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Additional Force Field Parameters

bond	Kr(kcal mol^{-1} Å^{-2})	r_{eq} (Å)
EA-CA	430.9	1.43
NX-CA	441.6	1.37
EA-EA	430.9	1.43
NX-CT	337.0	1.49
EA-CB	438.3	1.42
CA-OM	450.0	1.364

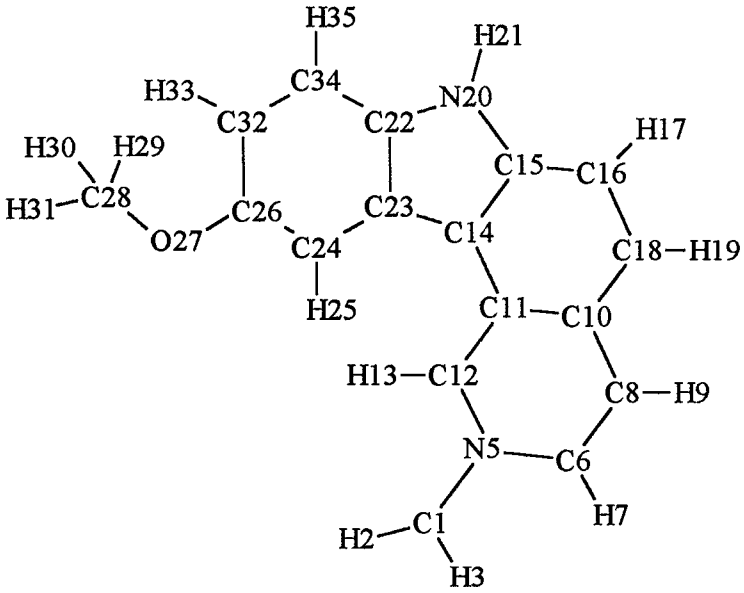
angle	K_Φ(kcal mol^{-1} rad^{-2})	Φ_{eq} (deg)
CT-CT-NX	80.	112.2
CB-CB-CN	85.	108.8
CA-EA-CA	85.	121.0
CA-EA-EA	85.	118.5
CA-CA-EA	85.	121.
NX-CA-EA	70.	122.
NX-CA-CA	70.	120.
EA-CA-HC	35.	119.
NX-CA-HC	35.	115.
CA-NX-CA	70.	120.
CA-NX-CT	70.	120.
NX-CT-HC	35.	108.5
EA-EA-CB	85.	120.
EA-CB-CN	85.	116.2
EA-CB-CB	85.	135.
CA-EA-CB	85.	123.4
CA-CA-OM	70.	120.
CA-OM-CT	70.	115.
CN-NA-CN	70.	111.6

dihedral angle	*idivf*	$V_n/2$(kcal mol^{-1})	γ (deg)	n
X-EA-CB-X	4	16.3	180.	2.
X-CA-EA-X	4	10.2	180.	2.
X-EA-EA-X	4	16.3	180.	2.
X-CA-NX-X	4	6.9	180.	2.
X-NX-CT-X	6	0.00	0.	2.
X-CA-OM-X	2	1.8	180.	2.

improper torsional angles	$V_n/2$(kcal mol^{-1})	γ (deg)	n
X-X-CA-OM	1.8	180.	2.
X-X-EA-EA	16.3	180.	2.
X-X-NX-CT	0.0	180.	2.

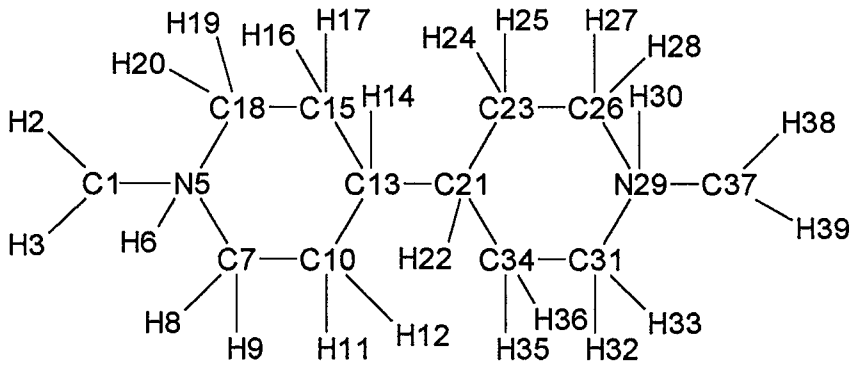
van der Waals	R* (Å)	ε(kcal mol^{-1})
EA	1.85	0.12
NX	1.75	0.16
OM	1.65	0.15
SW	5.0	0.1

