

Electronic Supplementary Information

for

Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study

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of Sciences, Leninskiy Prospekt 33, 119071 Moscow, Russian Federation

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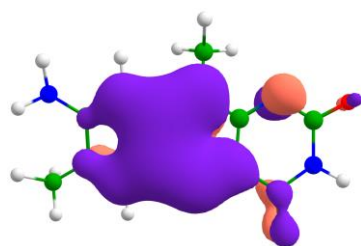
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Leninskie Gory 1/3, Moscow, 119991, Russian Federation

Phone: +7-495-939-20-35

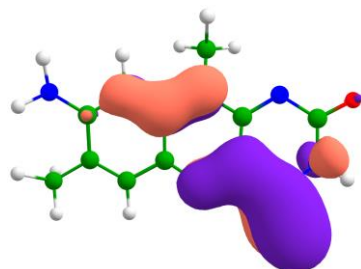
E-mail: khrenova.maria@gmail.com

Section S1. Active space orbitals for CASSCF(12/12) calculations of iLOV-a, iLOV-m and iLOV-d model systems.

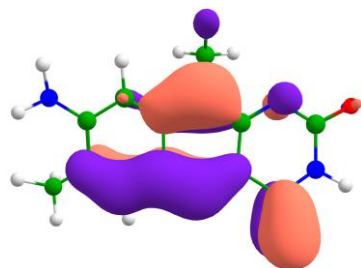
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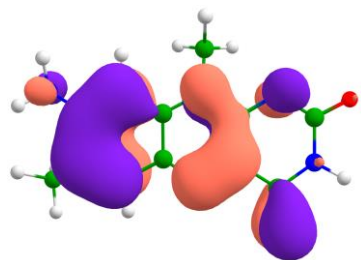
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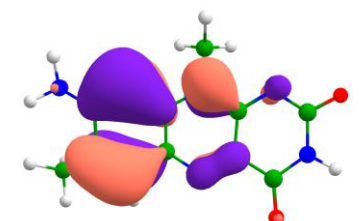
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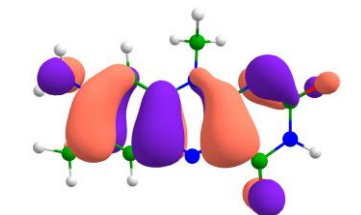
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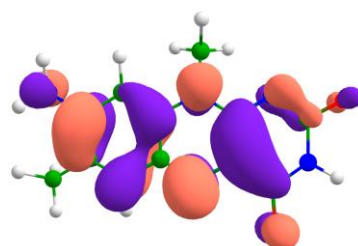
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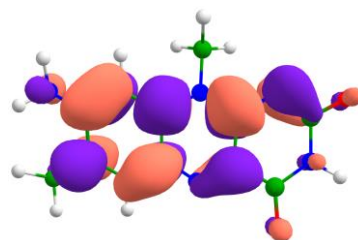
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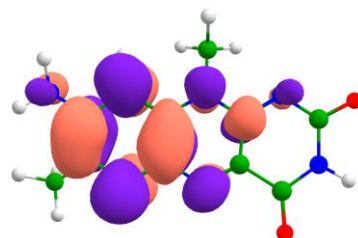
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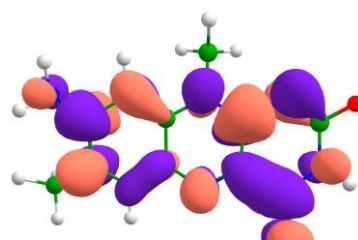
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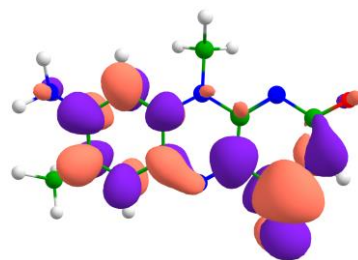
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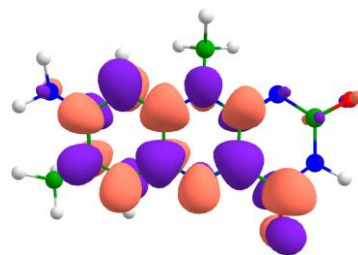
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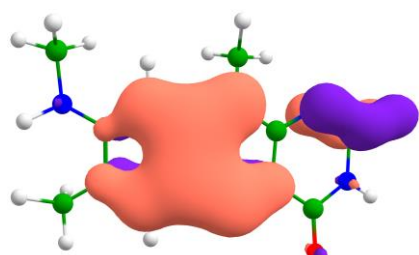
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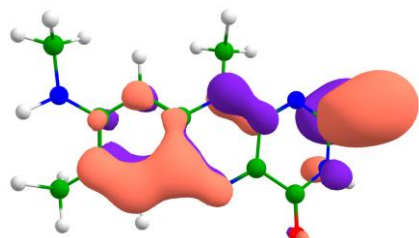
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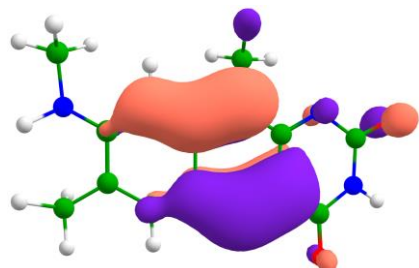
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iLOV-m

