Multiscale analysis of enantioselectivity in enzyme-catalysed 'lethal synthesis' using projector-based embedding

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1 Example input file for the generation of Projection-based embedding profiles with QM/MM

```
memory,500, m

geomtyp=xyz
nosym
noorient

geometry={
C1      -11.443994    13.530871     6.095726
C2      -12.615096    13.486453     5.089573
O3      -12.671857    12.450378     4.348016
O4      -13.430702    14.447066     5.075337
H5      -10.650551    12.835197     5.811858
H6      -11.818585    13.266354     7.090616
S7      -10.925788    11.825331     1.175627
C8      -12.619528    11.279574     1.352945
O9      -12.934846    10.086439     1.209463
C10     -13.531530    12.315282     1.834446
F11     -14.862996    11.935817     1.636166
H12     -13.361275    13.300507     1.382042
H13     -13.258648    12.428756     3.079395
C14     -10.092723    10.245621     1.547309
H15      -9.020619    10.432246     1.456436
H16     -10.359972     9.488339     0.810288
C17     -14.072663    13.444345    -2.071347
O18     -14.232385    14.586944    -1.555392
O19     -14.958103    12.697051    -2.546950
C20     -12.612932    12.910579    -2.146510
O21     -11.667764    13.680893    -2.045564
C22     -12.391333    11.432316    -2.358710
C23     -11.955042    11.047501    -3.788249
O24     -11.685646     9.818408    -3.973958
O25     -11.886566    11.944357    -4.665387
H26     -11.586959    11.120745    -1.683309
```

```
H27      -13.291369    10.861090    -2.119560
H28      -11.035825    14.561474     6.157823
H29      -10.336244     9.927175     2.565521
}
#Import the MM point charges for QM/MM, in this case a file called lattice
lattice,infile=lattice.

#Define the basis set.
basis={
default,aug-cc-pvdz
}

#Run initial low level method, any functional can be used here.
{ks,b3lyp,direct;wf,156,1,0}
#localise the orbitals.
{ibba,bonds=1,iborth='ZBD'}
#Run the projection embedding code.
{embed,proj,n_orbitals=40,aotrunc,denkeep=0.0001;atoms,C8,O9,C10,H12,H13,F11,O3,C2,O4
#Run the post embedding low-level method to determine type-in-type error.
{ks,b3lyp,direct;wf,80,1,0}
#Run pre-correlation mean field, usually HF.
{hf,direct;wf,80,1,0}
#Run the High-level correlation method.
{ccsd(t);core,5;wf,80,1,0}
```