Supporting Information

An electrostatic duel: subtle differences in catalytic performance of monoamine oxidase A and B isoenzymes elucidated at a residue level by quantum computations

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S1. Scheme of the rate-limiting step for the reaction between phenylethylamine (PEA) and the truncated monoamine oxidase (MAO) cofactor, lumiflavin (LFN). The reaction was modeled based on the presumed hydride transfer mechanism. More details about the reaction and its mechanism can be found in our previous work.[1-4]
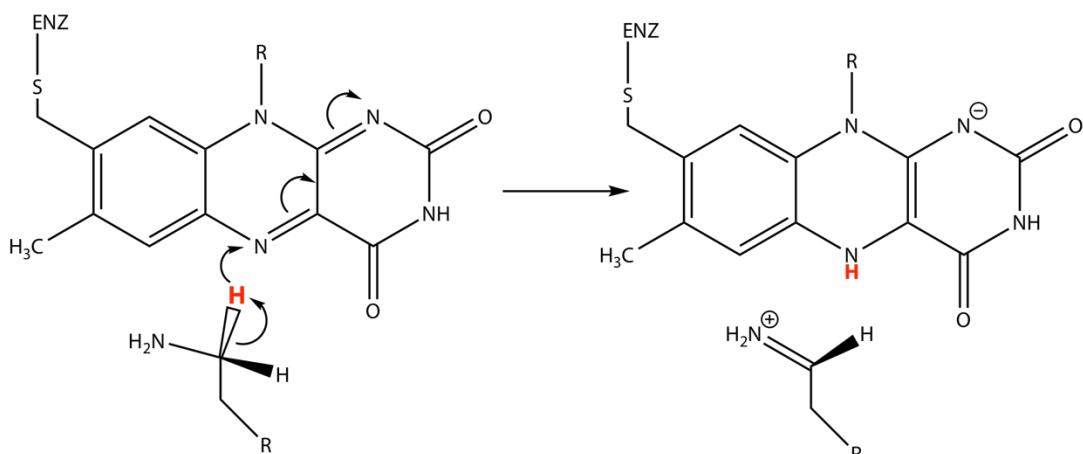
S2. Details on simulation of reactions.

Representative geometries of our system were derived from preceding molecular dynamics simulations of the rate-limiting step of PEA oxidation by the monoamine oxidase enzyme. For the MAO A isoenzyme, the simulation details were published in our previous work.[2] The simulations were based on crystallographic structures of both MAO enzymes, deposited in the Protein Data Bank (ID code 2Z5X for MAO A and 1GOS for MAO B). We used the OPLS-AA force field[5-7] for the description of our system, which was enclosed by a spherical simulation cell (30 Å radius, centered on the reacting N atom of the flavin cofactor), encompassing the enzyme with a manually docked PEA molecule and roughly 1900 water molecules. Both systems were primarily relaxed in 10 distinctive steps, where the temperature was slowly raised from 1 K to 300 K, the timestep was gradually increased from 0.1 fs to 1 fs and the restraints on the reactive subsystem were slowly relaxed. It is important to note that special care was taken in order to dock the PEA molecule as similarly as possible into both active sites (i.e., achieve a similar relative position of PEA to the flavin cofactor), so as to minimize the variation between the isoenzymes.

The simulation of the reaction was based on the Free Energy Perturbation/Umbrella Sampling approach,[8-9] along with the Empirical Valence Bond (EVB) protocol[10-12] in order to calculate the

pertinent free energy profiles. The force field of the reactants was linearly transformed into the force field of the products in 51 steps *via* the following equation:

$$H(\lambda) = \lambda \cdot H_R + (1 - \lambda) \cdot H_P,$$

where the coupling parameter λ was varied from 1 (reactants) to 0 (products). For both isoenzymes, 10 independent replicas were generated, all with 51 λ-steps of 10 ps. The EVB methodology was used to generate free energy profiles and calculate the average free energy barrier for both isoenzymes. As is common with the EVB protocol, the free energy profiles for the reaction in the enzyme were generated by using parameters derived from gas phase simulations of the reaction between PEA and LFN, described in our previous work.[13]

The calculated difference of 1.27 kcal/mol between the barriers of both isoenzymes was in excellent agreement with the experimentally determined difference of 1.28 kcal/mol. All simulations and free-energy calculations were performed with the *Q5* software package.[14]

Structures of our system corresponding to the state of reactants and the transition state were identified from the free energy profiles and extracted from the molecular dynamics trajectories.

S3. Details on evaluation of the effect of electrostatic environment.

The first value we calculated was the energy barrier difference, which is determined by the following equation:

$$\Delta E = E_{OFF} - E_{ON} = \left(\langle E_{OFF}^{TS} \rangle_{snapshots} - \langle E_{OFF}^{R} \rangle_{snapshots} \right) - \left(\langle E_{ON}^{TS} \rangle_{snapshots} - \langle E_{ON}^{R} \rangle_{snapshots} \right),$$

where E_{OFF} is the energy difference between the transition state (TS) and the state of reactants (R) when the charges are turned "OFF" (i.e., not present) and E_{ON} is the energy difference between the transition state (TS) and the state of reactants (R) when the charges are turned "ON" (i.e., present). All values were averaged over 100 snapshots.

For both isoenzymes, the inclusion of the electrostatic environment (charges "ON") results in a lower energy barrier compared to the state with charges "OFF". This barrier lowering effect amounts to 14.22 kcal/mol in the MAO A enzyme and 17.54 kcal/mol in MAO B, which means that the inclusion of the electrostatic environment lowers the barrier by 3.32 kcal/mol more in the MAO B isoenzyme. This is in fairly good agreement with the experimental values reported, where the free energy barrier for this reaction is 1.28 kcal/mol lower in the MAO B isoenzyme than in MAO A.[15]

In a similar manner to the calculated energy barrier difference, the influence of the electrostatic environment on the charge transfer between the two reacting moieties during the transition from R to TS was determined using the Natural Bond Orbital method. The charge transfer is defined as the difference between the sum of the atomic charges of all PEA atoms in the transition state and in the reactant state. The value given in Table 1 represents the increase in charge transfer when the electrostatic environment is included – i.e., in the state with the charges ON the amount of charge transferred is increased in both isoenzymes by 0.156 and 0.184 a. u., respectively. As mentioned above, the presumed mechanism of this rate-limiting step is hydride transfer from PEA to LFN, which means that negative charge is transferred from PEA to LFN. Therefore, an increase in the amount of charge transferred reflects an enhancement of the reaction due to the presence of the electrostatic environment. As evident with the energy barrier and in agreement with the experimental data, this increase in charge transfer when the electrostatic environment is included is more pronounced in the isoenzyme MAO B than in isoenzyme MAO A (by about 0.03 charge units).

Consistent with the increased charge transfer, the difference in dipole moments of TS and R of the reacting moiety also increases upon inclusion of the electrostatic environment in both isoenzymes. Again, this increase is more pronounced in the MAO B isoenzyme compared to the MAO A isoenzyme by about 0.4 D.

