The first step and the co(II)balamin cofactor inactive particles reactivation in the updated mechanism of the Methionine Synthase process.

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SUPPORTING INFORMATION

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Table S1. The methylcob(II)alamin, homocysteine ion, and histidine substrates common model CASSCF geometry optimization starting coordinates.

N	**0.27519597**	**-0.29617784**	**0.94237837**
Co	**-0.39204881**	**-1.22333468**	**-0.61651790**
N	**-0.93889149**	**-1.82879803**	**-2.39589541**
N	**1.29448249**	**-1.07718780**	**-1.52609227**
C	**1.53157297**	**0.33321970**	**0.98659049**
C	**-2.49994250**	**-1.22402740**	**1.38057652**
C	**-1.69687019**	**-0.59802106**	**2.31954652**
C	**-3.95109152**	**-1.60103632**	**1.61550036**
H	**-2.10860921**	**-0.40180207**	**3.29306977**
C	**-0.39861919**	**-0.12341603**	**2.05567614**
C	**0.35682716**	**0.76568382**	**3.02605836**
C	**1.59596060**	**1.20637722**	**2.22572135**
H	**2.52190369**	**1.04969150**	**2.76052029**
C	**2.51363927**	**0.20296039**	**0.06814836**
C	**2.39219439**	**-0.55409153**	**-1.14978183**
C	**3.49888370**	**-0.80812784**	**-2.15009566**
C	**2.71990880**	**-1.33081639**	**-3.38231206**

H	**2.52614785**	**-0.51530654**	**-4.07384803**
C	**1.41953704**	**-1.87536848**	**-2.76036241**
H	**1.56765190**	**-2.89834150**	**-2.46233519**
C	**-0.35084683**	**-2.91758182**	**-4.41147038**
C	**-1.85662904**	**-3.10502036**	**-4.09620660**
H	**-2.15740546**	**-4.14488195**	**-4.09422039**
C	**-1.97888862**	**-2.49759121**	**-2.71397688**
C	**-3.15433063**	**-2.21412090**	**-0.54729747**
C	**-3.10021010**	**-2.68319285**	**-1.82193195**
C	**-4.26641825**	**-2.52733779**	**0.43596136**
H	**-4.12187796**	**-2.05883589**	**2.57883297**
N	**-2.17690679**	**-1.45688245**	**0.10274109**
H	**4.16253896**	**-1.56707872**	**-1.74965068**
C	**0.07506797**	**-1.77068801**	**-3.47269914**
H	**0.18900578**	**-3.82559974**	**-4.16767562**
H	**-0.17104210**	**-2.69666756**	**-5.45564677**
H	**-2.49346769**	**-2.58298608**	**-4.80164156**
H	**-3.91556689**	**-3.28013500**	**-2.17567343**
H	**-5.24348311**	**-2.35246210**	**0.01527522**
H	**-4.20178282**	**-3.57131349**	**0.72583183**
H	**-4.55227598**	**-0.69953502**	**1.55884791**
H	**0.67602527**	**0.21178827**	**3.89649464**
H	**-0.29184947**	**1.56464913**	**3.33929931**
H	**3.44607187**	**0.69959984**	**0.26745424**
H	**1.55373905**	**2.25402131**	**1.92637800**
H	**3.26394634**	**-2.09400730**	**-3.91522700**
C	**-0.05127393**	**-3.09199855**	**0.05384107**
H	**-0.77141552**	**-3.15180934**	**0.85609926**

