Supplementary File

Identification of Novel AXL Kinase Inhibitors Using Ligand-Based Pharmacophore Screening and Molecular Dynamics Simulations

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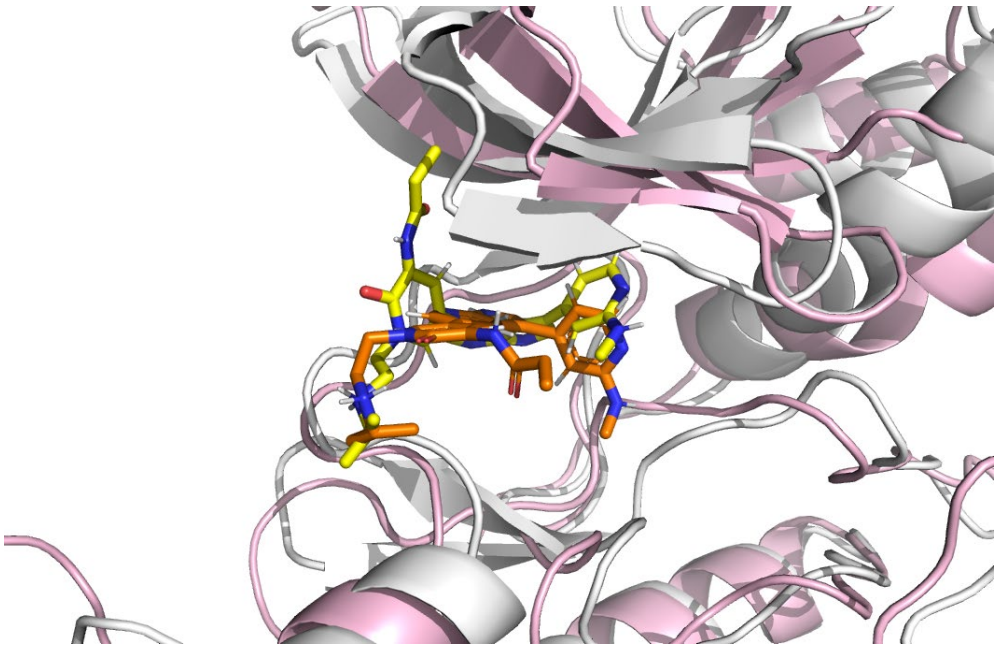

Figure S1: Structural alignment of PubChem-122421875 molecule complex docking (white) and representative conformation (light pink) of stable structures of last 5 nano seconds of total 100 nano seconds of Molecular dynamics simulations. The docking molecule is shown in orange sticks and the simulations out molecule shown in yellow sticks.

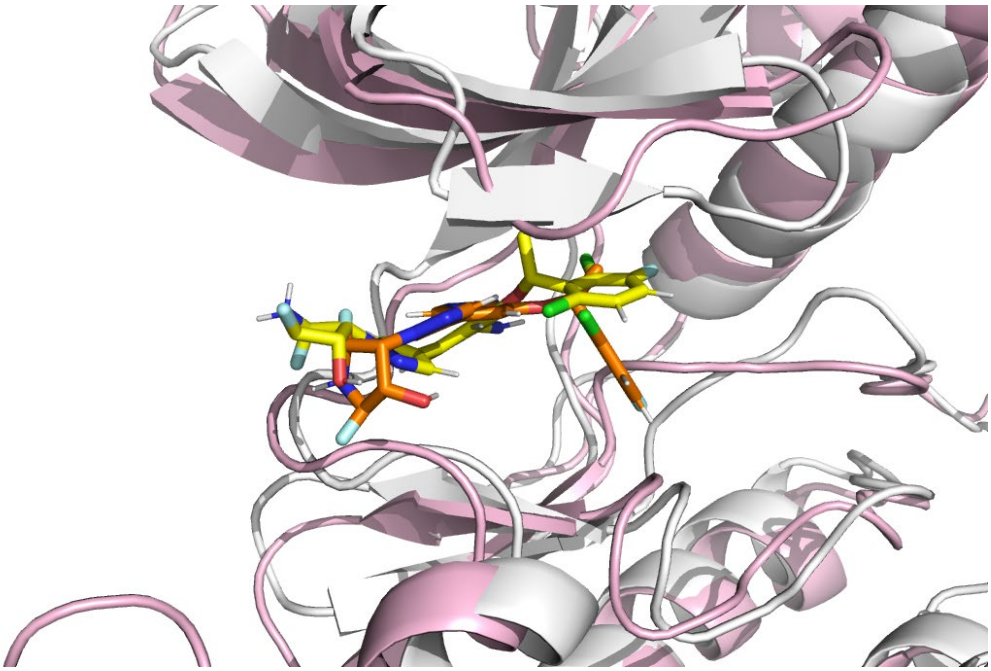

Figure S2: Structural alignment of PubChem-78160848 molecule complex docking (white) and representative conformation (light pink) of stable structures of last 5 nano seconds of total 100 nano seconds of Molecular dynamics simulations. The docking molecule is shown in orange sticks and the simulations out molecule shown in yellow sticks.

