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                                                paper/assay paper_id  \
66  http://dx.doi.org/10.1016/j.bmcl.2013.08.112       17B
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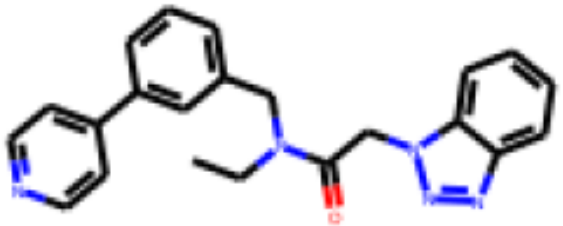
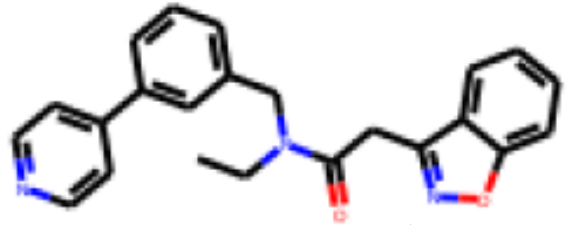
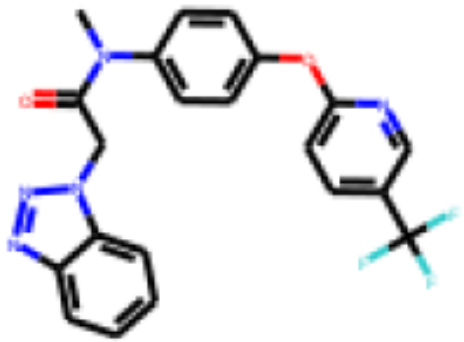
Focus on keeping benzotriazole, amide, and tertiary amine as pharmacophore

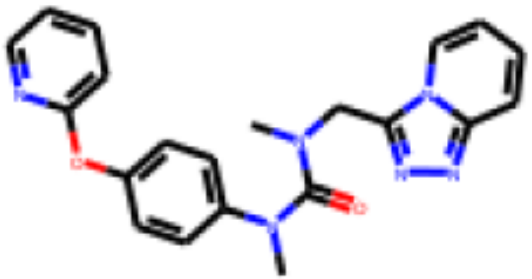
Then choose candidates with sufficient diversity and sufficient branching to fill P-1 or P2

