Electronic supplementary information (ESI)

Latin American Databases of Natural Products: Biodiversity and Drug Discovery against SARS-CoV-2.

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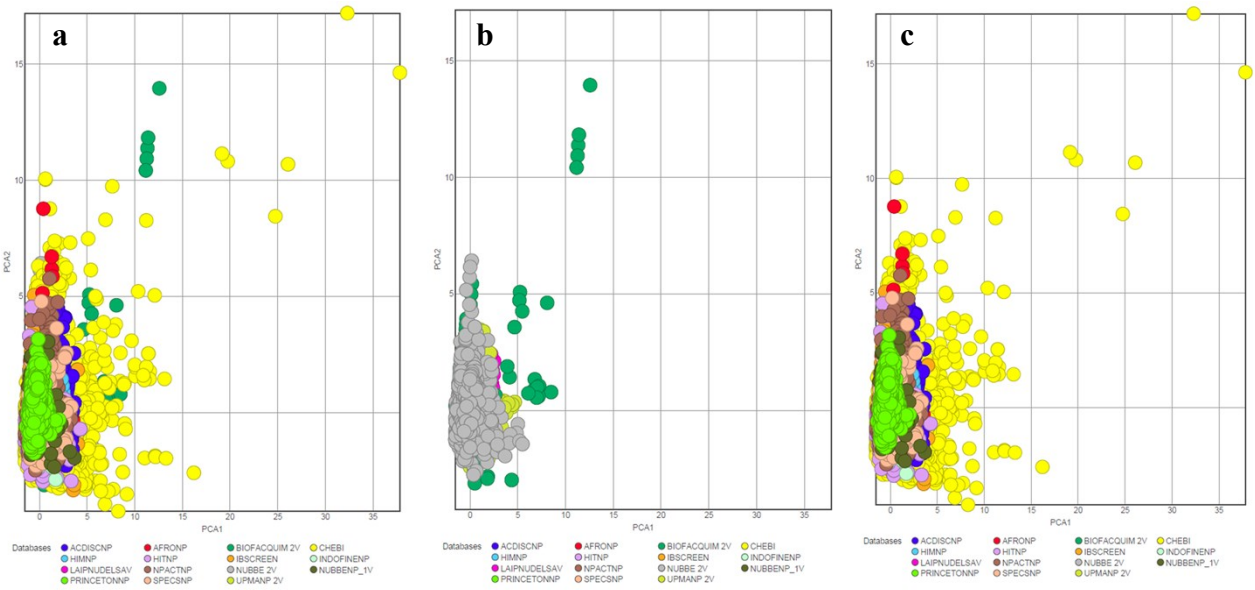


Figure S1 *Representation of the chemical space in 2D. All NPs (**a**), LATAM_DBS_NPs (**b**) and REF_NPs (**c**).*

Table S1. *Summary of Principal Component Analysis (PCA) of s ix physicochemical properties (PCP)*

PCP	PCA	Deviation	Condition	% Var
S log P	1	2.00036156e+000	1.00000000e+000	66.691
TPSA	2	1.15902870e+000	2.97871271e+000	89.080
Weight	3	6.13420952e-001	1.06340767e+001	95.351
a_acc	4	4.28659458e-001	2.17767056e+001	98.414
a_don	5	2.60168406e-001	5.91163876e+001	99.542
b_rotN	6	1.65783895e-001	1.45590261e+002	100.000

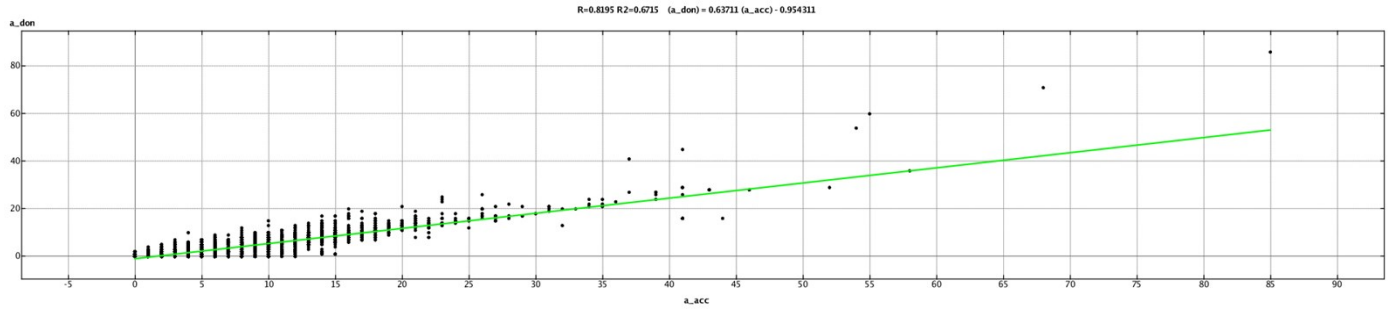


Figure S2 *Correlation scatter plot hydrogen bond acceptors (HBAs), and hydrogen bond donors (HBDs) in DBs*