Next, we considered the HOMO-LUMO gap between the two frontier molecular orbitals relevant to this reaction, i.e., the HOMO of PEA and the LUMO of LFN. A narrower HOMO-LUMO gap indicates higher reactivity between the two molecules. Again, the inclusion of the electrostatic environment (charges turned ON) in both isoenzymes causes the HOMO-LUMO gap to become narrower when going from R to TS. And in line with other parameters, this gap-narrowing effect is more pronounced (by about 23 %) in the MAO B isoenzyme.

S4. A more detailed version of Table 1. The experimental enzymatic free energy barrier is given for both isoenzymes. In addition, the calculated energy barriers for both enzymes and both states (charges ON and OFF) are given, as well as their differences (i.e., the barrier lowering effect of the enzymatic environment). For the charge transfer, dipole moment and HOMO-LUMO gap, the calculated values are given for both R and TS with charges turned ON or OFF in both enzymes (all values are averaged over 100 snapshots).

	MAO A				MAO B			
	ON		OFF		ON		OFF	
	R	TS	R	TS	R	TS	R	TS
$\Delta G^{\ddagger}_{exp}$ [kcal/mol]	18.57				17.29			
energy barrier [kcal/mol]	26.09		40.31		19.71		37.25	
	14.22				17.54			
charge transfer [a. u.]	0.0132	0.5617	0.0076	0.4001	0.0206	0.6109	0.0130	0.4191
	0.549		0.393		0.5903		0.4062	
	0.156				0.184			
dipole moment [D]	14.34	15.90	10.62	11.34	13.04	14.88	10.35	10.98
	1.56		0.72		1.84		0.63	
	0.84				1.21			
HOMO-LUMO gap [a. u.]	0.2037	0.1399	0.2147	0.1731	0.1988	0.1293	0.2152	0.1723
	0.0638		0.0416		0.0695		0.0429	
	0.022				0.027			

S5. Alignment of primary sequences of MAO A and MAO B isoenzymes. Amino acid residues marked in blue font color are positively charged, while residues marked in red are negatively charged. Green squares represent residue pairs where the MAO A residue is more catalytic, while orange squares mean the opposite. A lighter color denotes that $\left|\Delta\Delta G^{\ddagger}_{elec}(x)\right| > 0.05$, while a stronger color means that $\left|\Delta\Delta G^{\ddagger}_{elec}(x)\right| > 0.1$.

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MAOA   --HMFDVVVIGGGISGLSAAKLLTEYGVSVLVLEARDRVGGRTYTIRNEHVDYVDVGGAY
MAOB   MSNKCDVVVVGGGISGMAAAKLLHDSGLNVVVLEARDRVGGRTYTLRNQKVKYVDLGGSY

MAOA   VGPTQNRILRLSKELGIETYKVNVSERLVQYVKGKTYPFRGAFPPVWNPIAYLDYNNLWR
MAOB   VGPTQNRILRLAKELGLETYKVNEVERLIHHVKGKSYPFRGPFPPVWNPITYLDHNNFWR

MAOA   TIDNMGKEIPTDAPWEAQHADKWDKMTMKELIDKICWTKTARRFAYLFVNINVTSEPHEV
MAOB   TMDDMGREIPSDAPWKAPLAEEWDNMTMKELLDKLCWTESAKQLATLFVNLCVTAETHEV

MAOA   SALWFLWYVKQCGGTTRIFSVTNGGQERKFVGGSGQVSERIMDLLGDQVKLNHPVTHVDQ
MAOB   SALWFLWYVKQCGGTTRIISTTNGGQERKFVGGSGQVSERIMDLLGDRVKLERPVIYIDQ

MAOA   SSDNIIIETLNHEHYECKYVINAIPPTLTAKIHFRPELPAERNQLIQRLPMGAVIKCMMY
MAOB   TRENVLVETLNHEMYEAKYVISAIPPTLGMKIHFNPPLPMMRNQMITRVPLGSVIKCIVY

MAOA   YKEAFWKKKDYCGCMIIEDEDAPISITLDDTKPDGSLPAIMGFILARKADRLAKLHKEIR
MAOB   YKEPFWRKKDYCGTMIIDGEEAPVAYTLDDTKPEGNYAAIMGFILAHKARKLARLTKEER

MAOA   KKKICELYAKVLGSQEALHPVHYEEKNWCEEQYSGGCYTAYFPPGIMTQYGRVIRQPVGR
MAOB   LKKLCELYAKVLGSLEALEPVHYEEKNWCEEQYSGGCYTTYFPPGILTQYGRVLRQPVDR

MAOA   IFFAGTETATKWSGYMEGAVEAGERAAREVLNGLGKVTEKDIWVQEPESKDVPAVEITHT
MAOB   IYFAGTETATHWSGYMEGAVEAGERAAREILHAMGKIPEDEIWQSEPESVDVPAQPITTT

MAOA   FWERNLPSVSGLLKIIGFSTSV--TALGFVLYKYKLL---
MAOB   FLERHLPSVPGLLRLIGLTTIFSATALGFLAHKRGLLVRV
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S6. Difference in contributions to the barrier change $\Delta G^{\ddagger}_{elec}(x)$ (based on the interaction between the dipole moment of the reacting moiety and the electric field exerted by the enzymatic environment) between MAO A and MAO B, as a function of the average distance from the reacting moiety. Note that a negative value indicates that the MAO B residue is more catalytic of the two, while for the positive value the opposite is true. Red crosses mark residue pairs where at least one of the two residues is charged, while violet crosses mark pairs where both residues are neutral.
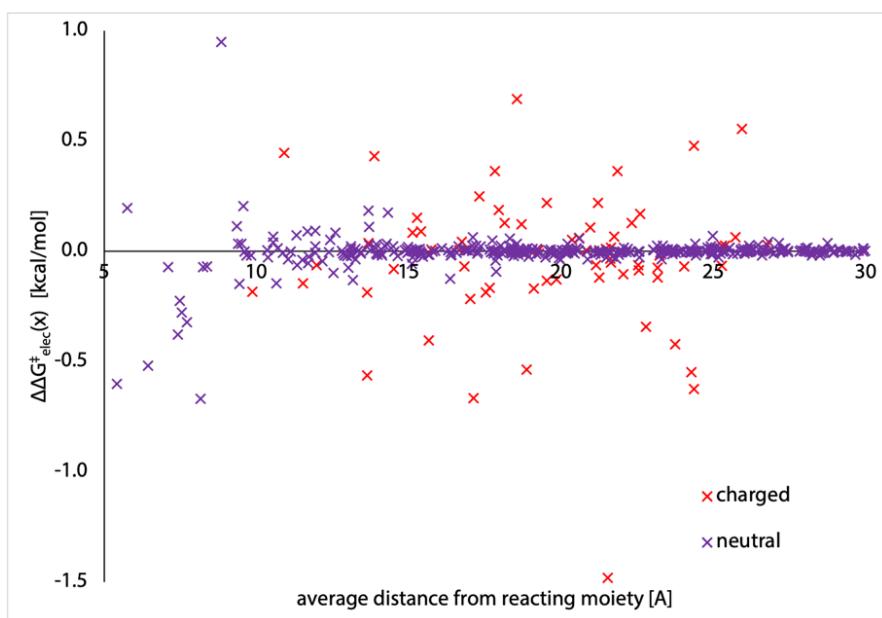
S7. List of all MAO A and MAO B residue pairs with corresponding calculated $\Delta G^{\ddagger}_{elec}(x)$ values. The name and residue number of all residues is given, as well as the average distance of the residue from the reacting moiety and its individual $\Delta G^{\ddagger}_{elec}(x)$ contribution, based on the interaction between the electric field of the enzymatic environment and the dipole moment of the reacting moiety. A negative value of $\Delta G^{\ddagger}_{elec}(x)$ denotes the lowering of the barrier (a catalytic effect of the residue), while the opposite is true for a positive value of $\Delta G^{\ddagger}_{elec}(x)$. Finally, the difference in $\Delta G^{\ddagger}_{elec}(x)$ i.e., $\Delta\Delta G^{\ddagger}_{elec}(x)$ between the isoenzymes is calculated. A negative value in this case means that the MAO B residue provides a more significant lowering of the barrier than the corresponding MAO A residue and vice versa for the positive value. Entries are sorted by $\Delta\Delta G^{\ddagger}_{elec}(x)$. The red lines are drawn at ±0.1 kcal/mol.

