Supporting information for:

Effect of a Tertiary Butyl Group on Polar Solvation Dynamics in Aqueous Solution: A Computational Approach

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1 Forcefields of chromophores

Table S1 lists the partial charges in the ground and excited state of all chromophores employed in this study. The full forcefields and geometries are available at the end of this document (Appendix A: forcefields, Appendix B: geometries). Please note that the geometries were calculated separately for each derivative, so that the equilibrium bond lengths and angles in each forcefield differ. Thus, the current setup supports only the use of one type of derivate per simulation.

2 TDSS using the linear response approximation

The time-dependent Stokes shift can in many cases be approximated as the correlation function of the fluctuations in interaction energy between solute and solvent. This relation can be derived from linear response theory (LRT), see for example Ref. [1]. Fig. S1 shows the nonequilibrium (NEQ) and linear response (EQ) relaxation curves, where we calculated the response both on the ground state (𝕊0) and on the excited state (𝕊1). In the left panel, the large discrepancy between both EQ curves and the true NEQ results become clear.

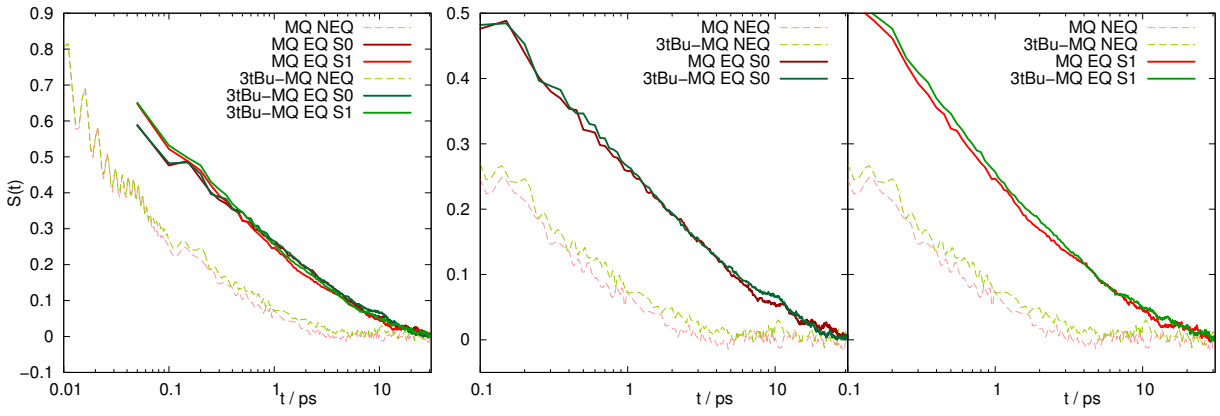

Figure S1: Time-dependent Stokes shift S(t) of MQ and 3tBu-MQ (light dashed lines) compared to the respective linear response curves in the ground and excited state at 27 °C. The middle and right figure show enlarged parts of the left figure to enable comparison between the two chromophores in the linear response approximation.

Table S1: Partial charges of chromophores MQ, EQ, iPrQ, 3iPr-MQ, 3Am-MQ, 3tBu-MQ and 3tBu-1tBuQ calculated quantum-mechanically using the ωB97xD functional and the aug-cc-pVTZ basis set.

