Supporting information

Tuning the Fluorescence of Calcium-discharged Photoprotein Obelin via Mutating at the His22-Phe88-Trp92 Triad– a QM/MM Study

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CONTENTS

Computational details

Force Field Parameters

The AMBER Parm99SB force field[1] was used to model the amino acid residues and water. The atom types of the substrate molecule CLM were assigned according to the standard AMBER atom type. The equilibrium bond lengths, angles, dihedral angles, force constants, and van der Waals parameters for the atom types of CLM were similar to those defined in the AMBER Parm99SB force field. The restricted electrostatic potential (RESP) charges were determined by the RESP fitting protocol implemented in the ANTECHAMBER module of the Amber10 package[2] after the calculations of ESP of CLM at the HF/6-31G(d,p) level. Calcium ion parameter used in this study was based on this paper (*J. Chem. Soc. Faraday Trans.* 1998, **94**, 1603-1611).[3]

MM Minimization

The crystal structures of Calcium-discharged obelin (WT, PDB: 2F8P)[4] and its F88Y mutant (PDB: 4N1G)[5] were downloaded from the Protein Data Bank. Basing on the crystal structure of WT, we constructed the mutants H22F, H22R, H22E, W92A, W92Y, and W92R. The mutants F88A and F88E were constructed according to the crystal structure of F88Y. Now our targeted systems are WT and its nine mutants. For each starting structure, the missing residues were added by the ModLoop.[6] The H++ program[7] was used to identify the protonation state of histidine residue. Herein, the His64 was protonated and the His22 held electronic neutrality in these proteins according to our previous study.[8] The identification of protonation states of the ionizable amino acid residues as well as the C−/N−terminal, and the addition of hydrogen atoms were performed by the LEAP module of the AMBER10 package.[2] Sodium ions were added in order to ensure the electric neutrality of the whole system by Amber tools. Each structure was immersed in a octahedral TIP3P[9] water box with a minimum solute wall distance of 10 Å using the LEAP module. The energies of these systems were minimized as follows. First, the heavy atoms were frozen, permitting the hydrogen atoms to move during a 4000-step minimization. Second, the protein and CLM were frozen, and the water molecules were allowed to move during a 4000-step minimization. The MM minimizations were performed via using the AMBER Parm99SB force field.[10]

MD Simulation

The optimized structures above were heated stepwise to 300 K in 50 ps with protein fixed. The Molecular Dynamics (MD) simulation was performed using the periodic boundary conditions at constant temperature T = 300 K and pressure P = 1 atm. The time step used for the MD simulations was 2 fs. A default cutoff radius of 10 Å was introduced for nonbonding interactions. The electrostatic interactions were calculated by means of the Particle Mesh Ewald method.[11] The SHAKE algorithm[12] was used to constrain all the bonds involving hydrogen atoms. The coordinates of the simulated systems were collected every 1 ps during MD simulation.

QM/MM Calculations

We extracted CLM, water molecules within 10 Å of CLM, photoprotein residues from the selected snapshot structures. CLM and triad His22-Phe88-Trp92 (or triad variants) comprised the QM region, while the remaining atoms were included in the

MM region. Herein, CLM was a phenolate anion and His22 held electronic neutrality, which was based on our previous study.[8] The covalent bond between C_β and C_α of triad was cut. QM/MM boundary was treated by link atom approach,[13] and hydrogen atom was used as link atom. The calculations of QM subsystem were performed using density functional theory (DFT) and time-dependent DFT (TDDFT).[14] The Coulomb-attenuated hybrid exchange-correlation functional (CAM-B3LYP)[15] and 6-31G(d,p) basis set were employed.[16, 17] The validity of QM system was also tested. (See Table S1) The side chains of nine amino acids (Ala46, His64, Ile111, Trp114, Tyr138, Thr172, His175, Trp179, and Tyr190) and the selected water molecules were allowed to relax in the MM subsystem, while the other atoms of MM region were kept frozen. The AMBER Parm99SB force field[10] was used for the MM optimization. The microiterations technique[18] was used to converge the MM subsystem geometry at every QM optimization step. The QM/MM calculations were performed using the coupling scheme implemented between Gaussian 09 A.02[19] and TINKER 4.2.[20]

Table S1 The maximum wavelengths of fluorescence (λ_{max} in nm) and absorption spectra (λ_{abs} in nm) as well as their oscillator strengths (f) of the QM subsystem (CLM+triad) of the wild-type calcium-discharged photoprotein obelin (CaDP-obelin) calculated at the TD CAM-B3LYP/6-31G(d,p)/MM level starting from three different initial equilibrium structures from the MD trajectory

Snapshots	λ_{max}	f	λ_{abs}	f
original	516	0.11	381	0.44
1000 ps	506	0.15	374	0.44
1900 ps	508	0.12	371	0.46
2600 ps	521	0.12	388	0.38

Table S2 The maximum wavelength of fluorescence (λ_{max} in nm) and oscillator strengths (f) of CLM with His22, Phe88 or Trp92 as QM subsystem in WT calculated at the TD CAM-B3LYP/6-31G(d,p)/MM level

QM area	λ_{max}	f
CLM	580	0.07
CLM+His22	534	0.10
CLM+His22+Phe88	523	0.13
CLM+His22+Trp92	519	0.13
CLM+triad (His22+Phe88+Trp92)	516	0.11
WT FL in experiment[21]	510	--

To test the validity of QM subsystem (CLM+triad), the S_1-state geometries and the maximum wavelength of fluorescence (λ_{max}) with oscillator strength f of additional four different QM subsystems, i.e., CLM, CLM+His22, CLM+His22+Phe88, CLM+His22+Phe88, and CLM+His22+Trp92 were calculated. As shown in Table S2, the λ_{max} of CLM+triad (516 nm) is closest to the value measured in the experimental study (510 nm).[21] Hence, it is reasonable to select (CLM+triad) as QM subsystem to investigate the color-tuning of calcium-discharged obelin.

Table S3 The maximum wavelengths of fluorescence (λ_{max} in nm) and oscillator strength (f) of the QM subsystem (CLM+triad) in ten CaDPs using larger basis sets, 6-311G(d,p), 6-31+G(d,p), and 6-311+G(d,p) based on the optimized S_1 structure using 6-31G(d,p) calculated at the TD CAM-B3LYP/MM level

CaDPs	6-31G(d,p)		6-311G(d,p)		6-31+G(d,p)		6-311+G(d,p)	
	λ_{max}	f	λ_{max}	f	λ_{max}	f	λ_{max}	f
WT	516	0.11	516	0.12	530	0.13	532	0.13
H22F	550	0.12	548	0.13	565	0.13	567	0.13
H22R	430	0.20	431	0.21	440	0.21	443	0.21
H22E	656	0.09	654	0.09	674	0.09	677	0.10
F88A	529	0.11	529	0.11	537	0.12	540	0.12
F88Y	483	0.14	486	0.15	495	0.16	498	0.16
F88E	662	0.07	665	0.07	674	0.08	678	0.08
W92A	509	0.13	510	0.13	519	0.14	522	0.14
W92Y	478	0.16	481	0.16	491	0.17	495	0.17
W92R	375	0.41	379	0.40	387	0.39	390	0.39

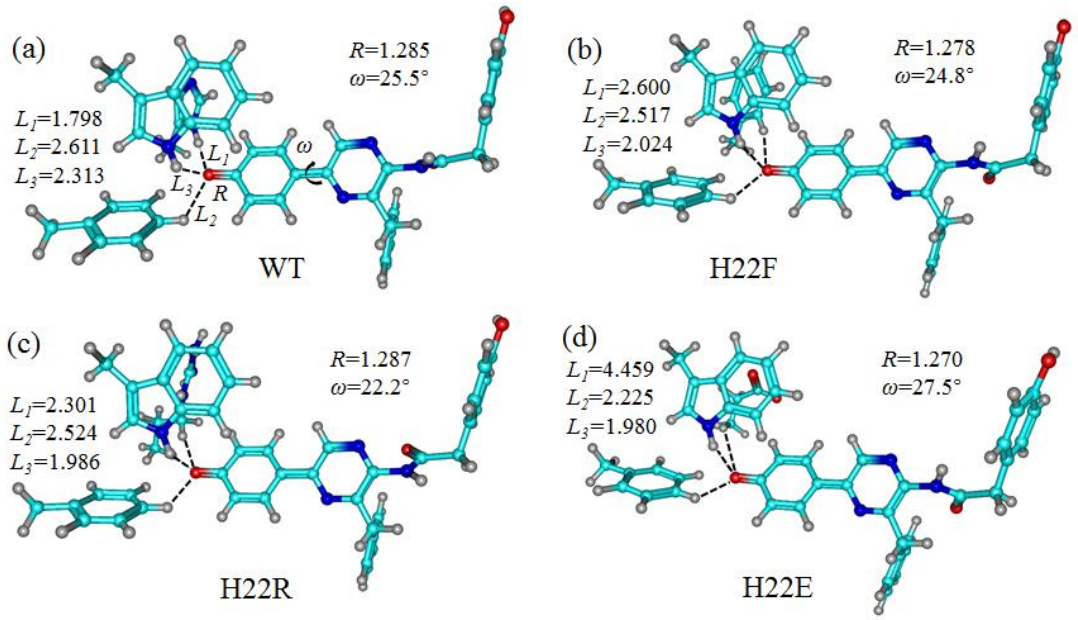


Fig. S1 The optimized S_0-state geometries of CLM with triad in WT (a), H22F (b), H22R (c), and H22E (d) calculated at the CAM-B3LYP/6-31G(d,p)/MM level.

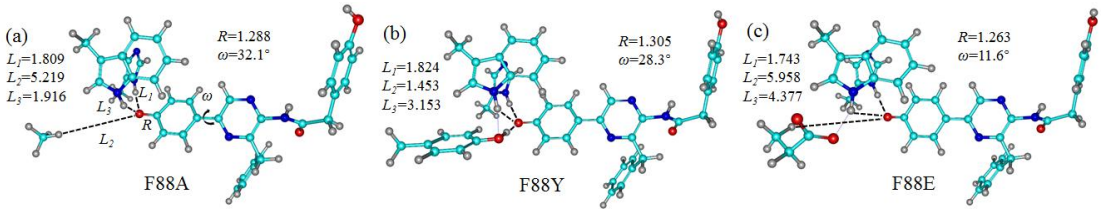


Fig. S2 The optimized S_0 geometries of CLM with triad in F88A (a), F88Y (b), and F88E (c) calculated at the CAM-B3LYP/6-31G(d,p)/MM level.

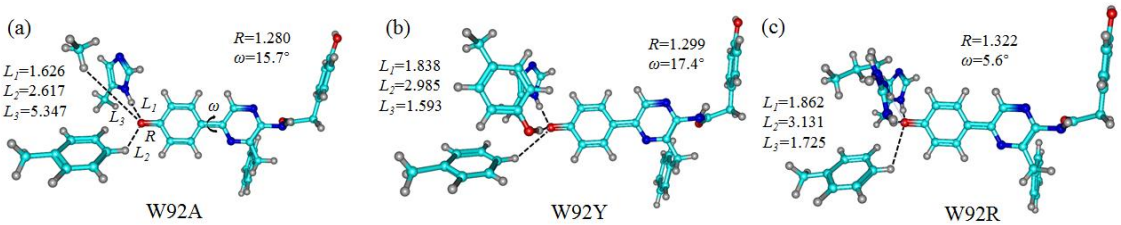
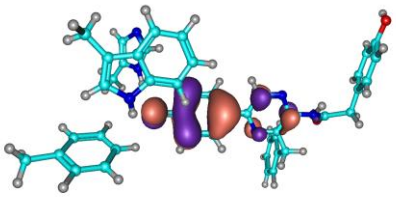
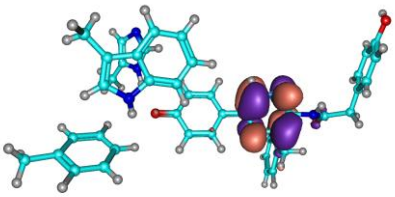


Fig. S3 The optimized S_0 geometries of CLM with triad in W92A (a), W92Y (b), and W92R (c) calculated at the CAM-B3LYP/6-31G(d,p)/MM level.

Table S4 The natural transition orbitals of CLM together with triad at the S_1 state in WT and its mutants calculated at the TD CAM-B3LYP/6-31G(d,p)/MM level

Name	occ.	virt.
WT		
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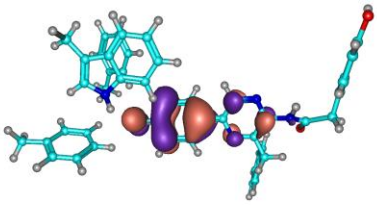
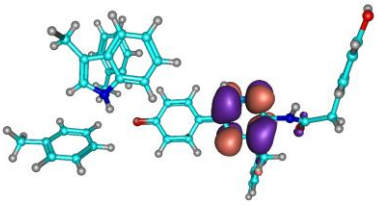
H22F		
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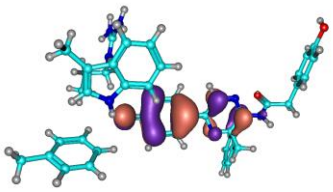
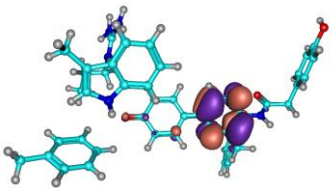
H22R		
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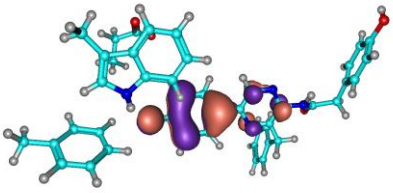
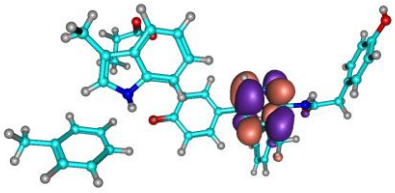
H22E		
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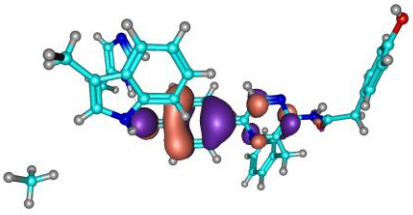
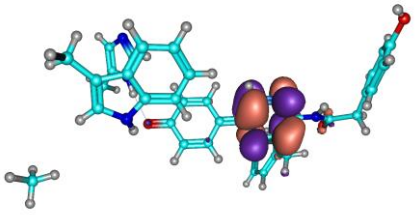
F88A		
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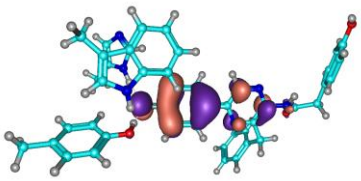
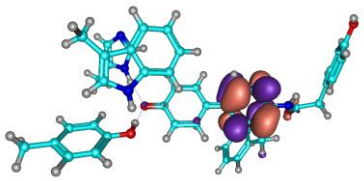
F88Y		
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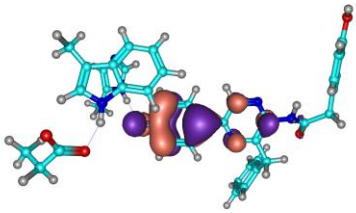
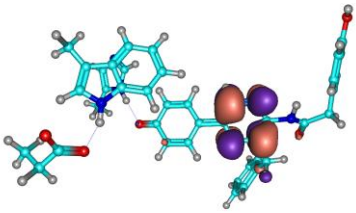
F88E		
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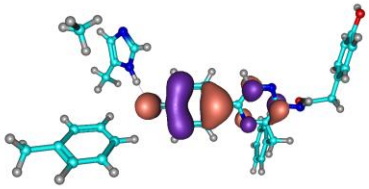
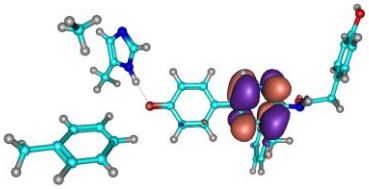
W92A		
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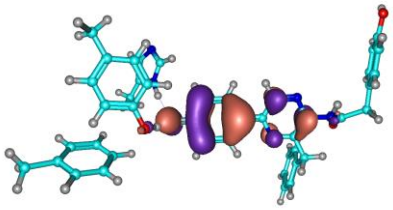
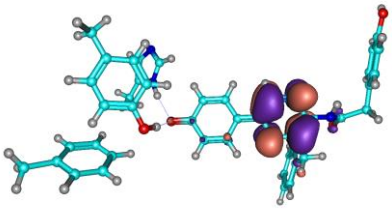
W92Y		
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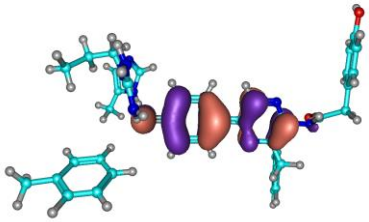
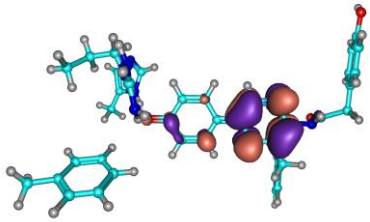
W92R		
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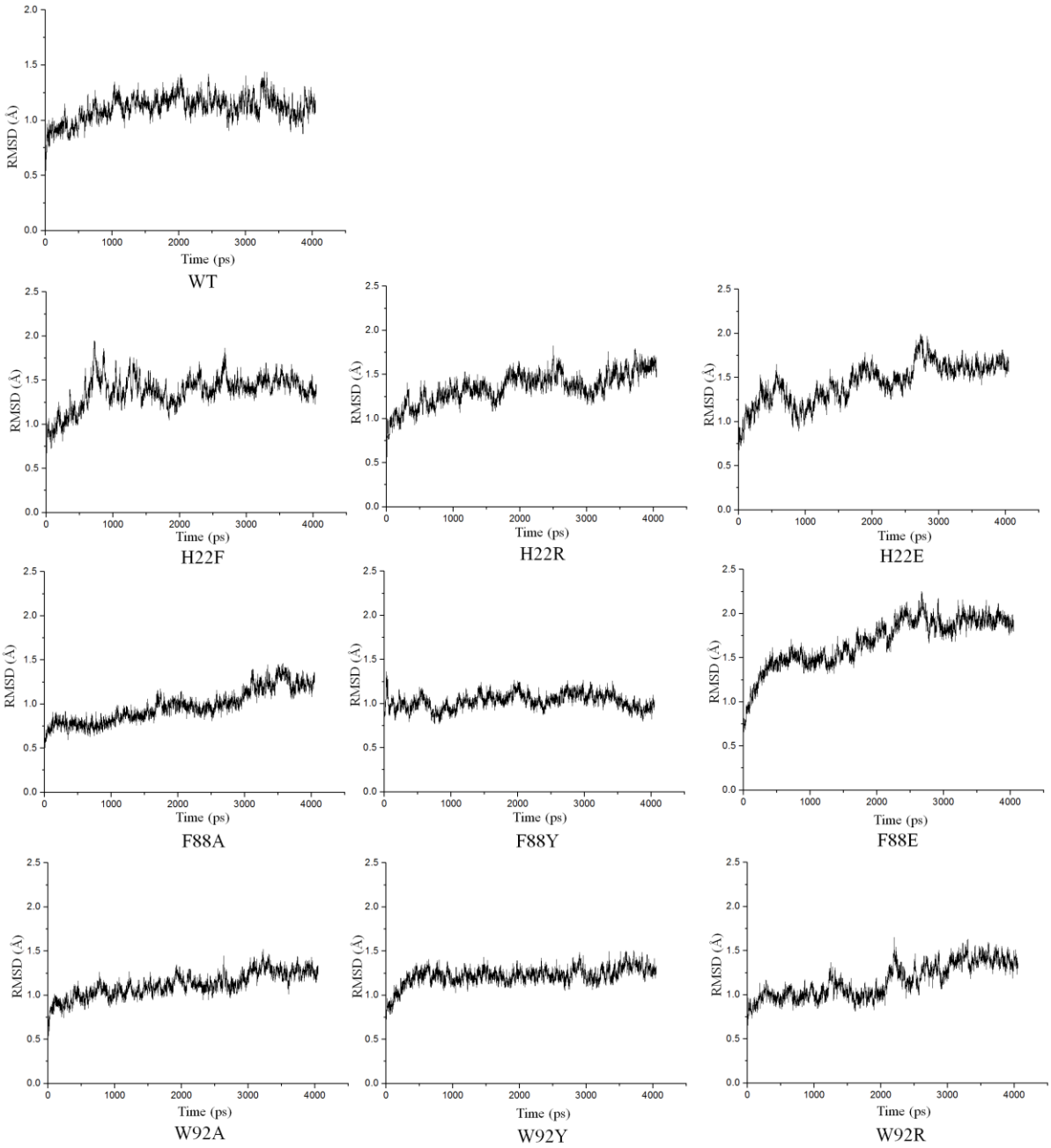