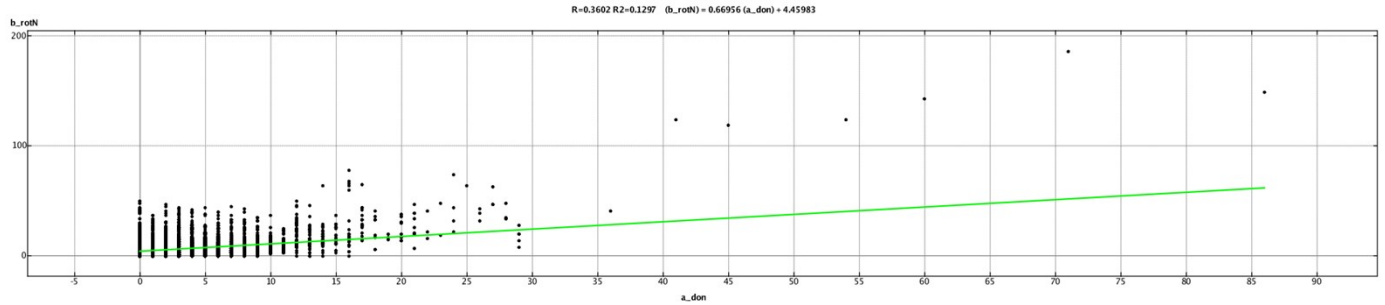


Figure S3 *Correlation scatter plot hydrogen bond donors and number of rotatable bonds (NRBs) in data set.*

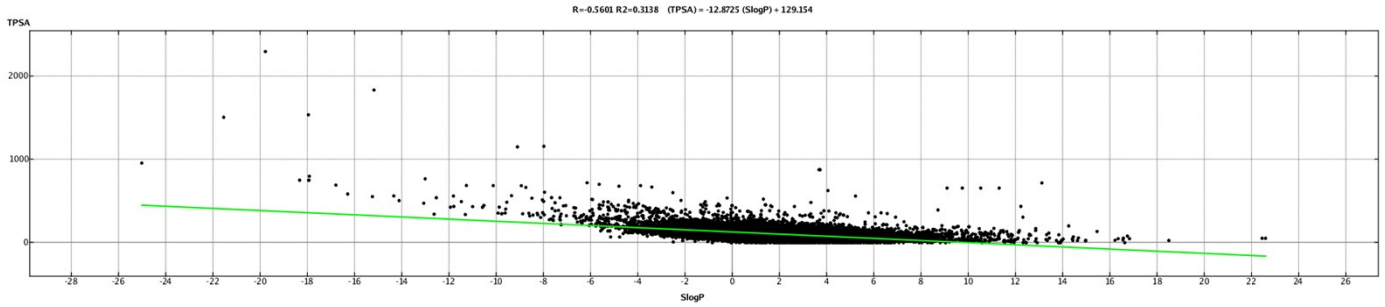


Figure S4 *Correlation scatter plot S Log P and TPSA in DBs*

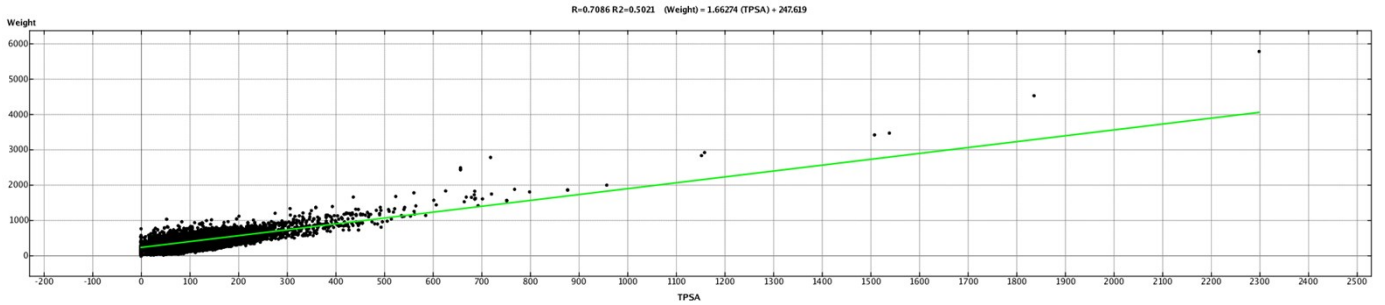
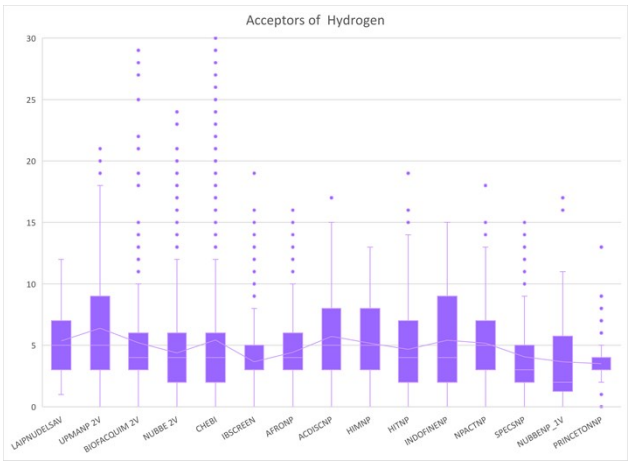


Figure S5 *Correlation scatter plot TPSA and Weight Molecular in DBs*

Figure S1-S5 *Correlation Scatter Plot of Physicochemical properties of the databases.* ***Note:*** *These correlation scatter graphs show that the groups of hydrogen acceptors / donors, the partition coefficient / TPSA, were adjusted to the regression model, observing a great association between these physicochemical properties of therapeutic interest.*



