Supplementary Table 1 - List of studies for the construction of the meta-data

Access ID	Samples	Platform
GSE13911	69	Affymetrix Human Genome U133 Plus 2.0 array
GSE54129	132	Affymetrix Human Genome U133 Plus 2.0 array
GSE66229	400	Affymetrix Human Genome U133 Plus 2.0 array

Supplementary Table 2 - List of RNAm, NCBI Reference Sequences and Primer sequences (forward and reverse complement) for the PCR

GENE	CÓDIGO NCBI	SEQUENCE
AJUBA	NM_001289097.2 NM_032876.6	F-GATGCTGTGGGATTCCTGGC R-GAACTTCTCCAGCAGGCGAC
GPNMB	NM_001005340.2 NM_002510.3	F-AGCCCTGTGGATGTGGATGA R-GAGCCAGGCTTGTGTCATCC
CD80	NM_005191.4	F-GGATTGTCATCAGCCCTGCC R-GAGAAAGACCAGCCAGCACC
FBXL13	NM_001111038.2 NM_001287150.2 NM_001394494.2 NM_145032.3	F-ACAGCAGCCTCAGATCCCTT R-TTAGCCGCACACAGTTGCTT
PDILT	NM_174924.2	F-GTGGATGCAGACGAACCCAG R-CCCACGAGCTGCTTAACCAG
CCDC69	NM_015621.3	F-GGCCGTCCAGTCCTGATAGT R-GGGAGGGGTATGGAAAGCCT
KNL1	NM_144508.5 NM_170589.5	F-CTACCACCCCTTCCAGAGCA R-TGGCGGTAGAGAGGTGGTTT
IL13RA2	NM_000640.3	F-ACCTTTGCCGCCAGTCTATC R-GGTCTTCACCTTCCCAGCATT
NOLC1	NM_001284388.2 NM_004741.5 NM_001284389.2	F-GCTCTCCAAGACCACAAGCC R-CCTCCCTGACCCTTCGGAAT

Supplementary Table 3 – List of top 10 ligands identified by screening MCULE's purchasable library using AutoDock Vina for the AJUBA target. Results were obtained by applying the RO5 violations filter with a value of zero (first column) and a maximum value of one violation of Lipinski's rules (fourth column).

MCULE ID ***RO5 violations* 0**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**	**MCULE ID** ***RO5 violations* 1**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**
MCULE-2386589557-0-6*	-7.3	5	**MCULE-1346978245-0-5***	-7.5	4
MCULE-8494477087-0-5*	-7.1	5	**MCULE-3807948532-0-1***	-7.5	5
MCULE-8618831675-0-4	-7.1	3	**MCULE-3063637254-0-1***	-7.3	4
MCULE-4680685315-0-2	-7.1	4	MCULE-5100808095-0-2	-7.2	4
MCULE-3694094262-0-3	-7.1	4	MCULE-3351135747-0-1	-7.2	4
MCULE-8663038790-0-3	-6.9	4	MCULE-4204800704-0-1	-7.2	3
MCULE-6320162783-0-1	-6.9	4	MCULE-1828307804-0-10	-7.1	3
MCULE-8680129923-0-1	-6.9	4	MCULE-6778694814-0-1	-7.0	3
MCULE-5479669360-0-2*	-6.9	4	MCULE-1079488332-0-2	-7.0	5
MCULE-4497233309-0-6	-6.8	3	MCULE-7588444166-0-2	-7.0	4

*: Compounds selected for the molecular docking step on the DockThor server. Compounds with favorable toxicological properties were chosen as a selection criterion, without prediction for the toxicity endpoint models and with a prediction of toxicity class equal to or greater than 4.

Supplementary Table 4 – List of top 10 ligands identified by screening MCULE's purchasable library using AutoDock Vina for the FBXL13 target. Results were obtained by applying the RO5 violations filter with a value of zero (first column) and a maximum value of one violation of Lipinski's rules (fourth column).

