Computational prediction of absorbance maxima for a structurally diverse series of engineered green fluorescent protein chromophores

Supporting Information

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Table S1. Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with TD-PBE.

	TD-PBE/6-31+G(d,p)				TD-PBE/6-311++G(2df,2p)			
	gas phase		PCM water		gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*
Y66$_{12}$	2.97	0.79	2.86	0.93	2.95	0.77	2.85	0.93
Y66$_{2.3}$	3.30	0.62	3.11	0.76	3.27	0.61	3.09	0.75
Y66W	3.07	0.41	2.91	0.54	3.05	0.40	2.89	0.54
Y66F	3.40	0.48	3.26	0.56	3.38	0.49	3.24	0.56
Y66H$_7$	3.47	0.42	3.30	0.51	3.43	0.41	3.27	0.50
Y66H$_{2.3}$	3.39	0.29	3.32	0.40	3.37	0.30	3.30	0.41
Y66H$_{12}$	3.32	0.63	3.23	0.72	3.30	0.61	3.22	0.72
Y66D$_7$	1.98	0.01	3.63	0.19	1.97	0.01	3.62	0.18
Y66S	3.98	0.09	5.71	0.25	3.94	0.09	5.68	0.25
Y66L$_{ox2}$	3.56	0.30	3.42	0.35	3.53	0.30	3.39	0.34

Table S2 Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with.

	TD-B3LYP/6-31+G(d,p)				TD-B3LYP/6-311++G(2df,2p)			
	gas phase		PCM water		gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*
Y66$_{12}$	3.10	0.90	2.99	1.03	3.07	0.88	2.97	1.01
Y66$_{2.3}$	3.54	0.70	3.34	0.83	3.50	0.68	3.31	0.82
Y66W	3.34	0.53	3.14	0.67	3.31	0.52	3.12	0.66
Y66F	3.65	0.60	3.49	0.69	3.61	0.59	3.46	0.67
Y66H$_7$	3.69	0.49	3.49	0.59	3.64	0.48	3.45	0.58
Y66H$_{2.3}$	3.68	0.40	3.57	0.53	3.64	0.39	3.54	0.52
Y66H$_{12}$	3.46	0.75	3.36	0.83	3.42	0.74	3.33	0.82
Y66D$_7$	2.76	0.01	3.93	0.25	2.75	0.01	3.90	0.25
Y66S	6.19	0.22	6.02	0.27	6.14	0.21	5.98	0.26
Y66L$_{ox2}$	3.85	0.44	3.69	0.49	3.81	0.42	3.66	0.47

Table S3 Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with TD-BLYP.

	TD-BLYP/6-31+G(d,p)				TD-BLYP/6-311++G(2df,2p)			
	gas phase		PCM water		gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*
Y66$_{12}$	2.95	0.78	2.84	0.93	2.93	0.72	2.83	0.91
Y66$_{2.3}$	3.28	0.62	3.09	0.75	3.26	0.61	3.08	0.75
Y66W	3.04	0.40	2.88	0.53	3.02	0.39	2.87	0.53
Y66F	3.39	0.49	3.25	0.58	3.37	0.50	3.23	0.58
Y66H$_7$	3.45	0.42	3.28	0.51	3.41	0.41	3.26	0.52
Y66H$_{2.3}$	3.37	0.29	3.30	0.41	3.36	0.30	3.29	0.42
Y66H$_{12}$	3.29	0.62	3.21	0.72	3.27	0.60	3.20	0.72
Y66D$_7$	2.00	0.01	3.62	0.19	2.16	0.01	3.60	0.19
Y66S	3.96	0.09	5.67	0.25	3.93	0.09	5.63	0.25
Y66L$_{ox2}$	3.55	0.31	3.41	0.36	3.52	0.31	3.38	0.35

Table S4 Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with TD-TPSSh.

	TD-TPSSh /6-31+G(d,p)				TD-TPSSh/6-311++G(2df,2p)			
	gas phase		PCM water		gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*
Y66$_{12}$	3.10	0.88	2.99	1.02	3.08	0.86	2.97	1.00
Y66$_{2.3}$	3.49	0.68	3.30	0.82	3.46	0.67	3.27	0.80
Y66W	3.29	0.50	3.11	0.64	3.27	0.49	3.09	0.63
Y66F	3.60	0.57	3.45	0.65	3.57	0.55	3.42	0.64
Y66H$_7$	3.66	0.47	3.47	0.57	3.61	0.46	3.43	0.56
Y66H$_{2.3}$	3.62	0.36	3.53	0.49	3.59	0.36	3.49	0.49
Y66H$_{12}$	3.46	0.72	3.36	0.80	3.43	0.71	3.33	0.79
Y66D$_7$	2.47	0.01	3.87	0.22	2.47	0.01	3.84	0.22
Y66S	6.14	0.22	5.99	0.27	6.09	0.22	5.95	0.27
Y66L$_{ox2}$	3.80	0.39	3.64	0.44	3.76	0.38	3.61	0.43

Table S5 Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with TD-TPSS.

	TD-TPSS /6-31+G(d,p)				TD-TPSS/6-311++G(2df,2p)			
	gas phase		PCM water		gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*	ΔE, eV	*f*
$Y66_{12}$	3.04	0.82	2.92	0.96	3.02	0.81	2.90	0.96
$Y66_{2.3}$	3.37	0.65	3.18	0.78	3.35	0.64	3.16	0.77
Y66W	3.15	0.43	2.98	0.56	3.13	0.43	2.97	0.57
Y66F	3.48	0.51	3.33	0.59	3.46	0.52	3.31	0.60
$Y66H_7$	3.54	0.44	3.37	0.53	3.51	0.43	3.34	0.54
$Y66H_{2.3}$	3.47	0.31	3.40	0.44	3.46	0.32	3.38	0.44
$Y66H_{12}$	3.39	0.65	3.29	0.75	3.36	0.64	3.28	0.75
$Y66D_7$	2.10	0.01	3.72	0.20	2.44	0.00	3.71	0.19
Y66S	4.08	0.10	5.82	0.26	4.04	0.09	5.79	0.26
$Y66L_{ox2}$	3.65	0.33	3.50	0.37	3.62	0.32	3.48	0.37

Table S6 Excitation energies of the model chromophores and oscillator strengths in the gas phase and water calculated with TD-SVWN.

