Supplementary Information: *From bioavailability scarcity to energy barriers limitations of anaerobic microbial reductive defluorination*

Supplementary information for binding free energy calculation, MMPBSA method

The binding free energies of the protein with ligand in solvent can be expressed as in Eq. (1) and Eq. (2) [1, 2]:

$$\Delta G_{bind} = \Delta G_{complex} - [\Delta G_{protein} + \Delta G_{lig}] \quad (1)$$

$$\Delta G_{bind} = \Delta H - T\Delta S \quad (2)$$

Eq. (2) can be then approximated as shown in Eq. (3):

$$\Delta G_{bind} = \Delta E_{MM} + \Delta G_{sol} - T\Delta S \quad (3)$$

where $^{\Delta E_{MM}}$ is composed of the bonded energy, the van der Waals ($^{\Delta E_{vdw}}$) energy and the electrostatic ($^{\Delta E_{ele}}$) energy, where the bonded energy is assumed to be zero for single trajectory approach. Therefore, $^{\Delta E_{MM}}$ can be expressed as in Eq. (4):

$$\Delta E_{MM} = \Delta E_{vdw} + \Delta E_{ele} \quad (4)$$

The solvation free energy $^{\Delta G_{sol}}$ can be computed by the contributions from polar solvation energy ($^{\Delta G_{polar}}$)and ($^{\Delta G_{nonpolar}}$), which are the electrostatic and non-electrostatic contributions to the solvation free energy, respectively, shown as in Eq. (5):

$$\Delta G_{solvation} = \Delta G_{polar} + \Delta G_{nonpolar} \quad (5)$$

The $^{\Delta G_{polar}}$ is estimated by solving the Poisson−Boltzmann (PB) equation. $^{\Delta G_{nonpolar}}$ is calculated by using solvent accessible surface area (SASA) model.

Table S1 Molecular mechanics parameters for selected ligands for molecular dynamics simulation

Tetrachloroethene	Bonds	Distance r0 (nm)	k (kJ/mol/nm^2)
	C1-C2	0.133430	4.764739E+05
	C1-Cl3	0.173080	2.688638E+05
	C1-Cl4	0.173080	2.688638E+05
	C2-Cl5	0.173080	2.688638E+05
	C2-Cl6	0.173080	2.688638E+05

	Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)	
	C2-C1-Cl3	123.110	4.853440E+02	
	C2-C1-Cl4	123.110	4.853440E+02	
	Cl3-C1-Cl4	114.340	4.610768E+02	
	C1-C2-Cl5	123.110	4.853440E+02	
	C1-C2-Cl6	123.110	4.853440E+02	
	Cl5-C2-Cl6	114.340	4.610768E+02	
	Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	Cl3-C1-C2-Cl5	180.000	27.82360	2
	Cl3-C1-C2-Cl6	180.000	27.82360	2
	Cl4-C1-C2-Cl5	180.000	27.82360	2
	Cl4-C1-C2-Cl6	180.000	27.82360	2
	Improper Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	C2-Cl3-C1-Cl4	180.000	4.60240	2
	C1-Cl5-C2-Cl6	180.000	4.60240	2
Trichlorofluoroethene	Bonds	Distance r0 (nm)	k (kJ/mol/nm^2)	
	C1-C2	0.133430	4.764739E+05	
	C1-Cl3	0.173080	2.688638E+05	
	C1-Cl4	0.173080	2.688638E+05	
	C2-F5	0.133850	3.101181E+05	
	C2-Cl6	0.173080	2.688638E+05	
	Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)	
	C2-C1-Cl3	123.110	4.853440E+02	
	C2-C1-Cl4	123.110	4.853440E+02	
	Cl3-C1-Cl4	114.340	4.610768E+02	
	C1-C2-F5	122.870	5.681872E+02	
	C1-C2-Cl6	123.110	4.853440E+02	
	F5-C2-Cl6	113.162	5.000000E+02	
	Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	Cl3-C1-C2-F5	180.000	27.82360	2
	Cl3-C1-C2-Cl6	180.000	27.82360	2
	Cl4-C1-C2-F5	180.000	27.82360	2
	Cl4-C1-C2-Cl6	180.000	27.82360	2
	Improper Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	C2-Cl3-C1-Cl4	180.000	4.60240	2
	C1-F5-C2-Cl6	180.000	4.60240	2
Dichlorodifluoroethene	Bonds	Distance r0 (nm)	kd (kJ/mol)	
	C1-C2	0.133430	4.764739E+05	
	C1-F3	0.133850	3.101181E+05	
	C1-Cl4	0.173080	2.688638E+05	
	C2-F5	0.133850	3.101181E+05	
	C2-Cl6	0.173080	2.688638E+05	
	Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)	
	C2-C1-F3	122.870	5.681872E+02	
	C2-C1-Cl4	123.110	4.853440E+02	
	F3-C1-Cl4	114.661	5.000000E+02	
	C1-C2-F5	122.870	5.681872E+02	
	C1-C2-Cl6	123.110	4.853440E+02	
	F5-C2-Cl6	114.661	5.000000E+02	

	Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	F3-C1-C2-F5	180.000	27.82360	2
	F3-C1-C2-Cl6	180.000	27.82360	2
	Cl4-C1-C2-F5	180.000	27.82360	2
	Cl4-C1-C2-Cl6	180.000	27.82360	2
	Improper Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	C2-F3-C1-Cl4	180.000	4.60240	2
	C1-F5-C2-Cl6	180.000	4.60240	2
Chlorotrifluoroethene	Bonds	Distance r0 (nm)	k (kJ/mol/nm^2)	
	C1-C2	0.133430	4.764739E+05	
	C1-F3	0.133850	3.101181E+05	
	C1-F4	0.133850	3.101181E+05	
	C2-F5	0.133850	3.101181E+05	
	C2-Cl6	0.173080	2.688638E+05	
	Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)	
	C2-C1-F3	122.870	5.681872E+02	
	C2-C1-F4	122.870	5.681872E+02	
	F3-C1-F4	111.640	5.865968E+02	
	C1-C2-F5	122.870	5.681872E+02	
	C1-C2-Cl6	115.602	5.000000E+02	
	Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	F3-C1-C2-F5	180.000	27.82360	2
	F3-C1-C2-Cl6	180.000	27.82360	2
	F4-C1-C2-F5	180.000	27.82360	2
	F4-C1-C2-Cl6	180.000	27.82360	2
	Improper Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	C2-F3-C1-F4	180.000	4.60240	2
	C1-F5-C2-Cl6	180.000	4.60240	2
Tetrafluoroethene	Bonds	Distance r0 (nm)	k (kJ/mol/nm^2)	
	C1-C2	0.133430	4.764739E+05	
	C1-F3	0.133850	3.101181E+05	
	C1-F4	0.133850	3.101181E+05	
	C2-F5	0.133850	3.101181E+05	
	C2-F6	0.133850	3.101181E+05	
	Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)	
	C2-C1-F3	122.870	5.681872E+02	
	C2-C1-F4	122.870	5.681872E+02	
	F3-C1-F4	111.640	5.865968E+02	
	C1-C2-F5	122.870	5.681872E+02	
	C1-C2-F6	122.870	5.681872E+02	
	F5-C2-F6	111.640	5.865968E+02	
	Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	F3-C1-C2-F5	180.000	27.82360	2
	F3-C1-C2-F6	180.000	27.82360	2
	F4-C1-C2-F5	180.000	27.82360	2
	F4-C1-C2-F6	180.000	27.82360	2
	Improper Dihedrals	Angle a0 (Deg.)	kd (kJ/mol)	Multiplicity
	C2-F3-C1-Cl4	180.000	4.60240	2
	C1-F5-C2-Cl6	180.000	4.60240	2

Table S2 Molecular mechanics parameters of Cobalamin cofactor are calculated at B3LYP/ 6-311G(d,p) level of theory using Gaussian 09.

Cobalamin	Bonds	Distance r0 (nm)	k (kJ/mol/nm^2)
	P1-O10	0.168432	1.435555E+05
	P1-O14	0.162309	2.074604E+05
	P1-O18	0.15065	4.547930E+05
	P1-O22	0.149647	4.822287E+05
	C2-C3	0.152066	1.880194E+05
	C2-N84	0.146062	2.060285E+05
	C2-H90	0.109302	2.902079E+05
	C2-H91	0.108998	2.981623E+05
	C3-O14	0.142911	1.872643E+05
	C3-H92	0.109327	2.930088E+05
	C3-H93	0.109451	2.901647E+05
	C4-C7	0.159338	1.078546E+05
	C4-C44	0.1573	1.352165E+05
	C4-C45	0.153607	1.606226E+05
	C4-N46	0.148781	1.163437E+05
	C5-N6	0.148077	1.659440E+05
	C5-C9	0.154819	1.609055E+05
	C5-O25	0.140729	1.785645E+05
	C5-H94	0.109131	2.964871E+05
	N6-C8	0.136454	2.816376E+05
	N6-C31	0.13937	2.428004E+05
	C7-C11	0.158468	1.182475E+05
	C7-C50	0.15393	1.577023E+05
	C7-C51	0.155797	1.402655E+05
	C8-N13	0.131467	3.865079E+05
	C8-H95	0.107518	3.347700E+05
	C9-C12	0.154772	1.552299E+05
	C9-O29	0.139124	2.516765E+05
	C9-H96	0.110123	2.694010E+05
	O10-C12	0.14213	1.990860E+05
	C11-C15	0.151184	1.625195E+05
	C11-C55	0.155709	1.373060E+05
	C11-H97	0.109134	2.896392E+05
	C12-C16	0.153032	1.733606E+05
	C12-H98	0.109367	2.895782E+05
	N13-C34	0.138106	2.628651E+05
	C15-C19	0.145377	2.076909E+05
	C15-N46	0.129292	4.568943E+05
	C16-C21	0.152365	1.938888E+05
	C16-O25	0.14601	1.304497E+05

C16-H99	0.109167	2.938909E+05
N17-C20	0.13261	3.426758E+05
N17-C34	0.134272	3.162095E+05
C19-C23	0.136694	3.731029E+05
C19-C60	0.151465	1.874472E+05
C20-N24	0.134451	2.858693E+05
C20-H100	0.108662	3.022795E+05
C21-O32	0.14234	2.061561E+05
C21-H101	0.109784	2.780806E+05
C21-H102	0.109848	2.782120E+05
C23-C26	0.154198	1.427932E+05
C23-N47	0.140395	1.983828E+05
N24-C27	0.133832	3.007531E+05
C26-C30	0.156792	1.297937E+05
C26-C61	0.153536	1.665003E+05
C26-C62	0.156969	1.318175E+05
C27-N28	0.136993	3.274588E+05
C27-C31	0.140835	2.665630E+05
N28-H103	0.101107	4.129947E+05
N28-H168	0.10217	3.769363E+05
O29-H104	0.100778	3.104257E+05
C30-C33	0.150901	1.715259E+05
C30-C66	0.154975	1.538879E+05
C30-H105	0.109448	2.838883E+05
C31-C34	0.140518	2.637235E+05
O32-H106	0.097091	4.502024E+05
C33-C35	0.139173	3.050013E+05
C33-N47	0.133938	3.156975E+05
C35-C36	0.138883	3.115421E+05
C35-H107	0.108103	3.180181E+05
C36-C37	0.152145	1.666174E+05
C36-N48	0.134982	2.934090E+05
C37-C38	0.155287	1.439999E+05
C37-C71	0.155089	1.453897E+05
C37-C72	0.153364	1.641019E+05
C38-C39	0.151953	1.614514E+05
C38-C73	0.155763	1.348903E+05
C38-H108	0.109134	2.894835E+05
C39-C40	0.137533	3.389891E+05
C39-N48	0.138711	2.271734E+05
C40-C41	0.144538	2.314316E+05
C40-C78	0.151826	1.839459E+05
C41-C42	0.153541	1.530316E+05
C41-N49	0.130544	4.130161E+05
C42-C43	0.157424	1.240947E+05
C42-C79	0.154664	1.533576E+05
C42-C80	0.154748	1.493486E+05
C43-C44	0.154577	1.512605E+05