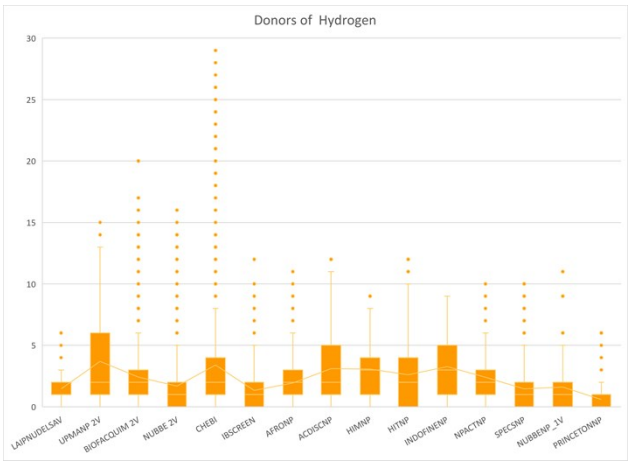
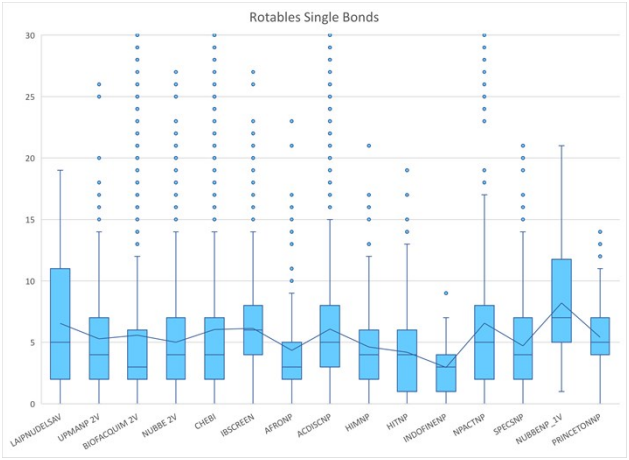


Figure S6 *Box plot of hydrogen bond acceptors (HBAs), hydrogen bond donors (HBDs) in Dbs.*



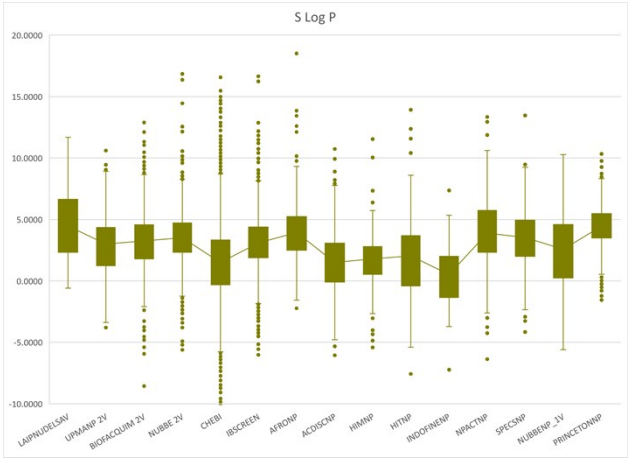
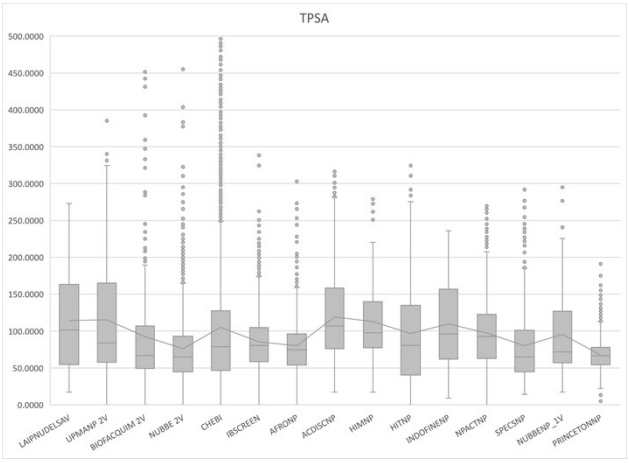


Figure S7 *Box plot of rotatable bonds (NRBs) and the octanol/water partition coefficient (w/o; S Log P) in databases*



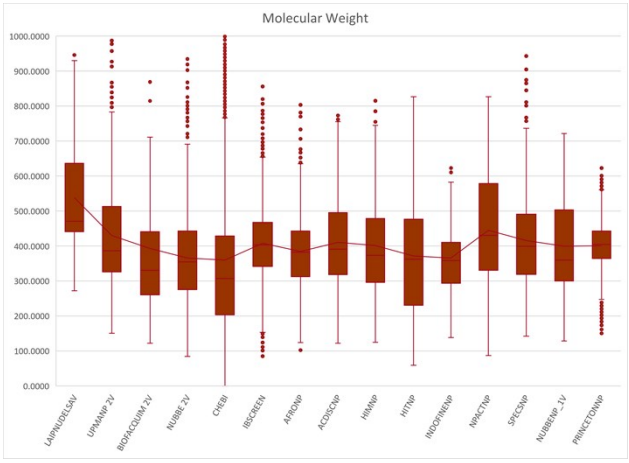


Figure S8 *Box plot of topological polar surface area (TPSA and molecular weight (MW)in dataset.*