	TD-SVWN/6-31+G(d,p)			
	gas phase		PCM water	
Chromophore	ΔE, eV	*f*	ΔE, eV	*f*
Y66$_{12}$	2.99	0.79	2.87	0.92
Y66$_{2.3}$	3.29	0.62	3.10	0.76
Y66W	3.05	0.40	2.89	0.53
Y66F	3.40	0.48	3.26	0.56
Y66H$_7$	3.47	0.41	3.29	0.51
Y66H$_{2.3}$	3.39	0.29	3.32	0.40
Y66H$_{12}$	3.34	0.63	3.24	0.71
Y66D$_7$	1.97	0.01	3.62	0.18
Y66S	5.86	0.21	5.72	0.25
Y66L$_{ox2}$	3.56	0.30	3.42	0.34

Table S7. Correlation parameters between the experimental and calculated excitation energies for GFP-like chromophores

	Gas phase				PCM water			
	Chromophores excluded	intercept	slope	R^2	Chromophores excluded	intercept	slope	R^2
CIS/6-31+G(d,p)	$Y66L_{ox2}$	-0.38	1.49	0.882	$Y66L_{ox2}$	0.35	1.27	0.853
CIS/6-311++G(2df,2p)	$Y66L_{ox2}$	-0.28	1.45	0.881	$Y66L_{ox2}$	0.40	1.24	0.853
	Y66S, $Y66L_{ox2}$				Y66S, $Y66L_{ox2}$	1.00	1.05	0.909
CIS(D)/6-31+G(d,p)	$Y66L_{ox2}$	-1.75	1.72	0.923	$Y66L_{ox2}$	-0.69	1.39	0.950
CIS(D)/6-311++G(2df,2p)	$Y66L_{ox2}$	-1.46	1.61	0.923	$Y66L_{ox2}$	-0.47	1.30	0.948
	Y66S, $Y66L_{ox2}$				Y66S, $Y66L_{ox2}$	0.42	1.03	0.960
PBE0/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.28	0.71	0.896	Y66S, $Y66L_{ox2}$	0.88	0.79	0.919
PBE0/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.30	0.69	0.902	Y66S, $Y66L_{ox2}$	0.88	0.78	0.921
PBE/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.54	0.54	0.768	Y66S, $Y66L_{ox2}$	1.13	0.63	0.828
PBE/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.52	0.54	0.783	Y66S, $Y66L_{ox2}$	1.12	0.63	0.828
B3LYP/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.28	0.69	0.893	Y66S, $Y66L_{ox2}$	0.89	0.77	0.912
B3LYP/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.30	0.67	0.899	Y66S, $Y66L_{ox2}$	0.90	0.76	0.913
BLYP/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.46	0.56	0.788	Y66S, $Y66L_{ox2}$	1.08	0.64	0.834
BLYP/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.43	0.56	0.812		1.08	0.64	0.834
TPSSh/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.46	0.62	0.856	Y66S, $Y66L_{ox2}$	1.11	0.65	0.842
TPSSh/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.47	0.61	0.865	Y66S, $Y66L_{ox2}$	1.03	0.71	0.884
TPSS/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.55	0.56	0.789	Y66S, $Y66L_{ox2}$	1.13	0.65	0.840
TPSS/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.53	0.56	0.814	Y66S, $Y66L_{ox2}$	1.04	0.71	0.888
SVWN/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	1.58	0.53	0.733	Y66S, $Y66L_{ox2}$	1.14	0.62	0.814

Table S8. Correlation parameters between the experimental and calculated oscillator strengths for GFP-like chromophores

	Gas phase				PCM water			
	Chromophores excluded	intercept	slope	R^2	Chromophores excluded	intercept	slope	R^2
CIS/6-31+G(d,p)	$Y66L_{ox2}$			0.348				0.371
CIS/6-311++G(2df,2p)	$Y66L_{ox2}$			0.350				0.189
PBE0/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.01	1.17	0.620	Y66S, $Y66L_{ox2}$	0.03	1.29	0.841
PBE0/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.01	1.15	0.623	Y66S, $Y66L_{ox2}$	0.03	1.27	0.845
PBE/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.13	1.15	0.659	Y66S, $Y66L_{ox2}$	-0.07	1.24	0.847
PBE/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.09	1.08	0.636	Y66S, $Y66L_{ox2}$	-0.07	1.25	0.844
B3LYP/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.01	1.13	0.609	Y66S, $Y66L_{ox2}$	0.02	1.27	0.833
B3LYP/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.03	1.18	0.717	Y66S, $Y66L_{ox2}$	-0.01	1.29	0.833
BLYP/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.11	1.11	0.631	Y66S, $Y66L_{ox2}$	-0.07	1.30	0.906
BLYP/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.03	0.95	0.600	Y66S, $Y66L_{ox2}$	-0.07	1.29	0.912
TPSS/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.06	1.18	0.638	Y66S, $Y66L_{ox2}$	-0.05	1.27	0.842
TPSS/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.06	1.16	0.644	Y66S, $Y66L_{ox2}$	-0.05	1.27	0.850
TPSSh/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.12	1.18	0.649	Y66S, $Y66L_{ox2}$	-0.02	1.31	0.848
TPSSh/6-311++G(2df,2p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.08	1.11	0.622	Y66S, $Y66L_{ox2}$	-0.03	1.29	0.854
SVWN/6-31+G(d,p)	Y66S, $Y66L_{ox2}$, $Y66D_7$	-0.13	1.16	0.647	Y66S, $Y66L_{ox2}$	-0.09	1.32	0.913