C43-C85	0.154537	1.627429E+05
C43-H109	0.109041	2.903877E+05
C44-N49	0.149445	1.173889E+05
C44-H110	0.109406	2.837580E+05
C45-H111	0.108831	2.989695E+05
C45-H112	0.108892	2.999802E+05
C45-H113	0.109175	2.895167E+05
N46-Co89	0.186555	1.167639E+05
N47-Co89	0.190632	1.005997E+05
N48-Co89	0.190951	9.779004E+04
N49-Co89	0.188518	1.039842E+05
C50-H114	0.109024	2.944928E+05
C50-H115	0.108737	3.004873E+05
C50-H116	0.108722	3.033149E+05
C51-C52	0.152764	1.694560E+05
C51-H117	0.10941	2.866621E+05
C51-H118	0.108665	3.013635E+05
C52-O53	0.123319	5.761214E+05
C52-N54	0.134646	3.573648E+05
N54-H119	0.101889	3.944099E+05
N54-H164	0.100907	4.226893E+05
C55-C56	0.154076	1.600660E+05
C55-H120	0.109083	2.928350E+05
C55-H121	0.109242	2.888968E+05
C56-C57	0.152807	1.658924E+05
C56-H122	0.10901	2.945689E+05
C56-H123	0.10929	2.913081E+05
C57-N58	0.135765	3.343252E+05
C57-O59	0.122458	6.098995E+05
N58-H124	0.101453	4.085304E+05
N58-H170	0.100915	4.210133E+05
C60-H125	0.109112	2.934085E+05
C60-H126	0.108533	3.055404E+05
C60-H127	0.109327	2.887728E+05
C61-H128	0.108801	3.000477E+05
C61-H129	0.109472	2.846938E+05
C61-H130	0.109025	2.972506E+05
C62-C63	0.152495	1.667847E+05
C62-H131	0.109489	2.840276E+05
C62-H132	0.109169	2.931784E+05
C63-O64	0.121692	6.394249E+05
C63-N65	0.136727	3.143421E+05
N65-H133	0.100558	4.363162E+05
N65-H163	0.100881	4.246775E+05
C66-C67	0.154108	1.687397E+05
C66-H134	0.10926	2.884981E+05
C66-H135	0.109344	2.893949E+05
C67-C68	0.152258	1.718023E+05

C67-H136	0.109085	2.943031E+05
C67-H137	0.109527	2.827370E+05
C68-O69	0.122451	6.093408E+05
C68-N70	0.135609	3.380116E+05
N70-H138	0.100535	4.376008E+05
N70-H166	0.100884	4.250134E+05
C71-H139	0.109291	2.910531E+05
C71-H140	0.10937	2.888253E+05
C71-H141	0.109272	2.909100E+05
C72-H142	0.109286	2.908454E+05
C72-H143	0.109005	2.963766E+05
C72-H144	0.109312	2.881649E+05
C73-C74	0.153547	1.766088E+05
C73-H145	0.109094	2.929820E+05
C73-H146	0.109391	2.861840E+05
C74-C75	0.154089	1.541286E+05
C74-H147	0.109242	2.880551E+05
C74-H148	0.109461	2.832516E+05
C75-O76	0.123483	5.630791E+05
C75-N77	0.133816	3.672961E+05
N77-H149	0.101097	4.191717E+05
N77-H167	0.103433	3.405608E+05
C78-H150	0.108832	2.977166E+05
C78-H151	0.109227	2.884495E+05
C78-H152	0.108941	2.958494E+05
C79-H153	0.109175	2.920247E+05
C79-H154	0.109094	2.935363E+05
C79-H155	0.1093	2.897381E+05
C80-C81	0.153969	1.690472E+05
C80-H156	0.109278	2.857072E+05
C80-H157	0.10897	2.939795E+05
C81-C82	0.152931	1.695460E+05
C81-H158	0.108923	2.983662E+05
C81-H159	0.109558	2.813309E+05
C82-O83	0.123678	5.517634E+05
C82-N84	0.134311	3.465324E+05
N84-H169	0.101772	3.992591E+05
C85-C86	0.153187	1.653691E+05
C85-H160	0.109053	2.940828E+05
C85-H161	0.109366	2.857929E+05
C86-N87	0.133943	3.678772E+05
C86-O88	0.123614	5.637013E+05
N87-H162	0.101998	3.893749E+05
N87-H165	0.101986	3.902548E+05
Angles	Angle a0 (Deg.)	(kJ/mol/rad^2)
O10-P1-O14	98.125	7.930648E+02
O10-P1-O18	105.602	7.033504E+02

O10-P1-O22	108.162	9.804159E+02
O14-P1-O18	112.129	8.038566E+02
O14-P1-O22	107.043	7.638910E+02
O18-P1-O22	122.875	6.885093E+02
C3-C2-N84	112.252	9.125102E+02
C3-C2-H90	109.314	4.323415E+02
C3-C2-H91	110.19	4.222340E+02
N84-C2-H90	108.197	5.472160E+02
N84-C2-H91	107.729	5.637321E+02
H90-C2-H91	109.087	3.191664E+02
C2-C3-O14	106.168	8.362003E+02
C2-C3-H92	110.453	5.500660E+02
C2-C3-H93	110.538	5.589935E+02
O14-C3-H92	110.53	4.489004E+02
O14-C3-H93	110.296	3.834149E+02
H92-C3-H93	108.844	3.222491E+02
C7-C4-C44	121.037	8.998268E+02
C7-C4-C45	112.297	8.945332E+02
C7-C4-N46	103.098	9.249266E+02
C44-C4-C45	109.682	9.405335E+02
C44-C4-N46	101.667	1.140683E+03
C45-C4-N46	107.433	7.887602E+02
N6-C5-C9	115.299	7.084665E+02
N6-C5-O25	110.334	8.497937E+02
N6-C5-H94	105.918	3.573845E+02
C9-C5-O25	104.961	9.724897E+02
C9-C5-H94	111.643	5.263007E+02
O25-C5-H94	108.598	5.567847E+02
C5-N6-C8	125.134	7.948584E+02
C5-N6-C31	127.714	7.943109E+02
C8-N6-C31	105.077	7.006528E+02
C4-C7-C11	102.567	1.050551E+03
C4-C7-C50	113.111	9.399099E+02
C4-C7-C51	110.566	1.026338E+03
C11-C7-C50	113.081	1.011017E+03
C11-C7-C51	108.23	8.874564E+02
C50-C7-C51	109.076	9.806722E+02
N6-C8-N13	114.692	5.761719E+02
N6-C8-H95	120.439	2.530760E+02
N13-C8-H95	124.868	2.419767E+02
C5-C9-C12	102.53	1.124260E+03
C5-C9-O29	114.014	7.789825E+02
C5-C9-H96	104.775	5.449149E+02
C12-C9-O29	118.994	9.906738E+02
C12-C9-H96	106.108	5.217512E+02
O29-C9-H96	109.232	4.994065E+02
P1-O10-C12	116.142	1.273370E+03
C7-C11-C15	103.167	1.044804E+03

C7-C11-C55	118.016	9.506584E+02
C7-C11-H97	107.912	4.435066E+02
C15-C11-C55	111.066	8.780770E+02
C15-C11-H97	109.359	4.210697E+02
C55-C11-H97	107.091	3.208137E+02
C9-C12-O10	113.025	7.431318E+02
C9-C12-C16	102.149	8.425811E+02
C9-C12-H98	111.731	4.942070E+02
O10-C12-C16	108.536	8.998817E+02
O10-C12-H98	109.882	4.243982E+02
C16-C12-H98	111.273	5.452839E+02
C8-N13-C34	104.493	1.211073E+03
P1-O14-C3	122.755	1.047600E+03
C11-C15-C19	124.416	6.994654E+02
C11-C15-N46	112.686	6.122804E+02
C19-C15-N46	122.853	6.163368E+02
C12-C16-C21	116.194	8.558839E+02
C12-C16-O25	106.695	8.381648E+02
C12-C16-H99	108.792	5.282352E+02
C21-C16-O25	107.672	8.423599E+02
C21-C16-H99	108.562	4.321402E+02
O25-C16-H99	108.714	4.768982E+02
C20-N17-C34	112.88	1.304564E+03
C15-C19-C23	119.925	7.514234E+02
C15-C19-C60	116.428	5.946835E+02
C23-C19-C60	123.641	5.572766E+02
N17-C20-N24	128.607	5.216433E+02
N17-C20-H100	116.342	2.204435E+02
N24-C20-H100	115.041	2.244276E+02
C16-C21-O32	108.798	9.686978E+02
C16-C21-H101	107.719	5.422979E+02
C16-C21-H102	110.429	5.709494E+02
O32-C21-H101	111.084	4.642298E+02
O32-C21-H102	111.225	4.622712E+02
H101-C21-H102	107.528	3.532424E+02
C19-C23-C26	128.141	5.669662E+02
C19-C23-N47	124.315	6.161168E+02
C26-C23-N47	107.535	5.730397E+02
C20-N24-C27	118.799	1.293839E+03
C5-O25-C16	111.253	1.515921E+03
C23-C26-C30	99.511	8.575939E+02
C23-C26-C61	117.404	1.009033E+03
C23-C26-C62	110.653	7.690387E+02
C30-C26-C61	112.594	9.845015E+02
C30-C26-C62	105.766	1.034863E+03
C61-C26-C62	109.967	7.586322E+02
N24-C27-N28	118.954	7.274780E+02
N24-C27-C31	117.578	6.218381E+02

N28-C27-C31	123.457	6.563137E+02
C27-N28-H103	112.095	4.148181E+02
C27-N28-H168	114.594	3.959062E+02
H103-N28-H168	114.864	2.602798E+02
C9-O29-H104	112.483	6.526681E+02
C26-C30-C33	100.215	7.987473E+02
C26-C30-C66	114.437	7.080236E+02
C26-C30-H105	110.639	4.956791E+02
C33-C30-C66	110.403	8.903194E+02
C33-C30-H105	111.818	4.708883E+02
C66-C30-H105	109.138	3.281931E+02
N6-C31-C27	135.991	6.778088E+02
N6-C31-C34	105.808	6.321304E+02
C27-C31-C34	118.182	7.445557E+02
C21-O32-H106	106.483	6.277396E+02
C30-C33-C35	124.46	5.999254E+02
C30-C33-N47	110.393	5.300112E+02
C35-C33-N47	125.137	6.467822E+02
N13-C34-N17	126.314	6.083842E+02
N13-C34-C31	109.92	6.561433E+02
N17-C34-C31	123.753	6.894041E+02
C33-C35-C36	125.226	8.084263E+02
C33-C35-H107	117.272	2.666141E+02
C36-C35-H107	117.456	2.617429E+02
C35-C36-C37	123.635	6.897572E+02
C35-C36-N48	124.601	6.502075E+02
C37-C36-N48	111.665	6.008452E+02
C36-C37-C38	100.631	8.354323E+02
C36-C37-C71	107.63	8.439696E+02
C36-C37-C72	114.677	1.000061E+03
C38-C37-C71	109.142	9.124331E+02
C38-C37-C72	115.36	1.028577E+03
C71-C37-C72	108.912	7.490609E+02
C37-C38-C39	102.467	9.017524E+02
C37-C38-C73	117.309	7.383461E+02
C37-C38-H108	109.301	4.717844E+02
C39-C38-C73	109.128	8.424808E+02
C39-C38-H108	111.988	4.380483E+02
C73-C38-H108	106.731	3.167759E+02
C38-C39-C40	124.137	6.673703E+02
C38-C39-N48	109.083	6.450610E+02
C40-C39-N48	126.379	6.239872E+02
C39-C40-C41	121.307	8.112673E+02
C39-C40-C78	118.133	5.668228E+02
C41-C40-C78	120.424	6.418858E+02
C40-C41-C42	126.024	7.361702E+02
C40-C41-N49	122.701	6.720836E+02
C42-C41-N49	111.225	6.312541E+02

C41-C42-C43	100.917	7.628905E+02
C41-C42-C79	108.659	8.053736E+02
C41-C42-C80	115.721	1.087488E+03
C43-C42-C79	111.975	8.946805E+02
C43-C42-C80	108.917	1.064572E+03
C79-C42-C80	110.374	8.204323E+02
C42-C43-C44	102.987	9.242793E+02
C42-C43-C85	113.048	8.465647E+02
C42-C43-H109	105.769	3.978320E+02
C44-C43-C85	119.585	9.964196E+02
C44-C43-H109	107.253	4.769605E+02
C85-C43-H109	107.304	3.873230E+02
C4-C44-C43	123.332	9.106347E+02
C4-C44-N49	104.475	1.065523E+03
C4-C44-H110	107.663	4.666938E+02
C43-C44-N49	102.486	8.682388E+02
C43-C44-H110	110.458	3.990496E+02
N49-C44-H110	107.123	3.929285E+02
C4-C45-H111	110.775	3.730143E+02
C4-C45-H112	111.302	3.946714E+02
C4-C45-H113	110.636	3.687671E+02
H111-C45-H112	107.958	2.301331E+02
H111-C45-H113	108.322	3.276610E+02
H112-C45-H113	107.723	2.969043E+02
C4-N46-C15	113.911	7.872910E+02
C4-N46-Co89	114.196	6.649788E+02
C15-N46-Co89	131.444	6.059782E+02
C23-N47-C33	110.408	8.413863E+02
C23-N47-Co89	125.038	7.224761E+02
C33-N47-Co89	124.339	6.860782E+02
C36-N48-C39	110.096	8.445101E+02
C36-N48-Co89	124.545	7.004622E+02
C39-N48-Co89	125.089	7.326023E+02
C41-N49-C44	112.824	7.901352E+02
C41-N49-Co89	131.362	6.523989E+02
C44-N49-Co89	115.74	6.578457E+02
C7-C50-H114	110.281	4.626413E+02
C7-C50-H115	113.005	4.163972E+02
C7-C50-H116	111.526	4.130193E+02
H114-C50-H115	107.272	2.786366E+02
H114-C50-H116	106.262	2.725392E+02
H115-C50-H116	108.18	3.051526E+02
C7-C51-C52	113.135	8.681520E+02
C7-C51-H117	110.365	4.062121E+02
C7-C51-H118	109.442	4.132621E+02
C52-C51-H117	107.113	4.331677E+02
C52-C51-H118	108.094	5.274265E+02
H117-C51-H118	108.558	2.998336E+02

