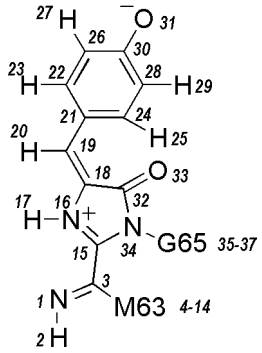
Table 2. Changed/added force field parameters



Nonbonded parameters					
Atomic charges					
Atom	OPLS type	Atom type	Charges*		
			$q_{trans, g}$	$q_{trans, e}$	$q_{cis, g}$
1	opls_966	N	-0.776	-0.686	-0.702
2	opls_290	H	0.357	0.334	0.333
3	opls_973	CA1	0.405	0.428	0.449
4	opls_136	CB1	-0.084	-0.086	-0.076
5	opls_140	HB1	0.060	0.060	0.060
6	opls_140	HB2	0.060	0.060	0.060
7	opls_210	CG1	0.098	0.098	0.098
8	opls_140	HG1	0.060	0.060	0.060
9	opls_140	HG2	0.060	0.060	0.060
10	opls_202	SD1	-0.435	-0.435	-0.435
11	opls_209	CE3	0.038	0.038	0.038
12	opls_140	HF1	0.060	0.060	0.060
13	opls_140	HF2	0.060	0.060	0.060
14	opls_140	HF3	0.060	0.060	0.060
15	opls_967	C1	0.217	0.144	0.111
16	opls_970	N2	-0.679	-0.484	-0.552
17	opls_513	H2	0.452	0.363	0.415

Nonbonded parameters					
Atomic charges					
Atom	**OPLS type**	**Atom type**	**Charges***		
			$q_{trans, g}$	**$q_{trans, e}$**	**$q_{cis, g}$**
18	opls_968	CA2	0.354	0.171	0.266
19	opls_972	CB2	-0.504	-0.283	-0.365
20	opls_140	HB	0.179	0.144	0.134
21	opls_145	CG2	0.365	0.217	0.249
22	opls_145	CD1	-0.239	-0.185	-0.151
23	opls_146	HD1	0.142	0.133	0.160
24	opls_145	CD2	-0.229	-0.171	-0.184
25	opls_146	HD2	0.189	0.109	0.114
26	opls_145	CE1	-0.296	-0.251	-0.275
27	opls_146	HE1	0.146	0.123	0.125
28	opls_145	CE2	-0.303	-0.250	-0.257
29	opls_146	HE2	0.147	0.120	0.122
30	opls_166	CZ	0.786	0.671	0.694
31	opls_167	OH	-0.691	-0.618	-0.621
32	opls_969	C2	0.423	0.376	0.311
33	opls_236	O2	-0.546	-0.543	-0.525
34	opls_971	N3	-0.073	-0.014	-0.013
35	opls_223 B	CA3	0.010	0.010	0.010
36	opls_140	HA1	0.064	0.054	0.054
37	opls_140	HA2	0.064	0.054	0.054
38	opls_235	C	0.500	0.500	0.500
39	opls_236	O	-0.500	-0.500	-0.500

Lennard-Jones parameters			
OPLS type	**Atom type**	**V**	**W**
opls_966	NN	0.325	0.711756
opls_967	CE	0.355	0.293076
opls_968	CF	0.355	0.293076
opls_969	CG	0.355	0.293076
opls_970	NF	0.325	0.711756
opls_971	NG	0.325	0.711756
opls_972	TH	0.355	0.318197
opls_973	CC	0.355	0.292880

Bonded parameters			
Bonds[†]			
Atom types		**b_0, nm**	**f_c, kJ mol^{-1} nm^{-2}**
NN	H3	0.1024	363414.2
NN	CC	0.1299	408631.7
CC	CE	0.1417	322168.0
CE	NF	0.1353	404000.0
NF	CF	0.1368	350000.0
CF	CG	0.1386	435427.2
CG	O	0.1250	477295.2
CG	NG	0.1351	350000.0
NG	CT_2	0.1446	282190.3
NG	CE	0.1337	404000.0
CF	TH	0.1404	459710.6
TH	HC	0.0999	284702.4
TH	CA	0.1366	357552.7
CC	CT	0.1510	265265.6
H	NF	0.1000	363171.2