Atom Nomenclature and Atomic Charges for the Chromophores



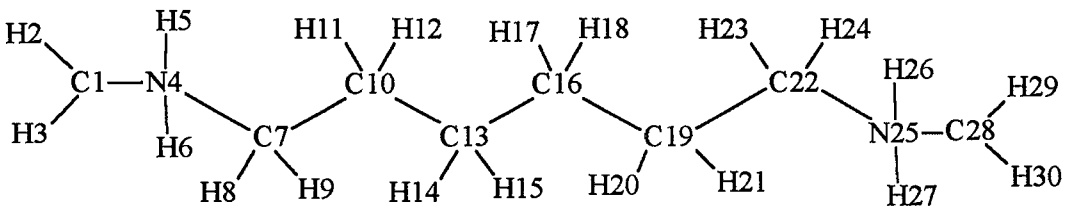
Atom #	Atom Type	Charge
C1	CT	-0.1429
H2	HC	0.1689
H3	HC	0.1689
N5	NX	-0.0023
C6	CA	-0.0322
H7	HC	0.1994
C8	CA	-0.3125
H9	HC	0.2228
C10	EA	0.3359
C11	EA	-0.1926
C12	CA	0.1863
H13	HC	0.1550
C14	CB	-0.0060
C15	CN	0.2674
C16	CA	-0.1401
H17	HC	0.2046
C18	CA	-0.3248
H19	HC	0.2071
N20	NA	-0.6146
H21	HC	0.4230
C22	CN	0.2731
C23	CB	-0.0098
C24	CA	-0.4034
H25	HC	0.1854
C26	CA	0.4423
O27	OM	-0.4022
C28	CT	0.0663
H29	HC	0.0569
H30	HC	0.0569
H31	HC	0.0569
C32	CA	-0.2609
H33	HC	0.1992
C34	CA	-0.2327
H35	HC	0.2005

