Electronic Supplementary Information for Quantum chemical (QM:MM) investigation on the mechanism of enzymatic reaction of tryptamine and N,N-dimethyltryptamine by monoamine oxidase A

Károly Kubicskó, Ödön Farkas

Table 1 Geometry optimization results at ONIOM(M06-2X/6-31++G(d,p):UFF=QEq) level. The $E^{\mathrm{Total}}_{\mathrm{opt,freq}}$ total energies, $\Delta E^{\ddagger}_{\mathrm{opt,freq}}$ activation energy barriers, lowest computed IR $\tilde{\nu}$ wavenumbers are shown for structures of reactant complexes (**RCs**) and product complexes (**PCs**). The frequency analysis of the optimized structures proved that **RCs** and **PCs** have real frequency modes, each **TS** structure has only one imaginary frequency. In case of structures of transition states (**TSs**), the imaginary wavenumbers are listed. The $G^{\mathrm{Corr}}_{\mathrm{opt,freq}}$ corrections to Gibbs free energies are also listed

Fig 7. subfigures	Label of structure	$E^{\mathrm{Total}}_{\mathrm{opt,freq}}/[\mathrm{Eh}]$	$\Delta E^{\ddagger}_{\mathrm{opt,freq}}/[\mathrm{kcal\cdot mol^{-1}}]$	$\tilde{\nu}/[\mathrm{cm^{-1}}]$	$G^{\mathrm{Corr}}_{\mathrm{opt,freq}}/[\mathrm{Eh}]$
(a)	$\mathbf{RC^{T}_{FAD}}$	-976.0258821		29.8206	2.6105970
(b)	$\mathbf{TS^{T}_{FAD}}$	-975.9714394	34.1633173	1101.9649 i	2.6065480
(c)	$\mathbf{PC^{imT^{+}}_{FADH^{-}}}$	-976.0080617		15.9576	2.6150790
(d)	$\mathbf{RC^{T}_{FADH^{+}}}$	-976.4871783		29.8279	2.6253510
(e)	$\mathbf{TS^{T}_{FADH^{+}}}$	-976.4551260	20.1131262	1338.5083 i	2.6217110
(f)	$\mathbf{PC^{imT^{+}}_{FADH_2}}$	-976.5130532		37.8155	2.6227840
(g)	$\mathbf{RC^{DMT}_{FAD}}$	-1054.6004033		27.0436	2.6690840
(h)	$\mathbf{TS^{DMT}_{FAD}}$	-1054.5541290	29.0375679	1215.6165 i	2.6659600
(i)	$\mathbf{PC^{imDMT^{+}}_{FADH^{-}}}$	-1054.5938877		30.5310	2.6707080
(j)	$\mathbf{RC^{DMT}_{FADH^{+}}}$	-1055.0670350		32.5769	2.6835630
(k)	$\mathbf{TS^{DMT}_{FADH^{+}}}$	-1055.0383041	18.0289158	1346.7944 i	2.6810490
(l)	$\mathbf{PC^{imDMT^{+}}_{FADH_2}}$	-1055.0995307		33.3502	2.6835950

Table 2 The ESI contains Gaussian input files for single point energy computation at ONIOM(M06-2X/6-311++G(3df,3pd):UFF=QEq) level using the optimized structures at ONIOM(M06-2X/6-31++G(d,p):UFF=QEq) level. The $E^{\mathrm{Total}}_{\mathrm{spe}}$ single point energies at the optimized geometries were calculated at ONIOM(M06-2X/6-311++G(3df,3pd):UFF=QEq) level. The G^{Total} Gibbs free energies were calculated using the $G^{\mathrm{Total}} = E^{\mathrm{Total}}_{\mathrm{spe}} + G^{\mathrm{Corr}}_{\mathrm{opt,freq}}$ formula. The $\Delta G^{\ddagger}$ activation Gibbs free energies are listed

Fig 7. subfigures	Label of structure	Gaussian input file of structure	$E^{\mathrm{Total}}_{\mathrm{spe}}/[\mathrm{Eh}]$	$G^{\mathrm{Total}}/[\mathrm{Eh}]$	$\Delta G^{\ddagger}/[\mathrm{kcal\cdot mol^{-1}}]$
(a)	$\mathbf{RC^{T}_{FAD}}$	RC_FAD_T.gjf	-976.4907860	-973.8801890	
(b)	$\mathbf{TS^{T}_{FAD}}$	TS_FAD_T.gjf	-976.4349315	-973.8283835	32.5084490
(c)	$\mathbf{PC^{imT^{+}}_{FADH^{-}}}$	PC_FADH-_imT+.gjf	-976.4726010	-973.8575220	
(d)	$\mathbf{RC^{T}_{FADH^{+}}}$	RC_FADH+_T.gjf	-976.9543955	-974.3290445	
(e)	$\mathbf{TS^{T}_{FADH^{+}}}$	TS_FADH+_T.gjf	-976.9209932	-974.2992822	18.6761292
(f)	$\mathbf{PC^{imT^{+}}_{FADH_2}}$	PC_FADH2_imT+.gjf	-976.9815615	-974.3587775	
(g)	$\mathbf{RC^{DMT}_{FAD}}$	RC_FAD_DMT.gjf	-1055.0868814	-1052.4177974	
(h)	$\mathbf{TS^{DMT}_{FAD}}$	TS_FAD_DMT.gjf	-1055.0395001	-1052.3735401	27.7718810
(i)	$\mathbf{PC^{imDMT^{+}}_{FADH^{-}}}$	PC_FADH-_imDMT+.gjf	-1055.0820594	-1052.4113514	
(j)	$\mathbf{RC^{DMT}_{FADH^{+}}}$	RC_FADH+_DMT.gjf	-1055.5555831	-1052.8720201	
(k)	$\mathbf{TS^{DMT}_{FADH^{+}}}$	TS_FADH+_DMT.gjf	-1055.5262704	-1052.8452214	16.8164417
(l)	$\mathbf{PC^{imDMT^{+}}_{FADH_2}}$	PC_FADH2_imDMT+.gjf	-1055.5905275	-1052.9069325	