Table S1: Top 100 molecules selected from virtual screening of 408 molecules set into the AXL active site. Binding energies are shown in kcal/mol.

S.No	Molecule	Binding Energy
1	PubChem-86622644	-9.1
2	PubChem-87083194	-8.3
3	PubChem-78160848	-8.3
4	PubChem-54673081	-8.3
5	PubChem-59105506	-8.3
6	PubChem-87624595	-8.3
7	PubChem-91161419	-8.3
8	PubChem-68651527	-8.3
9	PubChem-68651279	-8.3
10	PubChem-59496934	-8.3

11	PubChem-86647548	-8.2
12	PubChem-68650592	-8.2
13	PubChem-76973938	-8.2
14	PubChem-68651815	-8.2
15	PubChem-68651884	-8.2
16	PubChem-87130086	-8.2
17	PubChem-68651864	-8.2
18	PubChem-68650778	-8.2
19	PubChem-46215820	-8.2
20	PubChem-67095038	-8.2
21	PubChem-91571058	-8.2
22	PubChem-59291637	-8.2
23	PubChem-68651547	-8.2
24	PubChem-71726787	-8.2
25	PubChem-86622836	-8.2
26	PubChem-68652004	-8.2
27	PubChem-118893848	-8.2
28	PubChem-11487431	-8.1
29	PubChem-123758792	-8.1
30	PubChem-90805470	-8.1
31	PubChem-67363082	-8.1
32	PubChem-87238440	-8.1
33	PubChem-57974178	-8.1
34	PubChem-122421875	-8.1
35	PubChem-24771111	-8.1
36	PubChem-89770312	-8.1

37	PubChem-89770356	-8.1
38	PubChem-123781824	-8.1
39	PubChem-87689658	-8.1
40	PubChem-54674207	-8.1
41	PubChem-68650407	-8.1
42	PubChem-87636284	-8.1
43	PubChem-87240593	-8.1
44	PubChem-68650511	-8.1
45	PubChem-90028383	-8
46	PubChem-91026614	-8
47	PubChem-68651953	-8
48	PubChem-89254356	-8
49	PubChem-89254396	-8
50	PubChem-68651123	-8
51	PubChem-54674209	-8
52	PubChem-68651841	-8
53	PubChem-134203387	-8
54	PubChem-68650813	-8
55	PubChem-87240181	-8
56	PubChem-44454763	-8
57	PubChem-69043445	-8
58	PubChem-124099582	-8
59	PubChem-57463219	-8
60	PubChem-90163766	-8
61	PubChem-46241028	-7.9
62	PubChem-134203514	-7.9

63	PubChem-91230843	-7.9
64	PubChem-89254389	-7.9
65	PubChem-71727044	-7.9
66	PubChem-67364965	-7.9
67	PubChem-89254325	-7.9
68	PubChem-57928218	-7.9
69	PubChem-11516065	-7.9
70	PubChem-126726905	-7.9
71	PubChem-121494162	-7.9
72	PubChem-68650944	-7.9
73	PubChem-89254050	-7.9
74	PubChem-68651602	-7.9
75	PubChem-89254356	-7.9
76	PubChem-68651319	-7.9
77	PubChem-54674981	-7.9
78	PubChem-89254102	-7.9
79	PubChem-68651553	-7.8
80	PubChem-76167946	-7.8
81	PubChem-78160852	-7.8
82	PubChem-68651430	-7.8
83	PubChem-66830616	-7.8
84	PubChem-86643676	-7.8
85	PubChem-89254010	-7.8
86	PubChem-123546428	-7.8
87	PubChem-25224351	-7.8
88	PubChem-68651927	-7.8

89	PubChem-87659671	-7.8
90	PubChem-50996689	-7.8
91	PubChem-89254052	-7.8
92	PubChem-71727607	-7.7
93	PubChem-127040635	-7.7
94	PubChem-68650375	-7.7
95	PubChem-87945151	-7.7
96	PubChem-68651653	-7.7
97	PubChem-68650645	-7.7
98	PubChem-69271388	-7.7
99	PubChem-68651266	-7.7
100	PubChem-87240187	-7.7