Table S1. Structures of NDM-1, their native ligands and predicted RMSD values

Cross validation of native ligands from crystallographic structures of NDM-1 based on RMSD values							
		4RL2	**6NY7**	**6O3R**	**4EYB**	**6TWT**	**5ZGE**
Native ligands	**3S3**	3.19	3.2	2.50	1.20	2.68	3.29
	L8J	1.50	2.87	1.76	1.13	1.50	1.61
	XJE	2.10	0.68	1.55	1.10	1.20	0.70
	0WO	3.20	3.15	4.46	2.55	1.02	1.52
	EPE	0.80	0.88	0.92	0.81	0.78	0.60
	Z27	1.11	1.21	1.47	1.34	1.97	0.30

Following criteria has been adopted as reported in study (Bajda et al., 2013).

RMSD ≤ 1.0 Å, good pose. (Green)

RMSD ≤ 2.0 Å, close pose. (Blue)

RMSD ≤ 3.0 Å, pose with errors. (Red)

RMSD >3 .0 Å, bad pose. (Pink)

Bajda, M., Więckowska, A., Hebda, M., Guzior, N., Sotriffer, C. A., & Malawska, B. (2013). Structure-based search for new inhibitors of cholinesterases. International Journal of Molecular Sciences, 14(3), 5608-5632.