47301	1.20074
N	3.10816	1.49366	0.00868
N	1.21486	0.26257	-0.04993
N	4.52708	-1.00660	0.04586
H	-3.22394	-1.53551	-0.22897
H	-0.98289	-0.52906	-0.16181
H	-2.73200	3.38180	0.14620
H	-4.99707	2.37206	0.08358
H	-0.39955	3.22733	0.09942
H	-7.80164	-1.13971	-0.94359
H	-5.31616	-1.86258	-1.12364
H	-5.29952	-2.00692	0.65394
H	-8.93505	-2.73156	0.53777
H	-7.32223	-3.13665	1.35490
H	1.97447	-2.24664	-1.29220
H	3.02134	-3.16878	-0.19927
H	1.59394	-2.27329	0.42177
H	5.39812	-2.57439	2.04599
H	6.64850	-3.39640	1.05648
H	6.77543	-1.65709	1.44339



H	5.02375	1.53887	0.87802
H	4.50119	2.98208	-0.03979
H	5.00541	1.49279	-0.89507
O	2.21848	3.64463	0.10312
O	-5.53484	-0.08436	-0.09674
O	5.49369	-2.72639	-1.11386
Coordinates for Model Number 18			
C	-3.86979	-1.71358	-0.02142
C	-2.76840	-0.88132	-0.03410
C	-2.91548	0.52245	0.01938
C	-1.81595	1.44595	0.00718
C	-4.22709	1.03618	0.08675
C	-5.33399	0.20943	0.10250
C	-5.17528	-1.18683	0.04696
C	0.51281	2.32042	-0.03570
C	1.46924	0.29570	-0.07205
C	-0.47279	1.21717	-0.02850
C	2.99673	2.36743	-0.10426
C	2.48776	-0.76710	-0.08599
C	4.77943	-1.32990	-0.04876
C	1.97141	-2.17071	-0.21060
C	5.60451	-1.40866	1.20886
N	1.73992	1.65178	-0.06270
N	0.19528	0.00414	-0.05555
N	-6.26385	-2.02113	0.10228
N	3.71711	-0.43089	0.02929
H	-3.73220	-2.79165	-0.06067
H	-1.76904	-1.29995	-0.08695
H	-4.37060	2.11332	0.12664
H	-6.33237	0.63603	0.15924
H	-6.14499	-2.97966	-0.18250
H	-2.07476	2.50445	0.03246
H	-7.17277	-1.63148	-0.08802
H	1.24773	-2.37325	0.58314
H	1.43702	-2.28293	-1.15850
H	2.78631	-2.89377	-0.18108
H	4.96809	-1.56017	2.08637
H	6.33014	-2.21756	1.11828
H	6.13262	-0.46025	1.35344
H	3.59213	2.16741	0.78831
H	2.73749	3.42790	-0.15011
H	3.57876	2.08632	-0.98395
O	0.36536	3.53174	-0.02458
O	5.06987	-1.90732	-1.07933
Coordinates for Model Number 19			
C	-0.98632	1.47295	-0.05706
C	1.35088	2.31935	-0.07752
C	2.28293	0.28543	-0.10045
C	0.34887	1.22337	-0.08502
C	3.83584	2.33980	-0.11329
C	-2.10393	0.55776	-0.05465
C	-3.38177	1.09234	0.05679
C	-1.95863	-0.85942	-0.16084
C	-4.53242	0.27461	0.07540
C	-3.06074	-1.67132	-0.15414
C	-4.37391	-1.14005	-0.03490
C	-5.83832	0.81550	0.19996
C	-5.52644	-1.96063	-0.02017
C	-6.93887	-0.00771	0.21412
C	-6.78114	-1.40781	0.10226
C	3.29531	-0.78766	-0.09164
C	5.57488	-1.36959	0.04158
C	2.77798	-2.18259	-0.28146
C	6.32863	-1.49601	1.33852

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N	2.56976	1.63799	-0.08667
N	1.00774	0.00364	-0.10509
N	4.51767	-0.45869	0.08848
H	-1.23195	2.53398	-0.02488
H	-3.50583	2.17036	0.13632
H	-0.96068	-1.27369	-0.24704
H	-2.94183	-2.74865	-0.23996
H	-5.95368	1.89310	0.28486
H	-5.40576	-3.03757	-0.10608
H	-7.93453	0.41518	0.31044
H	-7.65790	-2.04901	0.11347
H	1.92137	-2.35795	0.37320
H	2.42170	-2.30206	-1.30979
H	3.55959	-2.92113	-0.10195
H	5.64444	-1.69980	2.16861
H	7.07051	-2.29030	1.25288
H	6.83016	-0.54813	1.56066
H	4.43249	2.03628	-0.97529
H	4.40884	2.14849	0.79538
H	3.59030	3.40206	-0.18313
O	1.21254	3.52949	-0.06864
O	5.90829	-1.91993	-0.98972
Coordinates for Model Number 20			
C	-1.27512	0.89162	0.09447
C	0.90741	2.09412	0.07778
C	2.14054	0.22529	-0.01028
C	0.09091	0.86673	0.06930
C	3.35748	2.49222	-0.03930
C	-2.17968	-0.20893	0.06684
C	-3.63235	-0.19194	0.01995
C	-1.81482	-1.55103	0.12855
C	-4.06146	-1.53510	0.07714
C	-4.61003	0.82267	-0.08235
C	-5.39939	-1.92961	0.08323
C	-5.95253	0.43412	-0.06647
C	-6.33723	-0.90954	0.02097
C	3.29666	-0.68162	-0.07428
C	5.63985	-0.92531	-0.12224
C	2.98173	-2.13938	-0.24892
C	6.53574	-0.90496	1.08756
N	2.21699	1.60489	0.02857
N	0.91710	-0.24046	0.01250
N	-4.25874	2.16452	-0.14365
N	-2.92643	-2.32205	0.13669
N	4.47075	-0.18021	0.02772
H	-1.68631	1.89513	0.16621
H	-0.81901	-1.96698	0.17739
H	-2.92875	-3.32751	0.19061
H	-5.69059	-2.97387	0.13384
H	-6.71930	1.20203	-0.13574
H	-7.39565	-1.15265	0.02425
H	-3.42931	2.38196	-0.67584
H	-5.01982	2.78507	-0.37813
H	2.20863	-2.44331	0.46004
H	2.57986	-2.30677	-1.25303
H	3.87497	-2.75301	-0.13137
H	5.99331	-1.24897	1.97446
H	7.40619	-1.53669	0.90828
H	6.85824	0.12189	1.28740
H	4.00581	2.37105	0.83044
H	2.94849	3.50522	-0.06134
H	3.94388	2.30541	-0.94091
O	0.58946	3.27328	0.10442
O	5.94432	-1.45338	-1.17531

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Coordinates for Model Number 21			
C	-0.66422	1.71469	-0.04093
C	1.72316	2.41036	-0.05921
C	2.51837	0.32054	-0.10654
C	0.65065	1.38093	-0.07262
C	4.20349	2.26922	-0.10415
C	-1.83629	0.86977	-0.03792
C	-3.08801	1.45664	0.05500
C	-1.79006	-0.55871	-0.12443
C	-4.25429	0.66576	0.06849
C	-4.07366	-0.74567	-0.02478
C	-5.55425	1.22114	0.17049
C	-5.23125	-1.57950	-0.01627
C	-6.64554	0.38734	0.17792
C	-6.48680	-1.01049	0.08388
C	3.45593	-0.81998	-0.11698
C	5.69362	-1.55500	0.01617
C	2.84127	-2.17414	-0.31176
C	6.37181	-1.79865	1.33763
N	2.89440	1.65124	-0.07849
N	1.22824	0.12156	-0.10822
N	-2.85004	-1.32652	-0.12012
N	4.69724	-0.57676	0.06256
H	-0.84700	2.78854	-0.00663
H	-3.17904	2.53898	0.12256
H	-0.82313	-1.04779	-0.19915
H	-5.67014	2.29875	0.24213
H	-7.64763	0.79857	0.25613
H	-7.36614	-1.65143	0.09062
H	-5.87995	-3.36290	-0.09151
H	2.10375	-2.36625	0.47238
H	3.60413	-2.95290	-0.31726
H	2.29950	-2.20240	-1.26135
H	5.63551	-2.04808	2.10874
H	7.09624	-2.60643	1.23091
H	6.88135	-0.88584	1.66250
H	4.76529	2.03612	0.80192
H	4.02675	3.34548	-0.16605
H	4.77765	1.93394	-0.96961
O	1.65936	3.62593	-0.03970
O	-5.02980	-2.91041	-0.10755
O	6.03721	-2.07425	-1.02712
Coordinates for Model Number 21-H (with H-capping)			
C	-0.60369	-1.69151	0.01384
C	1.79348	-2.38307	0.03666
C	2.56321	-0.27831	-0.00029
C	0.71147	-1.34981	0.01244
C	-1.78157	-0.85884	-0.00551
C	-3.02821	-1.46591	0.00137
C	-1.75077	0.57325	-0.03161
C	-4.20468	-0.69174	-0.01673
C	-4.03967	0.72458	-0.04293
C	-5.49964	-1.26792	-0.00939
C	-5.20786	1.54305	-0.06176
C	-6.60171	-0.44857	-0.02778
C	-6.45843	0.95363	-0.05406
C	3.52994	0.80331	-0.01556
C	5.68117	1.61210	0.03120
N	2.94146	-1.59881	0.02681
N	1.27412	-0.08162	-0.01133
N	-2.82150	1.32476	-0.04984
N	4.78210	0.53851	-0.03313
H	-0.77809	-2.76742	0.03291
H	3.89524	-1.92827	0.03497

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H	-3.10580	-2.55121	0.02136
H	-0.78966	1.07911	-0.03645
H	-5.60323	-2.34891	0.01092
H	-7.60037	-0.87518	-0.02230
H	-7.34622	1.58261	-0.06835
H	-5.87623	3.32097	-0.09445
H	3.12186	1.81874	-0.02276
H	6.54063	1.48404	-0.64787
O	1.73254	-3.59551	0.05860
O	-5.02091	2.87803	-0.08637
O	5.57818	2.55111	0.78522
Coordinates for Model Number 22			
C	-3.38903	-1.19183	-0.01122
C	-2.21672	-0.45346	-0.01895
C	-2.25823	0.95522	0.01461
C	-1.07085	1.78611	0.01189
C	-3.51223	1.59522	0.05453
C	-4.69087	0.86584	0.06199
C	-4.60940	-0.52239	0.02949
C	1.33442	2.42612	-0.01473
C	2.07859	0.32003	-0.08232
C	0.23475	1.42128	-0.02282
C	3.81128	2.22615	-0.08732
C	2.99042	-0.84282	-0.12075
C	5.21161	-1.62958	-0.03426
C	2.34368	-2.17929	-0.33235
C	5.90048	-1.91842	1.27135
N	2.48741	1.63873	-0.05051
N	0.78304	0.15006	-0.06954
N	-5.84748	-1.30356	0.03872
N	4.23793	-0.62775	0.04558
H	-3.37686	-2.27545	-0.03628
H	-1.25412	-0.95041	-0.05095
H	-3.55442	2.68056	0.08026
H	-5.66204	1.34584	0.09213
H	-1.23301	2.86276	0.04249
H	1.59797	-2.36146	0.44616
H	1.80947	-2.18545	-1.28686
H	3.08686	-2.97644	-0.34150
H	5.16895	-2.17567	2.04468
H	6.60915	-2.73574	1.13508
H	6.42959	-1.02333	1.61390
H	4.37680	1.97439	0.81132
H	3.65943	3.30655	-0.14096
H	4.36709	1.88256	-0.96130
O	1.29806	3.64069	0.01200
O	-6.90331	-0.68947	0.07397
O	-5.74831	-2.52113	0.01099
O	5.52469	-2.13209	-1.09443