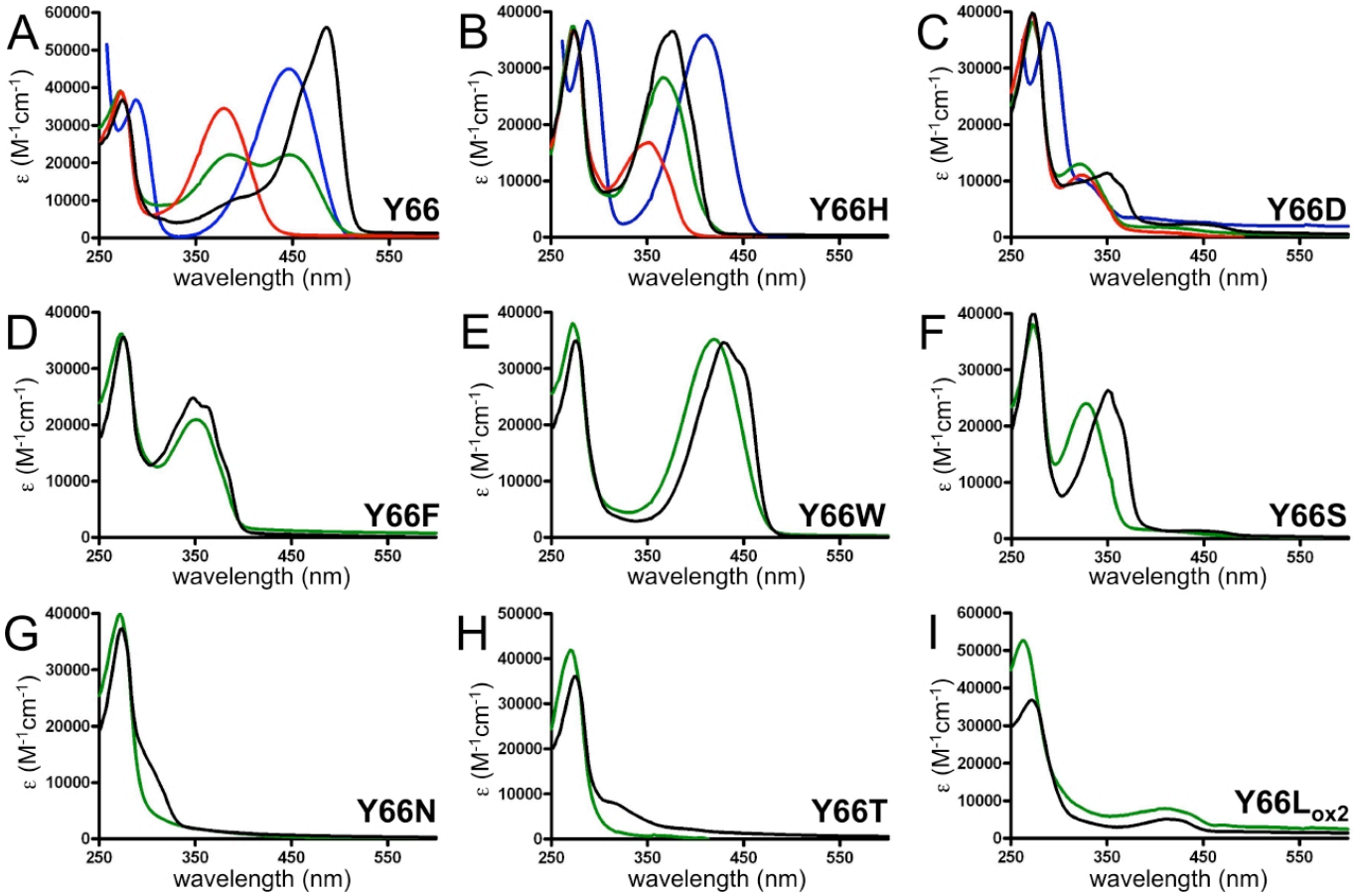

Figure S1. Absorbance spectra for all GFP variants investigated in this work. (A) EGFP (**Y66**); (B) EBFP (**Y66H**); (C) EGFP-T65A/Y66D (**Y66D**); (D) EGFP-T65A/Y66F (**Y66F**); (E) ECFP (**Y66W**); (F) EGFP-T65A/Y66S (**Y66S**); (G) EGFP-T65A/Y66N (**Y66N**); (H) EGFP-T65A/Y66T (**Y66T**); and (I) EGFP-T65A/Y66L (**Y66L$_{ox2}$**). For all GFP variant the absorption spectrum for both the native protein (black) and denatured protein at pH 7 (green) is provided. For those variants with ionizable chromophores, the absorption spectrum for denatured protein at both pH 2.3 (red) and pH 12 or 13 (blue) is also provided.

