

Electronic Supplementary Information for:

Entropic Effect Makes a More Tightly Folded Conformer of a β -Amino Acid
Less Stable: UV-UV Hole Burning and IR Dip Spectroscopy of L- β^3 -
Homotryptophan by Laser Desorption Supersonic Jet Technique

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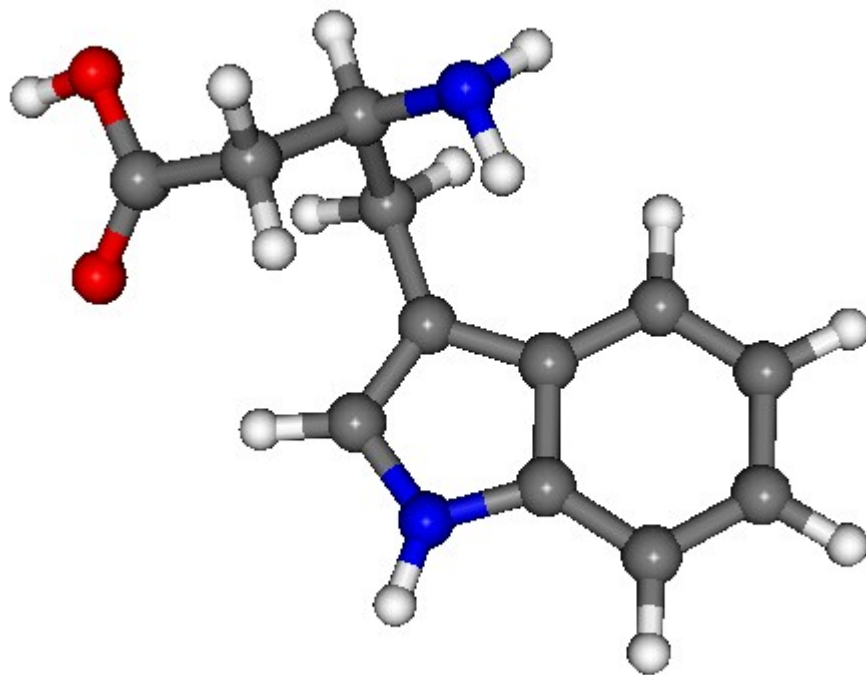
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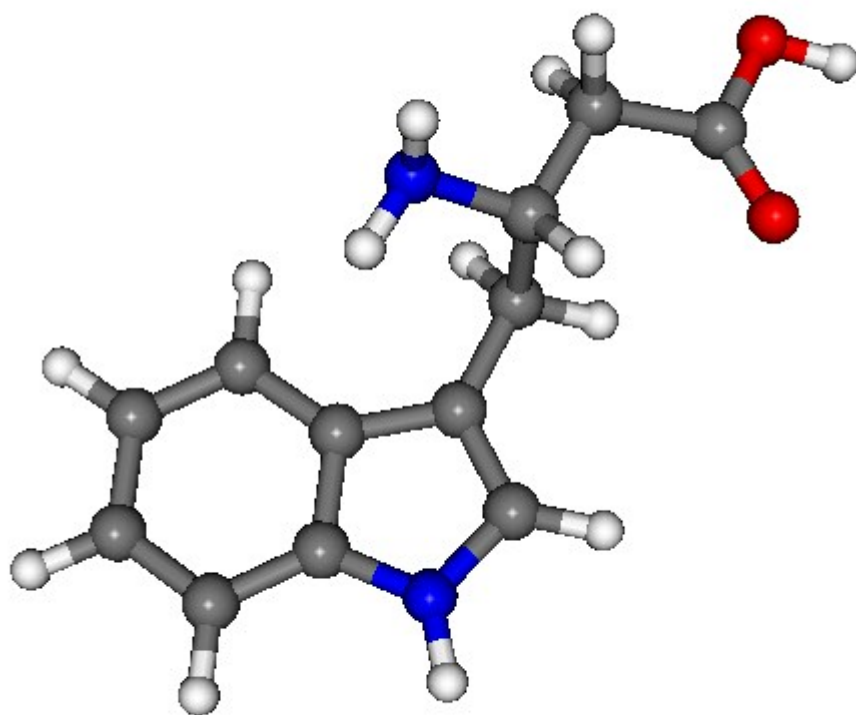
Table S1. Zero point corrected relative energies M05-2X and MP2 with 6-31G** basis set

Conformer	ΔE /kJmol ⁻¹ (M05-2X)	ΔE /kJmol ⁻¹ (MP2)
O 15	0.80	0.44
O 01	0.00	0.00
O 12	4.0	4.6
O 04	2.7	1.8
O 11	2.5	1.5
O 07	4.4	4.9
N 25	7.5	6.1
O 14	5.8	4.0
N 35	10	8.3
N 26	8.7	7.4
N 20	10	8.1
O 05	9.5	8.5
N 40	8.8	6.9
N 24	9.8	7.2
N 09	10	8.2
N 48	12	9.8
O 06	8.0	8.0
N 36	13	11
N 22	12	9.7
N 05	10	6.7
N 21	13	9.7
N 13	11	8.1
O 03	12	11
N 08	13	12
O 16	10	7.6
N 12	13	9.8
N 28	14	12
O 24	13	15

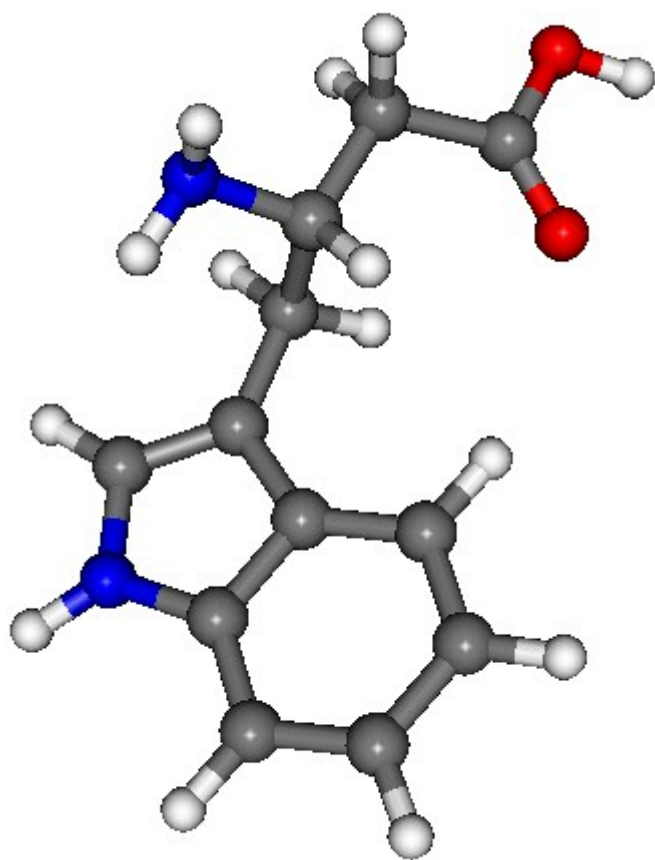
Figure S1. Geometries of 37 stable conformers of L- β^3 -homotryptophan at MP2/6-31G**. The names indicate hydrogen bonding patterns and relative stability obtained by force-field calculation. (See text.)