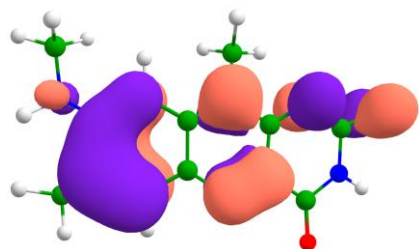
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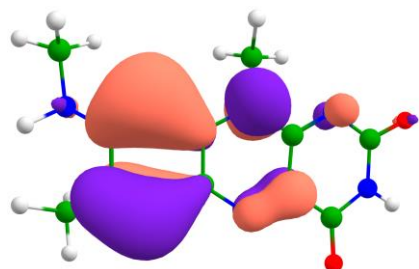
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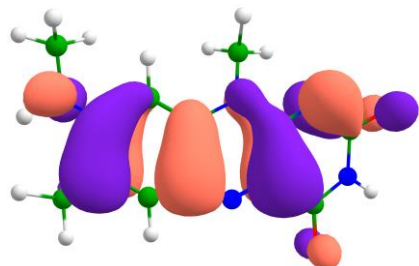
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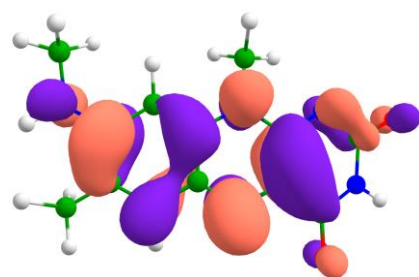
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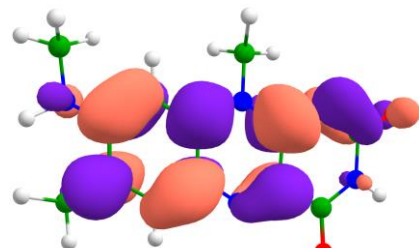
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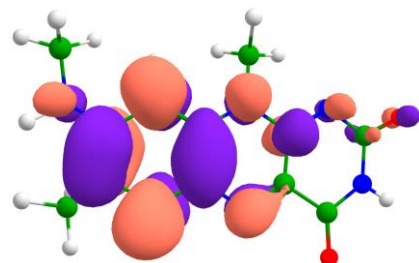
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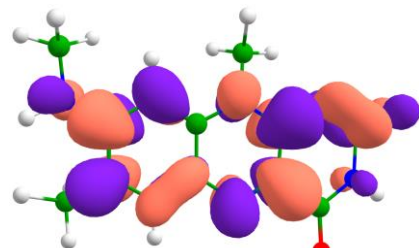
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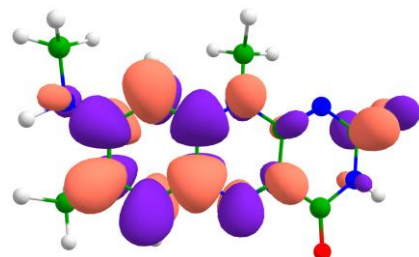
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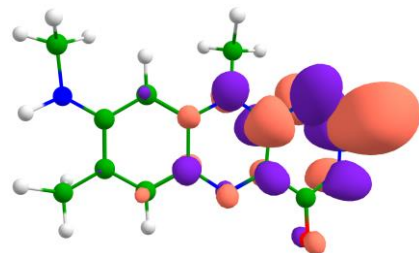
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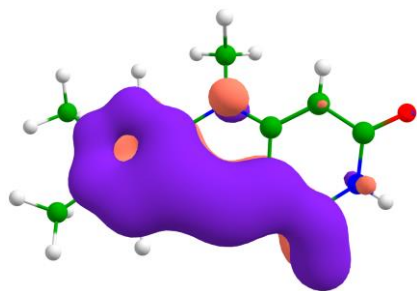
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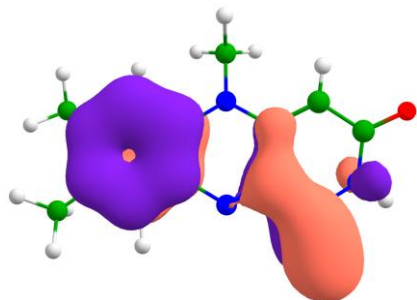
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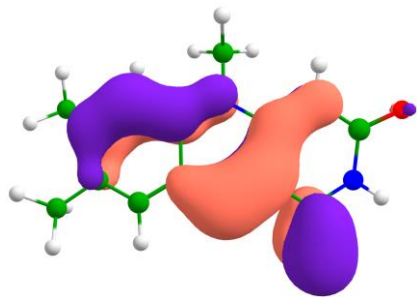
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iLOV-d