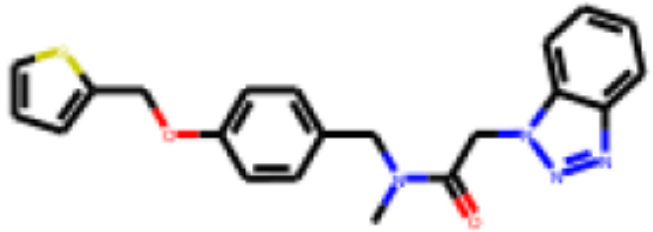




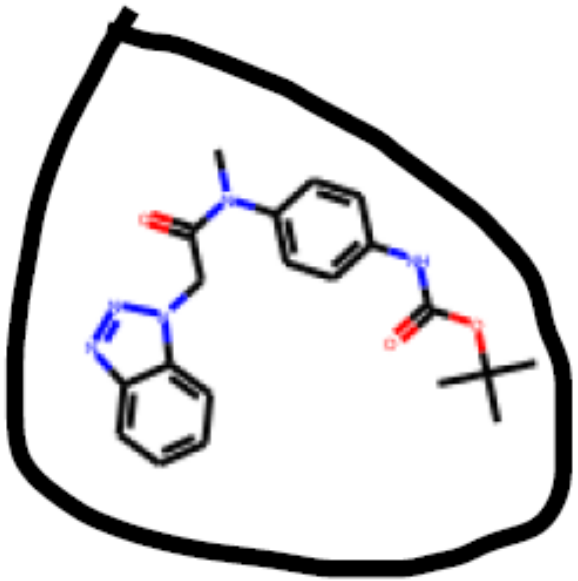
New ring system might be interesting

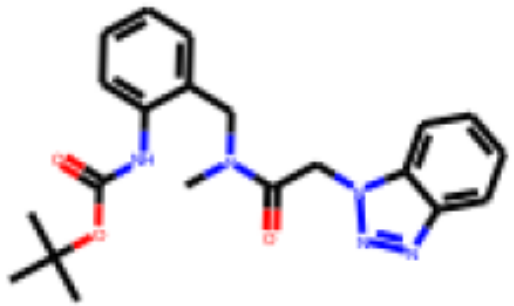


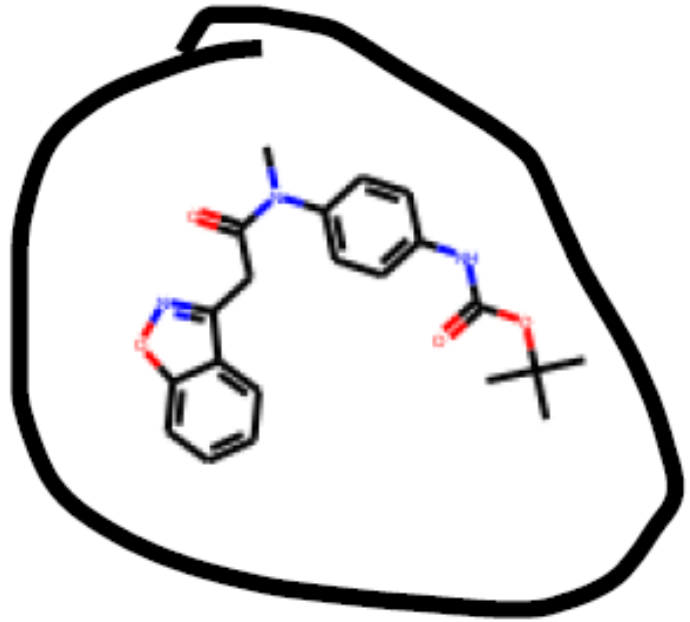




		paper/assay	paper_id
70	http://dx.doi.org/10.1016/j.bmcl.2013.08.112		16B

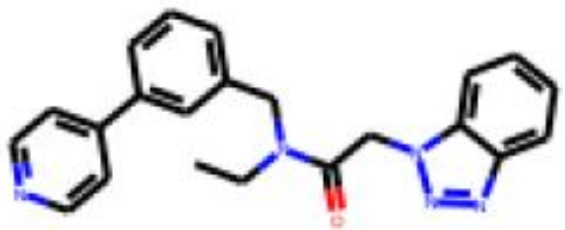
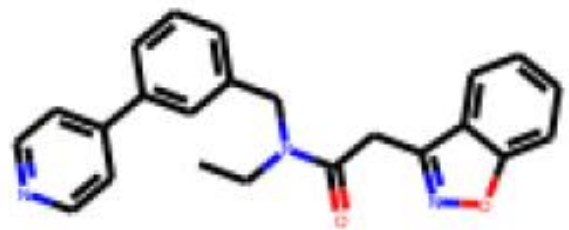
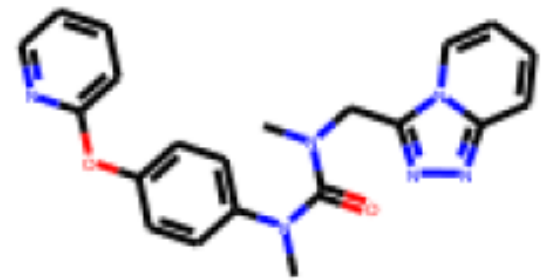
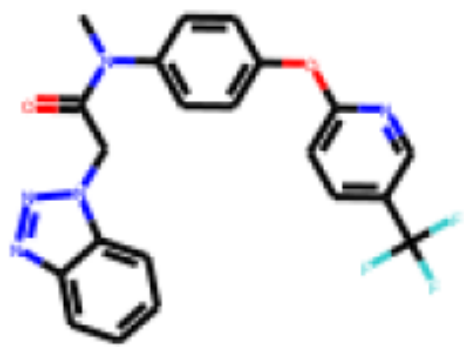
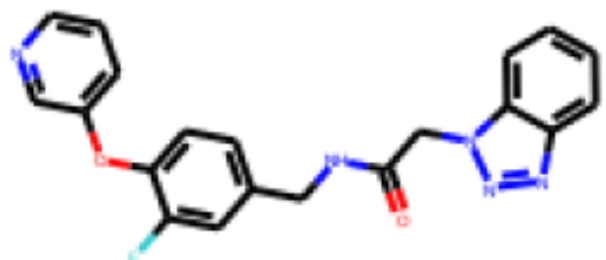
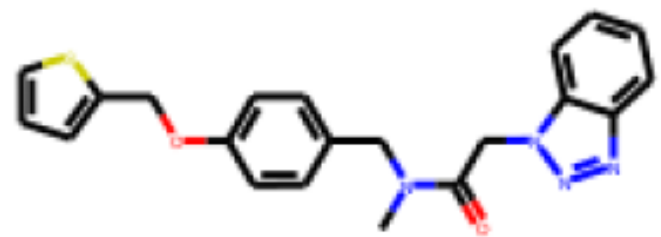






