Title: Classification of small molecule protein kinase inhibitors based upon the structures of their drug-enzyme complexes

Author: Robert Roskoski

PII: S1043-6618(15)30129-8
DOI: http://dx.doi.org/doi:10.1016/j.phrs.2015.10.021
Reference: YPHRS 2965

To appear in: *Pharmacological Research*

Received date: 25-10-2015
Revised date: 26-10-2015
Accepted date: 27-10-2015

Please cite this article as: Roskoski Robert.Classification of small molecule protein kinase inhibitors based upon the structures of their drug-enzyme complexes.*Pharmacological Research* http://dx.doi.org/10.1016/j.phrs.2015.10.021

Classification of small molecule protein kinase inhibitors based upon the structures of their drug-enzyme complexes

Robert Roskoski Jr.

Blue Ridge Institute for Medical Research

3754 Brevard Road, Suite 116, Box 19

Horse Shoe, North Carolina 28742-8814, United States

Phone: 1-828-891-5637

Fax: 1-828-890-8130

E-mail address: rrj@brimr.org

Key words: ATP-binding site; Catalytic spine; K/E/D/D; Protein kinase structure; Regulatory spine; Residence time

Chemical compounds studied in this article

Afatinib (PubMed CID: 10184653), Crizotinib (PubMed CID: 11626560), Erlotinib (PubMed CID: 176870), Gefitinib (PubMed CID: 123631), Imatinib (PubMed CID: 5291), Nilotinib (PubMed CID: 644241), Sorafinib (PubMed CID: 216239), Sunitinib (PubMed CID: 5329102); Tofacitinib (PubMed CID: 9926791); Vemurafenib (PubMed CID: 42611257)

Abbreviations: ALL, acute lymphoblastic leukemia; AS, activation segment; CDK, cyclin-dependent kinase; CML, chronic myelogenous leukemia; CS or C-spine, catalytic spine; EGFR or ErbB1, epidermal growth factor receptor; FGFR, fibroblast growth factor receptor; GIST, gastrointestinal stromal tumor; HER2, human epidermal growth factor receptor-2 or human ErbB2; HGFR or c-Met, hepatocyte growth factor receptor; HP, hydrophobic; JAK, Janus kinase; NSCLC, non-small cell lung cancer; PDGFR, platelet-