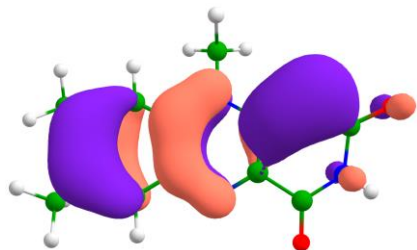
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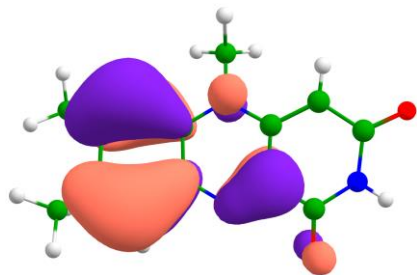
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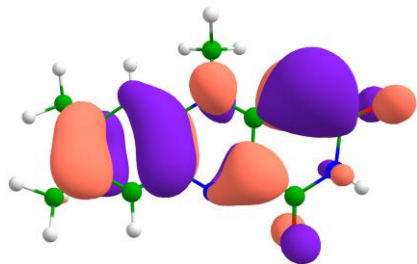
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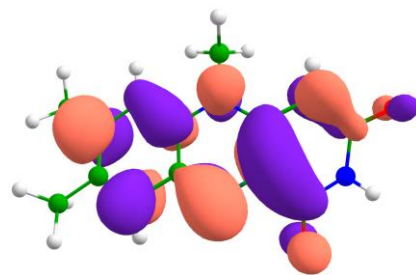
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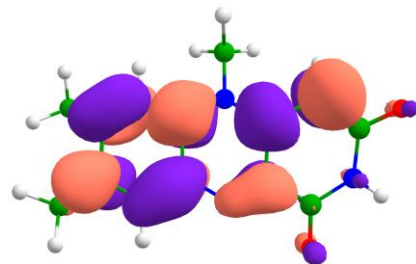
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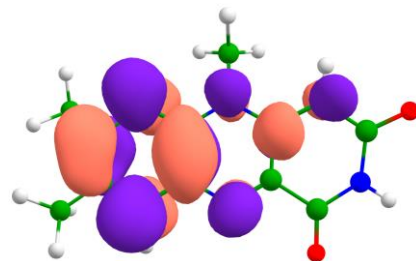
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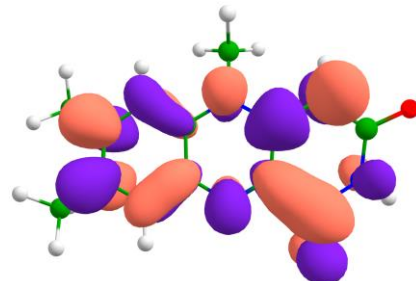
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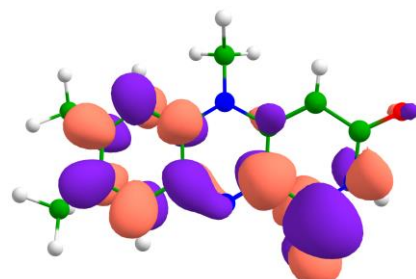
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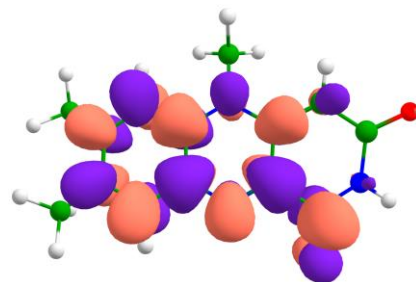
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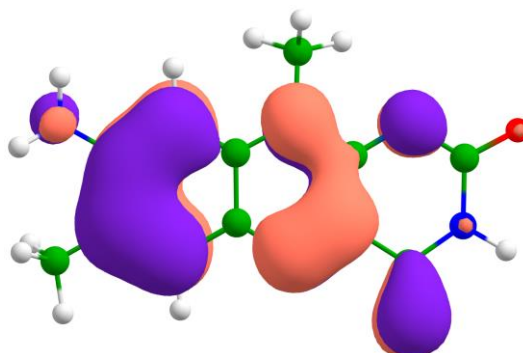
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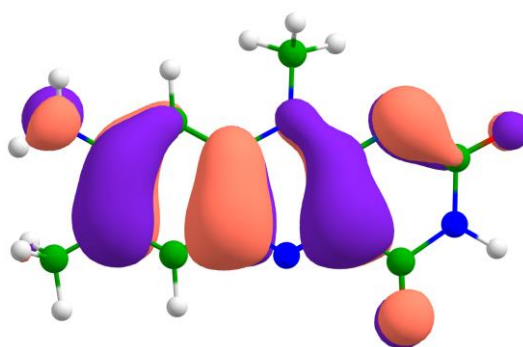
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Section S2. Active space orbitals for CASSCF(4/4) calculations of iLOV-a, iLOV-m and iLOV-d model systems and their mutants.

