Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary materials

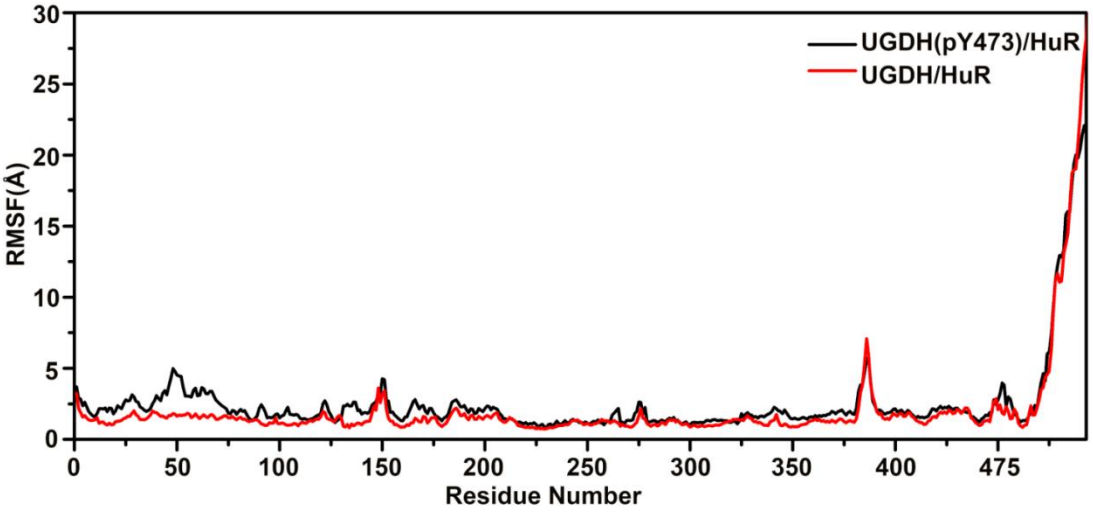


Figure S1. Comparison of the root mean square fluctuation (RMSF) of UGDH in wild type and Y473 phosphorylated UGDH/HuR complex

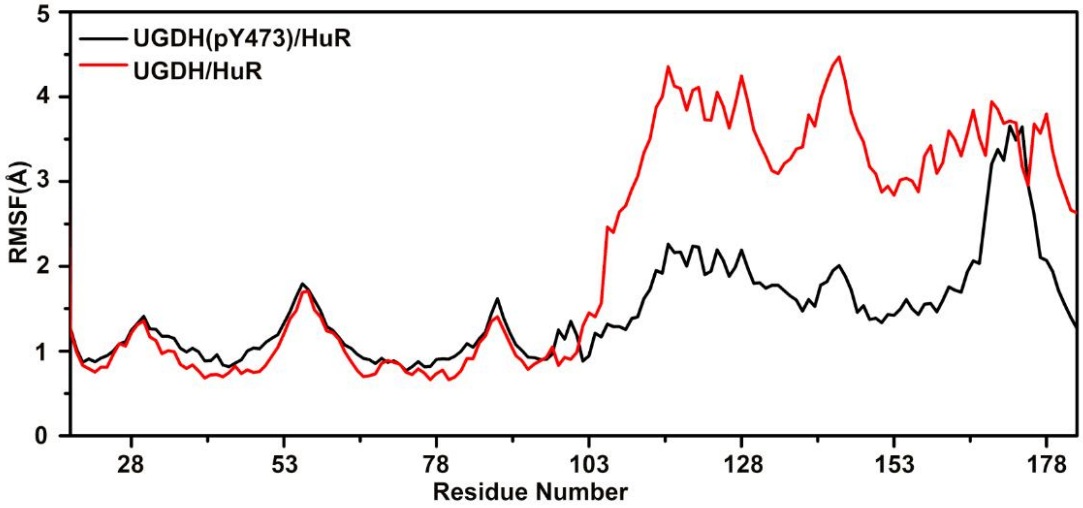


Figure S2. Comparison of the root mean square fluctuation (RMSF) of HuR in wild type and Y473 phosphorylated UGDH/HuR complex