Atom Nomenclature and Atomic Charges for the Ditercalinium Linker

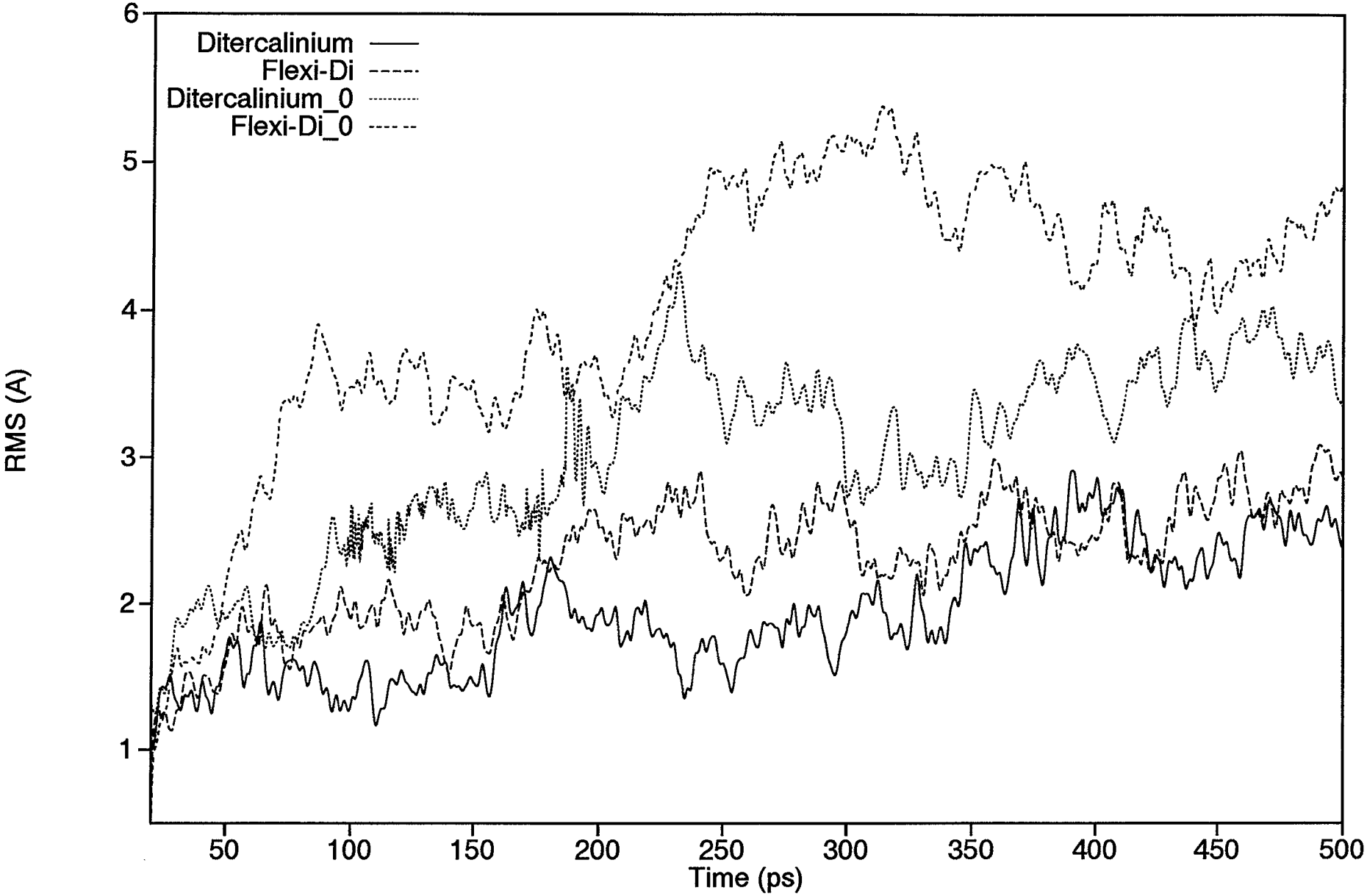


Atom #	Atom Type	Charge
C1	CT	-0.2708
H2	HC	0.2296
H3	HC	0.2296
N5	N3	-0.0955
H6	H3	0.3735
C7	CT	0.1000
H8	HC	0.1400
H9	HC	0.1492
C10	CT	-0.1253
H11	HC	0.1028
H12	HC	0.0756
C13	CT	-0.0453
H14	HC	0.0944
C15	CT	-0.1254
H16	HC	0.1028
H17	HC	0.0756
C18	CT	-0.1000
H19	HC	0.1400
H20	HC	0.1492
C21	CT	-0.0453
H22	HC	0.0944
C23	CT	-0.1253
H24	HC	0.1028
H25	HC	0.0756
C26	CT	-0.1000
H27	HC	0.1400
H28	HC	0.1492
N29	N3	-0.0955
H30	H3	0.3735
C31	CT	-0.1000
H32	HC	0.1400
H33	HC	0.1492
C34	CT	-0.1254
H35	HC	0.1028
H36	HC	0.0756
C37	CT	-0.2708
H38	HC	0.2296
H39	HC	0.2296

