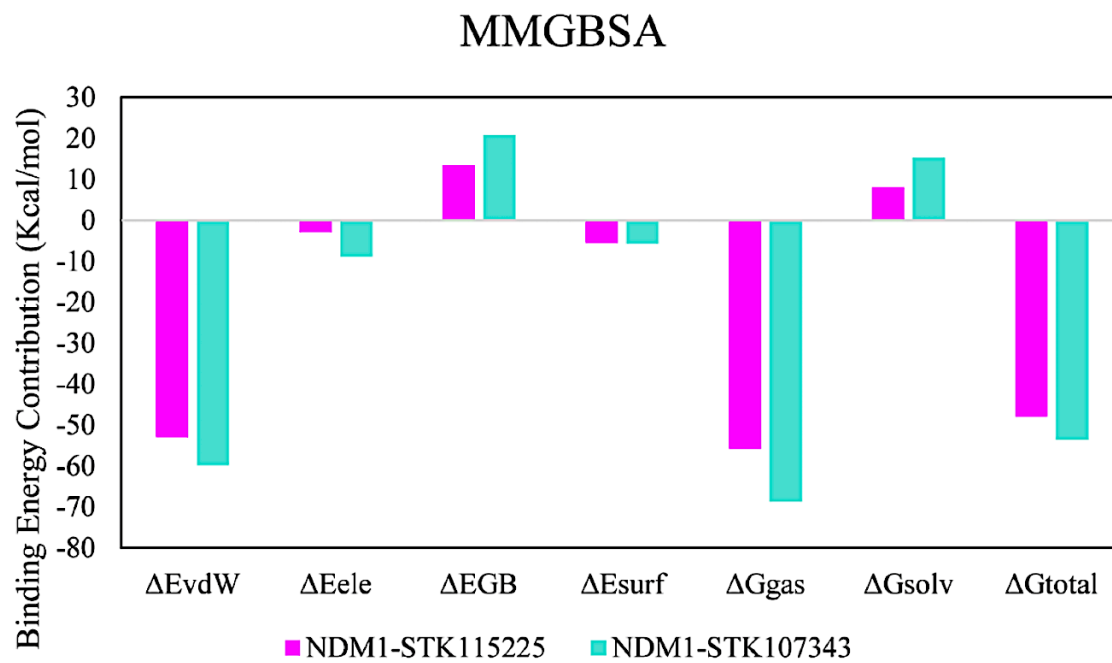


## SUPPLEMENTARY INFORMATION

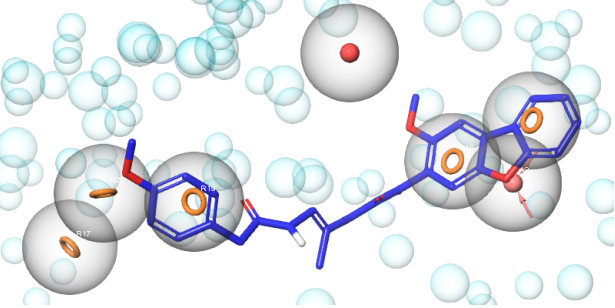
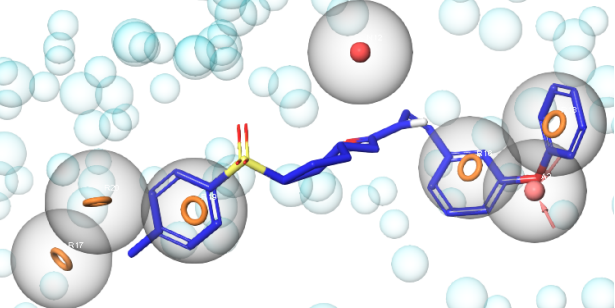
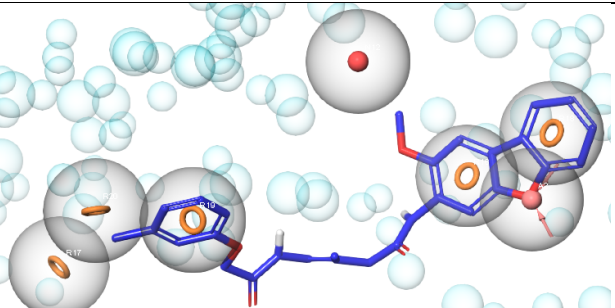
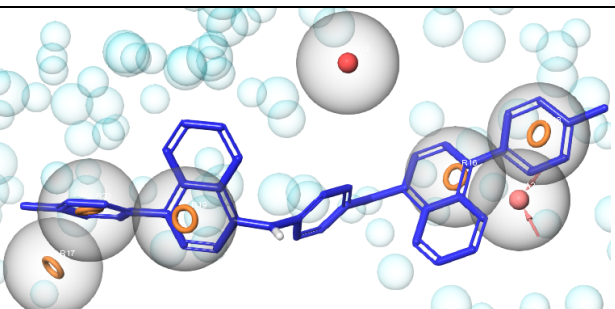


**Supplementary Figure 1.** Contribution of each binding energy component in the calculation of  $\Delta G_{total}$  for the two ligands, STK115225 (magenta) and STK107343 (cyan).