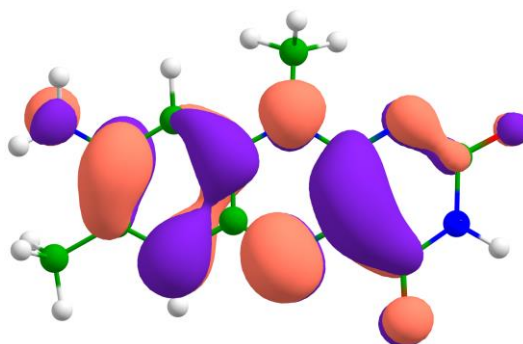
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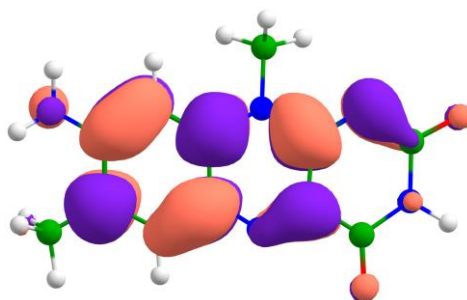
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HOMO

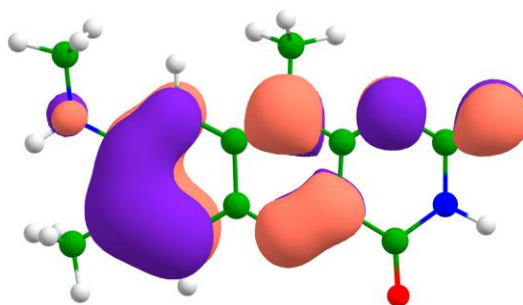


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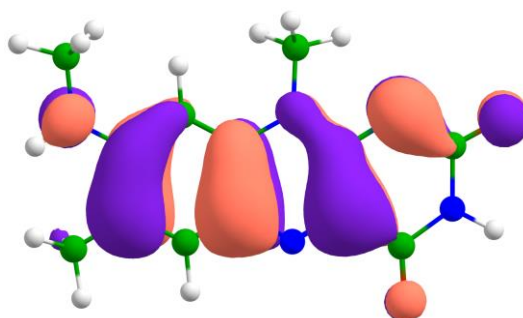


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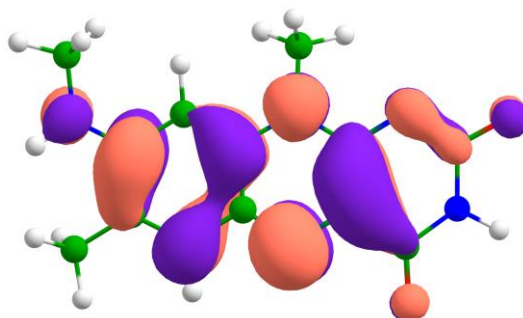
iLOV-m



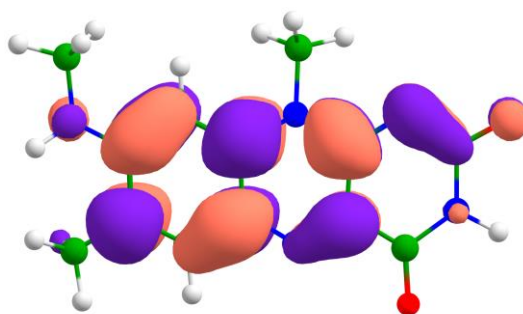
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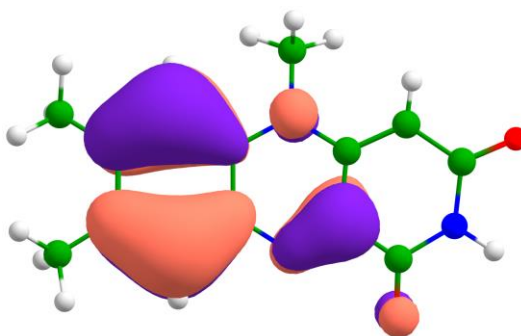