MCULE ID ***RO5 violations* 0**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**	**MCULE ID** ***RO5 violations* 1**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**
MCULE-1421958665-0-2	-8.9	4	MCULE-2834940013-0-1	-9.5	4
MCULE-9793153865-0-1	-8.7	4	**MCULE-4837473549-0-1***	-9.4	4
MCULE-6762186979-0-1	-8.4	4	MCULE-2856220621-0-15	-8.9	4
MCULE-7343047040-0-1*	-8.3	6	MCULE-3031349951-0-8	-8.5	4
MCULE-7134467177-0-19	-8.3	4	MCULE-4329088478-0-13	-8.3	4
MCULE-7485237354-0-2	-8.2	4	**MCULE-1240068246-0-3***	-8.2	5
MCULE-5801701072-0-1	-8.2	4	**MCULE-7674523665-0-10***	-8.1	5
MCULE-7839530280-0-2*	-8.1	4	MCULE-1589361690-0-3	-8.1	4
MCULE-9497113862-0-1*	-8.1	4	MCULE-6462715004-0-1	-8.1	4
MCULE-1376851564-0-1	-8.1	3	MCULE-4627906027-0-1	-8.1	4

*: Compounds selected for the molecular docking step on the DockThor server. Compounds with favorable toxicological properties were chosen as a selection criterion, without prediction for the toxicity endpoint models and with a prediction of toxicity class equal to or greater than 4.

Supplementary Table 5 – List of top 10 ligands identified by screening MCULE's purchasable library using AutoDock Vina for the CCDC69 target. Results were obtained by applying the RO5 violations filter with a value of zero (first column) and a maximum value of one violation of Lipinski's rules (fourth column).

MCULE ID ***RO5 violations* 0**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**	**MCULE ID** ***RO5 violations* 1**	**Vina Docking Score (Kcal mol−1)**	**Predicted Toxicity Class**
MCULE-3357521706-0-2	-6.1	4	MCULE-6567370457-0-1	-6.1	3
MCULE-7291884843-0-1	-6.1	4	**MCULE-2466636342-0-1***	-5.9	5
MCULE-6245522375-0-3	-5.8	5	MCULE-7061391609-0-3	-5.9	4
MCULE-1779314389-0-1	-5.7	4	MCULE-2229168061-0-14	-5.9	4
MCULE-2550805052-0-11	-5.6	5	MCULE-9565803118-0-2	-5.8	4
MCULE-5230409338-0-3*	-5.6	4	MCULE-6712895418-0-1	-5.8	5
MCULE-8983182958-0-3	-5.6	5	MCULE-7912008497-0-1	-5.7	4
MCULE-6589791340-0-1*	-5.5	4	MCULE-7005897344-0-5	-5.7	4
MCULE-3852950789-0-1*	-5.5	5	MCULE-4361650137-0-1	-5.7	4
MCULE-5463099531-0-1	-5.5	3	MCULE-4709007350-0-1	-5.7	3

*: Compounds selected for the molecular docking step on the DockThor server. Compounds with favorable toxicological properties were chosen as a selection criterion, without prediction for the toxicity endpoint models and with a prediction of toxicity class equal to or greater than 4.

Supplementary Table 6 – List of top 10 ligands identified by screening MCULE's purchasable library using AutoDock Vina for the CD80 target. Results were obtained by applying the RO5 violations filter with a value of zero (first column) and a maximum value of one violation of Lipinski's rules (fourth column).