	MQ		EQ		iPrQ		3iPr-MQ		3Am-MQ		3tBu-MQ		3tBu-tBuQ	
	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$	$\mathbb{S}0$	$\mathbb{S}1$
C_N	-0.1027	-0.1790	0.1781	0.1713	0.2638	0.2257	-0.1382	-0.1544	-0.0835	-0.0868	-0.1425	-0.1398	0.4523	0.4002
H_{N1}	0.0996	0.1000	0.0479	0.0148	0.0688	0.0751	0.1109	0.0952	0.0960	0.0758	0.1113	0.0897		
HN_2	0.0996	0.1000	0.0479	0.0148			0.1109	0.0952	0.0960	0.0758	0.1113	0.0897		
H_{N3}	0.0996	0.1000					0.1109	0.0952	0.0960	0.0758	0.1113	0.0897		
N_1	0.0273	0.1388	-0.0890	0.0164	-0.1222	-0.0265	0.0478	0.1406	0.0834	0.1653	0.0188	0.1041	-0.1291	-0.0030
C_2	0.0231	-0.1851	0.0802	-0.1270	0.1464	-0.0972	-0.0712	-0.2628	-0.2270	-0.4591	-0.0634	-0.2425	0.0288	-0.1950
H_2	0.1473	0.1580	0.1325	0.1402	0.1066	0.1049	0.1520	0.1521	0.2165	0.2295	0.1781	0.1913	0.1376	0.1569
C_3	-0.1788	-0.1201	-0.1994	-0.1454	-0.2415	-0.1758	0.0130	0.1196	0.3818	0.4863	-0.0740	0.0381	-0.0897	0.0144
H_3	0.1511	0.1266	0.1494	0.1260	0.1429	0.1201								
C_4	-0.0863	-0.2404	-0.0633	-0.2287	0.0397	-0.1869	-0.1758	-0.3578	-0.2717	-0.4161	-0.1508	-0.3360	-0.1349	-0.3340
H_4	0.1433	0.1277	0.1390	0.1259	0.1305	0.1258	0.1785	0.1713	0.1926	0.1777	0.1491	0.1368	0.1458	0.1330
C_{4A}	0.1894	0.1871	0.1614	0.1712	0.0563	0.1291	0.1499	0.1617	0.1540	0.1605	0.1466	0.1870	0.1769	0.2051
C_5	-0.5888	-0.3337	-0.5586	-0.3194	-0.4648	-0.3026	-0.5298	-0.2694	-0.5286	-0.2619	-0.5264	-0.2665	-0.5572	-0.3169
H_5	0.1746	0.1524	0.1700	0.1494	0.1757	0.1604	0.1565	0.1342	0.1539	0.1351	0.1656	0.1429	0.1632	0.1459
C_6	0.7151	0.6980	0.6747	0.6605	0.6896	0.6855	0.6584	0.6366	0.6728	0.6533	0.6507	0.6251	0.6802	0.6671
O_6	-0.8385	-0.6610	-0.8347	-0.6502	-0.9088	-0.6521	-0.8280	-0.6454	-0.8351	-0.6627	-0.8104	-0.6400	-0.8380	-0.6527
C_7	-0.2820	-0.3645	-0.2475	-0.3304	-0.2955	-0.4012	-0.2524	-0.3423	-0.2698	-0.3574	-0.2553	-0.3629	-0.2911	-0.3871
H_7	0.1346	0.1342	0.1261	0.1249	0.1204	0.1291	0.1241	0.1254	0.1249	0.1295	0.1271	0.1314	0.1227	0.1256
C_8	-0.1973	-0.2041	-0.2100	-0.2226	-0.2204	-0.1631	-0.1732	-0.1735	-0.1760	-0.1819	-0.1924	-0.1666	-0.1551	-0.1402
H_8	0.1731	0.1902	0.1543	0.1757	0.2196	0.2237	0.1520	0.1687	0.1551	0.1721	0.1573	0.1672	0.1902	0.2100
C_{8A}	0.0967	0.0749	0.1243	0.1109	0.1931	0.1610	0.0944	0.0643	0.0637	0.0446	0.1215	0.0452	0.0905	0.0522
C_{A1} to C_{A3}			-0.2146	-0.1664	-0.2118	-0.1992							-0.2962	-0.2848
H_{A1} to H_{A9}			0.0771	0.0627	0.0539	0.0439							0.0815	0.0736
C_C							0.2502	0.1460			0.4995	0.4695	0.4704	0.4474
H_{C1}							0.0027	0.0209						
N_C									-0.4396	-0.4924				
C_{B1} to C_{B3}							-0.2134	-0.1585	0.0001	0.0305	-0.3048	-0.2957	-0.3053	-0.2968
H_{B1} to H_{B9}							0.0472	0.0326	0.0574	0.0460	0.0646	0.0593	0.0675	0.0615

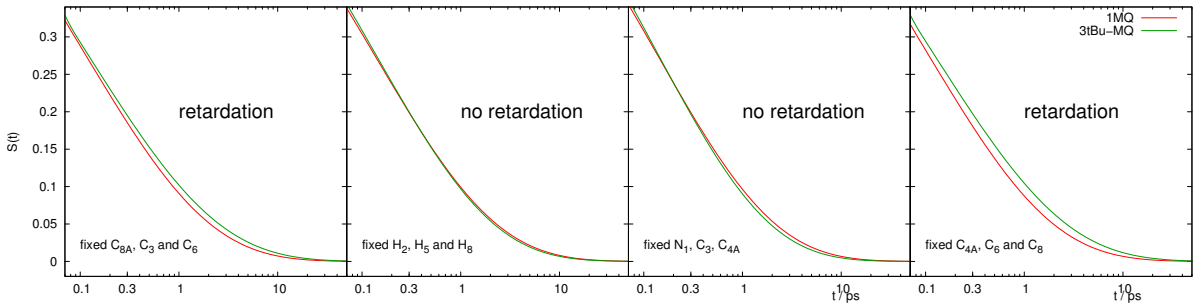

Figure S2: Fitting functions of relaxation curves of restrained nonequilibrium simulations to omit translation and rotation.