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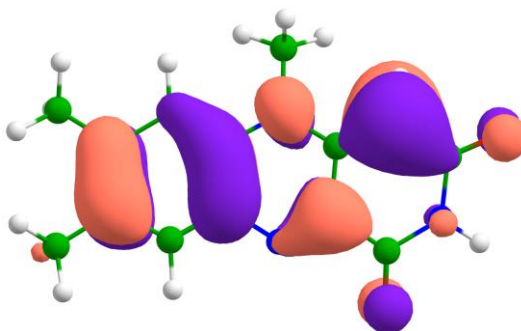


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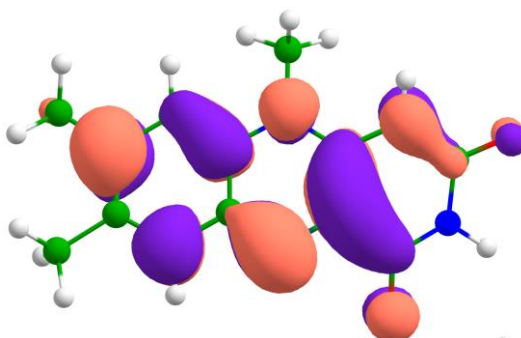
iLOV-d



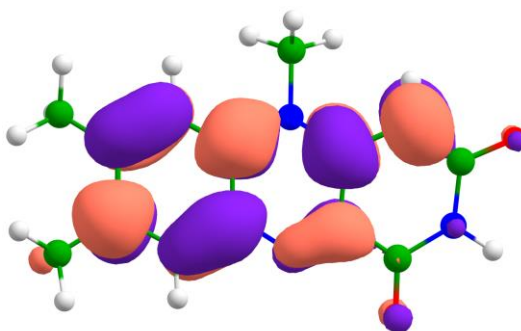
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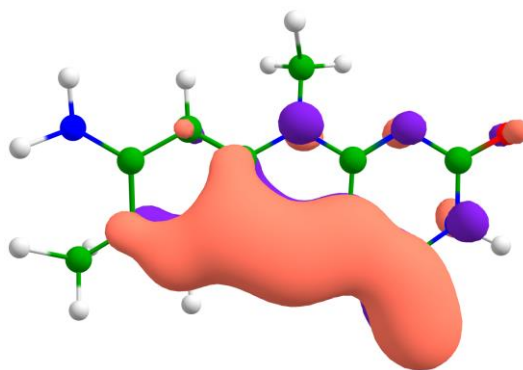


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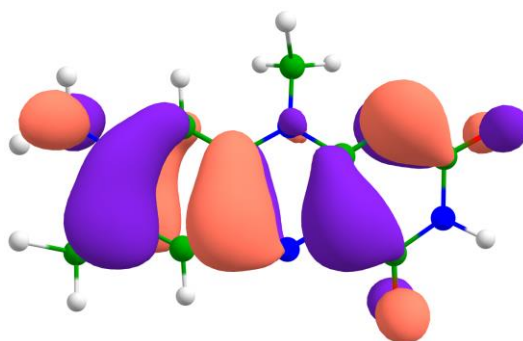


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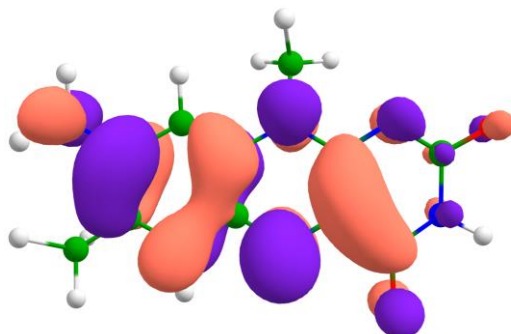
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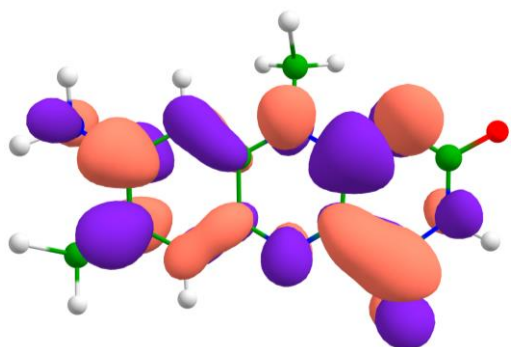
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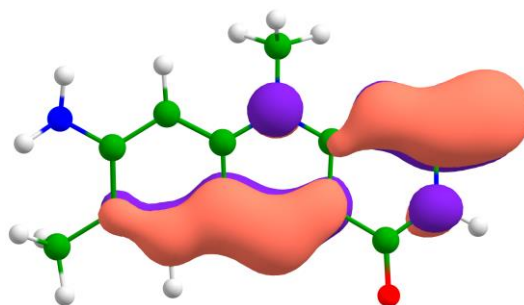