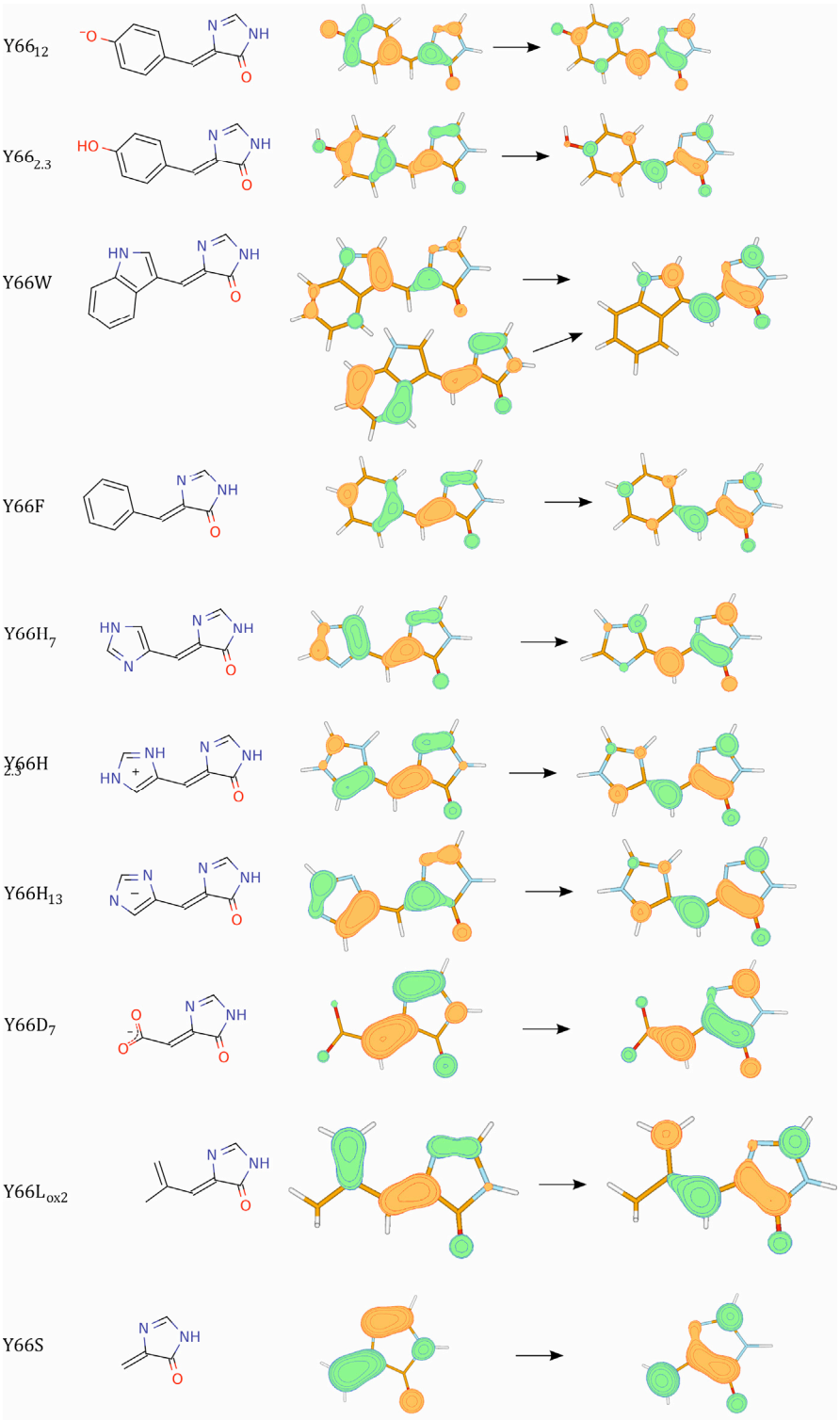

Figure S2. Structures of the model chromophores and the orbital transitions corresponding to the S_0 → S_1 transition as predicted by the CIS/6-31+G(d,p) calculations.

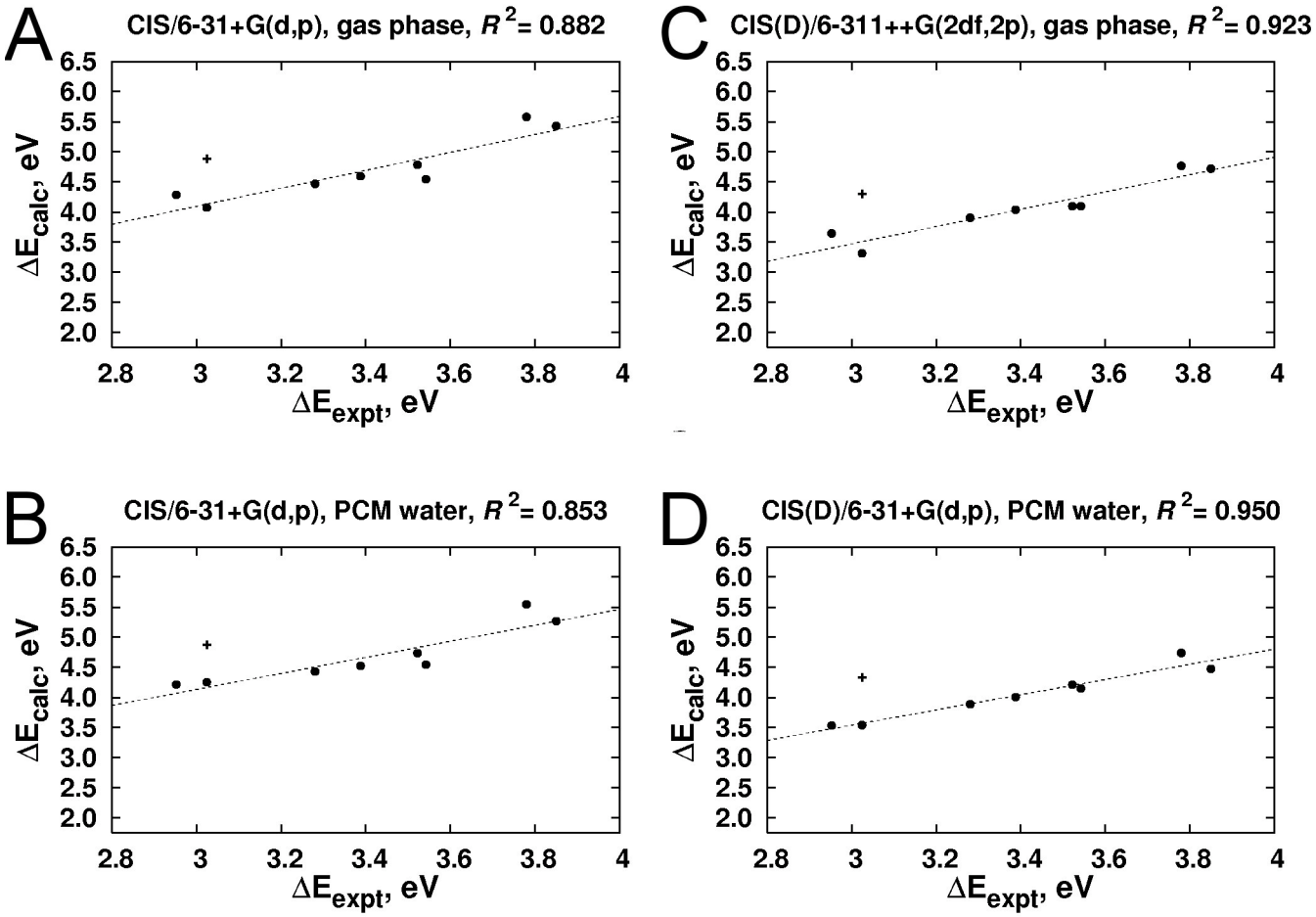

Figure S3. Correlation between calculated and experimental exaction energies (A) and oscillator strengths (B) of the model chromophores: CIS/6-31+G(d,p) and CIS(D)/6-31+G(d,p) calculations. **Y66L$_{ox2}$** is excluded from the correlation and shown as "**+**".