Fig. S4 RMS deviation of WT and its mutants during MD simulation.

Cartesian coordinates (in Å) of optimized equilibrium structures (only QM region)

Wild-type Ca^{2+}-discharged obelin (**WT**)

TD CAM-B3LYP/6-31G(d,p)/MM

Coelenteramide (CLM) (S_1)

O	40.113917	32.085764	32.593867
H	40.441329	32.520976	31.787008
C	38.809890	31.734009	32.482361
C	38.168069	31.262800	33.626018
C	36.856601	30.820970	33.550347
H	36.380311	30.450298	34.455353
H	38.697339	31.280415	34.570635
C	38.115533	31.779460	31.275001
H	38.610571	32.155427	30.383875
C	36.797639	31.346708	31.217712
H	36.260745	31.388030	30.274549
C	36.150753	30.843963	32.345564
C	34.733989	30.326032	32.236310
H	34.588208	29.839112	31.270460
H	34.553818	29.588028	33.027231
C	33.643215	31.399050	32.332851
O	33.026348	31.760598	31.346686
N	33.411439	31.817651	33.608467
H	34.168495	31.662594	34.264563
C	32.626151	32.951111	34.016190
N	33.381694	33.956021	34.459074
C	32.637535	34.957927	35.081135
H	33.192640	35.771800	35.529469
C	31.243222	32.884564	34.068173
C	30.421924	31.730997	33.565363
C	29.552722	32.024710	32.351314
C	28.271779	31.482528	32.248876
C	27.497214	31.704682	31.113685
C	27.980804	32.485204	30.070897
C	29.253728	33.036605	30.171870
C	30.029428	32.809552	31.300661
H	31.029167	33.220512	31.373512
H	29.641381	33.650529	29.365135
H	27.376819	32.672427	29.188321
H	26.500377	31.273802	31.052298
H	27.872491	30.884022	33.063783
H	31.083444	30.891256	33.326155
H	29.764680	31.396479	34.376768
N	30.526536	33.897488	34.675056
C	31.271860	34.893652	35.162485

C	30.476065	35.987332	35.806226
C	30.905576	37.323165	35.727235
H	31.798801	37.534432	35.164225
C	30.231046	38.332647	36.352788
H	30.573482	39.356957	36.272082
C	29.039772	38.070979	37.128010
O	28.430356	38.989274	37.730028
C	28.595081	36.692891	37.157208
H	27.684262	36.482453	37.707696
C	29.285943	35.702903	36.511252
H	28.941813	34.675219	36.517166

Wild-type Ca^{2+}-discharged obelin (**WT**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 (S_1)

O	40.107318	32.100103	32.601963
H	40.434518	32.538883	31.796915
C	38.804207	31.747666	32.488753
C	38.163919	31.264198	33.628234
C	36.853526	30.819247	33.548848
H	36.380395	30.435727	34.450227
H	38.692182	31.278120	34.573403
C	38.107576	31.806755	31.283228
H	38.599421	32.198407	30.397104
C	36.791999	31.367950	31.221770
H	36.255375	31.417947	30.278808
C	36.148231	30.847483	32.343685
C	34.739051	30.311040	32.224632
H	34.603856	29.825165	31.256920
H	34.565982	29.565313	33.009756
C	33.624258	31.357998	32.325347
O	32.948311	31.653988	31.355771
N	33.439031	31.828418	33.590275
H	34.224343	31.716378	34.221251
C	32.647118	32.956419	33.989358
N	33.404533	33.959966	34.443610
C	32.657160	34.962354	35.055020
H	33.215189	35.774624	35.502980
C	31.262582	32.898024	34.026321
C	30.443745	31.733123	33.541344
C	29.550398	32.005524	32.340086
C	28.278022	31.438979	32.262859
C	27.480251	31.636412	31.139345
C	27.933044	32.413278	30.080221

C	29.197417	32.987998	30.154791
C	29.996375	32.784719	31.272008
H	30.990342	33.212291	31.320532
H	29.562044	33.598582	29.335013
H	27.311744	32.580026	29.205533
H	26.490013	31.188059	31.100411
H	27.903673	30.838485	33.087770
H	31.108279	30.897934	33.297475
H	29.802630	31.396432	34.365106
N	30.543646	33.913247	34.622590
C	31.289742	34.915093	35.109075
C	30.501997	36.003691	35.767598
C	30.970363	37.330733	35.768981
H	31.891003	37.548150	35.254285
C	30.305709	38.328121	36.422974
H	30.679549	39.344542	36.418070
C	29.084545	38.062491	37.144741
O	28.491049	38.964221	37.798184
C	28.596200	36.702534	37.094083
H	27.667815	36.492311	37.614578
C	29.278513	35.724093	36.420501
H	28.907441	34.707540	36.365417
C	28.043106	42.952558	37.683661
H	27.832160	44.021257	37.773321
H	27.457079	42.433937	38.451005
C	29.497032	42.699180	37.891386
N	30.002303	41.423303	37.981888
H	29.462897	40.549297	37.970177
C	31.350046	41.543544	38.081528
H	31.996349	40.681316	38.159099
N	31.741049	42.794707	38.071764
C	30.586167	43.526785	37.951302
H	30.600712	44.607766	37.924950
H	27.697629	42.617726	36.694967

Wild-type Ca^{2+}-discharged obelin (**WT**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 (S_1)

O	40.118097	32.090926	32.581270
H	40.440483	32.527051	31.772704
C	38.813673	31.740681	32.479725
C	38.182768	31.265972	33.627999
C	36.870441	30.825590	33.563349
H	36.402909	30.451492	34.471284

H	38.721524	31.281764	34.567266
C	38.108327	31.789212	31.278589
H	38.593987	32.170183	30.384464
C	36.791422	31.352082	31.231142
H	36.247579	31.393291	30.291845
C	36.155341	30.846588	32.364028
C	34.741137	30.319838	32.268912
H	34.596481	29.801945	31.318815
H	34.568319	29.606891	33.083504
C	33.642571	31.386301	32.337683
O	33.001747	31.695964	31.348264
N	33.433341	31.860040	33.596752
H	34.200511	31.732544	34.247179
C	32.631464	32.983930	33.988898
N	33.378399	33.995850	34.443685
C	32.622761	34.990187	35.053166
H	33.171886	35.806341	35.505077
C	31.247708	32.914781	34.025339
C	30.442022	31.743697	33.533128
C	29.561245	32.008314	32.321256
C	28.276761	31.469757	32.248941
C	27.492191	31.655899	31.113980
C	27.971464	32.392610	30.037946
C	29.248289	32.940039	30.107822
C	30.034454	32.746988	31.235671
H	31.037636	33.152837	31.280239
H	29.632931	33.519680	29.274742
H	27.361811	32.549642	29.153400
H	26.491595	31.231105	31.080806
H	27.880751	30.901505	33.086630
H	31.116218	30.913865	33.296934
H	29.796090	31.403277	34.351491
N	30.518030	33.923064	34.619394
C	31.256998	34.931467	35.109479
C	30.464495	36.012548	35.772084
C	30.917490	37.345665	35.769400
H	31.820832	37.573858	35.229049
C	30.253719	38.334499	36.437850
H	30.619135	39.354077	36.429320
C	29.054527	38.050316	37.190685
O	28.470679	38.940247	37.872002
C	28.573959	36.687868	37.131734
H	27.653483	36.464241	37.660992
C	29.252984	35.719543	36.440873

H	28.890784	34.699715	36.386989
C	28.068985	42.951877	37.675293
H	27.865074	44.022226	37.765367
H	27.490824	42.433554	38.448565
C	29.528192	42.696230	37.865461
N	30.031030	41.421991	37.997280
H	29.488628	40.553099	38.036488
C	31.382580	41.537069	38.052960
H	32.028173	40.676565	38.153003
N	31.778952	42.783628	37.972113
C	30.624643	43.517356	37.855509
H	30.647482	44.595388	37.774362
C	25.093319	40.633253	43.812935
H	24.327713	40.017526	44.292662
H	24.576872	41.479608	43.365069
C	25.757922	39.838242	42.713436
C	25.934889	38.460534	42.833222
H	25.649983	37.962912	43.754168
C	26.425222	37.711301	41.770773
H	26.531645	36.636252	41.876084
C	26.753641	38.333224	40.571688
H	27.129832	37.770033	39.724640
C	26.603113	39.711047	40.445995
H	26.869840	40.183769	39.506485
C	26.105254	40.455165	41.509290
H	25.966169	41.528522	41.403280
H	27.723866	42.618221	36.686754
H	25.771449	41.002195	44.590018

Wild-type Ca^{2+}-discharged obelin (**WT**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Trp92 (S_1)

O	40.067646	32.079192	32.579682
H	40.406737	32.505539	31.773334
C	38.767147	31.720681	32.451558
C	38.114554	31.239583	33.585309
C	36.804411	30.794648	33.494397
H	36.324135	30.413288	34.392978
H	38.634623	31.249736	34.535131
C	38.083426	31.769635	31.237971
H	38.584697	32.153029	30.353490
C	36.769510	31.326936	31.164648
H	36.249733	31.362207	30.211391
C	36.108981	30.817618	32.282469

C	34.709144	30.262854	32.141970
H	34.582214	29.814674	31.155334
H	34.555258	29.474485	32.888981
C	33.538408	31.244649	32.292475
O	32.701636	31.347246	31.410532
N	33.488408	31.858258	33.504675
H	34.355926	31.861717	34.028329
C	32.665426	32.948551	33.936175
N	33.416932	33.962116	34.389033
C	32.676087	34.949248	35.021462
H	33.237672	35.764548	35.459677
C	31.282331	32.878174	34.003383
C	30.446876	31.726228	33.517494
C	29.541452	32.037055	32.335130
C	28.275823	31.458510	32.241478
C	27.468131	31.693118	31.132081
C	27.903493	32.519526	30.103774
C	29.160926	33.107017	30.194999
C	29.969702	32.864556	31.296692
H	30.955037	33.309875	31.359733
H	29.511507	33.758082	29.400495
H	27.274541	32.715251	29.240723
H	26.483456	31.234096	31.079958
H	27.913336	30.819490	33.042574
H	31.090743	30.887358	33.240802
H	29.813697	31.390316	34.347119
N	30.566467	33.885386	34.615740
C	31.310800	34.894267	35.095859
C	30.530476	35.980180	35.759980
C	31.004160	37.305242	35.756138
H	31.914597	37.511649	35.221059
C	30.359983	38.305217	36.425151
H	30.747444	39.316660	36.421984
C	29.160313	38.041128	37.182871
O	28.592641	38.941915	37.862416
C	28.654113	36.687787	37.124232
H	27.732521	36.481964	37.658525
C	29.315879	35.706700	36.432866
H	28.937094	34.692762	36.381351
C	28.077637	42.955924	37.671611
H	27.867628	44.024786	37.763896
H	27.513706	42.437193	38.454251
C	29.541887	42.713938	37.842790
N	30.061561	41.444227	37.957796

H	29.533705	40.563922	37.983059
C	31.411303	41.576552	38.020221
H	32.067713	40.725582	38.131273
N	31.791001	42.830049	37.956734
C	30.627424	43.549977	37.845198
H	30.637585	44.629469	37.781805
C	31.692302	41.956460	42.365612
H	30.900209	42.696633	42.495316
H	32.437672	42.410207	41.703406
C	31.180510	40.720738	41.700777
C	29.918649	40.212135	41.707306
H	29.027680	40.582705	42.190985
N	29.870286	39.040644	40.972942
H	29.012688	38.688173	40.573915
C	31.110504	38.824427	40.410937
C	31.533915	37.849522	39.509980
H	30.865282	37.070388	39.162569
C	32.835661	37.927755	39.048003
H	33.180387	37.203037	38.317728
C	33.707862	38.931296	39.499831
H	34.712012	38.971930	39.090957
C	33.294091	39.875477	40.423783
H	33.967511	40.661377	40.753088
C	31.969006	39.843755	40.872956
H	27.713840	42.617202	36.691064
H	32.148418	41.757472	43.344460

Wild-type Ca^{2+}-discharged obelin (**WT**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_1)

O	40.100617	32.096054	32.602689
H	40.434947	32.511373	31.788566
C	38.803742	31.725882	32.478706
C	38.158060	31.235848	33.612388
C	36.852952	30.776841	33.520692
H	36.373539	30.396487	34.420119
H	38.676180	31.254190	34.563143
C	38.118928	31.772437	31.265872
H	38.613497	32.170950	30.384442
C	36.810084	31.316921	31.192040
H	36.285342	31.355630	30.241834
C	36.157851	30.796180	32.308898
C	34.758183	30.241051	32.169313
H	34.635945	29.764680	31.195362

H	34.587531	29.482697	32.942268
C	33.613850	31.254172	32.281466
O	32.852060	31.446455	31.348305
N	33.499012	31.800111	33.520744
H	34.325237	31.749890	34.105776
C	32.687573	32.909821	33.926727
N	33.433614	33.917805	34.381933
C	32.689202	34.911788	35.008681
H	33.242134	35.727883	35.456497
C	31.305196	32.838068	33.977905
C	30.480651	31.686980	33.475287
C	29.569092	32.017771	32.304188
C	28.286958	31.475722	32.224606
C	27.471061	31.742516	31.128488
C	27.914649	32.566999	30.102361
C	29.190455	33.116094	30.178957
C	30.007589	32.841445	31.266512
H	31.008773	33.251881	31.317313
H	29.548871	33.762701	29.384314
H	27.277817	32.789208	29.251724
H	26.475930	31.306513	31.082021
H	27.918041	30.841963	33.027024
H	31.136655	30.864570	33.176177
H	29.856154	31.319320	34.298909
N	30.585594	33.843084	34.590324
C	31.323027	34.846724	35.080628
C	30.527033	35.907085	35.769693
C	30.932679	37.253138	35.742308
H	31.795159	37.504838	35.147409
C	30.286150	38.215431	36.466251
H	30.613283	39.247832	36.453179
C	29.169952	37.872410	37.319405
O	28.639355	38.714570	38.087356
C	28.714638	36.499283	37.260636
H	27.843349	36.242950	37.854035
C	29.371574	35.563912	36.508512
H	29.040821	34.532214	36.466911
C	27.995929	42.987532	37.667481
H	27.805232	44.064549	37.736750
H	27.459438	42.490866	38.490344
C	29.458580	42.722146	37.811335
N	29.973642	41.450507	37.957452
H	29.430512	40.592376	38.030162
C	31.329070	41.557363	38.026318

