Probe Report
NIH Chemical Genomics Center

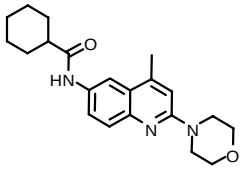
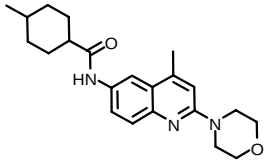
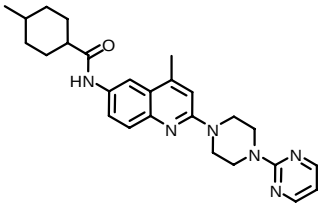
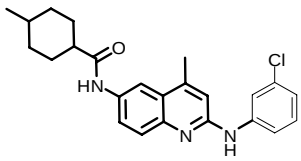
Glucocerebrosidase

Target and assay description:
Glucocerebrosidase (GC), a lysosomal enzyme, catalyzes the hydrolysis of β-glucocerebroside to glucose and ceramide. The inherited deficiency of glucocerebrosidase activity results in Gaucher disease. These novel small molecule inhibitors of glucocerebrosidase were identified from a quantitative high throughput screen at the NCGC.

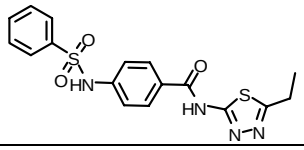
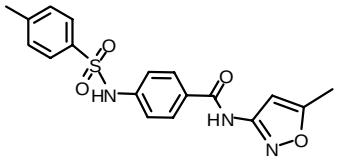
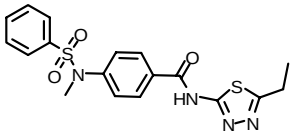
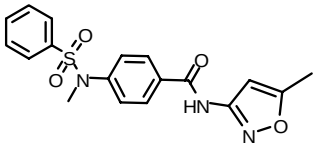
PubChem Assay ID: 361
Link: http://pubchem.ncbi.nlm.nih.gov/assay/assay.cgi?aid=360

Date of Report: November 15, 2006

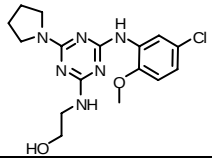
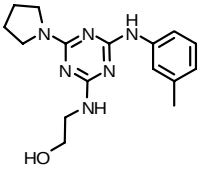
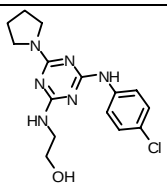
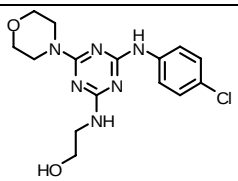
Inhibitor Probe Series 1:

PubChem ID NCGC ID	STRUCTURE	K_i (M)	IC_{50} (M) E_{max} Hill Coef.	%Purity (PDA) Purity (ELSD) NMR	CLogP	Supplier - ID
NCGC00092410 ***PROBE***		3.7E-08	3.50E-09 96% 0.67	~100 ~100 Yes	4.204	ChemDiv-C095-0200
CID4243169 NCGC00045406		6.7E-08	1.79E-08 97% 0.66	99 ~100 Yes	4.723	ChemDiv-C095-0224
NCGC00092411		2.2E-06	9.56E-07 78% 0.79	99 ~100 ND	5.002	ChemDiv-C095-0480
NCGC00092414		122E-06	2.89E-05 27% 1.47	~99 ~99 ND	7.990	ChemDiv-C129-0096

Inhibitor Probe Series 2:

PubChem ID NCGC ID	STRUCTURE	K_i (M)	IC_{50} (M) E_{max} Hill Coef.	%Purity (PDA) %Purity (ELSD) NMR	CLogP	Supplier - ID
CID4264637 NCGC00060210 ***PROBE***		5.16E-08	7.46E-08 99% 0.67	99 99 Yes	2.86	ChemBridge-7818198
CID4261164 NCGC00058635		1.06E-07	1.76E-07 98% 0.66	~100 ~100 Yes	2.86	ChemBridge-7889323
CID4255797 NCGC00055675		8.44E-06	2.26E-06 78% 0.79	96 ~99 ND	ND	ChemBridge-7475785
CID421898 NCGC00055633		1.92E-05	2.39E-05 62% 0.94	98 99 ND	2.55	ChemBridge-7480417

Inhibitor Probe Series 3:

PubChem ID NCGC ID	STRUCTURE	K_i (M)	IC_{50} (M) E_{max} Hill Coef.	%Purity (PDA) %Purity (ELSD) NMR	CLogP	Supplier - ID
CID847960 NCGC00029010		3.17E-7	5.05E-07 100% 0.91	~100 ~100 Yes	3.60	Asinex- BAS 05604353
NCGC00092397		2.77E-06	5.12E-06 91% 1.00	~99 ~99 ND	3.41	Asinex- BAS 03224400
NCGC00093501		4.23E-06	7.76E-06 87% 1.07	~99 ~99 ND	3.63	ChemNavigator-19767522
NCGC00092396		ND	1.11E-04 59% 1.29	96* ND ND	2.81	Asinex- BAS 02534286

* According to Vendor's QC data