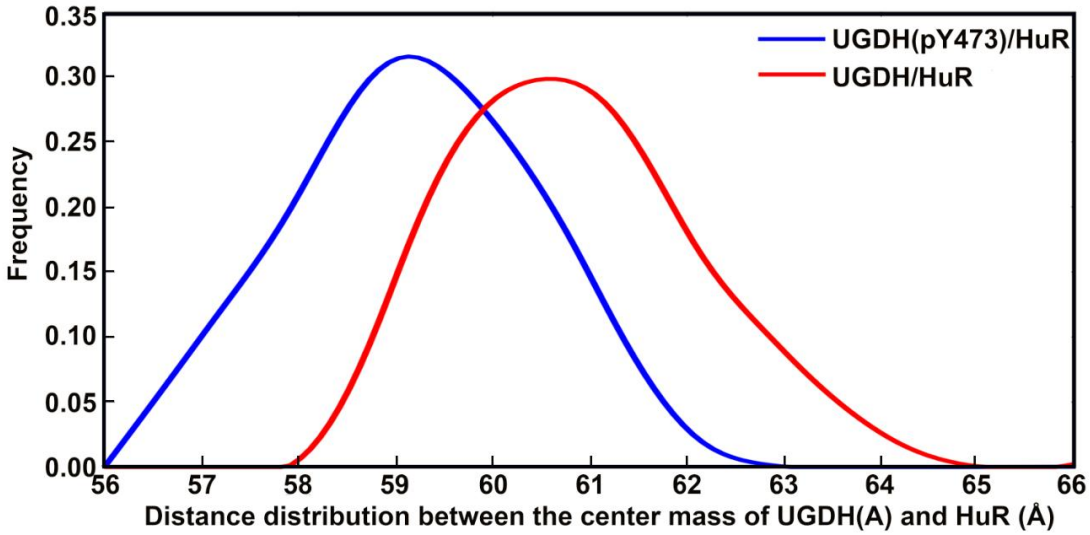
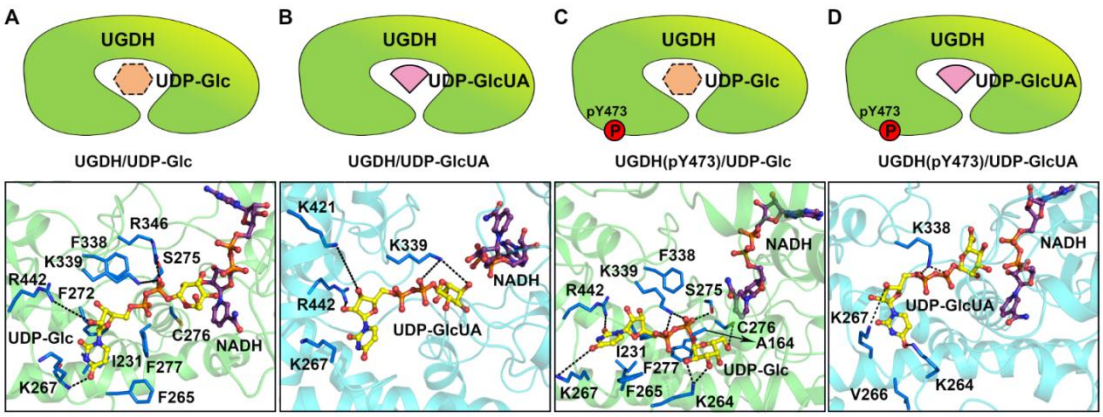


Figure S3. Comparison of the distance between UGDH and HuR in wild type and Y473 phosphorylated UGDH/HuR complex.



The binding free enegy between free UGDH and UDP-Glc or UDP-GluUA

UGDH/UDP-Glc	UGDH/UDP-GlcUA	UGDH(pY473)/UDP-Glc	UGDH(pY473)/UDP-GlcUA
△G: -42.66 kcal/mol	△G: -25.15 kcal/mol	△G: -46.41 kcal/mol	△G: -28.40 kcal/mol

Figure S4. The binding modes of UDP-Glc with UGDH (A), UDP-GlcUA with UGDH (B), UDP-Glc with Y473 phosphorylated UGDH (C) and UDP-GlcUA with Y473 phosphorylated UGDH (D). Schematic of each binding model was showed on the upper. The wide type and Y473 phosphorylated UGDH were shown as green and cyan cartoon respectively. The dominant residues and two ligands were shown in sticks. UDP-Glc and UDP-GlcUA were coloured in cyan and pink, respectively. The color of dominant residues in the two complexes were consistent with the color of cartoon. The numbers represent the binding free energy (kcal/mol) between molecules.

Table S1 The binding free energy between UGDH hexamer and HuR (kcal/mol).