H	31.971081	40.697375	38.153389
N	31.727752	42.802083	37.936694
C	30.565027	43.534990	37.816196
H	30.593040	44.611619	37.717636
C	25.072356	40.643083	43.831408
H	24.345704	39.988710	44.321342
H	24.512804	41.486424	43.432826
C	25.712950	39.910293	42.679941
C	25.972551	38.543260	42.762966
H	25.781630	38.015675	43.692948
C	26.433873	37.848438	41.652396
H	26.616888	36.780150	41.724697
C	26.630279	38.510995	40.445235
H	26.985896	37.989997	39.565029
C	26.396280	39.881032	40.355177
H	26.542155	40.396830	39.410349
C	25.940980	40.573253	41.471731
H	25.740102	41.639123	41.396701
C	31.684139	41.950811	42.368423
H	30.861537	42.656180	42.506237
H	32.406923	42.436749	41.703444
C	31.214802	40.700876	41.700257
C	29.964875	40.163209	41.686170
H	29.055107	40.528289	42.140039
N	29.951346	38.990599	40.949980
H	29.113029	38.672319	40.480991
C	31.204063	38.814452	40.400038
C	31.656625	37.859071	39.492944
H	31.008378	37.066489	39.138354
C	32.952727	37.982431	39.025078
H	33.317766	37.276672	38.285934
C	33.792480	39.010154	39.481630
H	34.789546	39.091787	39.062025
C	33.355484	39.928735	40.421289
H	34.005210	40.733401	40.753717
C	32.034683	39.849677	40.875590
H	27.410926	42.665537	36.761263
H	25.770519	41.010568	44.593018
H	32.161967	41.770261	43.341916

Wild-type Ca^{2+}-discharged obelin (**WT**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_0)

O	40.138816	32.074429	32.557451

H	40.468271	32.520695	31.756361
C	38.835772	31.729880	32.449115
C	38.199044	31.263095	33.598240
C	36.885553	30.830437	33.531310
H	36.411136	30.465107	34.439383
H	38.737752	31.273217	34.537377
C	38.134353	31.779697	31.245267
H	38.626416	32.148781	30.350020
C	36.814124	31.353598	31.195592
H	36.269229	31.402053	30.257408
C	36.174782	30.858985	32.330488
C	34.744195	30.376665	32.250041
H	34.567006	29.871979	31.297564
H	34.552665	29.665147	33.061392
C	33.729424	31.513348	32.331692
O	33.325594	32.086060	31.338503
N	33.301271	31.779192	33.605960
H	33.885705	31.434788	34.358402
C	32.514454	32.916203	33.971801
N	33.198058	34.004523	34.343516
C	32.511623	34.995892	34.877266
H	33.071941	35.859971	35.216020
C	31.129622	32.847089	34.089803
C	30.310420	31.673191	33.605754
C	29.525495	31.939645	32.330395
C	28.207051	31.499377	32.212015
C	27.497986	31.709382	31.032670
C	28.085154	32.372115	29.961971
C	29.396838	32.817244	30.078088
C	30.111944	32.599513	31.248598
H	31.141267	32.934355	31.318017
H	29.864650	33.340267	29.250511
H	27.530955	32.552681	29.046212
H	26.470751	31.362736	30.956365
H	27.726050	30.992374	33.044184
H	30.972359	30.813441	33.459404
H	29.605372	31.411167	34.397416
N	30.447470	33.850740	34.645909
C	31.108736	34.935764	35.073933
C	30.394883	35.997061	35.767736
C	30.897129	37.310026	35.804272
H	31.796549	37.547757	35.254197
C	30.268667	38.314507	36.495095
H	30.690756	39.312249	36.488743

C	29.107579	38.070831	37.291668
O	28.596670	38.968783	38.055640
C	28.576228	36.743478	37.197533
H	27.673431	36.521544	37.759715
C	29.194809	35.755671	36.460292
H	28.777876	34.753511	36.428480
C	28.075910	42.944039	37.675278
H	27.875954	44.015037	37.768272
H	27.505310	42.427213	38.455088
C	29.536488	42.684325	37.846702
N	30.040600	41.410880	37.978290
H	29.499571	40.523736	38.029667
C	31.390943	41.532752	38.017267
H	32.040721	40.677075	38.127856
N	31.787245	42.781491	37.921962
C	30.629751	43.510725	37.815673
H	30.647282	44.589136	37.732005
C	25.087002	40.640813	43.815529
H	24.313461	40.039983	44.301068
H	24.584116	41.493293	43.364745
C	25.731174	39.827123	42.718347
C	25.889214	38.448978	42.853811
H	25.612002	37.971123	43.787388
C	26.363128	37.680079	41.798690
H	26.464488	36.606149	41.920504
C	26.685259	38.282415	40.588797
H	27.057543	37.709763	39.747156
C	26.548386	39.659388	40.443833
H	26.827437	40.105732	39.494757
C	26.070930	40.424524	41.502225
H	25.950363	41.499218	41.385909
C	31.692048	41.945278	42.361949
H	30.862729	42.643069	42.495407
H	32.420019	42.445206	41.713233
C	31.239643	40.701003	41.666152
C	29.983189	40.179092	41.601390
H	29.071050	40.539519	42.055120
N	29.972332	39.029019	40.831421
H	29.160950	38.752156	40.288669
C	31.239696	38.845383	40.323355
C	31.694535	37.899756	39.407819
H	31.035077	37.135629	39.014327
C	33.000562	38.014538	38.970309
H	33.370958	37.323775	38.219520

C	33.842185	39.025461	39.460323
H	34.843945	39.106610	39.051583
C	33.401468	39.930548	40.412241
H	34.052259	40.723932	40.769303
C	32.072106	39.857595	40.843618
H	27.708591	42.603057	36.696359
H	25.777881	41.002438	44.584939
H	32.152968	41.754175	43.340826

Wild-type Ca^{2+}-discharged obelin (**WT**) 1000 ps
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_1)

O	39.563781	32.351443	32.838434
H	39.800408	32.681754	33.737792
C	38.278783	31.915277	32.837761
C	37.657370	31.403587	33.973739
C	36.382919	30.864372	33.885383
H	35.936559	30.427293	34.774286
H	38.186376	31.392745	34.919237
C	37.580688	31.948836	31.631674
H	38.063078	32.390855	30.765859
C	36.304133	31.415416	31.556452
H	35.769924	31.437251	30.611140
C	35.690487	30.850019	32.675914
C	34.311110	30.252626	32.569350
H	34.180506	29.751975	31.607948
H	34.162876	29.509167	33.360358
C	33.160402	31.247212	32.678583
O	32.256153	31.238100	31.846519
N	33.198801	32.040810	33.765839
H	34.084838	32.085991	34.255040
C	32.318432	33.093248	34.170329
N	32.971008	34.250183	34.334722
C	32.208054	35.230233	34.945488
H	32.715073	36.152852	35.196302
C	30.996434	32.869417	34.514299
C	30.317383	31.534703	34.441157
C	29.121586	31.448227	33.508377
C	29.255468	31.620396	32.127553
C	28.184180	31.378338	31.277176
C	26.956395	30.975043	31.792886
C	26.781649	30.911877	33.167734
C	27.860387	31.145572	34.013055

H	27.726795	31.090174	35.087497
H	25.817863	30.642456	33.584107
H	26.135013	30.731898	31.126749
H	28.316885	31.482382	30.204508
H	30.218280	31.914373	31.730866
H	31.049218	30.772017	34.165802
H	29.967816	31.290410	35.452325
N	30.235836	33.873760	35.068891
C	30.893014	35.026956	35.263276
C	30.100965	36.102716	35.915616
C	30.431083	37.456815	35.714360
H	31.200461	37.690192	34.996678
C	29.831730	38.450741	36.430911
H	30.117525	39.487494	36.299932
C	28.829581	38.147448	37.423419
O	28.339947	39.047870	38.163139
C	28.427557	36.763023	37.533505
H	27.621359	36.524896	38.219579
C	29.047576	35.785779	36.802800
H	28.769565	34.741842	36.885507
C	28.037665	43.195941	37.717760
H	27.953384	44.285153	37.695223
H	27.464022	42.831000	38.577251
C	29.477372	42.812943	37.839940
N	29.887884	41.517075	38.062527
H	29.293224	40.689755	38.182760
C	31.245731	41.524212	38.042599
H	31.828044	40.627611	38.200052
N	31.731616	42.723112	37.824582
C	30.631050	43.536620	37.696891
H	30.729857	44.599673	37.523035
C	24.905793	40.832798	43.967413
H	24.230875	40.183310	44.530264
H	24.294555	41.637655	43.547664
C	25.541319	40.071403	42.828774
C	25.674178	38.690480	42.903243
H	25.321637	38.185932	43.791895
C	26.185462	37.959801	41.838324
H	26.263091	36.880276	41.916110
C	26.564253	38.612473	40.674274
H	26.938008	38.076528	39.811517
C	26.453185	39.997542	40.589384
H	26.757461	40.491611	39.673127
C	25.943248	40.722347	41.657683

H	25.832892	41.800905	41.574901
C	31.509817	41.452446	42.274548
H	30.605922	42.052644	42.423410
H	32.151808	42.028466	41.596604
C	31.187578	40.170018	41.584843
C	29.988441	39.530185	41.521033
H	29.047288	39.786133	41.986617
N	30.083630	38.421191	40.702862
H	29.275840	38.005142	40.266853
C	31.351087	38.379264	40.161917
C	31.894000	37.539626	39.187781
H	31.311442	36.742752	38.739773
C	33.198041	37.779308	38.791864
H	33.640433	37.153169	38.024370
C	33.957959	38.809033	39.374235
H	34.980328	38.961172	39.043351
C	33.419777	39.636071	40.343367
H	34.006299	40.444648	40.769861
C	32.088662	39.439260	40.731951
H	27.585925	42.792672	36.799598
H	25.628899	41.271638	44.665096
H	31.983008	41.316238	43.256705

Wild-type Ca^{2+}-discharged obelin (**WT**) 1000 ps
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_0)

O	39.535470	32.350898	32.824720
H	39.772600	32.677831	33.725450
C	38.257186	31.899786	32.827859
C	37.650245	31.372327	33.964855
C	36.379691	30.825042	33.883846
H	35.948494	30.373718	34.773529
H	38.187450	31.359647	34.905336
C	37.549797	31.933894	31.626997
H	38.020873	32.387205	30.760856
C	36.275283	31.394470	31.559347
H	35.730310	31.423322	30.620209
C	35.676157	30.819193	32.681383
C	34.287023	30.238855	32.590977
H	34.142930	29.723499	31.639734
H	34.124646	29.516422	33.397854
C	33.186536	31.286761	32.673717
O	32.380827	31.436009	31.762272

N	33.154549	31.975131	33.839673
H	33.932924	31.841278	34.473430
C	32.274288	33.036487	34.201661
N	32.851341	34.233958	34.320892
C	32.138970	35.218128	34.831934
H	32.640550	36.167288	34.977306
C	30.952421	32.835666	34.590159
C	30.259089	31.501269	34.518582
C	29.112622	31.427341	33.527130
C	29.322054	31.622787	32.159245
C	28.293528	31.409440	31.250336
C	27.042793	30.992339	31.693443
C	26.799006	30.886790	33.055523
C	27.831009	31.101973	33.961910
H	27.636900	31.025448	35.025476
H	25.816233	30.604997	33.414522
H	26.255082	30.776599	30.979349
H	28.475456	31.546514	30.188999
H	30.300856	31.930348	31.812948
H	30.996115	30.727425	34.291528
H	29.869125	31.293950	35.518994
N	30.236611	33.836344	35.104294
C	30.800600	35.042836	35.251680
C	30.068994	36.110632	35.912788
C	30.447195	37.454097	35.759089
H	31.236129	37.704491	35.063804
C	29.838031	38.465846	36.459153
H	30.165533	39.490447	36.325857
C	28.828929	38.198540	37.429701
O	28.361954	39.112710	38.208625
C	28.402357	36.836094	37.518634
H	27.599018	36.597563	38.209329
C	29.004219	35.836296	36.788229
H	28.685853	34.804683	36.900560
C	28.029093	43.178277	37.729100
H	27.954509	44.268722	37.716692
H	27.439265	42.806982	38.575231
C	29.464554	42.784827	37.874154
N	29.882974	41.488110	38.077046
H	29.310192	40.623591	38.179342
C	31.239011	41.519609	38.099011
H	31.827981	40.625955	38.247463
N	31.720047	42.729834	37.925564
C	30.611641	43.528585	37.784170

H	30.694871	44.597719	37.639619
C	24.904704	40.831951	43.970027
H	24.221660	40.196903	44.540094
H	24.304178	41.639666	43.540473
C	25.534840	40.046532	42.845179
C	25.649509	38.666220	42.946459
H	25.273911	38.185990	43.839187
C	26.173564	37.910248	41.906226
H	26.247462	36.832586	42.008120
C	26.578005	38.536682	40.736967
H	26.973344	37.982658	39.895556
C	26.476073	39.919907	40.620383
H	26.806704	40.381237	39.696446
C	25.958231	40.670937	41.667605
H	25.863990	41.749708	41.565925
C	31.514721	41.459492	42.275150
H	30.600843	42.041139	42.433802
H	32.145615	42.059001	41.606166
C	31.209448	40.189877	41.556623
C	29.988135	39.621322	41.373766
H	29.028469	39.921995	41.768964
N	30.070763	38.538828	40.518919
H	29.293825	38.350546	39.887545
C	31.376451	38.451538	40.075994
C	31.934685	37.622131	39.103208
H	31.335177	36.879355	38.589575
C	33.266489	37.819324	38.783874
H	33.725243	37.207363	38.013856
C	34.035889	38.795842	39.439468
H	35.073702	38.924898	39.149125
C	33.487245	39.600339	40.423089
H	34.083932	40.365632	40.911698
C	32.131533	39.444597	40.737622
H	27.599403	42.789935	36.794143
H	25.635300	41.269162	44.661532
H	32.002260	41.314930	43.249800

Wild-type Ca^{2+}-discharged obelin (**WT**) 1900 ps
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_1)

O	39.247903	31.893955	32.883403
H	39.357284	32.214919	33.808158
C	37.940702	31.598119	32.649417

C	37.053110	31.254157	33.668996
C	35.733915	30.961962	33.363591
H	35.061579	30.695539	34.173938
H	37.392206	31.216310	34.698791
C	37.494395	31.623215	31.330903
H	38.190838	31.899917	30.547352
C	36.169608	31.330128	31.040099
H	35.828519	31.377489	30.010023
C	35.267591	31.003046	32.049811
C	33.811867	30.741118	31.739146
H	33.686544	30.455955	30.692532
H	33.439818	29.922582	32.364045
C	32.960019	31.988837	31.958574
O	32.775788	32.805766	31.059133
N	32.428319	32.081475	33.198893
H	32.724453	31.386271	33.870444
C	31.782056	33.233088	33.769217
N	32.559182	34.304194	33.945816
C	31.908105	35.318740	34.637051
H	32.493483	36.197701	34.871458
C	30.471419	33.103053	34.198620
C	29.636532	31.873611	33.974621
C	28.694955	31.946682	32.783600
C	29.125986	32.454457	31.556393
C	28.269939	32.473514	30.462093
C	26.967733	31.996007	30.575737
C	26.531177	31.489058	31.793131
C	27.388803	31.474476	32.887349
H	27.038480	31.073831	33.833877
H	25.524376	31.098015	31.898900
H	26.304248	32.013976	29.717208
H	28.620835	32.868027	29.513160
H	30.137133	32.839812	31.461586
H	30.291926	31.003556	33.850878
H	29.039998	31.707246	34.878570
N	29.841848	34.119399	34.883280
C	30.611643	35.209886	35.055757
C	29.925996	36.324901	35.769944
C	30.257356	37.671604	35.527043
H	30.981666	37.890407	34.761125
C	29.723040	38.685584	36.270683
H	30.019837	39.714596	36.107151
C	28.790766	38.411065	37.337431
O	28.372962	39.321911	38.109927

C	28.382312	37.034880	37.496448
H	27.633353	36.819645	38.251609
C	28.938501	36.040370	36.739676
H	28.662012	35.001365	36.866210
C	28.146448	43.556723	37.653369
H	28.085913	44.646838	37.644742
H	27.593068	43.193804	38.526007
C	29.584889	43.137596	37.728550
N	29.965284	41.819584	37.893532
H	29.358272	41.006426	38.027772
C	31.322921	41.789899	37.846570
H	31.878956	40.870498	37.964984
N	31.839577	42.980618	37.661842
C	30.759141	43.829533	37.589776
H	30.888950	44.893891	37.455808
C	25.160639	41.070720	44.190743
H	24.499481	40.455636	44.804472
H	24.542685	41.840601	43.722584
C	25.807043	40.221264	43.121071
C	26.026608	38.862181	43.334371
H	25.768188	38.428649	44.293714
C	26.531061	38.054470	42.323386
H	26.662891	36.991695	42.503534
C	26.827956	38.600435	41.081708
H	27.184593	37.977590	40.269310
C	26.647680	39.962093	40.861740
H	26.902930	40.377907	39.892606
C	26.143528	40.764452	41.878008
H	25.983711	41.824677	41.699205
C	31.824185	41.812035	42.006808
H	30.995807	42.521145	42.081030
H	32.603733	42.305470	41.413293
C	31.412337	40.575622	41.282664
C	30.156357	40.063705	41.187409
H	29.244090	40.411089	41.650795
N	30.154666	38.937694	40.388373
H	29.323562	38.659747	39.883297
C	31.428737	38.749252	39.899407
C	31.903610	37.828462	38.965013
H	31.246966	37.098621	38.504297
C	33.244564	37.889677	38.631315
H	33.638268	37.199614	37.892147
C	34.101395	38.820743	39.240946
H	35.150690	38.816277	38.963446

C	33.627870	39.738176	40.163694
H	34.296051	40.467977	40.613166
C	32.263336	39.729375	40.482809
H	27.666196	43.179776	36.739975
H	25.884510	41.562980	44.850624
H	32.232981	41.620174	43.010337

Wild-type Ca^{2+}-discharged obelin (**WT**) 1900 ps
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_0)