C51-C52-O53	122.008	4.972214E+02
C51-C52-N54	114.754	6.223406E+02
O53-C52-N54	123.236	5.818226E+02
C52-N54-H119	120.443	3.449566E+02
C52-N54-H164	117.769	3.467546E+02
H119-N54-H164	119.584	2.130291E+02
C11-C55-C56	113.888	9.142743E+02
C11-C55-H120	110.407	4.187521E+02
C11-C55-H121	109.549	4.677927E+02
C56-C55-H120	109.557	3.752307E+02
C56-C55-H121	107.154	3.606391E+02
H120-C55-H121	105.935	3.182121E+02
C55-C56-C57	111.408	1.069468E+03
C55-C56-H122	111.372	3.572945E+02
C55-C56-H123	108.721	3.866658E+02
C57-C56-H122	111.141	5.061981E+02
C57-C56-H123	106.185	5.017308E+02
H122-C56-H123	107.78	2.969424E+02
C56-C57-N58	115.812	6.175420E+02
C56-C57-O59	121.021	4.782882E+02
N58-C57-O59	123.167	5.701091E+02
C57-N58-H124	121.117	3.514522E+02
C57-N58-H170	116.745	3.526002E+02
H124-N58-H170	118.162	2.128804E+02
C19-C60-H125	109.509	4.616257E+02
C19-C60-H126	111.605	4.213901E+02
C19-C60-H127	113.982	3.990707E+02
H125-C60-H126	106.007	2.887618E+02
H125-C60-H127	106.726	2.583418E+02
H126-C60-H127	108.599	2.768339E+02
C26-C61-H128	112.167	4.360127E+02
C26-C61-H129	109.351	4.892936E+02
C26-C61-H130	112.387	3.693263E+02
H128-C61-H129	107.153	2.822453E+02
H128-C61-H130	107.465	3.147577E+02
H129-C61-H130	108.104	2.527828E+02
C26-C62-C63	115.542	8.737360E+02
C26-C62-H131	107.498	3.562327E+02
C26-C62-H132	109.231	4.074954E+02
C63-C62-H131	111.315	5.182966E+02
C63-C62-H132	105.342	4.326983E+02
H131-C62-H132	107.648	3.061862E+02
C62-C63-O64	121.664	4.739955E+02
C62-C63-N65	115.981	5.980666E+02
O64-C63-N65	122.348	5.629960E+02
C63-N65-H133	122.443	3.252481E+02
C63-N65-H163	117.916	3.174387E+02
H133-N65-H163	118.5	1.947276E+02

C30-C66-C67	113.539	1.184738E+03
C30-C66-H134	109.152	4.177106E+02
C30-C66-H135	109.438	4.914680E+02
C67-C66-H134	108.639	4.130074E+02
C67-C66-H135	108.807	4.237318E+02
H134-C66-H135	107.061	2.693186E+02
C66-C67-C68	110.941	8.216443E+02
C66-C67-H136	110.208	4.133746E+02
C66-C67-H137	110.134	3.236166E+02
C68-C67-H136	106.316	4.578156E+02
C68-C67-H137	111.149	5.600419E+02
H136-C67-H137	107.982	3.063992E+02
C67-C68-O69	121.946	4.759962E+02
C67-C68-N70	116.402	6.009582E+02
O69-C68-N70	121.63	5.553310E+02
C68-N70-H138	122.563	3.212505E+02
C68-N70-H166	118.426	3.117460E+02
H138-N70-H166	118.939	1.944965E+02
C37-C71-H139	111.448	4.914337E+02
C37-C71-H140	109.852	3.568353E+02
C37-C71-H141	111.007	4.739558E+02
H139-C71-H140	108.195	2.648470E+02
H139-C71-H141	108.074	2.428399E+02
H140-C71-H141	108.156	3.098036E+02
C37-C72-H142	110.076	4.510235E+02
C37-C72-H143	112.544	4.037501E+02
C37-C72-H144	110.87	4.667523E+02
H142-C72-H143	108.071	2.485219E+02
H142-C72-H144	106.958	2.873480E+02
H143-C72-H144	108.116	2.761284E+02
C38-C73-C74	117.299	8.558335E+02
C38-C73-H145	108.019	4.519373E+02
C38-C73-H146	108.643	3.872270E+02
C74-C73-H145	106.713	4.124409E+02
C74-C73-H146	109.781	3.559946E+02
H145-C73-H146	105.763	3.180639E+02
C73-C74-C75	112.086	1.353913E+03
C73-C74-H147	112.234	3.678724E+02
C73-C74-H148	110.357	4.029828E+02
C75-C74-H147	110.054	5.601038E+02
C75-C74-H148	105.452	4.209255E+02
H147-C74-H148	106.283	2.396052E+02
C74-C75-O76	120.001	4.223831E+02
C74-C75-N77	115.058	4.929713E+02
O76-C75-N77	124.931	5.551938E+02
C75-N77-H149	119.376	3.634727E+02
C75-N77-H167	122.699	3.845976E+02
H149-N77-H167	115.587	2.293581E+02

C40-C78-H150	111.308	4.425176E+02
C40-C78-H151	113.457	3.793885E+02
C40-C78-H152	110.527	4.351667E+02
H150-C78-H151	107.55	2.359329E+02
H150-C78-H152	106.302	2.657326E+02
H151-C78-H152	107.353	2.975927E+02
C42-C79-H153	110.625	4.587489E+02
C42-C79-H154	111.316	4.083190E+02
C42-C79-H155	111.901	4.232018E+02
H153-C79-H154	107.241	2.893766E+02
H153-C79-H155	108.107	2.493993E+02
H154-C79-H155	107.455	2.881014E+02
C42-C80-C81	115.726	9.273527E+02
C42-C80-H156	106.67	4.850288E+02
C42-C80-H157	110.47	3.485172E+02
C81-C80-H156	107.699	3.479596E+02
C81-C80-H157	110.094	4.991634E+02
H156-C80-H157	105.595	2.389441E+02
C80-C81-C82	112.427	1.139240E+03
C80-C81-H158	112.794	4.131821E+02
C80-C81-H159	111.112	4.386046E+02
C82-C81-H158	109.668	4.765557E+02
C82-C81-H159	105.653	4.188782E+02
H158-C81-H159	104.674	2.162847E+02
C81-C82-O83	120.876	5.555998E+02
C81-C82-N84	115.547	6.955717E+02
O83-C82-N84	123.574	5.379132E+02
C2-N84-C82	122.399	7.241501E+02
C2-N84-H169	117.912	3.037043E+02
C82-N84-H169	118.618	3.199349E+02
C43-C85-C86	115.097	1.020867E+03
C43-C85-H160	112.087	3.030852E+02
C43-C85-H161	108.017	3.561455E+02
C86-C85-H160	107.81	5.465926E+02
C86-C85-H161	106.498	5.034253E+02
H160-C85-H161	106.89	2.899652E+02
C85-C86-N87	115.52	6.783558E+02
C85-C86-O88	120.716	5.174412E+02
N87-C86-O88	123.75	5.661122E+02
C86-N87-H162	122.255	3.467472E+02
C86-N87-H165	121.558	3.411342E+02
H162-N87-H165	116.185	2.165290E+02
N46-Co89-N47	89.705	6.900396E+02
N46-Co89-N48	169.669	9.406187E+02
N46-Co89-N49	83.331	7.560495E+02
N47-Co89-N48	95.306	7.416455E+02
N47-Co89-N49	172.473	7.663071E+02
N48-Co89-N49	92.024	7.403389E+02

Dihedrals	Angle a0 (Deg.)	k (kJ/mol/rad^2)
P1-O10-C12-C9	91.342	8.244285E+02
P1-O10-C12-C16	-156.095	7.978024E+02
P1-O10-C12-H98	-34.213	3.921597E+02
P1-O14-C3-C2	-165.371	6.858432E+02
P1-O14-C3-H92	-45.565	4.212973E+02
P1-O14-C3-H93	74.848	4.030740E+02
C2-N84-C82-C81	-176.348	7.091876E+02
C2-N84-C82-O83	3.083	4.855882E+02
C3-C2-N84-C82	101.908	5.795064E+02
C3-C2-N84-H169	-66.084	1.473763E+02
C3-O14-P1-O10	61.216	6.933571E+02
C3-O14-P1-O18	-49.353	6.422580E+02
C3-O14-P1-O22	173.123	6.587319E+02
C4-C7-C11-C15	-19.353	1.232727E+03
C4-C7-C11-C55	103.509	9.208501E+02
C4-C7-C11-H97	-135.036	5.180777E+02
C4-C7-C50-H114	-175.378	4.697651E+02
C4-C7-C50-H115	-55.327	4.594416E+02
C4-C7-C50-H116	66.803	4.277601E+02
C4-C7-C51-C52	-175.241	1.138305E+03
C4-C7-C51-H117	64.764	4.401069E+02
C4-C7-C51-H118	-54.645	4.922830E+02
C4-C44-C43-C42	146.03	1.072576E+03
C4-C44-C43-C85	-87.603	8.921094E+02
C4-C44-C43-H109	34.704	4.052133E+02
C4-C44-N49-C41	-149.028	6.446664E+02
C4-C44-N49-Co89	28.204	8.737069E+02
C4-N46-C15-C11	1.837	8.652356E+02
C4-N46-C15-C19	-175.803	7.122644E+02
C4-N46-Co89-N47	156.567	8.129394E+02
C4-N46-Co89-N48	37.397	8.180320E+01
C4-N46-Co89-N49	-26.296	7.331810E+02
C5-N6-C8-N13	164.545	6.079050E+02
C5-N6-C8-H95	-15.148	2.479610E+02
C5-N6-C31-C27	18.319	3.530201E+02
C5-N6-C31-C34	-163.402	5.769681E+02
C5-C9-C12-O10	83.244	9.752677E+02
C5-C9-C12-C16	-33.169	1.316190E+03
C5-C9-C12-H98	-152.202	6.035327E+02
C5-C9-O29-H104	-117.996	6.157982E+01
C5-O25-C16-C12	-1.194	8.489115E+02
C5-O25-C16-C21	124.202	8.171286E+02
C5-O25-C16-H99	-118.367	3.993602E+02
N6-C5-C9-C12	-88.062	1.175968E+03
N6-C5-C9-O29	41.925	1.200958E+03
N6-C5-C9-H96	161.294	6.647699E+02
N6-C5-O25-C16	104.296	6.821553E+02

N6-C8-N13-C34	-0.572	6.219322E+02
N6-C31-C27-N24	-176.904	3.975939E+02
N6-C31-C27-N28	1.916	4.544899E+02
N6-C31-C34-N13	-1.078	6.076961E+02
N6-C31-C34-N17	177.644	4.837449E+02
C7-C4-C44-C43	87.2	9.108664E+02
C7-C4-C44-N49	-156.885	9.713069E+02
C7-C4-C44-H110	-43.225	4.783947E+02
C7-C4-C45-H111	-68.28	4.588073E+02
C7-C4-C45-H112	51.843	5.387885E+02
C7-C4-C45-H113	171.577	4.615891E+02
C7-C4-N46-C15	-14.734	6.416680E+02
C7-C4-N46-Co89	172.053	8.634333E+02
C7-C11-C15-C19	-170.402	8.655146E+02
C7-C11-C15-N46	12.001	6.103883E+02
C7-C11-C55-C56	91.593	9.668439E+02
C7-C11-C55-H120	-32.144	5.235230E+02
C7-C11-C55-H121	-148.436	5.070942E+02
C7-C51-C52-O53	-72.608	5.583118E+02
C7-C51-C52-N54	107.917	6.700495E+02
C8-N6-C5-C9	109.934	6.752582E+02
C8-N6-C5-O25	-8.732	6.170336E+02
C8-N6-C5-H94	-126.078	4.167820E+02
C8-N6-C31-C27	-177.584	4.052959E+02
C8-N6-C31-C34	0.695	7.310845E+02
C8-N13-C34-N17	-177.672	4.584286E+02
C8-N13-C34-C31	1.009	6.359900E+02
C9-C5-N6-C31	-88.942	6.808036E+02
C9-C5-O25-C16	-20.507	7.204845E+02
C9-C12-C16-C21	-97.937	1.103379E+03
C9-C12-C16-O25	22.112	7.632885E+02
C9-C12-C16-H99	139.233	5.359179E+02
O10-C12-C9-O29	-43.611	6.107947E+02
O10-C12-C9-H96	-167.116	5.464453E+02
O10-C12-C16-C21	142.447	8.774038E+02
O10-C12-C16-O25	-97.503	6.478615E+02
O10-C12-C16-H99	19.618	4.763319E+02
C11-C7-C4-C44	132.78	1.118517E+03
C11-C7-C4-C45	-95.03	1.198105E+03
C11-C7-C4-N46	20.302	1.250714E+03
C11-C7-C50-H114	-59.338	4.603459E+02
C11-C7-C50-H115	60.713	4.504279E+02
C11-C7-C50-H116	-177.157	4.199360E+02
C11-C7-C51-C52	73.152	1.071850E+03
C11-C7-C51-H117	-46.843	4.298038E+02
C11-C7-C51-H118	-166.252	4.794278E+02
C11-C15-C19-C23	-157.095	7.407113E+02
C11-C15-C19-C60	23.725	8.811360E+02