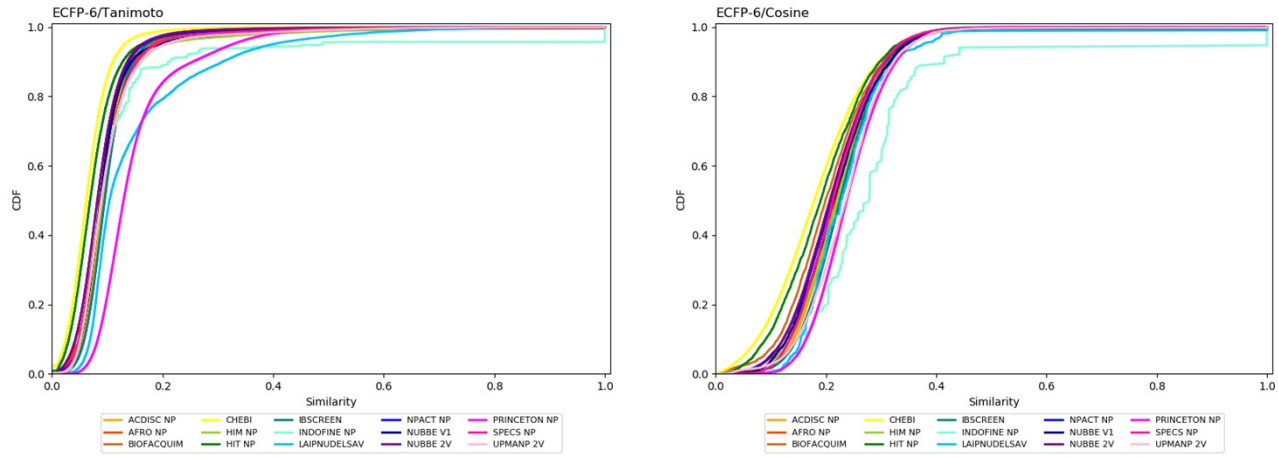


Figure S9 *Cumulative distribution function of the pairwise-similarity of the different data sets computed with ECFP-6-Tanimoto and Cosine.*

Table S2 *Summary statistics of the pairwise similarity computed with Tanimoto-ECFP-6*

NPs_DBs	mean	SD	min	1st Q	median	3rdQ	max
ACDISCNP	0.0998	0.0504	0.0	0.0714	0.0909	0.1154	1.0
AFRONP	0.0966	0.0558	0.0	0.0641	0.0873	0.1167	1.0
BIOFACQUIM	0.0944	0.0567	0.0	0.0654	0.0862	0.1104	1.0
CHEBI	0.6726	0.0413	0.0	0.0421	0.0625	0.0849	1.0
HIM_NP	0.1079	0.0925	0.0	0.0682	0.0903	0.1176	1.0
HIT_NP	0.0809	0.7522	0.0	0.0476	0.0691	0.0948	1.0
IBSCREEN	0.1026	0.0494	0.0	0.0753	0.0955	119	1.0
INDOFINE NP	0.1385	0.1942	0.0108	0.0614	0.0821	0.1259	1.0
LAIPNUDELSAV	0.1526	0.1207	0.0161	0.0824	0.1043	0.1718	1.0
NPACT NP	0.0960	0.0590	0.0	0.0677	0.0879	0.1103	1.0
NUBBE 1V	0.1010	0.0717	0.0	0.0685	0.0876	0.1111	1.0
NUBBE 2V	0.0893	0.0517	0.0	0.0610	0.0822	0.1068	1.0
PRINCETON NP	0.1532	0.0815	0.0099	0.1045	0.1314	0.1698	1.0
SPECSNP	0.1017	0.0704	0.0	0.0657	0.0889	0.1189	1.0
UPMANP 2V	0.1051	0.0747	0.0	0.0676	0.0893	0.1189	1.0

Min: Minimum; Max: Maximum; Q: Quartile; SD, Standard Deviation.

Table S3 *Summary statistics of the pairwise similarity computed with Cosine-ECFP-6*

NPS_DBS	mean	SD	min	1st Q	median	3rdQ	max
ACDISC NP	0.2252	0.0694	0.0143	0.1766	0.2201	0.2680	1.0
AFRO NP	0.2226	0.0775	0.0129	0.1719	0.2178	0.2651	1.0
BIOFACQUIM	0.2061	0.0878	0.0022	0.1518	0.1990	0.2524	1.0
CHEBI	0.1084	0.0865	0.0001	0.1232	0.1790	0.2587	1.0
HIM NP	0.2274	0.0935	0.0328	0.1740	0.2201	0.2690	1.0
HIT NP	0.1970	0.1000	0.0122	0.1358	0.1904	0.2472	1.0
IBSCREEN	0.2288	0.0665	0.0118	0.1832	0.2253	0.2707	1.0
INDOFINE NP	0.3052	0.1889	0.0615	0.2045	0.2789	0.3142	1.0
LAIPNUDELSAV	0.2406	0.1032	0.1070	0.1823	0.2280	0.2732	1.0
NPACTNP	0.2106	0.0768	0.0123	0.1606	0.2080	0.2559	1.0
NUBBE 1V	0.2195	0.0808	0.0387	0.1677	0.2125	0.2622	1.0
NUBBE 2V	0.2123	0.0756	0.0079	0.1613	0.2072	0.2580	1.0
PRINCETON NP	0.2415	0.0637	0.0298	0.1962	0.2365	0.2813	1.0
SPECSNP	0.2182	0.0787	0.0431	0.1688	0.2122	0.2581	1.0
UPMANP 2V	0.2364	0.0805	0.0071	0.1881	0.2363	0.2790	1.0

Min: Minimum; Max: Maximum; Q: Quartile; SD, Standard Deviation.

