Table H1 The RNA-Ligand binding information of test sets

Test sets	PDBID	Ligand
Test18	1ddy	B12,NME
	1f1t	ROS
	1fmn	FMN
	1nem	BDR,BDG,NEB,IDG
	1q8n	MGR
Test18	2juk	G0B
	2mis	MG
	2pwt	LHA
	2tob	TOA,2TB,TOC
	4f8u	SIS
	4pqv	MG
	4yaz	4BW,MG
	5bjo	MG,747
	5v3f	74G
	6ez0	U37
	364d	MG
	379d	CO
	430d	MG
Test3	1y26	ADE,MG
	3d2x	D2X,MG
	3gx2	SFG,MG
CL1	4tzx	ADE,MG
	4xnr	ADE,MG
	5swe	ADE
CL2	1j7t	PAR
	1mwl	GET
	2be0	JS5
	2et3	LLL
	2et4	NMY
CL3	1uts	P13
	1uud	P14
	2l8h	R, L8H
	1uui	P12
	1arj	ARG

Table H2. Performance of MultiModRLBP with differentlearning rate and dropout on Test18 and Test3 set.

learning rate	dropout	Test18-AUC	Test3-AUC
0.001	0.1	0.781	0.843
0.001	0.2	0.753	0.831
0.03	0.1	0.72	0.82
0.005	0.1	0.737	0.935

Table H3. The hyperparameter configuration of MultiModRLBP

Neural network component	Hyperparameters	Value of hyperparameter
RGCN Module	Number of RGCN layers in RGCN Module	3
	Number of neurons for the dense layers	192
	Activation function of the dense layers	ReLU
RNABert Module	Maximum sequence embedding length	440
	Number of Transformer blocks	6
	Activation function of the dense layers	GELU
	Number of neurons for the laste dense layer	120
ELBFS Module	Convolutional kernel size of the CNN layer	17×71
	Sliding window size	11
	Activation function of CNN layer	ReLU
MFFusion Module	Number of dense layers	3
	Number of neurons for the first dense layer	192
	Activation function of the first dense layer	ReLU
	Number of neurons for the second dense layer	96
	Activation function of the second dense layer	ReLU
	Number of neurons for the third dense layer	1
	Activation function of the third dense layer	Sigmod
Overall architecture	Loss function	Binary Cross-Entropy Loss

Neural network component	Hyperparameters	Value of hyperparameter
Overall architecture	Optimizer	Adam
	Adam learning rate	0.001
	Adam decay	0
	Adam bata_1	0.9
	Adam bata_2	0.999
	Dropout rate	0.1
	Batch size	5
	Epochs	80

Table H4 Performance of RLBind with different local window sizes on Test18 set.

Sizes of local windows (nts)	Precision	Recall	MCC	AUC
7	0.568	0.389	0.296	0.733
9	0.769	0.435	0.326	0.742
11	0.644	0.523	0.378	0.78
13	0.56	0.461	0.323	0.738
15	0.585	0.417	0.323	0.715

Table H5 Performance of MultiModRLBP with different convolution kernel sizes on Test18 set .

convolution kernel sizes	Precision	Recall	MCC	AUC
13×71	0.678	0.351	0.315	0.722
17×71	0.644	0.523	0.378	0.78
21×71	0.648	0.473	0.356	0.768