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	∼1382.4	[2]
H-REMD	-	single strands (6-mers), duplexes (12-mers)	MM	1.68	[3]
T-REMD	-	AAAA, CAAU, CCCC, GACC, UUUU	MM	264	[4]
METAD, T-REMD, RECT	α,β,γ,ϵ,ζ,Z_x,χ, distance (COM)	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 (6,8-mers)	MM	96	[7]
RECT	α,β,γ,ϵ,ζ,Z_x,Z_y,χ, distance (COM)	A, C, AA, AC, CA, CC	MM	∼35	[8]
RECT, T-REMD+METAD	α,β,γ,ϵ,ζ,Z_x,Z_y,χ, distance (COM), ϵRMSD	GACC, CCCC, AAAA, CAAA, UUCG-TL (8-mer)	MM	∼504	[9]
US	α,β,γ,ϵ,ζ,χ	16 dinucleotides	MM	16.128	[10]
Conformational Landscapes					
RECT, H-REMD, T-REMD	α,β,γ,δ,ϵ,ζ,Z_x,Z_y,χ, distance (COM)	GACC	MM	∼14.4	[11]
METAD	H-bonds, RGyr, RMSD, χ	GAGA-TL, UUCG-TL (10-mers)	MM	4.44	[12]
T-REMD	-	SAM-II riboswitch	MM	6	[13]
T-REMD, SMD	distance (COM)	(cgauUCUaugc) duplex (22-mer)	MM	∼5	[14]
T-REMD	-	SVL loop (17-mer)	MM	57.6	[15]
A-REMD	Z_x, Z_y, χ	U nucleoside	QM/MM	∼0.1	[16]
BE-METAD	H-bonds, RGyr, energy	gene32 mRNA pseudoknot (32-mer)	MM	3	[17]
US	distance (COM)	*add* riboswitch	MM	1.177	[18]
US	χ	U and 2-thio-U nucleosides	MM	0.144	[19]
US	χ, pseudodihedral (COM)	A, G, U, and C nucleosides, duplex with CUG (18-mer)	MM	6.016	[20]
US+pseudo-spring method	distance (COM)	duplex (32-mer)	MM	∼0.3	[21]
T-REMD	-	GCAA -TL (8-mer)	MM	448	[22]
T-REMD	-	pT181 RNA hairpins (48-mers)	MM	17.16	[23]
RAM	H-bonds, distance (COM)	TAR (29-mer) in RNA:peptide complex	MM	0.8	[24]
REMD+US	distance, RMSD	U-singlestrand (5-mer) in RNA:protein complex	MM	3.6	[25]
US	distance (COM)	GTPase center of rRNA	MM	4.494	[26]
RAM	α,β,δ,ϵ,ζ, H-bonds	UUCG-TL (14-mer)	MM	1.04	[27]
T-REMD	-	theophylline-binding aptamer (33-mer)	MM	1.6	[28]
GaMD, TMD	RMSD	CRISPR-Cas9 RNA complex	MM	∼12	[29]
METAD	distance (COM), stacking	PNAs (6-mers), PNA:RNA duplex (12-mer)	MM	∼1.2	[30]
T-REMD+METAD	H-bonds, RGyr	polio viral RNA hairpin (22-mer)	MM	16	[31]
US	pseudodihedral (COM)	hairpin from group-II intron (35-mer)	MM	1.008	[32]
METAD	χ, pseudodihedral (COM)	duplexes with A-A mismatches (18-mers)	MM	∼0.6	[33]
T-REMD	-	gcGCAAgc-TL (8-mer)	MM	356	[34]
Ion Interactions and Ion/ligand Induced Conformational Changes					
METAD	distance (COM), hydrophobic contacts, H-bonds	duplex with A-A mismatches (20-mer)	MM	1.4	[35]
US+TI	distance	mononucleotides, hammerhead ribozyme	MM	∼3.5	[36]
SMD	distance	preQ$_1$-III riboswitch	MM	0.1	[37]
BE-METAD	distance, coordination	nucleosides, GpG dinucleotide, GC duplex (8-mer)	MM	82	[38]
GCMC-MD	distance, coordination	BWYV pseudoknot, VS ribozyme, 23S rRNA, Mg^{2+} riboswitch	MM	4	[39]
US	distance (COM)	GTPase center of rRNA	MM	20.488	[40]
TI	distance	guanine riboswitch	MM	0.576	[41]
T-REMD, METAD	distance (COM)	siRNA duplex (42-mer)	MM	28.8	[42]
Reactivity and Catalysis					
A-REMD	distance	HDV ribozyme	QM/MM	∼0.235	[43]
US+string method	distance	*glmS* riboswitch	QM/MM	0.00225, ∼0.00015	[44]
T-REMD	-	hammerhead ribozyme	MM	5	[45]
US+string method	distance, angle	HDV ribozyme	MM, QM/MM	0.0465, ∼0.00019	[46]
US, TI	distance	twister ribozyme	MM	0.525	[47]
US+string method	distance	*glmS* riboswitch	QM/MM	∼0.000098	[48]
TI	distance	group-II introns	QM/MM	∼0.0001	[49]
METAD	distance	GAAA-TL, UUCG-TL (10-mers), GC duplex (16-mer)	QM/MM	0.72	[50]
US+string method	distance	*glmS* riboswitch	QM/MM	∼0.0072	[51]
T-REMD	-	hairpin ribozyme	MM	25.6	[52]
US, TI	distance	hammerhead ribozyme	MM, QM/MM	∼0.33, ∼0.0004	[53]

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