For oxyquinolinium betains LRT is not applicable, as the nonequilibrium event of exciting the chromophore leads to a large change in solvent structure close to the oxygen site of MQ. Such changes cannot be described by linear response approaches, as those inherently neglect changes in structure that do not occur in equilibrium. Fig. S1 furthermore shows that the difference between solvation behavior around MQ and 3tBu-MQ vanished completely in the ground state. In the excited state, the difference is visible, but too small to be significant.

3 Restrained nonequilibrium simulations: Contribution of solute

In addition to the restrained simulation where translation and rotation was omitted by freezing the coordinates of the atoms C_{8A}, C_3 and C_6, different sets of atoms where chosen, too. The corresponding relaxation curves are shown in Fig. S2. As described in the main

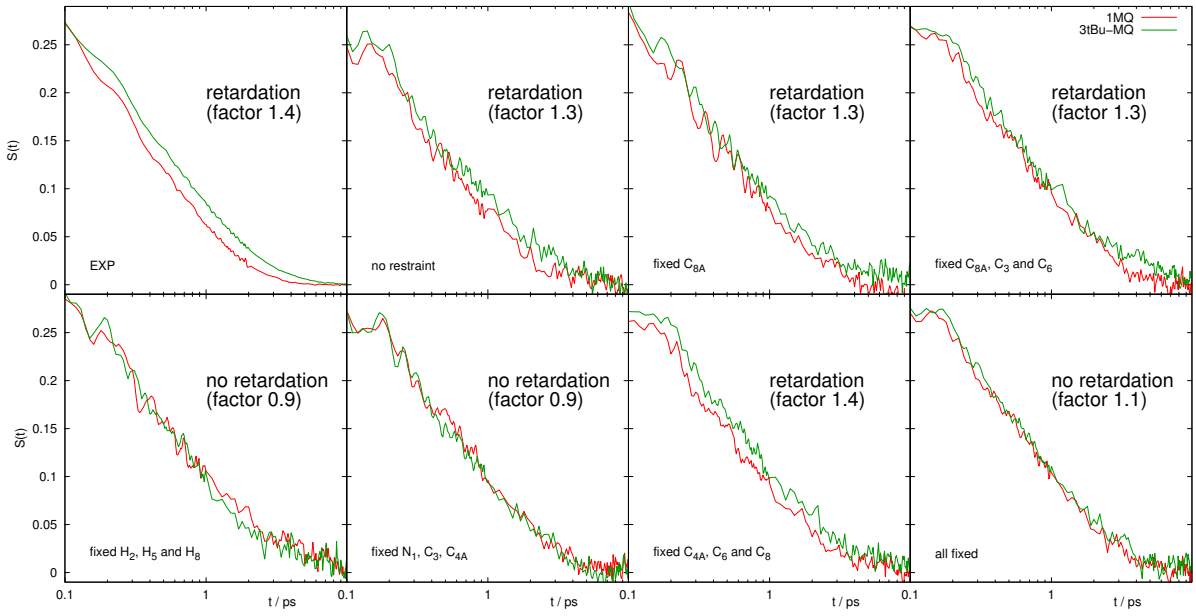

Figure S3: Unprocessed relaxation curves of restrained nonequilibrium simulations to omit translation, rotation or vibration.

article, the omission of solute rotation slows down the respective curves but does not affect

