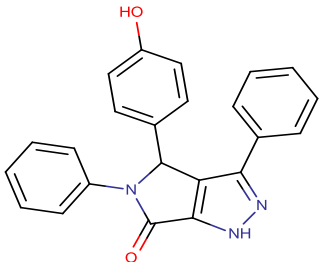
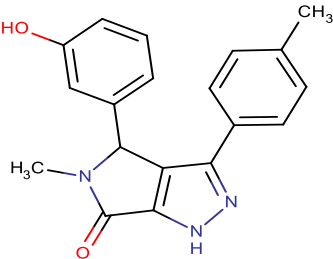
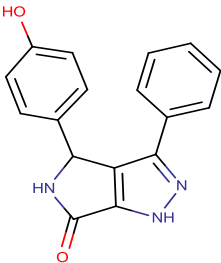
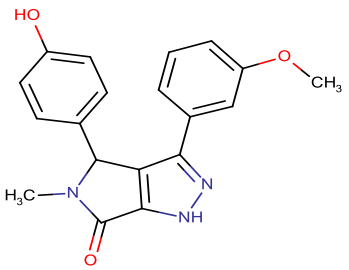
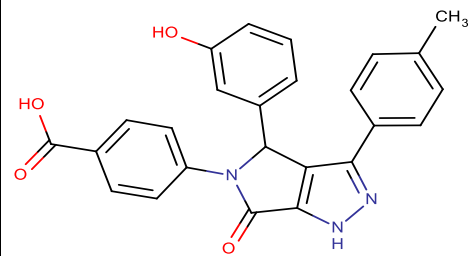
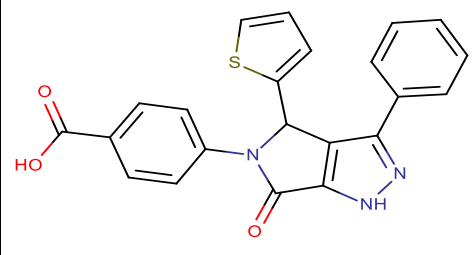
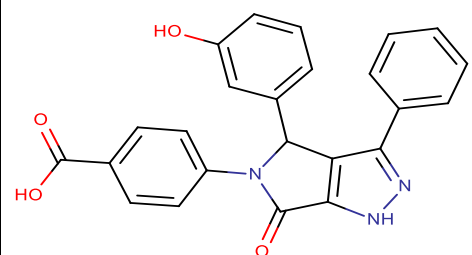
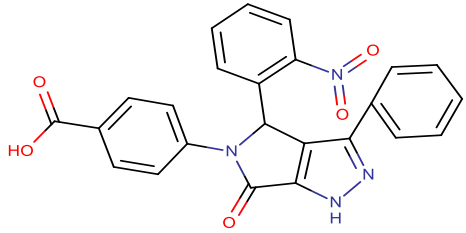
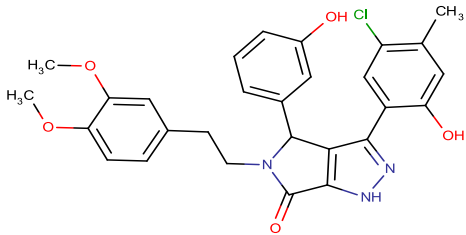
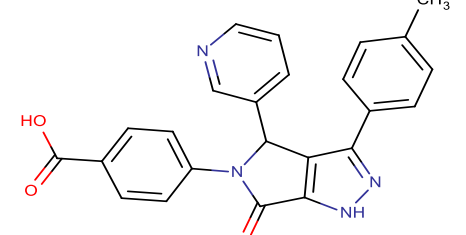
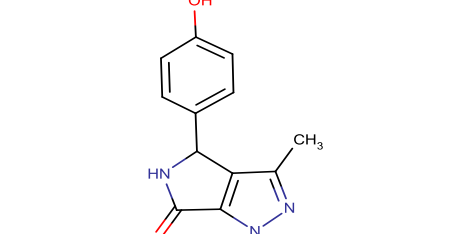
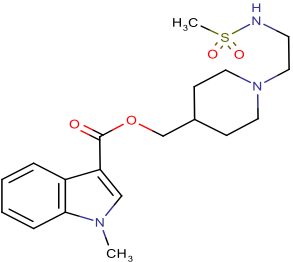
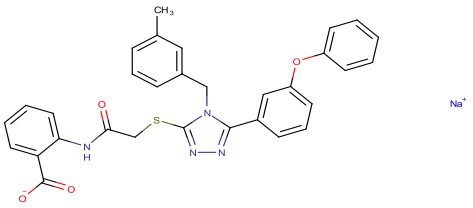
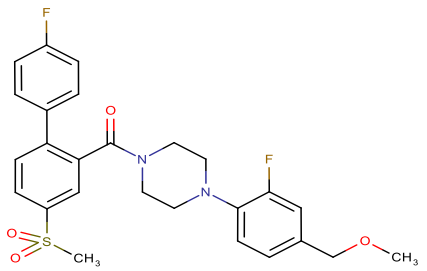
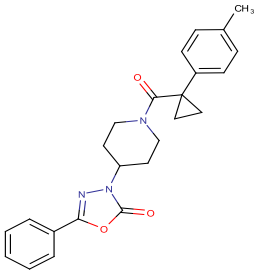


