APPENDIX A:
Simulation parameters for aminocinnamates

We report here the parameters determining the Force Field for phenylalkyl-4-(4'-cyanobenzylidene) aminocinnamates as described in chapter 3.

Atom types

atom type	description
C	any sp2 carbonyl carbon
CA	any sp2 aromatic carbon
C=C	any sp2 olefinic carbon
C=N	any sp2 imminic (amidic) carbon
CT	any sp3 carbon(four explicit substituents)
CY	sp cyanidic carbon
HA	any hydrogen attached to aromatic carbon
HC	any hydrogen attached to aliphatic carbon
HC=N	any hydrogen attached to imminic carbon
N=C	any sp2 imminic nitrogen
NY	sp cyanidic nitrogen
O	sp2 carbonyl oxygen
OS	any etheric/esteric oxygen

Atomic Charges for the homologue N=0

atom	type	charge (au)	atom	type	charge (au)
N1	NY	-.4245	C2	CY	0.3973
C3	CA	-.0610	C4	CA	-.1494
H5	HA	0.1384	C6	CA	0.0081
H7	HA	0.0691	C9	CA	-.1347
H10	HA	0.1260	C11	CA	-.0994
H12	HA	0.1251	C8	CA	-.0228
C13	C=N	0.2629	H14	HC=N	0.0078
N15	N=C	-.4580	C16	CA	0.3410
C17	CA	-.2073	H18	HA	0.1543
C19	CA	-.1751	H20	HA	0.1377
C22	CA	-.2364	H23	HA	0.1562
C24	CA	-.1794	H25	HA	0.1416
C21	CA	0.1781	C26	C=C	-.1078
H27	HC	0.1137	C28	C=C	-.3612
H29	HC	0.1856	C30	C	0.7936
O31	O	-.4577	O32	OS	-.5129
C33	CA	0.4266	C34	CA	-.2580
H35	HA	0.1544	C36	CA	-.0759
H37	HA	0.1088	C38	CA	-.1425
H39	HA	0.1093	C40	CA	-.0605
H41	HA	0.1047	C42	CA	-.2804
H43	HA	0.1646			

Stretching parameters (AMBER 99 parameters)

atom1	atom2	K $_{(Kcal/(mol\,Å^2)}$	r (Å)
C	O	570.0	1.229
C	OS	450.0	1.323
CA	CA	469.0	1.400
CA	C=C	317.0	1.510
CA	C=N	299.5	1.495
CA	CT	317.0	1.510
CA	CY	400.0	1.458
CA	HA	367.0	1.080
C=C	C=C	549.0	1.350
C=C	HC	367.0	1.080
C=N	HC=N	367.0	1.080
C=N	N=C	502.0	1.324
CT	CT	310.0	1.526
CT	HC	340.0	1.090
CT	OS	320.0	1.410
CY	NY	600.0	1.150
C	C=C	278.5	1.535
CA	N=C	299.5	1.495
CA	OS	364.1	1.436

Bending parameters (parameters: AMBER99; angles: ab initio averages)

atom1	atom2	atom3	K $_{(Kcal/mol*rad*rad)}$	Θ (°)
C=C	C	OS	80.0	108.
C=C	C	O	80.0	126.7
O	C	OS	80.0	125.
CA	CA	CA	63.0	120.
CA	CA	CT	70.0	120.
CA	CA	CY	63.0	120.
CA	CA	C=C	63.0	120.
CA	CA	C=N	63.0	120.
CA	CA	HA	50.0	120.
CA	CA	N=C	70.0	120.
CA	CA	OS	70.0	120.
CA	CT	CT	63.0	111.
CA	CT	HC	50.0	109.5
CA	CT	OS	50.0	112.6
CT	CT	HC	50.0	109.5
HC	CT	HC	35.0	109.5
HC	CT	OS	50.0	109.5
CA	CY	NY	80.0	180.
C	C=C	C=C	63.0	120.5
C	C=C	HC	50.0	116.7
CA	C=C	HC	50.0	115.9
CA	C=C	C=C	70.0	126.7
C=C	C=C	HC	50.0	122.8
CA	C=N	HC=N	50.0	120.
CA	C=N	N=C	70.0	119.8
HC=N	C=N	N=C	50.0	120.
CA	N=C	C=N	70.0	113.2
C	OS	CA	60.0	114.1
C	OS	CT	60.0	117.

Amber torsional parameters

atom1	atom2	atom3	atom4	K $_{(Kcal/mol)}$	n	γ (°)
x	CA	CA	x	1.50	2	180.
NY	CY	CA	CA	0.00	1	180.
CA	CA	C=N	x	20.00	2	180.
x	C=N	N=C	CA	20.00	2	180.
x	C=C	C=C	x	6.65	2	180.
CA	CA	C=C	x	1.50	2	180.
x	C	OS	CA	3.01	1	180.
x	C=C	C	x	2.52	2	180.
x	C	OS	CT	5.83	1	0.
x	OS	CT	x	0.56	3	0.

Fourier-like torsional parameters

atom1	atom2	atom3	atom4	V $_{(Kcal/mol)}$	C_0	C_1	C_2	C_3	C_4	C_5
C=N	N=C	CA	CA	0.5	2.6367	-2.3663	1.8672	-0.9117	1.7877	-0.4618
C	OS	CA	CA	0.5	2.1393	0.0000	1.7479	0.0000	1.9696	0.0000

Non bonded parameters

atom	r_{LJ} (Å)	ϵ_{LJ} $_{(Kcal/mol)}$	mass
HC	0.600	0.016	1.008
HC=N	0.600	0.016	1.008
HA	1.459	0.015	1.008
C	1.908	0.086	12.010
C=C	1.908	0.086	12.010
NY	1.824	0.170	14.010
N=C	1.824	0.170	14.010
CY	1.908	0.086	12.010
C=N	1.908	0.086	12.010
OS	1.661	0.210	16.000
O	1.661	0.210	16.000
CA	1.908	0.086	12.010
CT	1.908	0.109	12.010

Note that $r_{LJ} = \frac{1}{2}\sigma 2^{\frac{1}{6}}$ is half the distance of maximum LJ interaction.