H	**-0.42381487**	**-3.78603726**	**-0.69903140**
H	**4.08806296**	**0.08064975**	**-2.34243723**
H	**-1.37801698**	**-10.78438373**	**2.22368466**
C	**-1.75867785**	**-10.02303348**	**2.89300269**
H	**-1.21623071**	**-10.05047079**	**3.83100263**
C	**-1.67111574**	**-8.62778164**	**2.21987964**
O	**-1.84518183**	**-8.62052686**	**0.98917041**
O	**-1.47076292**	**-7.66004120**	**2.97732005**
H	**-2.80121898**	**-10.25870362**	**3.09989314**
C	**1.19959089**	**-3.73674981**	**0.67756251**
O	**1.97462907**	**-2.81933176**	**1.46644300**
C	**2.26656077**	**-4.50973067**	**-0.10713391**
H	**0.81354645**	**-4.48654619**	**1.36730589**
C	**3.23862930**	**-3.40155086**	**1.76838053**
C	**3.27186428**	**-4.73679578**	**1.01591551**
H	**1.89020770**	**-5.42949506**	**-0.54073934**
H	**3.99954766**	**-2.74509854**	**1.36830963**
H	**2.92983284**	**-5.54211476**	**1.65833138**
O	**2.90050060**	**-3.72459336**	**-1.10847721**
H	**3.76799969**	**-4.08575343**	**-1.22407536**
O	**4.55061799**	**-5.03671320**	**0.49504216**
H	**5.15526535**	**-5.11182171**	**1.22388455**
N	**3.49887495**	**-3.59273984**	**3.16277971**
H	**2.88060461**	**-4.22362842**	**3.62876939**
H	**3.67273661**	**-2.76826717**	**3.69181529**
C	**-1.69001445**	**2.88635248**	**-1.41994490**
C	**-0.38219354**	**1.30151199**	**-2.25264949**
C	**-1.78527462**	**1.71461340**	**-0.65781411**

C	**-2.36666156**	**4.08357734**	**-1.07206551**
H	**0.36549918**	**0.84498871**	**-2.85725971**
C	**-2.60419726**	**1.68880478**	**0.47388345**
C	**-3.16111266**	**4.03586158**	**0.07526662**
H	**-2.26439250**	**4.97245588**	**-1.65907352**
C	**-3.28334379**	**2.84849039**	**0.82572481**
H	**-2.68560180**	**0.81564132**	**1.07282219**
N	**-0.79179037**	**2.58279178**	**-2.44676469**
N	**-0.94344641**	**0.72761100**	**-1.23633371**
H	**-3.69091543**	**4.90800599**	**0.40425863**
H	**-3.91244998**	**2.83157771**	**1.69007139**
H	**2.07765612**	**4.94109711**	**-1.99774718**
C	**2.00115338**	**5.26352130**	**-0.98862052**
N	**1.82599364**	**6.56628070**	**-0.60863214**
N	**2.10342815**	**4.49286767**	**0.05629388**
C	**1.80012061**	**6.60126415**	**0.77579878**
H	**1.65969638**	**7.32862892**	**-1.21865836**
C	**1.99121179**	**5.31221371**	**1.16860742**
C	**1.78840357**	**7.86400574**	**1.58946832**
H	**2.04191576**	**4.91469834**	**2.15260721**
C	**0.52825407**	**8.80017107**	**1.66950396**
H	**2.60458887**	**8.50271283**	**1.26795052**
H	**2.01467287**	**7.55514998**	**2.60511120**
N	**0.61518543**	**9.97887568**	**0.85389919**
H	**0.47655109**	**9.13920897**	**2.69080849**
C	**-0.80735794**	**8.11049739**	**1.46108564**
H	**0.63009128**	**10.87727980**	**1.26931540**
O	**-1.59475609**	**7.88378778**	**2.32915462**

H	**0.56510738**	**9.93543971**	**-0.13628663**
O	**-1.08031855**	**7.82637470**	**0.17016764**
H	**-1.90766003**	**7.37051155**	**0.13939085**
H	**-0.48413319**	**3.19048058**	**-3.16614659**
H	**-0.00747701**	**-0.81651519**	**-3.98992158**

Table S2. The cob(II)alamin bio inactive particle plus AdoMet substrate common model CASSCF geometry optimization starting coordinates.