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Model	RFP-derived Chromophores					GFP-derived Chromophores				
	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]
1a	2.977	417	0.64	820	2.66	3.455	359	0.640	42	0.19
1b	2.987	415	0.61	618	2.02	3.468	358	0.679	15	0.07
2a	2.968	418	0.67	1335	4.31	3.473	357	0.652	13	0.06
2b	2.995	414	0.63	983	3.23	3.452	359	0.557	20	0.09
3	2.968	418	0.68	1425	4.60	3.463	358	0.705	24	0.11
4	2.923	424	0.75	1162	3.64	3.387	366	0.787	11	0.05
5	2.945	421	0.70	2062	6.56	3.467	358	0.704	180	0.79
6	2.881	430	0.83	527	1.60	3.197	388	0.912	342	1.28
7	2.819	440	0.88	450	1.31	3.200	388	0.927	339	1.27
8	2.883	430	0.75	395	1.20	3.304	375	0.796	370	1.48
9	2.897	428	0.82	4254	13.09	3.403	364	0.841	609	2.59
10	2.898	428	0.81	3776	11.62	3.369	368	0.848	763	3.18
11	2.859	434	0.78	498	1.49	3.256	381	0.812	1049	4.08
12	2.772	447	0.92	6135	17.28	3.210	386	0.984	1358	5.13
13	2.785	445	0.83	7024	19.98	3.289	377	0.853	1751	6.94
14	2.801	443	0.85	7205	20.72	3.310	375	0.894	1744	7.00
15	2.840	437	0.80	724	2.14	3.222	385	0.837	1879	7.15
16a	2.733	454	0.64	7938	21.75	3.218	385	0.577	2046	7.77
16b	2.783	446	0.77	7197	20.44	3.260	380	0.711	1882	7.33
17	2.775	447	0.86	7918	22.36	3.284	378	0.901	2067	8.17
18	2.630	471	0.91	9944	25.23	3.137	395	0.927	2540	9.16
19	2.732	454	0.80	12564	34.39	3.138	395	0.553	2908	10.50
20	2.239	554	0.48	27128	49.88	2.689	461	0.363	5738	15.21
21	2.654	467	0.46	16899	43.64	2.985	415	0.298	5258	17.19
22	2.710	458	0.69	6876	18.52	2.965	418	0.638	8834	28.47

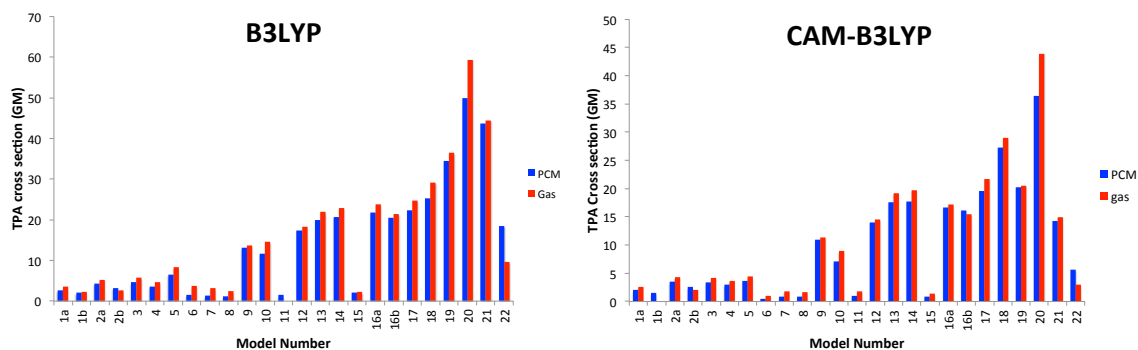
**Table S3** One-photon excitation energies [in eV] and the corresponding wavelengths [in nm], OPA oscillator strengths ( $f$ ), TPA transition moments ( $\delta^{\text{TPA}}$ ) and TPA cross-sections [in GM] for the transition to  $S_1$  as determined at the B3LYP/6-31G+(d,p) Level of Theory and PCM with parameters for  $\text{H}_2\text{O}$ . The properties for RFP-derived chromophores (Figure S1) are computed in this study, while the GFP-derived ones were previously reported.<sup>1</sup>

Model	$\Delta$ Energy [eV]	$\Delta$ Wavelength (nm)	$\Delta f$	$\Delta\delta^{\text{TPA}}$	$\Delta$ TPA [GM]	% increase in $f$	% increase in TPA
1a	-0.478	58	0.001	778	2.48	0.2	1339.8
1b	-0.481	58	-0.070	603	1.96	-10.3	2984.8
2a	-0.505	61	0.020	1322	4.25	3.1	7356.3
2b	-0.457	55	0.077	963	3.14	13.8	3630.8
3	-0.495	60	-0.028	1401	4.50	-4.0	4243.4
4	-0.464	58	-0.034	1151	3.60	-4.3	7951.8
5	-0.522	63	-0.003	1882	5.77	-0.4	728.5
6	-0.316	43	-0.084	184	0.32	-9.2	24.9
7	-0.381	52	-0.052	111	0.04	-5.6	3.0
8	-0.421	55	-0.049	25	-0.28	-6.2	-18.7
9	-0.506	64	-0.026	3645	10.51	-3.1	406.5
10	-0.471	60	-0.037	3013	8.45	-4.4	266.0
11	-0.397	53	-0.031	-551	-2.59	-3.8	-63.4
12	-0.438	61	-0.066	4777	12.15	-6.7	236.8
13	-0.504	68	-0.019	5274	13.03	-2.2	187.7
14	-0.509	68	-0.042	5461	13.72	-4.7	195.9
15	-0.382	52	-0.037	-1155	-5.01	-4.4	-70.1
16a	-0.485	68	0.063	5892	13.98	10.9	179.9
16b	-0.477	65	0.058	5315	13.10	8.2	178.7
17	-0.509	69	-0.043	5851	14.18	-4.8	173.5
18	-0.507	76	-0.016	7404	16.06	-1.7	175.3
19	-0.406	59	0.242	9655	23.89	43.8	227.5
20	-0.450	93	0.118	21391	34.67	32.5	227.9
21	-0.331	52	0.165	11641	26.46	55.4	154.0
22	-0.255	39	0.051	-1958	-9.95	8.0	-35.0

**Table S4** Differences between the properties computed for the RFP-derived chromophore and those previously computed for the corresponding GFP-derived chromophore for the transition to  $S_1$  as in Table S3.

Model	B3LYP					CAM-B3LYP				
	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]
1a	3.032	409	0.53	1042	3.51	3.384	366	0.66	616	2.59
2a	3.050	407	0.51	661	2.25	3.371	368	0.70	1025	4.27
1b	3.016	411	0.55	1580	5.27	-	-	-	-	-
2b	3.059	405	0.51	779	2.67	3.400	365	0.64	474	2.01
3	3.023	410	0.56	1708	5.72	3.371	368	0.70	1017	4.23
4	2.982	416	0.63	1445	4.71	3.323	373	0.77	917	3.71
5	2.991	415	0.56	2551	8.37	3.374	368	0.76	1049	4.38
6	2.949	420	0.68	1175	3.75	3.339	371	0.86	254	1.04
7	2.890	429	0.76	1033	3.16	3.256	381	0.90	474	1.84
8	2.959	419	0.64	756	2.43	3.304	375	0.77	417	1.67
9	2.962	419	0.66	4240	13.64	3.305	375	0.81	2846	11.40
10	2.956	419	0.67	4546	14.57	3.315	374	0.80	2213	8.92
11	2.931	423	0.66	737	2.32	3.283	378	0.80	469	1.85
12	2.857	434	0.76	6134	18.36	3.206	387	0.90	3850	14.51
13	2.872	432	0.67	7243	21.91	3.219	385	0.81	5051	19.19
14	2.874	431	0.70	7581	22.96	3.225	385	0.85	5156	19.66
15	2.915	425	0.68	719	2.24	3.274	379	0.83	351	1.38
16a	2.832	438	0.52	8071	23.73	3.242	382	0.73	4465	17.21
16b	2.901	428	0.62	6914	21.33	3.277	378	0.78	3915	15.42
17	2.854	435	0.70	8271	24.70	3.204	387	0.85	5764	21.69
18	2.777	446	0.73	10315	29.18	3.119	398	0.89	8115	28.95
19	2.841	436	0.69	12303	36.42	3.251	381	0.99	5278	20.45
20	2.366	524	0.39	28912	59.35	2.869	432	0.65	14550	43.93
21	2.718	456	0.29	16415	44.46	3.296	376	0.92	3756	14.96
22	2.881	430	0.60	3171	9.65	3.276	378	0.75	754	2.97

**Table S5** One-photon excitation energies [in eV] and the corresponding wavelengths [in nm], OPA oscillator strengths ( $f$ ), TPA transition moments ( $\delta^{\text{TPA}}$ ) and TPA cross-sections [in GM] for the transition to  $S_1$  as determined at the B3LYP and CAM-B3LYP/6-31G+(d,p) Level of Theory in the gas phase for the RFP-derived chromophores given in Figure S1.

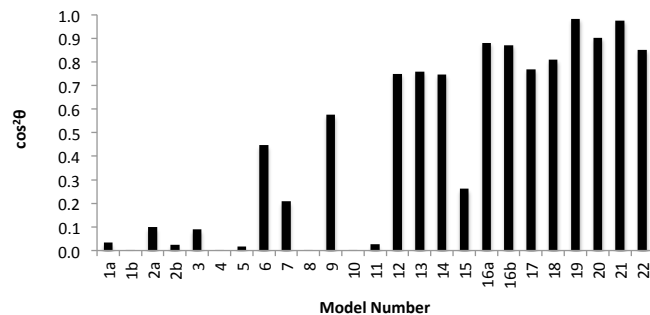
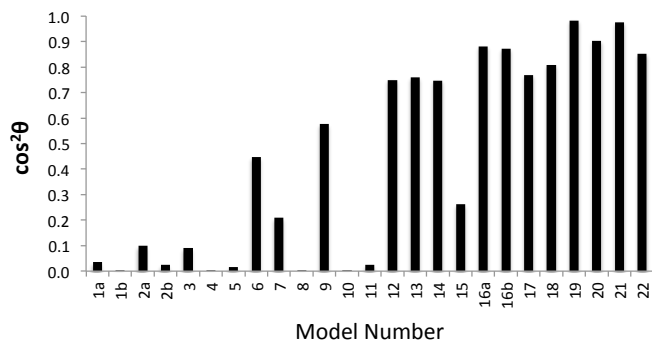
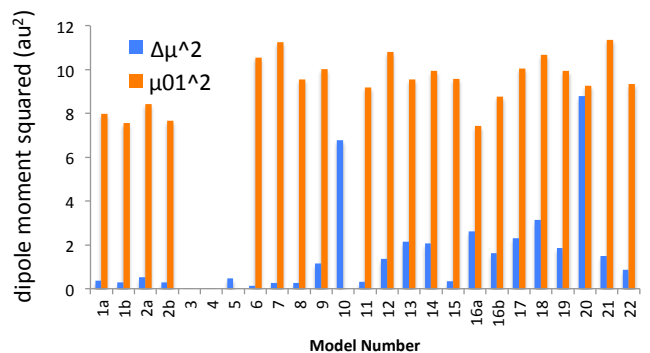
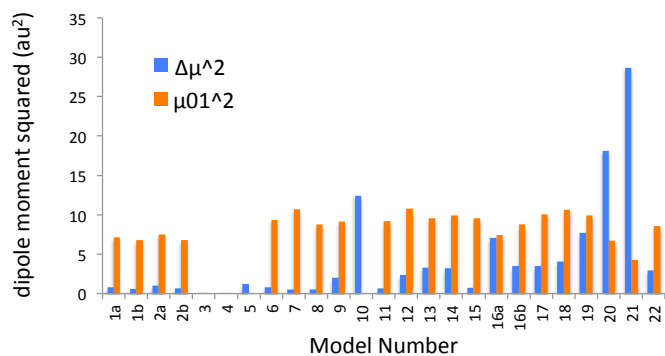
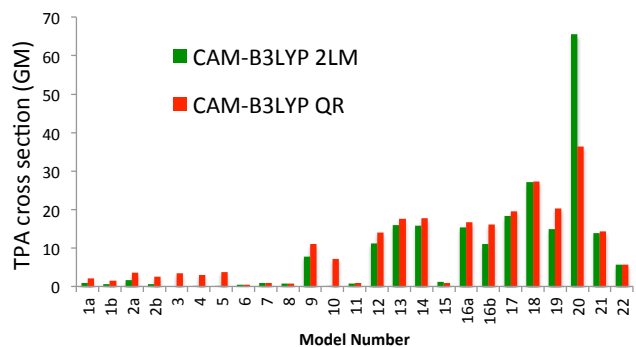
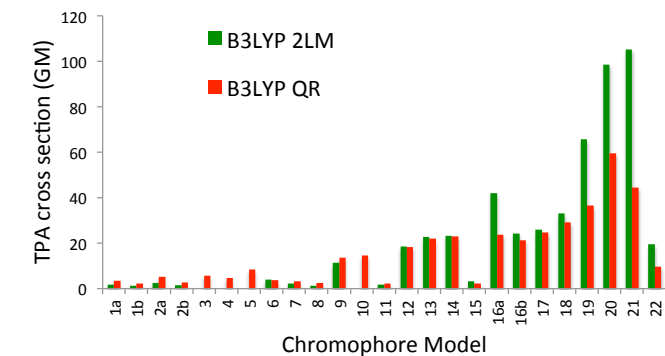


