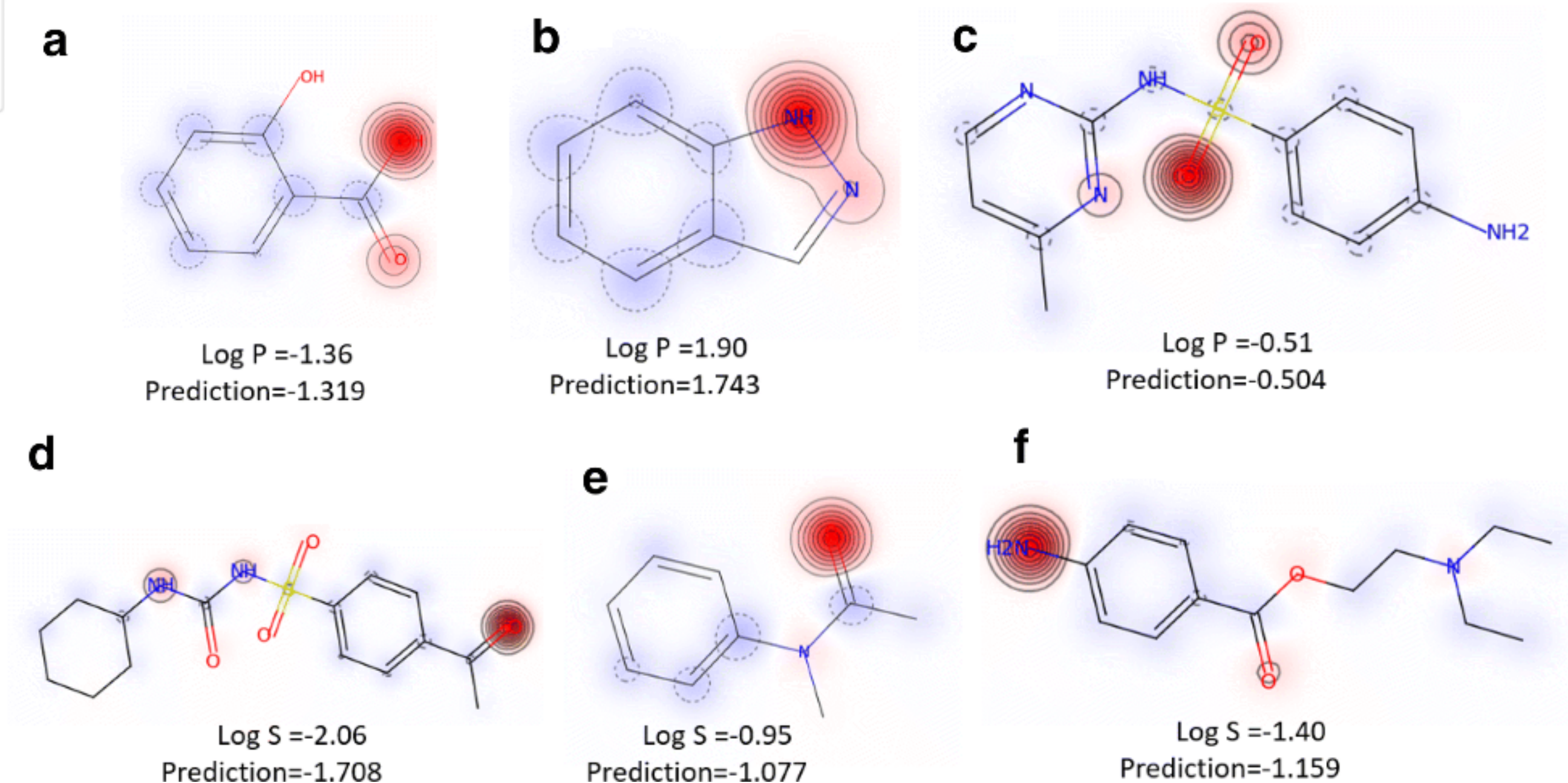
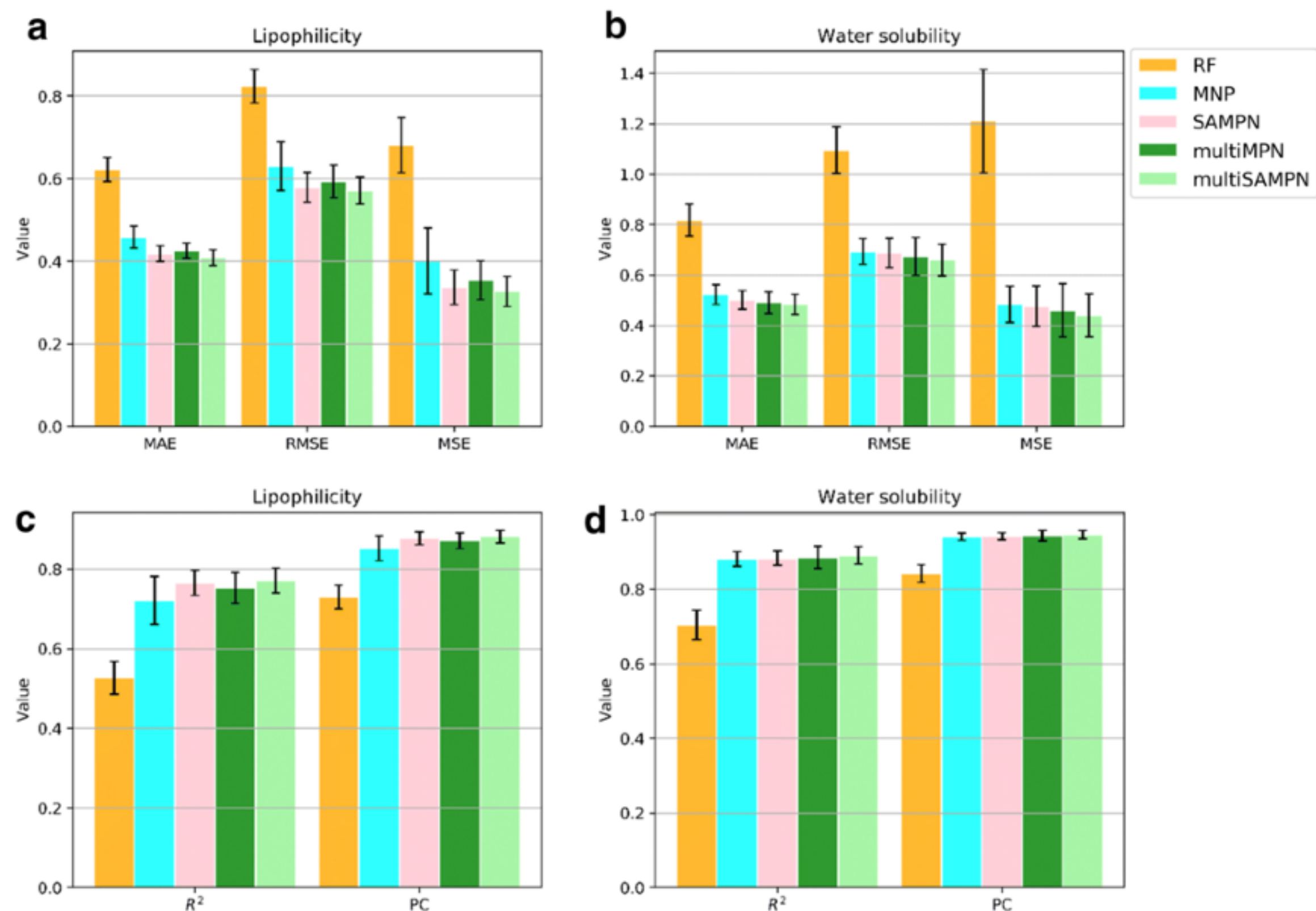


Opening the black box?



Recent deep learning method seems to perform well in solubility prediction and also highlights moieties that contribute to (red) or detract from (blue) solubility. See Ref. [7].

Free energy calculations of solubility