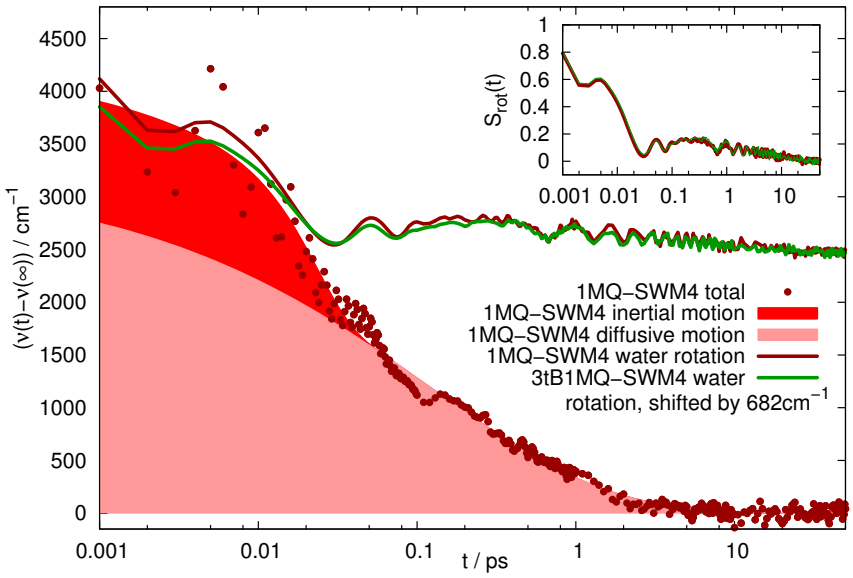

Figure S4: Rotational relaxation of water around MQ.

the relative retardation between MQ and 3tBu-MQ. However, this is only true for freezing the set C_{8A}, C_3 and C_6 or C_{4A}, C_6 and C_3. When freezing more atoms in the pyridinium part of the chromophore, or some hydrogen atoms (sets N_1, C_3 and C_{4A} or H_2, H_5 and H_8), the retardation vanishes. The freezing of some atoms affects the possible normal modes, so that the freezing of some sets may forbid specific solute vibrational modes that couple to solvation and are responsible for the retardation. In addition to Fig. S2 and the corresponding section in the main article, where in both cases the fitting functions of the actual data is shown for the sake of clearness, Fig. S3 shows the unprocessed Stokes shift relaxation functions of experiment, free simulation and all restrained simulations. The retardation is clearly visible, although small.

4 Restrained nonequilibrium simulations: Contribution of solvent

Fig. S4 shows the relaxation after solute excitation solely via water rotation, where the solute was fixed, as well as the water oxygens. The relaxation corresponds well to the Gaussian function of the overall relaxation as shown in Fig. S4. The inset in Fig. S4 shows the normalized relaxation function arising from water rotation around MQ and 3tBu-MQ, where no difference could be detected. If the retardation in the Stokes shift would stem from hydrophobic contributions, a retardation would also be visible for relaxation via solvent rotation. As this is not the case, the observed slowing down of dynamics upon addition of sidechains must stem from a different source (vibrational relaxation, as pointed out in the main article).

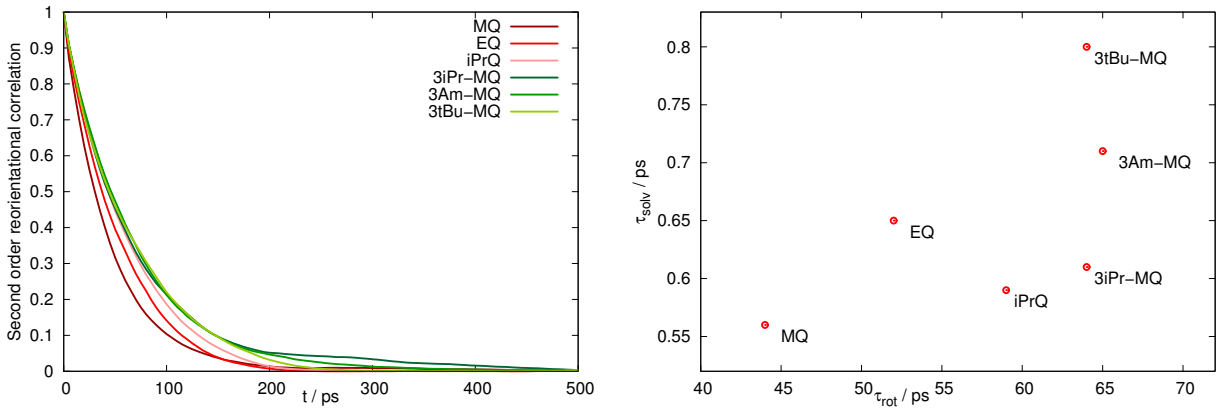

Figure S5: Second order reorientational correlation functions of different solutes and their correlation to solvation time.