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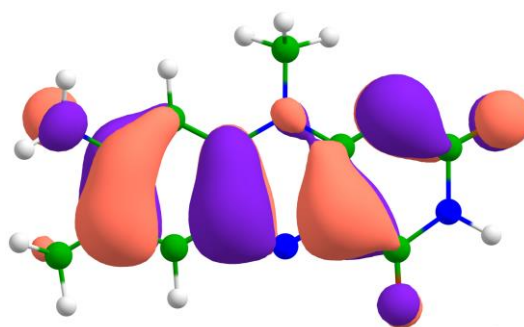


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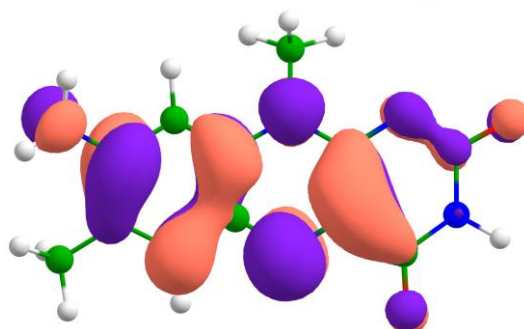
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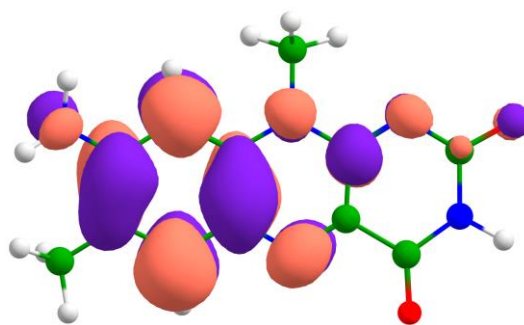
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HOMO

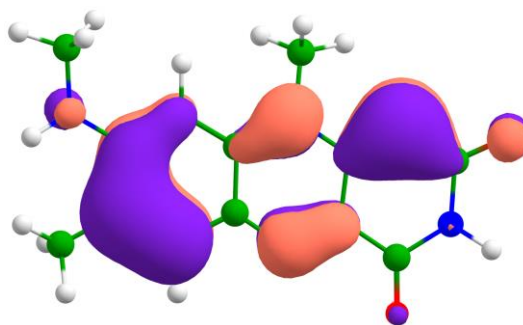


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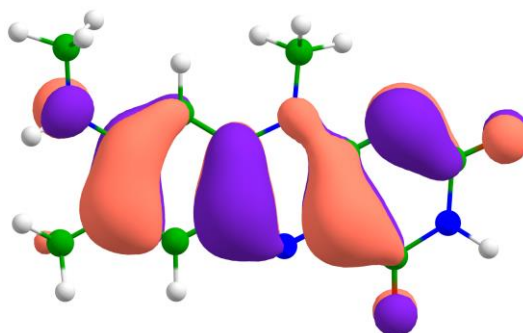


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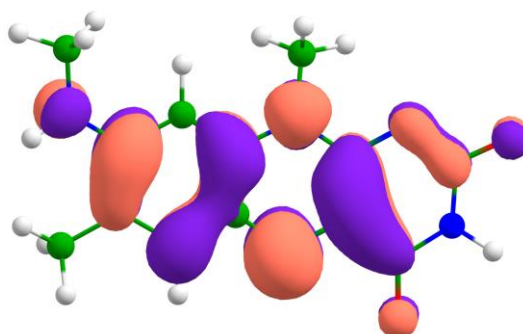
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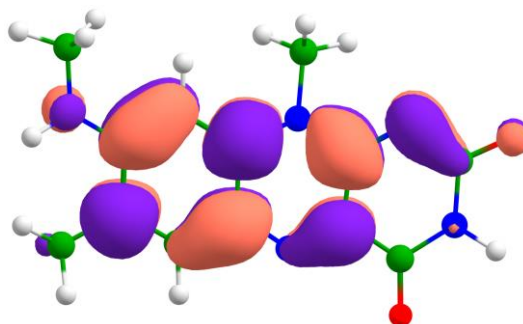
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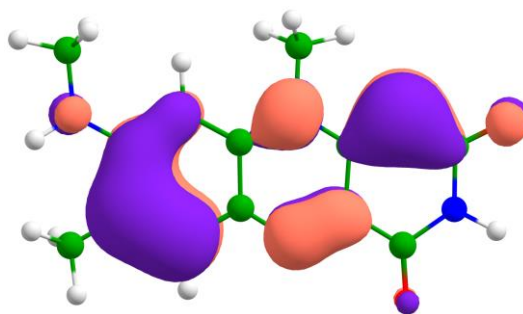