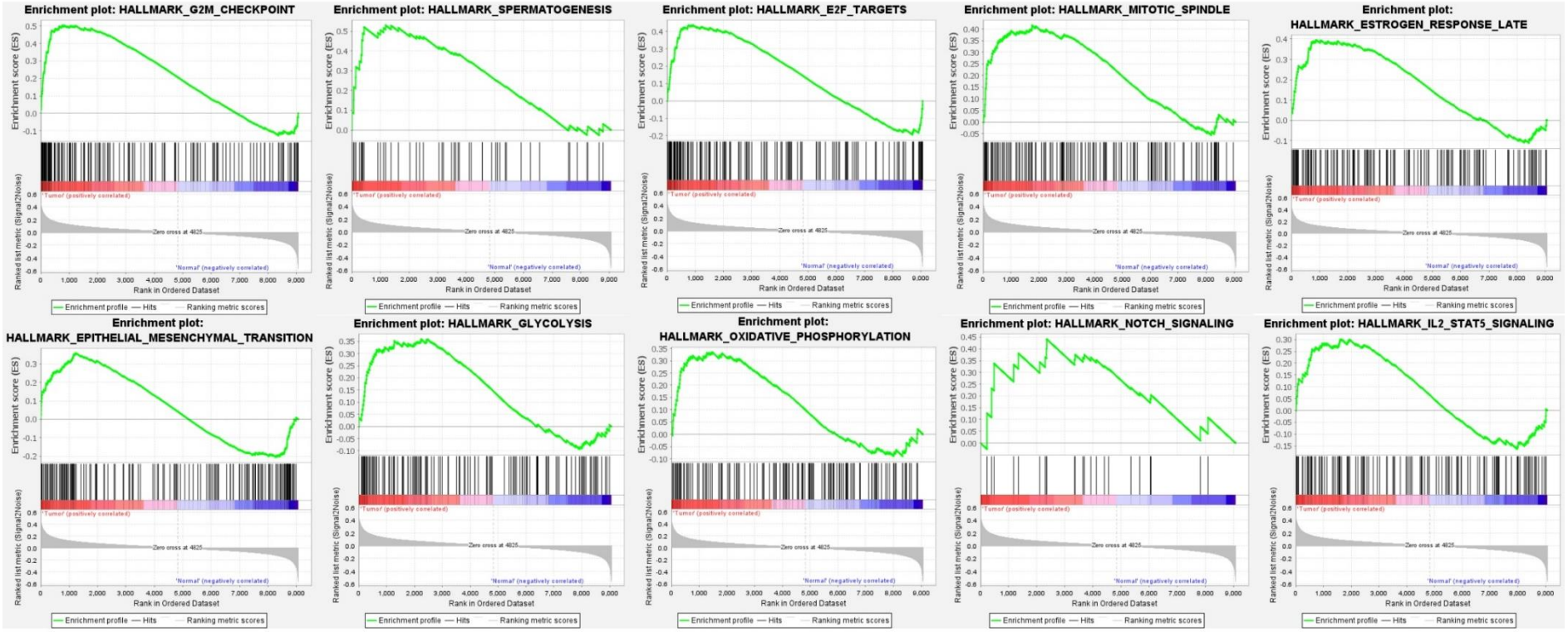
MCULE ID ***RO5 violations* 0**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**	**MCULE ID** ***RO5 violations* 1**	**Vina Docking Score (Kcal mol−1)**	**Predicted Toxicity Class**
MCULE-9029233932-0-3	-6.5	4	**MCULE-5603330835-0-4***	-6.2	5
MCULE-2278849636-0-73	-5.8	4	MCULE-6803888312-0-2	-6.1	4
MCULE-7527853534-0-1	-5.7	3	MCULE-8687320609-0-2	-6.0	3
MCULE-7110142890-0-1	-5.7	4	MCULE-3297909584-0-5	-5.9	4
MCULE-4428265531-0-1	-5.7	4	**MCULE-8352206143-0-1***	-5.9	5
MCULE-2625873551-0-8*	-5.6	4	MCULE-5153818617-0-1	-5.9	4
MCULE-9178344200-0-1*	-5.6	4	**MCULE-4926494876-0-3***	-5.9	5
MCULE-5779193146-0-2	-5.6	3	MCULE-7734390487-0-3	-5.9	4
MCULE-4809120560-0-2*	-5.6	4	MCULE-7803762894-0-3	-5.9	4
MCULE-2768743746-0-1	-5.6	4	MCULE-3841426087-0-2	-5.8	5

*: Compounds selected for the molecular docking step on the DockThor server. Compounds with favorable toxicological properties were chosen as a selection criterion, without prediction for the toxicity endpoint models and with a prediction of toxicity class equal to or greater than 4.