Angles				
Atom types			θ_0, deg	f_c, kJ mol^{-1} rad^{-2}
H3	NN	CC	109.692	293.076
CE	CC	NN	121.897	669.888
CT	CC	NN	114.114	669.888
CC	CT	HC	109.784	314.010
CC	CT	CT	109.351	488.600
CT	CC	CE	123.944	669.440
NG	CE	CC	126.450	293.076
NG	CE	NF	111.601	586.152
CC	CE	NF	121.834	293.076
CE	NF	CF	106.104	586.152
NF	CF	CG	107.114	586.152
NF	CF	TH	119.645	293.076
TH	CF	CG	133.057	293.076
CF	CG	O	133.201	293.076
CF	CG	NG	108.795	586.152
O	CG	NG	117.996	293.076
CG	NG	CT_2	122.132	293.076
CG	NG	CE	106.330	586.152
CT_2	NG	CE	131.412	293.076
H	NF	CE	126.126	293.076
H	NF	CF	126.234	293.076
CF	TH	HC	111.975	293.076
HC	TH	CA	112.023	293.076
CF	TH	CA	136.002	711.756
TH	CA	CA	120.000	586.152
HC	CT_2	NG	106.948	293.076
C	CT_2	NG	114.300	527.537

Proper dihedrals							
Atom types				Ryckaert-Bellemans constants, kJ mol^{-1}			
				C_0	C_1	C_2	C_3
CE	NF	CF	CG	20.0966	0	-20.0966	0
CE	NF	CF	TH	20.0966	0	-20.0966	0
NF	CF	CG	NG	30.3543	0	-30.3543	0
TH	CF	CG	NG	30.3543	0	-30.3543	0
NF	CF	CG	O	30.3543	0	-30.3543	0
TH	CF	CG	O	30.3543	0	-30.3543	0
O	CG	NG	CE	19.4686	0	-19.4686	0
O	CG	NG	CT_2	19.4686	0	-19.4686	0
CF	CG	NG	CE	19.4686	0	-19.4686	0
CF	CG	NG	CT_2	19.4686	0	-19.4686	0
CT_2	NG	CE	NF	19.4686	0	-19.4686	0
CT_2	NG	CE	CC	19.4686	0	-19.4686	0
CG	NG	CE	NF	19.4686	0	-19.4686	0
CG	NG	CE	CC	19.4686	0	-19.4686	0
NG	CE	NF	CF	41.8680	0	-41.8680	0
CC	CE	NF	CF	41.8680	0	-41.8680	0
H	NF	CE	CC	13.3888	0	-13.3888	0
H	NF	CE	NG	19.4556	0	-19.4556	0
H	NF	CF	CG	11.7152	0	-11.7152	0
H	NF	CF	TH	11.7152	0	-11.7152	0
NN	CC	CE	NF	8.7923	0	-8.7923	0
CT	CC	CE	NF	0.8374	0	-0.8374	0
NN	CC	CE	NG	8.7923	0	-8.7923	0
CT	CC	CE	NG	0.8374	0	-0.8374	0
CT	CT	CC	CE	4.8358	-7.6577	1.6831	1.1388
CT	CT	CC	NN	4.8818	0	-4.8818	0
HC	CT	CC	CE	0.0000	0	0.0000	0

Proper dihedrals							
Atom types				Ryckaert-Bellemans constants, kJ mol^{-1}			
				C_0	C_1	C_2	C_3
HC	CT	CC	NN	0.0000	0	0.0000	0
H3	NN	CC	CE	8.4992	0	-8.4992	0
H3	NN	CC	CT	8.4992	0	-8.4992	0
S	CT	CT	CC	3.4269	-3.8623	2.5958	-2.1604
HC	CT	CT	CC	0.6280	1.8841	0.0000	-2.5121
C	CT_2	NG	CE	3.8037	-6.9564	-1.0174	4.1701
C	CT_2	NG	CG	3.8037	-6.9564	-1.0174	4.1701
HC	CT_2	NG	CG	0.3705	1.1116	0.0000	-1.4821
HC	CT_2	NG	CE	0.3705	1.1116	0.0000	-1.4821
N	C	CT_2	NG	10.3707	-6.6110	-10.5005	6.7408
O	C	CT_2	NG	0.0000	0	0.0000	0
HC	TH	CF	CG	58.6152	0	-58.6152	0
CA	TH	CF	CG	58.6152	0	-58.6152	0
HC	TH	CF	NF	58.6152	0	-58.6152	0
CA	TH	CF	NF	58.6152	0	-58.6152	0
CA	CA	TH	CF	46.0375	-4.3941	-44.0383	2.3949
CA	CA	TH	HC	8.7864	0	-8.7864	0

Improper dihedrals					
Atom types				θ_0, deg	f_c, kJ mol^{-1} rad^{-2}
C1	CA1	N2	N3	180	4.6024
N3	C1	C2	CA3	180	4.1840
CA2	N2	CB2	C2	180	4.6024
C2	CA2	O2	N3	180	4.6024
TH	CA2	HB	CG2	180	62.7600
N2	C1	H2	CA2	180	4.1840

[*]Charges were obtained from QM calculations of the chromophore model in the trans ground and excited state ($q_{trans,g,}$ and $q_{trans,e}$) and the cis ground state ($q_{cis,g}$)

[†]Distances were adopted from the asFP595 crystal structure, bonds involving hydrogens from QM calculations.