C11-C15-N46-Co89	173.568	6.400593E+02
C11-C55-C56-C57	75.07	1.037869E+03
C11-C55-C56-H122	-49.641	4.323987E+02
C11-C55-C56-H123	-168.251	4.650431E+02
C12-C9-C5-O25	33.549	1.037407E+03
C12-C9-C5-H94	151.013	5.498309E+02
C12-C9-O29-H104	3.232	6.175544E+01
C12-O10-P1-O14	171.007	8.180716E+02
C12-O10-P1-O18	-73.211	7.203659E+02
C12-O10-P1-O22	60.004	7.499719E+02
C12-C16-C21-O32	-80.135	7.496442E+02
C12-C16-C21-H101	159.356	6.121674E+02
C12-C16-C21-H102	42.202	6.019000E+02
N13-C8-N6-C31	-0.085	5.459720E+02
N13-C34-N17-C20	178.471	5.132810E+02
N13-C34-C31-C27	177.566	5.520197E+02
O14-C3-C2-N84	58.027	9.933982E+02
O14-C3-C2-H90	-62.034	5.568892E+02
O14-C3-C2-H91	178.094	4.506472E+02
C15-C11-C7-C50	-141.502	9.555475E+02
C15-C11-C7-C51	97.541	1.103899E+03
C15-C11-C55-C56	-149.626	9.536542E+02
C15-C11-C55-H120	86.636	5.196315E+02
C15-C11-C55-H121	-29.656	5.034422E+02
C15-C19-C23-C26	170.105	8.997389E+02
C15-C19-C23-N47	-8.666	5.967293E+02
C15-C19-C60-H125	33.743	4.946729E+02
C15-C19-C60-H126	150.806	4.105838E+02
C15-C19-C60-H127	-85.715	4.829229E+02
C15-N46-C4-C44	-140.79	6.122117E+02
C15-N46-C4-C45	104.04	6.217329E+02
C15-N46-Co89-N47	-15.146	4.473485E+02
C15-N46-Co89-N48	-134.316	7.558721E+01
C15-N46-Co89-N49	161.991	4.220817E+02
C16-C12-C9-O29	-160.024	7.290647E+02
C16-C12-C9-H96	76.471	6.392152E+02
C16-C21-O32-H106	179.673	9.316803E+01
C16-O25-C5-H94	-140.027	4.285187E+02
N17-C20-N24-C27	-1.398	4.414519E+02
N17-C34-C31-C27	-3.713	4.477929E+02
C19-C15-C11-C55	62.22	9.152085E+02
C19-C15-C11-H97	-55.758	4.135211E+02
C19-C15-N46-Co89	-4.072	5.523111E+02
C19-C23-C26-C30	-150.773	5.558826E+02
C19-C23-C26-C61	-29.061	5.448715E+02
C19-C23-C26-C62	98.275	5.332793E+02
C19-C23-N47-C33	167.525	4.752719E+02
C19-C23-N47-Co89	-17.621	5.185842E+02

C20-N17-C34-C31	-0.038	5.642004E+02
C20-N24-C27-N28	178.434	6.132255E+02
C20-N24-C27-C31	-2.691	4.991433E+02
C21-C16-C12-H98	21.419	4.944083E+02
C23-C19-C15-N46	20.265	4.365838E+02
C23-C19-C60-H125	-145.403	4.194791E+02
C23-C19-C60-H126	-28.339	3.574074E+02
C23-C19-C60-H127	95.139	4.109992E+02
C23-C26-C30-C33	-32.46	1.143350E+03
C23-C26-C30-C66	85.638	1.117040E+03
C23-C26-C30-H105	-150.586	4.913570E+02
C23-C26-C61-H128	79.773	3.823232E+02
C23-C26-C61-H129	-161.502	4.381016E+02
C23-C26-C61-H130	-41.446	3.990530E+02
C23-C26-C62-C63	-54.321	1.249543E+03
C23-C26-C62-H131	-179.285	4.861292E+02
C23-C26-C62-H132	64.186	4.891933E+02
C23-N47-C33-C30	-11.931	7.589330E+02
C23-N47-C33-C35	166.935	5.050910E+02
C23-N47-Co89-N46	24.958	6.922708E+02
C23-N47-Co89-N48	-164.091	6.517946E+02
C23-N47-Co89-N49	2.705	3.602600E+01
N24-C20-N17-C34	2.772	4.727721E+02
N24-C27-N28-H103	-9.885	3.286237E+02
N24-C27-N28-H168	-143.111	3.618243E+02
N24-C27-C31-C34	4.975	6.019748E+02
O25-C5-N6-C31	152.392	6.216606E+02
O25-C5-C9-O29	163.536	1.056806E+03
O25-C5-C9-H96	-77.094	6.181011E+02
O25-C16-C12-H98	141.468	4.121275E+02
O25-C16-C21-O32	160.344	7.508757E+02
O25-C16-C21-H101	39.835	6.129885E+02
O25-C16-C21-H102	-77.32	6.026937E+02
C26-C23-C19-C60	-10.778	7.858485E+02
C26-C23-N47-C33	-11.461	8.173155E+02
C26-C23-N47-Co89	163.392	9.543934E+02
C26-C30-C33-C35	-149.719	6.251648E+02
C26-C30-C33-N47	29.157	7.271412E+02
C26-C30-C66-C67	177.752	8.919481E+02
C26-C30-C66-H134	56.398	4.909045E+02
C26-C30-C66-H135	-60.47	4.881396E+02
C26-C62-C63-O64	78.825	5.882032E+02
C26-C62-C63-N65	-100.232	6.567624E+02
C27-N24-C20-H100	179.771	3.216320E+02
N28-C27-C31-C34	-176.205	7.427550E+02
O29-C9-C5-H94	-79.001	5.552328E+02
O29-C9-C12-H98	80.943	4.407689E+02
C30-C26-C23-N47	28.163	7.512640E+02

C30-C26-C61-H128	-165.56	4.133208E+02
C30-C26-C61-H129	-46.834	4.792907E+02
C30-C26-C61-H130	73.221	4.329430E+02
C30-C26-C62-C63	-161.174	1.209296E+03
C30-C26-C62-H131	73.862	4.799152E+02
C30-C26-C62-H132	-42.667	4.829013E+02
C30-C33-C35-C36	178.738	5.323644E+02
C30-C33-C35-H107	1.265	2.276038E+02
C30-C33-N47-Co89	173.172	8.467477E+02
C30-C66-C67-C68	172.584	1.050397E+03
C30-C66-C67-H136	55.107	4.676766E+02
C30-C66-C67-H137	-63.928	4.583614E+02
C31-N6-C5-H94	35.046	4.188880E+02
C31-N6-C8-H95	-179.778	2.369952E+02
C31-C27-N28-H103	171.31	3.164713E+02
C31-C27-N28-H168	38.084	3.471472E+02
O32-C21-C16-H99	42.815	5.061572E+02
C33-C30-C26-C61	-157.573	1.086868E+03
C33-C30-C26-C62	82.306	1.140153E+03
C33-C30-C66-C67	-70.11	9.884316E+02
C33-C30-C66-H134	168.536	5.187749E+02
C33-C30-C66-H135	51.669	5.156881E+02
C33-C35-C36-C37	-173.279	5.217942E+02
C33-C35-C36-N48	2.8	4.261467E+02
C33-N47-Co89-N46	-160.887	5.292053E+02
C33-N47-Co89-N48	10.065	5.052214E+02
C33-N47-Co89-N49	176.861	3.545743E+01
C34-N13-C8-H95	179.106	2.249173E+02
C34-N17-C20-H100	-178.41	3.215728E+02
C35-C33-C30-C66	89.249	5.702844E+02
C35-C33-C30-H105	-32.465	3.748876E+02
C35-C33-N47-Co89	-7.961	5.425373E+02
C35-C36-C37-C38	-164.022	6.559801E+02
C35-C36-C37-C71	81.79	6.148643E+02
C35-C36-C37-C72	-39.562	6.290117E+02
C35-C36-N48-C39	177.025	4.413515E+02
C35-C36-N48-Co89	2.747	4.349741E+02
C36-C35-C33-N47	0.027	4.021647E+02
C36-C37-C38-C39	-23.245	1.192061E+03
C36-C37-C38-C73	96.217	1.151142E+03
C36-C37-C38-H108	-142.174	4.749645E+02
C36-C37-C71-H139	56.804	4.260584E+02
C36-C37-C71-H140	176.707	4.002619E+02
C36-C37-C71-H141	-63.721	4.450657E+02
C36-C37-C72-H142	-173.911	4.917057E+02
C36-C37-C72-H143	-53.293	4.715243E+02
C36-C37-C72-H144	67.944	4.635487E+02
C36-N48-C39-C38	-10.232	7.113545E+02

C36-N48-C39-C40	176.823	4.976488E+02
C36-N48-Co89-N46	111.115	6.945626E+01
C36-N48-Co89-N47	-7.612	5.549182E+02
C36-N48-Co89-N49	174.104	5.755338E+02
C37-C36-C35-H107	4.19	2.043661E+02
C37-C36-N48-C39	-6.487	6.480293E+02
C37-C36-N48-Co89	179.235	6.343729E+02
C37-C38-C39-C40	-165.112	8.104304E+02
C37-C38-C39-N48	21.75	8.729995E+02
C37-C38-C73-C74	-67.506	1.105231E+03
C37-C38-C73-H145	171.951	4.710773E+02
C37-C38-C73-H146	57.669	4.978835E+02
C38-C37-C36-N48	19.45	7.515230E+02
C38-C37-C71-H139	-51.569	4.450262E+02
C38-C37-C71-H140	68.333	4.169574E+02
C38-C37-C71-H141	-172.095	4.658049E+02
C38-C37-C72-H142	-57.65	5.005958E+02
C38-C37-C72-H143	62.968	4.796936E+02
C38-C37-C72-H144	-175.795	4.714416E+02
C38-C39-C40-C41	-157.991	8.007546E+02
C38-C39-C40-C78	17.78	7.278609E+02
C38-C39-N48-Co89	164.007	7.316565E+02
C38-C73-C74-C75	-157.31	1.072165E+03
C38-C73-C74-H147	78.243	5.110422E+02
C38-C73-C74-H148	-40.101	5.081000E+02
C39-C38-C37-C71	89.794	1.260903E+03
C39-C38-C37-C72	-147.236	1.067543E+03
C39-C38-C73-C74	48.358	1.080108E+03
C39-C38-C73-H145	-72.185	4.664530E+02
C39-C38-C73-H146	173.533	4.927208E+02
C39-C40-C41-C42	167.412	7.024860E+02
C39-C40-C41-N49	-9.771	4.483800E+02
C39-C40-C78-H150	146.633	3.900686E+02
C39-C40-C78-H151	-91.896	4.058608E+02
C39-C40-C78-H152	28.744	4.136931E+02
C39-N48-Co89-N46	-62.314	6.984614E+01
C39-N48-Co89-N47	178.959	5.808209E+02
C39-N48-Co89-N49	0.675	6.034453E+02
C40-C39-C38-C73	69.858	7.131189E+02
C40-C39-C38-H108	-48.089	3.832616E+02
C40-C39-N48-Co89	-8.937	5.075003E+02
C40-C41-C42-C43	-158.919	6.691710E+02
C40-C41-C42-C79	83.218	6.392138E+02
C40-C41-C42-C80	-41.571	6.563080E+02
C40-C41-N49-C44	177.779	5.985620E+02
C40-C41-N49-Co89	1.102	4.317336E+02
C41-C40-C39-N48	13.946	5.684336E+02
C41-C40-C78-H150	-37.557	4.086349E+02