res name MAO A	res ID MAO A	dist. MAO A [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO B [kcal/mol]	$\Delta\Delta G^{\ddagger}_{elec}(x)$ [kcal/mol]
ASN	181	8.64	-1.51	CYS	172	9.06	-0.57	0.95
ASP	359	19.24	-0.11	ARG	350	17.88	0.58	0.69
ASN	241	26.29	-0.02	GLU	232	25.60	0.54	0.55
ASH	343	24.43	-0.01	GLU	334	24.32	0.47	0.48
ASP	64	11.15	2.93	ASP	55	10.66	3.37	0.44
ASP	339	14.25	1.42	ASP	330	13.49	1.85	0.43
GLU	399	18.17	0.32	GLU	390	17.49	0.68	0.36
LYS	370	22.25	-0.39	LEU	361	21.47	-0.02	0.36
ARG	76	17.95	-0.03	ARG	67	16.66	0.21	0.25
GLU	329	20.19	-0.80	GLU	320	22.22	-0.58	0.22
GLU	228	19.95	1.06	GLU	219	19.13	1.28	0.22
MET	350	9.43	-0.35	MET	341	9.70	-0.15	0.20
GLY	67	5.90	-2.13	GLY	58	5.60	-1.94	0.20
GLU	185	17.91	-0.86	GLU	176	18.00	-0.68	0.18
TYR	53	13.72	-0.05	TYR	44	13.63	0.14	0.18
CYS	323	14.19	-0.03	THR	314	14.45	0.14	0.17
ASP	46	22.89	0.71	ASP	37	22.33	0.88	0.17
GLU	400	15.30	1.20	GLU	391	15.25	1.35	0.15
LYN	372	22.34	-0.03	LYS	363	22.29	0.10	0.13
LYS	90	18.35	-0.05	LYS	81	17.93	0.08	0.13
LYS	199	18.76	0.73	LYS	190	18.62	0.85	0.12
THR	183	9.47	0.21	THR	174	9.26	0.32	0.11
ALA	409	13.40	-0.13	THR	400	14.01	-0.02	0.11
GLU	43	21.12	0.86	GLU	34	20.80	0.97	0.11
VAL	65	11.58	-0.06	LEU	56	12.27	0.03	0.09
GLN	74	11.81	0.43	GLN	65	11.56	0.52	0.09
ARG	206	15.27	0.77	ARG	197	15.54	0.85	0.09
ARG	217	15.28	-0.22	ARG	208	14.95	-0.13	0.08
THR	336	12.19	-0.34	THR	327	12.99	-0.26	0.08
SER	223	11.76	-0.20	SER	214	10.86	-0.13	0.07
HID	488	24.01	-0.04	THR	479	25.96	0.03	0.07
LYS	316	21.46	-0.31	ARG	307	22.03	-0.24	0.07
GLY	351	10.66	0.24	GLY	342	10.45	0.31	0.07
TYR	62	17.04	-0.09	TYR	53	17.16	-0.03	0.06
ASP	232	25.92	0.49	ASP	223	25.55	0.55	0.06
GLU	453	20.71	0.27	GLU	444	20.49	0.33	0.06
THR	340	18.53	-0.02	THR	331	18.08	0.04	0.06
GLN	99	20.13	0.00	HIE	90	21.08	0.06	0.06
GLY	301	12.74	0.18	GLY	292	12.09	0.23	0.05
GLU	87	20.76	0.53	GLU	78	19.96	0.58	0.05
ASN	212	17.88	-0.08	ASN	203	17.60	-0.03	0.05
GLU	393	16.70	0.99	GLU	384	16.80	1.03	0.04
ASH	162	26.32	0.00	ASH	153	27.30	0.04	0.04
LEU	354	10.49	0.14	LEU	345	10.61	0.18	0.04
GLH	492	26.54	-0.04	GLH	483	27.78	0.00	0.04
GLU	436	13.69	-0.05	GLU	427	13.65	-0.01	0.04
GLN	418	28.88	0.00	GLN	409	28.61	0.03	0.04
VAL	303	9.77	0.06	VAL	294	9.02	0.10	0.03
VAL	48	18.61	0.01	VAL	39	18.48	0.05	0.03
THR	408	9.55	-0.08	THR	399	9.46	-0.05	0.03
GLN	474	24.80	0.00	SER	465	24.01	0.03	0.03
GLN	401	20.27	-0.03	GLN	392	20.15	0.00	0.03
ILE	333	14.37	0.01	VAL	324	14.19	0.04	0.03
GLY	49	13.91	0.12	GLY	40	13.94	0.15	0.03
THR	417	26.86	0.00	THR	408	26.09	0.03	0.03
PHE	177	13.54	-0.36	PHE	168	13.85	-0.33	0.03
GLU	458	26.81	-0.02	GLH	449	26.74	0.00	0.03
SER	345	23.53	0.02	ASN	336	23.16	0.05	0.03
ARG	457	25.61	-0.13	ARG	448	25.16	-0.10	0.03
GLU	367	25.36	0.29	GLU	358	25.19	0.31	0.03
SER	81	17.36	-0.05	ALA	72	17.07	-0.03	0.02
LEU	294	23.02	-0.01	MET	285	23.28	0.01	0.02
THR	211	17.17	-0.05	THR	202	17.00	-0.03	0.02
ASN	92	18.26	-0.05	ASN	83	17.77	-0.03	0.02
ASN	125	26.09	-0.03	ASN	116	26.25	-0.01	0.02
THR	105	24.51	0.01	SER	96	25.32	0.03	0.02
GLY	447	11.98	0.03	GLY	438	11.88	0.06	0.02
GLY	50	13.08	0.09	GLY	41	13.13	0.12	0.02
VAL	178	14.34	-0.33	VAL	169	14.64	-0.31	0.02
ALA	355	14.45	0.08	ALA	346	14.02	0.10	0.02
PRO	186	18.11	0.01	THR	177	18.61	0.03	0.02
GLN	147	31.55	-0.01	PRO	138	30.32	0.01	0.02
THR	204	16.37	-0.11	THR	195	16.90	-0.09	0.02
ASN	75	17.55	0.05	ASN	66	17.15	0.07	0.02
ASN	396	15.22	0.06	ASN	387	14.73	0.08	0.02
ASN	133	25.44	0.00	ASH	124	25.62	0.02	0.02
ARG	454	21.83	0.04	ARG	445	21.46	0.05	0.02
HID	388	28.02	-0.01	HID	379	28.15	0.00	0.02
GLH	375	24.71	-0.02	GLH	366	25.42	0.00	0.02
LYN	136	24.77	0.01	ARN	127	24.84	0.02	0.02
ASN	57	22.08	-0.01	ASN	48	22.05	0.01	0.01
PRO	347	20.74	0.00	ALA	338	20.30	0.01	0.01
GLN	200	13.90	0.34	GLN	191	13.92	0.35	0.01
VAL	473	25.26	-0.01	GLN	464	25.23	0.01	0.01
SER	38	33.04	-0.01	ASN	29	33.82	0.00	0.01
LYN	151	30.39	0.00	GLH	142	30.10	0.01	0.01
TRP	397	10.78	0.01	TRP	388	10.61	0.03	0.01
TYR	89	16.33	0.11	TYR	80	15.85	0.13	0.01
GLY	21	18.75	0.02	GLY	12	18.12	0.03	0.01
LEU	298	18.53	0.03	VAL	289	19.24	0.05	0.01
GLY	414	25.73	0.01	GLY	405	25.28	0.02	0.01
TYR	106	25.50	-0.02	TYR	97	26.47	-0.01	0.01
GLH	290	29.80	-0.01	MET	281	30.03	0.00	0.01
TRP	166	32.33	0.00	TRP	157	32.61	0.01	0.01
ARN	493	29.79	0.00	ARN	484	30.58	0.01	0.01
ASH	123	27.61	-0.03	ASH	114	28.44	-0.02	0.01
GLH	262	33.98	-0.01	GLH	253	33.41	0.00	0.01
ASN	126	27.04	-0.04	ASN	117	27.70	-0.03	0.01
CYS	145	26.11	-0.01	CYS	156	26.30	0.00	0.01
LEU	78	15.55	0.05	LEU	69	15.18	0.06	0.01
LEU	277	19.34	-0.01	LEU	268	19.08	0.00	0.01
VAL	220	18.83	0.04	VAL	211	17.90	0.05	0.01
TYR	124	22.67	-0.07	HIE	115	24.66	-0.06	0.01
LEU	361	18.60	0.02	LEU	352	19.17	0.03	0.01
ASP	480	21.78	0.34	ASP	471	21.14	0.35	0.01
GLY	213	13.19	0.19	GLY	204	13.00	0.20	0.01
ILE	353	12.91	0.03	ILE	344	13.61	0.04	0.01
LYN	318	26.84	-0.01	LYN	309	27.77	0.00	0.01
ALA	358	15.07	0.06	ALA	349	14.78	0.07	0.01
THR	278	21.76	0.01	GLY	269	22.61	0.02	0.01
PHE	173	18.02	-0.11	LEU	164	19.20	-0.10	0.01
SER	497	31.50	0.02	SER	488	32.49	0.03	0.01
ASH	150	30.00	-0.02	GLH	141	30.42	-0.01	0.01
MET	157	18.91	0.06	MET	148	19.21	0.07	0.01
GLN	237	29.98	-0.01	ARN	228	29.86	0.00	0.01
THR	130	24.80	0.02	THR	121	25.01	0.03	0.01
GLN	293	28.32	-0.02	GLN	284	29.43	-0.01	0.01
TRP	472	24.41	0.01	TRP	463	24.00	0.01	0.01
THR	489	28.07	-0.03	THR	480	29.14	-0.02	0.01
ASN	292	28.48	0.00	ASN	283	29.80	0.01	0.01
PRO	413	23.78	0.02	PRO	404	23.22	0.02	0.01
GLN	384	29.27	0.00	LEU	375	30.88	0.01	0.01
TRP	128	19.44	-0.02	TRP	119	19.89	-0.01	0.01
LYN	239	29.02	0.01	LYN	230	28.69	0.01	0.01
PRO	299	17.83	-0.08	PRO	290	17.50	-0.07	0.01
THR	156	23.06	0.02	THR	147	22.97	0.03	0.01
PRO	412	20.64	-0.01	PRO	403	20.35	0.00	0.01
LEU	463	34.43	0.00	MET	454	34.36	0.00	0.01
ALA	120	28.75	-0.02	THR	111	29.48	-0.01	0.01
LYN	371	25.94	-0.01	LYN	362	26.32	0.00	0.01
TRP	152	25.92	-0.03	TRP	143	25.91	-0.02	0.01