**Supplementary Table 1.** The seven features of the pharmacophore model with their respective scores as well as coordinates

<b>Rank</b>	<b>Feature label</b>	<b>Score</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
1	R16	-1.62	-1.6473	-37.3508	5.1067
2	R19	-1.16	2.8594	-45.2797	-1.6987
3	R18	-1.13	-4.9237	-35.1183	4.524
4	N12	-1.09	0.3111	-36.8595	-1.1857
5	R20	-1.02	6.6019	-46.3632	-2.8173
6	R17	-0.86	10.4897	-47.5495	0.399
7	A2	-0.72	-4.2899	-37.2535	6.14

**Supplementary Table 2.** Phase scores for the alignment of the ligands selected as hits for binding to NDM1.

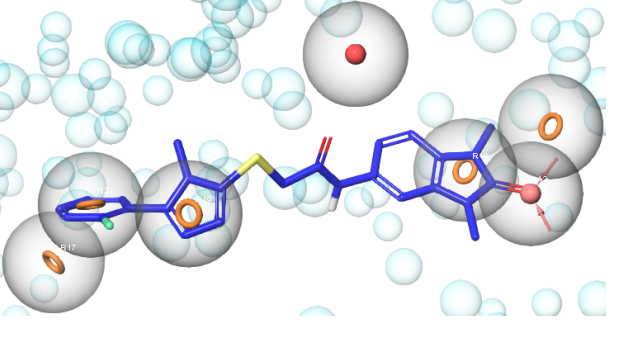
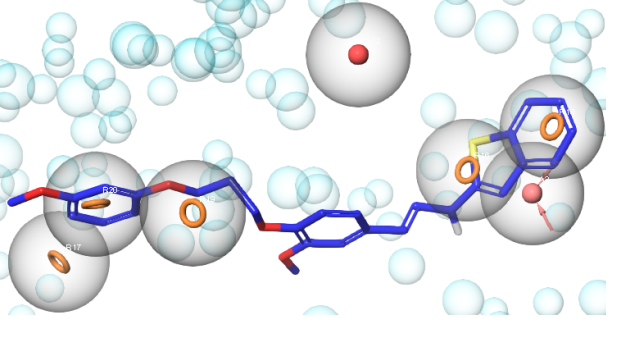
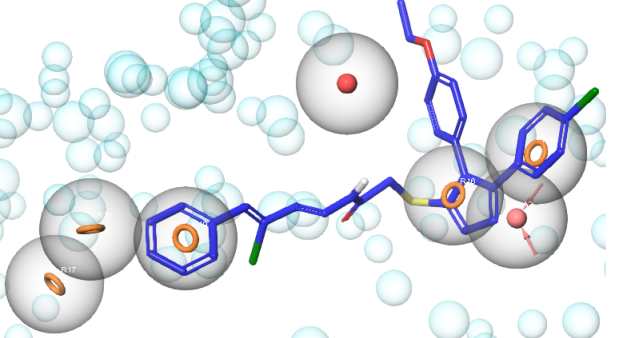
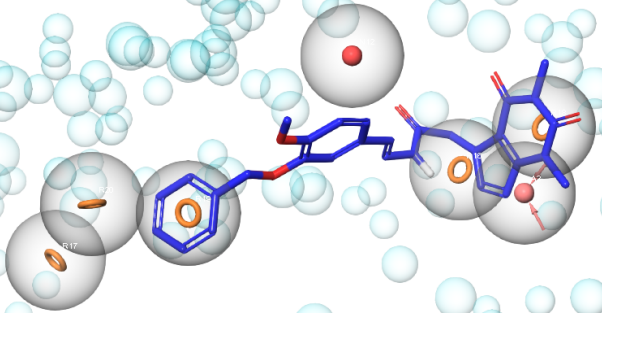
S. No.	Compound ID	Alignment	Phase score
1	STK116979		1.539
2	STK107657		1.53
3	STK118152		1.482
4	STK070333		1.478