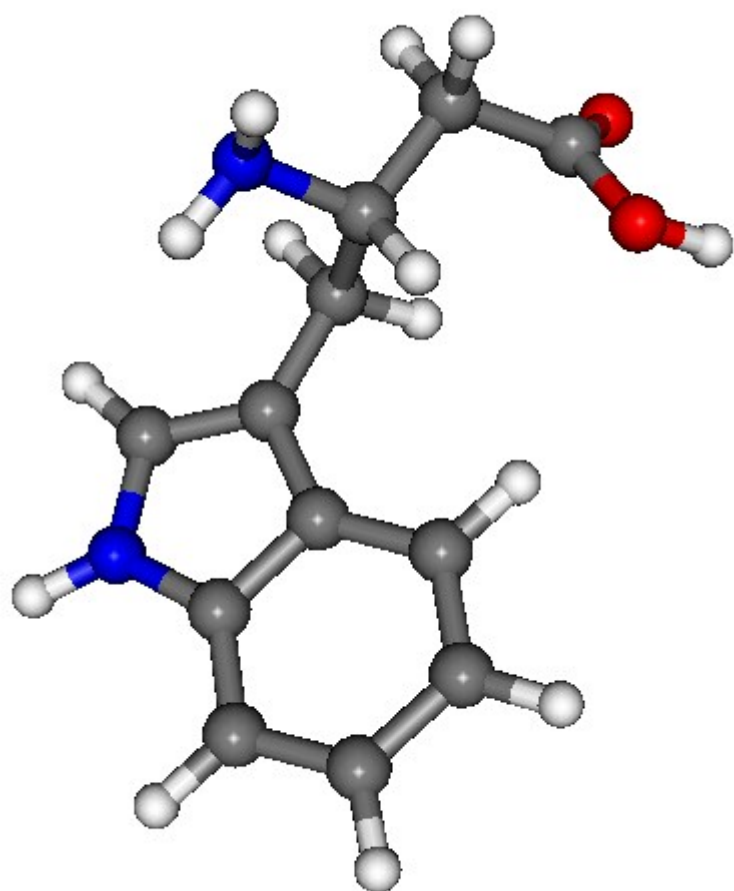
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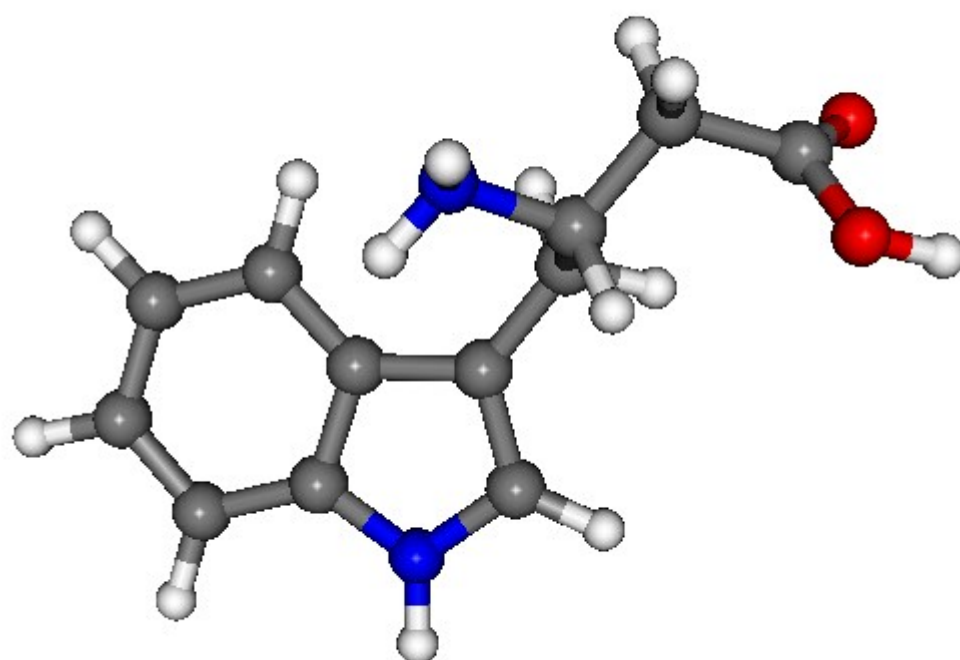
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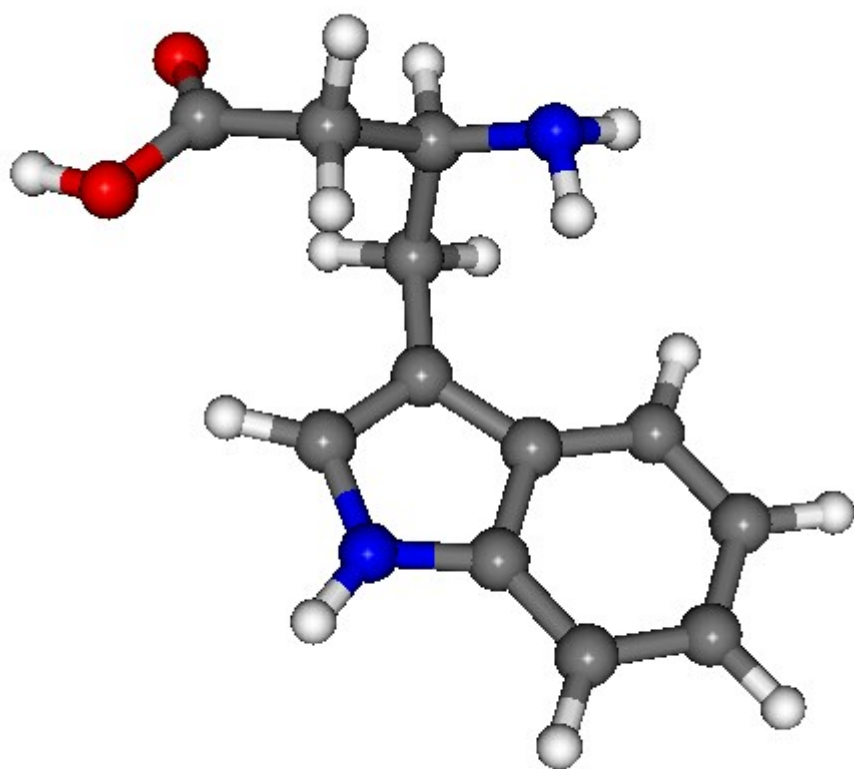
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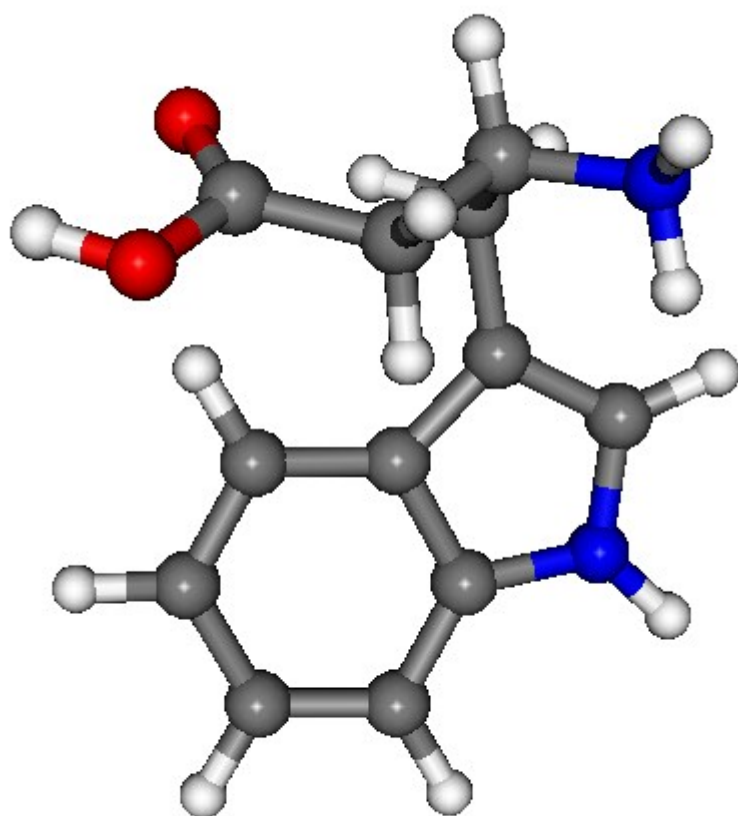
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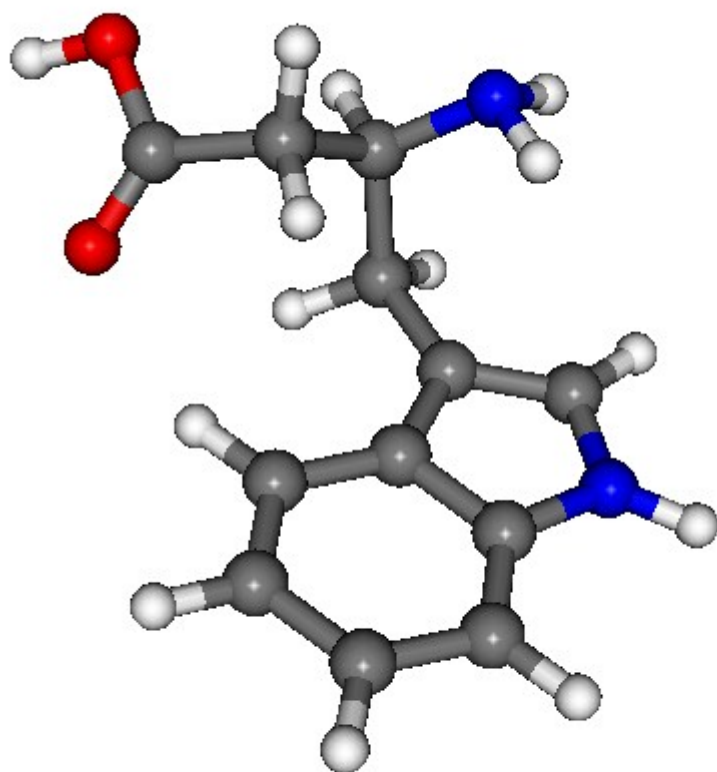
