

mISOFORM 1	mISOFORM 1	PIE	ΔE^{es}	ΔE^{ex}	ΔE^{ct+mix}	ΔE^{di}	ΔG^{sol}
THR472	ILE474	-11.216	-7.074	3.504	-2.638	-4.119	-0.890
GLY473	GLU478	-4.675	-4.573	0.000	0.000	0.000	-0.102
ILE474	GLU476	-6.971	-3.625	0.502	-1.161	-1.557	-1.130
	GLU479	-6.370	-4.171	0.919	-0.937	-1.719	-0.462
GLU476	ARG480	-15.023	-50.706	0.002	-0.012	-0.512	36.205
GLU477	ARG480	-22.321	-60.466	4.925	-2.696	-4.273	40.189
	SER481	-9.035	-4.296	0.026	-0.299	-0.626	-3.840
GLU478	ARG480	-13.600	-26.281	0.329	-0.868	-1.735	14.954
	SER481	-24.402	-20.429	8.232	-3.539	-4.987	-3.679
	GLN482	-16.224	-12.205	0.320	-0.351	-1.352	-2.636
GLU479	SER481	-10.914	-6.700	0.534	-1.642	-1.866	-1.240
	GLN482	-20.027	-11.410	4.671	-3.016	-4.725	-5.545
ARG480	GLU483	-12.545	-36.423	6.620	-4.233	-5.712	27.202
SER481	GLU483	-8.896	-3.052	0.874	-1.177	-2.233	-3.307

1 **Table 1.** PIEDA of mANO2 isoform 1 dimer

2 All energies are expressed in kcal/mol. The calculation had an FMO-MP2/6-31G**/PCM level.

mISOFORM 2	mISOFORM 2	PIE	ΔE^{es}	ΔE^{ex}	$\Delta E^{\text{ct+mix}}$	ΔE^{di}	ΔG^{sol}
THR472	ILE474	-11.159	-7.046	2.371	-2.836	-3.752	0.103
ILE474	GLU476	-3.818	-2.704	1.365	-1.541	-2.380	1.442
GLU478	HIS480	-4.012	0.227	0.038	-0.453	-0.908	-2.917
GLU479	SER481	-3.000	3.072	0.013	-0.792	-0.901	-4.391

1 **Table 2.** PIEDA of mANO2 isoform 2 dimer

2 All energies are expressed in kcal/mol. The calculation has the FMO-MP2/6-31G**/PCM level.