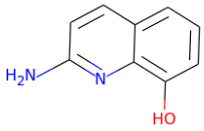
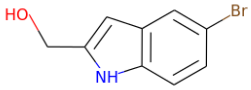
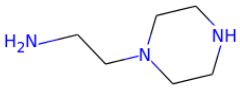
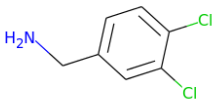
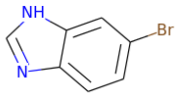
Table 1. Statistics of data collection and refinement of Mab3862 (7r22)

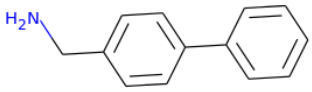
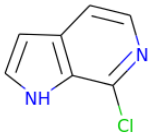
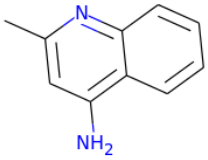
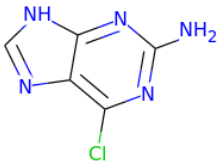
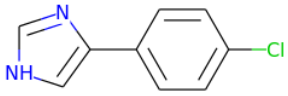
Data collection and processing	
Diffraction source	I04 beamline at Diamond Light Source
Wavelength	0.9795 Å
Temperature	100K
Detector	PIXEL (DECTRIS EIGER2 XE 16M)
Total rotation range per image	0.1°
Total rotation range	360°
Exposure time per image	0.008s
Space group	$P4_132$
Unit cell parameters	106.89 Å 106.89 Å 106.89 Å 90.00° 90.00° 90.00°
Resolution range	47.80-2.73 Å
Rmerge	0.12
Total reflections	405313
Unique reflections	5963
Multiplicity	68
<I/σ>	0.6 at 2.73Å
Overall B factor from Wilson plot	94.0 $Å^2$
Structure refinement	
Resolution range	2.72-2.76 Å
Completeness in resolution range	75.5%
Working set reflections	4059 (90%)
Test set reflections	451 (10.02%)
Final R_{work}	0.347
Final R_{free}	0.299
Molecules in asymmetric unit	1
RMSD Bond/Angles	0.6013°/ 2.036 Å
Ramachandran plot	
Favoured regions	68%
Allowed	17%
Outliers	14%
Rotamer outliers	6%
Solvent contents	72.46%
Matthew coefficient	$4.47Å^3$
Average B factor	98.3 $Å^2$

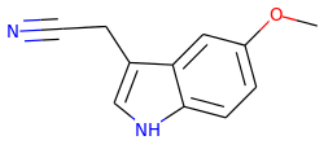
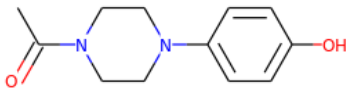
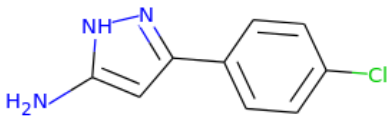
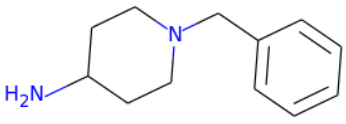
Table 2. Mab3862 dimer interface interaction

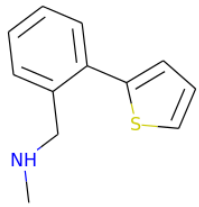
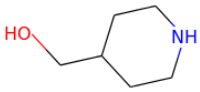
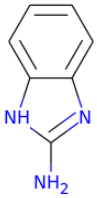
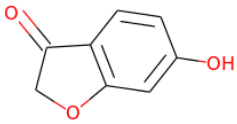
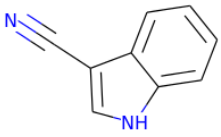
Number of residues		
Interface	36	35.6%
Surface	100	99.0%
Total	101	100.0%
Solvent accessible area (Å)		
Interface	1454.1	19%
Total	7633.4	100%
Solvation energy, kcal/mol		
Isolated structure	-62.8	100%
Gain on complex formation	-13.5	21.5%
Average gain	-3.4	5.5%
P-value	0.017	-

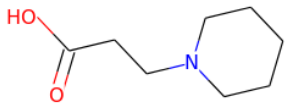
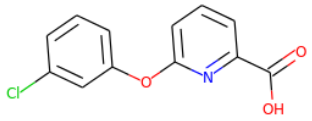
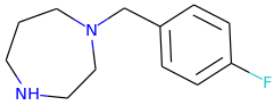
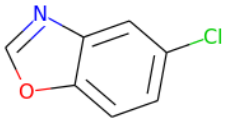
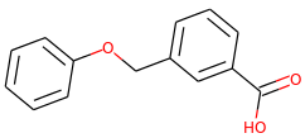
Table 3. A list of putative positive hits from SPR and TSA with 2d structure and glide score annotated in each site.