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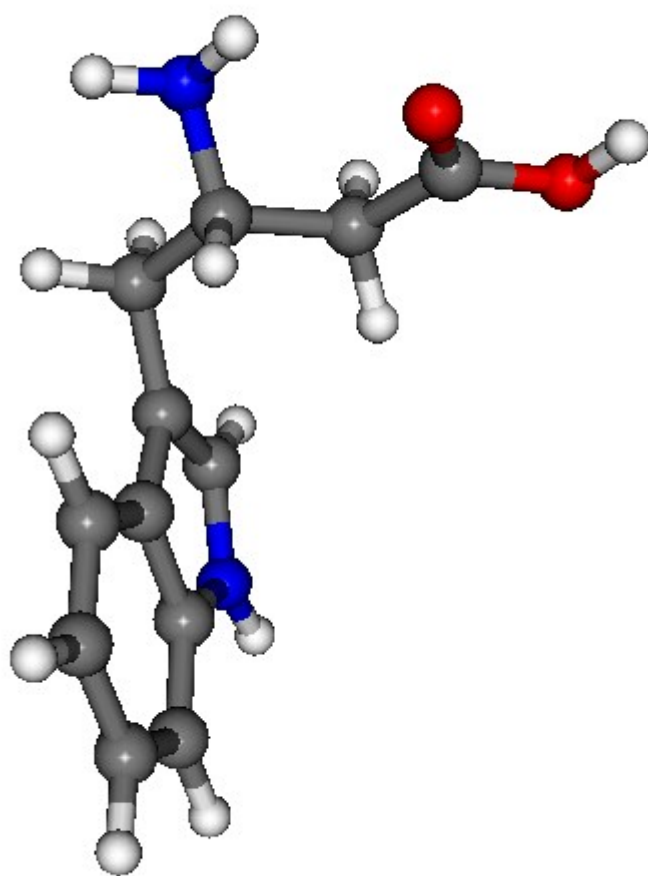
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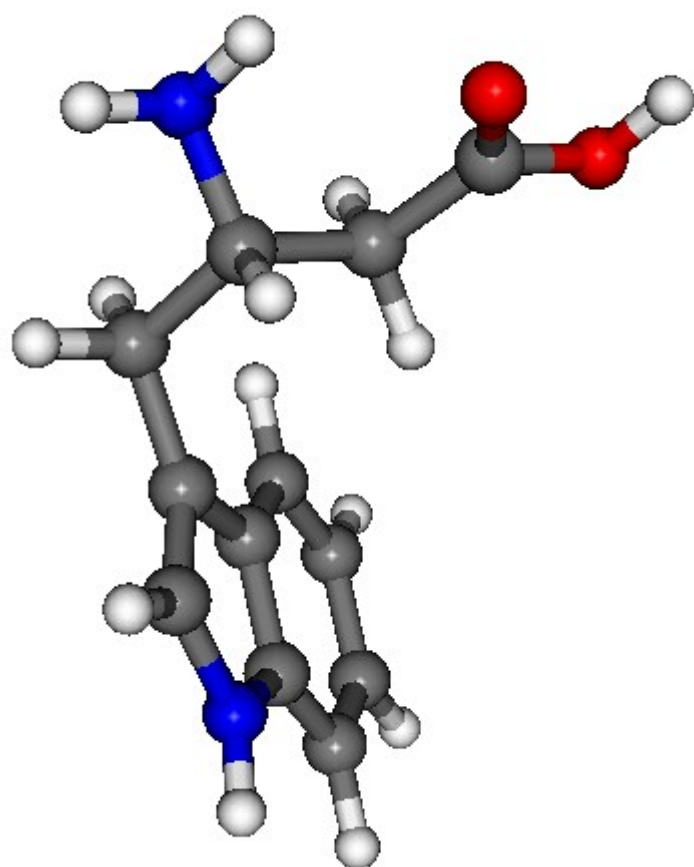
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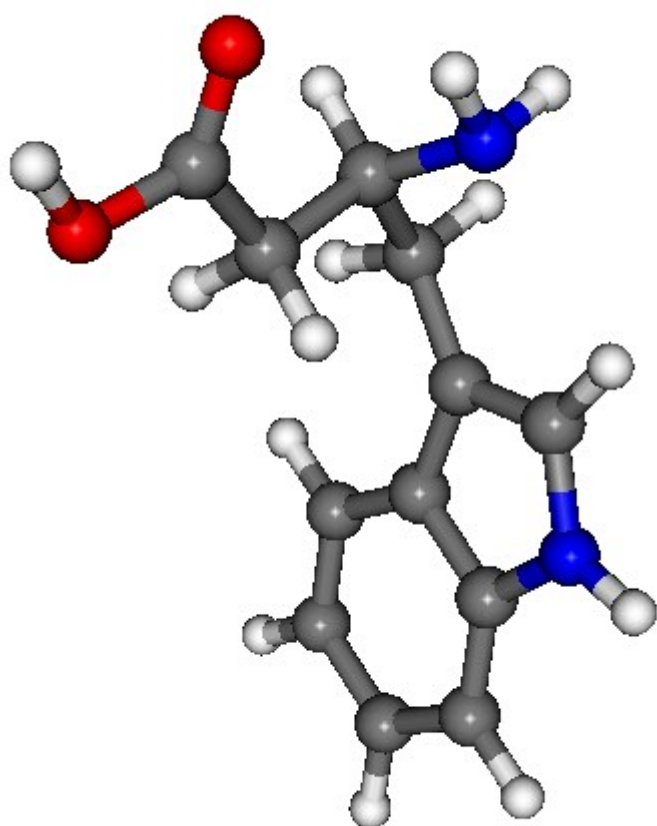
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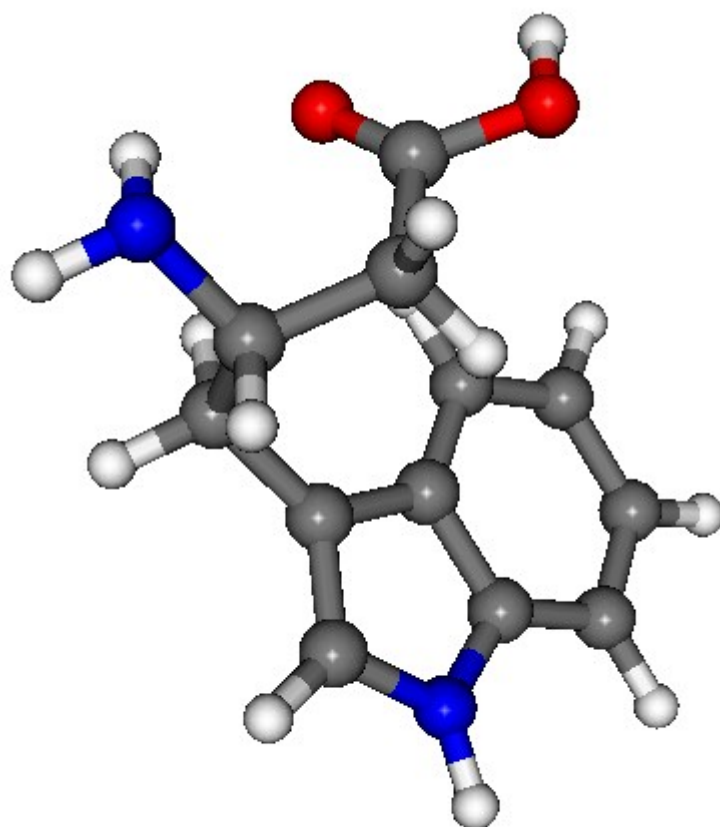
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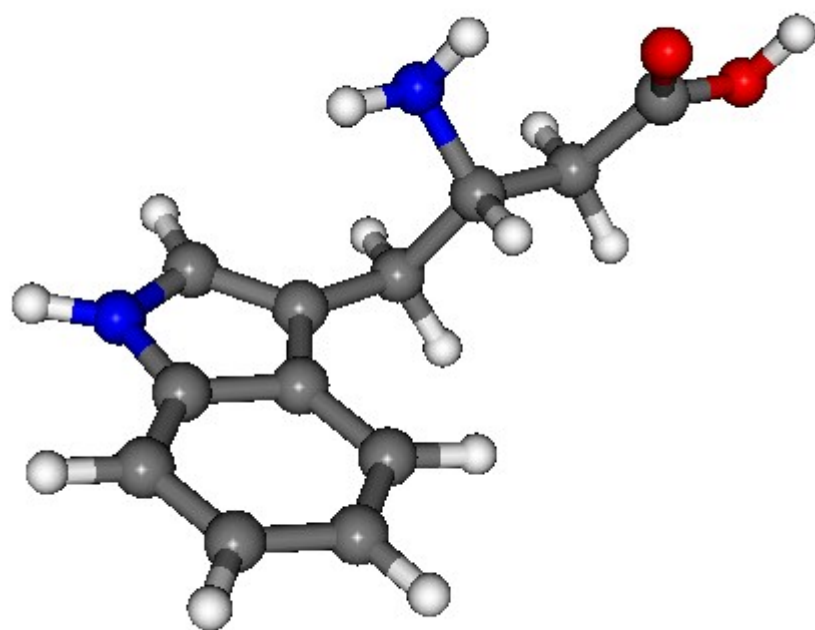