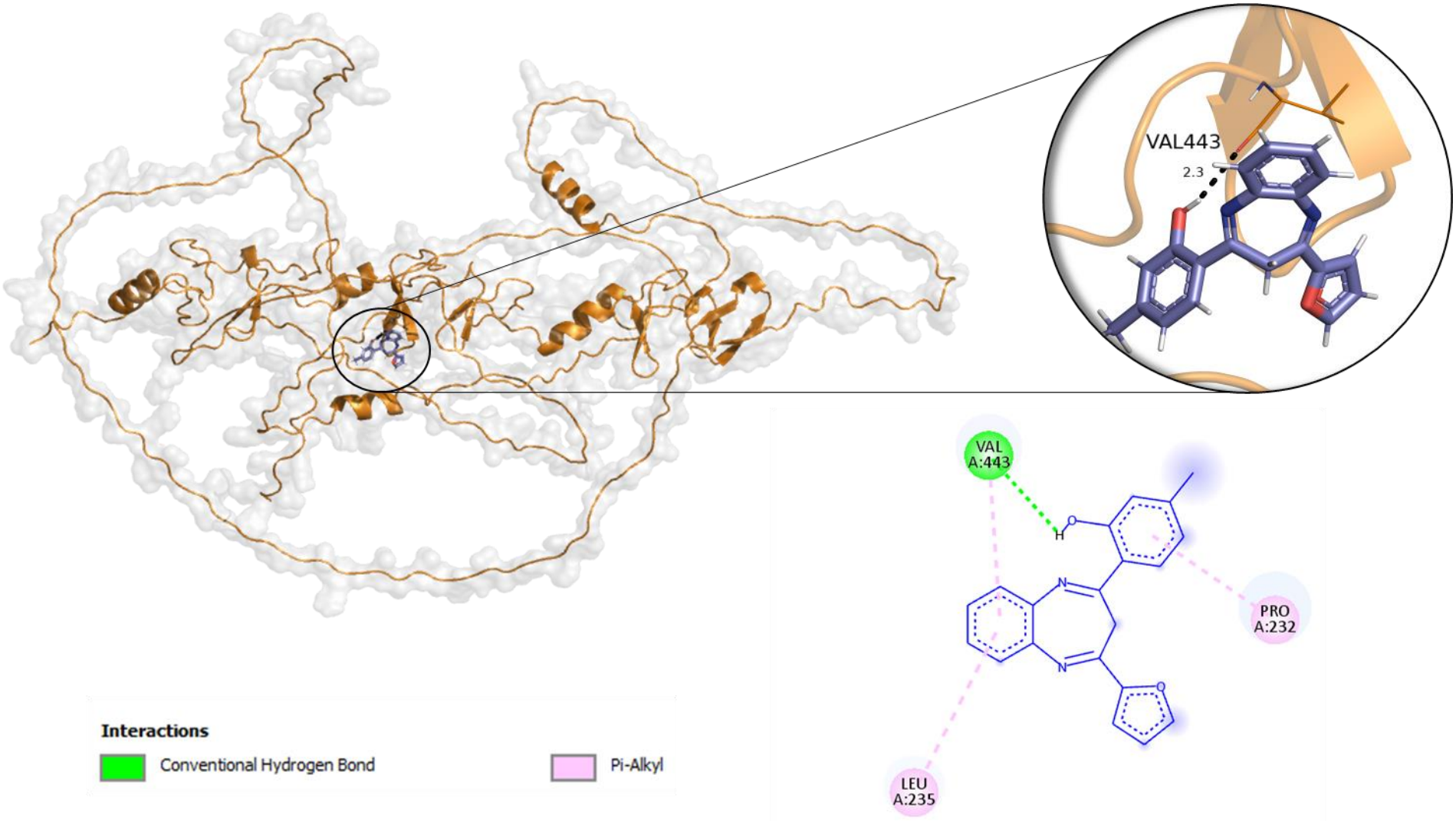
Supplementary Table 7 – List of top 10 ligands identified by screening MCULE's purchasable library using AutoDock Vina for the NOLC1 target. Results were obtained by applying the RO5 violations filter with a value of zero (first column) and a maximum value of one violation of Lipinski's rules (fourth column).

MCULE ID ***RO5 violations* 0**	**Vina Docking Score (Kcal mol^{-1})**	**Predicted Toxicity Class**	**MCULE ID** ***RO5 violations* 1**	**Vina Docking Score (Kcal mol−1)**	**Predicted Toxicity Class**
MCULE-5664033778-0-1*	-8.6	4	MCULE-9308263243-0-1	-8.0	4
MCULE-1565012771-0-2	-8.0	3	MCULE-3124833010-0-6	-7.9	4
MCULE-3493609194-0-3	-7.8	4	**MCULE-3208354401-0-1***	-7.8	4
MCULE-7733662288-0-1	-7.7	4	MCULE-9637835211-0-1	-7.8	4
MCULE-5092204522-0-3	-7.7	5	MCULE-7319692064-0-1	-7.7	5
MCULE-7508528499-0-3	-7.6	4	MCULE-5732820926-0-1	-7.7	5
MCULE-2888284016-0-4*	-7.6	4	MCULE-4931306065-0-11	-7.7	4
MCULE-5881513100-0-29*	-7.5	4	MCULE-5201794719-0-3	-7.6	4
MCULE-6651045318-0-2	-7.5	4	**MCULE-5283295284-0-4***	-7.5	4
MCULE-5189774934-0-5	-7.4	4	**MCULE-2195033842-0-2***	-7.5	4

