Supplementary Material (ESI) for Analyst

Inhibitor screening of protein kinases using MALDI-TOF MS combined with separation and enrichment of phosphopeptides by TiO_2 nanoparticle deposited capillary column

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Electronic Supplementary Information

Figures S1: Standard work curve for quantification of phosphopeptides by MALDI-TOF MS

Figure S2: Ranking of inhibitory potency of imatinib and its analogues towards Abl kinase

Figure S3-S9: The docked conformers/poses of imatinib and its analogues at the active site of Abl kinase as generated via Surflex docking-scoring combinations

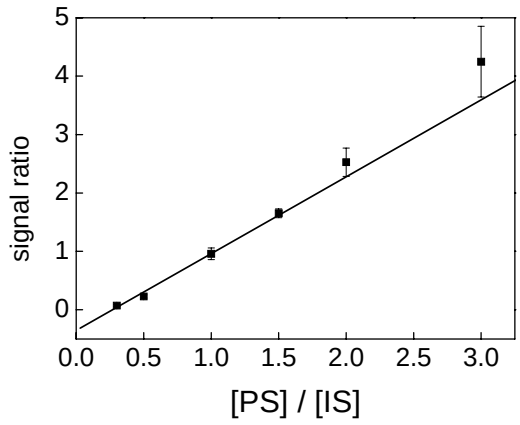

Figure S1. Standard work curve by plotting the ratio of signal intensities of phosphorylated substrate to standard phophopeptide as function of the molar ratio of phosphorylated substrate (PS) to internal standard (IS).

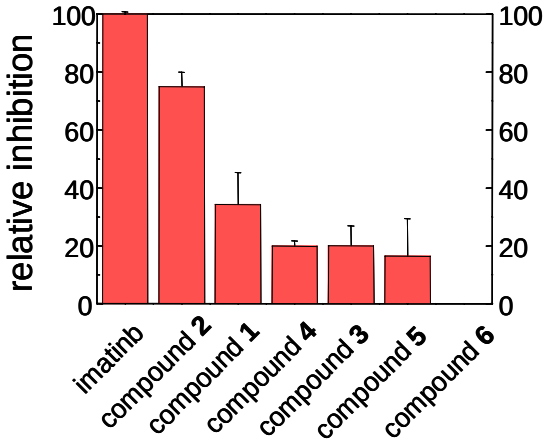

Figure S2. Ranking order of inhibitory potency of imatinib and its analogs towards Abl.

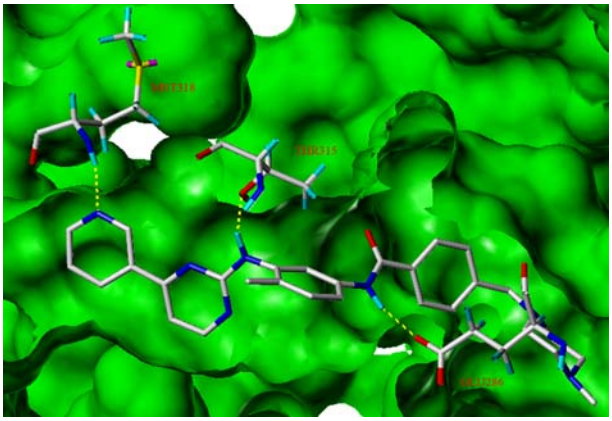

Figure S3. The docked conformers/poses of imatinib inhibitor (IC_{50}: 0.234 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

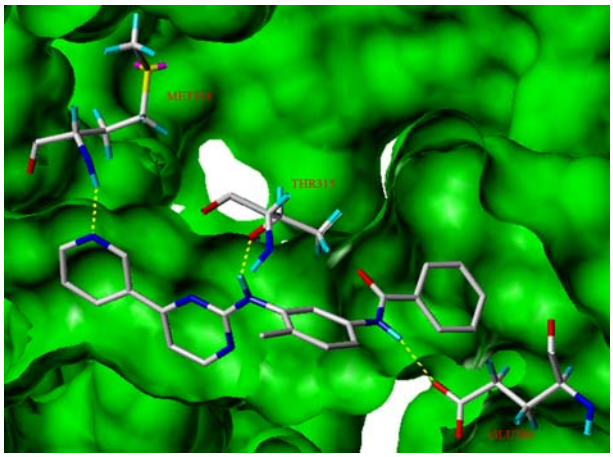

Figure S4. The docked conformers/poses of compound **1** (IC_{50}: 12.7 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