**Fig. S2** A visual representation for the TPA cross sections computed in the gas phase for the RFP-derived chromophores as given in Table S5 with the corresponding PCM values as given in Tables S3 and S7.

Model	B3LYP					CAM-B3LYP				
	2LM (GM)	QR (GM)	$\Delta\mu$ (au)	$\mu_{01}$ (au)	$\cos^2\theta$	2LM (GM)	QR (GM)	$\Delta\mu$ (au)	$\mu_{01}$ (au)	$\cos^2\theta$
1a	1.70	3.51	0.88	2.67	0.03	0.85	2.03	0.60	2.83	0.01
1b	1.16	2.25	0.77	2.60	0.00	0.60	1.50	0.52	2.75	0.00
2a	2.54	5.27	0.99	2.73	0.10	1.61	3.52	0.72	2.90	0.14
2b	1.38	2.67	0.82	2.61	0.03	0.66	2.55	0.53	2.77	0.02
3	0.00	5.72	0.05	0.02	0.09	0.00	3.42	0.05	0.02	0.00
4	0.00	4.71	0.17	0.06	0.00	0.00	2.94	0.19	0.06	0.00
5	0.00	8.37	1.09	0.03	0.02	0.00	3.69	0.69	0.07	0.00
6	3.95	3.75	0.88	3.06	0.45	0.44	0.49	0.38	3.25	0.00
7	2.18	3.16	0.70	3.27	0.21	0.85	0.89	0.51	3.35	0.00
8	1.36	2.43	0.73	2.96	0.00	0.73	0.80	0.51	3.09	0.02
9	11.26	13.64	1.41	3.02	0.58	7.80	10.97	1.07	3.16	0.67
10	0.06	14.57	3.53	0.12	0.00	0.03	7.13	2.60	0.12	0.00
11	1.83	2.32	0.81	3.03	0.03	0.81	0.94	0.55	3.03	0.00
12	18.50	18.36	1.54	3.29	0.75	11.18	13.94	1.16	3.29	0.82
13	22.63	21.91	1.81	3.09	0.76	15.98	17.62	1.46	3.09	0.85
14	23.29	22.96	1.80	3.15	0.75	15.84	17.69	1.43	3.15	0.84
15	3.11	2.24	0.86	3.09	0.26	1.22	0.92	0.58	3.09	0.16
16a	41.99	23.73	2.66	2.72	0.88	15.34	16.62	1.61	2.72	0.87
16b	24.26	21.33	1.87	2.96	0.87	11.08	16.14	1.28	2.96	0.84
17	25.86	24.70	1.87	3.17	0.77	18.29	19.58	1.52	3.17	0.86
18	33.00	29.18	2.02	3.27	0.81	27.11	27.28	1.77	3.27	0.90
19	65.60	36.42	2.78	3.15	0.98	14.89	20.30	1.36	3.15	0.90
20	98.51	59.35	4.26	2.59	0.90	65.57	36.39	2.96	3.04	0.89
21	105.19	44.46	5.35	2.08	0.97	13.86	14.28	1.22	3.37	0.91
22	19.38	9.65	1.70	2.92	0.85	5.61	5.65	0.93	3.06	0.71

**Table S6** TPA cross sections via the truncated SOS approach using 2 states; i.e. the 2-level model (2LM), and via quadratic response (QR), and the contributing components to the 2LM expression ((Equation 5 in the main text)) determined at the B3LYP and CAM-B3LYP/6-31+G(d,p) levels of theory in the gas phase.





**Fig. S3** Plots for the B3LYP (left) and CAM-B3LYP (right) data given in Table S6. Top figures compare the TPA cross sections computed via quadratic response (QR) to those obtained from the 2LM approximation. Middle figures compare the magnitudes of the transition dipole moment ( $\mu_{01}$ ) and the difference between permanent moments of excited and ground states ( $\Delta\mu$ ). The alignment between the  $\mu_{01}$  and  $\Delta\mu$  vectors is plotted in the bottom figures in terms of  $\cos^2\theta$  (the vectors are perfectly aligned when  $\cos^2\theta = 1$ ).

Model	RFP-derived Chromophores					GFP-derived Chromophores				
	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]	Energy [eV]	Wavelength (nm)	$f$	$\delta^{\text{TPA}}$	TPA [GM]
1a	3.306	375	0.78	507	2.03	3.707	334	0.730	1	0.01
1b	3.312	374	0.74	372	1.50	3.714	334	0.720	11	0.06
2a	3.295	376	0.81	884	3.52	3.702	335	0.743	76	0.38
2b	3.315	374	0.76	634	2.55	3.705	335	0.752	33	0.17
3	3.292	377	0.81	862	3.42	3.695	336	0.769	76	0.38
4	3.242	383	0.89	763	2.94	3.625	342	0.853	19	0.09
5	3.292	377	0.87	929	3.69	3.688	336	0.758	263	1.31
6	3.246	382	0.98	126	0.49	3.506	354	0.994	146	0.66
7	3.168	391	1.01	242	0.89	3.508	353	1.009	150	0.68
8	3.212	386	0.89	211	0.80	3.573	347	0.883	85	0.40
9	3.215	386	0.95	2894	10.97	3.624	342	0.889	688	3.31
10	3.235	383	0.93	1860	7.13	3.625	342	0.889	454	2.19
11	3.194	388	0.93	252	0.94	3.544	350	0.906	166	0.76
12	3.103	400	1.05	3949	13.94	3.466	358	1.029	1252	5.51
13	3.112	398	0.97	4963	17.62	3.522	352	0.900	1623	7.38
14	3.131	396	0.99	4922	17.69	3.542	350	0.938	1609	7.40
15	3.183	390	0.95	249	0.92	3.525	352	0.941	379	1.73
16a	3.127	397	0.87	4636	16.62	3.537	351	0.789	1483	6.80
16b	3.147	394	0.93	4443	16.14	3.548	349	0.852	1424	6.58
17	3.106	399	1.00	5536	19.58	3.517	353	0.948	1882	8.54
18	2.950	420	1.07	8551	27.28	3.364	369	0.988	2953	12.25
19	3.142	395	1.16	5606	20.30	3.511	353	0.999	1458	6.59
20	2.730	454	0.77	13314	36.39	3.139	395	0.630	3413	12.33
21	3.198	388	1.06	3808	14.28	3.535	351	0.871	1301	5.96
22	3.140	395	0.88	1564	5.65	3.432	361	0.862	2579	11.14

**Table S7** One-photon excitation energies [in eV] and the corresponding wavelengths [in nm], OPA oscillator strengths ( $f$ ), TPA transition moments ( $\delta^{\text{TPA}}$ ) and TPA cross-sections [in GM] for the transition to  $S_1$  as determined at the CAM-B3LYP/6-31G+(d,p) Level of Theory and PCM with parameters for  $\text{H}_2\text{O}$ . Models for the RFP-derived chromophores are given in Figure S1. Equivalent GFP-derived chromophores are given in Figure 2 of our previous study.<sup>1</sup>

Model	$\Delta$ Energy [eV]	$\Delta$ Wavelength (nm)	$\Delta f$	$\Delta\delta^{\text{TPA}}$	$\Delta$ TPA [GM]	% increase in $f$	% increase in TPA
1a	-0.402	41	0.048	506	2.03	6.6	28419.8
1b	-0.402	41	0.019	361	1.44	2.6	2603.6
2a	-0.407	41	0.071	808	3.14	9.6	818.1
2b	-0.390	39	0.012	601	2.39	1.6	1439.5
3	-0.403	41	0.041	786	3.04	5.3	805.1
4	-0.383	40	0.036	745	2.85	4.2	3120.5
5	-0.397	41	0.116	666	2.38	15.3	181.6
6	-0.260	28	-0.013	-20	-0.17	-1.3	-26.0
7	-0.341	38	-0.002	92	0.22	-0.2	31.9
8	-0.361	39	0.008	126	0.40	0.9	101.1
9	-0.408	43	0.060	2206	7.66	6.7	231.0
10	-0.391	41	0.037	1405	4.94	4.2	225.8
11	-0.350	38	0.019	86	0.18	2.1	23.2
12	-0.363	42	0.016	2697	8.43	1.6	152.9
13	-0.410	46	0.065	3340	10.24	7.2	138.8
14	-0.411	46	0.050	3314	10.29	5.3	139.0
15	-0.342	38	0.006	-130	-0.80	0.6	-46.5
16a	-0.410	46	0.080	3153	9.82	10.1	144.3
16b	-0.401	45	0.081	3019	9.56	9.5	145.4
17	-0.412	47	0.049	3654	11.04	5.2	129.3
18	-0.415	52	0.081	5598	15.02	8.2	122.6
19	-0.369	41	0.156	4149	13.71	15.6	208.1
20	-0.408	59	0.138	9900	24.06	21.9	195.2
21	-0.338	37	0.189	2506	8.31	21.7	139.4
22	-0.292	34	0.020	-1016	-5.49	2.3	-49.2

**Table S8** Differences between the properties computed for the RFP-derived chromophore and those previously computed for the corresponding GFP-derived chromophore for the transition to  $S_1$  as in Table S7.

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Model	B3LYP	CAM-B3LYP
1a	0.804	0.801
1b	0.804	0.799
2a	0.802	0.796
2b	0.804	0.798
3	0.803	0.797
4	0.807	0.801
5	0.788	0.787
6	0.791	0.788
7	0.803	0.796
8	0.811	0.807
9	0.787	0.775
10	0.793	0.780
11	0.808	0.804
12	0.776	0.755
13	0.756	0.738
14	0.764	0.748
15	0.804	0.801
16a	0.722	0.716
16b	0.730	0.715
17	0.757	0.740
18	0.712	0.690
19	0.738	0.726
20	0.615	0.608
21	0.660	0.670
22	0.738	0.743

**Table S9** The  $\Lambda$ -diagnostic for the first excited state computed at the B3LYP and CAM-B3LYP/6-31+G(d,p) level of theory in PCM (H<sub>2</sub>O) for the RFP-derived models (see Figure S1).

