

List of 23 pre-step 5 hit compounds (which successfully completed MD simulations), marked (with *) are those which are lead compounds (successfully completed QM/MM) :

DB07831*

DB07943

DB08439*

DB08557*

DB07181

DB14668*

DB12812^(a)

CNP0048157

CNP0049103

CNP0061106*

CNP0083976*

CNP0105092

CNP0151817

CNP0153569*

CNP0167760

CNP0191444

CNP0295631

CNP0304461*

CNP0330896

CNP0361420*

CNP0364174

CNP0364473*

CNP0375239

^(a) See Supplementary information note 1 regarding this compound.