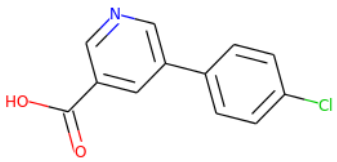
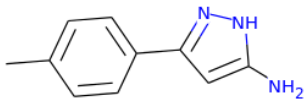
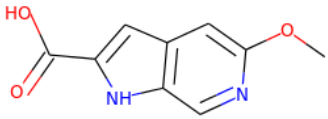
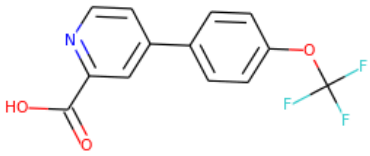
AFL Sample	Source	site 1	site 2	chemical name	structure 2D
15	SPR	-7.073	-4.979	2-Amino-8-quinolinol	
447	SPR	-6.966	-5.047	5-Bromo-2-(hydroxymethyl)indole	
137	TSA	-6.496	-6.177	1-(2-Aminoethyl)piperazine	
93	SPR	-6.298	-5.824	3,4-Dichlorobenzylamine	
459	SPR	-6.293	-5.474	6-Bromo-1H-benzimidazole	

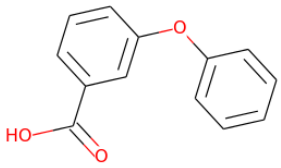
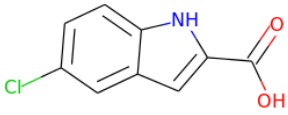
428	SPR	-6.235	-5.198	4-Phenylbenzylamine, 97%	
391	SPR	-6.177	-7.412	7-Chloro-6-azaindole	
277	SPR	-5.920	-3.936	4-Aminoquinaldine	
146	TSA	-5.889	-4.923	2-Amino-6-chloropurine	
441	SPR	-5.525	-5.185	4-(4-Chlorophenyl)-1H-imidazole	

201	SPR	-5.383	-4.292	5-Methoxy-3-indolylacetonitrile	
303	TSA	-5.329	-4.727	1-Acetyl-4-(4-hydroxyphenyl)piperazine	
65	SPR	-5.221	-5.435	3-(4-Chlorophenyl)-1H-pyrazol-5-amine	
158	SPR	-5.182	-4.692	4-Amino-1-benzylpiperidine	

175	SPR	-5.137	-4.430	N-Methyl-N-(2-thien-2-ylbenzyl)amine	
127	TSA	-5.096	-5.408	4-Piperidinemethanol	
16	SPR	-5.092	-5.995	2-Aminobenzimidazole	
80	SPR	-4.966	-4.986	6-Hydroxy-2,3-dihydrobenzo[b]furan-3-one	
352	SPR	-4.948	-4.290	Indole-3-carbonitrile	

177	TSA	-4.922	-4.694	1-Piperidinepropionic acid	
452	SPR	-4.809	-4.000	6-(3-Chlorophenoxy)pyridine-2-carboxylic acid	
342	SPR	-4.795	-4.394	1-(4-Fluorobenzyl)homopiperazine	
373	SPR	-4.779	-3.740	5-Chlorobenzoxazole	
66	SPR	-4.770	-4.647	3-(Phenoxymethyl)benzoic acid	

443	SPR	-4.761	-3.959	5-(4-Chlorophenyl)pyridine-3-carboxylic acid	
245	SPR	-4.641	-5.007	3-(4-Methylphenyl)-1H-pyrazol-5-amine	
450	SPR	-4.537	-4.105	5-Methoxy-1H-pyrrolo[2,3-c]pyridine-2-carboxylic acid	
449	SPR	-4.192	-3.957	4-(4-Trifluoromethoxyphenyl)picolinic acid	

375	SPR	-4.174	-4.016	3-Phenoxybenzoic acid	
448	SPR	-3.986	-4.058	5-Chloroindole-2-carboxylic acid	
387	SPR	-3.553	-4.549	4-Phenoxyphenylacetic acid