

Table S1. The docking results of all docked compounds.

Sr No	Compounds	CDocker Energy (kcal/mol)	CDocker Interaction Energy (kcal/mol)
1	Z2242870510	-56.1411	-72.0739
2	Z1459964184	-56.1093	-65.4403
3	Z1450394746	-52.6466	-56.5756
4	Z1528724474	-52.2466	-69.9404
5	Z1528728414	-51.9493	-73.4986
6	Z1459911657	-50.9891	-66.7749
7	Z1459944817	-49.8452	-52.6715
8	Z1528733448	-49.6324	-63.3844
9	Z1528732470	-49.4855	-67.4339
10	Z1528730729	-48.544	-58.1347
11	Z1486429255	-47.0096	-56.6088
12	BMS-561392	-46.8811	-84.7487
13	Z1528724087	-45.5471	-56.6246
14	Z1528722648	-45.0183	-58.5849
15	Z1459955640	-44.7217	-64.3175
16	Z1528732297	-44.5959	-54.4538
17	Z1491313606	-43.8655	-50.3304
18	Z1528733542	-43.8502	-57.9296
19	Z1459955208	-43.4574	-59.0217
20	Z1459953090	-43.1834	-62.9099
21	Z1528725731	-43.0169	-60.2798
22	Z1459952980	-42.9628	-59.5152
23	Z1458553178	-42.6636	-52.0732
24	Z1528734250	-42.3583	-69.7425
25	Z1491321704	-42.2492	-60.9035
26	Z1528729529	-42.2076	-55.3135
27	Z1528726287	-42.0067	-59.5588
28	Z1528737526	-41.6156	-55.3821
29	Z1528726184	-40.6665	-53.6412
30	Z1622768502	-39.9682	-48.3745
31	Z1450135453	-39.6709	-47.2973
32	Z1491241365	-39.3967	-52.7198
33	Z1621453431	-39.2137	-50.9913
34	Z667709452	-39.2060	-44.0101
35	Z1528740074	-39.0508	-67.6253
36	Z1528730817	-38.8585	-59.1904
37	Z1528729903	-38.5904	-59.9200
38	Z979204300	-38.1088	-48.2060
39	Z1459953672	-37.6721	-64.0687
40	Z56763116	-37.6049	-47.9984
41	Z1459952715	-36.9106	-53.6551
42	Z1695669925	-36.6018	-52.6710
43	Z56802949	-35.2797	-49.6022
44	Z1528726887	-35.2758	-61.4161
45	Z1486428487	-34.9859	-43.8406
46	Z1528731677	-34.7250	-58.2018
47	Z1528722614	-33.0695	-55.3592

48	Z1459910880	-32.6047	-53.4811
49	Z1459306382	-32.5517	-49.2233
50	Z1459945323	-32.4056	-51.8606
51	Z1459914020	-32.1744	-51.5033
52	Z1528736538	-31.9258	-54.5133
53	Z1528732695	-31.9127	-48.6324
54	Z1528723401	-31.6443	-57.6362
55	Z1528734882	-31.6401	-60.8797
56	Z1458344695	-31.4082	-51.6604
57	Z1528732030	-31.3666	-58.3274
58	Z1528730876	-31.3521	-53.3940
59	Z1528727670	-31.2591	-54.8110
60	Z1528724522	-30.8516	-59.8383
61	Z1457193774	-30.8079	-42.8165
62	Z1528738940	-30.7302	-52.4363
63	Z1528730067	-30.4646	-55.8875
64	Z1459081038	-30.4476	-48.5450
65	Z1528736555	-29.8198	-51.7578
66	Z1528722556	-29.6731	-57.4893
67	Z1528736331	-29.6270	-53.3223
68	Z1491321964	-29.4821	-46.6184
69	Z1528734470	-29.4425	-55.3997
70	Z1458074734	-29.0939	-51.2035
71	Z1457276435	-28.9624	-40.7601
72	Z1528728186	-28.2151	-48.9408
73	Z1459910377	-28.1492	-52.7709
74	Z1491221067	-28.1075	-51.9295
75	Z1491312739	-28.0775	-41.7890
76	Z1528726247	-27.8184	-52.2633
77	Z1993928589	-27.4417	-41.7910
78	Z1528727868	-27.3812	-51.2344
79	Z1491220628	-27.3079	-42.9765
80	Z1491264267	-27.1198	-44.5754
81	Z1491215394	-26.3354	-42.8602
82	Z1491307303	-24.7848	-41.1394
83	Z1528729800	-24.7500	-50.7507
84	Z1443588461	-24.1052	-41.8651
85	Z1491321366	-23.9678	-41.0930
86	Z89390634	-22.8471	-38.6707
87	Z1491257605	-20.9383	-53.2652
88	Z1528730726	-20.2330	-52.5102
89	Z1491241327	-19.8711	-50.0200
90	Z1491262029	-19.7867	-50.8186
91	Z1491263672	-18.6922	-38.916
92	Z1528725798	-18.5928	-60.7712
93	Z1460003853	-16.8643	-58.3594
94	Z1491212758	-15.9168	-51.6058
95	Z1491300930	-15.3511	-52.1074
96	Z1491270786	-10.8387	-49.7823
97	Z1491353920	-9.61124	-46.2699
98	Z56849813	7.09941	-36.8655