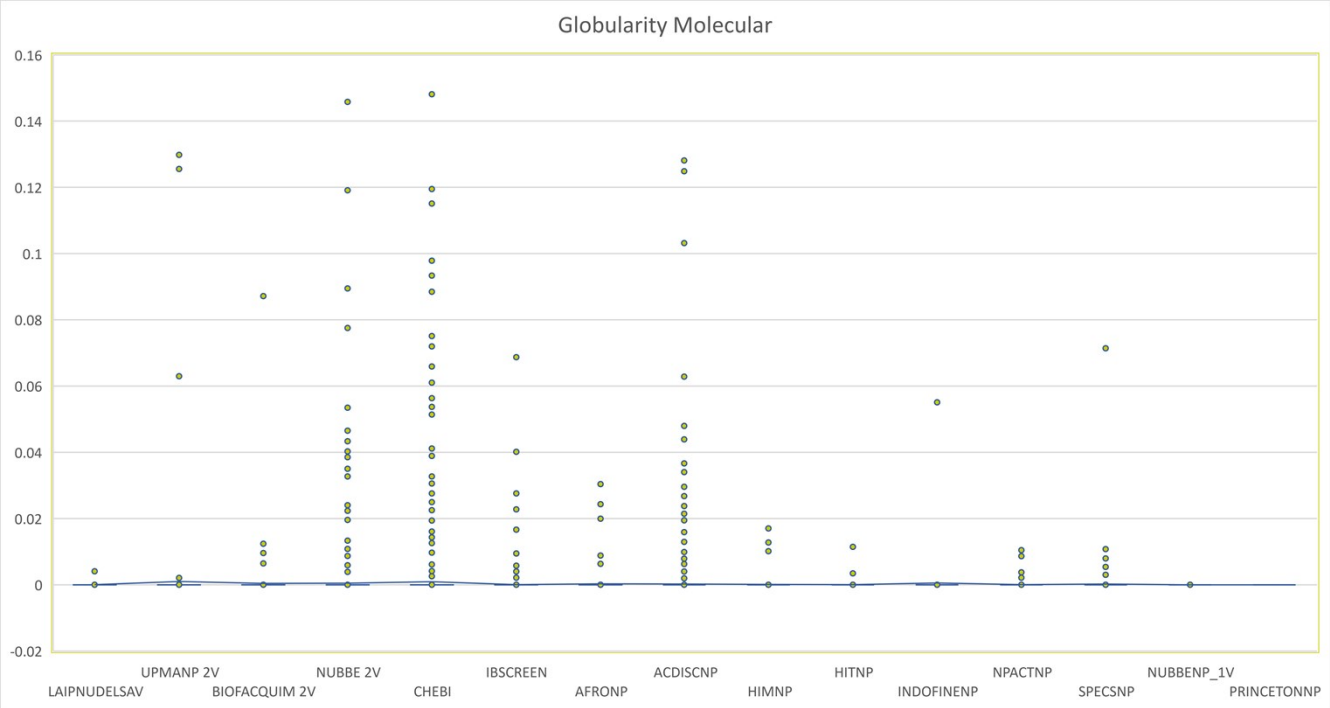


Figure S10 *Distribution of globularity molecular*

Table S4 *Metric of globularity molecular*

glob_mol	Mean	SD
LAIPNUDELSAV	0.0000	0.0004
UPMANP 2V	0.0010	0.0107
BIOFACQUIM_2V	0.0004	0.0055
NUBBE_2V	0.0005	0.0056
CHEBI	0.0009	0.0238
IBSCREEN	0.0000	0.0010
AFRONP	0.0003	0.0022
ACDISCNP	0.0002	0.0030
HIMNP	0.0001	0.0013
HITNP	0.0000	0.0007
INDOFINENP	0.0006	0.0055
NPACTNP	0.0001	0.0007
SPECSNP	0.0002	0.0029
NUBBE_1V	0.0000	0.0000
PRINCENTONNP	0.0000	0.0000

Mean; SD: Standard Deviation.