C41-C40-C78-H151	83.914	4.259996E+02
C41-C40-C78-H152	-155.446	4.346368E+02
C41-C42-C43-C44	-28.657	1.326553E+03
C41-C42-C43-C85	-159.104	1.228724E+03
C41-C42-C43-H109	83.764	4.585217E+02
C41-C42-C79-H153	179.93	4.522798E+02
C41-C42-C79-H154	-60.94	5.191855E+02
C41-C42-C79-H155	59.318	4.779958E+02
C41-C42-C80-C81	-46.086	7.723500E+02
C41-C42-C80-H156	-165.858	4.348290E+02
C41-C42-C80-H157	79.854	4.589768E+02
C41-N49-C44-C43	-19.355	6.135361E+02
C41-N49-C44-H110	96.928	3.526332E+02
C41-N49-Co89-N46	173.647	4.791204E+02
C41-N49-Co89-N47	-163.941	2.399092E+01
C41-N49-Co89-N48	2.904	4.508190E+02
C42-C41-C40-C78	-8.263	7.228186E+02
C42-C41-N49-C44	0.223	9.065327E+02
C42-C41-N49-Co89	-176.454	5.718610E+02
C42-C43-C44-N49	29.154	1.113361E+03
C42-C43-C44-H110	-84.703	4.857694E+02
C42-C43-C85-C86	-150.249	1.113374E+03
C42-C43-C85-H160	86.07	5.695878E+02
C42-C43-C85-H161	-31.427	4.664834E+02
C42-C80-C81-C82	-128.327	1.040177E+03
C42-C80-C81-H158	107.034	4.724905E+02
C42-C80-C81-H159	-10.147	4.384112E+02
C43-C42-C41-N49	18.538	6.467508E+02
C43-C42-C79-H153	69.332	4.541523E+02
C43-C42-C79-H154	-171.538	5.216545E+02
C43-C42-C79-H155	-51.28	4.800878E+02
C43-C42-C80-C81	66.701	9.049447E+02
C43-C42-C80-H156	-53.072	4.739236E+02
C43-C42-C80-H157	-167.359	5.027527E+02
C43-C44-C4-C45	-46.077	9.950591E+02
C43-C44-C4-N46	-159.577	9.447279E+02
C43-C44-N49-Co89	157.877	8.174911E+02
C43-C85-C86-N87	62.017	6.196909E+02
C43-C85-C86-O88	-116.657	5.818814E+02
C44-C4-C7-C50	-105.091	9.869405E+02
C44-C4-C7-C51	17.569	9.247484E+02
C44-C4-C45-H111	69.325	4.616833E+02
C44-C4-C45-H112	-170.552	5.427591E+02
C44-C4-C45-H113	-50.817	4.645003E+02
C44-C4-N46-Co89	45.997	8.109310E+02
C44-C43-C42-C79	86.759	1.073995E+03
C44-C43-C42-C80	-150.887	1.252169E+03
C44-C43-C85-C86	88.258	1.262833E+03

C44-C43-C85-H160	-35.423	6.062978E+02
C44-C43-C85-H161	-152.92	4.908221E+02
C44-N49-Co89-N46	-2.954	8.925437E+02
C44-N49-Co89-N47	19.459	2.456057E+01
C44-N49-Co89-N48	-173.697	7.990920E+02
C45-C4-C7-C50	27.099	1.048391E+03
C45-C4-C7-C51	149.759	9.784873E+02
C45-C4-C44-N49	69.838	1.067634E+03
C45-C4-C44-H110	-176.501	5.006424E+02
C45-C4-N46-Co89	-69.172	8.277212E+02
N46-C4-C7-C50	142.431	1.088453E+03
N46-C4-C7-C51	-94.909	1.013297E+03
N46-C4-C44-N49	-43.662	1.009907E+03
N46-C4-C44-H110	69.998	4.875732E+02
N46-C4-C45-H111	179.046	4.335175E+02
N46-C4-C45-H112	-60.831	5.042449E+02
N46-C4-C45-H113	58.903	4.360004E+02
N46-C15-C11-C55	-115.377	6.346924E+02
N46-C15-C11-H97	126.645	3.446879E+02
N46-C15-C19-C60	-158.914	4.818451E+02
N47-C23-C19-C60	170.451	5.444019E+02
N47-C23-C26-C61	149.875	7.312912E+02
N47-C23-C26-C62	-82.789	7.105608E+02
N47-C33-C30-C66	-91.875	6.539445E+02
N47-C33-C30-H105	146.41	4.093098E+02
N47-C33-C35-H107	-177.447	1.999308E+02
N48-C36-C35-H107	-179.731	1.878525E+02
N48-C36-C37-C71	-94.737	6.980462E+02
N48-C36-C37-C72	143.911	7.163373E+02
N48-C39-C38-C73	-103.28	7.611193E+02
N48-C39-C38-H108	138.773	3.967077E+02
N48-C39-C40-C78	-170.282	5.307047E+02
N49-C41-C40-C78	174.554	4.565776E+02
N49-C41-C42-C79	-99.325	6.187254E+02
N49-C41-C42-C80	135.886	6.347275E+02
N49-C44-C43-C85	155.521	9.201456E+02
N49-C44-C43-H109	-82.171	4.109001E+02
C50-C7-C11-C55	-18.64	7.568512E+02
C50-C7-C11-H97	102.815	4.617822E+02
C50-C7-C51-C52	-50.258	1.157257E+03
C50-C7-C51-H117	-170.253	4.429113E+02
C50-C7-C51-H118	70.338	4.957944E+02
C51-C7-C11-C55	-139.597	8.470102E+02
C51-C7-C11-H97	-18.142	4.938558E+02
C51-C7-C50-H114	61.138	4.611762E+02
C51-C7-C50-H115	-178.811	4.512228E+02
C51-C7-C50-H116	-56.681	4.206269E+02
C51-C52-N54-H119	-12.117	2.308170E+02

C51-C52-N54-H164	-175.182	2.221597E+02
O53-C52-C51-H117	49.23	4.067101E+02
O53-C52-C51-H118	166.033	3.959360E+02
O53-C52-N54-H119	168.416	1.932526E+02
O53-C52-N54-H164	5.35	1.871465E+02
N54-C52-C51-H117	-130.245	4.629486E+02
N54-C52-C51-H118	-13.442	4.490398E+02
C55-C56-C57-N58	-112.922	7.391544E+02
C55-C56-C57-O59	67.029	6.032584E+02
C56-C55-C11-H97	-30.282	4.358910E+02
C56-C57-N58-H124	17.794	2.239131E+02
C56-C57-N58-H170	174.942	2.454025E+02
C57-C56-C55-H120	-160.735	4.680459E+02
C57-C56-C55-H121	-46.243	4.592946E+02
N58-C57-C56-H122	11.918	4.406161E+02
N58-C57-C56-H123	128.864	4.457797E+02
O59-C57-C56-H122	-168.131	3.884527E+02
O59-C57-C56-H123	-51.185	3.924604E+02
O59-C57-N58-H124	-162.157	1.953366E+02
O59-C57-N58-H170	-5.008	2.114931E+02
C61-C26-C30-C66	-39.476	1.063066E+03
C61-C26-C30-H105	84.301	4.806232E+02
C61-C26-C62-C63	77.001	1.035580E+03
C61-C26-C62-H131	-47.963	4.499606E+02
C61-C26-C62-H132	-164.492	4.525846E+02
C62-C26-C30-C66	-159.596	1.113988E+03
C62-C26-C30-H105	-35.82	4.907657E+02
C62-C26-C61-H128	-47.894	4.271649E+02
C62-C26-C61-H129	70.832	4.980070E+02
C62-C26-C61-H130	-169.113	4.481570E+02
C62-C63-N65-H133	-8.642	8.776407E+01
C62-C63-N65-H163	-176.241	1.640800E+02
O64-C63-C62-H131	-158.207	3.646442E+02
O64-C63-C62-H132	-41.816	3.833805E+02
O64-C63-N65-H133	172.308	8.151756E+01
O64-C63-N65-H163	4.709	1.435194E+02
N65-C63-C62-H131	22.735	3.898746E+02
N65-C63-C62-H132	139.127	4.113698E+02
C66-C67-C68-O69	-77.937	6.224350E+02
C66-C67-C68-N70	100.358	5.724632E+02
C67-C66-C30-H105	53.176	4.399420E+02
C67-C68-N70-H138	3.792	2.236709E+01
C67-C68-N70-H166	-179.34	8.618700E+01
C68-C67-C66-H134	-65.774	5.490783E+02
C68-C67-C66-H135	50.455	5.853887E+02
O69-C68-C67-H136	41.891	3.966945E+02
O69-C68-C67-H137	159.16	3.846539E+02
O69-C68-N70-H138	-177.907	2.196792E+01

O69-C68-N70-H166	-1.039	8.054731E+01
N70-C68-C67-H136	-139.813	3.757880E+02
N70-C68-C67-H137	-22.545	3.649657E+02
C71-C37-C38-C73	-150.744	1.215211E+03
C71-C37-C38-H108	-29.135	4.855264E+02
C71-C37-C72-H142	65.441	4.824553E+02
C71-C37-C72-H143	-173.941	4.630111E+02
C71-C37-C72-H144	-52.703	4.553185E+02
C72-C37-C38-C73	-27.774	1.034607E+03
C72-C37-C38-H108	93.835	4.538711E+02
C72-C37-C71-H139	-178.309	4.222562E+02
C72-C37-C71-H140	-58.406	3.969044E+02
C72-C37-C71-H141	61.166	4.409184E+02
C73-C74-C75-O76	35.739	6.101451E+02
C73-C74-C75-N77	-145.341	6.490585E+02
C74-C73-C38-H108	169.562	4.693811E+02
C74-C75-N77-H149	-12.098	1.968104E+02
C74-C75-N77-H167	-173.961	2.581407E+02
C75-C74-C73-H145	-36.083	5.350453E+02
C75-C74-C73-H146	78.085	5.976670E+02
O76-C75-C74-H147	161.389	3.954426E+02
O76-C75-C74-H148	-84.37	3.935128E+02
O76-C75-N77-H149	166.76	1.700192E+02
O76-C75-N77-H167	4.897	2.139261E+02
N77-C75-C74-H147	-19.692	4.114293E+02
N77-C75-C74-H148	94.549	4.093408E+02
C79-C42-C43-C85	-43.689	1.008958E+03
C79-C42-C43-H109	-160.82	4.240538E+02
C79-C42-C80-C81	-169.985	9.552753E+02
C79-C42-C80-H156	70.243	4.873713E+02
C79-C42-C80-H157	-44.045	5.179125E+02
C80-C42-C43-C85	78.666	1.164642E+03
C80-C42-C43-H109	-38.466	4.492963E+02
C80-C42-C79-H153	-52.188	4.295082E+02
C80-C42-C79-H154	66.943	4.894003E+02
C80-C42-C79-H155	-172.799	4.526338E+02
C80-C81-C82-O83	28.897	5.926962E+02
C80-C81-C82-N84	-151.656	6.622152E+02
C81-C82-N84-H169	-8.436	1.867646E+02
C82-C81-C80-H156	-9.118	5.410892E+02
C82-C81-C80-H157	105.542	4.655487E+02
C82-N84-C2-H90	-137.383	3.504223E+02
C82-N84-C2-H91	-19.578	3.641865E+02
O83-C82-C81-H158	155.24	3.669091E+02
O83-C82-C81-H159	-92.456	3.645826E+02
O83-C82-N84-H169	170.994	1.665660E+02
N84-C2-C3-H92	-61.829	6.193306E+02
N84-C2-C3-H93	177.65	6.017217E+02

N84-C82-C81-H158	-25.313	3.924110E+02
N84-C82-C81-H159	86.991	3.897510E+02
C85-C43-C44-H110	41.664	4.449995E+02
C85-C86-N87-H162	9.282	1.326036E+02
C85-C86-N87-H165	-170.174	1.273515E+02
C86-C85-C43-H109	-34.025	5.911566E+02
N87-C86-C85-H160	-172.068	3.124440E+02
N87-C86-C85-H161	-57.649	3.975229E+02
O88-C86-C85-H160	9.258	3.025326E+02
O88-C86-C85-H161	123.677	3.816162E+02
O88-C86-N87-H162	-172.09	1.195817E+02
O88-C86-N87-H165	8.455	1.152938E+02
Co89-N49-C44-H110	-85.84	4.116638E+02
H90-C2-C3-H92	178.109	4.160270E+02
H90-C2-C3-H93	57.589	4.080065E+02
H90-C2-N84-H169	54.624	1.263672E+02
H91-C2-C3-H92	58.237	3.537279E+02
H91-C2-C3-H93	-62.283	3.479129E+02
H91-C2-N84-H169	172.43	1.281133E+02
H94-C5-C9-H96	40.369	4.044232E+02
H96-C9-C12-H98	-42.562	4.062463E+02
H96-C9-O29-H104	125.188	5.786703E+01
H97-C11-C55-H120	-154.019	3.154580E+02
H97-C11-C55-H121	89.689	3.094176E+02
H98-C12-C16-H99	-101.41	3.353150E+02
H99-C16-C21-H101	-77.694	4.395132E+02
H99-C16-C21-H102	165.152	4.341954E+02
H101-C21-O32-H106	-61.917	8.607397E+01
H102-C21-O32-H106	57.819	8.567141E+01
H105-C30-C66-H134	-68.179	3.135837E+02
H105-C30-C66-H135	174.954	3.124531E+02
H108-C38-C73-H145	49.018	2.986438E+02
H108-C38-C73-H146	-65.264	3.091975E+02
H109-C43-C44-H110	163.972	2.782345E+02
H109-C43-C85-H160	-157.705	3.922978E+02
H109-C43-C85-H161	84.798	3.404688E+02
H120-C55-C56-H122	74.554	2.868856E+02
H120-C55-C56-H123	-44.056	3.008995E+02
H121-C55-C56-H122	-170.954	2.835738E+02
H121-C55-C56-H123	70.436	2.972583E+02
H134-C66-C67-H136	176.748	3.325084E+02
H134-C66-C67-H137	57.713	3.277723E+02
H135-C66-C67-H136	-67.022	3.454857E+02
H135-C66-C67-H137	173.943	3.403756E+02
H145-C73-C74-H147	-160.531	3.456507E+02
H145-C73-C74-H148	81.125	3.443022E+02
H146-C73-C74-H147	-46.363	3.707458E+02
H146-C73-C74-H148	-164.706	3.691948E+02

H156-C80-C81-H158	-133.757	3.329788E+02
H156-C80-C81-H159	109.062	3.156851E+02
H157-C80-C81-H158	-19.097	3.027484E+02
H157-C80-C81-H159	-136.279	2.883845E+02

Table S3 Atom types of the selected ligands, with charges, $\mathscr{E}$ and σ.