**Table S10** One-photon excitation energies [in eV] and the corresponding wavelengths [in nm], OPA oscillator strengths ( $f$ ), TPA transition moments ( $\delta^{\text{TPA}}$ ) and TPA cross-sections [in GM] for the transition to  $S_1$  as determined at the B3LYP/6-31G+(d,p) Level of Theory (except where noted) and PCM with parameters for  $\text{H}_2\text{O}$ . The properties are computed for the RFP-derived chromophores (Figure S1) at varying Acylimine dihedral angle ( $\theta_{\text{acylimine}}$ ).

Model	$\theta_{\text{acylimine}}$	Energy [eV]	Wavelength [nm]	$f$	$\delta^{\text{TPA}}$	TPA [GM]
13	0°	2.526	491	0.717	15955	37.33
	10°	2.559	484	0.735	14871	35.72
	20°	2.597	477	0.750	13483	33.35
	30°	2.636	470	0.767	12077	30.77
	40°	2.678	463	0.785	10597	27.87
	50°	2.720	456	0.804	9181	24.91
	60°	2.756	450	0.820	7974	22.21
	70°	2.787	445	0.835	6957	19.81
	80°	2.809	441	0.844	6246	18.07
	90°	2.819	440	0.848	5921	17.25
	100°	2.814	441	0.843	6057	17.58
	110°	2.791	444	0.833	6782	19.37
	120°	2.750	451	0.815	8151	22.60
	130°	2.693	461	0.794	10149	26.98
	140°	2.630	471	0.775	12329	31.27
	150°	2.571	482	0.757	14133	34.25
	160°	2.539	488	0.746	15096	35.67
	170°	2.524	491	0.739	15669	36.61
	180°	2.525	491	0.735	15945	37.29
	190°	2.535	489	0.734	16150	38.06
	200°	2.565	483	0.736	15796	38.12
	210°	2.628	472	0.751	14012	35.50
	220°	2.703	459	0.779	11469	30.72
	230°	2.772	447	0.818	8936	25.17
	240°	2.828	438	0.866	6781	19.88
	250°	2.856	434	0.900	5653	16.91
	260°	2.849	435	0.899	5813	17.31
	270°	2.809	441	0.864	7244	20.96
	280°	2.750	451	0.819	9374	26.00
	290°	2.685	462	0.780	11783	31.14
	300°	2.619	473	0.746	14080	35.41
	310°	2.563	484	0.720	15802	38.05
	320°	2.523	491	0.702	16666	38.90
	330°	2.497	497	0.686	16886	38.60
	340°	2.490	498	0.677	16538	37.59
350°	2.500	496	0.690	16386	37.54	
14	0°	2.544	487	0.725	16363	38.82
	10°	2.577	481	0.746	15350	37.38
	20°	2.615	474	0.763	13884	34.81
	30°	2.655	467	0.781	12406	32.06
	40°	2.698	460	0.801	10856	28.97
	50°	2.740	453	0.821	9394	25.86
	60°	2.778	446	0.840	8092	22.90
	70°	2.809	441	0.856	7031	20.34
80°	2.831	438	0.866	6284	18.47	

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90°	2.840	437	0.870	5980	17.68
100°	2.834	438	0.867	6160	18.13
110°	2.812	441	0.856	6869	19.92
120°	2.774	447	0.838	8196	23.12
130°	2.720	456	0.816	10119	27.44
140°	2.659	466	0.794	12277	31.82
150°	2.599	477	0.772	14205	35.18
160°	2.566	483	0.759	15230	36.76
170°	2.545	487	0.750	16004	38.02
180°	2.540	488	0.746	16559	39.17
190°	2.555	485	0.748	16481	39.44
200°	2.600	477	0.758	15426	38.23
210°	2.662	466	0.778	13524	35.15
220°	2.730	454	0.806	11193	30.58
230°	2.797	443	0.847	8679	24.89
240°	2.849	435	0.892	6646	19.79
250°	2.875	431	0.923	5619	17.03
260°	2.869	432	0.922	5847	17.64
270°	2.831	438	0.889	7208	21.18
280°	2.775	447	0.847	9302	26.26
290°	2.710	458	0.805	11724	31.58
300°	2.647	468	0.770	13972	35.89
310°	2.591	479	0.741	15747	38.76
320°	2.549	487	0.718	16733	39.85
330°	2.521	492	0.697	16908	39.42
340°	2.511	494	0.674	16444	38.00
350°	2.519	492	0.684	16258	37.84

16a	0°	2.482	500	0.571	17136	38.71
	10°	2.513	493	0.580	15911	36.85
	20°	2.550	486	0.589	14462	34.47
	30°	2.589	479	0.599	12964	31.85
	40°	2.632	471	0.611	11389	28.92
	50°	2.674	464	0.623	9903	25.97
	60°	2.712	457	0.632	8630	23.27
	70°	2.740	453	0.639	7652	21.07
	80°	2.762	449	0.644	6944	19.42
	90°	2.773	447	0.646	6618	18.65
	100°	2.767	448	0.643	6801	19.09
	110°	2.744	452	0.636	7543	20.82
	120°	2.702	459	0.627	8868	23.73
	130°	2.652	468	0.616	10729	27.66
	140°	2.585	480	0.603	12933	31.69
	150°	2.531	490	0.592	14798	34.76
	160°	2.494	497	0.584	16020	36.55
	170°	2.476	501	0.580	16803	37.77
	180°	2.472	502	0.577	17234	38.60
	190°	2.480	500	0.577	17437	39.33
	200°	2.526	491	0.584	16337	38.22
	210°	2.596	478	0.600	14059	34.74
	220°	2.667	465	0.619	11659	30.40
	230°	2.736	453	0.646	9174	25.18

	240°	2.789	445	0.674	7245	20.66
	250°	2.814	441	0.691	6287	18.26
	260°	2.807	442	0.688	6479	18.72
	270°	2.768	448	0.667	7813	21.94
	280°	2.713	457	0.642	9792	26.43
	290°	2.648	468	0.616	12117	31.15
	300°	2.583	480	0.595	14449	35.36
	310°	2.528	490	0.578	16321	38.25
	320°	2.487	499	0.567	17500	39.69
	330°	2.464	503	0.560	18032	40.13
	340°	2.451	506	0.555	18137	39.96
	350°	2.459	504	0.560	17859	39.59
16b	0°	2.515	493	0.667	16785	38.94
	10°	2.547	487	0.682	15740	37.43
	20°	2.585	480	0.696	14282	34.99
	30°	2.627	472	0.711	12710	32.17
	40°	2.670	464	0.727	11182	29.24
	50°	2.714	457	0.744	9659	26.09
	60°	2.753	450	0.759	8317	23.12
	70°	2.785	445	0.771	7246	20.61
	80°	2.805	442	0.777	6565	18.95
	90°	2.813	441	0.780	6279	18.22
	100°	2.807	442	0.777	6460	18.67
	110°	2.784	445	0.769	7197	20.46
	120°	2.744	452	0.755	8564	23.64
	130°	2.688	461	0.737	10500	27.82
	140°	2.627	472	0.721	12612	31.91
	150°	2.572	482	0.706	14369	34.84
	160°	2.539	488	0.696	15452	36.52
	170°	2.514	493	0.686	16463	38.16
	180°	2.509	494	0.681	16963	39.16
	190°	2.523	492	0.681	16992	39.65
	200°	2.566	483	0.689	16032	38.71
	210°	2.633	471	0.707	14021	35.64
	220°	2.703	459	0.731	11634	31.18
	230°	2.770	448	0.764	9172	25.81
	240°	2.824	439	0.805	7090	20.73
	250°	2.850	435	0.831	6019	17.93
	260°	2.842	436	0.827	6233	18.46
	270°	2.804	442	0.798	7570	21.83
	280°	2.747	451	0.762	9679	26.78
	290°	2.683	462	0.729	12030	31.76
	300°	2.618	474	0.700	14336	36.04
	310°	2.563	484	0.677	16122	38.82
	320°	2.522	492	0.662	17116	39.92
	330°	2.495	497	0.648	17483	39.90
	340°	2.485	499	0.637	17267	39.09
	350°	2.493	497	0.645	17060	38.88
17	0°	2.520	492	0.737	17470	40.68
	10°	2.552	486	0.753	16331	38.99

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20°	2.591	479	0.770	14797	36.41
30°	2.631	471	0.789	13272	33.68
40°	2.675	464	0.810	11596	30.42
50°	2.718	456	0.831	10044	27.20
60°	2.753	450	0.848	8798	24.45
70°	2.785	445	0.864	7682	21.84
80°	2.806	442	0.875	6934	20.02
90°	2.816	440	0.879	6597	19.18
100°	2.811	441	0.876	6754	19.57
110°	2.789	445	0.864	7521	21.45
120°	2.747	451	0.845	9009	24.93
130°	2.692	461	0.823	11033	29.32
140°	2.633	471	0.801	13211	33.58
150°	2.574	482	0.780	15165	36.83
160°	2.542	488	0.768	16146	38.27
170°	2.520	492	0.758	17016	39.61
180°	2.518	492	0.754	17381	40.40
190°	2.530	490	0.755	17491	41.04
200°	2.571	482	0.763	16636	40.33
210°	2.634	471	0.781	14747	37.51
220°	2.702	459	0.809	12316	32.98
230°	2.769	448	0.849	9723	27.34
240°	2.825	439	0.900	7463	21.84
250°	2.852	435	0.934	6317	18.85
260°	2.844	436	0.930	6547	19.42
270°	2.806	442	0.896	8004	23.11
280°	2.749	451	0.852	10232	28.36
290°	2.685	462	0.809	12758	33.72
300°	2.621	473	0.774	15075	37.99
310°	2.567	483	0.748	16826	40.65
320°	2.523	492	0.727	18008	42.01
330°	2.497	497	0.711	18255	41.74
340°	2.487	499	0.701	18060	40.96
350°	2.496	497	0.712	17865	40.82

18	0°	2.367	524	0.789	20503	42.12
	10°	2.398	517	0.802	19229	40.55
	20°	2.436	509	0.817	17739	38.60
	30°	2.476	501	0.835	16164	36.33
	40°	2.521	492	0.854	14445	33.67
	50°	2.565	483	0.877	12632	30.48
	60°	2.605	476	0.897	10989	27.35
	70°	2.637	470	0.914	9638	24.58
	80°	2.662	466	0.927	8631	22.42
	90°	2.674	464	0.930	8169	21.41
	100°	2.668	465	0.927	8387	21.89
	110°	2.643	469	0.913	9376	24.02
	120°	2.600	477	0.892	11158	27.65
	130°	2.541	488	0.869	13523	32.02
	140°	2.478	500	0.848	15865	35.72
	150°	2.423	512	0.831	17555	37.80
	160°	2.384	520	0.819	18704	38.98



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170°	2.364	524	0.811	19463	39.89
180°	2.360	525	0.804	20081	41.00
190°	2.369	523	0.800	20614	42.41
200°	2.411	514	0.803	20205	43.07
210°	2.471	502	0.811	18802	42.09
220°	2.540	488	0.831	16345	38.66
230°	2.613	475	0.871	13024	32.60
240°	2.674	464	0.929	9942	26.07
250°	2.708	458	0.977	8151	21.92
260°	2.701	459	0.977	8371	22.39
270°	2.658	466	0.932	10389	26.92
280°	2.597	478	0.883	13351	33.01
290°	2.530	490	0.842	16374	38.42
300°	2.464	503	0.810	19024	42.35
310°	2.409	515	0.789	20816	44.30
320°	2.371	523	0.777	21708	44.73
330°	2.347	528	0.772	21959	44.35
340°	2.338	530	0.772	21838	43.78
350°	2.346	528	0.779	21337	43.07

