Supporting Information for

Predicting protein-ligand binding affinity and correcting crystal structures with quantum mechanical calculations: Lactate Dehydrogenase A.

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\textsuperscript{b) IMED Oncology and Discovery Sciences, AstraZeneca, c/o Darwin Building, 310 Cambridge Science Park, Milton Rd, Cambridge, CB4 0WG, UK.}

\textsuperscript{c) Sygnature Discovery Ltd, Bio City, Pennyfoot St, Nottingham, UK NG1 1GF}
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S1. Interaction potential curves for a range of functional groups computed at the M06/6-31+G** level.

Methane with Methane [non-polar – non-polar]
Methane with Water [non-polar – polar]
Methane with Benzene [non-polar – non-polar]
Methane with Pyridine [non-polar – polar]
Methane with Amide carbonyl [non-polar – polar]
Methane with Amide NH [non-polar – polar]
Water with Water [polar – polar]
Water with Benzene [polar – non-polar]
Water with Pyridine [polar – polar]
Water with Amide Carbonyl [polar – polar]
Water with Amide NH [polar – polar]
Benzene with Benzene [non-polar – non-polar]

Examples involving aromatic compounds such as this are likely to be in error thanks to known problems with reproducing the interaction curves for higher levels of theory which suggest that minima might be at -1.7 to -2.8 kcal/mol.¹
Benzene with Pyridine [non-polar – polar]
Benzene with Amide Carbonyl [non-polar – polar]
Benzene with Amide NH [non-polar – polar]
Pyridine with Pyridine [polar – polar MISMATCHED]
Pyridine with Amide Carbonyl [polar – polar MISMATCHED]
Pyridine with Amide NH [polar – polar]
Amide Carbonyl with Amide NH [polar – polar]
S2. Quantum mechanical binding energies, logPs and observed affinities used to create Table 1 in the main text

A – Mineralocorticoid Receptor.²

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<th>ΔE (kcal/mol)</th>
<th>logD (measured)</th>
<th>pKi</th>
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B – Inducible NO synthase.³

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<th>pIC₅₀</th>
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C – Beta-secretase inhibitors.

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<th>ΔE (kcal/mol)</th>
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<th>Free-Wilson contributions to pIC_{50}</th>
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An experimental value of $\Delta G$ for binding was converted to a $pK_D$ using $-\log_{10}(e^{-\Delta G/RT})$.

<table>
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<tr>
<th>$\Delta E$ (kcal/mol) TPSS/TZVPP</th>
<th>SlogP (calculated in MOE from Chemical Computing Group)</th>
<th>$pK_D$ (from experimental $\Delta G$ for binding)</th>
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C)
E – Octa-acid cavitand.\textsuperscript{6}
An experimental value of $\Delta G$ for binding was converted to a pK$_D$ using $-\log_{10}(e^{-\Delta G/RT})$.

<table>
<thead>
<tr>
<th>$\Delta E$ (kcal/mol) BP86/TZVP+COSMO</th>
<th>ALOGP computed in Chemdoodle</th>
<th>pK$_D$</th>
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F – Cyclodextrin.\textsuperscript{7}
An experimental value of $\Delta G$ for binding was converted to a pK$_D$ using $-\log_{10}(e^{-\Delta G/RT})$.

<table>
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<th>$\Delta E$ (kcal/mol)</th>
<th>ALOGP computed in Chemdoodle</th>
<th>pK$_D$</th>
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F)
**S3. Statistics and coefficients for approach employing Number of hydrophobic atoms in place of logP**

Number of hydrophobic atoms was computed in MOE but fluorines were subsequently removed from the count.

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<th>Label</th>
<th>System</th>
<th>$\Delta E + \text{random}$</th>
<th>$\Delta E + N_{\text{hydrophobic}}$</th>
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<th>$\beta$</th>
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<td>$R^2$</td>
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### S4. XYZ coordinates for the occeptor complexes

**Compound 1**

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S5. Density maps (2mFo-DFc) of ligands 1, 2, 5, 6 and 7 contoured at 1 \( \sigma \).

S6. References.