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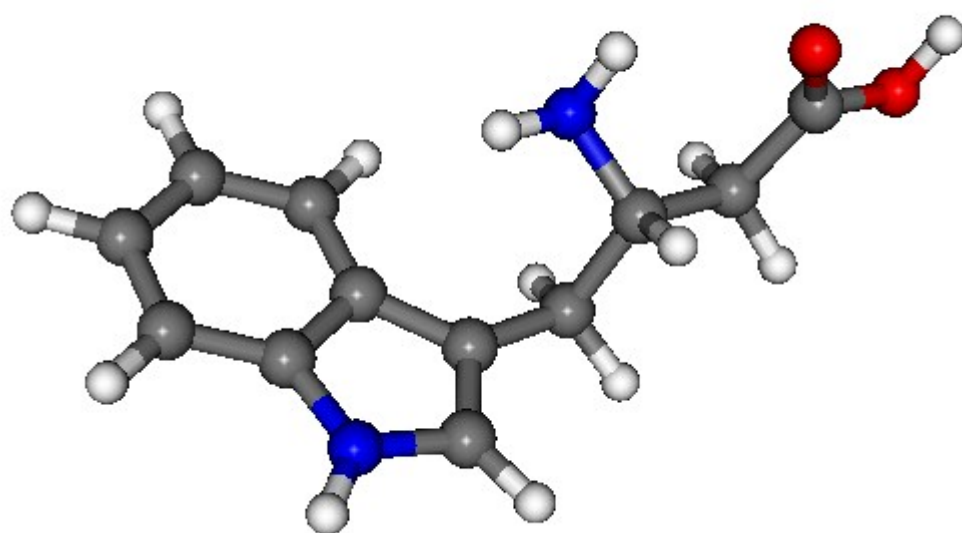
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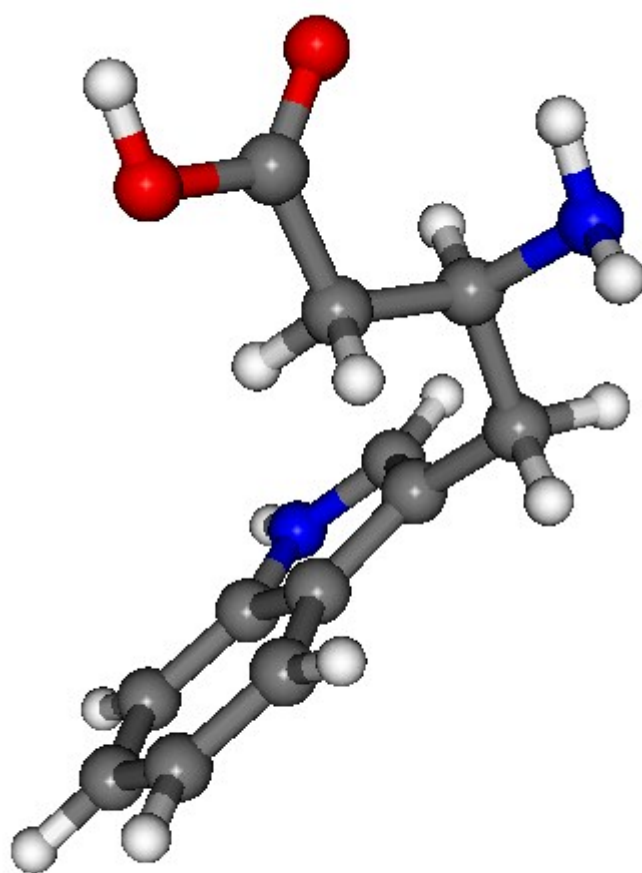
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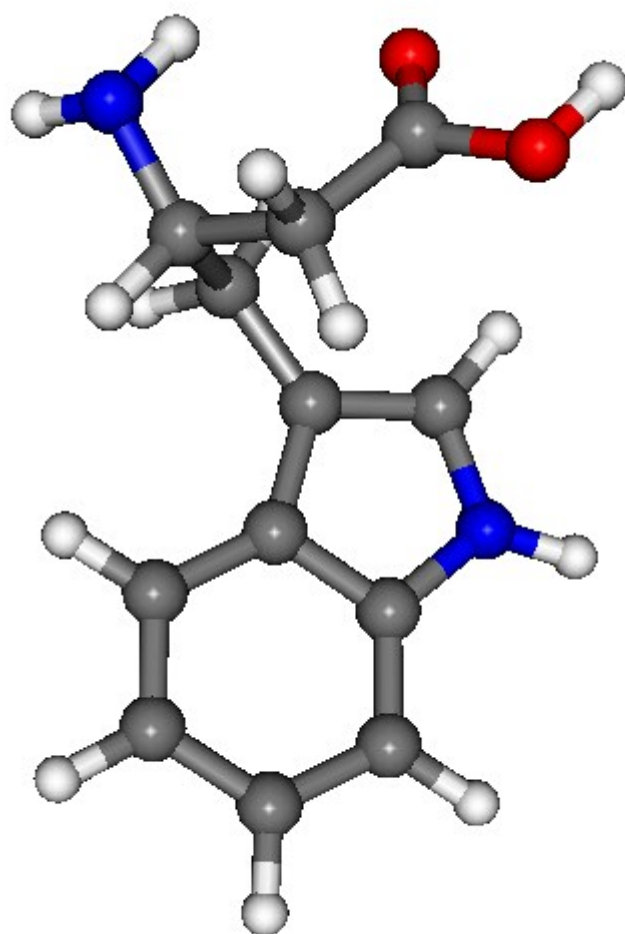
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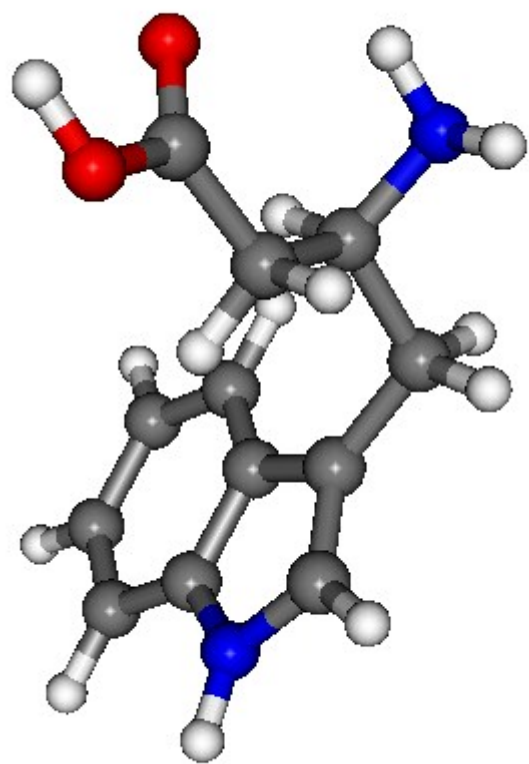