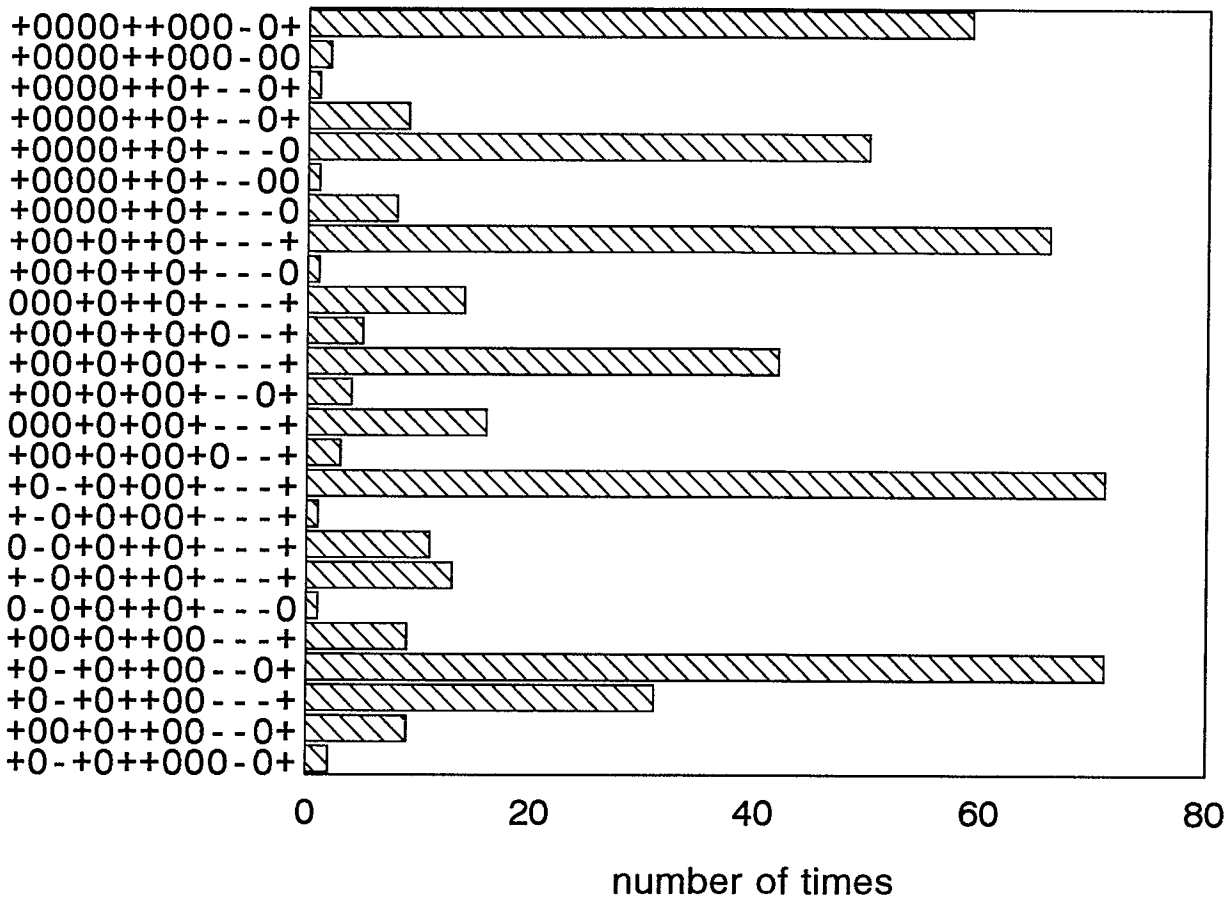
Atom Nomenclature and Atomic Charges for the Flexi-Di Linker