	paper/assay	paper_id
68	http://dx.doi.org/10.1016/j.bmcl.2013.08.112	17D

This is largely identical to the 17B selection

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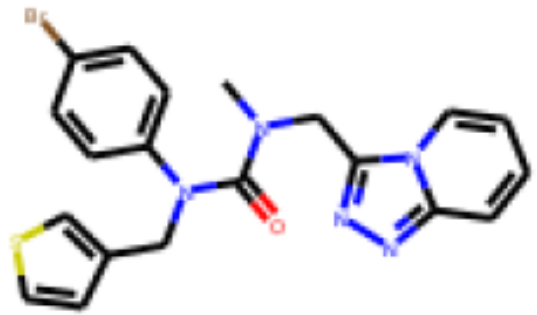
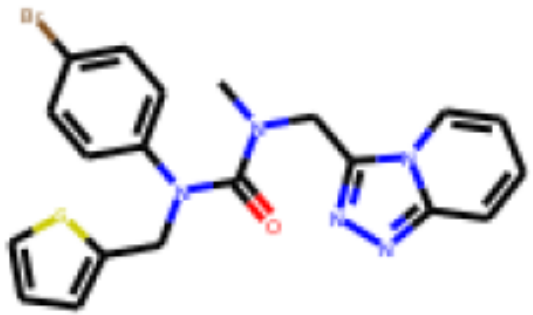
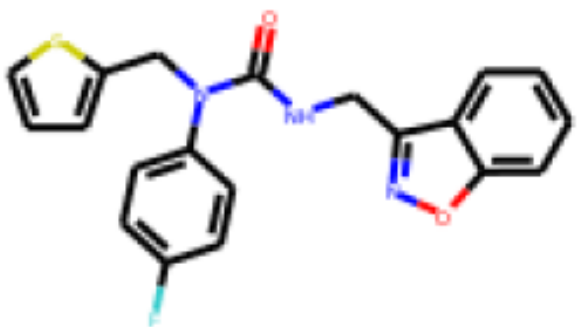
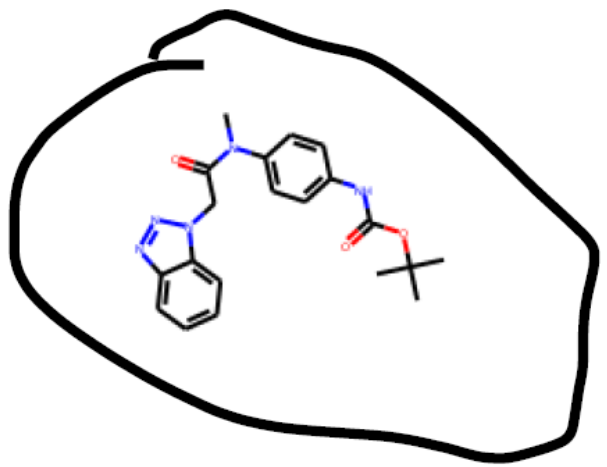
69	http://dx.doi.org/10.1016/j.bmcl.2013.08.112		16A