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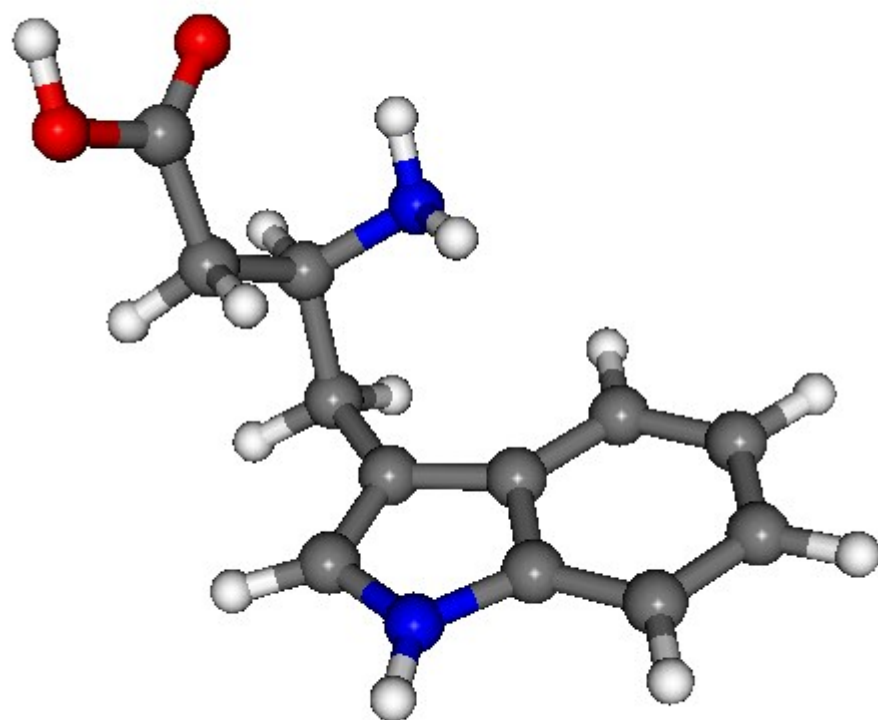
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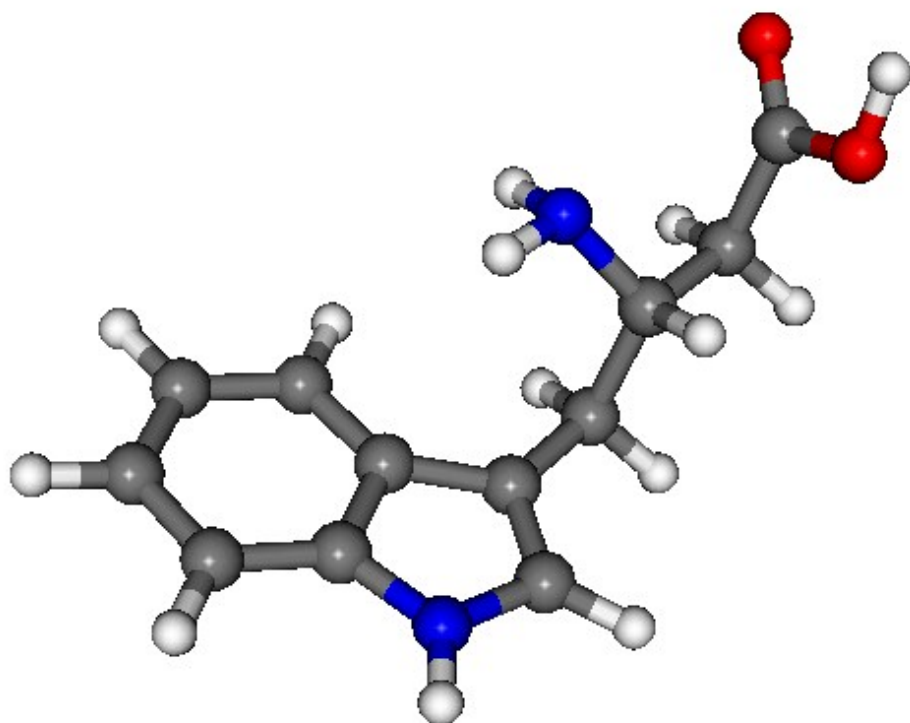
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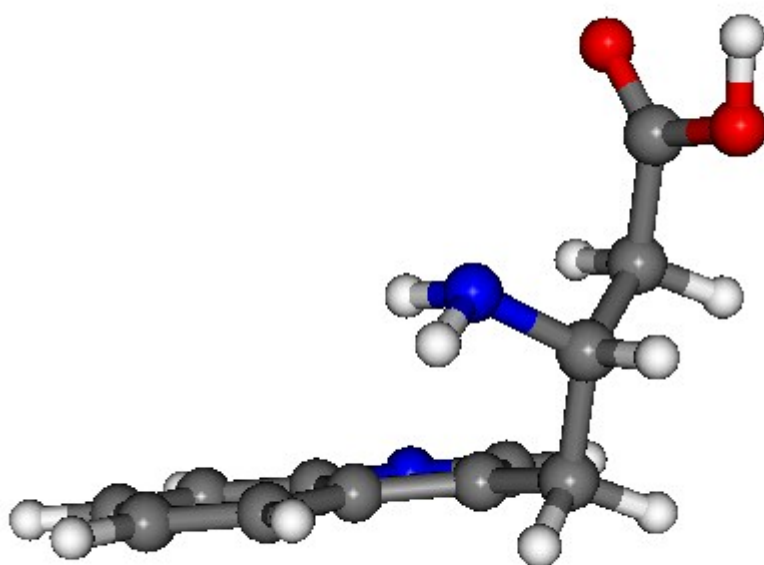
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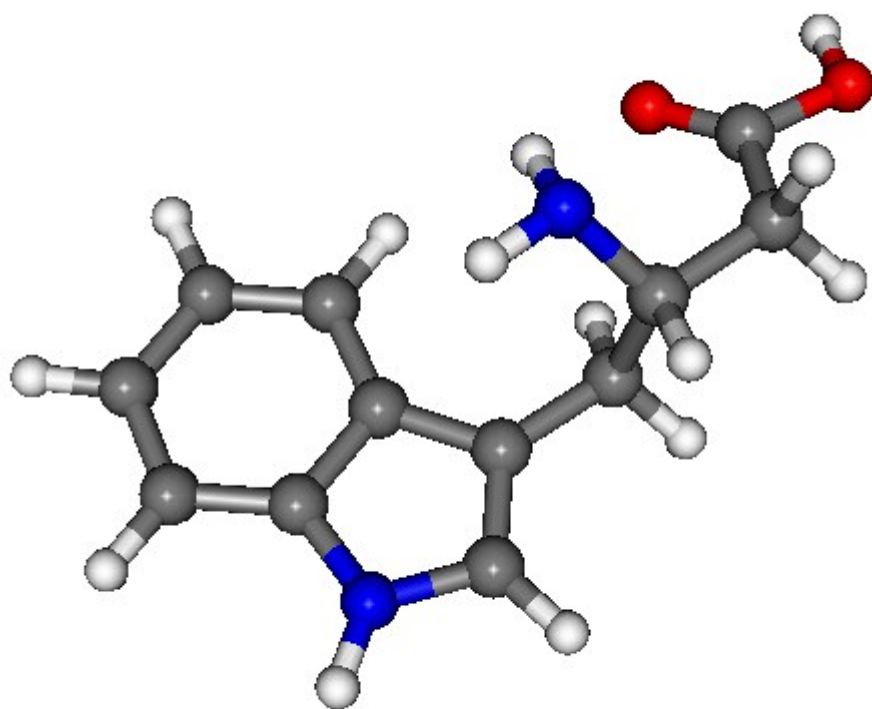
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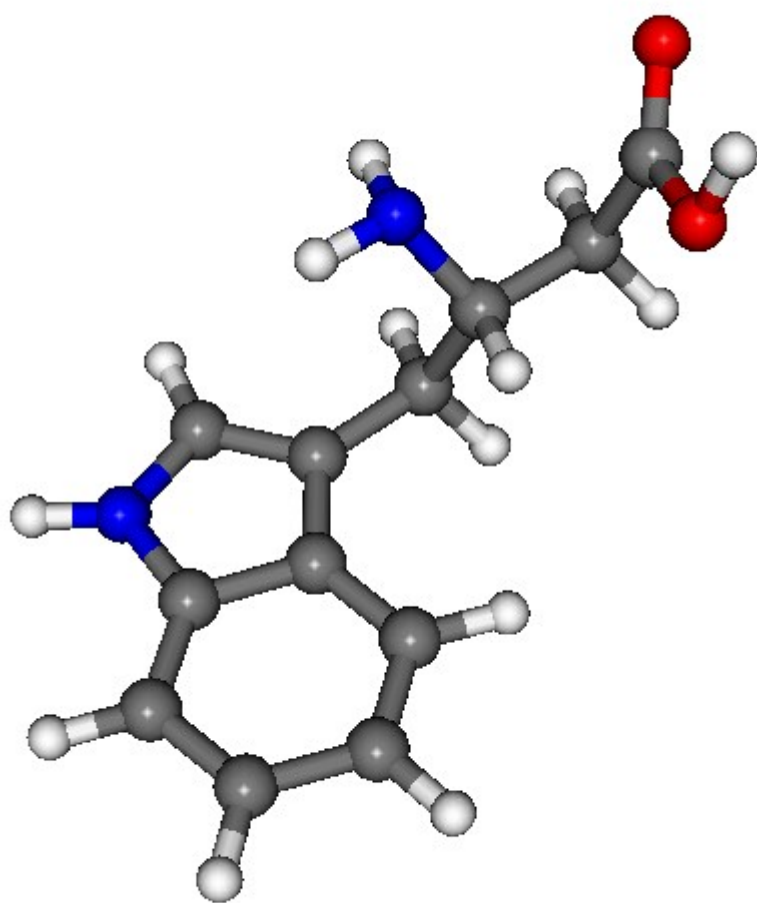