res name MAO A	res ID MAO A	dist. MAO A [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO B [kcal/mol]	$\Delta\Delta G^{\ddagger}_{elec}(x)$ [kcal/mol]	res name MAO A	res ID MAO A	dist. MAO A [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO B [kcal/mol]	$\Delta\Delta G^{\ddagger}_{elec}(x)$ [kcal/mol]	res name MAO A	res ID MAO A	dist. MAO A [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO B [kcal/mol]	$\Delta\Delta G^{\ddagger}_{elec}(x)$ [kcal/mol]
VAL	449	15.38	-0.03	VAL	440	15.18	-0.02	0.01	VAL	390	24.40	-0.01	VAL	381	24.67	-0.01	0.00	GLY	462	33.93	0.00	ALA	453	33.43	0.00	0.00
ILE	415	23.51	0.02	ILE	406	23.49	0.03	0.01	HID	242	27.81	0.01	ARN	233	28.10	0.01	0.00	ASH	252	40.46	0.00	GLH	243	41.97	0.00	0.00
GLU	394	15.78	0.61	GLU	385	15.71	0.62	0.01	GLH	58	25.95	0.03	GLN	49	26.29	0.03	0.00	PHE	432	23.33	-0.02	PHE	423	23.21	-0.02	0.00
GLY	103	26.42	0.01	GLY	94	26.58	0.02	0.01	PRO	285	35.92	0.00	PRO	276	36.30	0.00	0.00	ILE	505	42.39	0.01	ILE	496	43.71	0.01	0.00
HID	261	35.31	-0.01	HIE	252	35.67	0.00	0.01	LEU	376	19.87	-0.01	LEU	367	20.25	-0.01	0.00	LEU	42	26.34	0.01	LEU	33	26.08	0.01	0.00
TRP	144	25.03	-0.01	TRP	135	24.86	0.00	0.01	ILE	254	33.75	0.00	VAL	245	33.78	0.00	0.00	MET	13	37.67	0.01	LYN	4	38.80	0.01	0.00
ALA	483	20.20	0.03	ALA	474	19.86	0.04	0.01	GLY	382	26.32	0.00	GLY	373	27.31	0.01	0.00	VAL	247	29.90	0.00	ILE	238	29.95	0.00	0.00
LEU	337	10.42	-0.01	LEU	328	10.28	-0.01	0.01	GLY	235	28.14	0.01	GLY	226	27.87	0.01	0.00	TYR	410	15.54	0.11	TYR	401	14.75	0.11	0.00
ILE	486	19.71	0.02	ILE	477	20.04	0.03	0.01	ILE	55	16.66	0.06	LEU	46	17.50	0.06	0.00	ASN	253	39.01	-0.01	ASN	244	38.72	-0.01	0.00
VAL	18	23.93	0.00	VAL	9	23.52	0.00	0.01	GLY	428	32.65	0.00	ASH	419	33.64	0.00	0.00	ILE	119	33.41	-0.01	ILE	110	34.50	-0.01	0.00
LEU	364	23.58	0.01	LEU	355	23.13	0.01	0.01	ASH	319	25.50	-0.03	ASH	310	26.27	-0.03	0.00	TYR	268	32.12	0.00	TYR	259	32.17	0.00	0.00
ASN	494	33.05	-0.01	HIE	485	34.21	0.00	0.01	VAL	37	31.89	0.01	LEU	28	32.22	0.01	0.00	LYN	311	27.66	0.03	LYN	302	28.02	0.03	0.00
LEU	195	19.66	-0.07	LEU	186	19.50	-0.06	0.00	ILE	471	28.09	0.01	ILE	462	27.96	0.01	0.00	GLY	344	23.62	-0.02	GLY	335	23.05	-0.02	0.00
LEU	176	15.09	-0.18	LEU	167	15.35	-0.18	0.00	ASH	470	30.77	0.00	GLH	461	30.85	0.00	0.00	PRO	426	28.23	-0.01	PRO	417	28.16	-0.01	0.00
PRO	113	19.28	-0.01	PRO	104	20.46	-0.01	0.00	ARN	109	24.07	0.02	ARN	100	24.58	0.02	0.00	ALA	149	27.11	-0.02	ALA	140	27.32	-0.02	0.00
ILE	281	25.89	-0.01	ILE	272	26.32	-0.01	0.00	LEU	502	38.81	0.01	LEU	493	39.36	0.01	0.00	LEU	387	26.84	0.01	LEU	378	27.51	0.01	0.00
VAL	422	26.33	0.01	VAL	413	25.89	0.02	0.00	PHE	108	20.69	0.01	PHE	99	21.46	0.01	0.00	LEU	495	31.84	-0.01	LEU	486	33.04	-0.01	0.00
HIE	12	36.32	0.00	ASN	3	37.45	0.00	0.00	THR	467	34.63	0.00	PRO	458	34.77	0.00	0.00	ALA	44	21.58	-0.03	ALA	35	21.57	-0.03	0.00
CYS	266	33.25	-0.01	ALA	257	33.40	0.00	0.00	PHE	283	28.88	0.00	PHE	274	29.82	0.00	0.00	ALA	456	24.56	-0.01	ALA	447	24.43	-0.01	0.00
ILE	326	16.55	-0.05	ILE	317	17.28	-0.05	0.00	ILE	77	12.95	0.01	ILE	68	12.65	0.01	0.00	THR	437	17.28	-0.01	THR	428	17.29	-0.01	0.00
SER	403	13.70	0.00	SER	394	13.80	0.00	0.00	PRO	274	15.27	0.00	PRO	265	15.26	0.01	0.00	LEU	287	29.28	0.00	LEU	278	29.78	0.00	0.00
GLU	450	16.76	-0.26	GLU	441	16.54	-0.25	0.00	GLY	464	36.47	0.00	GLY	455	36.93	0.00	0.00	ALA	170	23.58	-0.05	ALA	161	24.26	-0.05	0.00
GLN	425	27.29	0.02	GLN	416	27.31	0.02	0.00	PRO	114	23.94	-0.01	PRO	105	24.92	-0.01	0.00	GLY	36	33.40	-0.01	GLY	27	33.19	-0.01	0.00
TRP	315	20.39	-0.04	TRP	306	20.77	-0.03	0.00	SER	250	38.89	0.00	THR	241	39.54	0.00	0.00	ILE	373	17.72	-0.04	LEU	364	17.89	-0.04	0.00
LYN	317	27.29	-0.01	LYN	308	28.47	-0.01	0.00	ASH	248	35.33	0.00	ASH	239	35.84	0.01	0.00	ASH	15	34.08	0.00	ASH	6	33.60	0.00	0.00
ILE	19	24.15	0.00	VAL	10	23.25	0.00	0.00	VAL	498	32.71	0.01	VAL	489	33.52	0.02	0.00	ILE	349	15.88	0.05	ILE	340	15.69	0.05	0.00
MET	324	15.96	-0.06	MET	315	16.64	-0.05	0.00	GLY	404	15.05	-0.06	GLY	395	15.10	-0.06	0.00	VAL	244	26.15	0.01	VAL	235	26.27	0.00	0.00
LEU	160	23.68	0.03	LEU	151	23.54	0.04	0.00	LEU	501	36.98	0.01	LEU	492	38.35	0.01	0.00	TRP	116	29.81	0.00	TRP	107	31.44	0.00	0.00
GLH	468	33.17	-0.01	GLH	459	33.04	-0.01	0.00	VAL	459	29.25	-0.01	ILE	450	29.05	-0.01	0.00	THR	509	48.58	0.00	THR	500	49.35	0.00	0.00
VAL	189	16.85	0.06	VAL	180	16.82	0.06	0.00	PRO	139	24.39	-0.03	PRO	130	24.13	-0.03	0.00	LEU	31	24.76	-0.01	LEU	22	24.75	-0.01	0.00
LYN	465	35.03	0.00	LYN	456	35.52	0.00	0.00	LEU	460	30.20	-0.01	LEU	451	30.35	0.00	0.00	PHE	507	46.50	0.01	LEU	498	46.45	0.01	0.00
GLU	475	21.00	0.14	GLU	466	20.67	0.15	0.00	GLH	265	36.82	0.01	GLH	256	36.92	0.01	0.00	GLY	214	9.76	0.41	GLY	205	9.47	0.40	0.00
ARN	129	26.44	-0.02	ARN	120	26.92	-0.02	0.00	THR	258	29.96	-0.02	THR	249	29.99	-0.02	0.00	ALA	142	24.36	0.01	ALA	133	24.33	0.01	0.00
LYN	469	34.00	-0.01	ASH	460	32.68	0.00	0.00	HID	263	36.15	0.00	MET	254	35.85	0.01	0.00	GLY	452	18.76	-0.04	GLY	443	18.43	-0.04	0.00
ILE	295	23.00	-0.01	ILE	286	23.76	-0.01	0.00	VAL	481	18.16	-0.01	VAL	472	17.41	-0.01	0.00	ARG	360	20.99	0.36	LYS	351	21.54	0.36	0.00
PRO	143	21.48	0.01	PRO	134	21.59	0.01	0.00	LEU	80	18.08	-0.03	LEU	71	17.80	-0.03	0.00	GLH	159	26.05	0.00	GLH	150	26.37	0.00	0.00
ARG	369	19.27	-0.45	ARG	360	19.26	-0.45	0.00	VAL	238	24.88	-0.02	VAL	229	24.68	-0.02	0.00	LEU	40	29.11	-0.01	VAL	31	28.87	-0.01	0.00
ALA	438	14.87	-0.04	ALA	429	14.87	-0.04	0.00	VAL	39	28.17	0.00	VAL	30	28.41	0.00	0.00	PRO	107	24.48	0.00	PRO	98	25.50	0.00	0.00
PRO	389	23.40	-0.02	PRO	380	24.00	-0.02	0.00	ASN	461	32.51	0.01	HIE	452	32.96	0.01	0.00	ILE	430	28.72	-0.01	ILE	421	28.12	-0.01	0.00
TRP	491	33.34	-0.01	LEU	482	33.48	0.00	0.00	PRO	118	33.59	-0.01	PRO	109	34.92	-0.01	0.00	PRO	496	33.79	-0.01	PRO	487	35.03	-0.01	0.00
ALA	146	26.59	0.02	ALA	137	26.66	0.02	0.00	LYN	102	26.82	0.01	LYN	93	28.08	0.01	0.00	TYR	35	31.03	-0.01	SER	26	30.79	-0.01	0.00
PHE	314	23.74	-0.01	PHE	305	24.27	-0.01	0.00	ALA	378	24.64	-0.01	ALA	369	25.23	-0.01	0.00	THR	276	18.79	0.02	THR	267	17.95	0.01	0.00
LEU	97	17.68	0.04	LEU	88	18.55	0.05	0.00	VAL	427	29.85	0.00	VAL	418	29.70	0.01	0.00	ARN	297	25.04	0.00	ARN	288	25.56	-0.01	0.00
VAL	98	19.70	-0.04	ILE	89	21.03	-0.04	0.00	PHE	490	33.69	-0.01	PHE	481	34.90	-0.01	0.00	LEU	233	26.12	-0.02	LEU	224	25.92	-0.03	0.00
TYR	264	32.64	0.00	TYR	255	32.16	0.00	0.00	ILE	255	36.34	0.00	LEU	246	36.53	0.00	0.00	ALA	313	22.54	-0.01	PRO	304	22.52	-0.02	0.00
TYR	309	18.47	0.03	TYR	300	18.45	0.03	0.00	LEU	122	31.22	-0.02	LEU	113	32.26	-0.02	0.00	ALA	191	20.84	-0.07	ALA	182	20.86	-0.07	0.00
ALA	451	16.94	-0.02	ALA	442	16.79	-0.01	0.00	GLY	506	45.01	0.01	GLY	497	45.97	0.01	0.00	TYR	197	11.11	0.34	TYR	188	11.12	0.34	0.00
GLY	420	23.62	0.02	GLY	411	23.11	0.02	0.00	VAL	466	31.85	0.00	ILE	457	32.29	0.00	0.00	GLY	135	21.30	0.04	GLY	126	21.39	0.03	0.00
ARN	429	34.17	0.01	ARN	420	34.20	0.01	0.00	THR	439	17.86	-0.03	THR	430	17.84	-0.03	0.00	LEU	32	27.34	-0.01	LEU	23	27.23	-0.01	0.00
ALA	362	19.33	0.02	ALA	353	18.75	0.02	0.00	THR	73	15.87	-0.09	THR	64	15.89	-0.09	0.00	PRO	476	24.09	0.00	PRO	467	23.66	0.01	0.00
MET	231	23.19	-0.01	MET	222	22.89	-0.01	0.00	LYN	267	35.90	0.00	LYN	258	36.02	0.00	0.00	VAL	269	28.00	-0.01	VAL	260	28.05	-0.02	0.00
VAL	115	25.48	0.00	VAL	106	27.03	0.00	0.00	VAL	16	29.55	0.01	VAL	7	29.09	0.01	0.00	ILE	161	21.56	0.03	LEU	152	22.25	0.03	0.00
THR	205	16.94	-0.08	THR	196	16.96	-0.08	0.00	GLY	500	35.62	0.01	GLY	491	36.65	0.01	0.00	GLN	249	34.04	0.00	GLN	240	34.13	0.00	0.00
VAL	380	20.89	0.00	VAL	371	21.61	0.00	0.00	ILE	504	40.36	0.01	LEU	495	41.81	0.01	0.00	GLY	85	22.92	0.01	GLY	76	22.25	0.01	0.00
LYN	479	25.78	-0.02	VAL	470	24.48	-0.01	0.00	PRO	243	25.18	-0.02	PRO	234	25.42	-0.02	0.00	TYR	419	27.40	0.02	TYR	410	26.34	0.02	0.00
PRO	288	31.40	0.00	PRO	279	31.97	0.00	0.00	ALA	279	23.83	0.00	MET	270	26.80	0.00	0.00	LEU	259	29.13	-0.01	LEU	250	29.72	-0.01	0.00
VAL	91	13.61	-0.03	VAL	82	13.05	-0.03	0.00	LEU	381	21.47	-0.01	LEU	372	22.57	-0.01	0.00	ALA	331	19.62	-0.03	ALA	322	19.64	-0.03	0.00
ILE	256	30.96	0.00	VAL	247	30.70	0.00	0.00	GLY	202	15.52	0.02	GLY	193	15.22	0.02	0.00	GLY	224	15.14	-0.05	GLY	215	13.92	-0.05	0.00
VAL	101	23.37	0.01	VAL	92	24.06	0.01	0.00	SER	510	50.49	0.01	ILE	501	51.22	0.00	0.00	LEU	234	25.52	-0.03	LEU	225	25.28	-0.03	0.00