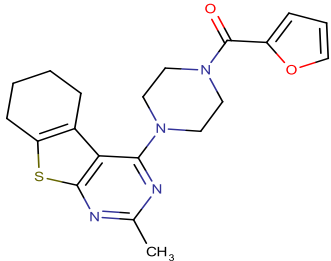
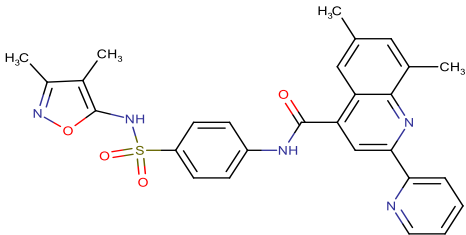
Supplementary Table 1: Compounds used in the study. GSK number (used internally within GlaxoSmithKline), notation of each compound used in the text, 2D representation of structure, and SMILES string identifiers are shown for all compounds.

GSK identifier	Notation in text	Structure	PubChem ID	SMILES
GSK875734A	1		ChemDiv1_028036	<chem>Oc1ccc(cc1)C1N(C(=O)c2[nH]nc(c12)-c1ccccc1)c1ccccc1</chem>
GSK1171747A	2		MolPort-002-791-313	<chem>CN1C(c2c([nH]nc2-c2ccc(C)cc2)C1=O)c1cccc(O)c1</chem>
GSK545023A	3		CID4204370	<chem>Oc1ccc(cc1)C1NC(=O)c2[nH]nc(c12)-c1ccccc1</chem>

GSK1402975A	4		CID23608256	<chem>COc1cccc(c1)-c1n[nH]c2C(=O)N(C)C(c12)c1ccc(O)cc1</chem>
GSK2725396A	CID 16020046		CID16020046	<chem>Cc1ccc(cc1)-c1n[nH]c2C(=O)N(C(c12)c1cccc(O)c1)c1ccc(cc1)C(O)=O</chem>
GSK866583A	5		MolPort-007-628-281	<chem>OC(=O)c1ccc(cc1)N1C(c2cccs2)c2c([nH]c2C1=O)-c1ccccc1</chem>
GSK545017A	6		CID19589042	<chem>OC(=O)c1ccc(cc1)N1C(c2c([nH]nc2-c2ccccc2)C1=O)c1cccc(O)c1</chem>

GSK866581A	7		CID19587840	<chem>OC(=O)c1ccc(cc1)N1C(c2c([nH]nc2-c2ccccc2)C1=O)c1ccccc1N(=O)=O</chem>
GSK1599375A	8		AC10B34I	<chem>COc1ccc(CCN2C(c3c(n[nH]c3C2=O)-c2cc(Cl)c(C)cc2O)c2ccccc(O)c2)cc1OC</chem>
GSK876334A	9		CID 19589028	<chem>Cc1ccc(cc1)-c1n[nH]c2C(=O)N(C(c12)c1cccnc1)c1ccc(cc1)C(O)=O</chem>
GSK866597A	10		AGN-PC-030Y99	<chem>Cc1n[nH]c2C(=O)NC(c12)c1ccc(O)cc1</chem>

GR113808	GR113808		CID119376	<chem>Cn1cc(C(=O)OCC2CCN(CCNS(C)(=O)=O)CC2)c2ccccc12</chem>
GSK260028B	GSK260028B		N/A	<chem>[Na+].Cc1cccc(Cn2c(SCC(=O)Nc3ccccc3C([O-])=O)nnc2-c2cccc(Oc3ccccc3)c2)c1</chem>
GSK522373A	GSK522373A		CID11855863	<chem>COCc1ccc(N2CCN(CC2)C(=O)c2cc(ccc2-c2ccc(F)cc2)S(C)(=O)=O)c(F)c1</chem>
GSK1421750A	ML191		CID23612552	<chem>Cc1ccc(cc1)C1(CC1)C(=O)N1CCC(CC1)n1nc(oc1=O)-c1ccccc1</chem>

GSK3175525A	ML192		CID1434953	<chem>Cc1nc(N2CCN(CC2)C(=O)c2ccco2)c2c3CCCCc3sc2n1</chem>
GSK3175526A	ML193		CID1261822	<chem>Cc1noc(NS(=O)(=O)c2ccc(NC(=O)c3cc(nc4c(C)cc(C)cc34)-c3cccn3)cc2)c1C</chem>