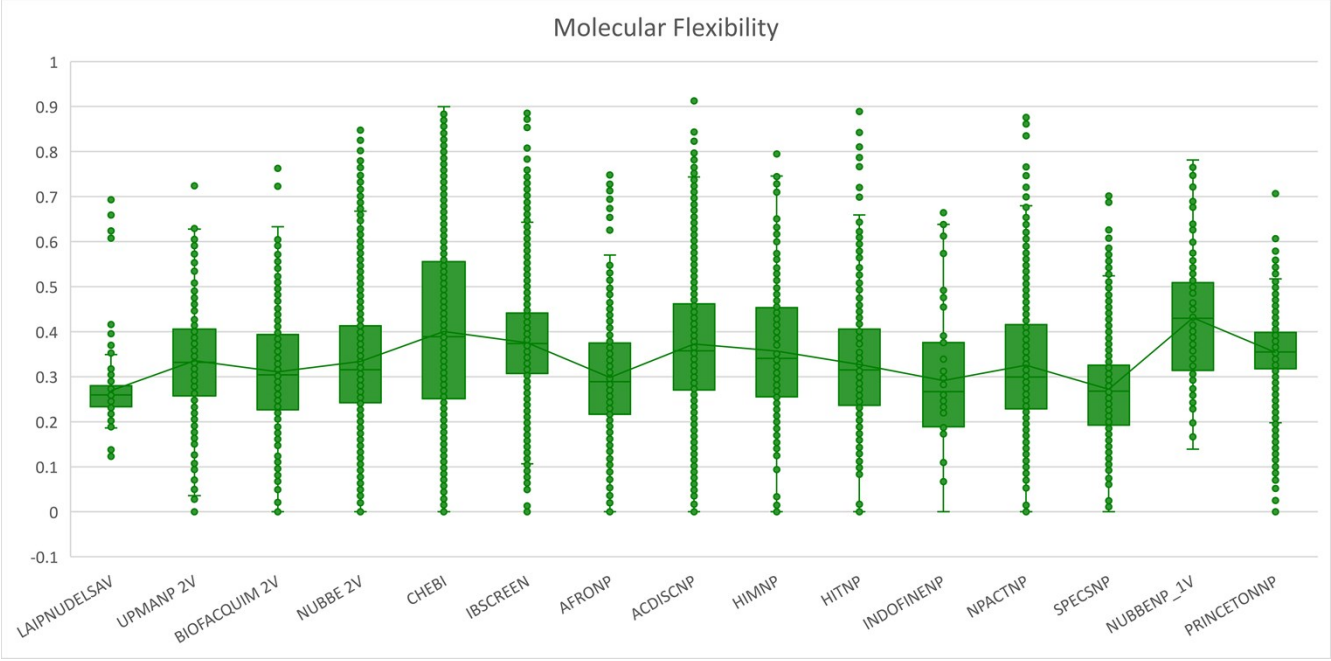


Figure S11. *Distribution of molecular flexibility*

Table S6. *Metric of flexibility molecular*

Molecular Flexibility	Min	1Qst	median	3Qst	Max	Mean	SD
LAIPNUDELSAV	0.1230	0.2336	0.2593	0.2790	0.6952	0.2688	0.0786
UPMANP 2V	0.0000	0.2582	0.3320	0.4055	0.7242	0.3354	0.1276
BIOFACQUIM_2V	0.0000	0.2268	0.3042	0.3934	0.7626	0.3110	0.1330
NUBBE_2V	0.0000	0.2423	0.3157	0.4124	0.8518	0.3339	0.1407
CHEBI	0.0000	0.2512	0.3888	0.5554	0.8999	0.4007	0.2058
IBSCREEN	-1.0000	0.3071	0.3738	0.4415	0.8854	0.3751	0.1140
AFRONP	0.0000	0.2172	0.2887	0.3745	0.7482	0.2982	0.1321
ACDISCNP	0.0000	0.2705	0.3573	0.4616	0.9126	0.3726	0.1424
HIMNP	0.0000	0.2559	0.3408	0.4531	0.8076	0.3569	0.1421
HITNP	0.0000	0.2365	0.3151	0.4051	0.8888	0.3569	0.1421
INDOFINENP	0.0000	0.1895	0.2671	0.3756	0.6642	0.2915	0.1235
NPACTNP	0.0000	0.2285	0.2995	0.4155	0.8759	0.3256	0.1439
SPECSNP	0.0000	0.1926	0.2680	0.3249	0.7017	0.2721	0.1062
NUBBE_1V	0.1389	0.3146	0.4298	0.5087	0.7813	0.4310	0.1447
PRINCENTONNP	0.0000	0.3177	0.3549	0.3981	0.7076	0.3536	0.0660

Min: Minimum; Max: Maximum; Q: Quartile; SD: Standard Deviation.