Ligand	Atom	Atom type	Charge	$\mathcal{E}$ (kJ/mol)	σ (nm)
Tetrachloroethene	C1	c2	0.0244283873	3.598240E-01	3.399670E-01
	C2	c2	0.0231595789	1.108760E+00	3.470941E-01
	Cl3	cl	-0.0118464596	1.108760E+00	3.470941E-01
	Cl4	cl	-0.0123700344	1.108760E+00	3.470941E-01
	Cl5	cl	-0.0115306264	1.108760E+00	3.470941E-01
	Cl6	cl	-0.0118408458	1.108760E+00	3.470941E-01
Trichlorofluoroethene	C1	c2	-0.1222272710	3.598240E-01	3.399670E-01
	C2	c2	0.2778824262	1.108760E+00	3.470941E-01
	Cl3	cl	-0.0076027402	1.108760E+00	3.470941E-01
	Cl4	cl	0.0237807706	1.108760E+00	3.470941E-01
	F5	f	-0.1420374753	2.552240E-01	3.118146E-01
	Cl6	cl	-0.0297957103	1.108760E+00	3.470941E-01
Dichlorodifluoroethene	C1	c2	0.1288906884	3.598240E-01	3.399670E-01
	C2	c2	0.1303143661	3.598240E-01	3.399670E-01
	F3	f	-0.1304644761	2.552240E-01	3.118146E-01
	Cl4	cl	0.0010970493	1.108760E+00	3.470941E-01
	F5	f	-0.1310184142	2.552240E-01	3.118146E-01
	Cl6	cl	0.0011807865	1.108760E+00	3.470941E-01
Chlorotrifluoroethene	C1	c2	0.4132618799	3.598240E-01	3.399670E-01
	C2	c2	-0.0491462395	3.598240E-01	3.399670E-01
	F3	f	-0.1631267707	2.552240E-01	3.118146E-01
	F4	f	-0.1311873332	2.552240E-01	3.118146E-01
	F5	f	-0.0805543561	2.552240E-01	3.118146E-01
	Cl6	cl	0.0107528196	1.108760E+00	3.470941E-01
Tetrafluoroethene	C1	c2	0.2335531635	3.598240E-01	3.399670E-01
	C2	c2	0.2298709233	3.598240E-01	3.399670E-01
	F3	f	-0.1164880499	2.552240E-01	3.118146E-01
	F4	f	-0.1161371019	2.552240E-01	3.118146E-01
	F5	f	-0.1154224463	2.552240E-01	3.118146E-01
	F6	f	-0.1153764887	2.552240E-01	3.118146E-01

Table S4 Atom types of the cobalamin cofactor, with charges, $\mathscr{E}$ and σ.

Cobalamin	Atom	Atom type	Charge	$\mathcal{E}$ (kJ/mol)	σ (nm)
	P1	p5	1.21476	8.368000E-01	3.741775E-01
	C2	c3	-0.00804	4.577296E-01	3.399670E-01
	C3	c3	0.161564	4.577296E-01	3.399670E-01
	C4	c3	-0.22799	4.577296E-01	3.399670E-01

C5	c3	0.28114	4.577296E-01	3.399670E-01
N6	na	0.131089	7.112800E-01	3.249999E-01
C7	c3	0.515853	4.577296E-01	3.399670E-01
C8	cc	0.193878	3.598240E-01	3.399670E-01
C9	c3	0.208463	4.577296E-01	3.399670E-01
O10	os	-0.55322	7.112800E-01	3.000012E-01
C11	c3	-0.05206	4.577296E-01	3.399670E-01
C12	c3	0.091287	4.577296E-01	3.399670E-01
N13	n2	-0.59793	7.112800E-01	3.249999E-01
O14	os	-0.41738	7.112800E-01	3.000012E-01
C15	ce	-0.05706	3.598240E-01	3.399670E-01
C16	c3	0.118575	4.577296E-01	3.399670E-01
N17	nb	-0.77442	7.112800E-01	3.249999E-01
O18	o	-0.72034	8.786400E-01	2.959922E-01
C19	ce	0.213632	3.598240E-01	3.399670E-01
C20	ca	0.614429	3.598240E-01	3.399670E-01
C21	c3	0.221986	4.577296E-01	3.399670E-01
O22	o	-0.75828	8.786400E-01	2.959922E-01
C23	c2	-0.28322	3.598240E-01	3.399670E-01
N24	nb	-0.79927	7.112800E-01	3.249999E-01
O25	os	-0.52375	7.112800E-01	3.000012E-01
C26	c3	0.258056	4.577296E-01	3.399670E-01
C27	ca	0.896048	3.598240E-01	3.399670E-01
N28	nh	-0.88742	7.112800E-01	3.249999E-01
O29	oh	-0.66389	8.803136E-01	3.066473E-01
C30	c3	-0.14015	4.577296E-01	3.399670E-01
C31	ca	-0.64573	3.598240E-01	3.399670E-01
O32	oh	-0.70218	8.803136E-01	3.066473E-01
C33	c2	0.261148	3.598240E-01	3.399670E-01
C34	ca	0.849704	3.598240E-01	3.399670E-01
C35	c2	-0.51267	3.598240E-01	3.399670E-01
C36	c2	0.228708	3.598240E-01	3.399670E-01
C37	c3	0.414693	4.577296E-01	3.399670E-01
C38	c3	-0.00956	4.577296E-01	3.399670E-01
C39	c2	-0.02623	3.598240E-01	3.399670E-01
C40	c2	0.034337	3.598240E-01	3.399670E-01
C41	c2	0.095434	3.598240E-01	3.399670E-01
C42	c3	0.239788	4.577296E-01	3.399670E-01
C43	c3	0.106086	4.577296E-01	3.399670E-01
C44	c3	-0.18099	4.577296E-01	3.399670E-01
C45	c3	-0.57678	4.577296E-01	3.399670E-01
N46	nh	0.084831	7.112800E-01	3.249999E-01
N47	nh	0.027701	7.112800E-01	3.249999E-01
N48	nh	-0.21885	7.112800E-01	3.249999E-01
N49	nh	-0.11441	7.112800E-01	3.249999E-01
C50	c3	-0.41691	4.577296E-01	3.399670E-01
C51	c3	-0.31575	4.577296E-01	3.399670E-01
C52	c	0.727595	3.598240E-01	3.399670E-01
O53	o	-0.60029	8.786400E-01	2.959922E-01
N54	n	-0.8647	7.112800E-01	3.249999E-01

C55	c3	-0.1678	4.577296E-01	3.399670E-01
C56	c3	-0.2363	4.577296E-01	3.399670E-01
C57	c	0.695444	3.598240E-01	3.399670E-01
N58	n	-0.85899	7.112800E-01	3.249999E-01
O59	o	-0.56814	8.786400E-01	2.959922E-01
C60	c3	-0.32213	4.577296E-01	3.399670E-01
C61	c3	-0.44391	4.577296E-01	3.399670E-01
C62	c3	-0.35606	4.577296E-01	3.399670E-01
C63	c	0.753321	3.598240E-01	3.399670E-01
O64	o	-0.53067	8.786400E-01	2.959922E-01
N65	n	-0.93334	7.112800E-01	3.249999E-01
C66	c3	0.062233	4.577296E-01	3.399670E-01
C67	c3	-0.34481	4.577296E-01	3.399670E-01
C68	c	0.754389	3.598240E-01	3.399670E-01
O69	o	-0.55782	8.786400E-01	2.959922E-01
N70	n	-0.92679	7.112800E-01	3.249999E-01
C71	c3	-0.41825	4.577296E-01	3.399670E-01
C72	c3	-0.50896	4.577296E-01	3.399670E-01
C73	c3	-0.15453	4.577296E-01	3.399670E-01
C74	c3	-0.07009	4.577296E-01	3.399670E-01
C75	c	0.653557	3.598240E-01	3.399670E-01
O76	o	-0.56462	8.786400E-01	2.959922E-01
N77	n	-0.86671	7.112800E-01	3.249999E-01
C78	c3	-0.47213	4.577296E-01	3.399670E-01
C79	c3	-0.46951	4.577296E-01	3.399670E-01
C80	c3	-0.02033	4.577296E-01	3.399670E-01
C81	c3	-0.19111	4.577296E-01	3.399670E-01
C82	c	0.531898	3.598240E-01	3.399670E-01
O83	o	-0.52126	8.786400E-01	2.959922E-01
N84	n	-0.41353	7.112800E-01	3.249999E-01
C85	c3	-0.54719	4.577296E-01	3.399670E-01
C86	c	0.794095	3.598240E-01	3.399670E-01
N87	n	-0.77769	8.786400E-01	2.959922E-01
O88	o	-0.6138	7.112800E-01	3.249999E-01
Co89	UF_Co	0.236163	5.857600E-02	2.558661E-01
H90	h1	0.071874	6.568880E-02	2.471353E-01
H91	h1	0.071874	6.568880E-02	2.471353E-01
H92	h1	0.041143	6.568880E-02	2.471353E-01
H93	h1	0.041143	6.568880E-02	2.471353E-01
H94	h2	0.074346	6.568880E-02	2.293173E-01
H95	h5	0.119438	6.276000E-02	2.421463E-01
H96	h1	0.033136	6.568880E-02	2.471353E-01
H97	hc	0.066511	6.568880E-02	2.649533E-01
H98	h1	0.113745	6.568880E-02	2.471353E-01
H99	h1	0.074742	6.568880E-02	2.471353E-01
H100	h5	0.015122	6.276000E-02	2.421463E-01
H101	h1	0.007655	6.568880E-02	2.471353E-01
H102	h1	0.007655	6.568880E-02	2.471353E-01
H103	hn	0.369101	6.568880E-02	1.069078E-01
H104	ho	0.454745	0.000000E+00	0.000000E+00

H105	hc	0.089523	6.568880E-02	2.649533E-01
H106	ho	0.43676	0.000000E+00	0.000000E+00
H107	ha	0.168701	6.276000E-02	2.599642E-01
H108	hc	0.053206	6.568880E-02	2.649533E-01
H109	hc	0.049828	6.568880E-02	2.649533E-01
H110	h1	0.15277	6.568880E-02	2.471353E-01
H111	hc	0.210751	6.568880E-02	2.649533E-01
H112	hc	0.210751	6.568880E-02	2.649533E-01
H113	hc	0.210751	6.568880E-02	2.649533E-01
H114	hc	0.104165	6.568880E-02	2.649533E-01
H115	hc	0.104165	6.568880E-02	2.649533E-01
H116	hc	0.104165	6.568880E-02	2.649533E-01
H117	hc	0.071256	6.568880E-02	2.649533E-01
H118	hc	0.071256	6.568880E-02	2.649533E-01
H119	hn	0.412731	6.568880E-02	1.069078E-01
H120	hc	0.090195	6.568880E-02	2.649533E-01
H121	hc	0.090195	6.568880E-02	2.649533E-01
H122	hc	0.090709	6.568880E-02	2.649533E-01
H123	hc	0.090709	6.568880E-02	2.649533E-01
H124	hn	0.3809	6.568880E-02	1.069078E-01
H125	hc	0.10889	6.568880E-02	2.649533E-01
H126	hc	0.10889	6.568880E-02	2.649533E-01
H127	hc	0.10889	6.568880E-02	2.649533E-01
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H129	hc	0.128921	6.568880E-02	2.649533E-01
H130	hc	0.128921	6.568880E-02	2.649533E-01
H131	hc	0.097691	6.568880E-02	2.649533E-01
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H133	hn	0.401712	6.568880E-02	1.069078E-01
H134	hc	0.038451	6.568880E-02	2.649533E-01
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H136	hc	0.097891	6.568880E-02	2.649533E-01
H137	hc	0.097891	6.568880E-02	2.649533E-01
H138	hn	0.406691	6.568880E-02	1.069078E-01
H139	hc	0.104738	6.568880E-02	2.649533E-01
H140	hc	0.104738	6.568880E-02	2.649533E-01
H141	hc	0.104738	6.568880E-02	2.649533E-01
H142	hc	0.130749	6.568880E-02	2.649533E-01
H143	hc	0.130749	6.568880E-02	2.649533E-01
H144	hc	0.130749	6.568880E-02	2.649533E-01
H145	hc	0.067	6.568880E-02	2.649533E-01
H146	hc	0.067	6.568880E-02	2.649533E-01
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H150	hc	0.147697	6.568880E-02	2.649533E-01
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H153	hc	0.125072	6.568880E-02	2.649533E-01
H154	hc	0.125072	6.568880E-02	2.649533E-01