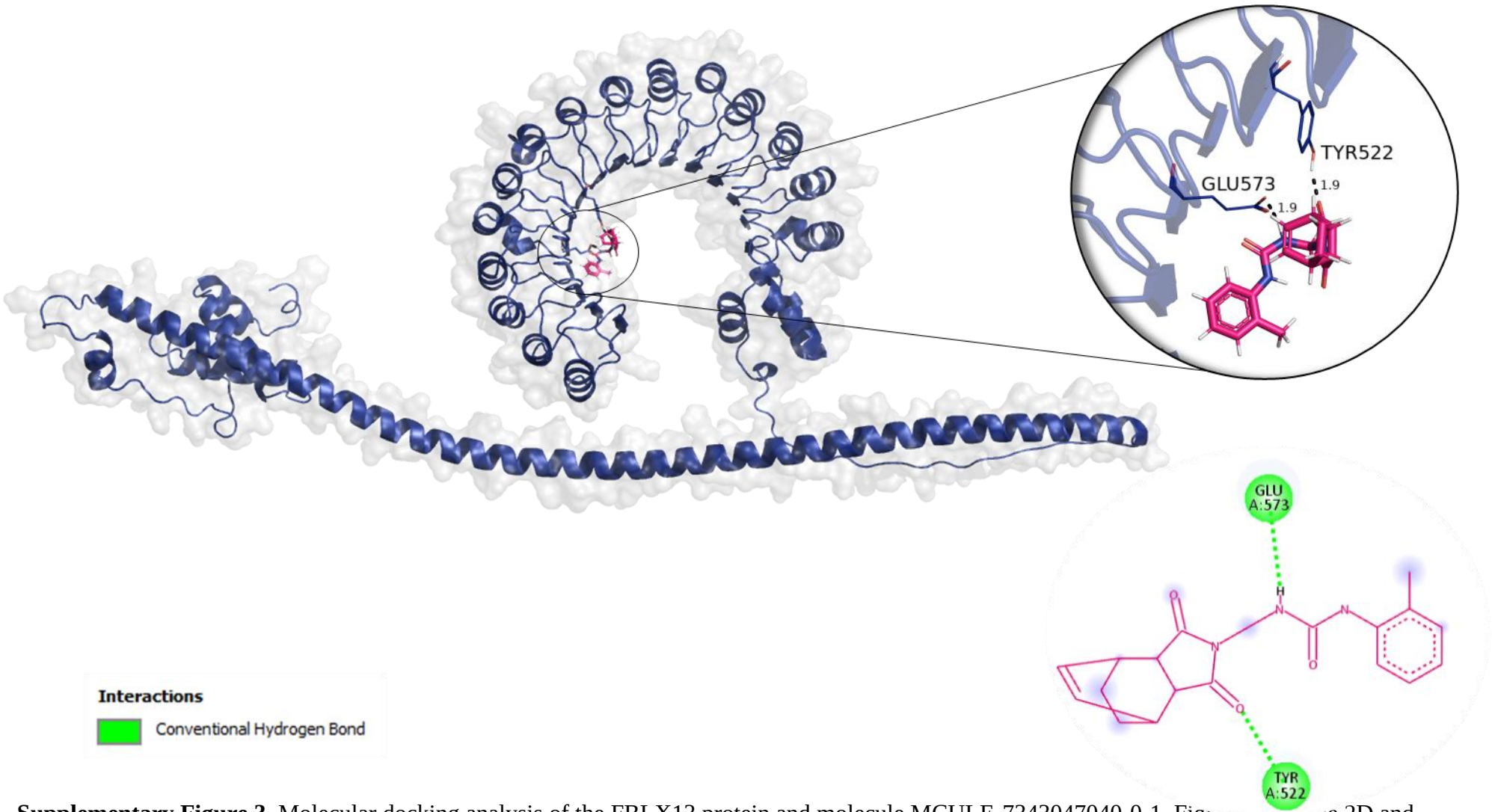
*: Compounds selected for the molecular docking step on the DockThor server. Compounds with favorable toxicological properties were chosen as a selection criterion, without prediction for the toxicity endpoint models and with a prediction of toxicity class equal to or greater than 4.