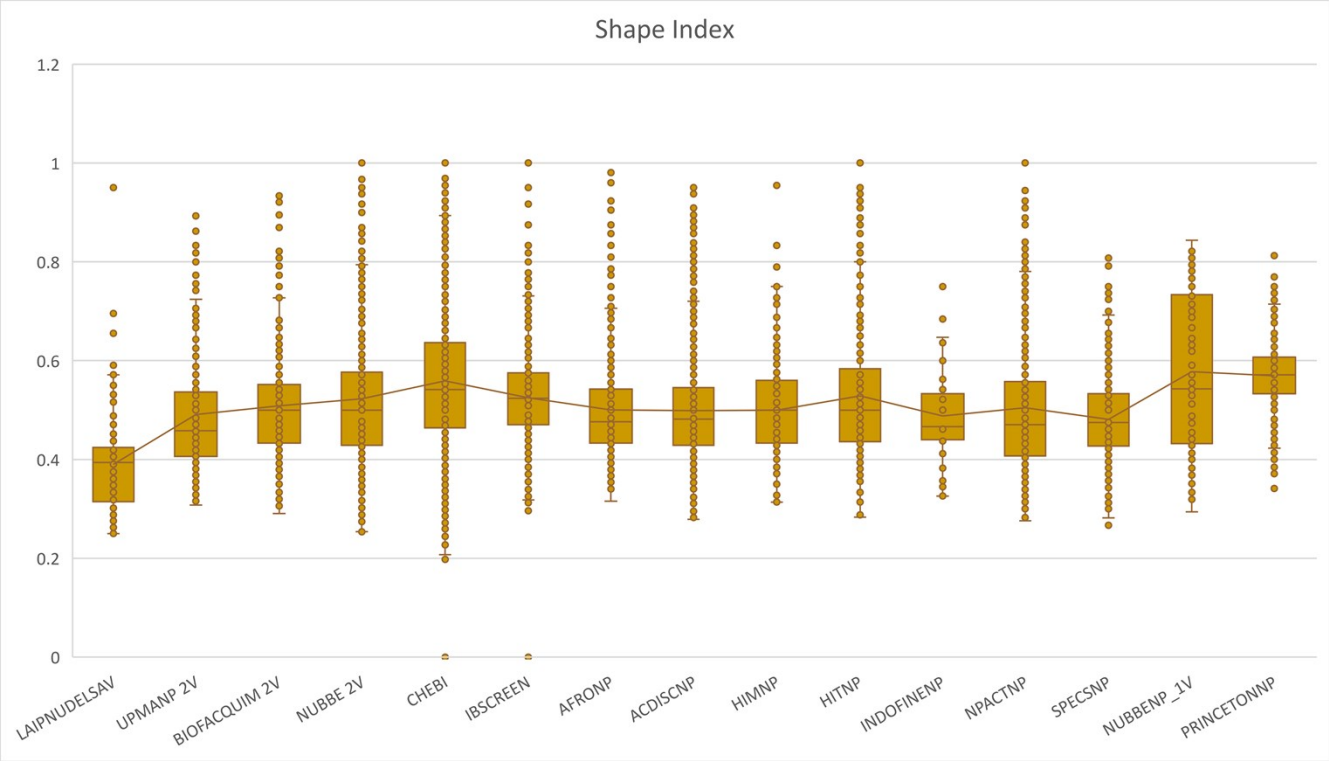


Figure S12 *Distribution of shape index*

Table S7 *Metric of shape index*

Shape Index	Min	1Qst	Median	3Qst	Max	Mean	SD
LAIPNUDELSAV	0.2500	0.3171	0.3939	0.4242	0.9500	0.3902	0.1009
UPMANP 2V	0.3077	0.4063	0.4583	0.5358	0.8929	0.4909	0.1169
BIOFACQUIM_2V	0.2906	0.4333	0.5000	0.5517	0.9375	0.5087	0.1238
NUBBE_2V	0.2537	0.4286	0.5000	0.5769	1.0000	0.5227	0.1369
CHEBI	0.0000	0.4643	0.5417	0.6364	1.0000	0.5592	0.1431
IBSCREEN	0.0000	0.4706	0.5238	0.5926	1.0000	0.5248	0.0753
AFRONP	0.3158	0.4333	0.4762	0.5417	0.9808	0.5005	0.1055
ACDISCNP	0.0000	0.4286	0.4815	0.5455	0.9583	0.4356	0.1397
HIMNP	0.2917	0.4333	0.5000	0.5600	0.9546	0.4994	0.0921
HITNP	0.2833	0.4369	0.5000	0.5833	1.0000	0.5285	0.1300
INDOFINENP	0.3261	0.4400	0.4667	0.5275	0.7500	0.4880	0.0877
NPACTNP	0.0000	0.4074	0.4706	0.5556	1.0000	0.4151	0.1663
SPECSNP	0.2667	0.4286	0.4750	0.5333	0.8077	0.4814	0.0818
NUBBE_1V	0.5417	0.5469	0.5521	0.5573	0.5625	0.5521	0.0147
PRINCENTONNP	0.3415	0.5333	0.5714	0.6071	0.8125	0.5693	0.0534

Min: Minimum; Max: Maximum; Q: Quartile; SD: Standard Deviation.