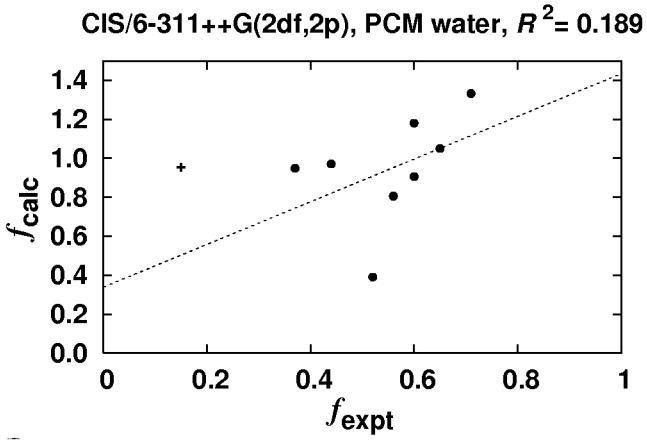

Figure S4. Correlation between calculated and experimental oscillator strengths of the model chromophores: CIS/6-311++G(2df,2p) calculations.

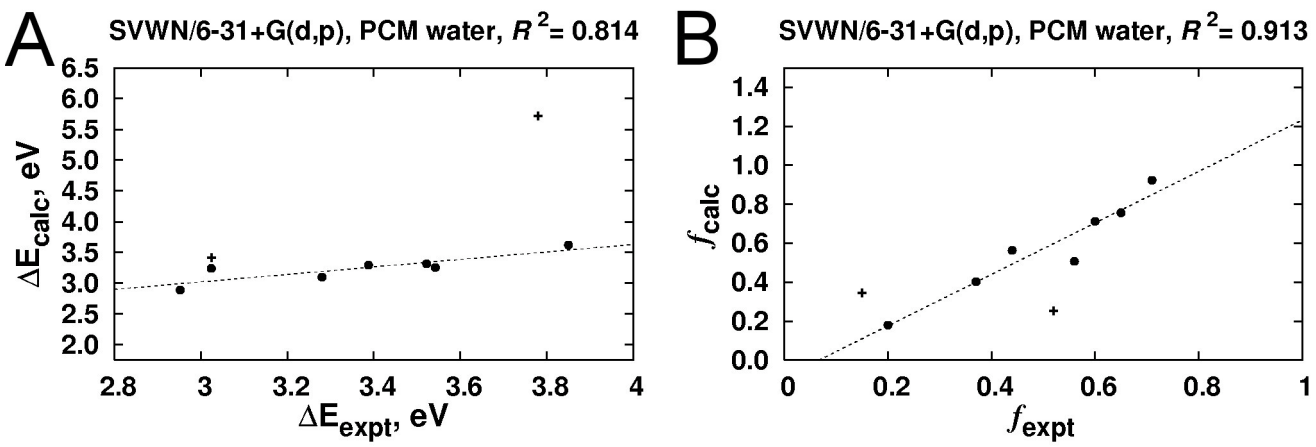

Figure S5. Correlation between calculated and experimental exaction energies (A) and oscillator strengths (B) of the model chromophores: SVWN/6-311++G(2df,2p) calculations. **Y66S** and **Y66L$_{ox2}$** are excluded from correlation. The excluded points are shown as "**+**".

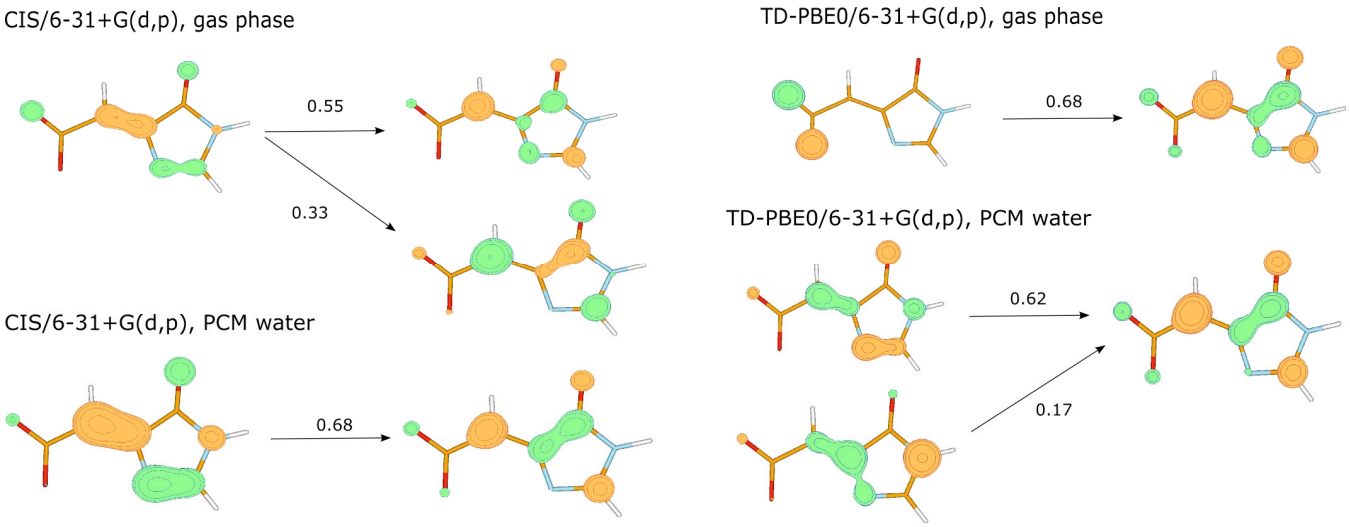

Figure S8. The orbital transitions corresponding to the $S_0 \rightarrow S_1$ transition of **Y66D$_7$** as predicted by the CIS and TD-PBE0 calculations in the gas phase and in water.