	H155	hc	0.125072	6.568880E-02	2.649533E-01
	H156	hc	0.025976	6.568880E-02	2.649533E-01
	H157	hc	0.025976	6.568880E-02	2.649533E-01
	H158	hc	0.067038	6.568880E-02	2.649533E-01
	H159	hc	0.067038	6.568880E-02	2.649533E-01
	H160	hc	0.161116	6.568880E-02	2.649533E-01
	H161	hc	0.161116	6.568880E-02	2.649533E-01
	H162	hn	0.352432	6.568880E-02	1.069078E-01
	H163	hn	0.412158	6.568880E-02	1.069078E-01
	H164	hn	0.395418	6.568880E-02	1.069078E-01
	H165	hn	0.363131	6.568880E-02	1.069078E-01
	H166	hn	0.424737	6.568880E-02	1.069078E-01
	H167	hn	0.470501	6.568880E-02	1.069078E-01
	H168	hn	0.389757	6.568880E-02	1.069078E-01
	H169	hn	0.287955	6.568880E-02	1.069078E-01
	H170	hn	0.385775	6.568880E-02	1.069078E-01

Charges and atom names of selected ligands for molecular dynamics simulations

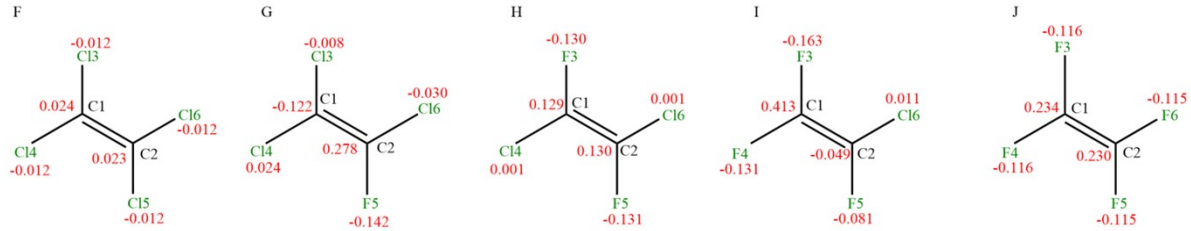

Fig. S1 The atom names and charges of halogenated ethene

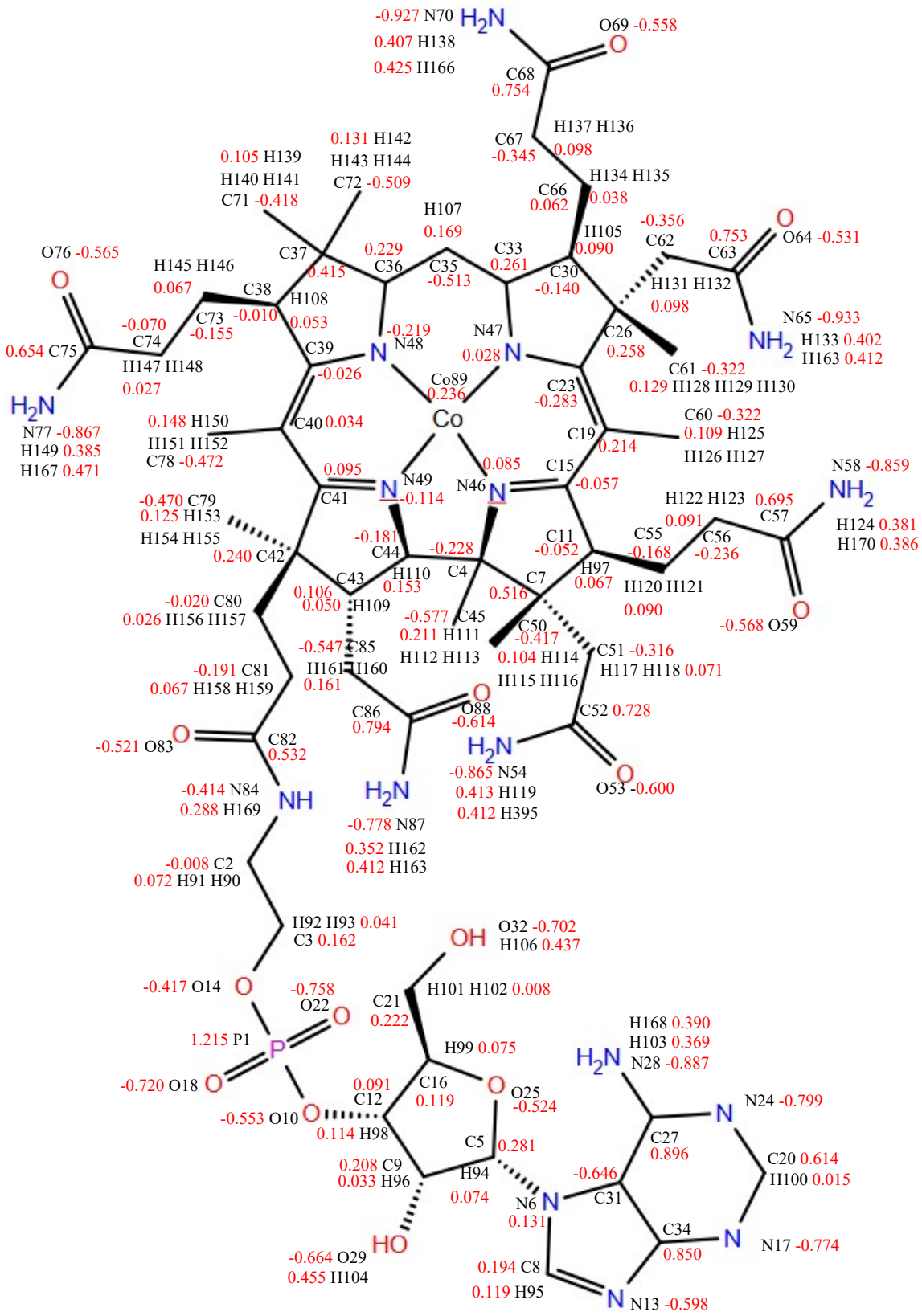

Fig. S2 The atom names and charges of cobalamin cofactor

Validation of cobalamin cofactor

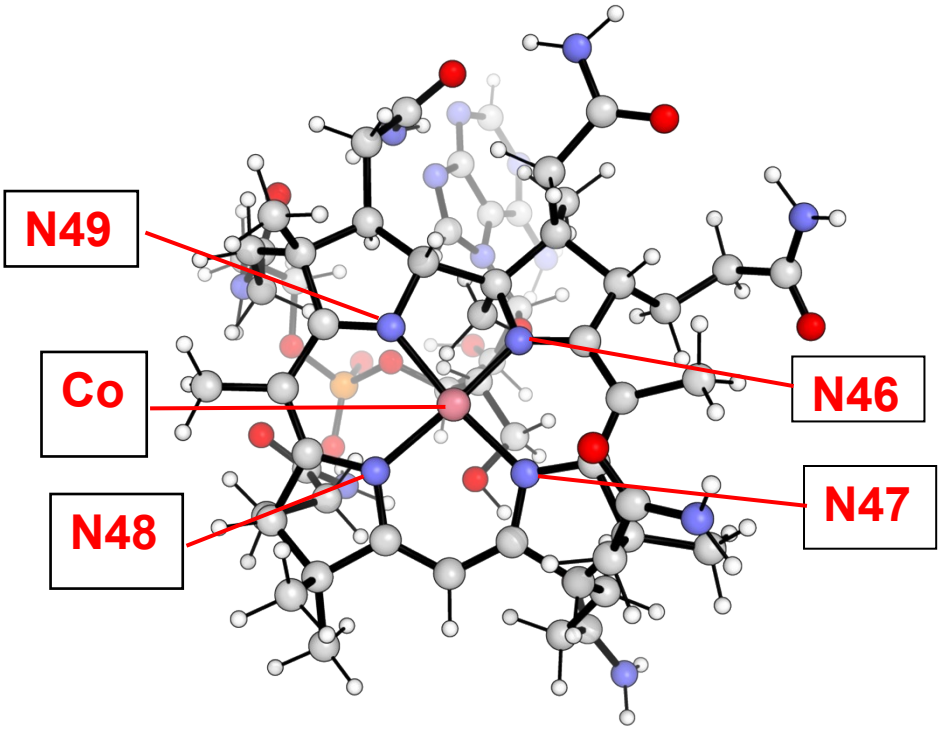

Fig. S3 The selected view of the cobalamin cofactor and atoms that are used to validate the structure in MD simulation.

Table S5 Optimized structure of cobalamin cofactor, calculated at B3LYP/ 6-311G(d,p) level of theory using Gaussian 09. The bonds and angles used to validate the geometry in MD simulation.

Optimized structure of Cobalt and nitrogen atom	
N46_Co_bond_distance (Å)	1.86555
N47_Co_bond_distance (Å)	1.90632
N48_Co_bond_distance (Å)	1.90951
N49_Co_bond_distance (Å)	1.88518
angle_N46_Co_N47 (Degree °)	89.70536
angle_N47_Co_N48 (Degree °)	95.30555
angle_N48_Co_N49 (Degree °)	92.02366
angle_N49_Co_N46 (Degree °)	83.33081

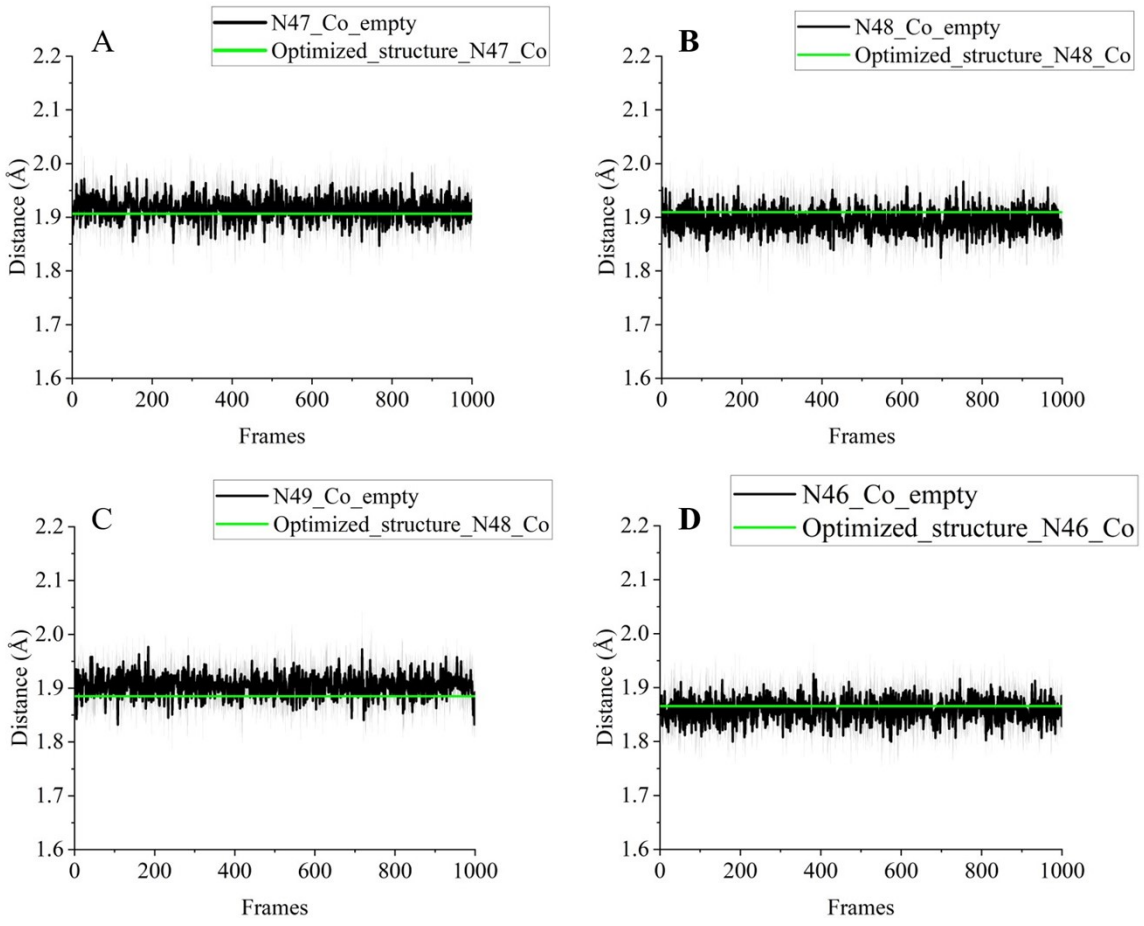

Fig. S4 The comparison between the selected bond distances during the MD simulation with the geometry optimized bond distances.