N	**0.43263415**	**1.44675684**	**-1.64148031**
Co	**0.08040848**	**1.87488928**	**0.22889985**
N	**-0.47579385**	**2.60961697**	**1.92132829**
N	**-1.83334305**	**1.56716477**	**0.01979705**
C	**-0.56961803**	**1.31171292**	**-2.59800364**
C	**2.96969668**	**2.07001810**	**-0.18419602**
C	**2.84690534**	**1.68314561**	**-1.52308854**
C	**4.29620593**	**2.47628176**	**0.44060727**
H	**3.74757718**	**1.66479268**	**-2.10825645**
C	**1.64509459**	**1.46903414**	**-2.20155569**
C	**1.56651071**	**1.25537248**	**-3.70345650**
C	**0.05339134**	**1.25687270**	**-3.98459409**
H	**-0.27098585**	**0.37962700**	**-4.53019171**
C	**-1.90951388**	**1.29458346**	**-2.35677026**
C	**-2.51905622**	**1.47711256**	**-1.05471164**
C	**-4.00955432**	**1.62233203**	**-0.79891794**
C	**-4.03759225**	**2.19912677**	**0.63961919**
H	**-4.13681616**	**3.27514679**	**0.59544135**
C	**-2.65706088**	**1.81868325**	**1.21438717**
H	**-2.72309797**	**0.89977807**	**1.79191429**

C	**-2.13514606**	**3.03090979**	**3.55305480**
C	**-0.74076613**	**3.48923444**	**4.06086652**
H	**-0.49091085**	**3.07664605**	**5.02915928**
C	**0.18294716**	**2.98433425**	**2.96784245**
C	**2.41586771**	**2.65778321**	**1.92482192**
C	**1.63220859**	**2.98305206**	**2.98621125**
C	**3.93277282**	**2.74901019**	**1.91124376**
H	**5.04329678**	**1.69851980**	**0.32894981**
N	**1.96363178**	**2.19870713**	**0.68037801**
H	**-4.49356312**	**0.65033820**	**-0.85695546**
C	**-1.91763728**	**2.89231404**	**2.03151569**
H	**-2.39253364**	**2.07159187**	**3.99054469**
H	**-2.92313067**	**3.72825851**	**3.80106166**
H	**-0.66953093**	**4.56834697**	**4.14137713**
H	**2.11463991**	**3.33320176**	**3.88207658**
H	**4.27494994**	**3.71464013**	**2.24630821**
H	**4.35813290**	**2.00894734**	**2.57811240**
H	**4.68570526**	**3.35676074**	**-0.04958973**
H	**2.03824789**	**0.31946483**	**-3.98315472**
H	**2.08479961**	**2.04258555**	**-4.23686982**
H	**-2.57349003**	**1.21732146**	**-3.19545428**
H	**-0.23656710**	**2.11801924**	**-4.56926086**
H	**-4.86228271**	**1.81218760**	**1.22223170**
C	**-0.64776415**	**-4.63035777**	**1.99242649**
H	**-0.33835791**	**-5.54793895**	**2.47283741**
H	**-4.49347686**	**2.25593130**	**-1.52531003**
C	**-1.08429992**	**-4.86188234**	**0.53965979**
O	**-2.19048146**	**-4.01587926**	**0.23695188**