Calculated Cartesian coordinates (in Å) and energies (in Hartrees) for the model chromophores

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Y6612 PBE0/6-311++G(2DF,2P)
-1,1
C,3.2206444757,-0.8562761081,0.
C,1.9193661636,-1.2519223486,0.
C,3.5937037538,0.5434543027,0.
C,2.4750729354,1.4675676438,0.
C,0.8355278449,-0.3284771578,0.
C,1.1793260076,1.0552715673,0.
C,-0.4750721681,-0.8206177387,0.
C,-1.7033533741,-0.1899753912,0.
N,-1.9597317758,1.1826296833,0.
C,-3.243198348,1.3030028618,0.
C,-2.9545239475,-0.9301493389,0.
N,-3.9035780089,0.0995664877,0.
O,4.7782047241,0.9241254131,0.
H,-4.8943952544,-0.0554059152,0.
H,-3.7764003891,2.2446147422,0.
O,-3.2283284603,-2.1264331987,0.
H,4.028753072,-1.5797538015,0.
H,1.6787753408,-2.3125047816,0.
H,2.7222581557,2.5240315389,0.
H,0.3708177298,1.7760710041,0.
H,-0.5706103316,-1.9052334542,0.
E=-644.7765676


Y662.3 PBE0/6-311++G(2DF,2P)
0,1
C,1.5971631972,3.103752046,0.
H,2.5948031431,3.5235375716,0.
C,-0.6448828471,3.101721667,0.
O,-1.7922536582,3.4801174462,0.
C,-0.0500091052,1.7420730004,0.
N,0.4905467623,3.9121732995,0.
N,1.3442588608,1.841974086,0.
H,0.4715618058,4.9162013144,0.
C,-0.8145787425,0.6300411931,0.
H,-1.8826351826,0.8325090331,0.
C,-0.4321013058,-0.7578086343,0.
C,-1.4418320326,-1.7314449003,0.
C,0.9007272258,-1.1956939294,0.
C,-1.1508647824,-3.0786433188,0.
H,-2.4781964096,-1.4129794745,0.
C,1.199331169,-2.5417960231,0.
H,1.6940009523,-0.4605942795,0.
C,0.1779059691,-3.4899022996,0.
H,-1.9340726466,-3.8254534438,0.
H,2.2349484743,-2.8672339346,0.
O,0.4224443282,-4.8182656885,0.
H,1.3692726673,-4.9736253517,0.
E=-645.3117645

