Table S1 Different types of train data are divided into quantities of metal and non-metal

Data	Metal	Non-Metal
Ligand	13	183
RNA-Ligand	374	477
RNA BindingSites	4923	5451

Table S2 Summary of the Datasets

| Datasets	PDBID_chain(lengths(nt))
Test18	1ddy_A(35),1f1t_A(38),1fmn_A(35),1nem_A(23),1q8n_A(38),2juk_A(22),2mis_A(26),2pwt_A(21),2tob_A(20),364d_C(31),379d_B(25),430d_A(29),4f8u_B(21),4pqv_A(68),4yaz_R(83),5bjo_E(35),5v3f_A(31),6ez0_A(22)
Test3	1y26_X(71),3d2x_A(77),3gx2_A(94)
CL1	4tzx_X(71),4xnr_X(71),5swe_X(71)
CL2	1j7t_A(21),1mwl_A(21),2be0_A(21),2bet3_A(21),2bet4_A(21)
CL3	1uts_B(29),1uud_B(29),2l8h_A(29),1uui_B(29),1arj_N(29)

Table S3 Prediction performance of "MultiModRLBP" and other competing methods on Test3set.

Model	Precision	Recall	MCC	F1	AUC
Rsite2	0.303	0.192	0.085	0.235	0.342
RBind	0.269	0.269	0.320	0.298	0.585
RNAsite	0.173	0.173	0.197	0.257	0.686
RLBind	0.519	0.519	0.421	0.540	0.783
MultiModRLBP	0.500	0.712	0.461	0.587	0.843

Table S4 Predictive performance of "MultiModRLBP" and model without different module on Test3 set.

Model	Precision	Recall	MCC	F1	AUC
without RGCN	0.285	0.942	0.269	0.438	0.725
Without RNABert	0.390	0.683	0.322	0.497	0.800
without ELBFS	0.370	0.654	0.296	0.473	0.779
MultiModRLBP	0.500	0.712	0.461	0.587	0.843

(a)

(b)

(c)

(d)
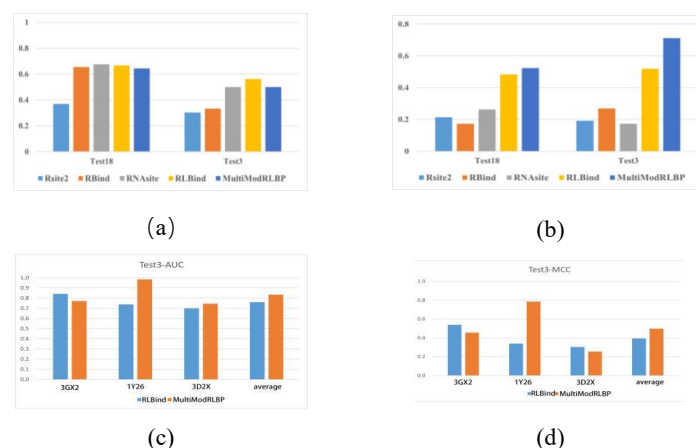
Fig S1. Comparison of the supplementary method indicators.(a) Precision of Test 18 and Test3. (b) Recall of Test18 and Test3.(c) AUC of theRNAs in Test3. (d) MCC of the RNAs in Test3.
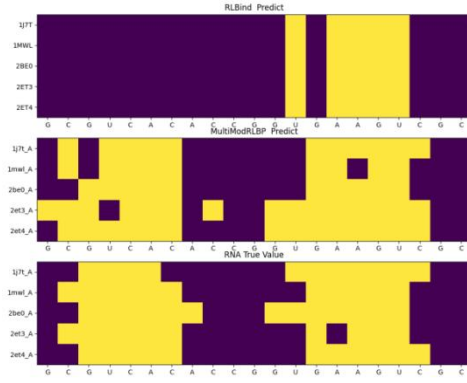
Fig S2.The predictive results of MultiModRLBP and RLBind on the CL2 dataset.

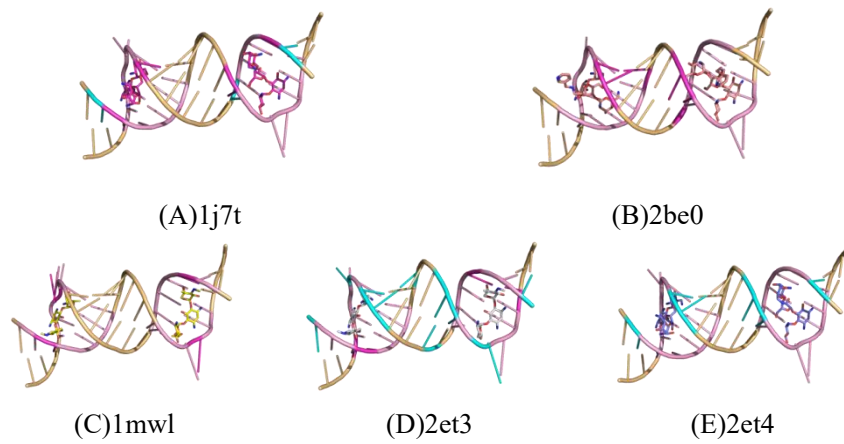(A)1j7t

(B)2be0

(C)1mwl

(D)2et3

(E)2et4

Fig S3. A (1j7t), B (2be0), C (1mwl), D (2et3), and E (2et4) provide visualizations of the binding interactions between the five RNAs and their respective ligands, as depicted using Pymol. In these figures, light pink represents true positives, light magenta indicates false negatives, and cyan signifies false positives. The small molecules are depicted as stick structures.
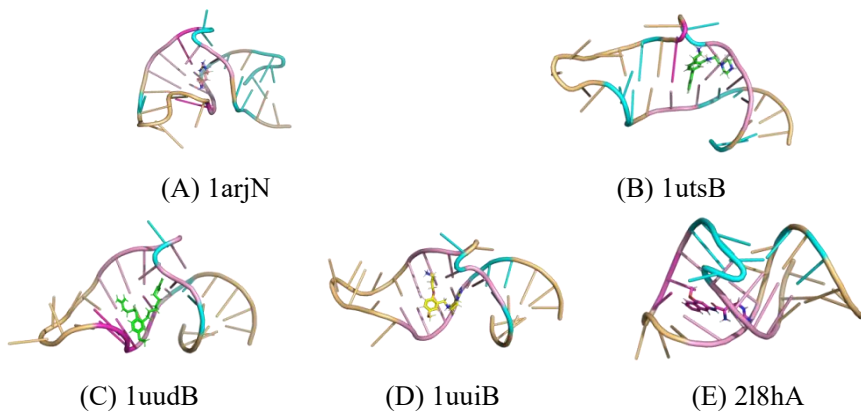

(A) 1arjN

(B) 1utsB

(C) 1uudB

(D) 1uuiB

(E) 2l8hA

Fig S4. A (1arjN), B (1utsB), C (1uudB), D (1uuiB), and E (2l8hA) provide visualizations of the binding interactions between the five RNAs and their respective ligands, as visualized using Pymol. In these figures, light pink represents true positives, light magenta indicates false negatives, and cyan signifies false positives. The small molecules are depicted as stick structures.