O	39.223408	31.889695	32.894722
H	39.324982	32.213193	33.820486
C	37.920226	31.592763	32.649016
C	37.024260	31.241405	33.659543
C	35.706727	30.956153	33.341537
H	35.026768	30.684202	34.143764
H	37.357157	31.190891	34.690749
C	37.485098	31.626811	31.326867
H	38.189153	31.907537	30.551711
C	36.161643	31.342680	31.023459
H	35.829379	31.400418	29.991249
C	35.251397	31.012195	32.024406
C	33.793919	30.770319	31.701652
H	33.672499	30.520903	30.645691
H	33.407131	29.936617	32.296417
C	32.971567	32.026989	31.953903
O	32.844396	32.903761	31.105717
N	32.403592	32.081847	33.188868
H	32.612321	31.323686	33.824268
C	31.726390	33.202558	33.747423
N	32.411774	34.339497	33.882816
C	31.811318	35.338235	34.502200
H	32.378338	36.250147	34.641397
C	30.430407	33.075832	34.241093
C	29.593368	31.836195	34.052885
C	28.714548	31.889629	32.813540
C	29.191155	32.385167	31.597681
C	28.372945	32.404011	30.474109
C	27.070150	31.920683	30.543655
C	26.591549	31.417682	31.746949
C	27.408515	31.408400	32.871478
H	27.017641	31.024005	33.808351
H	25.581918	31.027314	31.819575

H	26.434863	31.944895	29.664467
H	28.752116	32.807067	29.540520
H	30.198688	32.782258	31.524304
H	30.236050	30.950855	34.007206
H	28.956446	31.738736	34.935274
N	29.843382	34.080594	34.890913
C	30.505095	35.237531	35.033965
C	29.887504	36.328983	35.772213
C	30.272755	37.664857	35.574442
H	31.012197	37.897255	34.821472
C	29.725777	38.693838	36.302363
H	30.054598	39.712418	36.131457
C	28.778251	38.455037	37.339791
O	28.366829	39.388373	38.128926
C	28.356767	37.098844	37.492129
H	27.614886	36.883173	38.255628
C	28.894955	36.082448	36.734008
H	28.590033	35.054839	36.899184
C	28.138892	43.547315	37.661668
H	28.089107	44.638039	37.655544
H	27.573597	43.187028	38.528058
C	29.571542	43.113425	37.752361
N	29.941439	41.792093	37.903007
H	29.327630	40.965262	38.015708
C	31.297922	41.762122	37.882232
H	31.848910	40.839185	37.995134
N	31.826144	42.954608	37.728304
C	30.749506	43.806694	37.649600
H	30.881655	44.873583	37.536526
C	25.159880	41.059077	44.199403
H	24.503418	40.442185	44.817404
H	24.536131	41.822806	43.728638
C	25.812068	40.208360	43.134149
C	26.045237	38.852880	43.353524
H	25.789464	38.420135	44.313986
C	26.572071	38.049489	42.349854
H	26.723767	36.990334	42.538183
C	26.870653	38.593446	41.107722
H	27.268371	37.984389	40.304712
C	26.662900	39.949195	40.877753
H	26.913751	40.356306	39.903021
C	26.141496	40.748382	41.887790
H	25.967099	41.805653	41.704325
C	31.833003	41.824803	42.010229

H	30.999298	42.526398	42.092239
H	32.609256	42.333330	41.424266
C	31.430755	40.599788	41.268218
C	30.160557	40.160578	41.068121
H	29.238313	40.569952	41.454339
N	30.144051	39.055444	40.245713
H	29.350529	38.920798	39.608271
C	31.441083	38.804770	39.852538
C	31.925114	37.880708	38.926276
H	31.255889	37.204678	38.405918
C	33.283100	37.890115	38.664918
H	33.686824	37.202633	37.927880
C	34.147614	38.768561	39.339255
H	35.207284	38.728680	39.106100
C	33.669090	39.678896	40.266406
H	34.345117	40.367506	40.767101
C	32.289958	39.724788	40.512409
H	27.661418	43.174201	36.745390
H	25.874121	41.561158	44.863290
H	32.252587	41.627610	43.010114

Wild-type Ca^{2+}-discharged obelin (**WT**) 2600 ps
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_1)

O	39.470149	32.380101	32.934556
H	39.668965	32.777373	33.816644
C	38.163647	32.010133	32.876531
C	37.397025	31.764847	34.014003
C	36.084756	31.336249	33.887072
H	35.529474	31.104859	34.793354
H	37.834476	31.892826	34.997861
C	37.588288	31.848034	31.618627
H	38.191124	32.053572	30.740062
C	36.269471	31.430415	31.505768
H	35.835038	31.303582	30.518265
C	35.492927	31.163350	32.634321
C	34.072788	30.658451	32.503159
H	33.925215	30.175803	31.535576
H	33.890098	29.914381	33.287732
C	32.970245	31.721952	32.607510
O	32.198733	31.922727	31.682880
N	32.901039	32.316191	33.831503

H	33.727597	32.225536	34.409247
C	32.168516	33.486406	34.218830
N	32.965725	34.528151	34.491854
C	32.288134	35.588506	35.085975
H	32.892664	36.444361	35.356547
C	30.801975	33.440038	34.442882
C	29.923064	32.262607	34.119278
C	28.818256	32.591307	33.131491
C	29.131020	33.046306	31.848734
C	28.123490	33.350010	30.943418
C	26.786669	33.210581	31.305302
C	26.467244	32.759884	32.579386
C	27.479044	32.457616	33.485740
H	27.223916	32.102545	34.480593
H	25.428455	32.639489	32.873706
H	26.007498	33.458006	30.592911
H	28.378972	33.703257	29.949135
H	30.175056	33.146116	31.570271
H	30.529978	31.442269	33.728104
H	29.451931	31.912584	35.047951
N	30.153212	34.502478	35.028517
C	30.938865	35.551273	35.321266
C	30.205932	36.706085	35.918572
C	30.730721	38.011219	35.848085
H	31.660209	38.148751	35.322769
C	30.112496	39.078239	36.434208
H	30.546829	40.069799	36.386161
C	28.878788	38.899289	37.159081
O	28.283672	39.848191	37.743355
C	28.324870	37.571018	37.163711
H	27.365005	37.482885	37.654630
C	28.958831	36.519212	36.561847
H	28.535684	35.522972	36.545753
C	27.889965	43.741047	37.865561
H	27.728942	44.819305	37.934905
H	27.297704	43.255500	38.648832
C	29.330072	43.427173	38.064530
N	29.775711	42.129403	38.120704
H	29.202476	41.278226	38.001113
C	31.113476	42.178654	38.299613
H	31.718690	41.287830	38.380569
N	31.553240	43.414642	38.372514
C	30.440546	44.206176	38.230366
H	30.495240	45.285090	38.256113

C	25.104814	40.653580	43.715282
H	24.292681	40.149932	44.251272
H	24.647851	41.497628	43.190928
C	25.688305	39.694776	42.708989
C	25.803230	38.337381	43.010087
H	25.515773	37.982511	43.994851
C	26.242155	37.434508	42.052954
H	26.316886	36.383014	42.302161
C	26.567133	37.875423	40.774617
H	26.884896	37.164507	40.017237
C	26.476689	39.228978	40.462343
H	26.759225	39.573036	39.471696
C	26.037113	40.127020	41.429733
H	25.952646	41.182750	41.185731
C	31.647916	41.760347	42.121934
H	30.821283	42.453948	42.305697
H	32.293237	42.256499	41.388082
C	31.150950	40.493026	41.507848
C	29.916718	39.919481	41.593771
H	29.039381	40.230059	42.139281
N	29.873127	38.778550	40.822831
H	29.024211	38.277303	40.622732
C	31.073534	38.625297	40.175646
C	31.478429	37.691240	39.223488
H	30.815862	36.896755	38.897016
C	32.734881	37.848130	38.669031
H	33.063165	37.148947	37.906493
C	33.586411	38.890242	39.079462
H	34.571519	38.976040	38.631631
C	33.195949	39.793261	40.051254
H	33.854844	40.601602	40.355858
C	31.912589	39.678338	40.599952
H	27.528501	43.402055	36.884716
H	25.807382	41.033386	44.464785
H	32.217231	41.599899	43.049078

Wild-type Ca^{2+}-discharged obelin (**WT**) 2600 ps
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Trp92 (S_0)

O	39.459132	32.379153	32.965500
H	39.657575	32.791820	33.842825
C	38.155709	32.005880	32.908492
C	37.385517	31.763076	34.044829

C	36.076779	31.322526	33.915483
H	35.523295	31.079730	34.820267
H	37.821828	31.890611	35.029099
C	37.586505	31.834438	31.648813
H	38.191881	32.039831	30.772241
C	36.270666	31.411511	31.533384
H	35.841503	31.277947	30.544362
C	35.491349	31.143701	32.660285
C	34.074547	30.637863	32.510349
H	33.937187	30.178164	31.530189
H	33.878926	29.871236	33.270717
C	32.955523	31.679189	32.625083
O	32.073711	31.747544	31.782949
N	33.000644	32.424080	33.762321
H	33.847902	32.355983	34.309047
C	32.182736	33.518926	34.160380
N	32.877641	34.622483	34.461060
C	32.232855	35.637572	35.003845
H	32.826954	36.504644	35.268746
C	30.811197	33.447873	34.402546
C	29.950618	32.244971	34.088510
C	28.827054	32.571242	33.123732
C	29.116521	33.014546	31.831334
C	28.093210	33.319107	30.945215
C	26.764590	33.185978	31.336079
C	26.468777	32.743478	32.618444
C	27.495840	32.441384	33.507135
H	27.257298	32.094211	34.508222
H	25.436071	32.627194	32.933102
H	25.973037	33.433109	30.638168
H	28.330467	33.665977	29.944523
H	30.153029	33.102552	31.524981
H	30.566768	31.443781	33.679081
H	29.517405	31.892389	35.029999
N	30.173151	34.480764	34.955970
C	30.844086	35.597875	35.275373
C	30.148214	36.709943	35.905774
C	30.705089	38.001581	35.916463
H	31.656686	38.163264	35.432142
C	30.083937	39.073740	36.503898
H	30.557715	40.048138	36.480214
C	28.848755	38.923380	37.202031
O	28.274795	39.877487	37.834447
C	28.274286	37.615252	37.148358

H	27.305517	37.517793	37.623787
C	28.891429	36.556469	36.521145
H	28.418876	35.579616	36.493939
C	27.891381	43.717365	37.875739
H	27.743965	44.796887	37.955539
H	27.292278	43.233111	38.654727
C	29.327026	43.378884	38.074472
N	29.753729	42.075595	38.130871
H	29.164136	41.204896	38.010726
C	31.089346	42.114725	38.314799
H	31.685696	41.217766	38.396989
N	31.548831	43.346786	38.391151
C	30.444979	44.149057	38.244783
H	30.510847	45.227877	38.269277
C	25.100165	40.641737	43.725118
H	24.297816	40.131180	44.269222
H	24.633020	41.483724	43.206939
C	25.680890	39.690542	42.706938
C	25.761861	38.324853	42.979872
H	25.446514	37.952642	43.950044
C	26.205093	37.435833	42.011255
H	26.252767	36.377469	42.238148
C	26.572379	37.898448	40.752261
H	26.900641	37.201861	39.986120
C	26.511075	39.259417	40.463871
H	26.834049	39.615939	39.486412
C	26.062788	40.141796	41.442997
H	26.001956	41.204198	41.220782
C	31.643311	41.760358	42.127774
H	30.803443	42.436451	42.315383
H	32.278529	42.273683	41.396631
C	31.170282	40.489648	41.505250
C	29.930401	39.923187	41.542674
H	29.039645	40.239472	42.063656
N	29.903555	38.795840	40.751786
H	29.053965	38.329475	40.479146
C	31.123601	38.647593	40.140268
C	31.547899	37.742620	39.169266
H	30.885413	36.975731	38.782726
C	32.822450	37.907645	38.660616
H	33.168128	37.235888	37.881017
C	33.670549	38.929574	39.124521
H	34.669142	39.021527	38.707305
C	33.256634	39.807356	40.108737

H	33.908059	40.605204	40.453823
C	31.956444	39.684800	40.613297
H	27.518060	43.389443	36.895543
H	25.810888	41.028115	44.463284
H	32.221949	41.607121	43.051388

H22F Ca^{2+}-discharged obelin (**H22F**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + Phe22 + Phe88 + Trp92 (S_1)

O	40.241347	32.191262	32.421550
H	40.580070	32.654589	31.634808
C	38.951345	31.809092	32.257974
C	38.290902	31.275376	33.362862
C	36.992414	30.806796	33.231783
H	36.501397	30.391496	34.109088
H	38.795256	31.265635	34.321483
C	38.291848	31.880940	31.032408
H	38.801304	32.302909	30.170623
C	36.990054	31.413597	30.919538
H	36.485403	31.471454	29.959602
C	36.319089	30.860044	32.008974
C	34.927156	30.300670	31.828680
H	34.805979	29.901424	30.821037
H	34.771227	29.474061	32.532221
C	33.765785	31.284037	32.013184
O	32.963920	31.472287	31.114375
N	33.678998	31.807762	33.268389
H	34.540236	31.804231	33.802434
C	32.823487	32.865281	33.721888
N	33.523334	33.900324	34.198581
C	32.730783	34.842308	34.849264
H	33.249942	35.668927	35.317533
C	31.445566	32.725301	33.782581
C	30.673366	31.535219	33.280683
C	29.670894	31.838668	32.178671
C	28.385621	31.303040	32.222322
C	27.481475	31.532687	31.190497
C	27.841667	32.316942	30.103024
C	29.120046	32.864320	30.055644
C	30.025278	32.624343	31.080563
H	31.027833	33.032360	31.035219
H	29.413481	33.478278	29.210040
H	27.137889	32.507363	29.298663

H	26.489023	31.095219	31.246784
H	28.082252	30.701621	33.073408
H	31.364791	30.772569	32.911797
H	30.125035	31.092503	34.122272
N	30.681498	33.678546	34.419104
C	31.369666	34.708501	34.930155
C	30.519396	35.702131	35.658050
C	30.889566	37.057711	35.758339
H	31.783692	37.388506	35.252397
C	30.156971	37.949237	36.491557
H	30.457632	38.987185	36.565840
C	28.976239	37.536543	37.219412
O	28.317277	38.343298	37.928827
C	28.594279	36.150370	37.065838
H	27.700667	35.829491	37.589801
C	29.330614	35.283640	36.303343
H	29.035722	34.248426	36.178449
C	27.843839	42.754116	37.736839
H	27.437826	43.760931	37.871817
H	27.348699	42.091900	38.455458
C	29.331437	42.783292	37.983403
C	30.098790	41.620613	37.895626
H	29.606572	40.663834	37.739365
C	31.477927	41.680543	38.035920
H	32.068037	40.774191	37.957291
C	32.104053	42.895138	38.304563
H	33.181782	42.939518	38.419179
C	31.337533	44.043595	38.437168
H	31.794710	44.994379	38.662360
C	29.961735	43.986952	38.267085
H	29.377394	44.899472	38.331853
C	25.068448	40.916993	43.739356
H	24.228889	40.409733	44.222195
H	24.663535	41.788443	43.229029
C	25.684521	39.997447	42.712122
C	25.829336	38.632927	42.963527
H	25.547910	38.234795	43.934331
C	26.296655	37.773675	41.977572
H	26.385939	36.713426	42.190719
C	26.621576	38.266284	40.718476
H	26.970830	37.617595	39.922720
C	26.500804	39.627565	40.461739
H	26.778403	40.002086	39.482044
C	26.039145	40.486338	41.453608

H	25.937221	41.549136	41.248343
C	31.603934	42.092089	42.221923
H	30.768455	42.780537	42.372758
H	32.325568	42.616106	41.584527
C	31.167270	40.849424	41.513699
C	29.916697	40.317402	41.414947
H	28.981348	40.675174	41.819384
N	29.946219	39.157680	40.661634
H	29.139652	38.782094	40.180881
C	31.231035	38.968589	40.205934
C	31.736552	38.007180	39.333745
H	31.110046	37.217941	38.937745
C	33.061715	38.120251	38.956021
H	33.471035	37.411606	38.243216
C	33.879041	39.138001	39.475152
H	34.905438	39.206018	39.130927
C	33.386352	40.059030	40.383952
H	34.021010	40.852269	40.769682
C	32.034289	39.995756	40.742384
H	27.624918	42.420821	36.714620
H	25.759521	41.249520	44.521819
H	32.069447	41.887946	43.195827

H22F Ca^{2+}-discharged obelin (**H22F**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + Phe22 + Phe88 + Trp92 (S_0)

O	40.25581100	32.19700300	32.409956
H	40.58838600	32.65393900	31.616119
C	38.96617600	31.81275200	32.267501
C	38.32759100	31.28357600	33.387921
C	37.02776700	30.81488500	33.285161
H	36.55427900	30.39991500	34.172486
H	38.85202100	31.27282900	34.335310
C	38.28350500	31.87871500	31.054027
H	38.77657000	32.29371900	30.179714
C	36.97788700	31.41568700	30.969206
H	36.45112000	31.47272700	30.021138
C	36.33132000	30.86808500	32.076150
C	34.92325300	30.33484400	31.940729
H	34.77831300	29.88338600	30.958053
H	34.74723500	29.56291100	32.698845
C	33.83366700	31.39803000	32.070936
O	33.19894300	31.78470600	31.108146
N	33.60332200	31.80547000	33.356731