res name MAO A	res ID MAO A	dist. MAO A [A]	ΔG‡elec(x) MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	ΔG‡elec(x) MAO B [kcal/mol]	ΔΔG‡elec(x) [kcal/mol]
GLH	257	32.90	0.00	GLH	248	33.15	0.00	0.00
ALA	455	22.68	-0.01	ALA	446	22.42	-0.02	0.00
LYN	503	39.18	0.01	ARN	494	40.52	0.00	0.00
SER	508	46.73	0.01	THR	499	47.73	0.00	0.00
ALA	386	23.64	0.02	ALA	377	24.23	0.02	0.00
CYS	321	18.20	0.03	CYS	312	19.02	0.02	0.00
PHE	431	27.15	0.01	TYR	422	27.26	0.01	0.00
GLY	20	19.98	-0.04	GLY	11	19.69	-0.05	0.00
SER	251	40.38	0.00	ARN	242	42.09	0.00	0.00
SER	499	34.54	0.02	PRO	490	34.75	0.01	0.00
ASN	117	31.38	-0.02	ASN	108	32.90	-0.02	0.00
ALA	289	32.31	0.00	MET	280	33.74	-0.01	0.00
LEU	240	24.12	-0.03	LEU	231	24.12	-0.03	0.00
ILE	164	25.61	0.03	LEU	155	26.61	0.03	0.00
SER	94	21.84	-0.02	VAL	85	21.99	-0.03	0.00
CYS	374	22.02	0.00	CYS	365	22.50	-0.01	0.00
ALA	448	12.46	-0.14	ALA	439	12.28	-0.14	0.00
ARN	421	28.51	0.01	ARN	412	27.83	0.01	0.00
ALA	348	16.24	-0.02	ALA	339	16.54	-0.03	0.00
ILE	230	20.43	-0.05	ILE	221	20.32	-0.05	0.00
THR	167	28.55	-0.03	THR	158	29.31	-0.04	0.00
PHE	14	33.29	-0.01	CYS	5	33.56	-0.01	0.00
GLH	312	26.56	0.01	GLH	303	26.31	0.00	0.00
GLH	286	34.11	0.00	PRO	277	35.42	0.00	0.00
TYR	392	18.79	-0.03	TYR	383	18.59	-0.04	0.00
ILE	138	22.31	0.00	ILE	129	22.22	-0.01	-0.01
ALA	28	21.48	-0.02	ALA	19	21.24	-0.02	-0.01
TYR	121	27.84	-0.03	TYR	112	29.51	-0.03	-0.01
LEU	127	21.83	0.00	PHE	118	22.10	-0.01	-0.01
THR	245	28.76	0.00	ILE	236	29.99	0.00	-0.01
TYR	310	21.56	0.04	TYR	301	21.73	0.03	-0.01
LEU	346	21.94	0.05	TYR	337	22.00	0.04	-0.01
MET	308	17.68	0.04	VAL	299	17.71	0.04	-0.01
PHE	112	17.28	0.03	PHE	103	19.02	0.03	-0.01
ALA	302	13.74	-0.16	SER	293	13.09	-0.16	-0.01
GLH	385	27.03	0.01	GLH	376	27.88	0.01	-0.01
ALA	174	18.57	-0.11	ALA	165	18.82	-0.12	-0.01
ILE	270	23.99	0.01	ILE	261	23.83	0.01	-0.01
ALA	29	23.66	-0.03	ALA	20	23.26	-0.04	-0.01
VAL	17	28.54	-0.01	VAL	8	28.29	-0.01	-0.01
LEU	192	22.21	-0.04	LEU	183	22.09	-0.05	-0.01
PRO	482	21.39	0.00	PRO	473	21.07	-0.01	-0.01
ARN	96	24.06	0.02	ARN	87	24.87	0.02	-0.01
TRP	196	16.59	-0.05	TRP	187	16.55	-0.05	-0.01
GLY	405	11.97	0.14	GLY	396	11.89	0.14	-0.01
SER	27	18.54	-0.03	ALA	18	18.42	-0.04	-0.01
TRP	441	10.84	0.29	TRP	432	10.92	0.29	-0.01
MET	134	24.33	0.02	MET	125	24.18	0.01	-0.01
CYS	398	15.15	-0.01	CYS	389	14.75	-0.02	-0.01
VAL	41	23.96	-0.01	VAL	32	23.57	-0.01	-0.01
ALA	433	18.91	-0.04	ALA	424	18.78	-0.05	-0.01
ALA	111	17.69	-0.04	PRO	102	18.38	-0.04	-0.01
LYN	154	29.42	0.00	ASN	145	28.44	-0.01	-0.01
GLY	110	20.08	0.00	GLY	101	20.39	-0.01	-0.01
PRO	342	20.40	-0.03	PRO	333	19.92	-0.04	-0.01
THR	33	28.58	-0.01	HIE	24	28.61	-0.02	-0.01
LYN	168	28.55	-0.04	GLH	159	27.95	-0.05	-0.01
TYR	320	22.82	0.03	TYR	311	23.67	0.02	-0.01
HID	246	31.79	0.02	TYR	237	33.53	0.01	-0.01