5	STK107343		1.478
6	STK274045		1.473
7	STK124603		1.46
8	STK107402		1.458
9	STK215863		1.454

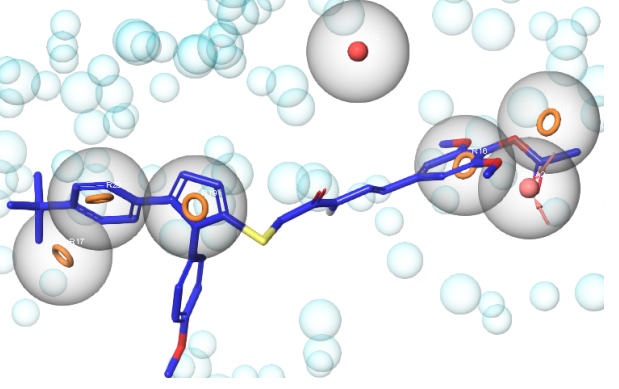
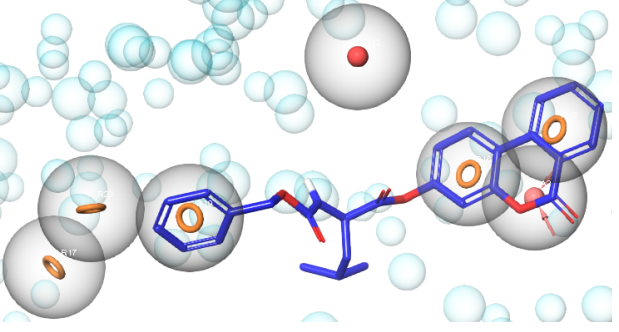
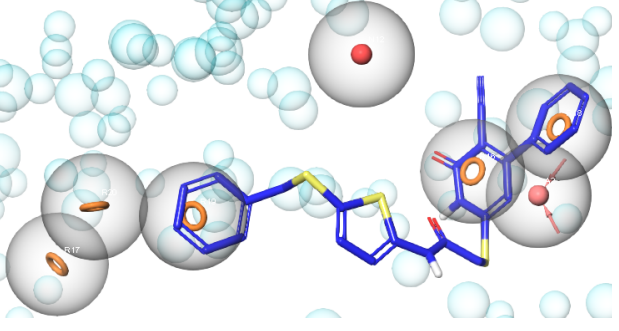
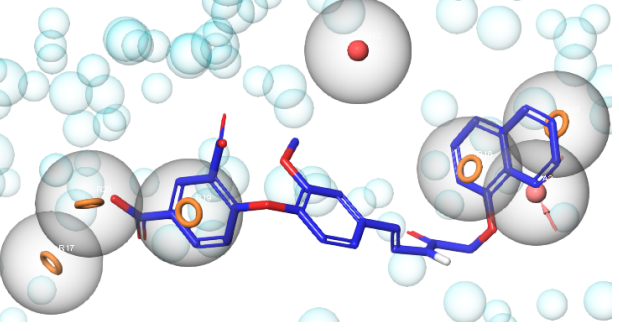
10	STK092412		1.453
11	STK215880		1.453
12	STK245606		1.449
13	STK005451		1.441
14	STK126037		1.436