C	**-1.53709731**	**-6.31089136**	**0.27830073**
H	**-0.28495916**	**-4.63525107**	**-0.15130441**
C	**-3.33599992**	**-4.81152213**	**-0.16705590**
C	**-2.69793863**	**-6.09516167**	**-0.68053034**
H	**-0.74199103**	**-6.90765248**	**-0.14119236**
H	**-3.93441472**	**-5.01500666**	**0.71118783**
H	**-2.32373305**	**-5.92646631**	**-1.68666351**
O	**-2.00406396**	**-6.86692118**	**1.49154382**
H	**-2.55190211**	**-7.61318281**	**1.27343072**
O	**-3.55776381**	**-7.20498501**	**-0.63778446**
H	**-4.27247378**	**-7.07879211**	**-1.24920485**
N	**-4.12933451**	**-4.15572864**	**-1.13435910**
H	**-4.81174403**	**-3.50401458**	**-0.81962511**
C	**0.52752092**	**6.96559929**	**-2.03172419**
C	**-1.36012841**	**6.17278329**	**-1.19534420**
C	**0.68314137**	**5.66780955**	**-1.65731647**
H	**-2.37286412**	**6.13532812**	**-0.87273817**
N	**-0.78188267**	**7.28330143**	**-1.73026673**
N	**-0.51160274**	**5.18754733**	**-1.13826079**
H	**-1.21987844**	**8.15831136**	**-1.88379957**
H	**-2.07603114**	**3.84716940**	**1.54215956**
H	**1.19976495**	**7.66032858**	**-2.47326281**
H	**1.54848693**	**5.05508209**	**-1.72118393**
S	**0.72687536**	**-3.46412784**	**2.25801050**
C	**0.35146009**	**-1.97044674**	**1.29657111**
H	**-0.50249547**	**-1.51659576**	**1.76171527**
H	**0.12581097**	**-2.17486103**	**0.27144312**
H	**1.17682948**	**-1.28635021**	**1.36648495**

C	**2.15367058**	**-4.27956194**	**1.47582937**
H	**2.96987727**	**-4.11824596**	**2.16213787**
H	**1.89916278**	**-5.32701538**	**1.48192973**
C	**2.50764465**	**-3.84196940**	**0.04634805**
H	**2.95781467**	**-2.85284822**	**0.03692394**
H	**1.61507027**	**-3.78272377**	**-0.55338387**
C	**3.39859445**	**-4.85260269**	**-0.66222081**
H	**3.49476183**	**-4.58426590**	**-1.70484816**
C	**2.88582223**	**-6.34637534**	**-0.60913269**
N	**4.81561418**	**-4.92916352**	**-0.11314279**
H	**4.84725157**	**-4.79042066**	**0.87710553**
H	**5.03417708**	**-5.92297110**	**-0.30489493**
O	**3.82118641**	**-7.15199214**	**-0.57627872**
O	**1.66709527**	**-6.46246730**	**-0.60500881**
H	**-3.68407789**	**-3.89585816**	**-1.98688164**
H	**5.46252701**	**-4.30366279**	**-0.54304639**
H	**-1.47024582**	**-4.22114024**	**2.55356763**

Figure S1. The active space orbitals surfaces, energy, and their electronic density population at the beginning of the CASSCF geometry optimization of the homocysteine negative ion methylcob(II)alamin cofactor and histidine common model: a) The Co-C bond distance is equal to 2.08 Å; b) The Co-N bond distance is equal to 2.35 Å.