H	34.32945000	31.60991600	34.034881
C	32.72798200	32.86683400	33.741351
N	33.33733400	33.96718700	34.199347
C	32.58050800	34.89256700	34.757663
H	33.08197000	35.76275300	35.165531
C	31.34449300	32.71906200	33.810298
C	30.60324700	31.51757000	33.266256
C	29.65898900	31.83286000	32.119213
C	28.35235600	31.34955100	32.126995
C	27.49982000	31.60170600	31.056734
C	27.93280300	32.35319700	29.972577
C	29.23395100	32.84426100	29.962322
C	30.08950000	32.58480400	31.024285
H	31.11185800	32.94301700	30.997598
H	29.58450900	33.43036400	29.119173
H	27.26830800	32.55817900	29.139365
H	26.48791000	31.20916200	31.077493
H	27.99187700	30.77189200	32.972916
H	31.32821700	30.76667200	32.938283
H	30.02653600	31.07520900	34.083654
N	30.59274900	33.65616700	34.388641
C	31.17598300	34.75242700	34.898716
C	30.38537600	35.71861000	35.643639
C	30.81722500	37.04812700	35.818284
H	31.71444200	37.38754600	35.315047
C	30.12062100	37.94596300	36.587522
H	30.48240400	38.96326900	36.683870
C	28.96185800	37.56828600	37.343831
O	28.39194400	38.35869700	38.170508
C	28.50668300	36.22748200	37.104859
H	27.61713900	35.90861900	37.639967
C	29.18339800	35.35311100	36.283668
H	28.81507300	34.34030500	36.147454
C	27.84653900	42.73346300	37.744032
H	27.43520800	43.73625900	37.892814
H	27.36691200	42.06799400	38.470537
C	29.33795400	42.76234800	37.959314
C	30.09735000	41.59210900	37.904944
H	29.60361400	40.62832800	37.798058
C	31.47910600	41.65356400	38.024007
H	32.06390000	40.74214100	37.972692
C	32.11380600	42.87398900	38.238802
H	33.19205700	42.91663800	38.347792
C	31.35460400	44.03108100	38.334137

H	31.81783500	44.98788400	38.515389
C	29.97684500	43.97434100	38.182973
H	29.39496500	44.88999600	38.220533
C	25.07359500	40.92088100	43.730265
H	24.20680800	40.45239200	44.205618
H	24.71012800	41.79177200	43.186229
C	25.68234700	39.95146000	42.743072
C	25.81995000	38.60011800	43.059067
H	25.53062400	38.24965400	44.045490
C	26.30719200	37.69598600	42.124141
H	26.40287300	36.64906800	42.393602
C	26.65339200	38.12687600	40.848812
H	27.04260500	37.45342600	40.093395
C	26.52181600	39.47159300	40.519704
H	26.82522300	39.78576500	39.525039
C	26.03921700	40.37572000	41.461359
H	25.93456200	41.42706300	41.202307
C	31.60590200	42.08193500	42.215725
H	30.75182200	42.74674900	42.367231
H	32.31637000	42.63078100	41.586052
C	31.20190400	40.83621400	41.487725
C	29.95077200	40.31721100	41.315022
H	29.00872200	40.68386500	41.698110
N	29.99757000	39.17431800	40.539232
H	29.23367300	38.83564000	39.947780
C	31.30192900	38.98399000	40.147727
C	31.82850900	38.03459500	39.274742
H	31.20467000	37.26704900	38.837247
C	33.15938400	38.15727100	38.926024
H	33.58384700	37.46566700	38.204701
C	33.96185500	39.17038800	39.475471
H	34.98810600	39.25564200	39.134713
C	33.45177900	40.06991200	40.397096
H	34.07703300	40.85938400	40.805847
C	32.09368600	39.99505800	40.732005
H	27.58478200	42.37846900	36.739073
H	25.75490700	41.25020700	44.522978
H	32.07987900	41.88406800	43.187351

H22R Ca^{2+}-discharged obelin (**H22R**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + Arg22 + Phe88 + Trp92 (S_1)

O	40.146259	32.069097	32.086993
H	40.455293	32.581076	31.321457

C	38.818920	31.776754	32.002425
C	38.180389	31.384062	33.176208
C	36.844392	31.021446	33.149416
H	36.354281	30.741981	34.078285
H	38.735542	31.411057	34.104952
C	38.102234	31.814976	30.809694
H	38.596961	32.116371	29.890047
C	36.757155	31.457661	30.800683
H	36.200387	31.498953	29.869573
C	36.109540	31.047022	31.962338
C	34.642348	30.685468	31.952073
H	34.340917	30.391261	30.942902
H	34.444802	29.842957	32.620934
C	33.795212	31.899364	32.330012
O	33.805116	32.909239	31.647290
N	33.057112	31.759640	33.466982
H	33.021066	30.854832	33.917310
C	32.375355	32.845361	34.092404
N	33.158206	33.879859	34.450940
C	32.441470	34.875706	35.083495
H	33.018098	35.731372	35.416255
C	31.006704	32.752050	34.317221
C	30.162933	31.607013	33.820460
C	29.424814	31.876295	32.516814
C	28.105957	31.454204	32.347624
C	27.441748	31.663050	31.141759
C	28.082497	32.295699	30.083777
C	29.397733	32.718913	30.244653
C	30.061775	32.510610	31.446675
H	31.085475	32.856618	31.560882
H	29.907399	33.218183	29.427282
H	27.568705	32.469132	29.143524
H	26.409019	31.339664	31.036953
H	27.586704	30.960697	33.165381
H	30.769054	30.706364	33.686225
H	29.421191	31.383439	34.592487
N	30.323632	33.731130	34.994300
C	31.098383	34.795659	35.329302
C	30.350612	35.895467	35.984733
C	30.815196	37.230519	35.972070
H	31.723175	37.454971	35.433717
C	30.146425	38.228305	36.620464
H	30.521365	39.245411	36.604822
C	28.944762	37.965580	37.381114

O	28.381953	38.866976	38.066824
C	28.451346	36.609072	37.325474
H	27.524819	36.393797	37.848988
C	29.121897	35.629653	36.642197
H	28.753846	34.612244	36.588280
C	27.615657	43.040662	37.853505
H	27.136284	44.017180	37.945146
H	27.139281	42.356994	38.562316
C	29.097291	43.181562	38.223280
H	29.499015	44.112431	37.815964
H	29.179681	43.270081	39.309822
C	29.944162	41.993109	37.777510
H	29.436773	41.048062	37.995282
H	30.110256	42.016056	36.694511
N	31.240396	41.929827	38.437135
H	31.359439	41.222048	39.155048
C	32.333066	42.574755	38.051458
N	32.294942	43.525958	37.102400
H	31.431025	44.017667	36.903934
H	33.129637	44.089294	36.999192
N	33.498946	42.245308	38.603995
H	33.547768	41.435785	39.216378
H	34.355027	42.604234	38.197318
C	25.080477	40.707885	44.032843
H	24.303529	40.111770	44.518694
H	24.586300	41.573354	43.593316
C	25.707338	39.892546	42.926206
C	25.940912	38.526450	43.084681
H	25.735854	38.056703	44.041072
C	26.404063	37.756172	42.026490
H	26.565938	36.692796	42.168805
C	26.634027	38.339418	40.784953
H	26.976014	37.754544	39.938261
C	26.421238	39.703990	40.616386
H	26.613788	40.145522	39.642710
C	25.962623	40.473365	41.681893
H	25.780347	41.537181	41.546182
C	31.535612	42.094849	42.485783
H	30.672769	42.740953	42.666817
H	32.233906	42.665200	41.861866
C	31.135597	40.870576	41.727344
C	29.876418	40.380547	41.526900
H	28.933979	40.758745	41.894759
N	29.921785	39.259922	40.730361

H	29.110738	38.866293	40.270482
C	31.223857	39.019838	40.369522
C	31.768610	38.045203	39.527722
H	31.150830	37.281300	39.072222
C	33.125877	38.097677	39.276010
H	33.565293	37.379302	38.592691
C	33.947488	39.052168	39.903371
H	35.008593	39.044484	39.681803
C	33.419735	39.981905	40.786067
H	34.067329	40.678395	41.315382
C	32.027108	39.999653	41.003501
H	27.485319	42.661265	36.833439
H	25.779041	41.047195	44.805632
H	31.987199	41.860164	43.457387

H22R Ca^{2+}-discharged obelin (**H22R**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + Arg22 + Phe88 + Trp92 (S_0)

O	40.14997200	32.08682700	32.082416
H	40.46125500	32.60097700	31.318447
C	38.82455800	31.79700400	32.005112
C	38.19558800	31.39873500	33.182906
C	36.86097000	31.03283600	33.165865
H	36.38348000	30.73773300	34.096447
H	38.76101500	31.41635500	34.105386
C	38.09556000	31.84781200	30.820048
H	38.58133200	32.15570300	29.898041
C	36.75053000	31.49071200	30.821369
H	36.18637400	31.53766000	29.894980
C	36.11552500	31.06832900	31.985859
C	34.65057000	30.69325100	31.984559
H	34.34186100	30.41375800	30.973578
H	34.46510700	29.83558100	32.637056
C	33.79192100	31.88336200	32.392868
O	33.76135600	32.90887700	31.735396
N	33.07685500	31.72456600	33.547867
H	33.08979700	30.83102800	34.022320
C	32.34605200	32.79414200	34.126896
N	33.04653900	33.86064600	34.518649
C	32.37958400	34.85316600	35.079867
H	32.96220000	35.70447800	35.416093
C	30.96449900	32.72927600	34.304767
C	30.12435800	31.57495600	33.810663
C	29.42724900	31.85810700	32.489479

C	28.10217000	31.46524100	32.300658
C	27.45800000	31.70882200	31.091129
C	28.12365100	32.34906500	30.053402
C	29.44701000	32.73593400	30.232757
C	30.09396800	32.49109500	31.437481
H	31.12536600	32.81073100	31.557794
H	29.97623500	33.23783300	29.429944
H	27.62151900	32.55524900	29.113790
H	26.41965300	31.41292300	30.968510
H	27.56262700	30.97248300	33.105346
H	30.73371400	30.67274000	33.710599
H	29.36388600	31.37786400	34.568100
N	30.30892400	33.72368300	34.907173
C	30.98667900	34.81033800	35.302786
C	30.27388700	35.89724600	35.979419
C	30.79361100	37.20035700	36.037093
H	31.71966600	37.43179100	35.524545
C	30.14898600	38.21295600	36.714258
H	30.58929700	39.20528900	36.740029
C	28.94198400	37.99608600	37.444791
O	28.39176400	38.90919600	38.166439
C	28.40287200	36.67562500	37.327911
H	27.46792000	36.46777200	37.841120
C	29.04232900	35.67737900	36.621664
H	28.61117300	34.68209300	36.571170
C	27.61263600	43.04270000	37.852741
H	27.15519900	44.03029000	37.942501
H	27.11854700	42.36526200	38.554697
C	29.09612000	43.14352200	38.227268
H	29.52345800	44.05808000	37.807807
H	29.18161400	43.24626700	39.312526
C	29.89043800	41.91252800	37.798965
H	29.36100300	40.99503400	38.088391
H	30.01422800	41.88588700	36.710245
N	31.21000100	41.82831000	38.408973
H	31.34699200	41.07756800	39.077357
C	32.29278000	42.49038600	38.032748
N	32.24200500	43.49302900	37.138040
H	31.37204600	43.98018400	36.959803
H	33.07129100	44.06688400	37.056389
N	33.47274000	42.12947200	38.541076
H	33.53436300	41.26139700	39.068145
H	34.31939700	42.51337700	38.136867
C	25.08205500	40.70189000	44.034122

H	24.30125400	40.11086100	44.520460
H	24.59123900	41.56536100	43.586048
C	25.71643700	39.87794300	42.938233
C	25.94692200	38.51273800	43.108494
H	25.71927500	38.04801700	44.062376
C	26.44076000	37.73873100	42.066025
H	26.60521300	36.67687800	42.219257
C	26.70815100	38.31854700	40.831282
H	27.09503600	37.74873800	39.995303
C	26.49262600	39.67975300	40.650594
H	26.72799700	40.11014200	39.682985
C	25.99805700	40.45184200	41.696901
H	25.81808200	41.51507000	41.552221
C	31.53050600	42.10326300	42.490137
H	30.65535500	42.72562800	42.692332
H	32.21012000	42.70851500	41.878259
C	31.15114400	40.89491700	41.697304
C	29.89176200	40.45352900	41.398693
H	28.94578600	40.85311600	41.735110
N	29.94326600	39.37165800	40.554567
H	29.15651000	39.02942700	39.995034
C	31.25659700	39.09289600	40.282945
C	31.81244100	38.12416700	39.442436
H	31.18609100	37.41191200	38.922380
C	33.17765500	38.14508300	39.257724
H	33.63117400	37.43563000	38.573403
C	33.99394300	39.06738400	39.942714
H	35.05987500	39.04208400	39.749713
C	33.45412200	39.98182200	40.832972
H	34.09289100	40.66799200	41.384319
C	32.05573800	40.02569000	40.992920
H	27.48411800	42.67546700	36.828014
H	25.77466000	41.04438700	44.810432
H	32.00563100	41.85764400	43.447326

H22E Ca^{2+}-discharged obelin (**H22E**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + Glu22 + Phe88 + Trp92 (S_1)

O	40.38531100	32.20277800	32.536588
H	40.76385100	32.72247500	31.804064
C	39.07992600	31.92473100	32.285753
C	38.31342400	31.38094000	33.312745
C	37.00491700	30.99550600	33.063134
H	36.43263000	30.55564500	33.876483

H	38.74651200	31.27774700	34.300270
C	38.50890300	32.12564100	31.032426
H	39.10182600	32.57052700	30.238143
C	37.19513100	31.74684900	30.802822
H	36.76434000	31.89649600	29.817199
C	36.42274300	31.15736100	31.802313
C	35.03557100	30.66224400	31.471486
H	34.95586200	30.46845400	30.401492
H	34.85425300	29.70790900	31.981338
C	33.83260100	31.55696500	31.796081
O	32.95336600	31.70705500	30.963843
N	33.79040100	32.00882900	33.078824
H	34.69127600	32.08663200	33.535869
C	32.86502900	32.94839100	33.650496
N	33.48759100	33.99035700	34.186634
C	32.65503200	34.83963200	34.914814
H	33.11814700	35.67755000	35.417598
C	31.50445800	32.69455700	33.738142
C	30.79620600	31.49864600	33.165219
C	29.71546400	31.84206800	32.152867
C	28.45324300	31.26248900	32.234578
C	27.47716600	31.54999900	31.287070
C	27.74158600	32.42564800	30.244108
C	28.99969200	33.01526100	30.160067
C	29.97506300	32.72493600	31.102962
H	30.95947200	33.17257900	31.033061
H	29.21840400	33.70642300	29.352392
H	26.98339600	32.66211700	29.503065
H	26.50161300	31.07410800	31.379869
H	28.22745400	30.58661500	33.052596
H	31.51341300	30.83551600	32.674275
H	30.32432700	30.93465200	33.982450
N	30.69719800	33.54627900	34.464791
C	31.30834500	34.59810800	35.012083
C	30.40323600	35.48078000	35.817014
C	30.63415800	36.86269900	35.963601
H	31.44251600	37.32274400	35.409974
C	29.88719800	37.62219600	36.827071
H	30.09024400	38.68019000	36.958827
C	28.84195100	37.02263300	37.632795
O	28.21507500	37.66971400	38.510402
C	28.56831500	35.62462100	37.389184
H	27.76499600	35.17530900	37.963309
C	29.31968500	34.89501700	36.511308

H	29.12531200	33.84287200	36.336850
C	28.27688900	42.83281500	37.547263
H	27.53781200	43.57695000	37.872987
H	28.24961600	42.01974100	38.281298
C	29.65634500	43.52755000	37.594067
H	29.62247900	44.43174100	36.970899
H	29.83922300	43.86510400	38.618422
C	30.90055200	42.71606100	37.125396
O	31.80967400	42.57155600	37.973373
O	30.88186600	42.35550800	35.924226
C	25.06681200	40.78214700	43.752670
H	24.15500700	40.38880900	44.216368
H	24.78145500	41.65775800	43.169817
C	25.64029800	39.73632200	42.830564
C	25.80417100	38.42177600	43.264425
H	25.55068700	38.16179200	44.287687
C	26.26947900	37.44301100	42.398664
H	26.39284600	36.42744000	42.759354
C	26.56427400	37.76074600	41.077842
H	26.93571000	37.02164500	40.378268
C	26.41259100	39.07020600	40.634893
H	26.68122000	39.31295600	39.612333
C	25.95841400	40.05129500	41.510145
H	25.84763300	41.07586500	41.163537
C	31.51806900	41.82716300	42.290991
H	30.66752100	42.49384200	42.460914
H	32.21217300	42.36755200	41.638509
C	31.09727700	40.57871800	41.579582
C	29.88536200	39.95468100	41.570878
H	28.95095700	40.25554800	42.022097
N	29.94906800	38.78365700	40.831228
H	29.15018300	38.38581800	40.348014
C	31.21641600	38.68698800	40.293130
C	31.75426900	37.72251400	39.443459
H	31.16850200	36.87437700	39.110997
C	33.05049400	37.91099900	39.002002
H	33.48228300	37.19929300	38.305402
C	33.81206200	39.00628200	39.436495
H	34.80967900	39.14099200	39.032290
C	33.28815600	39.93929800	40.312577
H	33.87205000	40.80232700	40.618187
C	31.96957900	39.78414000	40.751460
H	28.05372900	42.45578300	36.544622
H	25.73910300	41.09413200	44.559630

H 32.00675800 41.62744400 43.255375

H22E Ca^{2+}-discharged obelin (**H22E**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + Glu22 + Phe88 + Trp92 (S_0)

