

Supporting information for:

Structure-based design of targeted covalent inhibitors

Richard Lonsdale and Richard A. Ward

Chemistry, Oncology, IMED Biotech Unit, AstraZeneca, Cambridge, CB4 0WG, UK.

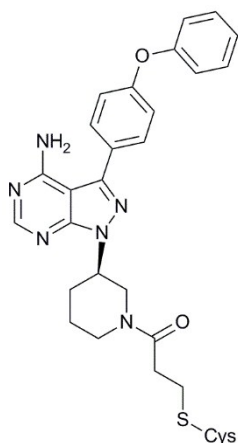


Figure S1 Covalent attachment formed between **5** and cysteine

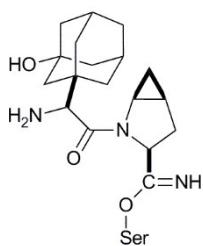


Figure S2 Covalent attachment formed between **10** and serine

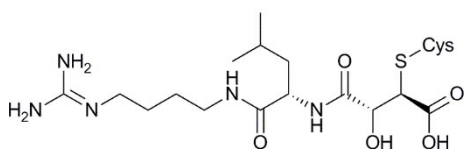


Figure S3 Covalent attachment formed between **11** and cysteine

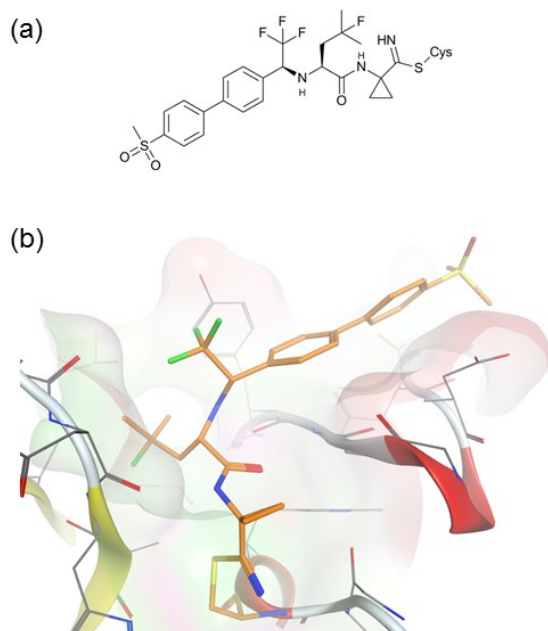


Figure S4 (a) Covalent attachment of **12** to cysteine. (b) X-ray crystal structure of **12** covalently bound to Cathepsin K (PDB: 5TDI)

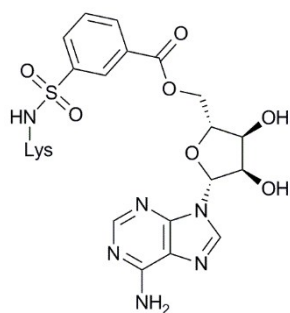


Figure S5 Covalent attachment of **20** to lysine.

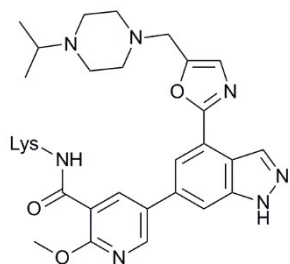


Figure S6 Proposed covalent attachment of **21** to lysine.

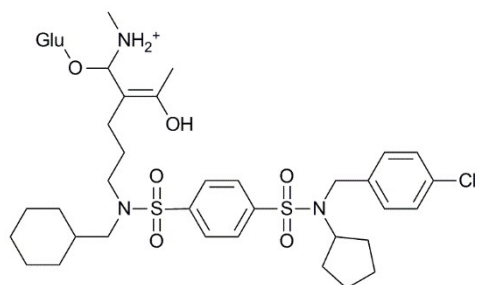


Figure S7 Covalent attachment of **22** to glutamate.