	Monomer/HuR		Trimer/HuR		Hexamer/HuR		Hexamer(pY473)/HuR	
	Total	STD	Total	STD	Total	STD	Total	STD
Pose1	-62.46	12.50	-66.32	15.21	-75.10	11.85	-83.39	13.05
Pose2	-62.43	14.26	-70.09	5.76	-85.38	10.45	-119.10	12.75
Pose3	-64.02	12.01	-45.05	13.34	-79.80	11.07	-115.42	13.54
Pose4					-70.96	11.80	-89.04	11.17
Pose5					-64.04	12.88	-83.35	10.03
Pose6					-67.71	11.28	-64.04	12.23

Table S2 Dominant residues in binding free energy contribution between UGDH and HuR (kcal/mol).

UGDH/HuR			UGDH(pY473)/HuR		
Residue	Total	STD	Residue	Total	STD
HuR:R37	-3.99	0.25	HuR:R19	-12.00	1.69
HuR:S42	-3.17	0.44	HuR:R147	-8.57	1.46
HuR:I103	-3.14	0.32	HuR:R76	-5.61	0.87
UGDH(A):R470	-3.00	0.14	HuR:S42	-4.95	0.67
UGDH(D):E200	-2.85	0.35	UGDH(A):D418	-4.94	0.76
HuR:R115	-2.75	0.16	UGDH(D):P186	-4.16	0.45
UGDH(D):P186	-2.73	0.31	UGDH(D):R205	-3.64	0.51
UGDH(D):Q193	-2.59	0.21	UGDH(A):R427	-3.51	0.39
HuR:R147	-2.46	0.24	HuR:R136	-3.30	0.24
HuR:L39	-2.34	0.27	HuR:I103	-3.26	0.32
HuR:F182	-2.31	0.41	UGDH(A):E250	-3.16	0.25
UGDH(A):P471	-2.30	0.33	UGDH(A):M419	-3.09	0.34
UGDH(A):L448	-2.22	0.47	HuR:F183	-3.03	0.33
HuR:R76	-2.14	0.11	HuR:R153	-2.93	0.19
			HuR:R85	-2.88	0.24
			HuR:L84	-2.83	0.22
			HuR:R115	-2.37	0.45
			HuR:K72	-2.31	0.35
			UGDH(D):Q189	-2.23	0.24
			HuR:L39	-2.18	0.13
			UGDH(D):Q193	-2.13	0.17
			HuR:T80	-2.12	0.22

Table S3 Hydrogen bond occupancies between UGDH(Hexamer) and HuR during MD simulations.

Hydrogen Bonds			
Acceptor	DonorH	Donor	Occupancy
UGDH(A):V494@OXT	HuR:R115@HH12	HuR:R115@NH1	83.45%
UGDH(A):V494@O	HuR:R115@HH22	HuR:R115@NH2	79.27%
UGDH(A):E478@OE1	HuR:R115@HH12	HuR:R115@NH2	74.53%
UGDH(A):E451@OE1	HuR:R136@HH12	HuR:R136@NH1	74.00%
UGDH(A):D446@OE1	HuR:Q141@HE22	HuR:Q141@NE22	72.21%
UGDH(A):E478@OE1	HuR:R115@HH12	HuR:R115@NH1	69.68%
UGDH(A):V494@OXT	HuR:R147@HH11	HuR:R147@NH1	49.54%
HuR:E47@OE2	UGDH(D):S476@HG	UGDH(D):S476@OG	50.91%
UGDH(A):Q453@OE1	HuR:Y26@H	HuR:Y26@N	50.00%
UGDH(A):V466@O	HuR:Q87@HE21	HuR:Q87@NE2	47.47%
UGDH(A):T454@OG1	HuR:Q29@HE22	HuR:Q29@NE2	43.64%
UGDH(A):Q453@OE1	HuR:N25@HD22	HuR:N25@ND2	38.55%
HuR:E47@OE1	UGDH(D):S476@HG	UGDH(D):S476@OG	36.36%
HuR:E47@OE2	UGDH(D):S476@H	UGDH(D):S476@N	35.82%
UGDH(A):E451@OE1	HuR:R136@HH22	HuR:R136@NH2	33.27%
UGDH(A):E451@OE2	HuR:R136@HH22	HuR:R136@NH2	31.64%
UGDH(A):V466@O	HuR:S88@HG	HuR:S88@OG	30.18%
UGDH(A):E451@OE2	HuR:D105@HD21	HuR:D105@ND2	28.18%
UGDH(A):Q458@OE1	HuR:Q29@HE22	HuR:Q29@NE2	28.02%
UGDH(A):G477@O	HuR:G112@H	HuR:G112@N	26.95%
HuR:E47@OE2	UGDH(D):S476@H	UGDH(D):S476@N	26.00%
HuR:Q29@OE1	UGDH(D):S468@HG	UGDH(D):S468@OG	25.09%