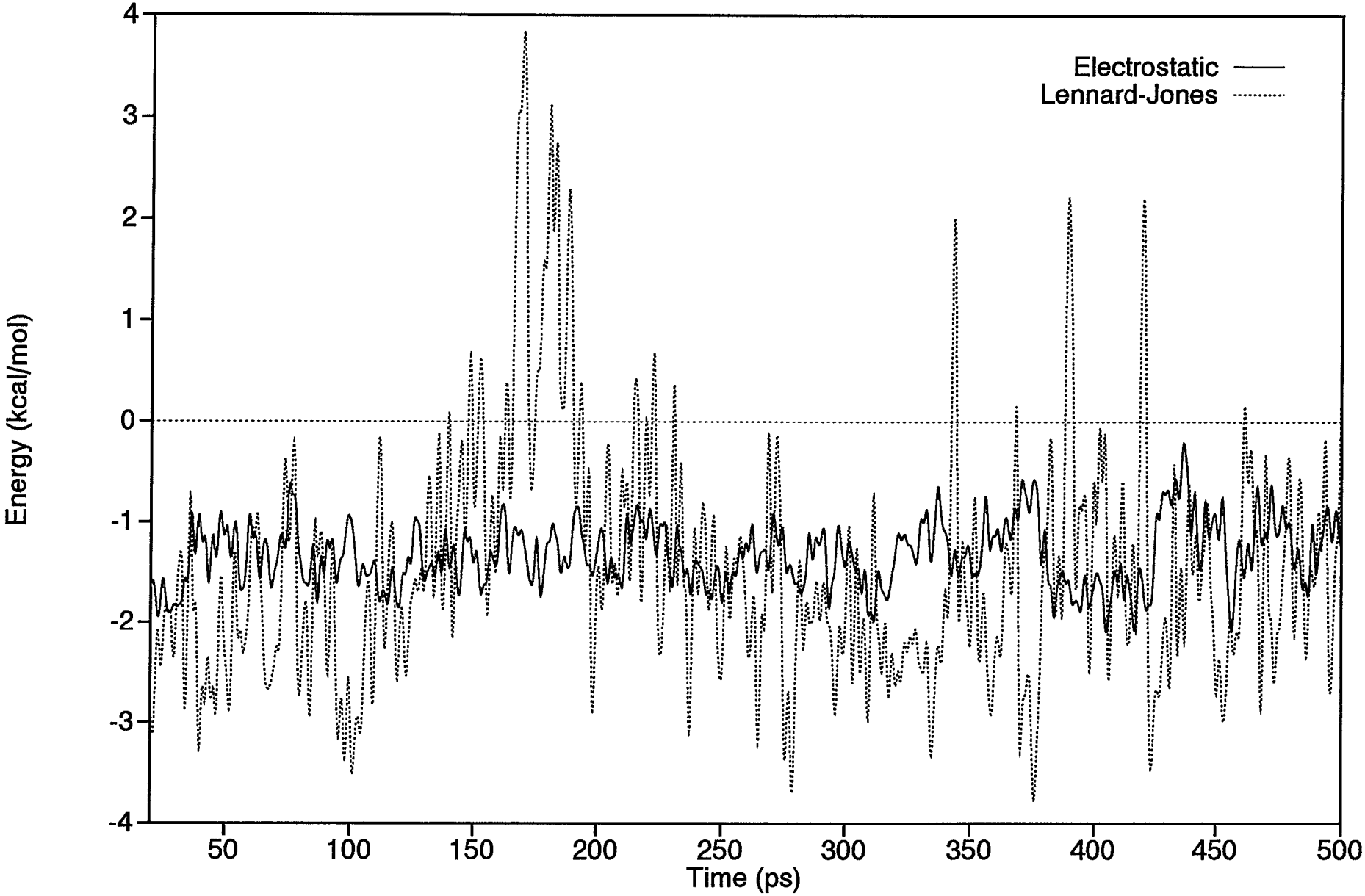
Atom #	Atom Type	Charge
C1	CT	-0.11839
H2	HC	0.17835
H3	HC	0.17835
N4	N3	-0.13679
H5	H3	0.30886
H6	H3	0.30886
C7	CT	-0.10528
H8	HC	0.13556
H9	HC	0.13556
C10	CT	-0.07863
H11	HC	0.07706
H12	HC	0.07706
C13	CT	-0.08489
H14	HC	0.06216
H15	HC	0.06216
C16	CT	-0.08489
H17	HC	0.06216
H18	HC	0.06216
C19	CT	-0.07863
H20	HC	0.07706
H21	HC	0.07706
C22	CT	-0.10528
H23	HC	0.13556
H24	HC	0.13556
N25	N3	-0.13679
H26	H3	0.30886
H27	H3	0.30886
C28	CT	-0.11839
H29	HC	0.17835
H30	HC	0.17835



