

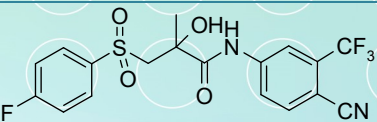
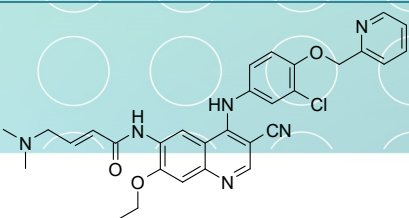
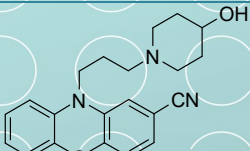
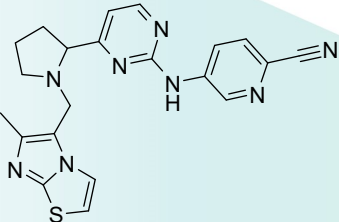
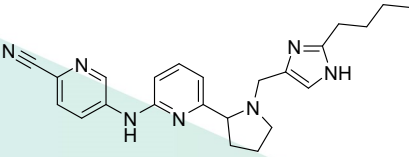
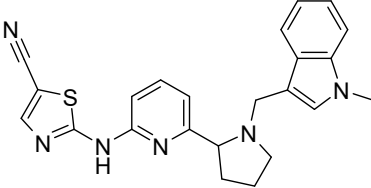
SL-37. Soft Electrophiles-5. Nitriles

Covalent inhibitors often possess an electrophilic “warhead” which interacts with a nucleophilic residue at the binding site under certain physiological conditions; examples of such electrophilic groups include acrylamides, epoxides, nitriles, and electron-deficient ketones.

Nitrile-containing molecules in which a nitrile group is attached to an aromatic core are quite widespread among pharmaceuticals and pesticides [2]. Due to the presence of the highly-polarized triple bond, nitriles can interact with Ser or Cys

residues of the proteins forming covalent adducts. Several nitrile-containing molecules have been developed as reversible covalent inhibitors of serine and cysteine proteases.

At ASINEX, we have created a library of heteroaromatic nitrile derivatives which have kinase-oriented pharmacophoric elements. These compounds are useful for the discovery of novel kinase inhibitors with improved safety, target selectivity, and pharmacokinetic properties.

		
<p>Bicalutamide non-steroidal antiandrogen</p>	<p>Neratinib Tyrosine kinase inhibitor</p>	<p>Periciazine Antipsychotic</p>
		

Signature Library 37

Formats	Supplementary Information
80 compounds per plate 0.1 mg; 1 mg; 2 mg dry film/powder 0.1 μmol; 1 μmol DMSO solutions	SL#37_Soft_Electrophiles_CN.sdf

References:

1. *Drug Discov Today*. 2015 Sep;20(9):1061-73. doi: 10.1016/j.drudis.2015.05.005
2. *J Med Chem*. 2010 November 25; 53(22): 7902–7917. doi:10.1021/jm100762r.

Contact us:

USA: +1 336 721 1617 mparisi@asinex.com
 Japan: +81-80-3401-9097 sota@asinex.com
 Europe/Global: lsadovenko@asinex.com