19	0°	2.501	496	0.739	26756	61.38
	10°	2.530	490	0.750	25089	58.88
	20°	2.563	484	0.759	22846	55.04
	30°	2.600	477	0.768	20447	50.69
	40°	2.638	470	0.777	18093	46.18
	50°	2.677	463	0.786	15797	41.50
	60°	2.711	457	0.793	13815	37.22
	70°	2.738	453	0.796	12263	33.70
	80°	2.755	450	0.797	11299	31.44
	90°	2.762	449	0.798	10884	30.44
	100°	2.758	450	0.798	11101	30.95
	110°	2.739	453	0.796	12141	33.39
	120°	2.704	459	0.790	14125	37.86
	130°	2.655	467	0.781	17021	43.99
	140°	2.600	477	0.771	20346	50.42
	150°	2.549	486	0.759	23296	55.51
	160°	2.518	493	0.752	25189	58.54
	170°	2.494	497	0.743	26892	61.33
	180°	2.489	498	0.739	27618	62.73
	190°	2.502	496	0.741	27345	62.78
	200°	2.547	487	0.756	25159	59.85
	210°	2.614	474	0.780	21369	53.53
	220°	2.679	463	0.807	17504	46.08
	230°	2.738	453	0.832	13957	38.36
	240°	2.782	446	0.854	11220	31.83
	250°	2.801	443	0.863	9949	28.63
	260°	2.793	444	0.857	10314	29.51
	270°	2.763	449	0.841	12038	33.70
	280°	2.716	457	0.820	14898	40.28
	290°	2.661	466	0.798	18235	47.33
	300°	2.602	477	0.775	21792	54.10
	310°	2.551	486	0.755	24738	59.01

	320°	2.513	494	0.740	26571	61.51
	330°	2.486	499	0.727	27479	62.28
	340°	2.475	501	0.715	27492	61.73
	350°	2.483	499	0.720	27070	61.18
20	0°	2.053	604	0.493	44252	68.40
	10°	2.062	601	0.493	43311	67.55
	20°	2.087	594	0.493	41174	65.78
	30°	2.120	585	0.492	38446	63.33
	40°	2.156	575	0.491	35288	60.16
	50°	2.199	564	0.490	31543	55.91
	60°	2.236	555	0.488	28105	51.53
	70°	2.267	547	0.486	25186	47.47
	80°	2.287	542	0.484	23282	44.63
	90°	2.292	541	0.482	22621	43.58
	100°	2.283	543	0.482	23366	44.66
	110°	2.258	549	0.483	25641	47.93
	120°	2.217	559	0.485	29371	52.92
	130°	2.166	572	0.488	33998	58.51
	140°	2.117	586	0.492	38377	63.08
	150°	2.074	598	0.494	41894	66.10
	160°	2.044	607	0.496	44178	67.67
	170°	2.030	611	0.496	45104	68.17
	180°	2.027	612	0.495	45298	68.24
	190°	2.038	608	0.493	44419	67.64
	200°	2.054	604	0.492	43071	66.63
	210°	2.076	597	0.490	41342	65.33
	220°	2.110	588	0.488	38743	63.23
	230°	2.155	575	0.486	34972	59.54
	240°	2.203	563	0.484	30689	54.61
	250°	2.247	552	0.483	26694	49.42
	260°	2.277	544	0.481	23944	45.54
	270°	2.292	541	0.481	22765	43.83
	280°	2.287	542	0.482	23299	44.68
	290°	2.266	547	0.483	25372	47.76
	300°	2.233	555	0.485	28571	52.25
	310°	2.193	565	0.488	32424	57.19
	320°	2.150	577	0.489	36433	61.77
	330°	2.109	588	0.490	40037	65.32
	340°	2.079	596	0.492	42515	67.39
	350°	2.058	602	0.493	44047	68.42
	360°	2.053	604	0.493	44252	68.40
21	0°	2.455	505	0.468	31199	68.94
	10°	2.479	500	0.468	29438	66.31
	20°	2.509	494	0.469	27071	62.48
	30°	2.541	488	0.470	24655	58.37
	40°	2.573	482	0.469	22363	54.29
	50°	2.605	476	0.469	20194	50.25
	60°	2.634	471	0.468	18309	46.56
	70°	2.655	467	0.465	16891	43.67
	80°	2.669	465	0.462	16008	41.81

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90°	2.674	464	0.460	15656	41.04
100°	2.669	465	0.461	15911	41.56
110°	2.653	467	0.462	16890	43.60
120°	2.624	473	0.463	18772	47.38
130°	2.581	480	0.463	21600	52.77
140°	2.531	490	0.461	25029	58.80
150°	2.486	499	0.460	28215	63.92
160°	2.461	504	0.461	30103	66.85
170°	2.442	508	0.459	31717	69.34
180°	2.440	508	0.459	32197	70.28
190°	2.454	505	0.461	31560	69.71
200°	2.497	497	0.472	28963	66.23
210°	2.559	485	0.486	25026	60.09
220°	2.619	473	0.498	21162	53.23
230°	2.669	465	0.504	17949	46.87
240°	2.704	459	0.506	15644	41.92
250°	2.716	456	0.503	14683	39.73
260°	2.708	458	0.498	15057	40.49
270°	2.683	462	0.494	16598	43.79
280°	2.642	469	0.490	19155	49.03
290°	2.595	478	0.486	22253	54.95
300°	2.545	487	0.480	25671	60.95
310°	2.499	496	0.475	28743	65.82
320°	2.466	503	0.472	30849	68.77
330°	2.442	508	0.469	32146	70.28
340°	2.433	510	0.466	32312	70.13
350°	2.438	509	0.466	32000	69.76

21-H	0°	2.185	568	0.328	40977	71.73
	10°	2.195	565	0.329	40302	71.23
	20°	2.227	557	0.333	38478	69.99
	30°	2.273	546	0.339	35865	67.94
	40°	2.329	532	0.345	32594	64.82
	50°	2.387	519	0.352	29097	60.80
	60°	2.438	509	0.355	25992	56.64
	70°	2.478	500	0.357	23551	53.01
	80°	2.500	496	0.357	22166	50.79
	90°	2.505	495	0.358	21918	50.43
	100°	2.492	498	0.358	22881	52.11
	110°	2.462	504	0.358	25008	55.57
	120°	2.418	513	0.357	28008	60.04
	130°	2.370	523	0.354	31229	64.34
	140°	2.324	534	0.351	34277	67.87
	150°	2.281	544	0.346	36898	70.37
	160°	2.247	552	0.342	38835	71.86
	170°	2.222	558	0.338	40135	72.69
	180°	2.216	560	0.337	40528	72.94
	190°	2.221	558	0.337	40304	72.87
	200°	2.240	554	0.340	39320	72.32
	210°	2.268	547	0.343	37759	71.21
	220°	2.310	537	0.348	35237	68.97
	230°	2.360	525	0.353	32099	65.54

	240°	2.409	515	0.356	28773	61.23
	250°	2.453	506	0.358	25721	56.75
	260°	2.486	499	0.358	23389	53.00
	270°	2.504	495	0.358	22098	50.82
	280°	2.504	495	0.358	22090	50.77
	290°	2.483	499	0.358	23384	52.84
	300°	2.447	507	0.357	25697	56.42
	310°	2.398	517	0.354	28831	60.78
	320°	2.341	530	0.349	32344	64.98
	330°	2.284	543	0.343	35702	68.30
	340°	2.234	555	0.336	38504	70.47
	350°	2.198	564	0.330	40371	71.54
22	0°	2.478	500	0.013	74	0.17
	10°	2.562	484	0.012	68	0.16
	20°	2.627	472	0.672	3697	9.35
	30°	2.646	469	0.678	4279	10.98
	40°	2.665	465	0.683	4988	12.99
	50°	2.682	462	0.685	5703	15.04
	60°	2.697	460	0.689	6327	16.88
	70°	2.709	458	0.689	6842	18.42
	80°	2.718	456	0.689	7172	19.42
	90°	2.722	456	0.688	7298	19.82
	100°	2.721	456	0.688	7140	19.38
	110°	2.714	457	0.688	6696	18.08
	120°	2.700	459	0.688	5931	15.86
	130°	2.680	463	0.687	4991	13.15
	140°	2.655	467	0.685	4071	10.52
	150°	2.628	472	0.679	3394	8.59
	160°	2.607	476	0.670	3076	7.67
	170°	2.596	478	0.668	2895	7.15
	180°	2.596	478	0.669	2875	7.10
	190°	2.607	476	0.678	3007	7.49
	200°	2.631	471	0.694	3594	9.12
	210°	2.660	466	0.710	4743	12.31
	220°	2.687	461	0.722	6187	16.38
	230°	2.709	458	0.728	7557	20.33
	240°	2.724	455	0.729	8552	23.26
	250°	2.730	454	0.727	8880	24.28
	260°	2.728	454	0.723	8598	23.47
	270°	2.719	456	0.718	7697	20.86
	280°	2.697	460	0.709	6662	17.77
	290°	2.673	464	0.699	5457	14.30
	300°	2.649	468	0.686	4286	11.03
	310°	2.620	473	0.659	3498	8.80
	320°	2.587	479	0.573	2711	6.65
	330°	2.532	490	0.231	1118	2.63
	340°	2.465	503	0.055	312	0.69
	350°	2.443	508	0.023	136	0.30
BLB	0°	2.642	469	0.020	160	0.41
	10°	2.735	453	0.090	921	2.53

20°	2.857	434	0.003	82	0.25
30°	2.812	441	0.634	4517	13.10
40°	2.852	435	0.648	3728	11.12
50°	2.890	429	0.661	3016	9.24
60°	2.928	424	0.674	2345	7.37
70°	2.957	419	0.682	1860	5.96
80°	2.977	416	0.687	1538	5.00
90°	2.986	415	0.689	1401	4.58
100°	2.981	416	0.686	1462	4.76
110°	2.960	419	0.679	1785	5.73
120°	2.920	425	0.668	2456	7.68
130°	2.866	433	0.654	3490	10.51
140°	2.806	442	0.639	4680	13.51
150°	2.752	451	0.624	5745	15.96
160°	2.718	456	0.614	6439	17.44
170°	2.700	459	0.609	6948	18.57
180°	2.698	460	0.608	7169	19.14
190°	2.710	458	0.610	7165	19.30
200°	2.752	451	0.620	6500	18.05
210°	2.824	439	0.640	5075	14.84
220°	2.898	428	0.666	3577	11.01
230°	2.963	419	0.695	2302	7.41
240°	3.010	412	0.721	1451	4.82
250°	3.028	410	0.733	1149	3.86
260°	3.016	411	0.728	1301	4.34
270°	2.981	416	0.709	1864	6.07
280°	2.929	423	0.684	2808	8.83
290°	2.870	432	0.657	3925	11.85
300°	2.809	441	0.629	5070	14.67
310°	2.755	450	0.597	5894	16.40
320°	2.710	458	0.519	5603	15.08
330°	2.657	467	0.251	2585	6.69
340°	2.601	477	0.065	542	1.34
350°	2.593	478	0.028	204	0.50