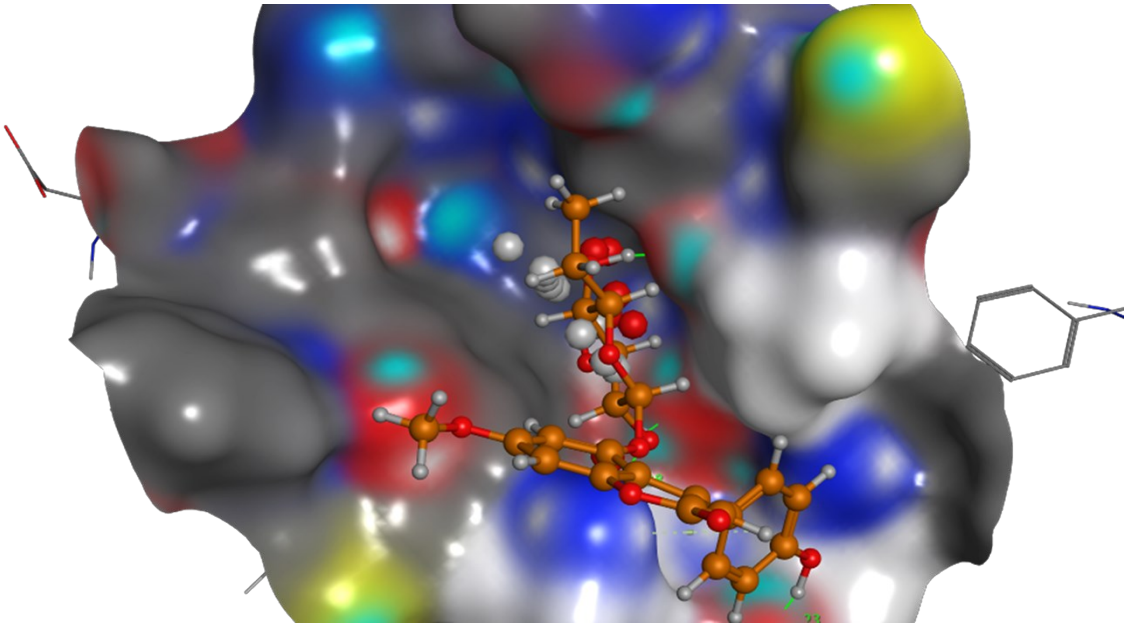


Figure S13 Ligand_LAIPNUDELSAV_29 in the pocket of protein NSP-15

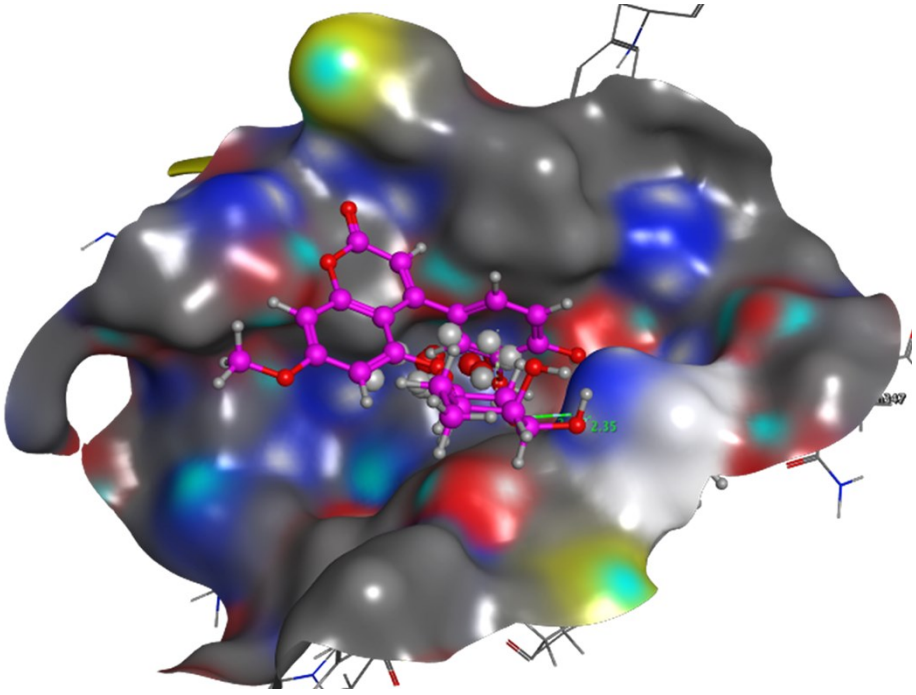


Figure S14 Ligand _LAIPNUDELSAV_31 in the binding site in endonucleases NSP-15

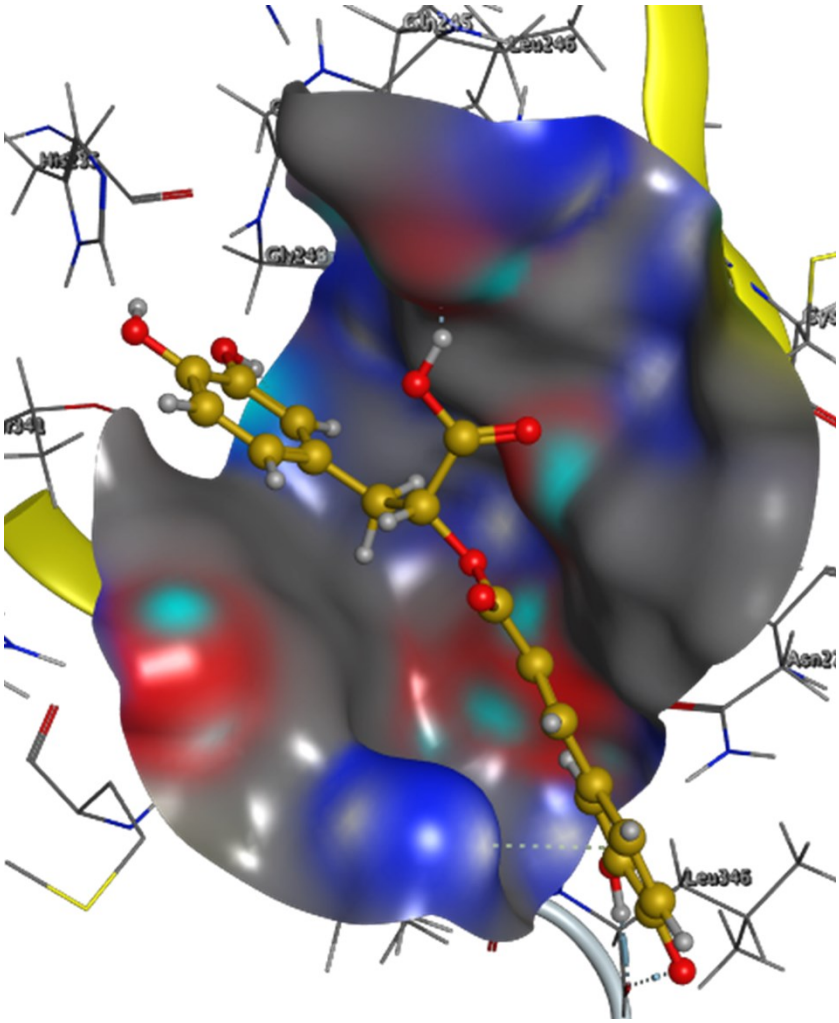


Figure S15 Ligand_UPMA_2V_266 in the site of protein NSP-15