O 40.38946700 32.18436000 32.531472
H 40.76526000 32.70733500 31.799809
C 39.08527000 31.90465400 32.289329
C 38.33081500 31.35034900 33.319795
C 37.01999000 30.96754800 33.081798
H 36.45739900 30.52137600 33.899117
H 38.77175500 31.24651400 34.303301
C 38.50252900 32.10934900 31.041126
H 39.08662000 32.55939100 30.243481
C 37.18711900 31.73166800 30.822015
H 36.74461000 31.88686600 29.842283
C 36.42611000 31.13904400 31.828446
C 35.02447200 30.67232200 31.519479
H 34.93243400 30.44017400 30.458151
H 34.80682800 29.75088500 32.073005
C 33.88260000 31.64687300 31.812608
O 33.06291600 31.91770700 30.952767
N 33.80084200 32.05621200 33.111353
H 34.65284500 31.98981600 33.653547
C 32.84573800 32.97846700 33.638358
N 33.37348200 34.08387700 34.185403
C 32.56194000 34.89821800 34.828650
H 32.99380900 35.77332200 35.301636
C 31.48592800 32.70227300 33.739128
C 30.81364800 31.49021700 33.128722
C 29.73686500 31.83927300 32.116411
C 28.45951600 31.29921900 32.229555
C 27.48480400 31.58603000 31.280728
C 27.76263400 32.42701400 30.213145
C 29.03413200 32.98020700 30.100817
C 30.01203500 32.68590600 31.040188
H 31.00875100 33.09861900 30.938330
H 29.26364100 33.64410100 29.273778
H 27.00352900 32.66622100 29.474198
H 26.50027600 31.13441000 31.387302
H 28.21908200 30.64792000 33.063091
H 31.55876200 30.85733600 32.640685
H 30.35468300 30.91287400 33.938636
N 30.67716400 33.51873400 34.411781

C	31.17433600	34.63219200	34.984325
C	30.32871900	35.45273600	35.817821
C	30.60037600	36.81827500	36.072729
H	31.41476100	37.31333800	35.552266
C	29.84641300	37.55448600	36.949694
H	30.07531900	38.60142100	37.119021
C	28.80384700	36.95439100	37.736888
O	28.20908000	37.56735600	38.676501
C	28.49851200	35.58930400	37.408679
H	27.70480500	35.11592200	37.978632
C	29.21900800	34.88228200	36.480199
H	28.97732100	33.84211700	36.276954
C	28.28799500	42.82859700	37.545023
H	27.53464800	43.54495000	37.899330
H	28.30180900	42.00637700	38.268528
C	29.64905100	43.56123700	37.565976
H	29.57918300	44.46272100	36.942157
H	29.83639500	43.90163300	38.588545
C	30.91127100	42.78184600	37.084668
O	31.79066200	42.57793100	37.950933
O	30.93645900	42.50284400	35.861899
C	25.06521100	40.78984900	43.751240
H	24.14420000	40.41122200	44.210000
H	24.79651900	41.66533600	43.159719
C	25.63765200	39.73129100	42.844847
C	25.80139000	38.42489600	43.300704
H	25.53482800	38.18117600	44.324832
C	26.27493000	37.43299500	42.454121
H	26.39750600	36.42310700	42.832129
C	26.58583800	37.73195900	41.133229
H	26.97834300	36.99688800	40.439841
C	26.42622200	39.03273200	40.666477
H	26.70771000	39.24882100	39.641150
C	25.95996100	40.02580500	41.520720
H	25.84471400	41.04423100	41.156743
C	31.51182500	41.81449700	42.286997
H	30.64994200	42.46672800	42.456986
H	32.19843500	42.37023800	41.639338
C	31.11023000	40.56584500	41.556978
C	29.89131900	39.95110400	41.481953
H	28.94078300	40.25112400	41.900471
N	29.97083200	38.79888100	40.718504
H	29.19914500	38.38774700	40.181572
C	31.25941500	38.69741500	40.243102

C	31.81623900	37.73936900	39.398175
H	31.22844200	36.90749400	39.033257
C	33.11995700	37.93280800	38.987684
H	33.56474500	37.23180100	38.287628
C	33.87219100	39.02252000	39.452250
H	34.87033000	39.17095500	39.053778
C	33.33323700	39.94032600	40.335245
H	33.91220000	40.79780900	40.665556
C	32.00558000	39.78033400	40.746769
H	28.04422900	42.45679400	36.544965
H	25.72441600	41.10305000	44.568839
H	31.99779000	41.61404800	43.252690

F88A Ca^{2+}-discharged obelin (**F88A**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Ala88 + Trp92 (S_1)

O	37.226300	31.493676	30.614524
H	37.102349	31.199513	31.526241
C	36.362016	32.508911	30.316776
C	36.802813	33.492637	29.435632
C	35.952824	34.520540	29.056742
H	36.308728	35.281298	28.367949
H	37.818747	33.436822	29.062342
C	35.058050	32.558931	30.799255
H	34.703263	31.795328	31.483465
C	34.215608	33.593363	30.411827
H	33.197831	33.601038	30.793010
C	34.642062	34.590828	29.532507
C	33.716631	35.680050	29.040281
H	34.070616	36.061371	28.081103
H	32.717764	35.253121	28.879833
C	33.512568	36.932059	29.914606
O	33.506121	38.038010	29.389439
N	33.243366	36.659319	31.209191
H	33.478916	35.724902	31.517409
C	33.024058	37.487933	32.354467
N	33.724971	37.011861	33.402048
C	33.427838	37.648850	34.595900
H	33.966147	37.303418	35.470715
C	32.093351	38.509725	32.413748
C	31.276420	39.037747	31.264246
C	31.443344	40.534702	31.091889
C	30.374558	41.404559	31.279606
C	30.545437	42.780736	31.167059

C	31.794992	43.308858	30.873996
C	32.867921	42.445008	30.668927
C	32.690792	41.072106	30.768909
H	33.522385	40.392812	30.610337
H	33.845642	42.849418	30.428882
H	31.940842	44.380728	30.804128
H	29.695793	43.440639	31.320141
H	29.398660	40.998104	31.530791
H	31.534770	38.536093	30.332625
H	30.221105	38.839920	31.480378
N	31.798217	39.109072	33.619518
C	32.508852	38.658897	34.666461
C	32.241763	39.402033	35.933448
C	30.951547	39.902963	36.233898
H	30.175807	39.776851	35.487518
C	30.694390	40.518632	37.429452
H	29.702544	40.876777	37.684304
C	31.735171	40.713884	38.412359
O	31.489704	41.204760	39.552874
C	33.060636	40.290787	38.034797
H	33.866840	40.451504	38.740497
C	33.281239	39.651882	36.847724
H	34.265974	39.300525	36.591403
C	33.708778	43.455860	42.430714
H	34.086382	43.915049	43.346193
H	32.619872	43.373713	42.519542
C	34.321370	42.102418	42.265686
N	33.832135	41.156566	41.390251
H	32.986801	41.214481	40.814264
C	34.677369	40.091407	41.449184
H	34.509371	39.190118	40.876423
N	35.667844	40.289498	42.284540
C	35.449699	41.540843	42.801683
H	36.101917	41.955509	43.555772
C	27.416527	42.148350	44.215659
H	27.984272	43.047870	44.453924
H	27.860035	41.661664	43.344710
H	26.383563	42.423558	43.990857
C	32.448070	37.838339	44.247569
H	32.276278	38.713949	44.879334
H	33.531955	37.701255	44.182427
C	31.939560	38.048305	42.861723
C	30.967460	38.889685	42.424636
H	30.369154	39.587384	42.992273

N	30.775245	38.750024	41.056125
H	30.507218	39.550225	40.493436
C	31.717800	37.847658	40.589668
C	32.009818	37.446412	39.287186
H	31.452246	37.826071	38.439161
C	33.072341	36.577446	39.105509
H	33.344526	36.280641	38.097797
C	33.804569	36.086147	40.196736
H	34.645683	35.426758	40.012184
C	33.489696	36.456926	41.492464
H	34.075893	36.090122	42.329879
C	32.443238	37.363962	41.696421
H	33.945814	44.123570	41.590150
H	27.392176	41.492720	45.089158
H	32.009769	36.954509	44.731126

F88A Ca^{2+}-discharged obelin (**F88A**)
CAM-B3LYP/6-31G(d,p)/MM
CLM+His22+Ala88+Trp92 (S_0)

O	37.26229700	31.48640200	30.555634
H	37.11026200	31.13751200	31.443520
C	36.38787200	32.49370500	30.275733
C	36.81867000	33.49594800	29.409607
C	35.96195800	34.52525700	29.051781
H	36.31118400	35.30076900	28.376353
H	37.83171800	33.45081800	29.028202
C	35.08603300	32.52850200	30.767004
H	34.73453900	31.74638600	31.431780
C	34.23565800	33.56184000	30.396302
H	33.21489900	33.54666700	30.771119
C	34.65422500	34.57840700	29.536614
C	33.72605800	35.68839300	29.095021
H	34.04752400	36.08613700	28.131082
H	32.71216200	35.28487800	28.977248
C	33.62157400	36.90590900	30.023525
O	33.84037200	38.03497400	29.614708
N	33.18305800	36.60850000	31.273331
H	33.17794900	35.63185500	31.533626
C	33.00374200	37.48283800	32.383501
N	33.68594200	37.11070800	33.471589
C	33.44889000	37.75618300	34.598125
H	33.99597800	37.43137800	35.476978
C	32.06841300	38.51468600	32.430614
C	31.28328200	39.01656200	31.237938

C	31.42913600	40.51435000	31.065271
C	30.34666600	41.36721200	31.250442
C	30.50441700	42.74509200	31.145515
C	31.75132400	43.28816700	30.868736
C	32.83601900	42.43957900	30.665155
C	32.67384900	41.06384400	30.752012
H	33.51533900	40.39731000	30.589573
H	33.81063700	42.85707600	30.437119
H	31.88670800	44.36224200	30.812796
H	29.64717500	43.39481000	31.294366
H	29.37346900	40.95145800	31.494483
H	31.59981000	38.50437900	30.329628
H	30.23119800	38.78097000	31.411911
N	31.81405400	39.13391400	33.584422
C	32.48700100	38.78940900	34.688973
C	32.21453700	39.46175000	35.952558
C	30.95593200	40.00170200	36.273324
H	30.14822900	39.91249900	35.551537
C	30.72563800	40.59865300	37.494957
H	29.73536300	40.95819000	37.758545
C	31.75589100	40.74338500	38.477467
O	31.51488200	41.20966600	39.653145
C	33.04569300	40.28363200	38.084082
H	33.86926800	40.39185200	38.779395
C	33.24291400	39.63177900	36.892518
H	34.22696600	39.25094200	36.661039
C	33.69552700	43.44897000	42.420403
H	34.07820700	43.89555800	43.340152
H	32.60593000	43.37273100	42.505596
C	34.29478300	42.09184700	42.238669
N	33.78970600	41.15434300	41.365492
H	32.93734300	41.21863700	40.771478
C	34.62765500	40.08628100	41.419582
H	34.45073000	39.18905400	40.843479
N	35.62783300	40.27025600	42.251091
C	35.42329900	41.52264300	42.769235
H	36.08271400	41.93495400	43.519291
C	27.41378200	42.14841600	44.214886
H	27.98982500	43.04369200	44.449446
H	27.84945500	41.66104200	43.341016
H	26.38015000	42.42635200	43.995262
C	32.45567400	37.82490800	44.233117
H	32.28446600	38.70812800	44.853722
H	33.53994200	37.68391300	44.173189

C	31.95601500	38.02644500	42.842013
C	31.03689700	38.92135900	42.394063
H	30.48598900	39.65734700	42.962373
N	30.85595200	38.81450900	41.024255
H	30.72006200	39.67294700	40.475600
C	31.74868300	37.85761900	40.568376
C	32.03248100	37.45587800	39.263998
H	31.50566200	37.88098000	38.418166
C	33.05825000	36.54534900	39.081803
H	33.33119200	36.25097600	38.072600
C	33.76384500	36.01480400	40.172235
H	34.58941600	35.33718900	39.980639
C	33.44929000	36.37782200	41.470501
H	34.01528000	35.98036300	42.308360
C	32.43765800	37.32424900	41.677840
H	33.92678400	44.12705300	41.585565
H	27.39854500	41.48776700	45.084674
H	32.01912000	36.94408900	44.726231

F88Y Ca^{2+}-discharged obelin (**F88Y**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM+His22+Tyr88+Trp92(S_1)

O	38.776434	32.457729	35.716008
H	38.585137	32.070105	34.853577
C	38.768416	33.816671	35.603213
C	38.736889	34.561311	36.779525
C	38.728648	35.946710	36.719711
H	38.701315	36.519364	37.641865
H	38.715421	34.040286	37.730451
C	38.818606	34.468793	34.375344
H	38.844456	33.899652	33.450612
C	38.813710	35.856953	34.333533
H	38.867877	36.338739	33.359913
C	38.765500	36.624276	35.498864
C	38.793314	38.136348	35.474789
H	39.089445	38.521888	36.451104
H	39.544908	38.472851	34.747178
C	37.485919	38.871254	35.127516
O	37.101088	39.806336	35.813883
N	36.913074	38.458568	33.969642
H	37.176300	37.531828	33.659680
C	35.643537	38.796514	33.408899
N	34.899061	37.691816	33.222181
C	33.719384	37.931387	32.547152

H	33.075518	37.074570	32.386050
C	35.310393	40.067409	32.976474
C	36.124802	41.311971	33.222730
C	35.285548	42.399151	33.864605
C	34.951488	43.554956	33.165627
C	34.119488	44.517815	33.726182
C	33.559572	44.310760	34.978222
C	33.944268	43.192495	35.717941
C	34.753818	42.218209	35.142822
H	35.017273	41.316643	35.686455
H	33.440703	42.982665	36.659551
H	32.872086	45.042211	35.381609
H	33.865491	45.405104	33.155777
H	35.364086	43.709959	32.173410
H	36.983701	41.092803	33.856643
H	36.502105	41.691220	32.266164
N	34.159127	40.272643	32.253817
C	33.382072	39.178382	32.107442
C	32.073283	39.467366	31.467962
C	31.939012	40.546064	30.559308
H	32.817604	41.146655	30.359478
C	30.737032	40.824603	29.971257
H	30.634311	41.618765	29.242302
C	29.556895	40.070095	30.302330
O	28.431233	40.328043	29.761615
C	29.701283	39.009248	31.260013
H	28.824542	38.428286	31.518178
C	30.922288	38.722760	31.797853
H	31.026197	37.907226	32.492738
C	24.144680	40.197935	30.385714
H	23.060257	40.076653	30.341639
H	24.464145	40.669893	29.449064
C	24.772712	38.847397	30.530863
N	26.123294	38.606132	30.384349
H	26.866271	39.267980	30.151245
C	26.310014	37.274076	30.593458
H	27.280785	36.806069	30.503911
N	25.189130	36.652168	30.862212
C	24.226148	37.626509	30.823710
H	23.183561	37.389565	30.973859
C	24.996638	41.714891	23.541998
H	25.282573	42.485978	22.818923
H	24.099242	42.064769	24.047911
C	26.086052	41.521801	24.559493

C	27.426190	41.497464	24.176530
H	27.681174	41.645249	23.133059
C	28.434186	41.307415	25.104657
H	29.476935	41.292294	24.807555
C	28.111505	41.140636	26.449829
O	29.124488	40.904950	27.320074
H	28.770505	40.794541	28.247587
C	26.778114	41.175105	26.855068
H	26.532264	41.032980	27.902596
C	25.780427	41.360278	25.908363
H	24.740393	41.372210	26.225232
C	25.943122	35.686921	26.408554
H	25.106545	36.351689	26.177217
H	25.645744	35.097346	27.280415
C	27.173319	36.445680	26.779679
C	27.626294	37.637347	26.301907
H	27.168354	38.308046	25.587978
N	28.840646	37.958858	26.889506
H	29.188520	38.909973	26.945927
C	29.139228	36.988827	27.824315
C	30.185197	36.910240	28.742419
H	30.946078	37.681214	28.801144
C	30.202616	35.825337	29.602854
H	30.990204	35.753944	30.346075
C	29.218374	34.825430	29.537394
H	29.246853	34.005114	30.246514
C	28.192158	34.897110	28.612518
H	27.421033	34.133517	28.586825
C	28.135031	36.001608	27.754439
H	24.389589	40.866065	31.223821
H	24.750439	40.804664	22.981626
H	26.094485	34.997051	25.566465

F88Y Ca^{2+}-discharged obelin (**F88Y**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Tyr88 + Trp92(S_0)

O	38.79250000	32.44091300	35.785814
H	38.62083600	32.02948900	34.930140
C	38.78258100	33.79469700	35.644258
C	38.74973300	34.56356300	36.805711
C	38.73914400	35.94712000	36.718746
H	38.71059300	36.53837300	37.629148
H	38.72974500	34.06233300	37.767071
C	38.83395200	34.42169800	34.402784

H	38.86428500	33.83433400	33.489888
C	38.82839000	35.80827200	34.333884
H	38.89221300	36.26921600	33.350088
C	38.77708000	36.59748600	35.483558
C	38.79461300	38.10912200	35.424156
H	39.10842500	38.52213000	36.383524
H	39.52132700	38.43542000	34.667968
C	37.46400000	38.79709800	35.095039
O	36.99769300	39.66521000	35.812863
N	36.92375800	38.42556500	33.900026
H	37.26184200	37.56012300	33.501748
C	35.64664300	38.79586300	33.392756
N	34.81869400	37.76583000	33.207886
C	33.66706100	37.99200600	32.602610
H	33.01441300	37.13947100	32.448788
C	35.30631700	40.08287900	32.979727
C	36.13940000	41.32078300	33.242297
C	35.29964900	42.41192900	33.876632
C	34.97853800	43.56890300	33.173474
C	34.14308500	44.53202300	33.727632
C	33.56434500	44.32127900	34.970921
C	33.93773700	43.20347700	35.716218
C	34.75542000	42.23042800	35.149602
H	35.01274900	41.33227000	35.702193
H	33.41918500	42.98599100	36.647669
H	32.86692000	45.04866500	35.364117
H	33.89876800	45.42020300	33.155599
H	35.40291800	43.72828700	32.187245
H	36.98425200	41.07710200	33.885834
H	36.53778900	41.68378700	32.290774
N	34.15930100	40.28725300	32.332624
C	33.30804400	39.27335100	32.136201
C	32.03910400	39.52842700	31.463187
C	31.87777900	40.60765400	30.580528
H	32.73057700	41.24500700	30.367507
C	30.66158800	40.86446900	29.985641
H	30.55881000	41.66184700	29.259661
C	29.50894600	40.08559700	30.277932
O	28.36502700	40.32546600	29.697292
C	29.67657500	39.02751200	31.200628
H	28.82170300	38.41098800	31.450064
C	30.90955200	38.74607900	31.743047
H	30.99632400	37.90909500	32.420996
C	24.15629000	40.20269600	30.379651