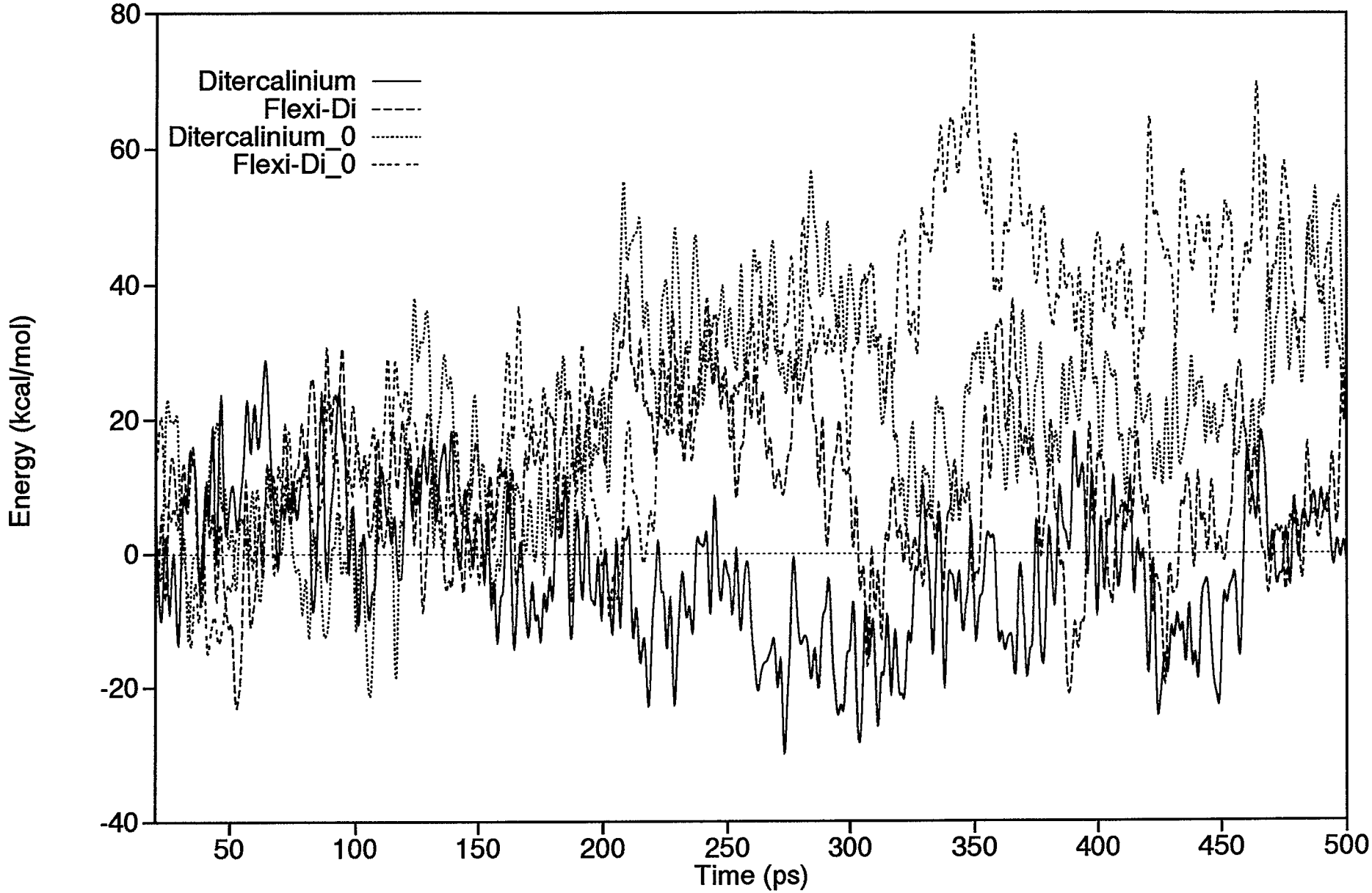
Evolution of the root-mean-square deviation (calculated for all non-hydrogen atoms after least-square fitting of the structures using the same atoms) from the corresponding refined initial structure along the sampling period of the molecular dynamics simulations for the complexes with ditercalinium (——), Flexi-Di (·····), ditercalinium with uncharged linker (——) and Flexi-Di with uncharged linker (-----).



Hypercubes visited by Flexi-Di in its complex with d(GCGCGC)$_2$ during the last 100 ps of the molecular dynamics simulations in water. 0, +, and − signs account for *anti*, *gauche* +, and *gauche* − dihedral angles in the 13-torsion Flexi-Di linker (*cf* Figure 1b).



Time evolution of the Lennard-Jones and electrostatic ($\varepsilon_{eff} = 3$) energy terms of the stacking interaction at the sandwiched GpC step. Values are relative to a canonical GpC step in the A-DNA conformation.



Time evolution of the intramolecular energy of the DNA molecule in the complexes along the dynamics simulations in water: ditercalinium (——), Flexi-Di (– – – –), ditercalinium with uncharged linker (-----), and Flexi-Di with uncharged linker (·····).