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## ACCEPTED MANUSCRIPT

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

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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-

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