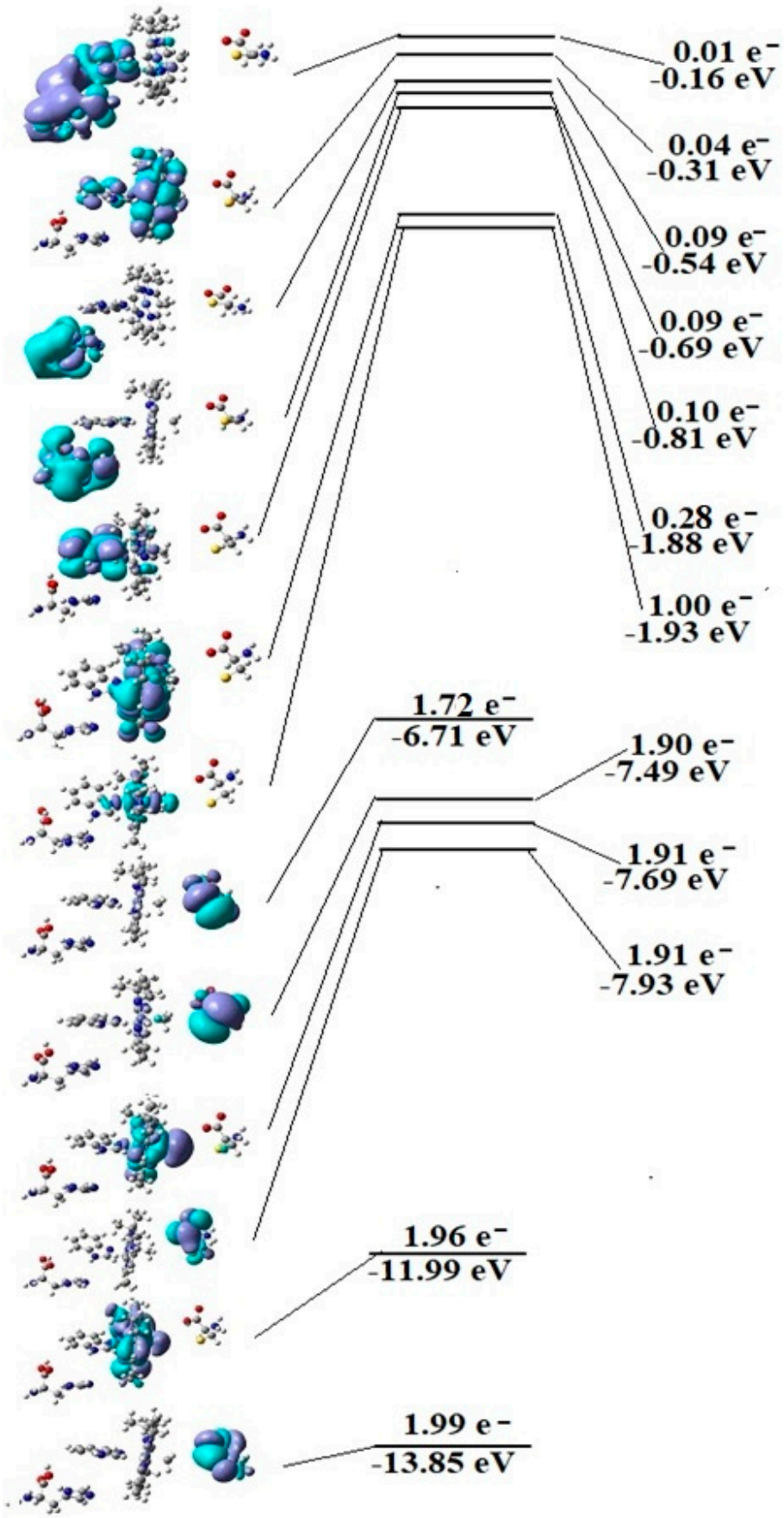
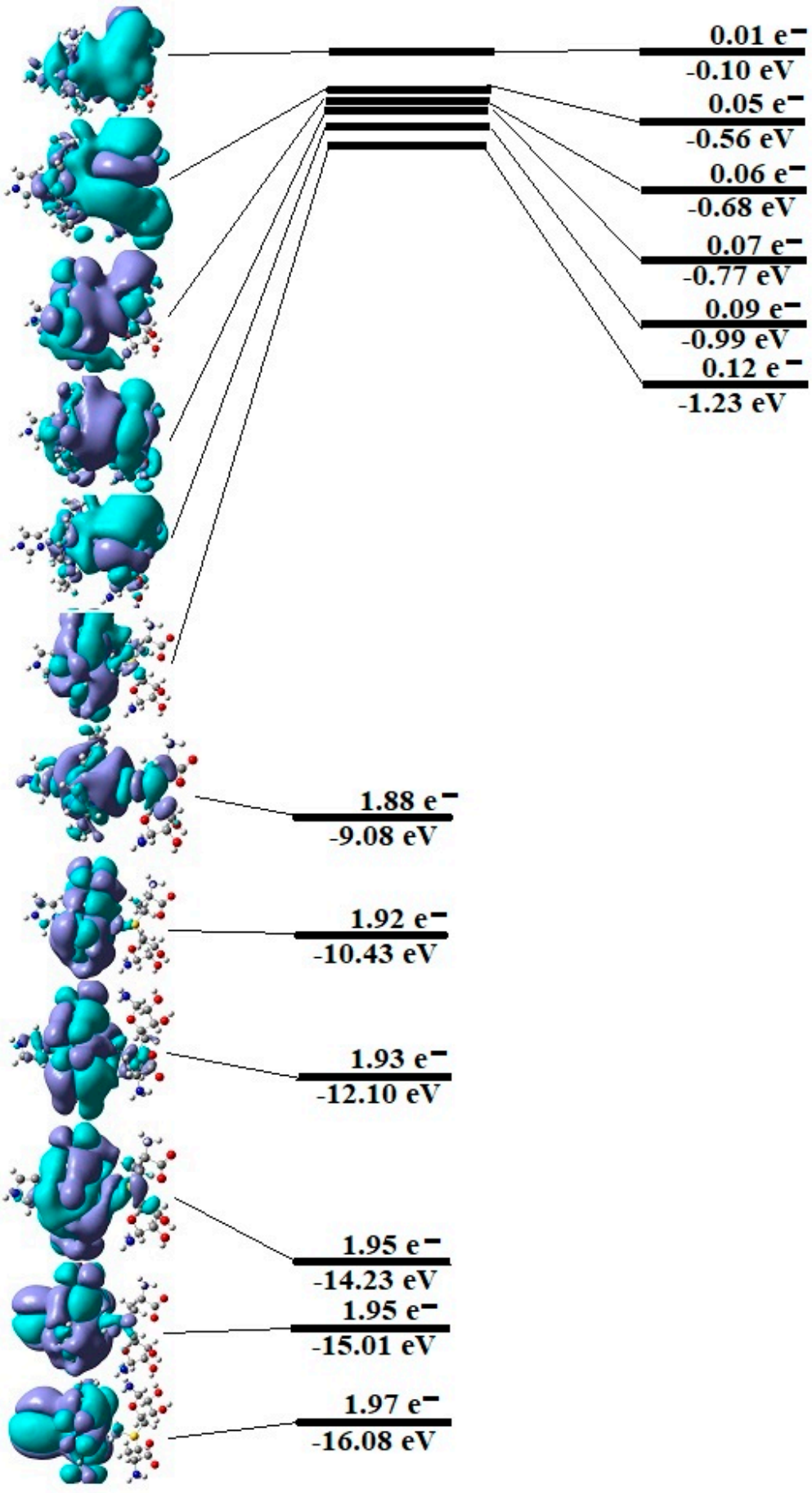

