Enhanced Sampling Method	CVs	RNA Systems	QM/MM	Total Timescale (μs)	Ref.
Refinements and Validations of Force Fields					
M-REMD	-	UUCG-TL (10,14-mers), CCCC, GACC	MM	∼7663	[1]
M-REMD	-	CCCC, GACC	MM	∼920	[2]
H-REMD	-	single strands, duplexes (12-mers)	MM	∼1.7	[3]
T-REMD	-	AAAA, CAAU, CCCC, GACC, UUUU	MM	264	[4]
METAD, T-REMD, RECT	α,β,γ,ϵ,ζ,Z_x,χ, distance	CC, AA, CA, AC, GACC, CCCC, AAAA	MM	∼206	[5]
METAD, T-REMD, REST2	H-bonds, RMSD	GAGA-TL (8,10-mers)	MM	966	[6]
T-REMD+METAD	ϵRMSD	GAGA-TL, UUCG-TL (8-mers)	MM	48	[7]
RECT	α,β,γ,ϵ,ζ,Z_x,Z_y,χ, distance	A, C, AA, AC, CA, CC	MM	∼35	[8]
RECT, T-REMD+METAD	α,β,γ,ϵ,ζ,Z_x,Z_y,χ, distance, ϵRMSD	GACC, CCCC, AAAA, CAAA, UUCG-TL (8-mer)	MM	∼420	[9]
US	α,β,γ,ϵ,ζ,χ	16 dinucleotides	MM	∼18	[10]
Conformational Landscapes					
RECT, H-REMD, T-REMD	α,β,γ,δ,ϵ,ζ,Z_x,Z_y,χ, distance	GACC	MM	∼14.4	[11]
METAD	H-bonds, RGyr, RMSD, χ	GAGA-TL, UUCG-TL (10-mers)	MM	0.84	[12]
T-REMD	-	SAM-II riboswitch	MM	6	[13]
T-REMD, SMD	distances (COM)	(cgauUCUaugc) duplex (22-mer)	MM	∼5	[14]
T-REMD	-	SVL loop (17-mer)	MM	∼58	[15]
A-REMD	Z_x, Z_y, χ	U	QM/MM	∼0.1	[16]
BE-METAD	H-bond, RGyr, energy	gene32 mRNA pseudoknot (32-mer)	MM	3	[17]
US	distance (COM)	*add* riboswitch	MM	∼0.9	[18]
US	χ	duplex, single strands with 2-thiouridines (14-mers)	MM	0.144	[19]
US	χ, pseudodihedral (COM)	duplexes with CUG repeats (9,11,19-mers)	MM	∼6	[20]
US - pseudo string method	distance (COM)	duplex (32-mer)	MM	∼0.06	[21]
T-REMD	-	GCAA -TL (8-mer)	MM	448	[22]
T-REMD	-	pT181 RNA hairpins (22-mers)	MM	∼9	[23]
RAM	H-bonds, distances	TAR (29-mer) in RNA:peptide complex	MM	0.8	[24]
REMD+US	distances, RMSD	U-singlestrand (5-mer) in RNA:protein complex	MM	3.6	[25]
US	distances	GTPase center of rRNA	MM	∼1.3	[26]
RAM	α,β,δ,ϵ,ζ, H-bonds	UUCG-TL (14-mer)	MM	∼1	[27]
T-REMD	-	theophylline aptamer (ligand-free)	MM	1.6	[28]
GaMD, TMD	RMSD	CRISPR-Cas9 RNA complex	MM	∼14.6	[29]
METAD	distance (COM), stacking	PNA:RNA duplex (12-mer)	MM	0.4	[30]
T-REMD+METAD	H-bonds, RGyr	polio viral RNA hairpin (22-mer)	MM	∼6.5	[31]
US	pseudodihedral (COM)	hairpin (35-mer)	MM	0.72	[32]
METAD	χ, pseudodihedral (COM)	duplexes (9,12-mers) with CAG repeats	MM	1.92	[33]
T-REMD	-	gcGCAAgc-TL (8-mer)	MM	6	[34]
Ion Interactions and Ion/ligand Induced Conformational Changes					
METAD	distance (COM), hydrophobic contacts, H-bonds	duplex (10-mer) with CAG repeats	MM	1.4	[35]
US+TI	distance, coordination	mononucleotides, hammerhead ribozyme	MM	∼11.5	[36]
SMD	distances	preQ$_1$-III riboswitch	MM	0.1	[37]
BE-METAD	distance, coordination	nucleosides, GpG dinucleotide, GC duplex (8-mer)	MM	82	[38]
GCMC-MD	distances, coordinations	BWYV pseudoknot, VS ribozyme, 23S rRNA, Mg^{2+} riboswitch	MM	∼4	[39]
US	distance (COM)	GTPase center of rRNA	MM	20.5	[40]
TI	distances	guanine riboswitch	MM	∼0.6	[41]
Reactivity and Catalysis					
A-REMD	distances	HDV ribozyme	QM/MM	0.235	[42]
US+string method	distances	*glmS* riboswitch	QM/MM	∼0.00017	[43]
T-REMD	-	hammerhead ribozyme	MM	5	[44]
US+string method	distances, angles	HDV ribozyme	MM, QM/MM	0.0465, 0.00019	[45]
US, TI	distances	twister ribozyme	MM	0.5	[46]
US+string method	distances	*glmS* riboswitch	QM/MM	∼0.00017	[47]
TI	distances	group-II introns	QM/MM	∼0.00001	[48]
METAD	distances	GAAA-TL, UUCG-TL (10-mers), GC duplex (14-mer)	QM/MM	∼0.001	[49]
US+string method	distances	*glmS* riboswitch	QM/MM	0.0072	[50]
T-REMD	-	hairpin ribozyme	MM	25.6	[51]
US, TI	distances	hammerhead ribozyme	MM, QM/MM	0.11, 0.0002	[52]

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