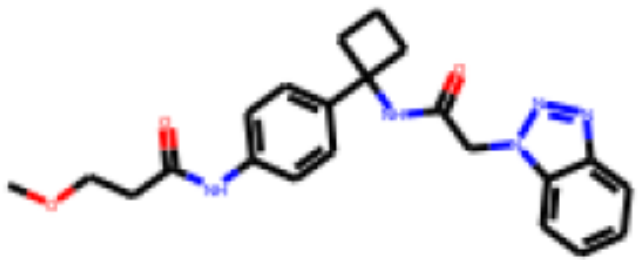


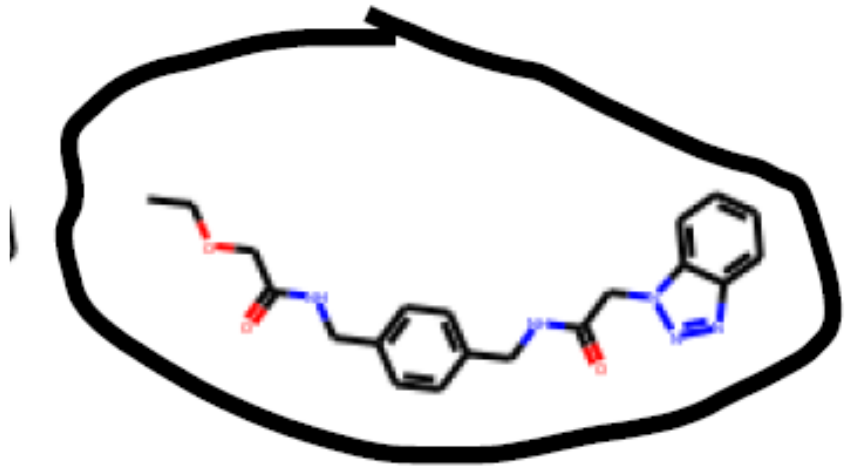
Because of reversed amide, the inhibitor might bind in a different way. Thiophenes might fit in P2 pocket, aryls towards P3?





		paper/assay	paper_id
71	http://dx.doi.org/10.1016/j.bmcl.2013.08.112		16D





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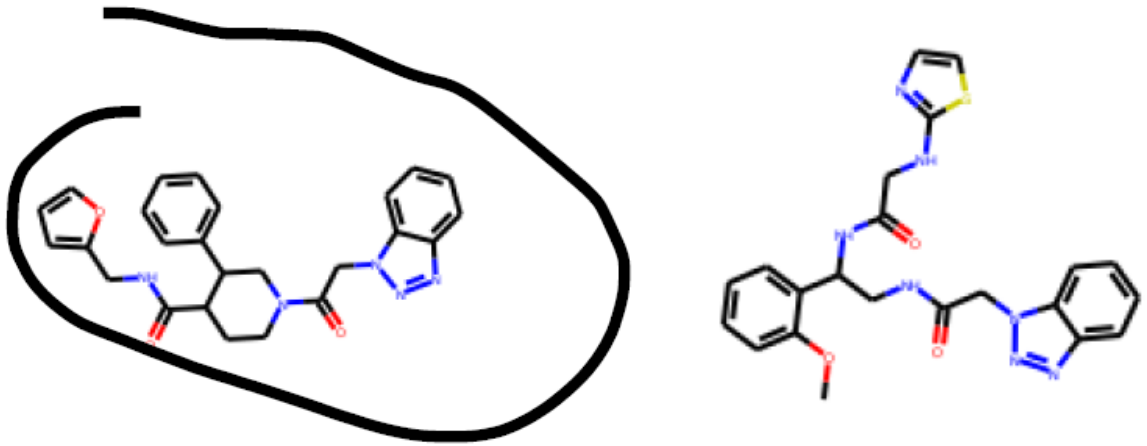

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67	http://dx.doi.org/10.1016/j.bmcl.2013.08.112		17C