

Identification of small molecule inhibitor of HBV replication via HBX interaction

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Table S1: Molecular properties of compound IR415

Property Name	Property Value
Molecular Weight	296.34 g/mol
Density:	1.3±0.1 g/cm ³
Boiling Point:	439.6±55.0 °C at 760 mmHg
Vapour Pressure:	0.0±1.1 mmHg at 25°C
Enthalpy of Vaporization:	69.7±3.0 kJ/mol
Flash Point	219.7±31.5 °C
Polarizability	30.7±0.5 10 ⁻²⁴ cm ³
Surface Tension	41.5±7.0 dyne/cm
Molar Volume	224.3±7.0 cm ³
Index of Refraction:	1.608
Molar Refractivity:	77.5±0.5 cm ³
Hydrogen Bond Donor Count	2
Hydrogen Bond Acceptor Count	4
Rotatable Bond Count	5
Topological Polar Surface Area	74 Å ²
Monoisotopic Mass	296.091 g/mol
Exact Mass	296.091 g/mol
XLogP3-AA	1.8
Compound Is Canonicalized	true
Formal Charge	0
Heavy Atom Count	20
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0