H	23.07358200	40.06561600	30.337366
H	24.46821700	40.68543100	29.446005
C	24.80808100	38.86291600	30.515760
N	26.15805300	38.63778700	30.347739
H	26.90921700	39.30710700	30.108230
C	26.35743200	37.30963600	30.556780
H	27.33242200	36.85336000	30.456564
N	25.24714100	36.67244800	30.844720
C	24.27541500	37.63762200	30.820089
H	23.23645300	37.39311300	30.986900
C	25.00694400	41.71638400	23.536094
H	25.30981700	42.47660900	22.807890
H	24.10841500	42.08395800	24.027458
C	26.08391100	41.51857900	24.567258
C	27.42969400	41.48952100	24.204632
H	27.70163800	41.64111400	23.165390
C	28.42213600	41.28379600	25.146425
H	29.46896200	41.26175100	24.862725
C	28.08642900	41.10177500	26.490599
O	29.07270900	40.83911500	27.365870
H	28.70409200	40.69342700	28.333640
C	26.74213700	41.14838400	26.871464
H	26.48242000	40.99955400	27.914241
C	25.76089100	41.35024500	25.912089
H	24.71621200	41.36764300	26.214604
C	25.95539300	35.68627700	26.410778
H	25.12364200	36.35797500	26.182513
H	25.65646300	35.09857400	27.283711
C	27.19256900	36.43679300	26.777721
C	27.63991600	37.63657500	26.313471
H	27.17551600	38.31405200	25.609924
N	28.85318200	37.95904500	26.900134
H	29.17322900	38.92108100	26.992224
C	29.15598700	36.98071500	27.824253
C	30.19923300	36.90589100	28.744912
H	30.93905500	37.69466200	28.825206
C	30.22335800	35.81543100	29.596920
H	31.00324400	35.75055700	30.349388
C	29.24740500	34.80825700	29.523551
H	29.27654800	33.98800000	30.233161
C	28.22122900	34.87832500	28.598335
H	27.45268400	34.11210000	28.571035
C	28.15810000	35.98701800	27.746054
H	24.39328200	40.87336600	31.218816

H	24.75284100	40.80389500	22.981777
H	26.09767000	34.99412200	25.567920

F88E Ca^{2+}-discharged obelin (**F88E**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Glu88 + Trp92 (S_1)

O	37.188588	31.362845	30.738312
H	36.642452	30.775118	31.275925
C	36.428567	32.415074	30.311102
C	37.043882	33.377012	29.513641
C	36.304694	34.448653	29.032881
H	36.789335	35.191419	28.406656
H	38.096869	33.271187	29.275805
C	35.076715	32.533571	30.615507
H	34.588133	31.798082	31.248725
C	34.354267	33.616134	30.129652
H	33.298522	33.678929	30.380183
C	34.946588	34.592485	29.325487
C	34.163065	35.742106	28.729930
H	34.704292	36.158878	27.879617
H	33.205817	35.363748	28.346519
C	33.827084	36.953269	29.625401
O	33.942319	38.085769	29.177241
N	33.307711	36.621128	30.828707
H	33.490328	35.671450	31.125867
C	33.102596	37.412260	32.013039
N	33.725629	36.857766	33.041761
C	33.457570	37.467410	34.267275
H	33.933675	37.020628	35.126392
C	32.256722	38.512088	32.081605
C	31.518317	39.118399	30.916656
C	31.733398	40.615950	30.795858
C	30.711519	41.510835	31.101390
C	30.913065	42.885276	31.037157
C	32.168132	43.390817	30.725556
C	33.181029	42.509279	30.346101
C	32.978951	41.135705	30.439054
H	33.774813	40.436694	30.205360
H	34.190937	42.894143	30.214109
H	32.322083	44.463638	30.727792
H	30.095231	43.550385	31.300457
H	29.731958	41.120810	31.362616
H	31.828670	38.637502	29.988143
H	30.439375	38.948598	31.033216

N	32.014164	39.104752	33.308495
C	32.631812	38.568918	34.354703
C	32.422549	39.294443	35.652832
C	31.421910	40.284471	35.806070
H	30.753454	40.453723	34.970114
C	31.328256	41.022746	36.956437
H	30.561854	41.771677	37.107542
C	32.268995	40.862575	38.041896
O	32.274494	41.617491	39.047325
C	33.212548	39.782687	37.893323
H	33.859904	39.561341	38.731021
C	33.268649	39.046330	36.745784
H	33.956085	38.221388	36.691235
C	33.668814	43.451712	42.267026
H	33.925974	43.954872	43.202545
H	32.582983	43.308307	42.238801
C	34.370429	42.135799	42.206986
N	34.108498	41.194244	41.239430
H	33.407283	41.262495	40.489153
C	34.964896	40.163631	41.455844
H	34.939402	39.257801	40.865939
N	35.757765	40.378894	42.479772
C	35.390140	41.610895	42.955125
H	35.843123	42.028875	43.842234
C	27.727034	41.837179	44.149610
H	27.319703	42.815332	44.429501
H	28.775214	42.001355	43.875473
C	26.969579	41.294550	42.919962
H	25.939447	41.054447	43.202457
H	26.932237	42.082020	42.160875
C	27.627292	40.043586	42.285223
O	28.197466	40.213058	41.168326
O	27.574936	38.987820	42.947883
C	32.409325	37.708597	44.303113
H	32.309877	38.574831	44.965871
H	33.482946	37.555382	44.149131
C	31.776464	37.953171	42.976999
C	30.570811	38.535195	42.701425
H	29.817411	38.945267	43.356092
N	30.300198	38.482935	41.360337
H	29.466769	39.006520	41.007360
C	31.344722	37.857000	40.730409
C	31.554926	37.525410	39.392498
H	30.847686	37.817972	38.625255

C	32.711007	36.834598	39.062075
H	32.883645	36.566429	38.024977
C	33.658939	36.481118	40.033945
H	34.560054	35.954131	39.734782
C	33.460302	36.811176	41.363215
H	34.203999	36.554345	42.113357
C	32.293970	37.494217	41.726332
H	33.965944	44.110384	41.436142
H	27.687600	41.147465	44.994911
H	32.001747	36.828670	44.824915

F88E Ca^{2+}-discharged obelin (**F88E**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Glu88 + Trp92(S_0)

O	37.27421900	31.37059000	30.659756
H	36.75499900	30.76073800	31.198966
C	36.48048300	32.40783500	30.262117
C	37.05699800	33.39519100	29.466195
C	36.28550100	34.45737300	29.017466
H	36.73909500	35.22069600	28.392450
H	38.10584400	33.31478100	29.202711
C	35.13312200	32.49058600	30.597468
H	34.67167000	31.73081200	31.221954
C	34.37627500	33.56064000	30.138366
H	33.32198000	33.58854400	30.403320
C	34.93094300	34.56188700	29.340137
C	34.10681700	35.71066600	28.800287
H	34.57837100	36.12430900	27.907982
H	33.11453400	35.33974000	28.512010
C	33.89589400	36.90515200	29.746203
O	34.22012100	38.03471300	29.414198
N	33.24189100	36.59316100	30.893835
H	33.17841600	35.60989300	31.119125
C	33.06715500	37.41968700	32.046682
N	33.69505800	36.95340500	33.138890
C	33.47928600	37.57030300	34.277202
H	33.98521900	37.17184100	35.147478
C	32.22364700	38.52087000	32.119025
C	31.52415400	39.11112300	30.906462
C	31.73967300	40.60560400	30.787139
C	30.72093500	41.50171500	31.100092
C	30.92965800	42.87446200	31.037522
C	32.18707300	43.37453600	30.724253
C	33.19499900	42.49115700	30.339086

C	32.98643200	41.11789100	30.424234
H	33.77834100	40.41685200	30.181535
H	34.20640300	42.87064100	30.204893
H	32.34573500	44.44660600	30.729873
H	30.11593400	43.54272700	31.303281
H	29.74207800	41.11711300	31.369310
H	31.87716800	38.61436800	30.001837
H	30.45133900	38.91553400	30.995390
N	31.98995400	39.12904900	33.281197
C	32.60525500	38.69336100	34.403763
C	32.40397200	39.35780400	35.660010
C	31.43367700	40.37465000	35.844897
H	30.74676800	40.57606200	35.027595
C	31.36092500	41.09969100	37.005175
H	30.58929100	41.84402100	37.164568
C	32.30626600	40.93034800	38.082806
O	32.32646800	41.68412400	39.096590
C	33.21228600	39.83250800	37.912091
H	33.85865100	39.57893600	38.741866
C	33.23932300	39.08909700	36.771946
H	33.91166400	38.24555500	36.741742
C	33.67112800	43.44030000	42.258290
H	33.93421600	43.93259500	43.198079
H	32.58545900	43.29477400	42.234323
C	34.37517300	42.12674000	42.168285
N	34.10921500	41.21045200	41.179615
H	33.40688200	41.31146500	40.412120
C	34.96929700	40.18040900	41.369016
H	34.94472900	39.29018000	40.755840
N	35.76715700	40.36835500	42.397786
C	35.39986100	41.58866500	42.902240
H	35.85692200	41.98984300	43.795916
C	27.72714400	41.83388500	44.147018
H	27.32387000	42.81466200	44.424584
H	28.77553800	41.99372100	43.871267
C	26.96632600	41.29279900	42.918282
H	25.93215600	41.06864700	43.200723
H	26.93870000	42.07664300	42.154947
C	27.60426500	40.02821500	42.285854
O	28.13925200	40.17472700	41.150237
O	27.56436900	38.98403000	42.968843
C	32.40338500	37.70216300	44.288781
H	32.29815900	38.57344200	44.943228
H	33.47823600	37.55828400	44.133983

C	31.76264800	37.92850900	42.962692
C	30.55742300	38.51137200	42.687241
H	29.80969000	38.93380200	43.340900
N	30.28309600	38.45030000	41.346826
H	29.45646900	38.97378600	40.988036
C	31.32845600	37.82352800	40.716653
C	31.54132500	37.49796500	39.378357
H	30.84443100	37.80787800	38.608835
C	32.69663200	36.80743400	39.049068
H	32.87789000	36.55490200	38.009119
C	33.64027100	36.44577900	40.021521
H	34.54235600	35.92003000	39.721299
C	33.44029700	36.77276100	41.351242
H	34.18187900	36.51240800	42.102151
C	32.27645700	37.46051100	41.713006
H	33.95135400	44.11273500	41.432242
H	27.68476400	41.14748100	44.994805
H	32.01929300	36.81414300	44.816551

W92A Ca^{2+}-discharged obelin (**W92A**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Ala92(S_1)

O	40.088070	31.960679	32.491145
H	40.425754	32.382999	31.681060
C	38.790425	31.594234	32.365299
C	38.145262	31.114726	33.503719
C	36.838874	30.661904	33.417906
H	36.359407	30.290020	34.320850
H	38.667172	31.138169	34.452354
C	38.103498	31.640942	31.154386
H	38.599978	32.028795	30.269361
C	36.790158	31.195024	31.086930
H	36.258511	31.239925	30.141060
C	36.141139	30.681885	32.208201
C	34.726295	30.158693	32.092454
H	34.564110	29.738695	31.098103
H	34.561318	29.367110	32.831104
C	33.651636	31.228836	32.286903
O	33.152602	31.803736	31.338890
N	33.287944	31.404190	33.598839
H	34.021115	31.179559	34.265297
C	32.577324	32.566894	34.067914
N	33.389870	33.513642	34.542376
C	32.701401	34.543053	35.177896

H	33.310251	35.308000	35.642211
C	31.193592	32.580433	34.114818
C	30.316363	31.490837	33.562565
C	29.478671	31.874501	32.351997
C	28.157111	31.442903	32.239681
C	27.402489	31.759034	31.113552
C	27.950788	32.514795	30.084912
C	29.267299	32.950210	30.193446
C	30.023357	32.632710	31.314092
H	31.054890	32.958152	31.387973
H	29.706322	33.542153	29.396625
H	27.364795	32.769218	29.207473
H	26.371452	31.419933	31.048708
H	27.708291	30.856336	33.037267
H	30.935808	30.624740	33.305428
H	29.631410	31.167216	34.354135
N	30.534370	33.612207	34.744361
C	31.333866	34.559127	35.259045
C	30.595415	35.651031	35.964634
C	31.180874	36.913248	36.197254
H	32.181807	37.097659	35.837012
C	30.506357	37.906463	36.847962
H	30.959592	38.880079	36.995225
C	29.161004	37.705065	37.334225
O	28.521091	38.620206	37.926432
C	28.582884	36.405613	37.092455
H	27.571756	36.243516	37.450240
C	29.272992	35.432517	36.421870
H	28.833909	34.465020	36.212455
C	27.943505	42.622272	37.947810
H	27.775362	43.702060	37.985339
H	27.315142	42.165695	38.721052
C	29.382961	42.334075	38.234928
N	29.865154	41.054482	38.385610
H	29.348367	40.169729	38.259591
C	31.186182	41.166420	38.668828
H	31.810111	40.300145	38.842037
N	31.586533	42.414375	38.716358
C	30.462538	43.153835	38.442217
H	30.490024	44.235381	38.429000
C	25.123036	40.534264	43.790778
H	24.334045	39.962194	44.285667
H	24.642495	41.381103	43.302145
C	25.783567	39.670416	42.743414

C	25.934952	38.298353	42.938392
H	25.600281	37.850769	43.869240
C	26.486687	37.497436	41.945801
H	26.590744	36.430184	42.114341
C	26.886133	38.056496	40.738181
H	27.311792	37.450123	39.947196
C	26.733783	39.422416	40.530234
H	27.046299	39.843139	39.580978
C	26.187607	40.221349	41.526553
H	26.068723	41.290006	41.363271
C	31.523571	42.004838	42.288888
H	31.061538	42.989939	42.353393
H	32.234717	42.006612	41.462187
H	30.745792	41.266628	42.086494
H	27.623259	42.243241	36.967749
H	25.807392	40.911949	44.558737
H	32.013751	41.759363	43.235388

W92A Ca^{2+}-discharged obelin (**W92A**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22+ Phe88 + Ala92 (S_0)

O	40.10335100	31.95688000	32.474321
H	40.44813200	32.37553400	31.663847
C	38.80772000	31.59365100	32.345152
C	38.16049400	31.11621100	33.484016
C	36.85208800	30.67170300	33.398460
H	36.36960400	30.30330600	34.301425
H	38.68159600	31.14078200	34.432894
C	38.12362000	31.63736500	31.132150
H	38.62293700	32.02010400	30.246829
C	36.80836100	31.19812600	31.064258
H	36.27822600	31.24353100	30.117681
C	36.15677500	30.69451900	32.187827
C	34.73093900	30.20181800	32.082688
H	34.54737600	29.79165900	31.087704
H	34.55236300	29.41034400	32.818693
C	33.70417900	31.31021500	32.288880
O	33.28448800	31.97579200	31.364277
N	33.27784100	31.43865100	33.590912
H	33.91612900	31.08000800	34.292384
C	32.53762700	32.57338500	34.054850
N	33.26930400	33.60097200	34.500426
C	32.63205200	34.59177200	35.090924
H	33.24066800	35.39927800	35.481554

C	31.15077400	32.57140000	34.153741
C	30.28001500	31.46052900	33.612450
C	29.48034400	31.82527900	32.372508
C	28.14639300	31.43389200	32.260469
C	27.41943300	31.73190100	31.112060
C	28.00684400	32.42857900	30.063419
C	29.33620900	32.82084100	30.171487
C	30.06740500	32.52010700	31.313404
H	31.10844500	32.81690200	31.380939
H	29.80571400	33.36674000	29.359747
H	27.44020400	32.67102900	29.170259
H	26.37824100	31.42821900	31.046358
H	27.66650400	30.89581000	33.073487
H	30.90609900	30.58757100	33.401662
H	29.58061500	31.17649800	34.400580
N	30.51623700	33.57865700	34.755340
C	31.22240100	34.60447100	35.258208
C	30.53655600	35.66356600	35.977204
C	31.16213500	36.89124200	36.269552
H	32.18331700	37.06792600	35.953635
C	30.50558500	37.91073400	36.911681
H	31.01372600	38.85415400	37.077486
C	29.14963600	37.78270400	37.347464
O	28.51762900	38.72505100	37.939030
C	28.53874200	36.51560700	37.073562
H	27.51372100	36.37953300	37.405974
C	29.19967700	35.51519600	36.401619
H	28.69663000	34.57733600	36.187682
C	27.94713900	42.61574700	37.947987
H	27.79615800	43.69861300	37.982597
H	27.30985400	42.16930500	38.719791
C	29.38129500	42.30411400	38.240817
N	29.84682400	41.01826000	38.374740
H	29.32151700	40.11297500	38.208074
C	31.15969300	41.11924400	38.684002
H	31.77422000	40.24466000	38.849447
N	31.57482900	42.36444800	38.765537
C	30.46139200	43.11580200	38.483862
H	30.49344500	44.19751600	38.494709
C	25.12800900	40.52582000	43.789512
H	24.34331200	39.94604700	44.282740
H	24.64011100	41.36886100	43.300380
C	25.80032400	39.66888100	42.742095
C	25.90864600	38.28883600	42.907421