RFP	0°	2.222	558	1.028	4389	7.94
	10°	2.238	554	1.031	4310	7.91
	20°	2.261	548	1.033	4299	8.05
	30°	2.287	542	1.036	4304	8.25
	40°	2.318	535	1.040	4226	8.32
	50°	2.354	527	1.046	3962	8.04
	60°	2.393	518	1.056	3428	7.19
	70°	2.430	510	1.066	2744	5.94
	80°	2.456	505	1.075	2170	4.79
	90°	2.465	503	1.079	1938	4.31
	100°	2.452	506	1.072	2188	4.82
	110°	2.418	513	1.058	2902	6.22
	120°	2.369	523	1.045	3818	7.85
	130°	2.317	535	1.037	4464	8.78
	140°	2.272	546	1.037	4546	8.60
	150°	2.241	553	1.042	4254	7.83
	160°	2.226	557	1.047	3918	7.11

	170°	2.217	559	1.050	3695	6.65
	180°	2.216	560	1.049	3676	6.61
	190°	2.218	559	1.044	3838	6.92
	200°	2.227	557	1.038	4141	7.52
	210°	2.241	553	1.031	4505	8.29
	220°	2.265	547	1.025	4836	9.09
	230°	2.301	539	1.021	4888	9.48
	240°	2.348	528	1.026	4435	8.96
	250°	2.397	517	1.041	3529	7.43
	260°	2.438	509	1.060	2612	5.69
	270°	2.460	504	1.073	2124	4.71
	280°	2.455	505	1.073	2270	5.01
	290°	2.427	511	1.061	3003	6.48
	300°	2.380	521	1.044	4029	8.36
	310°	2.326	533	1.029	4872	9.66
	320°	2.277	545	1.020	5216	9.91
	330°	2.241	553	1.017	5151	9.48
	340°	2.219	559	1.020	4849	8.75
	350°	2.213	560	1.024	4549	8.16
RFP-H	0°	2.227	557	1.149	677	1.23
	10°	2.230	556	1.148	704	1.28
	20°	2.243	553	1.146	794	1.46
	30°	2.262	548	1.142	926	1.74
	40°	2.289	542	1.138	1074	2.06
	50°	2.323	534	1.137	1157	2.29
	60°	2.359	526	1.137	1093	2.23
	70°	2.392	518	1.141	897	1.88
	80°	2.413	514	1.143	727	1.55
	90°	2.413	514	1.140	763	1.63
	100°	2.392	518	1.134	1033	2.17
	110°	2.360	526	1.134	1356	2.77
	120°	2.328	533	1.146	1463	2.91
	130°	2.303	538	1.164	1317	2.56
	140°	2.289	542	1.185	1065	2.05
	150°	2.281	544	1.203	837	1.60
	160°	2.277	545	1.218	679	1.29
	170°	2.277	545	1.227	597	1.13
	180°	2.277	545	1.230	575	1.09
	190°	2.278	544	1.227	599	1.14
	200°	2.278	544	1.218	678	1.29
	210°	2.280	544	1.204	826	1.58
	220°	2.289	542	1.185	1056	2.03
	230°	2.304	538	1.165	1310	2.55
	240°	2.329	532	1.146	1454	2.89
	250°	2.360	525	1.135	1352	2.76
	260°	2.393	518	1.134	1036	2.17
	270°	2.414	514	1.141	763	1.63
	280°	2.415	513	1.144	730	1.56
	290°	2.394	518	1.141	899	1.89
	300°	2.361	525	1.137	1099	2.25
	310°	2.324	533	1.137	1168	2.31

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	320°	2.291	541	1.139	1087	2.09
	330°	2.264	548	1.142	941	1.77
	340°	2.243	553	1.146	799	1.47
	350°	2.231	556	1.148	708	1.29
RFP (CAM-B3LYP)	0°	2.382	521	1.189	6552	13.62
	10°	2.396	517	1.193	6188	13.03
	20°	2.419	513	1.197	5763	12.37
	30°	2.445	507	1.202	5306	11.63
	40°	2.475	501	1.208	4753	10.67
	50°	2.506	495	1.215	4113	9.47
	60°	2.538	489	1.221	3420	8.08
	70°	2.564	484	1.224	2816	6.79
	80°	2.580	481	1.226	2411	5.89
	90°	2.585	480	1.226	2269	5.56
	100°	2.577	481	1.223	2436	5.93
	110°	2.555	485	1.219	2935	7.02
	120°	2.521	492	1.214	3744	8.72
	130°	2.478	500	1.210	4721	10.63
	140°	2.435	509	1.209	5554	12.07
	150°	2.400	517	1.209	6007	12.69
	160°	2.379	521	1.211	6100	12.66
	170°	2.366	524	1.213	6067	12.46
	180°	2.364	524	1.212	6057	12.41
	190°	2.369	523	1.209	6119	12.59
	200°	2.382	521	1.206	6164	12.83
	210°	2.402	516	1.203	6086	12.88
	220°	2.431	510	1.202	5754	12.47
	230°	2.468	502	1.203	5090	11.37
	240°	2.508	494	1.207	4195	9.68
	250°	2.545	487	1.214	3318	7.88
	260°	2.571	482	1.219	2693	6.53
	270°	2.583	480	1.223	2408	5.89
	280°	2.581	480	1.224	2499	6.10
	290°	2.564	484	1.220	2959	7.13
	300°	2.532	490	1.214	3759	8.84
	310°	2.491	498	1.205	4783	10.88
	320°	2.448	507	1.195	5774	12.68
	330°	2.412	514	1.187	6497	13.86
	340°	2.386	520	1.185	6820	14.24
350°	2.375	522	1.186	6804	14.07	

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Model	13	14	16a	16b	17	18	19	20	21	21-H	22	BLB	RFP	RFP-H	RFP (CAM-B3LYP)
0°	37.33	38.82	38.71	38.94	40.68	42.12	61.38	68.40	68.94	71.73	7.25	18.11	7.94	1.23	13.62
10°	35.72	37.38	36.85	37.43	38.99	40.55	58.88	67.55	66.31	71.23	8.06	14.42	7.91	1.28	13.03
20°	33.35	34.81	34.47	34.99	36.41	38.60	55.04	65.78	62.48	69.99	9.35	15.02	8.05	1.46	12.37
30°	30.77	32.06	31.85	32.17	33.68	36.33	50.69	63.33	58.37	67.94	10.98	13.10	8.25	1.74	11.63
40°	27.87	28.97	28.92	29.24	30.42	33.67	46.18	60.16	54.29	64.82	12.99	11.12	8.32	2.06	10.67
50°	24.91	25.86	25.97	26.09	27.20	30.48	41.50	55.91	50.25	60.80	15.04	9.24	8.04	2.29	9.47
60°	22.21	22.90	23.27	23.12	24.45	27.35	37.22	51.53	46.56	56.64	16.88	7.37	7.19	2.23	8.08
70°	19.81	20.34	21.07	20.61	21.84	24.58	33.70	47.47	43.67	53.01	18.42	5.96	5.94	1.88	6.79
80°	18.07	18.47	19.42	18.95	20.02	22.42	31.44	44.63	41.81	50.79	19.42	5.00	4.79	1.55	5.89
90°	17.25	17.68	18.65	18.22	19.18	21.41	30.44	43.58	41.04	50.43	19.82	4.58	4.31	1.63	5.56
100°	17.58	18.13	19.09	18.67	19.57	21.89	30.95	44.66	41.56	52.11	19.38	4.76	4.82	2.17	5.93
110°	19.37	19.92	20.82	20.46	21.45	24.02	33.39	47.93	43.60	55.57	18.08	5.73	6.22	2.77	7.02
120°	22.60	23.12	23.73	23.64	24.93	27.65	37.86	52.92	47.38	60.04	15.86	7.68	7.85	2.91	8.72
130°	26.98	27.44	27.66	27.82	29.32	32.02	43.99	58.51	52.77	64.34	13.15	10.51	8.78	2.56	10.63
140°	31.27	31.82	31.69	31.91	33.58	35.72	50.42	63.08	58.80	67.87	10.52	13.51	8.60	2.05	12.07
150°	34.25	35.18	34.76	34.84	36.83	37.80	55.51	66.10	63.92	70.37	8.59	15.96	7.83	1.60	12.69
160°	35.67	36.76	36.55	36.52	38.27	38.98	58.54	67.67	66.85	71.86	7.67	17.44	7.11	1.29	12.66
170°	36.61	38.02	37.77	38.16	39.61	39.89	61.33	68.17	69.34	72.69	7.15	18.57	6.65	1.13	12.46
180°	37.29	39.17	38.60	39.16	40.40	41.00	62.73	68.24	70.28	72.94	7.10	19.14	6.61	1.09	12.41
190°	38.06	39.44	39.33	39.65	41.04	42.41	62.78	67.64	69.71	72.87	7.49	19.30	6.92	1.14	12.59
200°	38.12	38.23	38.22	38.71	40.33	43.07	59.85	66.63	66.23	72.32	9.12	18.05	7.52	1.29	12.83
210°	35.50	35.15	34.74	35.64	37.51	42.09	53.53	65.33	60.09	71.21	12.31	14.84	8.29	1.58	12.88
220°	30.72	30.58	30.40	31.18	32.98	38.66	46.08	63.23	53.23	68.97	16.38	11.01	9.09	2.03	12.47
230°	25.17	24.89	25.18	25.81	27.34	32.60	38.36	59.54	46.87	65.54	20.33	7.41	9.48	2.55	11.37
240°	19.88	19.79	20.66	20.73	21.84	26.07	31.83	54.61	41.92	61.23	23.26	4.82	8.96	2.89	9.68
250°	16.91	17.03	18.26	17.93	18.85	21.92	28.63	49.42	39.73	56.75	24.28	3.86	7.43	2.76	7.88
260°	17.31	17.64	18.72	18.46	19.42	22.39	29.51	45.54	40.49	53.00	23.47	4.34	5.69	2.17	6.53
270°	20.96	21.18	21.94	21.83	23.11	26.92	33.70	43.83	43.79	50.82	20.86	6.07	4.71	1.63	5.89
280°	26.00	26.26	26.43	26.78	28.36	33.01	40.28	44.68	49.03	50.77	17.77	8.83	5.01	1.56	6.10
290°	31.14	31.58	31.15	31.76	33.72	38.42	47.33	47.76	54.95	52.84	14.30	11.85	6.48	1.89	7.13
300°	35.41	35.89	35.36	36.04	37.99	42.35	54.10	52.25	60.95	56.42	11.03	14.67	8.36	2.25	8.84
310°	38.05	38.76	38.25	38.82	40.65	44.30	59.01	57.19	65.82	60.78	8.80	16.40	9.66	2.31	10.88
320°	38.90	39.85	39.69	39.92	42.01	44.73	61.51	61.77	68.77	64.98	6.65	15.08	9.91	2.09	12.68
330°	38.60	39.42	40.13	39.90	41.74	44.35	62.28	65.32	70.28	68.30	4.80	13.80	9.48	1.77	13.86
340°	37.59	38.00	39.96	39.09	40.96	43.78	61.73	67.39	70.13	70.47	6.37	19.10	8.75	1.47	14.24
350°	37.54	37.84	39.59	38.88	40.82	43.07	61.18	68.42	69.76	71.54	6.73	19.21	8.16	1.29	14.07

**Table S11** TPA Cross-sections [in GM] extracted from Tables S10 and S12 as determined at the B3LYP/6-31G+(d,p) Level of Theory (except where noted) with PCM (H<sub>2</sub>O). The Cross-sections correspond to the S<sub>0</sub> to S<sub>1</sub> transition except for Models 22 and BLB at the near-planar conformations ( $\theta_{\text{acylimine}} = 0, 10, 20, 340$  and  $350$ ) where the transition is to the second excited state.