Table S2. Molecular docking comparison of screened compounds.

Compounds	CDocker energy (kcal/mol)	PyRex Docking (kcal/mol)	GNINA (kcal/mol)
Z2242870510	-56.1411	-5.9	-9.10
Z1459964184	-56.1093	-6.0	-9.45
Z1450394746	-52.6466	-5.7	-9.08
Z1528724474	-52.2466	-4.9	-8.33
Z1528728414	-51.9493	-5.4	-9.76
Z1459911657	-50.9891	-5.5	-8.68
Z1459944817	-49.8452	-5.1	-7.46
Z1528733448	-49.6324	-4.6	-8.12
Z1528732470	-49.4855	-5.4	-7.78
Z1528730729	-48.5440	-4.7	-6.75
Z1486429255	-47.0096	-5.4	-6.51
BMS-561392 (Ref)	-46.8811	-6.4	-12.1
Z1528724087	-45.5471	-5.0	-6.41
Z1528722648	-45.0183	-5.2	-8.68
Z1459955640	-44.7217	-4.7	-8.43

Ref: The reference compound BMS-561392.

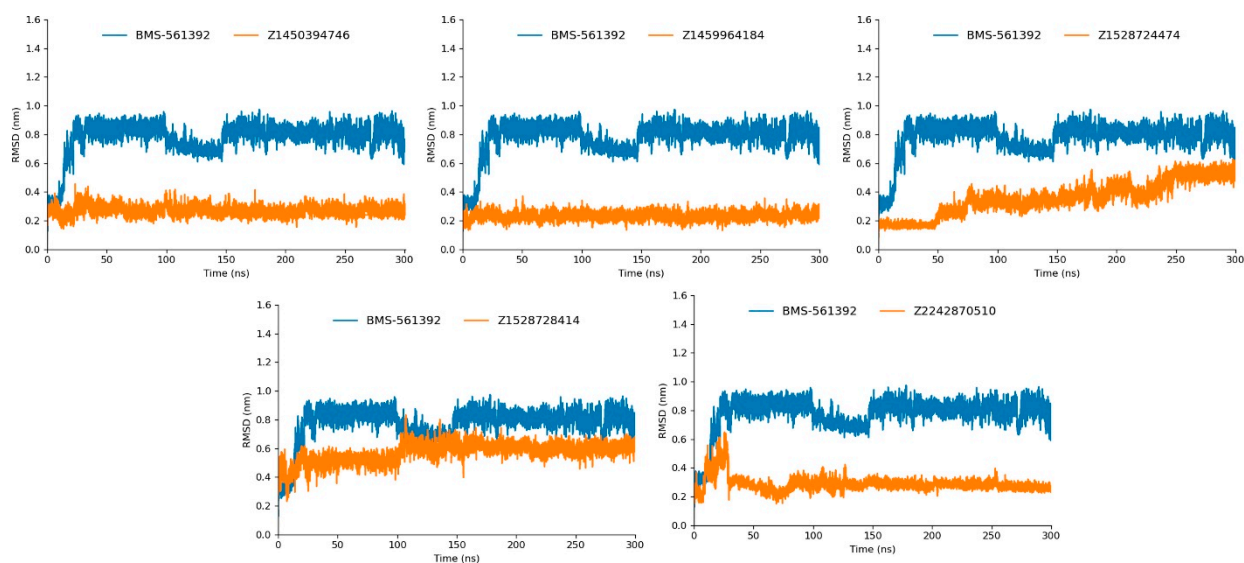


Figure S1. RMSD comparison of each screened enamine compound against the reference compound.