res name MAO A	res ID MAO A	dist. MAO A [A]	ΔG‡elec(x) MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	ΔG‡elec(x) MAO B [kcal/mol]	ΔΔG‡elec(x) [kcal/mol]
GLY	203	15.38	-0.08	GLY	194	15.47	-0.09	-0.01
MET	155	25.93	-0.02	MET	146	26.14	-0.03	-0.01
SER	209	12.93	-0.06	SER	200	13.27	-0.07	-0.01
TYR	175	20.13	-0.08	THR	166	18.41	-0.09	-0.01
PRO	275	17.46	0.02	PRO	266	18.09	0.01	-0.01
SER	478	20.58	-0.02	SER	469	20.29	-0.03	-0.01
ILE	23	13.07	-0.13	ILE	14	12.61	-0.14	-0.01
LYN	379	25.66	0.01	LYN	370	25.90	0.00	-0.01
THR	54	13.93	0.03	THR	45	14.28	0.01	-0.01
LYN	104	27.96	-0.01	LYN	95	29.11	-0.02	-0.01
TRP	193	15.51	-0.03	TRP	184	15.25	-0.04	-0.01
GLH	137	26.75	0.03	GLH	128	27.23	0.02	-0.01
TYR	402	19.69	-0.02	TYR	393	19.69	-0.04	-0.01
ARG	79	20.37	-0.28	ARG	70	19.98	-0.29	-0.01
SER	184	13.99	-0.11	ALA	175	13.88	-0.12	-0.01
ASN	179	13.37	-0.27	ASN	170	13.45	-0.29	-0.01
ARN	171	25.71	-0.04	LYN	162	24.75	-0.05	-0.01
GLY	221	17.50	0.01	GLY	212	17.02	0.00	-0.01
PHE	411	18.21	-0.02	PHE	402	18.54	-0.03	-0.01
GLY	434	15.30	-0.11	GLY	425	15.19	-0.12	-0.01
ILE	86	18.99	-0.03	LEU	77	18.54	-0.04	-0.01
LEU	84	21.31	-0.02	LEU	75	20.95	-0.03	-0.01
ARN	284	36.91	0.01	ASN	275	36.41	0.00	-0.01
LYN	158	23.09	0.00	LYN	149	23.50	-0.02	-0.01
ILE	273	19.10	-0.04	ILE	264	19.27	-0.05	-0.01
GLH	485	23.88	0.02	PRO	476	23.45	0.01	-0.01
GLY	22	15.71	-0.11	GLY	13	15.15	-0.12	-0.01
GLN	296	24.90	0.00	THR	287	25.06	-0.01	-0.01
THR	487	24.75	-0.04	THR	478	25.08	-0.06	-0.01
THR	169	25.42	-0.04	SER	160	25.85	-0.05	-0.01
SER	24	15.83	-0.07	SER	15	15.53	-0.09	-0.02
TYR	100	21.63	-0.01	HIE	91	22.16	-0.03	-0.02
VAL	60	20.31	0.02	VAL	51	19.23	0.00	-0.02
THR	88	16.84	-0.08	THR	79	15.98	-0.10	-0.02
HID	148	29.77	0.01	LEU	139	30.27	0.00	-0.02
HID	282	30.97	0.01	HIE	273	31.18	0.00	-0.02
HIE	391	21.01	-0.06	HIE	382	21.58	-0.08	-0.02
VAL	198	13.91	-0.04	VAL	189	14.06	-0.05	-0.02
LYN	163	29.59	0.03	LYN	154	29.75	0.01	-0.02
ASN	260	32.35	0.00	ASN	251	31.52	-0.02	-0.02
TYR	377	18.34	-0.06	TYR	368	18.85	-0.07	-0.02
ILE	325	14.94	0.08	ILE	316	16.35	0.07	-0.02
GLY	322	16.19	0.01	GLY	313	16.56	0.00	-0.02
VAL	70	10.01	0.21	VAL	61	9.64	0.19	-0.02
SER	383	26.53	0.01	SER	374	26.65	-0.01	-0.02
GLH	145	28.22	0.03	THR	136	28.75	0.01	-0.02
LYS	30	23.19	-0.49	LYS	21	23.27	-0.51	-0.02
HID	365	23.95	-0.01	THR	356	24.91	-0.03	-0.02
VAL	210	12.83	-0.07	THR	201	12.93	-0.08	-0.02
PRO	332	18.00	-0.05	PRO	323	17.83	-0.07	-0.02
GLY	222	14.41	-0.20	GLY	213	13.83	-0.22	-0.02
ASH	236	31.30	0.00	ASH	227	30.99	-0.02	-0.02
THR	52	9.68	-0.48	THR	43	9.68	-0.50	-0.02
GLH	34	28.16	0.01	ASH	25	28.31	-0.01	-0.02
PHE	194	14.33	-0.06	PHE	185	14.96	-0.08	-0.02
MET	300	13.05	0.04	LEU	291	12.92	0.02	-0.02
ILE	304	13.26	-0.17	ILE	295	12.94	-0.19	-0.02
GLY	25	18.71	-0.05	GLY	16	18.20	-0.07	-0.02
VAL	226	15.86	-0.12	VAL	217	15.07	-0.14	-0.02