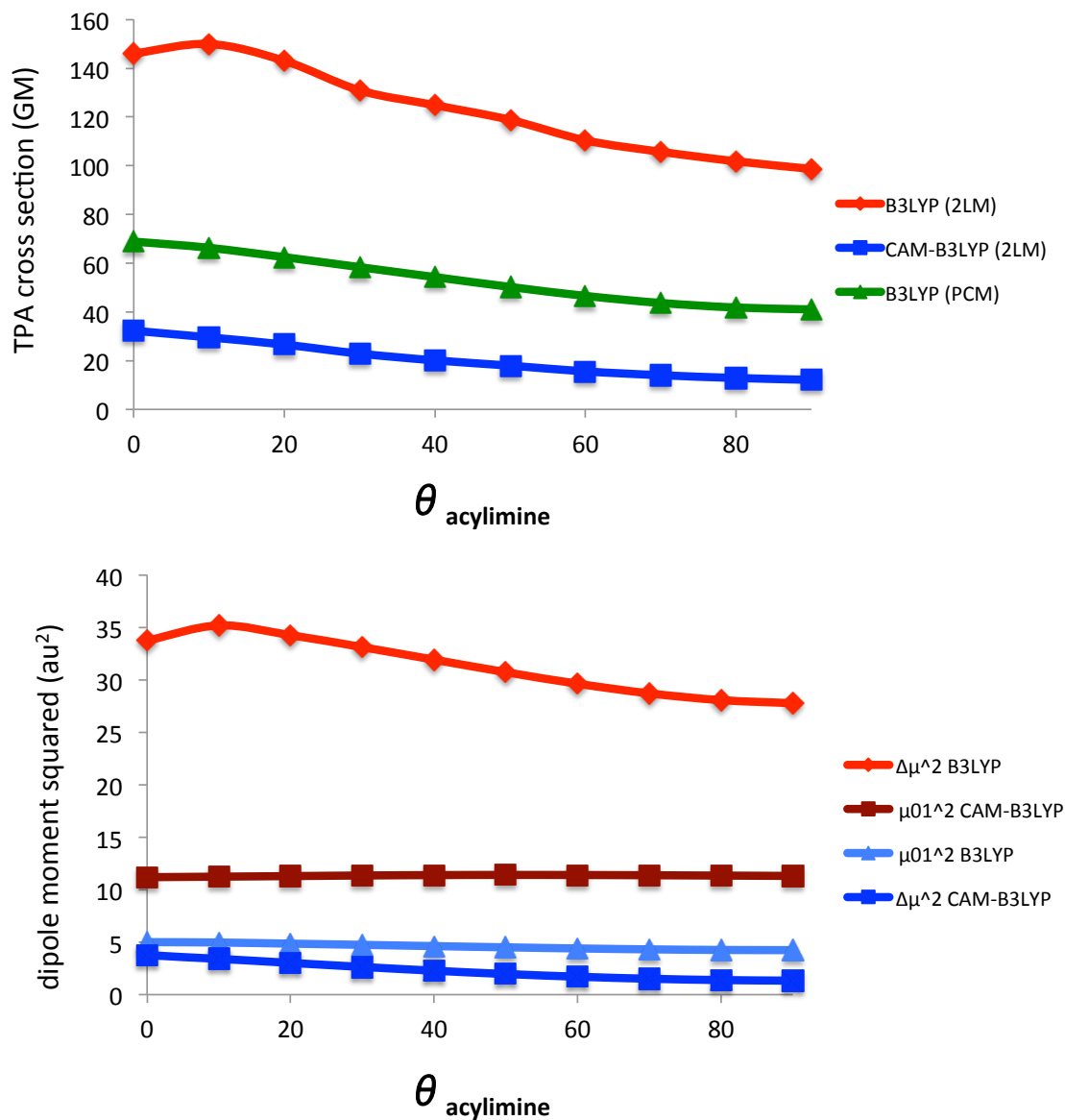


Model	$\theta_{\text{acylimine}}$	State	Energy [eV]	wavelength [nm]	$f$	$\delta^{\text{TPA}}$	TPA [GM]	
22	0°	1	2.478	500	0.014	75	0.17	
		2	2.596	478	0.650	2938	7.25	
		3	3.055	406	0.000	4	0.01	
	10°	1	2.562	484	0.012	68	0.16	
		2	2.61	475	0.656	3231	8.06	
		3	3.074	403	0.000	4	0.01	
	20°	1	2.627	472	0.672	3699	9.35	
		2	2.675	464	0.003	71	0.19	
		3	3.098	400	0.000	4	0.01	
	330°	1	2.532	490	0.231	1119	2.63	
		2	2.622	473	0.435	1907	4.80	
		3	3.065	405	0.001	2	0.01	
	340°	1	2.465	503	0.056	313	0.70	
		2	2.593	478	0.606	2585	6.37	
		3	3.049	407	0.001	2	0.01	
	350°	1	2.443	508	0.023	137	0.30	
		2	2.588	479	0.637	2744	6.73	
		3	3.045	407	0.000	3	0.01	
	BLB	0°	1	2.642	469	0.02	160	0.41
			2	2.718	456	0.585	6693	18.11
			3	3.246	382	0.001	3	0.01
10°		1	2.735	453	0.09	919	2.52	
		2	2.745	452	0.524	5226	14.42	
		3	3.272	379	0.001	3	0.01	
20°		1	2.776	447	0.621	5319	15.02	
		2	2.857	434	0.003	75	0.23	
		3	3.303	375	0.001	5	0.02	
330°		1	2.657	467	0.251	2584	6.68	
		2	2.735	453	0.352	5035	13.80	
		3	3.248	382	0.001	4	0.02	
340°		1	2.601	477	0.065	542	1.34	
		2	2.704	459	0.534	7132	19.10	
		3	3.232	384	0.001	4	0.02	
350°	1	2.593	478	0.028	204	0.50		
	2	2.703	459	0.572	7178	19.21		
	3	3.231	384	0.001	3	0.01		

**Table S12** TD-DFT data for the first 3 states of Models 22 and BLB at their near-planar conformations ( $\theta_{\text{acylimine}} = 0, 10, 20, 340$  and  $350$ ). Level of Theory is B3LYP/6-31G+(d,p) with PCM ( $\text{H}_2\text{O}$ ).

$\theta_{\text{acylimine}}$	B3LYP				CAM-B3LYP			
	$\Delta\mu$ (au)	$\mu_{01}$ (au)	$\cos^2\theta$	TPA (GM)	$\Delta\mu$ (au)	$\mu_{01}$ (au)	$\cos^2\theta$	TPA (GM)
0	5.81	2.24	0.99	146.05	1.93	3.35	0.84	32.25
10	5.93	2.23	0.99	149.94	1.85	3.35	0.84	29.56
20	5.85	2.20	0.99	143.05	1.74	3.36	0.85	26.60
30	5.75	2.18	0.99	130.93	1.62	3.37	0.86	22.88
40	5.65	2.15	0.99	124.85	1.51	3.38	0.87	20.12
50	5.54	2.12	0.98	118.80	1.40	3.38	0.89	17.96
60	5.44	2.10	0.98	110.40	1.31	3.38	0.90	15.58
70	5.36	2.08	0.97	105.71	1.23	3.37	0.91	14.03
80	5.30	2.06	0.97	101.80	1.18	3.37	0.91	12.88
90	5.27	2.06	0.97	98.68	1.15	3.36	0.92	12.12

**Table S13** Components contributing to the 2LM expression (Equation 5 in the main text) determined at the B3LYP and CAM-B3LYP/6-31+G(d,p) levels of theory in the gas phase for Model 21 at  $\theta_{\text{acylimine}}$  varying from 0° to 90°. All data is for the  $S_0$  to  $S_1$  transition except for the CAM-B3LYP data for conformers with  $\theta_{\text{acylimine}} = 0, 10$  in which data for the  $S_0$  to  $S_2$  is given because the first excited-state was dark.



**Fig. S4** Top: TPA cross sections computed for Model 21 (at  $\theta_{\text{acylimine}}$  varying from 0° to 90°) via the 2LM in the gas phase (as given in Table S13) versus the corresponding PCM values for B3LYP (given in Table S11). Bottom: The magnitudes of the dipole moments contributing to the 2LM expression (as given in Table S13).

**Table S14** Variation of TD-DFT properties with tilt and twist angles (see Table S1) for Model 21 at fixed  $\theta_{\text{acylimine}}$  of  $0^\circ$ ,  $90^\circ$ ,  $180^\circ$  and  $270^\circ$ . The TD-DFT values are for the transition to  $S_1$  as determined at the B3LYP/6-31G+(d,p) level of theory and PCM with parameters for  $\text{H}_2\text{O}$ .

$\theta_{\text{acylimine}}$	tilt	twist	Energy [eV]	wavelength [nm]	$f$	$\delta^{\text{TPA}}$	TPA [GM]
$0^\circ$	-30	160	2.401	516	0.317	30361	64.16
	-30	165	2.402	516	0.356	30743	65.04
	-30	170	2.401	516	0.391	30992	65.52
	-30	175	2.398	517	0.420	31296	65.99
	-30	180	2.392	518	0.441	31702	66.52
	-30	185	2.388	519	0.456	32059	67.03
	-30	190	2.391	519	0.471	32098	67.27
	-30	195	2.391	519	0.476	32374	67.85
	-30	200	2.389	519	0.471	32748	68.52
	-25	160	2.423	512	0.334	30060	64.69
	-25	165	2.422	512	0.371	30458	65.51
	-25	170	2.420	512	0.405	30766	66.08
	-25	175	2.414	514	0.428	31236	66.76
	-25	180	2.408	515	0.445	31741	67.46
	-25	185	2.407	515	0.461	31955	67.90
	-25	190	2.409	515	0.472	32079	68.27
	-25	195	2.406	515	0.469	32528	69.05
	-25	200	2.408	515	0.466	32560	69.21
	-20	160	2.437	509	0.351	30049	65.46
	-20	165	2.436	509	0.386	30461	66.27
	-20	170	2.431	510	0.414	30904	66.99
	-20	175	2.424	512	0.433	31461	67.78
	-20	180	2.420	512	0.450	31851	68.41
	-20	185	2.422	512	0.465	31971	68.77
	-20	190	2.421	512	0.467	32297	69.38
	-20	195	2.421	512	0.464	32433	69.68
	-20	200	2.425	511	0.459	32247	69.51
	-15	160	2.448	506	0.368	30161	66.29
	-15	165	2.445	507	0.400	30586	67.06
	-15	170	2.439	508	0.423	31096	67.83
	-15	175	2.433	510	0.440	31599	68.59
	-15	180	2.433	510	0.457	31772	68.97
	-15	185	2.434	509	0.466	31943	69.38
	-15	190	2.433	510	0.465	32149	69.77
	-15	195	2.437	509	0.462	31960	69.58
	-15	200	2.439	508	0.452	31898	69.58
	-10	160	2.457	505	0.386	30237	66.94
	-10	165	2.453	506	0.413	30662	67.65
	-10	170	2.446	507	0.432	31208	68.45
	-10	175	2.444	507	0.450	31462	68.90
	-10	180	2.445	507	0.463	31578	69.19
	-10	185	2.444	507	0.467	31750	69.54
	-10	190	2.447	507	0.466	31658	69.48
	-10	195	2.450	506	0.459	31476	69.25
	-10	200	2.445	507	0.436	31687	69.44
	-5	160	2.462	504	0.402	30399	67.54
	-5	165	2.456	505	0.424	30855	68.22
	-5	170	2.452	506	0.443	31205	68.77
	-5	175	2.452	506	0.459	31283	68.94
	-5	180	2.451	506	0.466	31420	69.22
	-5	185	2.452	506	0.467	31410	69.25
	-5	190	2.451	506	0.458	31362	69.10
	-5	195	2.456	505	0.450	31156	68.92
	-5	200	2.459	504	0.431	31030	68.78
	0	160	2.461	504	0.415	30599	67.97
	0	165	2.461	504	0.440	30787	68.36
	0	170	2.459	504	0.456	30895	68.48
	0	175	2.457	505	0.466	31009	68.65
	0	180	2.455	505	0.468	31199	68.94
	0	185	2.457	505	0.465	30996	68.62
	0	190	2.458	504	0.455	30893	68.46

