InFarmatik Kinase Fragment library fact sheet

1.) Name: InFarmatik kinase fragment library.

2.)Library design in brief:

- The library was built up based upon structural search in our building block, scaffold and intermediate database. In the search we used the structural review of kinase modulators accepted by many fellow researcher. (Nature reviews, 2009, p28-39).

- We generated new fragments to the library based upon permutation of the relevant kinase chemistry. Evaluation of the new fragments performed by using Molinspiration’s on-line Biology Data Prediction module.

- The kinase library was in silico and invitro screened to find dual inhibitors for CK2 & PIM1
  CompChem Solutions (UK) docked the optimized fragment structure into targets
  IOTA Pharmaceuticals performed invitro primary screening and IC 50 value
  Results and comapartive analysis to predicted values were presented on the following events: Agrinet 2012 (Bracknell, UK), FBLD 2012 (San Francisco, USA), UKQSAR 2012 , Fragments 2013 (Oxford, UK)

3.) Kinase fragment library contains 357 fragments. Currently about 80 % of the compounds are available from stock.

4.)Guaranteed purity is 90 % for screening quantities determined by LCMS at 220 nm wavelength. In case of ordering more than 100 mg the delivered purity is at least 95 % determined by proton NMR and by LCMS at 220 nm wavelength.

5.) Cherry picking is allowed. Be aware that price depends on the ordered quantity (number of compounds and weight).

6.)Some representative structures: