Supporting Information

Article

Identification of Potential Inhibitors for the Treatment of Alkaptonuria Using an Integrated In Silico Computational Strategy

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Supporting Information

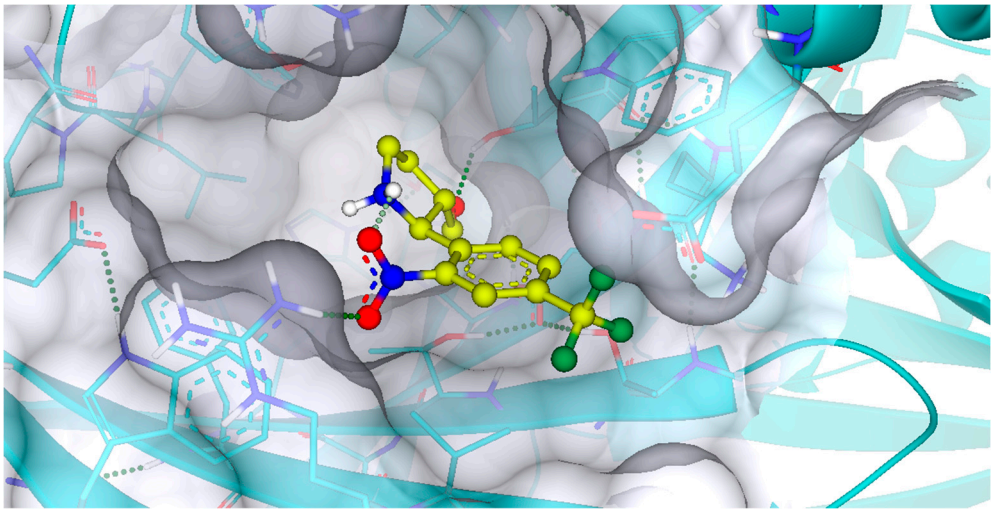

Figure S1. Docking complex of best hit of compound **a** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

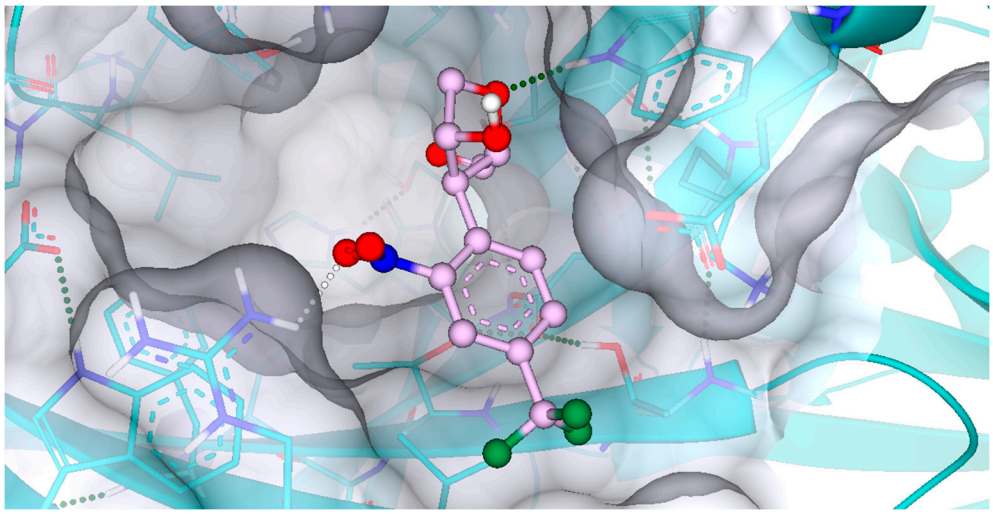

Figure S2. Docking complex of best hit of compound **b** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

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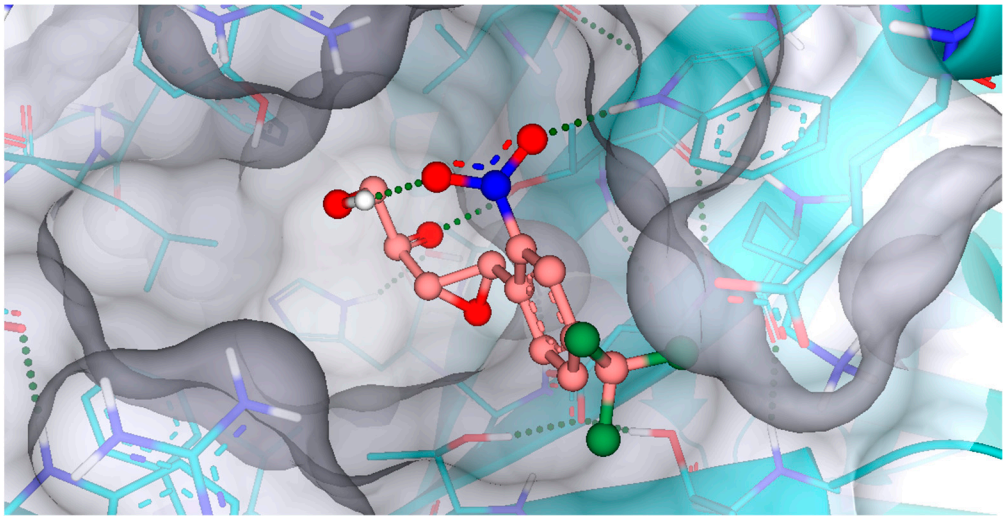