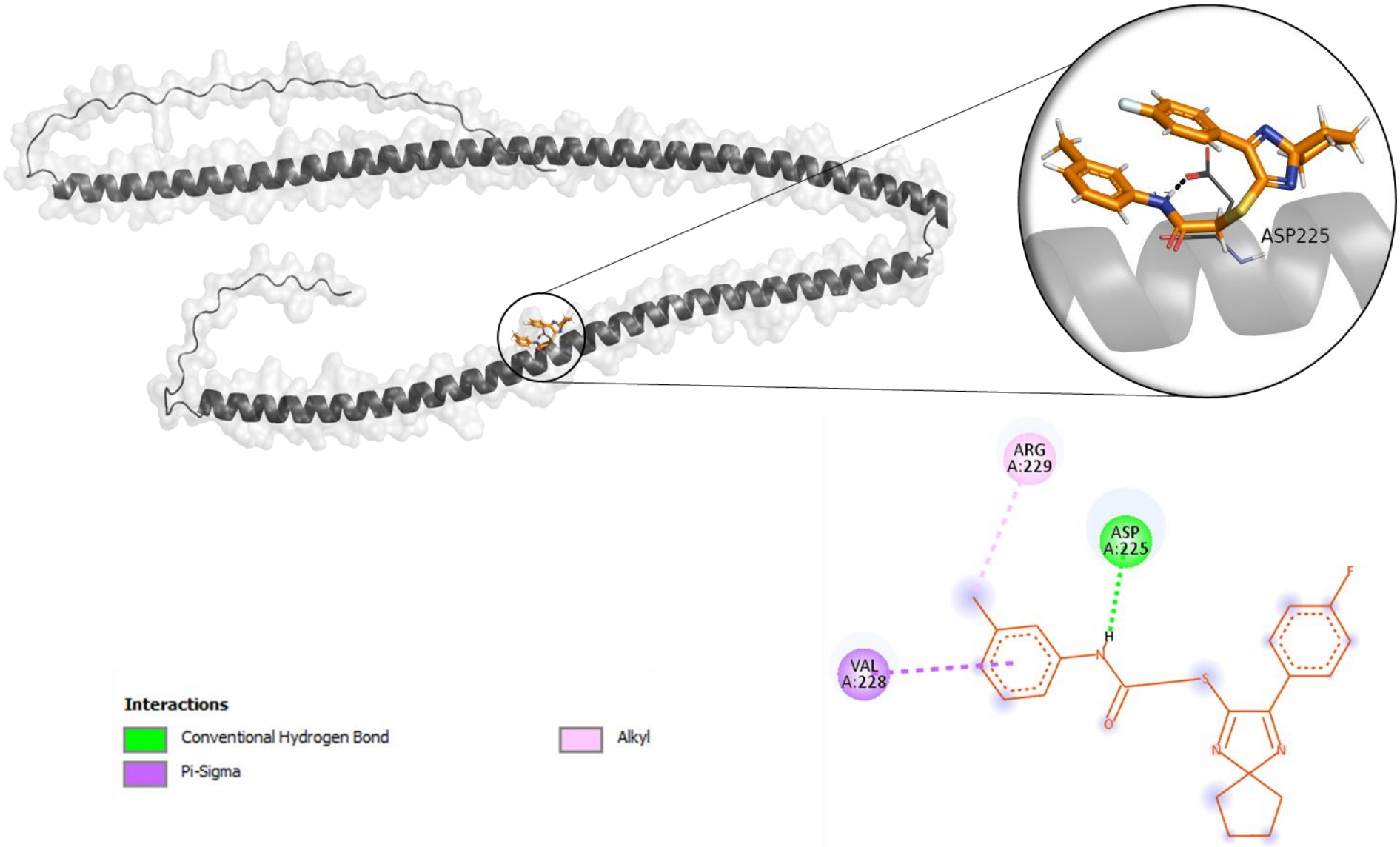
Supplementary Figure 1. Enrichment plots of genes were analyzed using Gene Set Enrichment Analysis (GSEA).