res name MAO A	res ID MAO A	dist. MAO A [A]	ΔG‡elec(x) MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	ΔG‡elec(x) MAO B [kcal/mol]	ΔΔG‡elec(x) [kcal/mol]
LEU	26	19.07	-0.06	MET	17	18.81	-0.09	-0.02
GLY	71	11.79	0.09	GLY	62	11.65	0.07	-0.02
HID	187	21.78	0.03	HIE	178	21.57	0.01	-0.03
VAL	484	22.17	-0.02	GLN	475	22.99	-0.04	-0.03
ILE	368	25.15	-0.01	GLH	359	25.18	-0.04	-0.03
PRO	72	15.19	-0.10	PRO	63	15.06	-0.12	-0.03
MET	416	21.80	0.06	LEU	407	21.18	0.03	-0.03
ILE	207	10.30	-0.24	ILE	198	10.46	-0.27	-0.03
ILE	131	19.31	0.03	MET	122	19.66	0.00	-0.03
SER	190	20.06	-0.08	SER	181	19.79	-0.11	-0.03
LYS	82	21.95	-0.37	LYS	73	21.28	-0.41	-0.03
ASN	271	21.75	0.00	SER	262	21.87	-0.03	-0.03
THR	435	11.06	-0.35	THR	426	10.99	-0.38	-0.04
ASH	328	20.81	0.01	GLY	319	20.96	-0.03	-0.04
PHE	219	13.63	0.02	PHE	210	12.86	-0.02	-0.04
ARN	172	23.57	-0.04	GLN	163	23.02	-0.08	-0.04
THR	140	20.19	0.01	SER	131	19.78	-0.03	-0.04
VAL	182	11.48	-0.03	VAL	173	11.52	-0.07	-0.04
ALA	272	18.11	0.04	ALA	263	17.59	0.00	-0.04
PHE	208	11.72	0.06	ILE	199	12.62	0.02	-0.05
ARG	291	21.27	0.38	ARG	415	22.00	0.33	-0.05
CYS	201	11.78	-0.07	CYS	192	11.61	-0.13	-0.05
VAL	63	15.64	-0.02	VAL	54	14.56	-0.07	-0.06
SER	442	11.39	-0.43	SER	433	11.28	-0.49	-0.06
GLU	446	12.10	0.24	GLU	437	11.87	0.17	-0.06
GLU	95	22.26	-0.01	GLU	86	22.79	-0.07	-0.06
LYS	366	21.16	-0.67	LYS	357	21.16	-0.74	-0.07
ARG	291	25.30	0.07	ARG	282	25.26	0.00	-0.07
LYS	357	16.34	0.92	LYS	348	17.34	0.85	-0.07
LYS	280	24.03	-0.21	LYS	271	24.07	-0.28	-0.07
MET	445	8.46	-0.53	MET	436	8.31	-0.60	-0.07
PHE	352	7.06	0.03	PHE	343	7.13	-0.05	-0.07
LYN	305	8.11	0.29	LYN	296	8.40	0.22	-0.07
GLU	83	23.23	0.40	GLU	74	23.10	0.33	-0.08
SER	334	12.71	0.19	ALA	325	13.33	0.11	-0.08
ASP	338	14.26	0.49	ASP	329	14.77	0.41	-0.08
GLH	477	21.96	0.01	GLU	468	23.14	-0.08	-0.08
GLN	225	18.52	-0.03	GLN	216	17.22	-0.12	-0.09
CYS	306	12.44	0.05	CYS	297	12.61	-0.05	-0.10
ARG	229	22.43	-0.74	ARG	220	21.67	-0.85	-0.10
ASP	132	21.09	-0.87	ASP	123	21.41	-0.99	-0.12
LYS	363	23.49	0.09	ARG	354	22.83	-0.03	-0.12
SER	227	16.43	-0.03	SER	218	16.30	-0.15	-0.13
GLU	327	19.65	-0.66	ASP	318	20.06	-0.79	-0.13
MET	307	13.35	0.12	ILE	298	12.97	-0.01	-0.13
ARG	56	19.63	-1.13	ARG	47	19.42	-1.27	-0.13
ILE	335	10.10	0.11	TYR	326	11.22	-0.04	-0.15
LYS	218	11.78	-2.69	LYS	209	11.27	-2.83	-0.15
ILE	180	9.63	-0.62	LEU	171	9.26	-0.77	-0.15
LYS	341	18.06	-1.40	LYS	332	17.24	-1.57	-0.17
GLU	188	19.52	-0.52	GLU	179	18.69	-0.69	-0.17
ARG	51	9.88	-0.45	ARG	42	9.85	-0.63	-0.18
GLU	216	13.69	0.01	GLU	207	13.57	-0.18	-0.19
ARG	45	17.68	-1.32	ARG	36	17.37	-1.50	-0.19
ARG	47	17.10	-1.86	ARG	38	16.94	-2.07	-0.22
TYR	69	7.72	0.11	TYR	60	7.25	-0.12	-0.23
GLY	443	7.64	0.13	GLY	434	7.44	-0.15	-0.28
GLY	66	7.73	-0.22	GLY	57	7.70	-0.54	-0.32