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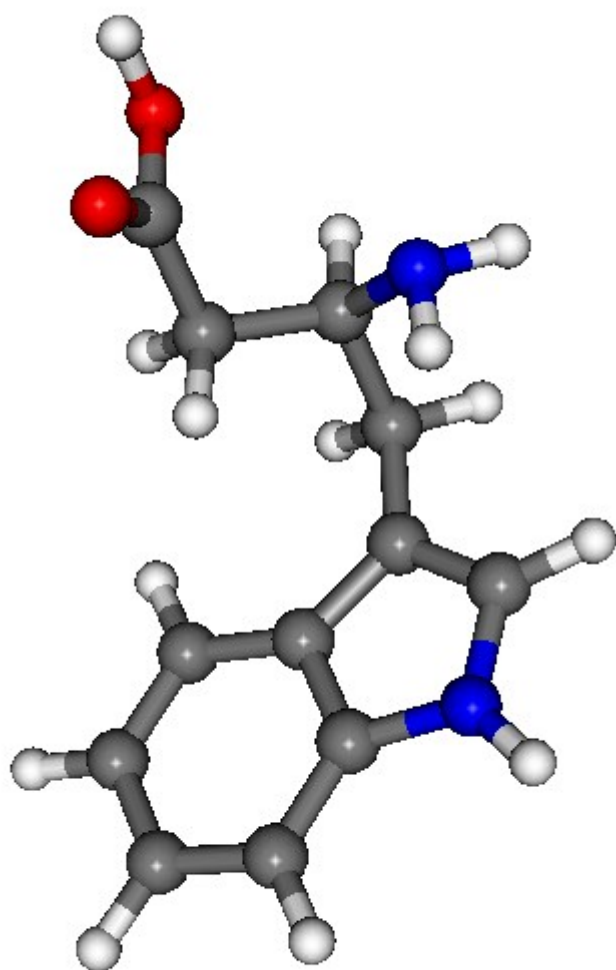
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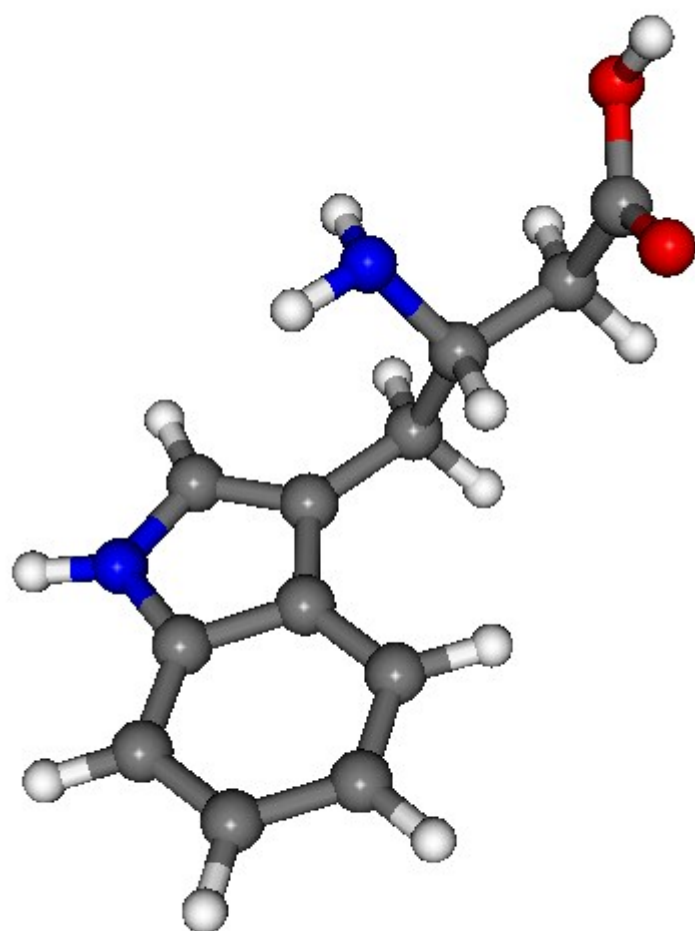
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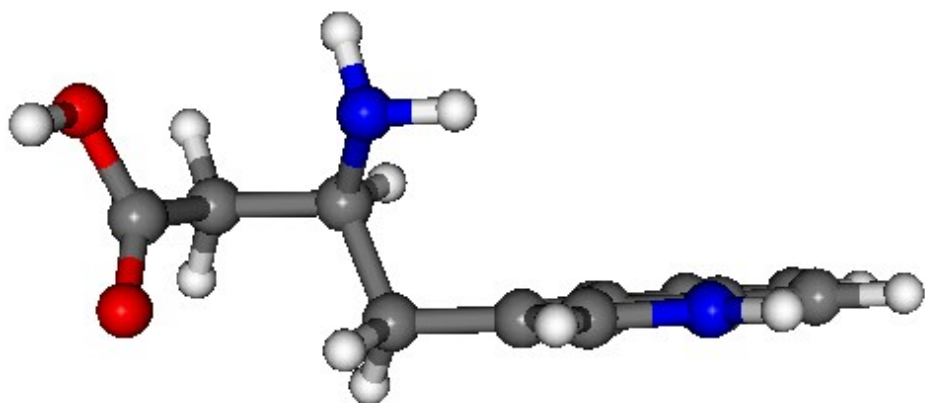
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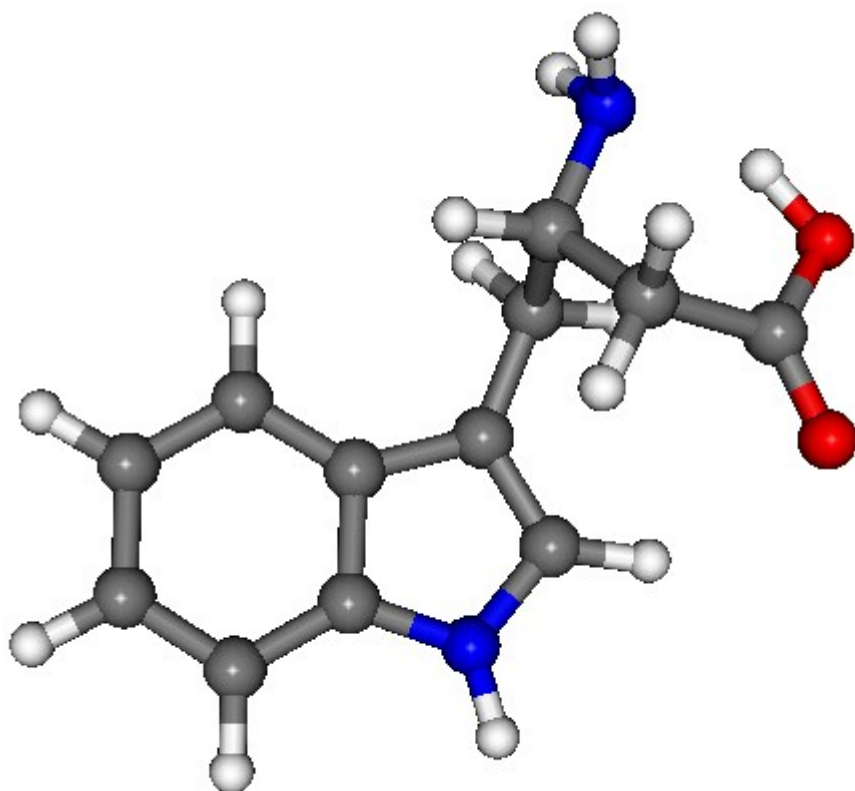
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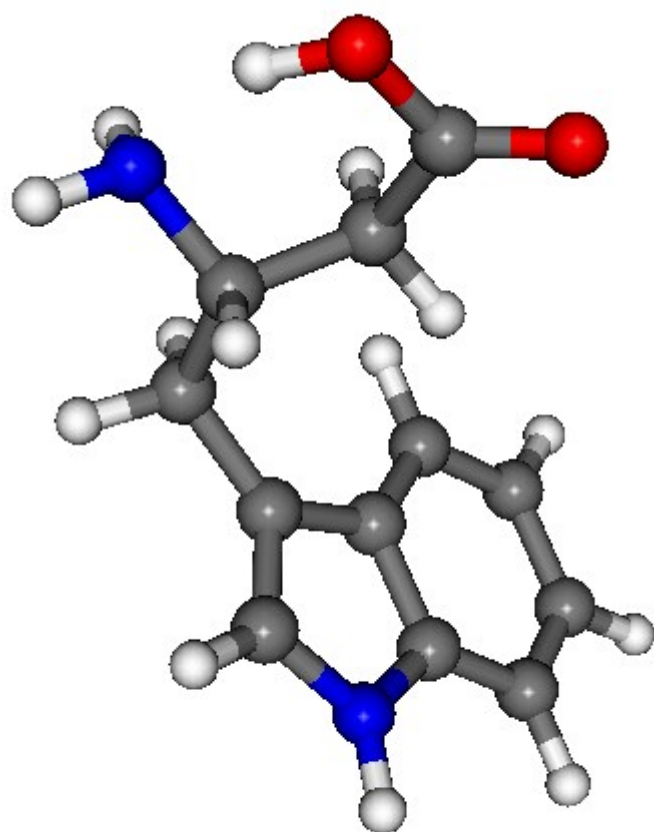