Y66W PBE0/6-311++G(2DF,2P)
0,1
C,3.4350275313,2.0868118837,0.
H,4.5139272759,2.0010011257,0.
C,1.439699034,3.11387386,0.
O,0.5962869598,3.9809990864,0.
C,1.346164912,1.6393589738,0.
```

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N,2.6278028187,1.0830855456,0.
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H,-0.7113149449,1.6099242903,0.
C,-0.0436500818,-0.4330435789,0.
C,-1.3218982619,-1.1037114425,0.
C,0.9125166263,-1.431398309,0.
C,-1.062685999,-2.4876259789,0.
C,-2.6468444077,-0.6671769783,0.
N,0.3059687633,-2.6432447567,0.
C,-2.0735458029,-3.4395677907,0.
C,-3.6589230549,-1.607186486,0.
H,-2.8826544544,0.3902996833,0.
H,0.7878704431,-3.5235036689,0.
C,-3.3763673029,-2.9788090652,0.
H,-1.8538310527,-4.5005582561,0.
H,-4.6915324818,-1.2809267748,0.
H,-4.1925575902,-3.6903924438,0.
H,1.9848009748,-1.3247608567,0.
E=-701.6069125

Y66F PBE0/6-311++G(2DF,2P)
0,1
C,1.5315066442,2.7418508159,0.
H,2.509473604,3.2058013536,0.
C,-0.7069960616,2.6421812167,0.
O,-1.8694422323,2.9664501553,0.
C,-0.0509281913,1.3064957849,0.
N,0.3906545461,3.5015477852,0.
N,1.3367208691,1.4700433154,0.
H,0.3281470746,4.5038812957,0.
C,-0.768121179,0.165904397,0.
H,-1.8436317597,0.3235151864,0.
C,-0.3281174365,-1.2107219034,0.
C,-1.3069833798,-2.2129952432,0.
C,1.0215447771,-1.5918386928,0.
C,-0.9571050883,-3.5510652156,0.
H,-2.3528539876,-1.9270974537,0.
C,1.3653624218,-2.9307753055,0.
H,1.783051971,-0.8242876675,0.
C,0.3823801304,-3.9137166238,0.
H,-1.7279134817,-4.3118759123,0.
H,2.410950746,-3.214129909,0.
H,0.6614299627,-4.9604612199,0.
E=-570.1311521

Y66H7 PBE0/6-311++G(2DF,2P)
0,1
C,1.5997900908,2.3381319181,0.
H,2.6049660019,2.7398462674,0.
C,-0.6440221444,2.3772345589,0.
O,-1.7823049724,2.7796637003,0.
C,-0.0733471483,1.0097333703,0.
N,0.5088347201,3.1666349988,0.
N,1.3231634636,1.0809087448,0.
C,-0.8249331155,-0.1085585143,0.
H,-1.9013422705,0.0256265941,0.
C,-0.3584866546,-1.4599184653,0.
H,-0.8814027187,-4.6068094958,0.
H,0.5083223866,4.1708456568,0.
C,-0.517523187,-3.5911262247,0.

C,0.9343551821,-1.9415192643,0.
N,-1.2473750047,-2.5160180936,0.
N,0.8132559549,-3.2935269662,0.
H,1.5708192283,-3.9534602608,0.
H,1.8769250767,-1.4232134229,0.
E=-564.135427

Y66H2.3 PBE0/6-311++G(2DF,2P)
1,1
C,1.6441250083,2.1439402049,0.
H,2.6899047573,2.4223495051,0.
C,-0.5777380363,2.4313245297,0.
O,-1.6616397941,2.9342853223,0.
C,-0.1640118923,0.9942840511,0.
N,0.6648039336,3.0800916638,0.
N,1.2262190589,0.9149726068,0.
C,-1.0127051358,-0.0469306021,0.
H,-2.0780325436,0.1454428898,0.
C,-0.5558272784,-1.4045726771,0.
C,0.9465860503,-3.0295903018,0.
N,-0.2655417325,-3.5794427035,0.
H,-0.4431450335,-4.5720778036,0.
N,0.7883598886,-1.7209513088,0.
H,1.882082341,-3.5632430492,0.
C,-1.222407533,-2.6000303727,0.
H,-2.2756958347,-2.8196812896,0.
H,0.7882131999,4.0794484808,0.
H,1.4847763308,-0.9597621125,0.
E=-564.5224976

Y66H12 PBE0/6-311++G(2DF,2P)
-1,1
C,1.6236785599,2.4557952491,0.
H,2.5923746184,2.939433183,0.
C,-0.6199148301,2.2977803566,0.
O,-1.7999663648,2.6335184633,0.
C,0.0532386782,1.0025344588,0.
N,0.4563904526,3.1876247973,0.
N,1.4379844073,1.1835509813,0.
C,-0.6574292061,-0.1738711107,0.
H,-1.7329908361,-0.0044863271,0.
C,-0.2881742619,-1.5223944874,0.
C,0.7411830576,-3.3614064157,0.
N,-0.5708342245,-3.7564992692,0.
N,0.9778324599,-2.0684796618,0.
H,1.5407549451,-4.0940472252,0.
C,-1.2142621578,-2.596447768,0.
H,-2.2963155277,-2.5298161218,0.
H,0.3563770134,4.1854491551,0.
E=-563.5871206

Y66D7 PBE0/6-311++G(2DF,2P)
-1,1
C,1.4823132904,1.877857106,0.
H,2.4123476207,2.4345054211,0.
C,-0.7424139865,1.5820957886,0.
O,-1.9315933094,1.825783984,0.
C,0.027642214,0.3056347673,0.
N,0.2678351677,2.5383061455,0.
N,1.4039011572,0.6023551085,0.
H,0.1077610982,3.5286027182,0.
C,-0.5871551367,-0.8903951531,0.

H,-1.6727282248,-0.8349395378,0.
C,-0.0307359046,-2.3186777708,0.
O,-0.9484461339,-3.1703590938,0.
O,1.1991097399,-2.4619106162,0.
E=-527.1646631

Y66S PBE0/6-311++G(2DF,2P)
0,1
C,1.593123464,-0.5223633107,0.
H,2.6452072805,-0.7786062335,0.
C,-0.1967171693,0.8289282823,0.
O,-0.8947049593,1.8095674618,0.
C,-0.5392017092,-0.6298913371,0.
N,1.1929793428,0.7948697001,0.
N,0.6430239184,-1.3841069444,0.
H,1.7830728902,1.6077297487,0.
C,-1.7804387918,-1.1077918447,0.
H,-2.6166195452,-0.420990908,0.
H,-1.9666385425,-2.1733023311,0.
E=-339.2736649

Y66Lox2 PBE0/6-311++G(2DF,2P)
0,1
C,1.3282911618,1.979790494,0.0426926294
H,2.2373617309,2.5669956485,0.0647716357
C,-0.8787341434,1.594973771,-0.0005018521
O,-2.0734470091,1.763662044,-0.0205019151
C,-0.0549699762,0.3528334871,0.0022399277
N,0.0973439631,2.5871972511,0.0270006777
N,1.3007338193,0.6944531272,0.0297061261
H,-0.0935684524,3.5731540199,0.0315198638
C,-0.6203201955,-0.8694652329,-0.0190198855
H,-1.7066108082,-0.8595216583,-0.0375727509
C,0.0098440223,-2.1714983492,-0.0206779064
C,-0.7915470029,-3.2476358941,-0.0477054646
C,1.5003174952,-2.3033006073,0.0068539929
H,-0.387126436,-4.2524004851,-0.0514897912
H,-1.8699881498,-3.1468238241,-0.0669818815
H,1.7909753162,-3.353284127,-0.0069219424
H,1.9538863144,-1.7950629363,-0.8446084368
H,1.9188139139,-1.8280916494,0.8950623479
E=-455.8901532

Y6612 PCM PBE0/6-311++G(2DF,2P)
-1,1
C,3.2197983747,-0.8509109472,0.
C,1.9120085877,-1.249180092,0.
C,3.584712397,0.5379437916,0.
C,2.4838838612,1.465114744,0.
C,0.8378657924,-0.3235395781,0.
C,1.1811066181,1.0532943862,0.
C,-0.4846225685,-0.8219410583,0.
C,-1.6994126099,-0.1876254107,0.
N,-1.9611876487,1.1871057468,0.
C,-3.2505082701,1.2935497468,0.
