

Table S1: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP/LANL2DZ. Italicized values are for PCM calculations in a water solvent. Structures **1A-1U** refer to [Carnosine + OxPt + H]⁺ in which direct Pt bonding to carnosine is observed. Structures **1V-1Y** refer to [Carnosine + OxPt + H]⁺ in which no direct Pt bonding to carnosine is observed. Structures **2A-2N**, **3A-3G**, **4A-4M** and **5A-5B** refer to [Carnosine + OxPt – CO₂ + H]⁺, [Carnosine – H + Pt(dach)]⁺, [Carnosine – NH₃ – H + Pt(dach)]⁺ and [OxPt – CO₂ + H]⁺ respectively.

Structure	Electronic energy (Hartrees)	ZPE (kcal mol ⁻¹)	H ₂₉₈ ^o – H ₀ ^o (kcal mol ⁻¹)	Entropy (cal mol ⁻¹ K ⁻¹)	Relative free energy at 298 K (kcal mol ⁻¹)
1A	-1639.2886242	312.6	19.6	196.8	0.0
	<i>-1639.4050202</i>	<i>314.6</i>	<i>19.9</i>	<i>201.1</i>	<i>0.8</i>
1B	-1639.2858222	312.8	20.0	203.4	0.4
	<i>-1639.3913698</i>	<i>314.5</i>	<i>20.1</i>	<i>204.5</i>	<i>8.5</i>
1C	-1639.2867573	314.4	19.6	197.5	2.7
	<i>-1639.3956112</i>	<i>315.2</i>	<i>19.8</i>	<i>200.1</i>	<i>7.6</i>
1D	-1639.2796868	312.7	20.0	205.4	3.4
	<i>-1639.4041530</i>	<i>314.2</i>	<i>20.0</i>	<i>204.7</i>	<i>0.0</i>
1E	-1639.2784107	313.5	19.8	203.6	5.4
	<i>-1639.4015638</i>	<i>314.5</i>	<i>19.7</i>	<i>201.5</i>	<i>2.6</i>
1F	-1639.2732867	312.9	20.7	213.8	5.9
	<i>-1639.3731196</i>	<i>312.8</i>	<i>20.8</i>	<i>215.6</i>	<i>15.6</i>
1G	-1639.2758092	312.9	20.1	204.4	6.5
	<i>-1639.3914762</i>	<i>314.0</i>	<i>20.3</i>	<i>207.1</i>	<i>7.3</i>
1H	-1639.2729851	312.2	20.1	207.4	6.7
	<i>-1639.3770276</i>	<i>314.2</i>	<i>20.5</i>	<i>213.3</i>	<i>14.9</i>
1I	-1639.2778140	312.9	19.7	198.0	6.7
	<i>-1639.3970803</i>	<i>313.9</i>	<i>20.1</i>	<i>203.7</i>	<i>4.5</i>
1J	-1639.2760210	313.7	19.8	202.3	7.4
	<i>-1639.3961354</i>	<i>314.9</i>	<i>19.9</i>	<i>202.4</i>	<i>6.3</i>
1K	-1639.2716859	312.5	20.2	204.9	8.7
	<i>-1639.3958654</i>	<i>314.3</i>	<i>20.3</i>	<i>214.4</i>	<i>2.7</i>
1L	-1639.2723656	312.9	20.3	206.1	8.3
	<i>-1639.3651803</i>	<i>312.2</i>	<i>20.3</i>	<i>207.8</i>	<i>21.9</i>