res name MAO A	res ID MAO A	dist. MAO A [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO A [kcal/mol]	res name MAO B	res ID MAO B	dist. MAO B [A]	$\Delta G^{\ddagger}_{elec}(x)$ MAO B [kcal/mol]	$\Delta\Delta G^{\ddagger}_{elec}(x)$ [kcal/mol]
ASH	141	22.79	0.01	ASP	132	22.79	-0.34	-0.34
ALA	68	7.42	-1.01	SER	59	7.40	-1.38	-0.38
LYS	440	16.00	0.58	HIE	431	15.32	0.18	-0.40
ASH	330	23.47	0.03	GLU	321	24.01	-0.39	-0.42
TYR	444	6.51	-1.46	TYR	435	6.36	-1.98	-0.52
ARG	356	19.46	0.55	HIE	347	18.30	0.01	-0.54
HIE	59	24.19	-0.01	LYS	50	24.39	-0.56	-0.55
LYS	395	14.05	-1.10	LYS	386	13.21	-1.66	-0.56
TYR	407	5.41	-1.55	TYR	398	5.44	-2.15	-0.60
ASH	153	24.34	0.00	ASP	144	24.38	-0.62	-0.63
VAL	93	16.96	-0.01	GLU	84	17.27	-0.67	-0.67
GLN	215	8.27	-0.55	GLN	206	8.04	-1.22	-0.67
ASP	61	21.26	0.80	LYS	52	21.79	-0.68	-1.48

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