C,-2.9627961318,-0.9196009551,0.
N,-3.9040182597,0.0922598223,0.
O,4.7892393758,0.9231641694,0.
H,-4.9153971278,-0.043786243,0.
H,-3.7986850645,2.2306495337,0.

O,-3.2136794679,-2.1268349173,0.
H,4.0217788727,-1.5849745876,0.
H,1.6742558913,-2.3120709498,0.
H,2.7242512669,2.5257807621,0.
H,0.3822154648,1.7852804938,0.
H,-0.5686735135,-1.9096997733,0.
E=-644.8729361

Y66W PCM PBE0/6-311++G(2DF,2P)
0,1
C,3.4435965628,2.127676981,0.
H,4.5287451197,2.0746848301,0.
C,1.4395608718,3.1059513657,0.
O,0.5654958343,3.964062765,0.
C,1.3614927456,1.6362867291,0.
N,2.8006046018,3.3348096278,0.
N,2.6541358553,1.1038408617,0.
H,3.2452613562,4.2545872378,0.
C,0.1890924507,0.9529454836,0.
H,-0.7022343327,1.5801134544,0.
C,-0.0279430175,-0.449376693,0.
C,-1.3160014108,-1.1054932308,0.
C,0.9161184128,-1.4700403183,0.
C,-1.06816178,-2.4925631275,0.
C,-2.6376301361,-0.6551052962,0.
N,0.2975621069,-2.6656334902,0.
C,-2.0870198607,-3.437800407,0.
C,-3.658441808,-1.5888550462,0.
H,-2.8659473449,0.4076464765,0.
H,0.7774832545,-3.567590057,0.
C,-3.3871287488,-2.964991543,0.
H,-1.8691442711,-4.5023457743,0.
H,-4.6913437749,-1.2526554461,0.
H,-4.2121032053,-3.6713987104,0.
H,1.9939928864,-1.3984725107,0.
E=-701.6424303

Y66F PCM PBE0/6-311++G(2DF,2P)
0,1
C,1.5246305577,2.7643136981,0.
H,2.4972346234,3.2495902712,0.
C,-0.6985668444,2.6448358627,0.
O,-1.8769139751,2.954883744,0.
C,-0.0435981125,1.3099736519,0.
N,0.3759547455,3.5066750471,0.
N,1.3433301002,1.4851687906,0.
H,0.319436118,4.5276767232,0.
C,-0.7568602816,0.1652202784,0.
H,-1.837559593,0.3090062189,0.
C,-0.3179574663,-1.2128628883,0.
C,-1.30562315,-2.2087590116,0.
C,1.0294730847,-1.6051682193,0.
C,-0.9644899275,-3.5504508049,0.
H,-2.3524718096,-1.9135817778,0.
C,1.3653755809,-2.9473937145,0.
H,1.8028376428,-0.8484400459,0.
C,0.3736428519,-3.9236876253,0.
H,-1.7433819593,-4.3077424683,0.
H,2.4121108206,-3.2389823844,0.
H,0.6459542807,-4.9756307164,0.
E=-570.1562992

Y66H7 PCM PBE0/6-311++G(2DF,2P)
0,1
C,1.5945780496,2.3861356236,0.
H,2.5902212246,2.8216501741,0.
C,-0.6344503994,2.3763434701,0.
O,-1.7970733983,2.7497175271,0.
C,-0.0483210181,1.0188881119,0.
N,0.4830394356,3.184158653,0.
N,1.345844136,1.1180179813,0.
C,-0.7908286725,-0.1089719634,0.
H,-1.8716285642,0.0256571025,0.
C,-0.3413980324,-1.4635031269,0.
H,-0.9200479479,-4.6126198027,0.
H,0.4748419793,4.2065065809,0.
C,-0.5389130141,-3.5984732808,0.
C,0.9410425798,-1.981754086,0.
N,-1.253302468,-2.5050176871,0.
N,0.7900879332,-3.324853048,0.
H,1.5458072873,-4.0150479562,0.
H,1.9074529916,-1.5020161003,0.
E=-564.1736515

Y66H2.3 PCM PBE0/6-311++G(2DF,2P)
1,1
C,1.6283598185,2.247766758,0.
H,2.658436505,2.595605947,0.
C,-0.5930290736,2.430258249,0.
O,-1.7176769262,2.8863252013,0.
C,-0.1190631184,1.0192338626,0.
N,0.5914064405,3.1356603487,0.
N,1.2748555028,1.0030948394,0.
C,-0.9260241503,-0.0551987519,0.
H,-2.0028024003,0.1016088114,0.
C,-0.4797688157,-1.4119380385,0.
C,0.9079049416,-3.1306569422,0.
N,-0.3336094185,-3.601342187,0.
H,-0.5779455279,-4.6019807076,0.
N,0.8417907005,-1.8124929712,0.
H,1.8143873645,-3.7255286758,0.
C,-1.2182016408,-2.5661989753,0.
H,-2.2902002765,-2.7138260837,0.
H,0.6740766124,4.1564111442,0.
H,1.6432927872,-1.1769292264,0.
E=-564.6310909

Y66H12 PCM PBE0/6-311++G(2DF,2P)
-1,1
C,1.6188784076,2.442276133,0.
H,2.5904097704,2.9271972897,0.
C,-0.6077526463,2.3086479575,0.
O,-1.7948536978,2.6369773354,0.
C,0.0390695284,0.9950043846,0.
N,0.4639621158,3.1779059884,0.
N,1.4284347455,1.1638669011,0.
C,-0.6826766559,-0.1647934141,0.
H,-1.761540762,-0.004578438,0.
C,-0.304234098,-1.5210121872,0.
C,0.7573705981,-3.3556158895,0.
N,-0.5453293205,-3.7538875559,0.
N,0.9699495897,-2.05164938,0.
H,1.5692742006,-4.0773261582,0.
C,-1.2135511356,-2.5957107934,0.

H,-2.2978764636,-2.5439972574,0.
H,0.3968189336,4.1964570607,0.
E=-563.6914813

Y66D7 PCM PBE0/6-311++G(2DF,2P)
-1,1
C,1.4715979298,1.8771413939,0.
H,2.4018308547,2.4402806764,0.
C,-0.7330130783,1.5914518448,0.
O,-1.9296875336,1.8027764786,0.
C,0.0291191553,0.2976426248,0.
N,0.2677367677,2.5321100197,0.
N,1.3988525879,0.5895174946,0.
H,0.1341405119,3.5461849054,0.
C,-0.605249312,-0.8826550144,0.
H,-1.6919064115,-0.8257556599,0.
C,-0.0427478167,-2.2825846828,0.
O,-0.9184436008,-3.1851424417,0.
O,1.1945771702,-2.4448939768,0.
E=-527.2883869

Y66S PCM PBE0/6-311++G(2DF,2P)
0,1
C,1.5950058393,-0.5167735493,0.
H,2.6544003785,-0.7620365336,0.
C,-0.1855080584,0.8236440461,0.
O,-0.8975637723,1.807063882,0.
C,-0.5407132263,-0.6306716227,0.
N,1.188120487,0.7938758269,0.
N,0.6427046127,-1.3847425724,0.
H,1.802057125,1.6126752837,0.
C,-1.7837438029,-1.1058800668,0.
H,-2.6235349766,-0.421080732,0.
H,-1.9784325568,-2.1719146994,0.
E=-339.2954226

Y66Lox2 PCM PBE0/6-311++G(2DF,2P)
0,1
C,1.3205659961,1.9991299052,0.0484902011
H,2.2211321306,2.6071681332,0.0741896932
C,-0.8684022833,1.5969040826,-0.0027760838
O,-2.0773091076,1.7497226367,-0.0274999508
C,-0.0459785823,0.3554570172,0.0025518228
N,0.0836475048,2.5883552689,0.0275738127
N,1.3077057029,0.7086856722,0.035085397
H,-0.1051316015,3.5932959908,0.0350396586
C,-0.6103307923,-0.8688850553,-0.0208877095
H,-1.6999984019,-0.8664987971,-0.0428611554
C,0.0128376093,-2.1749817252,-0.0208787676
C,-0.7985385765,-3.245001192,-0.0434660651
C,1.5020202018,-2.3238136114,0.0027567397
H,-0.401177504,-4.2541510379,-0.0446853336
H,-1.8772775556,-3.1324201273,-0.0611454271
H,1.7794161548,-3.3776084545,-0.002253377
H,1.9586630617,-1.8322022666,-0.8576398857
H,1.9303276164,-1.8475101239,0.8862535817
E=-455.9108004