0.01 e⁻
-0.16 eV
0.04 e⁻
-0.31 eV
0.09 e⁻
-0.54 eV
0.09 e⁻
-0.69 eV
0.10 e⁻
-0.81 eV
0.28 e⁻
-1.88 eV
1.00 e⁻
-1.93 eV
1.72 e⁻
-6.71 eV
1.90 e⁻
-7.49 eV
1.91 e⁻
-7.69 eV
1.91 e⁻
-7.93 eV
1.96 e⁻
-11.99 eV
1.99 e⁻
-13.85 eV

Figure S2. The active space orbitals surfaces, energy, and their electronic density population at the beginning of the CASSCF geometry optimization of the inactive particle of the cob(II)alamin cofactor and Adomet substrate common model. The Co-N bond distance is equal to 4.00 Å.


0.01 e⁻
-0.10 eV
0.05 e⁻
-0.56 eV
0.06 e⁻
-0.68 eV
0.07 e⁻
-0.77 eV
0.09 e⁻
-0.99 eV
0.12 e⁻
-1.23 eV
1.88 e⁻
-9.08 eV
1.92 e⁻
-10.43 eV
1.93 e⁻
-12.10 eV
1.95 e⁻
-14.23 eV
1.95 e⁻
-15.01 eV
1.97 e⁻
-16.08 eV