Figure S3. Docking complex of best hit of compound **d** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

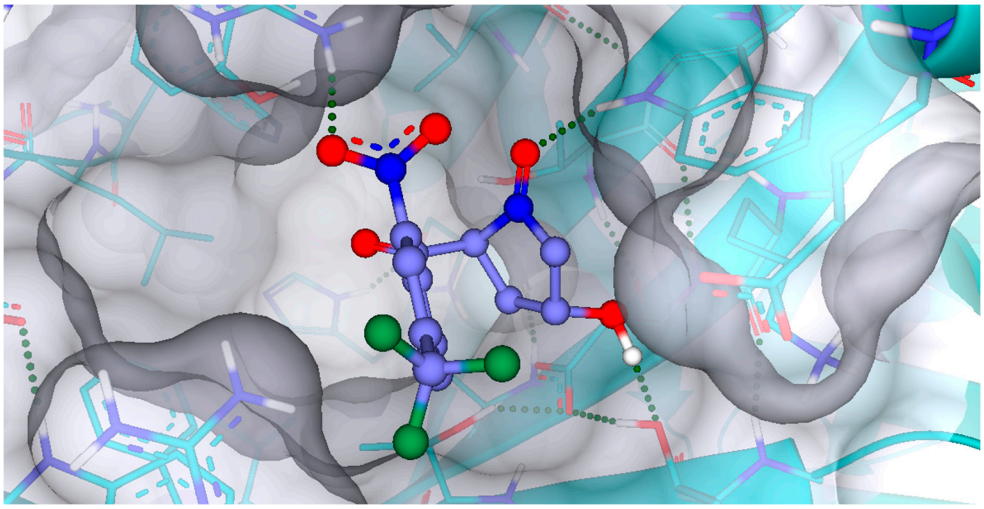

Figure S4. Docking complex of best hit of compound **e** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

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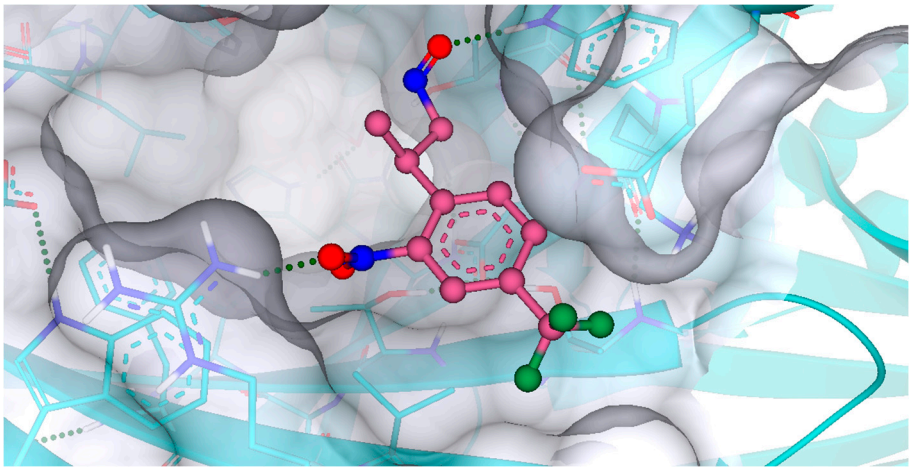

Figure S5. Docking complex of best hit of compound **g** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