	0	195	2.461	504	0.439	30722	68.22
	0	200	2.463	503	0.417	30528	67.93
	5	160	2.460	504	0.432	30916	68.59
	5	165	2.457	505	0.450	31055	68.74
	5	170	2.451	506	0.457	31183	68.71
	5	175	2.452	506	0.466	31094	68.56
	5	180	2.455	505	0.467	30880	68.24
	5	185	2.457	505	0.461	30775	68.11
	5	190	2.452	506	0.444	31068	68.49
	5	195	2.462	504	0.429	30362	67.46
	5	200	2.465	503	0.403	30101	67.05
	10	160	2.447	507	0.437	31363	68.83
	10	165	2.446	507	0.453	31351	68.76
	10	170	2.447	507	0.465	31147	68.39
	10	175	2.450	506	0.471	30888	67.95
	10	180	2.452	506	0.468	30686	67.66
	10	185	2.454	505	0.458	30552	67.45
	10	190	2.458	505	0.443	30209	66.91
	10	195	2.461	504	0.420	29997	66.60
	10	200	2.463	503	0.390	29741	66.14
	15	160	2.437	509	0.449	31583	68.79
	15	165	2.439	509	0.463	31333	68.32
	15	170	2.442	508	0.473	30939	67.63
	15	175	2.445	507	0.475	30608	67.08
	15	180	2.446	507	0.468	30488	66.90
	15	185	2.450	506	0.456	30134	66.33
	15	190	2.453	505	0.435	29900	65.98
	15	195	2.456	505	0.408	29657	65.61
	15	200	2.455	505	0.373	29523	65.26
	20	160	2.424	512	0.458	31766	68.45
	20	165	2.428	511	0.472	31237	67.52
	20	170	2.431	510	0.478	30824	66.81
	20	175	2.434	510	0.475	30610	66.47
	20	180	2.436	509	0.464	30370	66.09
	20	185	2.440	508	0.449	30021	65.54
	20	190	2.443	508	0.425	29809	65.25
	20	195	2.444	507	0.393	29635	64.92
	20	200	2.440	508	0.355	29594	64.63
	25	160	2.410	515	0.467	31771	67.64
	25	165	2.414	514	0.478	31175	66.62
	25	170	2.417	513	0.480	30847	66.07
	25	175	2.419	513	0.472	30641	65.75
	25	180	2.423	512	0.460	30297	65.20
	25	185	2.426	511	0.439	30051	64.85
	25	190	2.428	511	0.412	29872	64.58
	25	195	2.425	511	0.376	29907	64.50
	25	200	2.420	513	0.336	29904	64.19
	30	160	2.394	518	0.475	31555	66.33
	30	165	2.397	517	0.482	31149	65.63
	30	170	2.399	517	0.478	30928	65.27
	30	175	2.401	516	0.469	30694	64.89
	30	180	2.404	516	0.452	30421	64.49
	30	185	2.407	515	0.428	30279	64.31
	30	190	2.406	515	0.396	30282	64.25
	30	195	2.398	517	0.357	30540	64.40
	30	200	2.391	519	0.314	30540	64.04
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0	185	2.675	464	0.455	15651	41.05
0	190	2.677	463	0.446	15606	41.02
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5	160	2.682	462	0.428	15649	41.27
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5	170	2.669	465	0.449	15816	41.30
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5	200	2.688	461	0.401	15502	41.08
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	10	170	2.664	465	0.456	15786	41.08
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-15	165	2.430	510	0.393	31192	67.54
-15	170	2.423	512	0.414	31787	68.43
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0	170	2.444	507	0.446	31779	69.62
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0	190	2.440	508	0.445	32109	70.08
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0	200	2.452	506	0.410	31324	69.07
5	160	2.443	508	0.418	31810	69.60
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10	160	2.435	509	0.433	32371	70.40
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10	170	2.436	509	0.457	32045	69.72
10	175	2.438	509	0.462	31847	69.41
10	180	2.439	508	0.459	31738	69.25
10	185	2.441	508	0.449	31566	68.97
10	190	2.444	507	0.433	31319	68.61
10	195	2.447	507	0.411	31087	68.27
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15	160	2.424	512	0.438	32621	70.27
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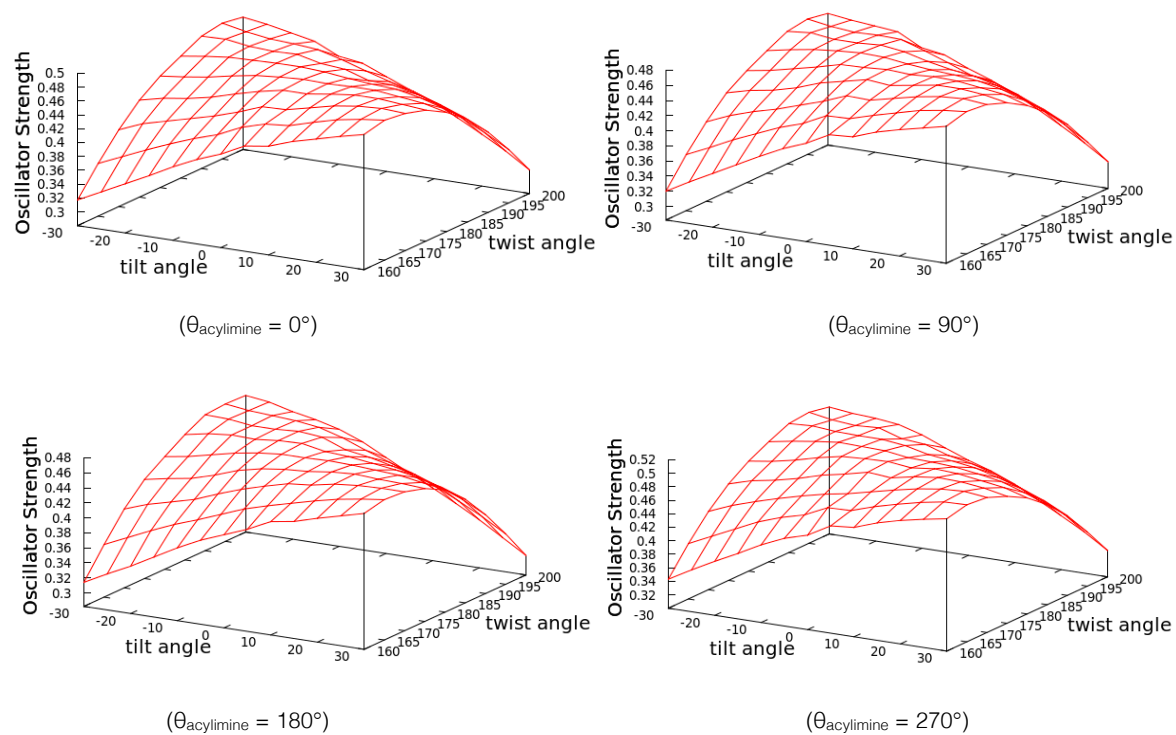
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	25	185	2.416	513	0.431	31228	66.81
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	-30	170	2.611	475	0.416	17491	43.72
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	-20	180	2.641	470	0.475	17202	43.98
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-10	185	2.671	464	0.492	16853	44.10
-10	190	2.673	464	0.489	16842	44.11
-10	195	2.671	464	0.476	16906	44.23
-10	200	2.680	463	0.468	16813	44.26
-5	160	2.694	460	0.430	16539	44.00
-5	165	2.685	462	0.451	16668	44.07
-5	170	2.678	463	0.468	16838	44.28
-5	175	2.678	463	0.484	16780	44.11
-5	180	2.680	463	0.493	16606	43.72
-5	185	2.678	463	0.491	16677	43.86
-5	190	2.681	463	0.485	16724	44.06
-5	195	2.683	462	0.473	16734	44.17
-5	200	2.687	461	0.454	16757	44.37
0	160	2.691	461	0.440	16673	44.26
0	165	2.690	461	0.467	16580	43.98
0	170	2.678	463	0.474	16891	44.42
0	175	2.684	462	0.492	16551	43.72
0	180	2.683	462	0.494	16598	43.80
0	185	2.682	462	0.486	16670	43.97
0	190	2.684	462	0.477	16621	43.92
0	195	2.689	461	0.462	16582	43.95
0	200	2.693	460	0.441	16579	44.10
5	160	2.690	461	0.459	16659	44.21
5	165	2.678	463	0.468	16910	44.47
5	170	2.678	463	0.482	16774	44.11
5	175	2.679	463	0.489	16692	43.91
5	180	2.681	462	0.490	16556	43.64
5	185	2.684	462	0.485	16477	43.53
5	190	2.687	461	0.473	16408	43.45
5	195	2.692	461	0.455	16366	43.50
5	200	2.697	460	0.430	16373	43.68
10	160	2.676	463	0.462	16911	44.42
10	165	2.674	464	0.479	16835	44.14
10	170	2.675	464	0.490	16663	43.72
10	175	2.677	463	0.496	16488	43.32
10	180	2.680	463	0.494	16350	43.06
10	185	2.682	462	0.483	16347	43.10
10	190	2.686	462	0.468	16249	42.99
10	195	2.690	461	0.445	16284	43.21
10	200	2.695	460	0.416	16315	43.44
15	160	2.665	465	0.474	17012	44.31
15	165	2.665	465	0.488	16816	43.79
15	170	2.667	465	0.497	16566	43.20
15	175	2.670	464	0.500	16343	42.72
15	180	2.672	464	0.492	16331	42.74
15	185	2.674	464	0.478	16251	42.62
15	190	2.678	463	0.459	16241	42.72
15	195	2.683	462	0.432	16294	43.00
15	200	2.685	462	0.398	16428	43.42
20	160	2.650	468	0.483	17085	43.99
20	165	2.652	468	0.496	16767	43.23
20	170	2.655	467	0.502	16471	42.57
20	175	2.657	467	0.499	16352	42.33
20	180	2.659	466	0.487	16328	42.32
20	185	2.663	466	0.472	16237	42.21
20	190	2.666	465	0.448	16322	42.54

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20	195	2.670	464	0.417	16409	42.88
20	200	2.670	464	0.380	16603	43.41
25	160	2.631	471	0.490	17135	43.49
25	165	2.635	471	0.502	16716	42.55
25	170	2.637	470	0.504	16485	42.05
25	175	2.639	470	0.495	16454	42.01
25	180	2.641	470	0.482	16394	41.93
25	185	2.644	469	0.461	16432	42.13
25	190	2.648	468	0.435	16529	42.50
25	195	2.650	468	0.401	16708	43.02
25	200	2.649	468	0.361	16953	43.61
30	160	2.609	475	0.496	17147	42.78
30	165	2.611	475	0.503	16841	42.10
30	170	2.612	475	0.500	16748	41.91
30	175	2.613	474	0.488	16742	41.92
30	180	2.616	474	0.472	16744	42.00
30	185	2.619	474	0.448	16848	42.37
30	190	2.621	473	0.418	17015	42.87
30	195	2.620	473	0.380	17332	43.62
30	200	2.617	474	0.339	17599	44.20

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**Fig. S5** Variation of OPA oscillator strengths with tilt and twist angles (see Figure 1 in the main text) for Model 21 at fixed  $\theta_{acylimine}$  of  $0^\circ$ ,  $90^\circ$ ,  $180^\circ$  and  $270^\circ$ . The OPA values are for the transition to  $S_1$  as determined at the B3LYP/6-31G+(d,p) level of theory and PCM with parameters for  $H_2O$ .

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## References

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