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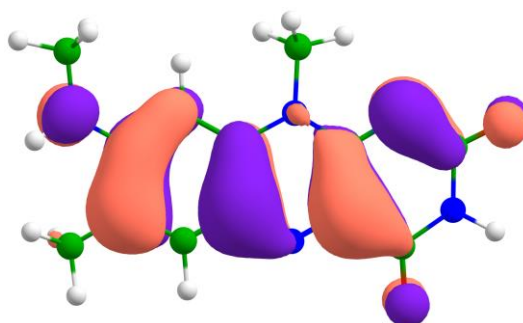


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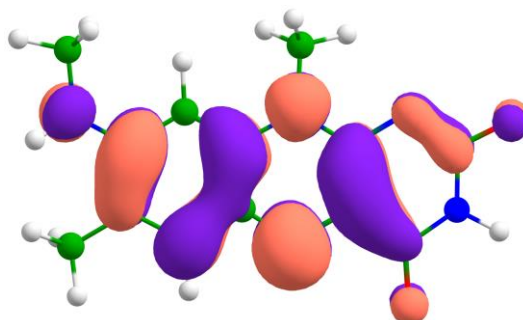
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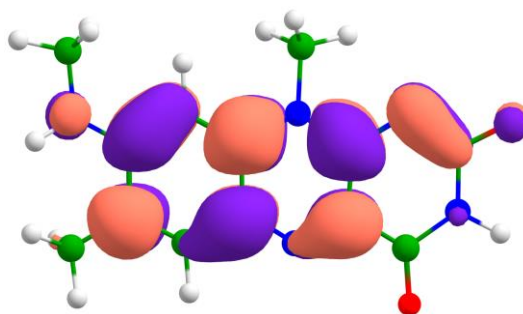
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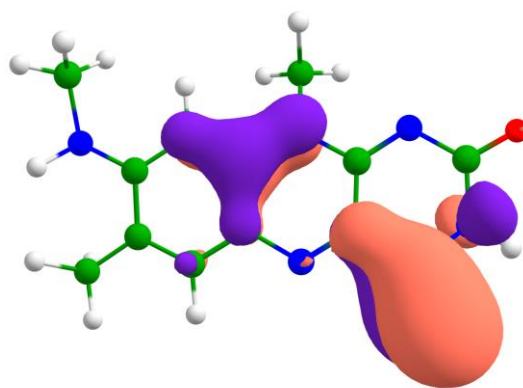


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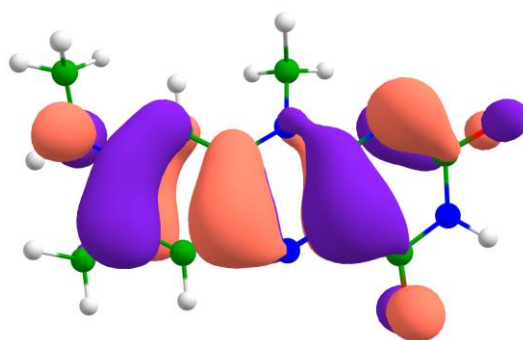


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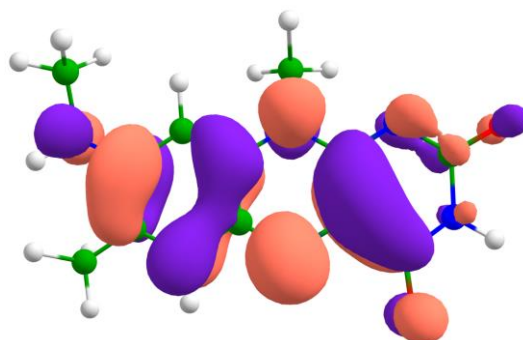
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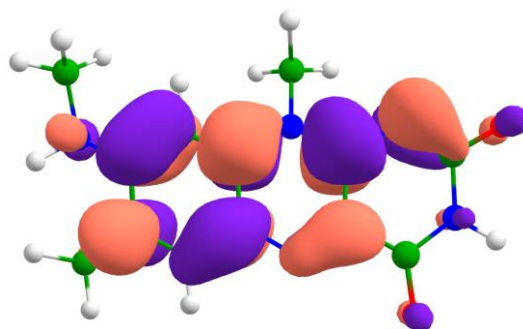
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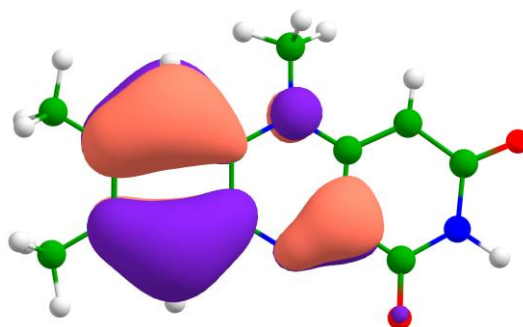