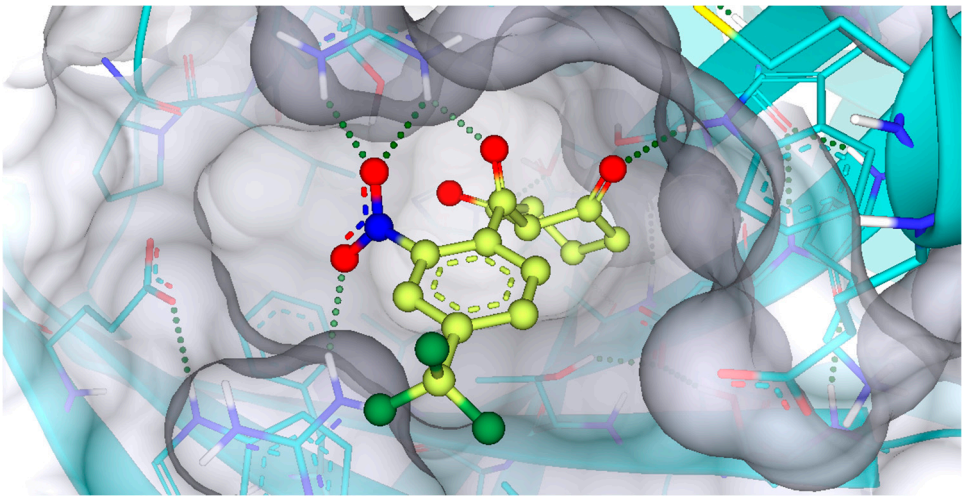

Figure S6. Docking complex of best hit of compound **h** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

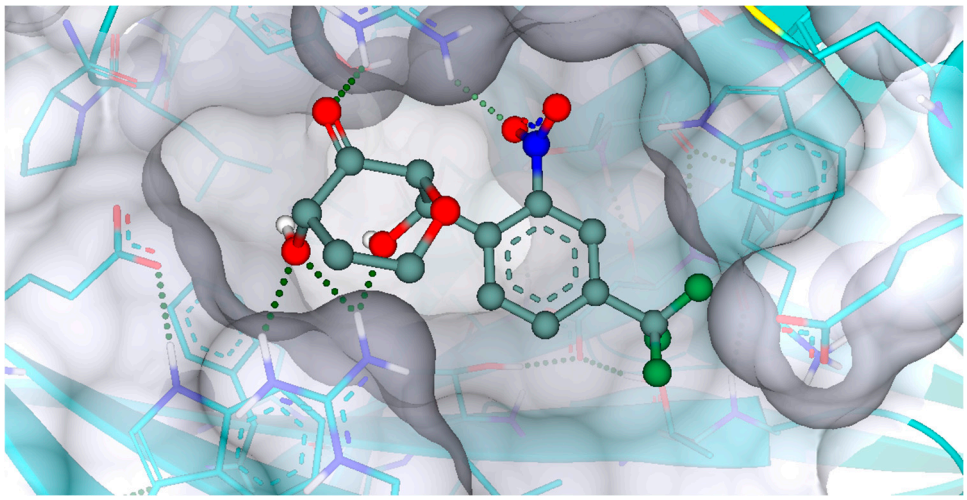

Figure S7. Docking complex of best hit of compound **i** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.

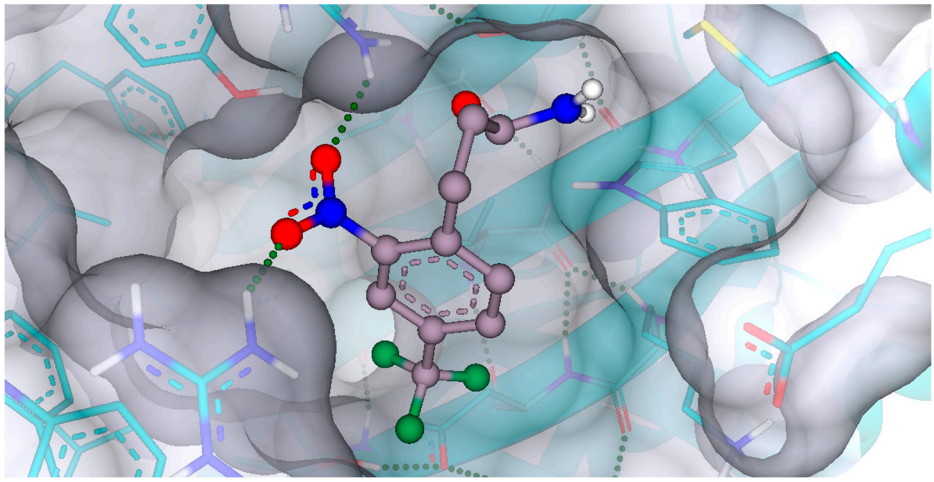

Figure S8. Docking complex of best hit of compound **j** on the basis of highest affinity, minimum binding energy, no or minimum torsion as well as the absence of any intra- and inter-molecular clashes.