H	25.53109100	37.82750300	43.815591
C	26.47395500	37.49754900	41.913205
H	26.54389100	36.42375700	42.058226
C	26.93313600	38.07477200	40.735862
H	27.37405900	37.48533200	39.940027
C	26.82544700	39.44945700	40.558388
H	27.19623000	39.87525900	39.633301
C	26.26320800	40.23753500	41.553935
H	26.17780000	41.31239300	41.411603
C	31.52599900	42.00049900	42.286846
H	31.06197300	42.98491700	42.347091
H	32.23814600	42.00004800	41.461253
H	30.75051700	41.26026800	42.083188
H	27.62076900	42.23810900	36.969063
H	25.80435300	40.91155300	44.560890
H	32.01427100	41.76076000	43.236563

W92Y Ca^{2+}-discharged obelin (**W92Y**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22+ Phe88 + Tyr92(S_1)

O	40.149862	32.135527	32.503430
H	40.544102	32.528282	31.702824
C	38.883645	31.716754	32.277826
C	38.186828	31.158180	33.348257
C	36.911930	30.651775	33.152591
H	36.399961	30.211212	34.005198
H	38.645308	31.153908	34.329688
C	38.279943	31.774604	31.022934
H	38.818554	32.212877	30.187627
C	36.999110	31.268790	30.845516
H	36.538393	31.318134	29.863083
C	36.293382	30.690614	31.899530
C	34.919850	30.104515	31.656898
H	34.819509	29.794262	30.616411
H	34.781693	29.215601	32.284011
C	33.747871	31.051615	31.921782
O	32.990673	31.386376	31.030467
N	33.600999	31.393109	33.244116
H	34.464557	31.343052	33.775207
C	32.856564	32.525148	33.719723
N	33.663385	33.483850	34.196580
C	32.972814	34.481476	34.867182
H	33.580635	35.233651	35.353669
C	31.472336	32.528674	33.778356

C	30.595540	31.427506	33.241364
C	29.612381	31.857549	32.164839
C	28.271973	31.484524	32.235067
C	27.384617	31.831405	31.220021
C	27.818329	32.569001	30.126180
C	29.154719	32.949343	30.052481
C	30.040977	32.596619	31.060600
H	31.085917	32.874773	30.995631
H	29.505328	33.522366	29.200143
H	27.130040	32.849805	29.334981
H	26.343339	31.532386	31.301157
H	27.913413	30.916281	33.088364
H	31.219489	30.628381	32.830145
H	30.021515	30.996513	34.071514
N	30.808383	33.549206	34.416584
C	31.605839	34.494658	34.947291
C	30.878201	35.569029	35.678230
C	31.489371	36.808926	35.966388
H	32.506081	36.978820	35.649621
C	30.820200	37.799313	36.621796
H	31.286559	38.758650	36.804758
C	29.469697	37.607765	37.079918
O	28.852657	38.519845	37.718311
C	28.863874	36.335010	36.793916
H	27.847954	36.185663	37.140395
C	29.541828	35.365862	36.104897
H	29.084955	34.414930	35.859462
C	28.105155	42.724196	37.565140
H	27.905967	43.789858	37.711009
H	27.605768	42.176133	38.370449
C	29.580684	42.489954	37.614421
N	30.135927	41.233090	37.705019
H	29.645495	40.338022	37.786488
C	31.483113	41.401352	37.672225
H	32.169072	40.570742	37.756570
N	31.829807	42.658745	37.555527
C	30.644070	43.349031	37.519441
H	30.621583	44.428157	37.447390
C	24.733491	40.900935	44.184205
H	24.126227	40.122935	44.650464
H	24.055038	41.720199	43.953897
C	25.288199	40.373343	42.878651
C	25.454352	39.001901	42.676107
H	25.282290	38.316359	43.500943

C	25.808284	38.500961	41.429685
H	25.944346	37.434066	41.294818
C	26.007175	39.365193	40.358773
H	26.305186	38.977810	39.391007
C	25.858873	40.731846	40.552734
H	26.015358	41.413865	39.724060
C	25.501127	41.233403	41.799585
H	25.373375	42.303673	41.929108
C	32.110516	42.149961	42.392186
H	31.516898	43.068991	42.417668
H	32.939077	42.321978	41.698210
C	31.271128	41.005619	41.878172
C	29.973875	40.819676	42.348643
H	29.582904	41.503199	43.086376
C	29.156016	39.810991	41.875442
H	28.144057	39.697194	42.241533
C	29.628983	38.955911	40.883097
O	28.791612	38.005771	40.377244
H	28.821195	38.071201	39.398884
C	30.939058	39.093889	40.428570
H	31.312666	38.406797	39.675449
C	31.748075	40.111543	40.924422
H	32.758382	40.223598	40.540366
H	27.686883	42.422287	36.594192
H	25.477888	41.250615	44.905347
H	32.481685	41.954123	43.407477

W92Y Ca^{2+}-discharged obelin (**W92Y**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22+ Phe88 + Tyr92 (S_0)

O	40.17456700	32.14153100	32.491532
H	40.57195000	32.54297500	31.695424
C	38.90539800	31.73840800	32.271065
C	38.20993800	31.18630600	33.346621
C	36.93492200	30.68074500	33.156535
H	36.42913700	30.23125800	34.008800
H	38.67782400	31.17160100	34.323386
C	38.29441700	31.80492600	31.019907
H	38.83393300	32.23468700	30.181014
C	37.00887200	31.30936500	30.849567
H	36.54089300	31.36326100	29.870849
C	36.31125800	30.72774300	31.906677
C	34.92896800	30.15493500	31.678168
H	34.80936800	29.85138700	30.637729

H	34.78384900	29.26895300	32.306823
C	33.80347300	31.14165700	31.962102
O	33.14893000	31.64897600	31.075294
N	33.56192900	31.35326100	33.307477
H	34.36561400	31.18891700	33.904309
C	32.80377600	32.47527400	33.773303
N	33.53319500	33.48588000	34.253918
C	32.89019700	34.47632600	34.842653
H	33.49717600	35.26242700	35.276442
C	31.41270800	32.49148500	33.825916
C	30.54451000	31.38699600	33.262412
C	29.59659300	31.82315900	32.159340
C	28.24467100	31.49318400	32.220340
C	27.38574400	31.84934400	31.184978
C	27.85823500	32.55421700	30.085809
C	29.20693800	32.88662300	30.020652
C	30.06754300	32.52549700	31.048095
H	31.12248900	32.76344400	30.982373
H	29.58703900	33.43320200	29.163968
H	27.19023900	32.84119900	29.280186
H	26.33508700	31.58588800	31.254831
H	27.85431200	30.95195300	33.077002
H	31.18674500	30.58531500	32.885009
H	29.95490400	30.96840400	34.083544
N	30.77547000	33.50184800	34.419711
C	31.48099200	34.50377300	34.963567
C	30.79488700	35.56511400	35.691189
C	31.43856700	36.77645900	35.989977
H	32.46020000	36.94335000	35.675807
C	30.79921100	37.79358200	36.656156
H	31.31669400	38.72732600	36.835311
C	29.46174600	37.66431500	37.110574
O	28.86502700	38.61049900	37.770075
C	28.82391300	36.42443000	36.822066
H	27.80718300	36.29227200	37.177295
C	29.46418900	35.42229200	36.125914
H	28.94642800	34.49293700	35.909581
C	28.11269700	42.70640900	37.565602
H	27.92682500	43.77271200	37.724486
H	27.60973400	42.15187600	38.364043
C	29.58565100	42.45198600	37.606676
N	30.12853300	41.18952700	37.677360
H	29.63223100	40.28091300	37.751275
C	31.47415900	41.35181000	37.639201

H	32.15326200	40.51456900	37.710691
N	31.83489000	42.60913400	37.536600
C	30.65386700	43.30690300	37.515017
H	30.63592200	44.38730700	37.459549
C	24.73783100	40.89288700	44.184262
H	24.13609400	40.11265800	44.654354
H	24.05505900	41.70906200	43.955980
C	25.29296300	40.36568100	42.878418
C	25.46763300	38.99561200	42.674098
H	25.28886100	38.30676100	43.495042
C	25.84766100	38.50063100	41.432593
H	26.00058300	37.43590200	41.297942
C	26.06264100	39.36811300	40.367126
H	26.39869600	38.98710500	39.409198
C	25.89779700	40.73279300	40.562734
H	26.07109500	41.42064300	39.742566
C	25.51512300	41.22886000	41.804264
H	25.38117200	42.29844900	41.934522
C	32.11104500	42.14449400	42.391377
H	31.50795500	43.05748400	42.416947
H	32.93787100	42.32556000	41.697345
C	31.28590700	40.99099800	41.873592
C	29.99976300	40.76971600	42.358785
H	29.60289900	41.43245600	43.112681
C	29.19109600	39.76192300	41.867845
H	28.18568100	39.62684800	42.245129
C	29.65297300	38.94489000	40.835185
O	28.82085400	38.02288700	40.293249
H	28.82131700	38.16238400	39.297923
C	30.95884000	39.11695000	40.372556
H	31.32390500	38.46423200	39.585676
C	31.76122900	40.12824400	40.890235
H	32.76243300	40.27065100	40.491499
H	27.68980000	42.42390600	36.590323
H	25.49375000	41.23936600	44.895290
H	32.48579100	41.95503100	43.407438

W92R Ca^{2+}-discharged obelin (**W92R**)
TD CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Arg92(S_1)

O	40.115776	32.096395	32.606174
H	40.488432	32.513214	31.808570

C	38.829439	31.716634	32.426850
C	38.157222	31.187833	33.528759
C	36.854751	30.736723	33.393718
H	36.353649	30.335051	34.271819
H	38.655550	31.170308	34.490161
C	38.173647	31.797825	31.199695
H	38.688099	32.219878	30.341152
C	36.864678	31.347672	31.081538
H	36.358996	31.422571	30.123426
C	36.186824	30.798835	32.168326
C	34.769922	30.287275	32.005570
H	34.616519	29.924165	30.987577
H	34.590456	29.456556	32.696841
C	33.725164	31.373886	32.242803
O	33.325278	32.083609	31.344912
N	33.279239	31.443770	33.552500
H	33.966257	31.093064	34.215153
C	32.709079	32.653871	34.067356
N	33.649526	33.513992	34.522989
C	33.117075	34.583507	35.171577
H	33.834958	35.267349	35.609298
C	31.335883	32.839813	34.178631
C	30.335539	31.826435	33.687382
C	29.599783	32.164836	32.399344
C	28.297849	31.699466	32.205782
C	27.635109	31.927781	31.004588
C	28.256931	32.630383	29.979096
C	29.549290	33.104365	30.169984
C	30.216554	32.871354	31.366991
H	31.235902	33.217344	31.494240
H	30.044896	33.654508	29.376574
H	27.744513	32.810050	29.039388
H	26.624053	31.555133	30.867634
H	27.797917	31.148267	32.998994
H	30.839525	30.863117	33.560566
H	29.592518	31.693613	34.480276
N	30.821346	33.931721	34.806353
C	31.766946	34.790874	35.305185
C	31.244224	35.915538	36.085132
C	32.087435	36.937139	36.599261
H	33.136981	36.947840	36.339650
C	31.598490	37.916645	37.409246
H	32.257648	38.680209	37.807433
C	30.207675	37.972172	37.767913

O	29.774408	38.876914	38.580279
C	29.355679	36.971296	37.206985
H	28.299131	37.013237	37.453656
C	29.857133	35.984703	36.394138
H	29.228158	35.208402	35.976341
C	28.352205	42.996281	37.566921
H	28.119381	44.054840	37.707111
H	27.851844	42.438535	38.366902
C	29.830284	42.792773	37.612978
N	30.393945	41.534441	37.554900
H	29.926255	40.639548	37.692374
C	31.738521	41.711057	37.450418
H	32.419792	40.878663	37.347633
N	32.073870	42.975295	37.447376
C	30.887938	43.661183	37.547157
H	30.861914	44.741228	37.561484
C	25.155099	40.698052	43.572269
H	24.299002	40.185717	44.019670
H	24.767956	41.574270	43.053390
C	25.814292	39.781776	42.567588
C	25.830037	38.400821	42.763027
H	25.402614	37.982992	43.670053
C	26.367439	37.552540	41.802659
H	26.345266	36.479886	41.964459
C	26.902025	38.075071	40.630545
H	27.305912	37.417513	39.867084
C	26.902008	39.450742	40.426566
H	27.330915	39.853421	39.514522
C	26.354412	40.294020	41.386180
H	26.339009	41.367929	41.218273
C	31.190160	42.096919	42.422445
H	30.413571	41.334390	42.322516
H	30.669415	43.023663	42.647835
C	31.953465	42.291483	41.110319
H	31.241131	42.596391	40.336242
H	32.656108	43.123373	41.187350
C	32.736910	41.093570	40.588246
H	33.194059	41.350459	39.632267
H	33.564530	40.837633	41.254576
N	31.882754	39.920050	40.389142
H	31.158510	39.953217	39.664851
C	31.880852	38.812305	41.110551
N	32.885084	38.522510	41.958957
H	33.565329	39.232629	42.173793

H	32.719224	37.852086	42.699214
N	30.865740	37.950514	40.981057
H	30.189656	38.154728	40.234272
H	30.990507	36.987935	41.257145
H	27.943707	42.679868	36.598933
H	25.817154	41.029490	44.378824
H	31.841602	41.834206	43.266022

W92R Ca^{2+}-discharged obelin (**W92R**)
CAM-B3LYP/6-31G(d,p)/MM
CLM + His22 + Phe88 + Arg92 (S_0)

O	40.13388400	32.08048800	32.595834
H	40.50903700	32.51160000	31.806064
C	38.84829600	31.70854000	32.411589
C	38.16908800	31.18350100	33.511936
C	36.86419700	30.74203800	33.372897
H	36.35859000	30.34050200	34.248758
H	38.66480300	31.15963800	34.474328
C	38.19698400	31.79443300	31.181815
H	38.71780200	32.21104300	30.324749
C	36.88579500	31.35346700	31.059266
H	36.38382300	31.43252100	30.099645
C	36.20129600	30.81244000	32.145478
C	34.77321000	30.33308400	31.985731
H	34.59915200	30.00140300	30.960312
H	34.57789300	29.48961300	32.657350
C	33.77428500	31.44822900	32.259579
O	33.44481200	32.24790200	31.411090
N	33.27404900	31.46187700	33.553448
H	33.88113700	31.02089400	34.236174
C	32.68443500	32.65653600	34.075928
N	33.55137500	33.55993700	34.529456
C	33.06591800	34.61918000	35.148430
H	33.79003600	35.31988800	35.544716
C	31.30691200	32.83269300	34.206897
C	30.29209200	31.82430800	33.726338
C	29.60296700	32.13760500	32.406457
C	28.29707200	31.68896400	32.199124
C	27.66212500	31.90265300	30.981183
C	28.31581000	32.57169000	29.952700
C	29.61257100	33.02582000	30.156708
C	30.25378700	32.80821500	31.371509
H	31.27470800	33.14893900	31.502987
H	30.13133600	33.55180600	29.362048

H	27.82282300	32.74246200	29.001199
H	26.64608600	31.54856100	30.835920
H	27.77065400	31.16683600	32.994532
H	30.77891700	30.84652600	33.654412
H	29.52872400	31.74428800	34.503908
N	30.83357000	33.91154300	34.839730
C	31.68524600	34.81455500	35.335014
C	31.16989600	35.94325200	36.126586
C	32.02826200	36.93043700	36.626544
H	33.08109300	36.93029200	36.372700
C	31.56728900	37.94142200	37.442898
H	32.26502000	38.67908500	37.825199
C	30.20812400	38.03830200	37.809749
O	29.78613800	38.97158700	38.645268
C	29.34032100	37.05868500	37.273675
H	28.28547900	37.11529300	37.527630
C	29.81157200	36.04310400	36.460626
H	29.13039400	35.28982000	36.079068
C	28.36122400	42.98661300	37.566187
H	28.13490800	44.04576400	37.714316
H	27.86015900	42.42403200	38.361984
C	29.83940300	42.77269900	37.605223
N	30.39651100	41.51132500	37.565520
H	29.94450400	40.61239800	37.780212
C	31.73704600	41.68460900	37.428909
H	32.41405900	40.84676600	37.343414
N	32.07912700	42.94812100	37.384453
C	30.89704400	43.63799000	37.494568
H	30.87339700	44.71804300	37.486745
C	25.16068200	40.69907900	43.568394
H	24.29934400	40.18815400	44.008155
H	24.77984400	41.57596800	43.045047
C	25.83167300	39.78140800	42.573197
C	25.82284900	38.39949300	42.760692
H	25.36784200	37.98295900	43.654924
C	26.37584600	37.54947400	41.810742
H	26.33621800	36.47622600	41.965910
C	26.95244900	38.07197100	40.659109
H	27.37842800	37.41702000	39.905788
C	26.97889500	39.44835400	40.463460
H	27.45452500	39.84491500	39.572471
C	26.41150100	40.29288900	41.410307
H	26.41689800	41.36780600	41.248532
C	31.19191000	42.09399600	42.419909

H	30.41442000	41.33211400	42.322936
H	30.67431200	43.02360800	42.641700
C	31.95474400	42.27944500	41.105479
H	31.24402400	42.59322300	40.333557
H	32.66874100	43.10181500	41.184875
C	32.72063300	41.07097800	40.578782
H	33.18197200	41.33031100	39.625071
H	33.54587100	40.80629100	41.246098
N	31.85579000	39.91194500	40.372520
H	31.13361100	39.92672100	39.633277
C	31.84976400	38.79145400	41.073365
N	32.85640200	38.47680200	41.918168
H	33.52095100	39.19237800	42.162039
H	32.67321800	37.80595100	42.653052
N	30.82630300	37.94834000	40.917572
H	30.17797500	38.20041900	40.138264
H	30.94695100	36.97624800	41.158757
H	27.95351500	42.68367600	36.592981
H	25.80421000	41.03362600	44.388965
H	31.84488100	41.83224000	43.263095

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