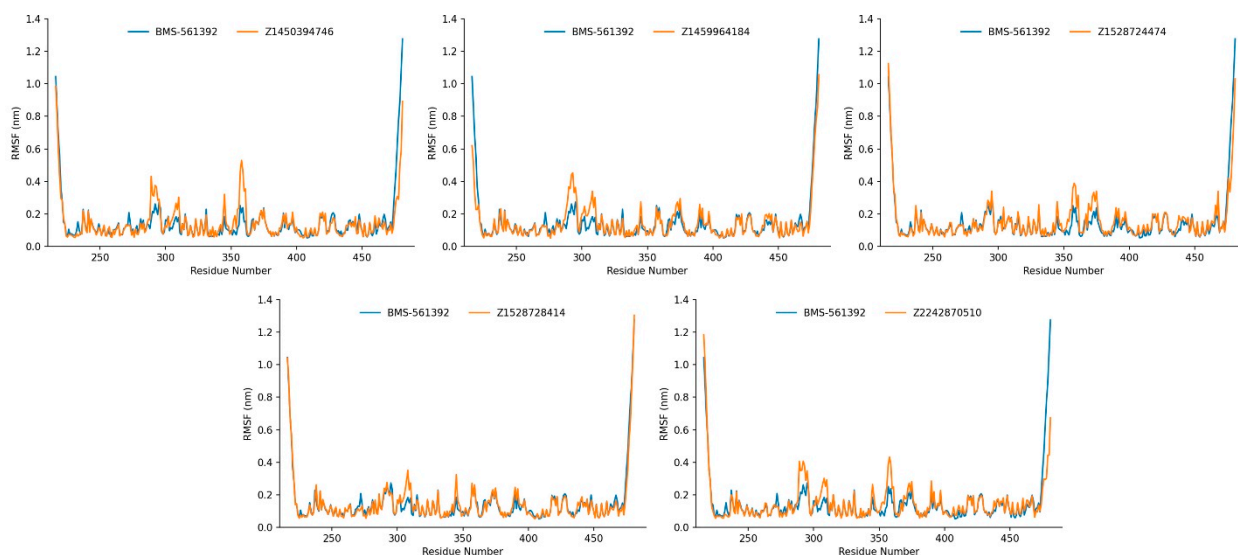


Figure S2. RMSF comparison of the top enamine compound against the reference compound.

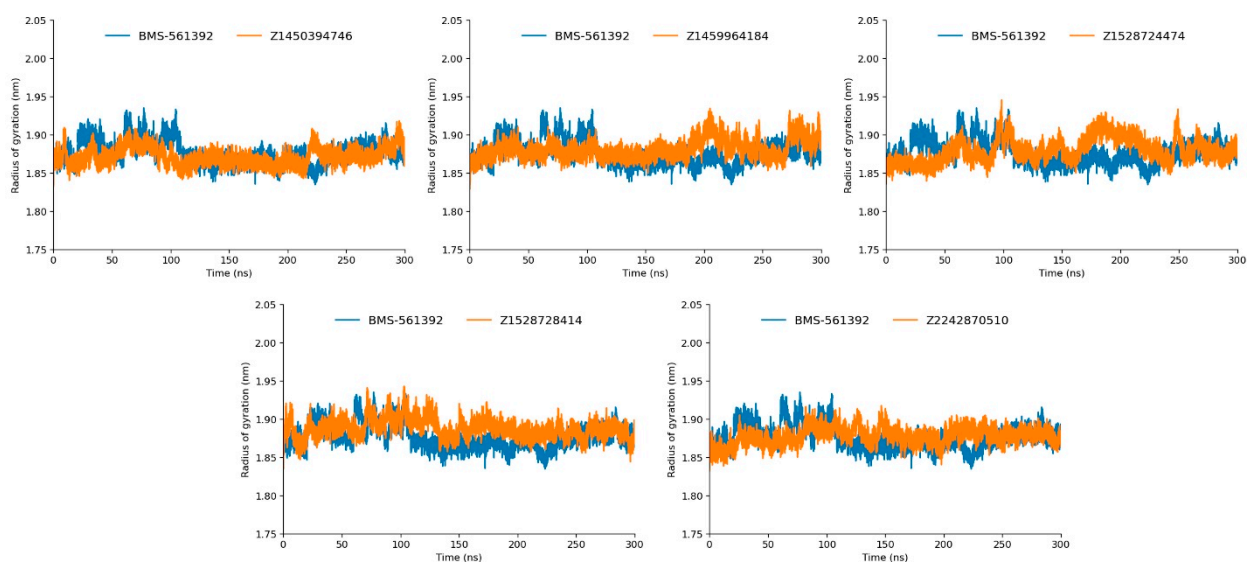


Figure S3. R_g comparison of the top screened enamine compound against the reference compound.