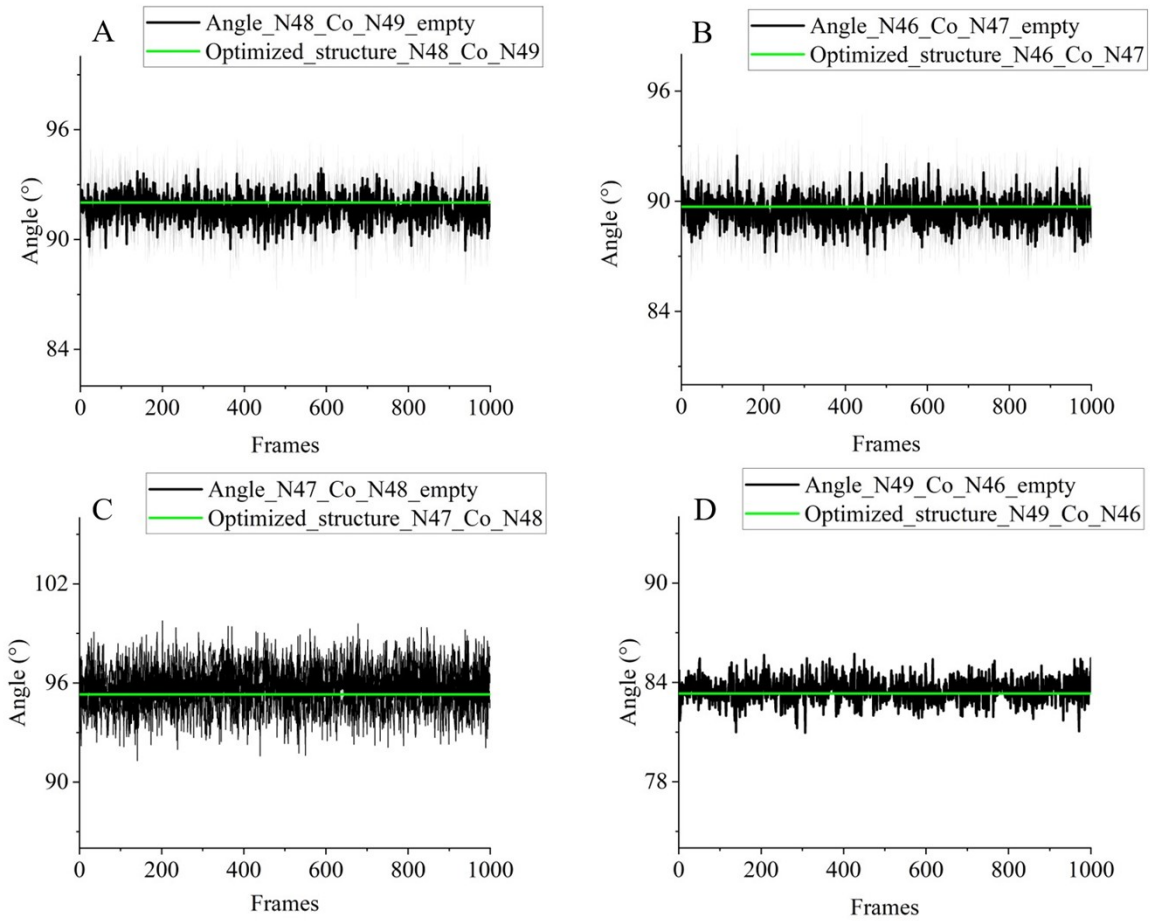

Fig. S5 The comparison between the selected angles during the MD simulation with the geometry optimized angles.

Validation of molecular dynamic simulation

The entire PceA chain-B of PDB id: 4UR0 was simulated in presence of the substrate trichloroethene (TCE), which is present in the crystal structure of PceA PDB id: 4UR0. Three independent simulations were conducted to assess the validity and reproducibility of the model. Each independent simulation was run 10 ns, subsequently, the representative structure was generated by using gmx cluster tool. Then, with the obtained representative structures from the three parallel molecular dynamics simulations of PceA, the RMSDs of all non-hydrogen atoms alignments with the PceA crystal structure chain-B are shown in Table 1. For the PceA-TCE complex, the RMSDs of all non-hydrogen atoms alignments are 1.524 Å, 1.427 Å, and 1.332 Å. All RMSD values are below the resolution of the crystal structure 1.65 Å, indicating that the simulated structures are in good agreement with the atomic positions in the crystallographic coordinates, and the results are reproducible.

Table S6. The RMSD (Å) results of alignment between the crystal structure and simulated structures PceA_trichloroethene. The active site includes residues Trp 56, Trp 96, Thr 242, Tyr 246, Arg 305, Trp376 and Tyr382.

System	Replication 1	Replication 2	Replication 3
PceA_trichloroethene	1.524	1.427	1.332
PceA_trichloroethene active site	0.953	0.581	0.9

The RMSDs of the all non-hydrogen atoms alignments between the active sites of the crystal structure and PceA-TCE, the values are reduced to 0.953 Å, 0.581 Å, and 0.900 Å. As shown in the Supplementary Information Figure S6, the alignments between the molecular dynamics simulated structures and the atomic positions of the PceA crystal structure demonstrate good agreement. These findings indicate that the molecular dynamics simulations reliably generate the influence of ligands association in the binding pocket between key residues, as compared to the crystal structure.

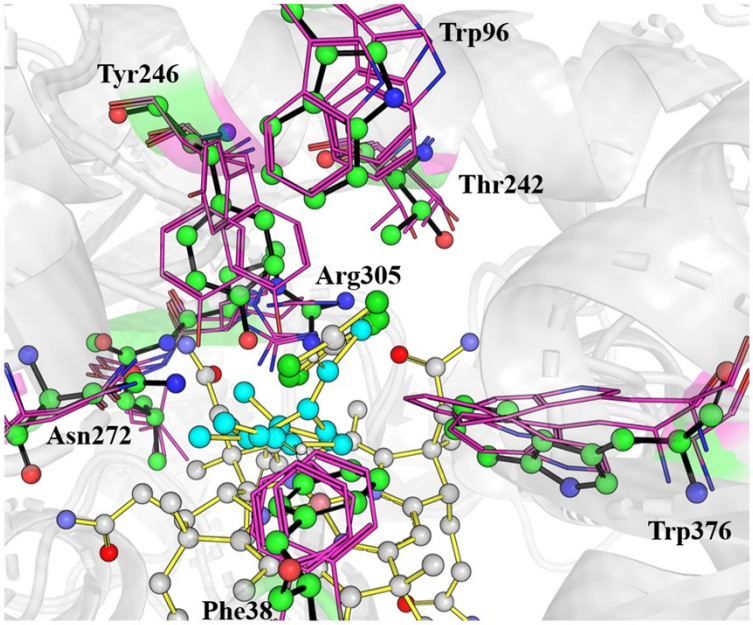

Fig. S6 The alignments for between the PceA crystal structure (shown in sticks, with green sphere) chain-B, with trichloroethene associated, and PceA_trichloroethene MD simulation structures (shown in line with purple color), and the trichloroethene ligands (shown in blue sphere).

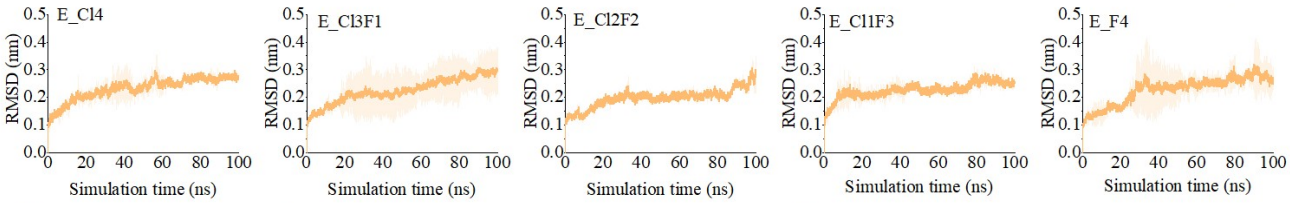

Fig. S7 The backbone atoms RMSD of 100 nano-seconds simulation MD trajectories for each ligand. The shaded areas are the standard deviation of three independent simulations.

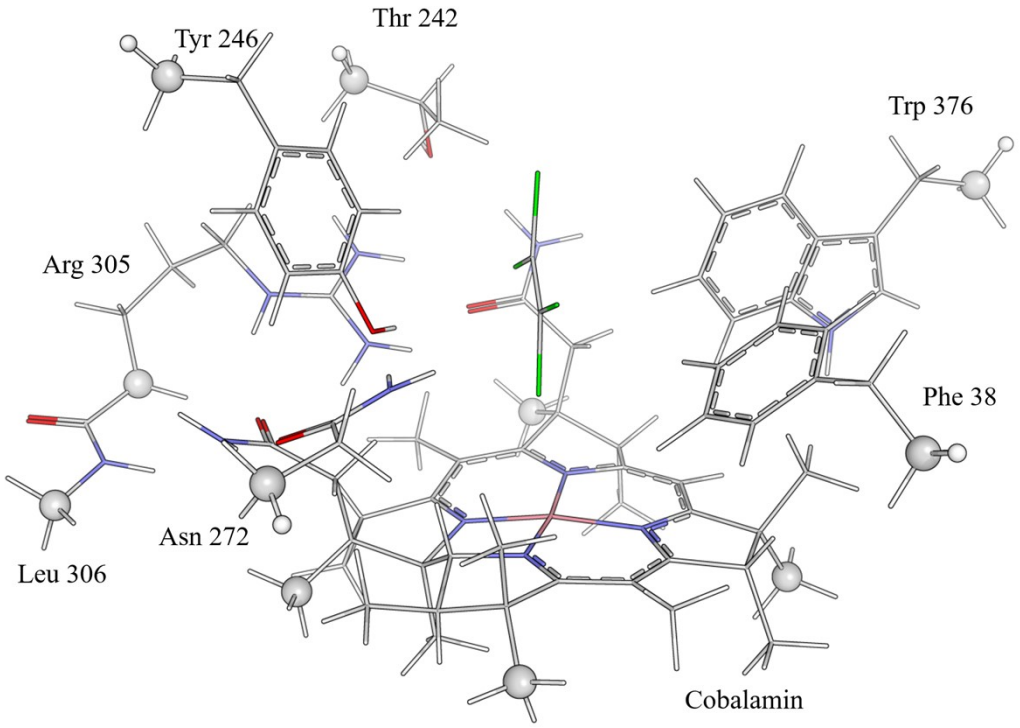

Fig. S8 The cluster model of PceA for QM calculation, the representation is the ligand Cl4 binding at the active site centre of PceA cluster, the atoms shown in sphere are the atoms fixed during the optimization.

Supplementary information for calculating energy difference between the unprotonated Tyr246, Co^{II} and the protonated Tyr246, Co^{I}

The proton-coupled electron transfer process is considered with following equation for calculating energy difference between the unprotonated Tyr246, Co^{II} and the protonated Tyr246, Co^{I}:

$$\left(\left(E_{deprotonated} - E_{protonnated}\right) - E_{proton} - \Delta H_{proton} - E_{pK_a}\right) \times 0.0433634 - 0.45$$

in which $E_{deprotonated}$ is the energy from the geometry optimized system before protonation (kcal/mol), $E_{protonated}$ is the energy from geometry optimized system after protonation (kcal/mol). E_{proton} is the proton transfer energy, 98.722 kcal/mol. ΔH_{proton} is the solvation enthalpy of the proton, 270.3kcal.mol [3]. E_{pK_a} is the energy of pK_a value in the gas phase, 7 x 1.364 [4]. 0.0433634 is the coefficient to convert kcal/mol to volt. 0.45 is the reference reduction potential when methyl viologen is used as electron donor [5, 6].

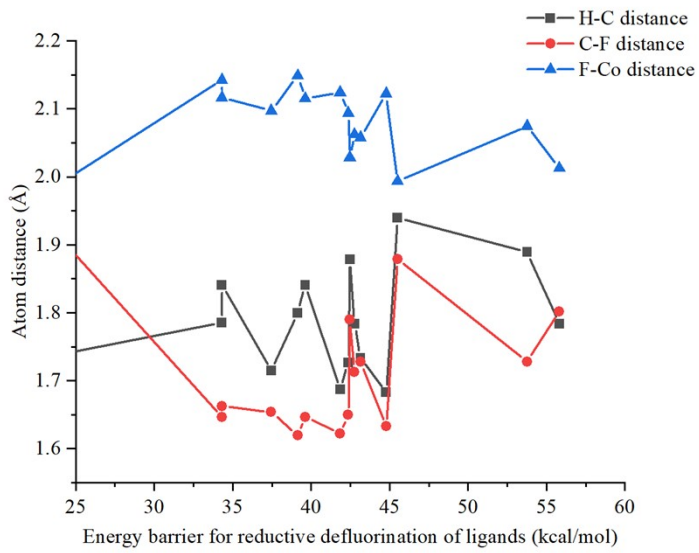

Figure S9 Correlation between transition-state geometry parameters and energy barriers for reductive defluorination. Three key distances were analysed relative to the calculated activation energy: H-C (Tyr246 H donor→substrate C, black squares), C-F (reacting bond, red circles), and F-Co (leaving F→cobalt, blue triangles).

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6. R. Z. Liao, S. L. Chen and P. E. Siegbahn, *Chemistry*, 2016, **22**, 12391-12399.