1M	-1639.2680874	312.9	20.4	210.2	9.9
	<i>-1639.3712658</i>	<i>312.5</i>	<i>20.5</i>	<i>212.7</i>	<i>17.0</i>
1N	-1639.2702447	314.2	20.1	202.5	11.8
	<i>-1639.3699854</i>	<i>314.1</i>	<i>20.3</i>	<i>206.5</i>	<i>21.1</i>
1O	-1639.2751572	314.9	19.4	192.0	11.9
	<i>-1639.3845742</i>	<i>313.7</i>	<i>19.7</i>	<i>197.0</i>	<i>13.7</i>
1P	-1639.2677622	313.4	20.2	204.1	12.2
	<i>-1639.3703845</i>	<i>313.5</i>	<i>20.4</i>	<i>205.0</i>	<i>20.8</i>
1Q	-1639.2640107	313.8	19.6	200.3	15.5
	<i>-1639.3799232</i>	<i>313.8</i>	<i>19.9</i>	<i>204.8</i>	<i>14.6</i>
1R	-1639.2631978	313.4	20.0	201.1	15.8
	<i>-1639.3842329</i>	<i>315.0</i>	<i>20.3</i>	<i>208.0</i>	<i>12.6</i>
1S	-1639.2554539	314.0	20.2	207.2	19.6
	<i>-1639.3634689</i>	<i>313.5</i>	<i>20.3</i>	<i>209.7</i>	<i>23.6</i>
1T	-1639.2554538	314.0	20.2	207.2	19.6
	<i>-1639.3634688</i>	<i>313.5</i>	<i>20.3</i>	<i>209.7</i>	<i>23.6</i>
1U	-1639.2500998	312.1	20.6	212.9	19.8
	<i>-1639.3468289</i>	<i>311.9</i>	<i>20.7</i>	<i>214.6</i>	<i>31.4</i>
1V	-1639.2855972	313.4	20.1	204.5	0.8
	<i>-1639.3803957</i>	<i>313.2</i>	<i>20.4</i>	<i>208.5</i>	<i>13.1</i>
1W	-1639.2750738	312.9	20.7	216.3	4.0
	<i>-1639.3730479</i>	<i>312.7</i>	<i>20.8</i>	<i>217.2</i>	<i>15.2</i>
1X	-1639.2806661	313.8	20.0	202.2	5.0
	<i>-1639.3792743</i>	<i>313.5</i>	<i>20.3</i>	<i>206.4</i>	<i>14.8</i>
1Y	-1639.2698582	313.8	20.6	219.8	7.1
	<i>-1639.3745151</i>	<i>314.0</i>	<i>20.7</i>	<i>218.0</i>	<i>15.1</i>
2A	-1450.7542132	304.6	18.5	192.5	0.0
2B	-1450.7521575	304.7	18.1	187.2	2.6
2C	-1450.7488908	305.0	18.2	184.3	5.9
2D	-1450.7396653	304.6	18.2	186.7	10.5
2E	-1450.7359210	304.2	18.4	189.4	11.9
2F	-1450.7356931	304.0	18.2	186.5	12.5

2G	-1450.7278354	303.5	18.6	198.1	13.9
2H	-1450.7225517	305.3	18.3	190.2	21.0
2I	-1450.7156471	305.4	18.5	193.8	24.6
2J	-1450.6987011	302.4	18.6	191.6	33.0
2K	-1450.6951026	303.3	18.8	199.0	34.1
2L	-1450.6961826	302.4	18.3	188.4	35.3
2M	-1450.6910914	302.8	18.4	189.3	38.6
2N	-1450.6692231	302.7	19.0	199.4	49.9
3A	-1260.9744123	282.5	15.8	168.1	0.0
3B	-1260.9646407	281.5	16.4	174.2	3.9
3C	-1260.9499510	283.0	15.7	171.6	14.8
3D	-1260.9471698	282.5	15.6	164.1	18.1
3E	-1260.9382042	283.1	15.3	159.5	25.4
3F	-1260.8792520	280.7	16.1	171.0	57.3
3G	-1260.8353995	281.2	15.5	163.5	86.9
4A	-1204.3891678	256.0	15.1	162.6	0.0
4B	-1204.3888797	256.2	14.7	157.3	1.6
4C	-1204.3795752	255.7	15.1	164.3	5.2
4D	-1204.3716679	255.2	15.1	166.1	9.3
4E	-1204.3753032	256.7	14.6	159.2	10.0
4F	-1204.3612046	255.2	14.9	161.7	16.8
4G	-1204.3318604	255.0	14.9	162.3	34.9
4H	-1204.3247413	254.8	15.1	166.2	38.2
4I	-1204.3241914	255.0	15.0	163.8	39.4
4J	-1204.3113922	254.7	14.8	158.9	48.4
4K	-1204.2953955	255.0	14.7	158.5	58.8
4L	-1204.2460587	253.0	15.6	169.7	85.3
4M	-1204.2346476	252.8	15.7	166.6	93.2
5A	-654.6722639	148.4	8.1	109.6	0.0
5B	-654.6344513	145.8	9.0	121.9	18.4