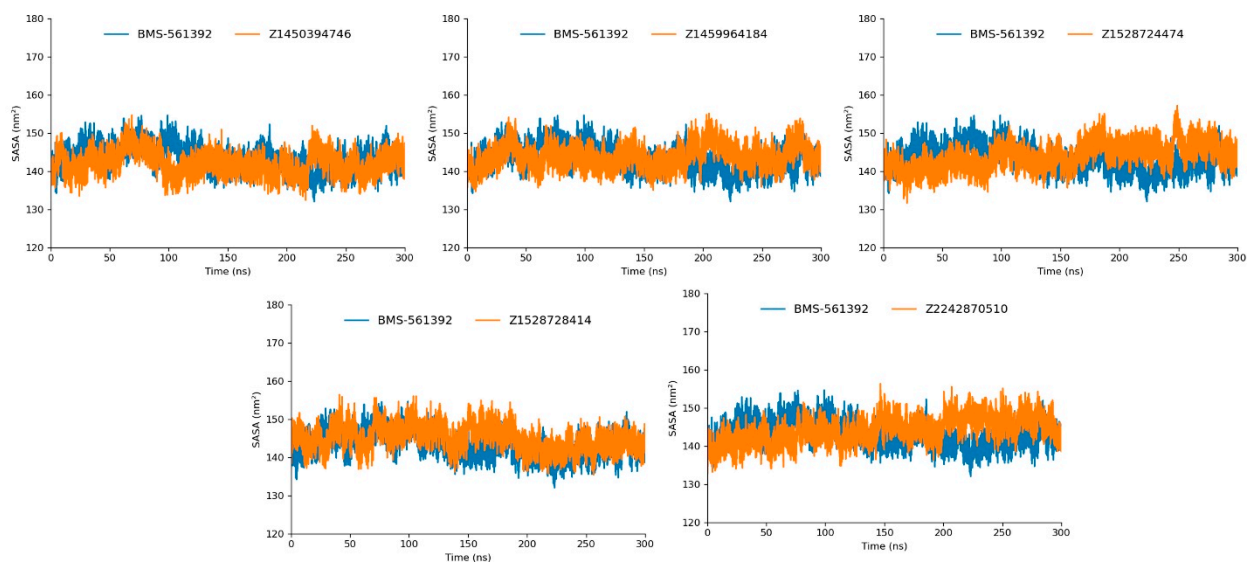


Figure S4. SASA plot comparison of the top screened enamine compound against the reference compound.

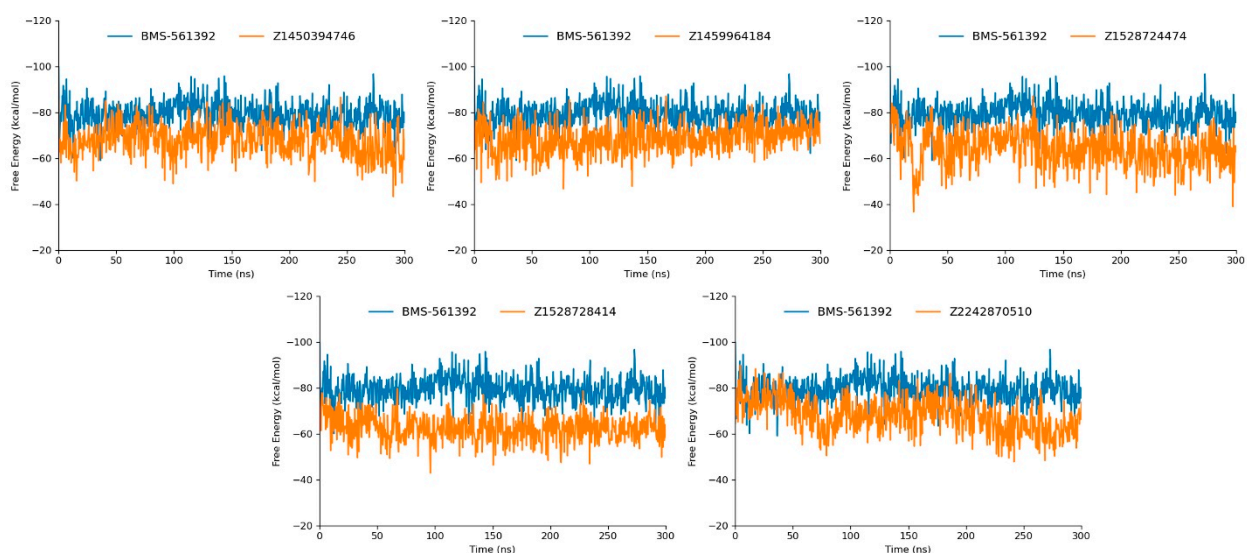


Figure S5. The graphs manifest the gmxMMPBSA free energy comparison of the screened enamine compounds with the reference compound.