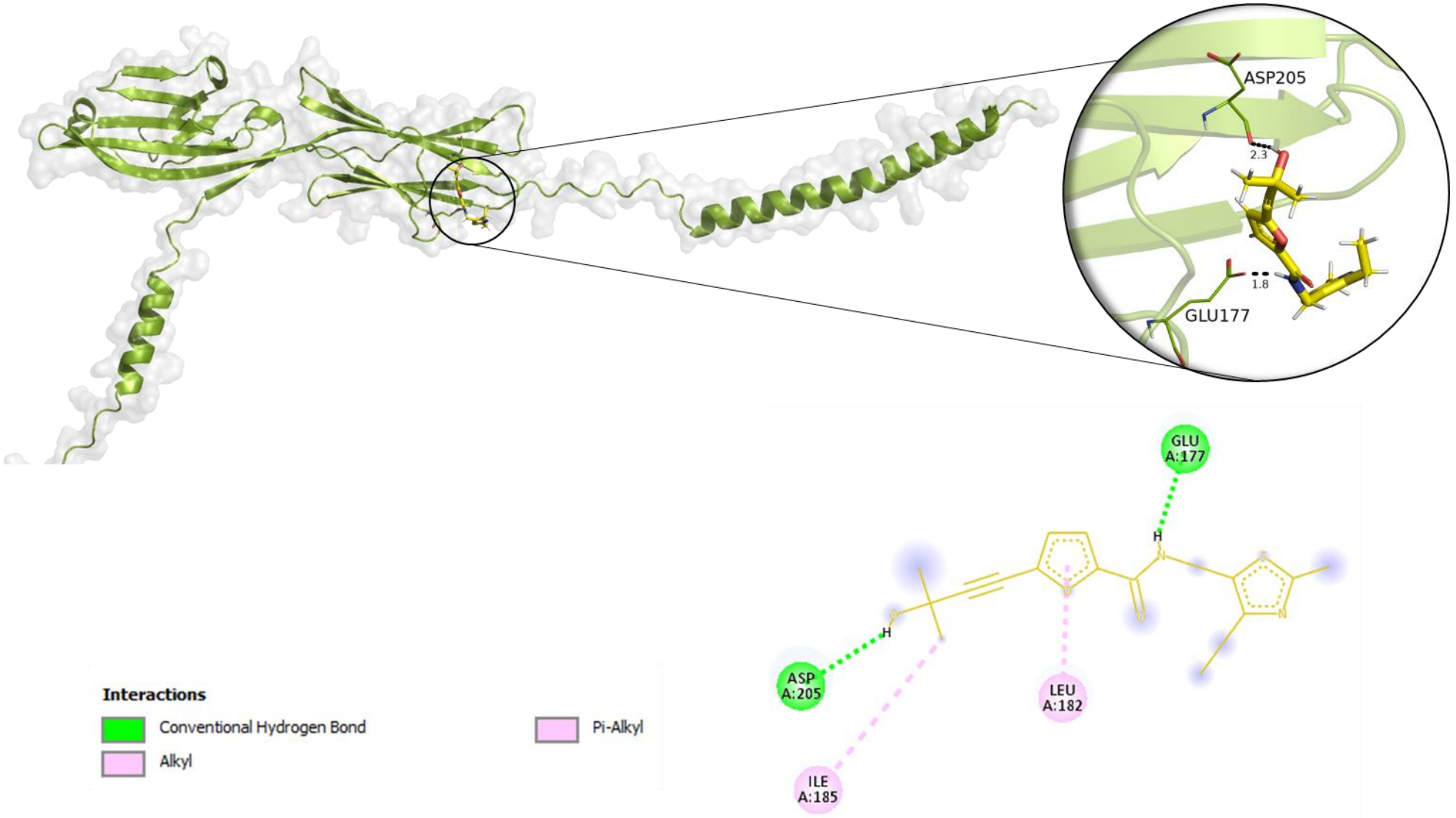
Supplementary Figure 2. Molecular docking analysis of the AJUBA protein and molecule MCULE-2386589557-0-6. Figure shows the 2D and 3D analysis of the interaction.



