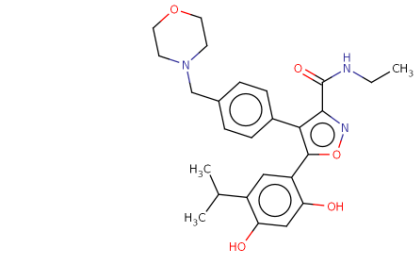
Compound synopsis

Type whole or part of the compound name into global search box and click ‘Search’.

Select ‘Compound’ tab on the top of the results page. This shows the list of compounds that match your search term, and indicates what data is available for them.

Click on the Compound Synopsis logo next to the compound you are interested in.



Compound Synopsis

- Compound Overview
- Bioactivity Data Summary
- Protein Affinity Profile
- Cellline Sensitivity Profile

480574 - Overview - Compound Synopsis

Synonyms	
2GJ	NVP-AUY922
VER-52296	
Molecular Formula	
C26H31N3O5	
IUPAC	
5-[2,4-dihydroxy-5-(propan-2-yl)phenyl]-N-ethyl-4-[4-(morpholin-4-ylmethyl)pheny...	
Standard InChI	
InChI=1S/C26H31N3O5/c1-4-27-26(32)24-23(18-7-5-17(6-8-18)15-29-9-11-33-12-10-29)...	
SD File	
SciTegic06031011152D 34 37 0 0 0 0 999 V2000 7.5319 -23...	
Smiles	
CCNC(=O)c1noc(c2cc(C(C)C)c(O)cc2O)c1c3ccc(CN4CCOCC4)cc3	
Cross References	
BindingDB	20926
PDB Het Code	2GJ
ChEMBL	CHEMBL252164

	MOLECULAR_WEIGHT	ALOGP	HBOND_DONORS	HBOND_ACCEPTORS	ATOMS	CONTAINS_TOXICOPHORE
Properties	465.54143	4.069	3	6	34	Yes

This takes you to the Compound Synopsis page for this compound. From here you can view data on the compound’s bioactivities, its protein affinity profile, cell line sensitivities, compounds with the same scaffold and more.