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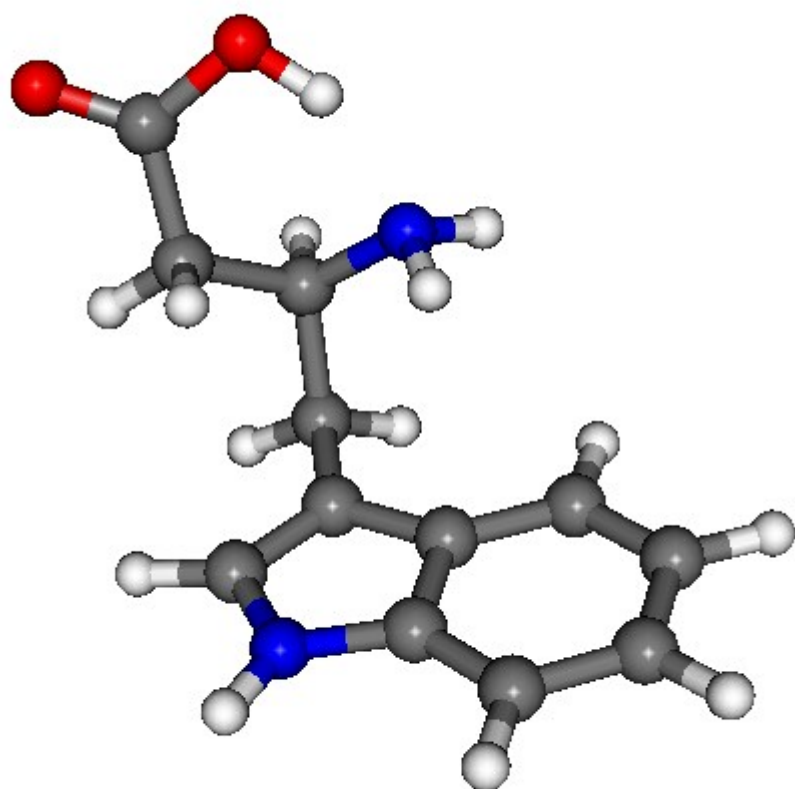
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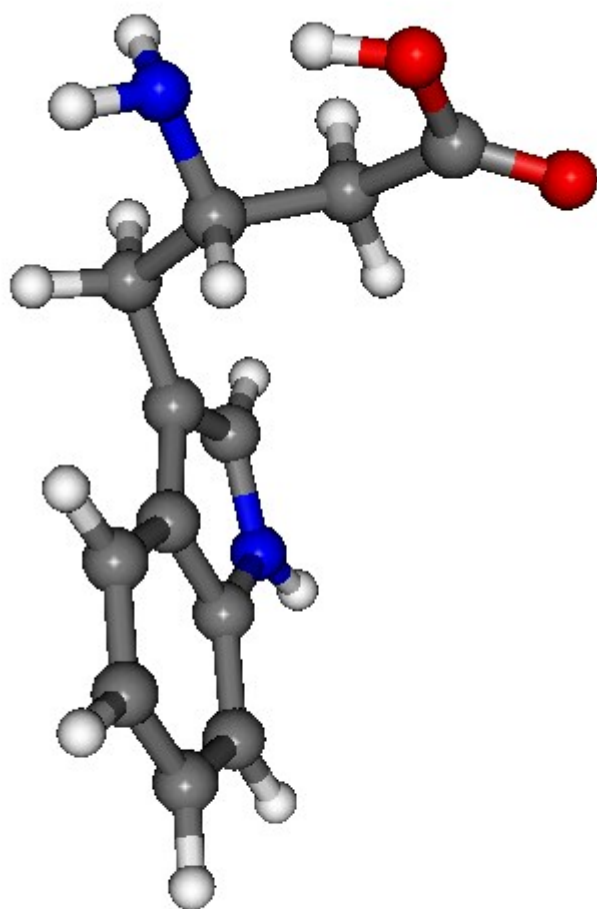
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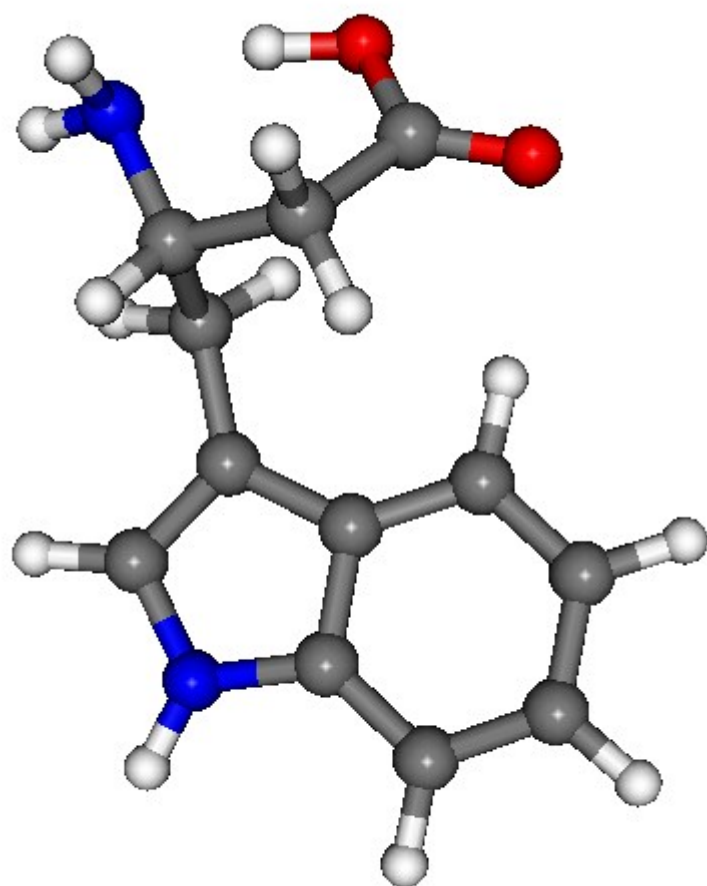
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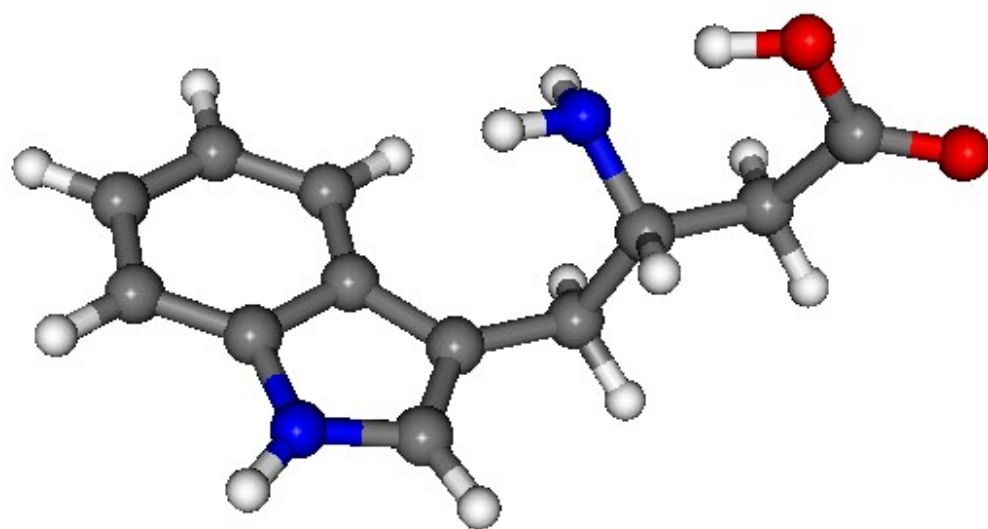