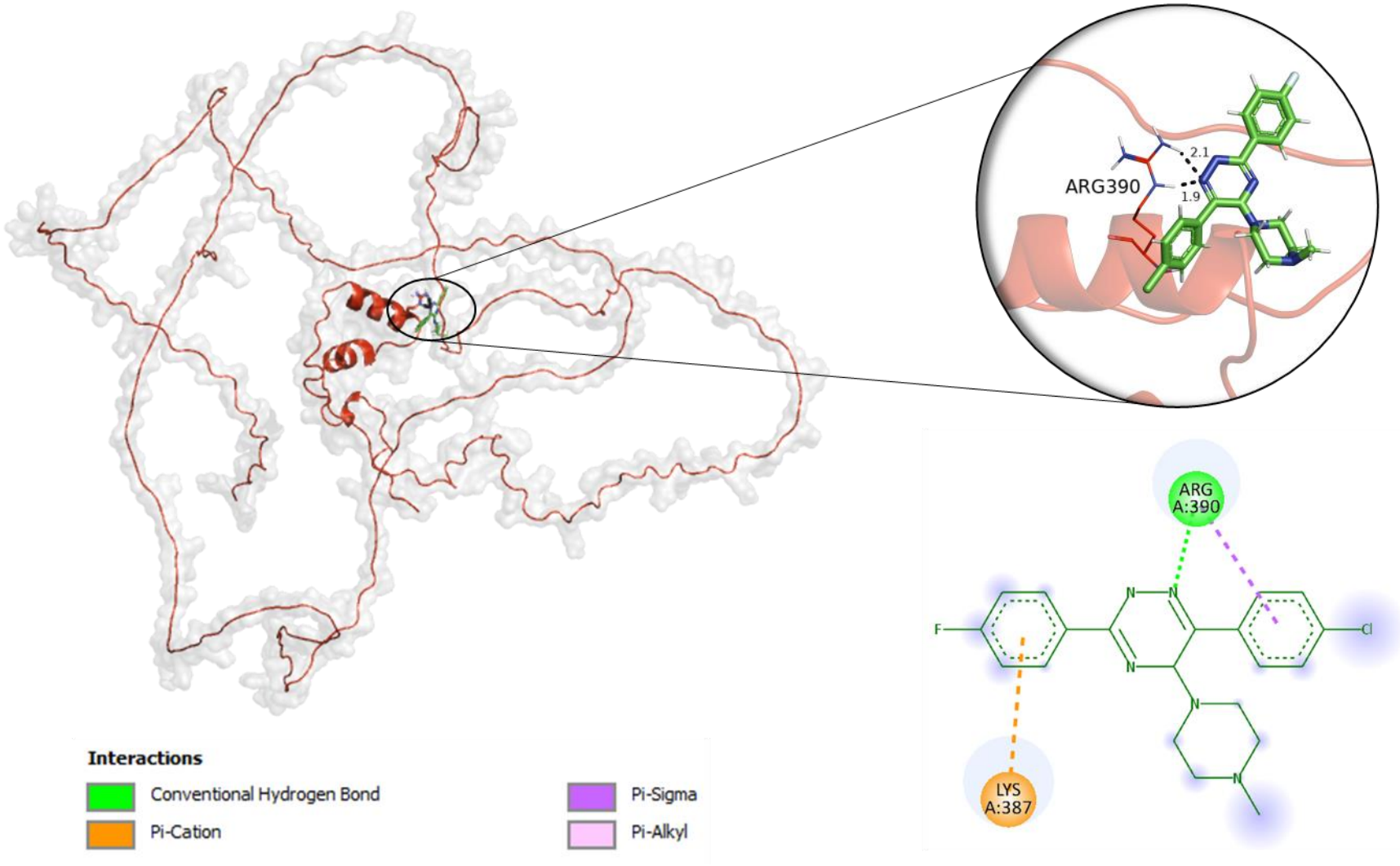
Supplementary Figure 3. Molecular docking analysis of the FBLX13 protein and molecule MCULE-7343047040-0-1. Figure shows the 2D and 3D analysis of the interaction.



Supplementary Figure 4. Molecular docking analysis of the CCDC69 protein and molecule MCULE-5230409338-0-3. Figure shows the 2D and 3D analysis of the interaction.



Supplementary Figure 5. Molecular docking analysis of the CD80 protein and molecule MCULE-9178344200-0-1. Figure shows the 2D and 3D analysis of the interaction.



Supplementary Figure 6]. Molecular docking analysis of the NOLC1 protein and molecule MCULE-5881513100-0-29. Figure shows the 2D and 3D analysis of the interaction.