15	STK230461		1.433
16	STK106993		1.43
17	STK101590		1.43
18	STK246068		1.429
19	STK107383		1.429

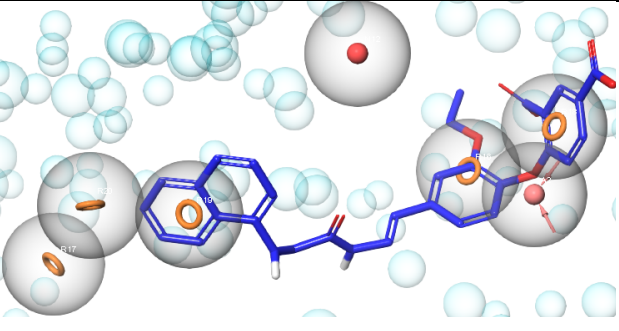
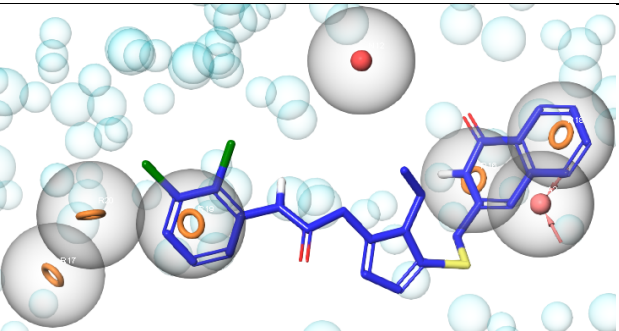
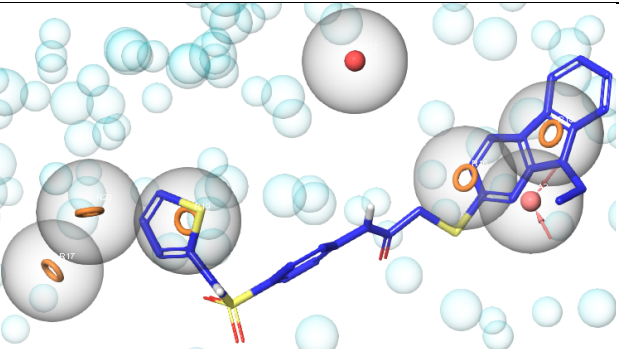
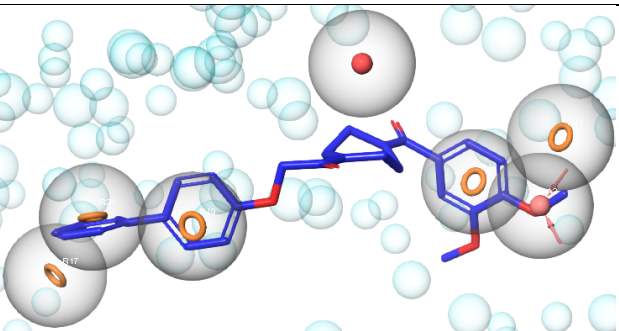
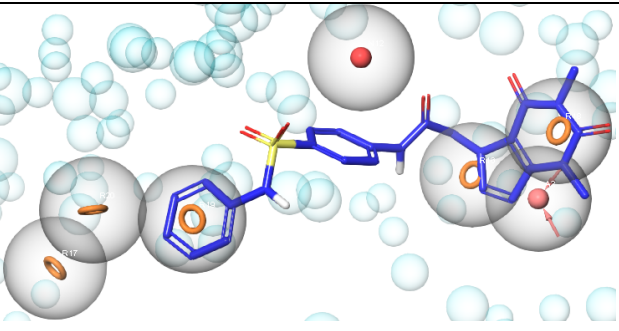
20	STK197820		1.428
21	STK115225		1.428
22	STK218557		1.427
23	STK219024		1.426
24	STK251382		1.426

25	STK221786		1.426
26	STK104366		1.425
27	STK105113		1.425
28	STK013244		1.424



29	STK106890	 <p>Molecular structure of STK106890, showing a complex molecule with a central blue ring system, a yellow sulfur atom, and a red nitrogen atom, surrounded by a light blue electron density map. The molecule is shown in a stick representation with orange and red spheres representing oxygen and nitrogen atoms, respectively. The structure is oriented horizontally, with the central ring system on the left and the nitrogen-containing group on the right.</p>	1.421
30	STK063204	 <p>Molecular structure of STK063204, showing a complex molecule with a central blue ring system, a red nitrogen atom, and a yellow sulfur atom, surrounded by a light blue electron density map. The molecule is shown in a stick representation with orange and red spheres representing oxygen and nitrogen atoms, respectively. The structure is oriented horizontally, with the central ring system on the left and the nitrogen-containing group on the right.</p>	1.42
31	STK211786	 <p>Molecular structure of STK211786, showing a complex molecule with a central blue ring system, a red nitrogen atom, and a yellow sulfur atom, surrounded by a light blue electron density map. The molecule is shown in a stick representation with orange and red spheres representing oxygen and nitrogen atoms, respectively. The structure is oriented horizontally, with the central ring system on the left and the nitrogen-containing group on the right.</p>	1.42
32	STK200966	 <p>Molecular structure of STK200966, showing a complex molecule with a central blue ring system, a red nitrogen atom, and a yellow sulfur atom, surrounded by a light blue electron density map. The molecule is shown in a stick representation with orange and red spheres representing oxygen and nitrogen atoms, respectively. The structure is oriented horizontally, with the central ring system on the left and the nitrogen-containing group on the right.</p>	1.418

33	STK084729		1.413
34	STK139857		1.41
35	STK100674		1.409
36	STK115575		1.408
37	STK104200		1.407

38	STK068819		1.407
39	STK219211		1.404
40	STK125344		1.403
41	STK194636		1.401
42	STK030716		1.401

43	STK218633		1.4
44	STK218604		1.4