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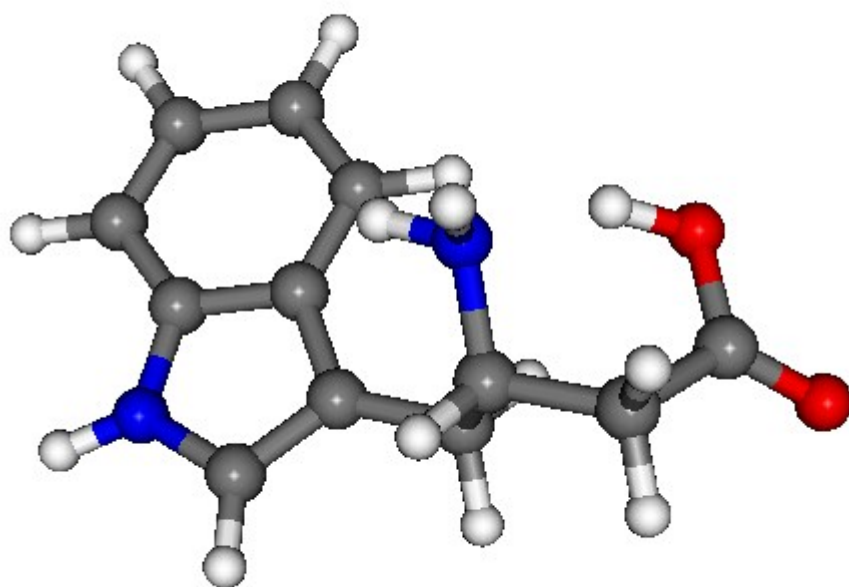
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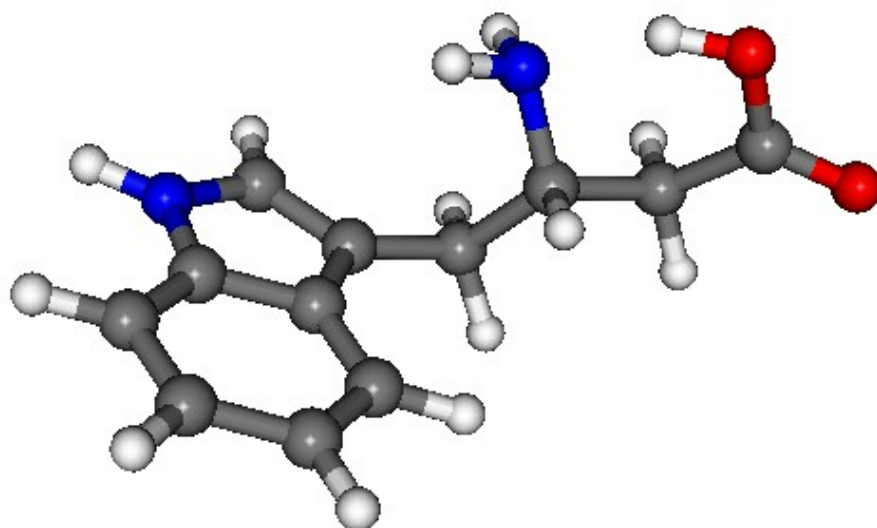
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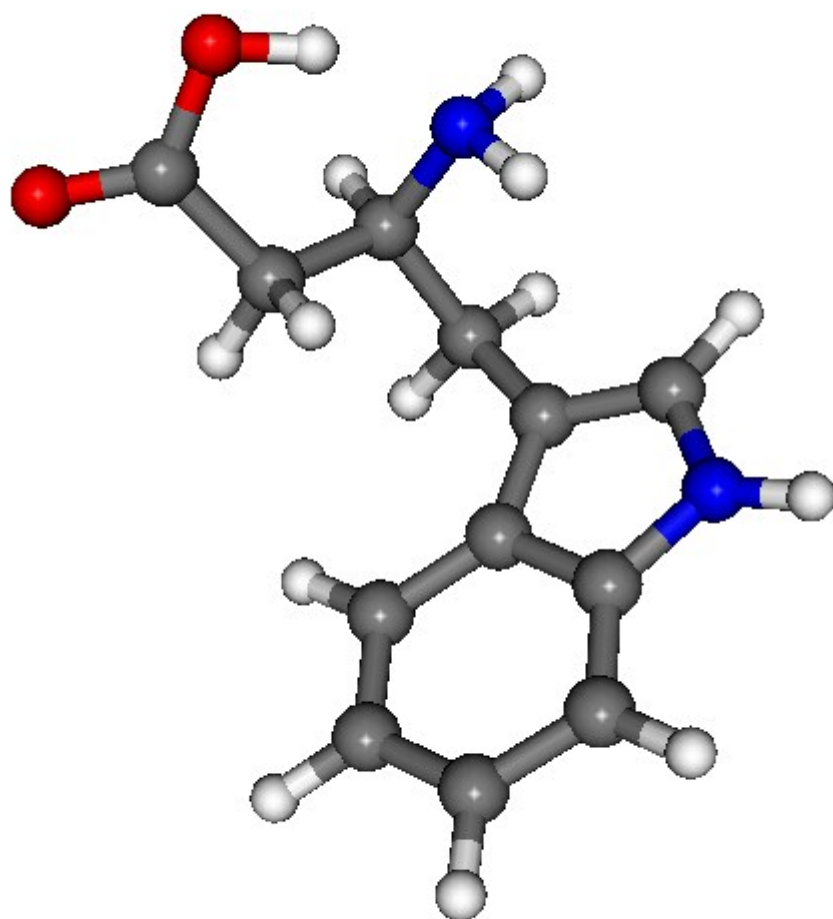
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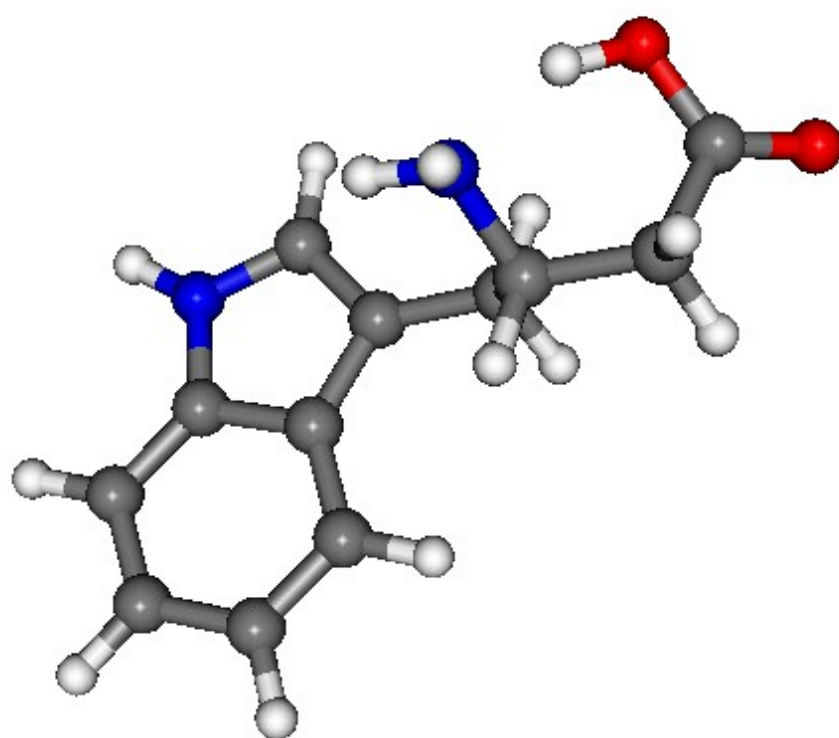
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O12



O14



O15