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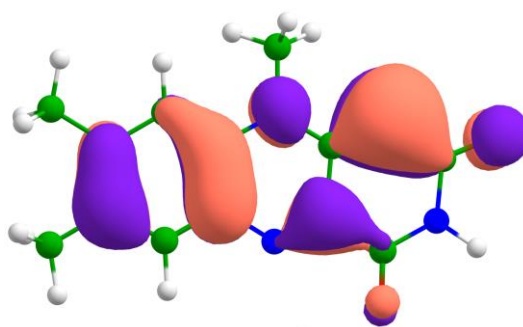


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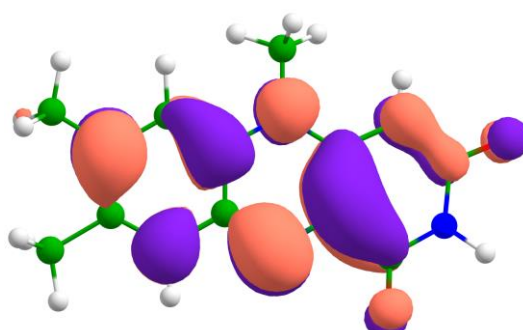
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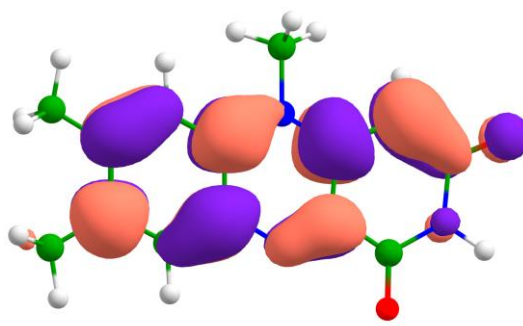
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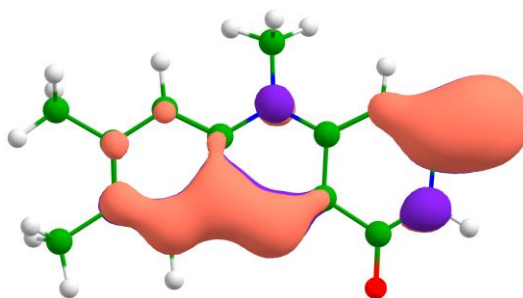


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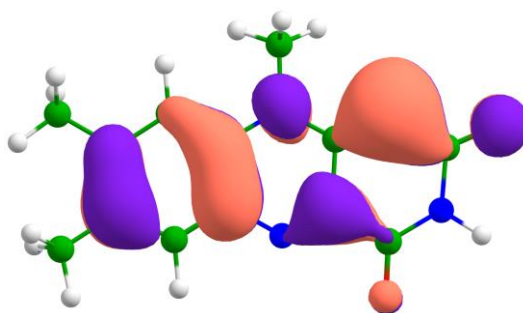


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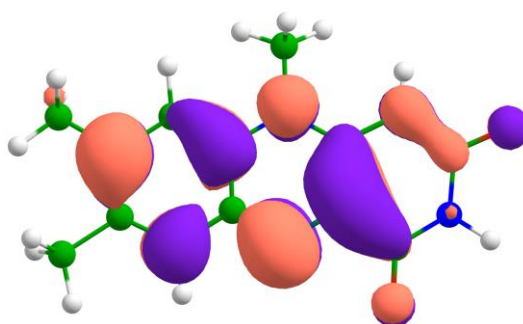
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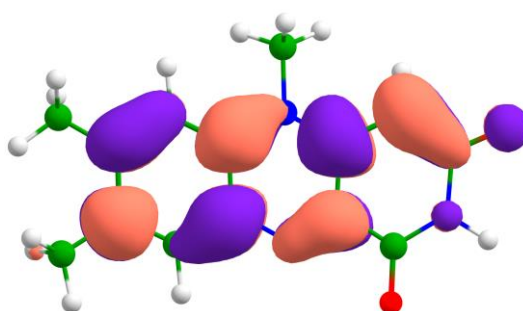
HOMO-1



HOMO



LUMO



LUMO+1