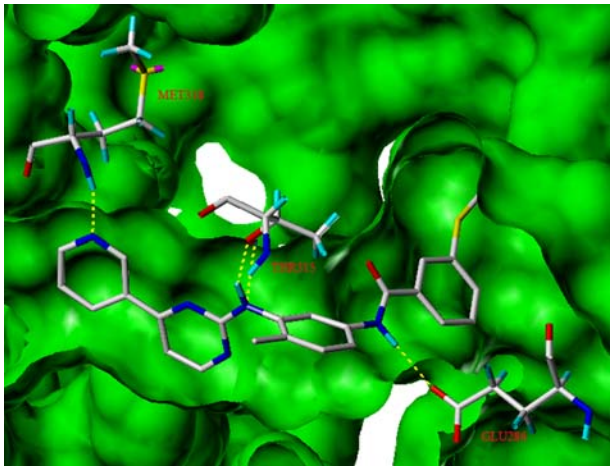

Figure S5. The docked conformers/poses of compound **2** (IC_{50}: 1.10 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

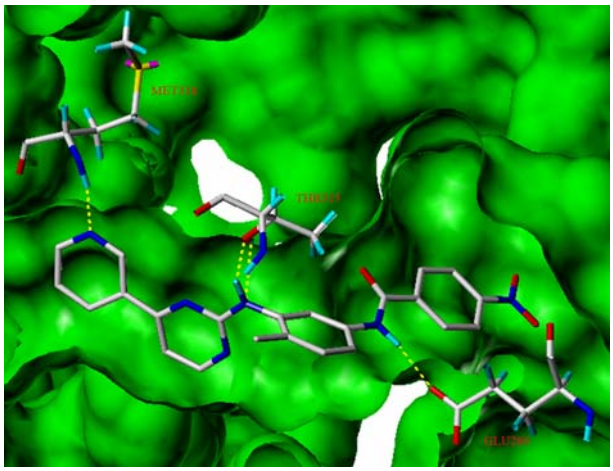

Figure S6. The docked conformers/poses of compound **3** (IC_{50} > 100 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

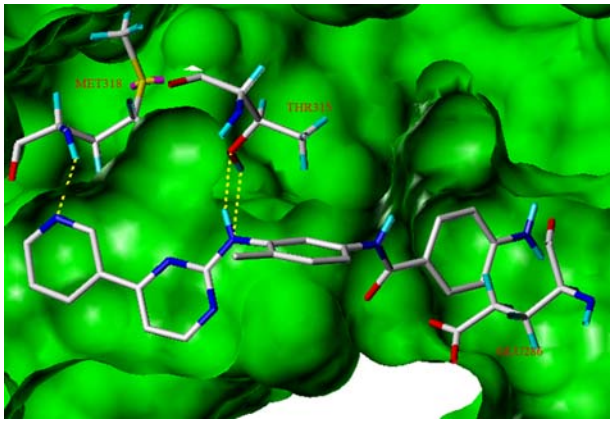

Figure S7. The docked conformers/poses of compound **4** (IC_{50} > 100 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

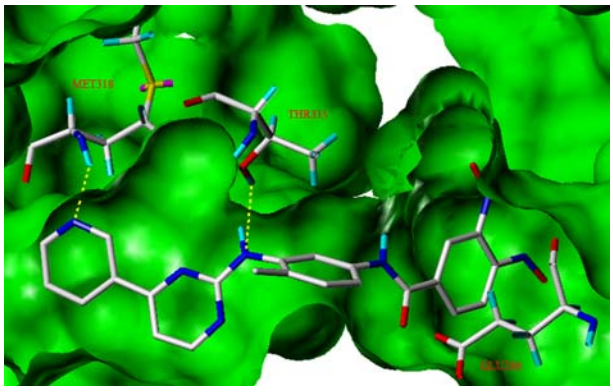

Figure S8. The docked conformers/poses of compound **5** (IC_{50} > 25 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.

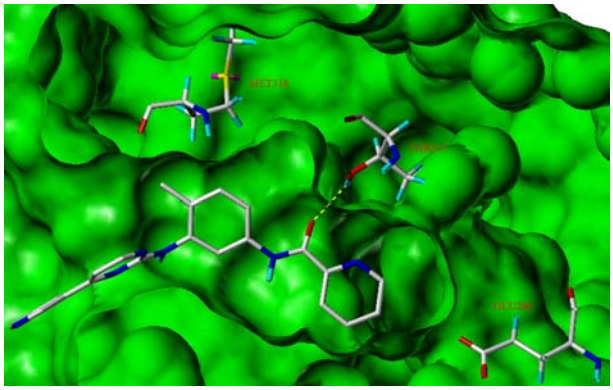

Figure S9. The docked conformers/poses of compound **6** (IC_{50} > 100 μM) at the active site of Abl kinase as generated via Surflex docking-scoring combinations. The dotted yellow lines illustrate the positions of probable hydrogen-bonding interactions as calculated by the H-Bond calculator imbedded in Surflex-Dock module in Sybyl X 1.0.