5 Correlation of rotation and solvation times

As discussed in the main article, the omission of solute rotation slightly slows down the solvation response but does not account fully for the retardation of larger chromophores. The left part of Fig. S5 shows the second legendre polynomials of the normalized correlation functions of the solute dipole moments. Larger chromophores show longer rotational correlation times. However, when plotted against the solvation times τ_{solv}, no direct proportionality could be found, as shown in the right part of Fig. S5.

6 Influence of partial charge distribution

To check on the influence of the partial charge distribution of 3tBu-MQ on the observed retardation of solvation dynamics we conducted two additional simulations. First, the change in partial charge upon excitation Δq was set to the one observed in MQ, so that $\Delta q_{3tBu-MQ} = \Delta q_{MQ}$. The ground state charge $q_{\mathbb{S}0}$ was left unchanged. The corresponding relaxation curve is shown in green in Fig. S6 and is slightly slower than the original 3tBu-MQ response (light green). Second, the partial charge distribution in the ground state, $q_{\mathbb{S}0}$ and its change Δq was set to the same values as encountered in MQ. Here, the ground state charges of the tertiary butyl sidechain were set to tabulated values and were not changed during excitation. The corresponding relaxation function is shown in dark green in Fig. S6 and is again slower than the original response. Thus, the attachment of the sidechain does not lead to an inductive effect that could cause the retardation. In contrast, if the partial charge distribution is artificially set to those observed in the unsubstituted chromophore, the retardation becomes significantly larger.

7 Adaption of geometry or dipole moment

As discussed in the main article, MQ can slightly adapt to the reaction field after excitation, where the dipole moment slightly rises, and the overall $\Delta\mu$ rises slightly, too. Different $\Delta\mu$ yield different solvation responses whenever linear response theory is not valid in a system, as is the case in the studied oxyquinolinium-water system. Whether such a de-

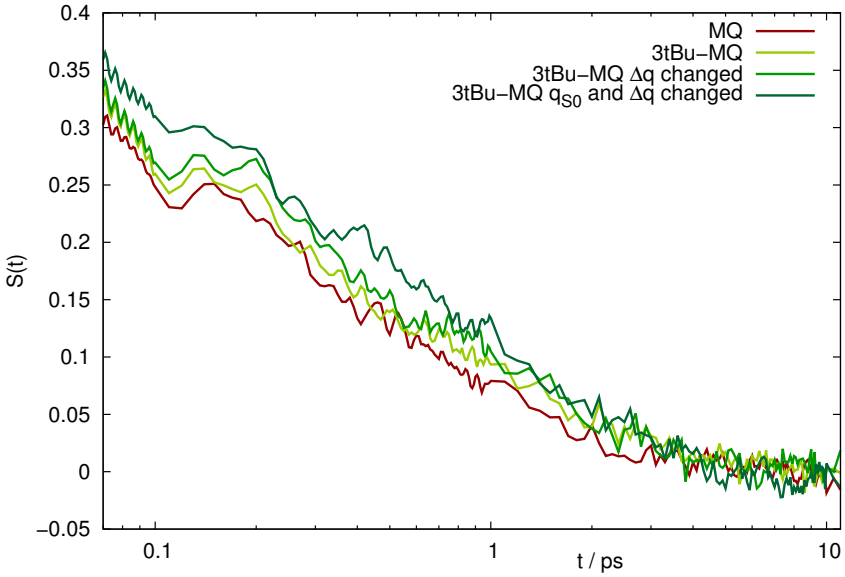

Figure S6: Solvation response of 3tBu-MQ with original charge distribution and two artificial ones, where either only Δq or both Δq and q_{S0} were set to the values observed in MQ.

crease speeds up the observed dynamics or slows them down depends on the direction of change. In a previous article, Ref. [1], we found that a decrease in $\Delta\mu$ (this is Δq) slows down solvation dynamics around solutes increasing their dipole moment (or quadrupole moment), but accelerates solvation dynamics around solutes decreasing their dipole moment (or quadrupole moment). The respective curves are shown in Fig. S7, and were calculated in water and methanol. An analogous finding, where a larger increase in charge leads to a slower solvation response, is also reported by Maroncelli and coworkers [2].
Oxyquinolinium betaine lowers its dipole moment upon excitation, so that an increase in $\Delta\mu$ might speed up the solvation response. As such a increase in the dipole moment is only found for MQ, but not for 3tBu-MQ, the former could show a small acceleration in solvation dynamics. However, the dipole moment increase for MQ in the ground state amounts only to 0.1 D, and is even less in $\Delta\mu$, so that the retardation of 3tBu-MQ cannot be explained by this effect.

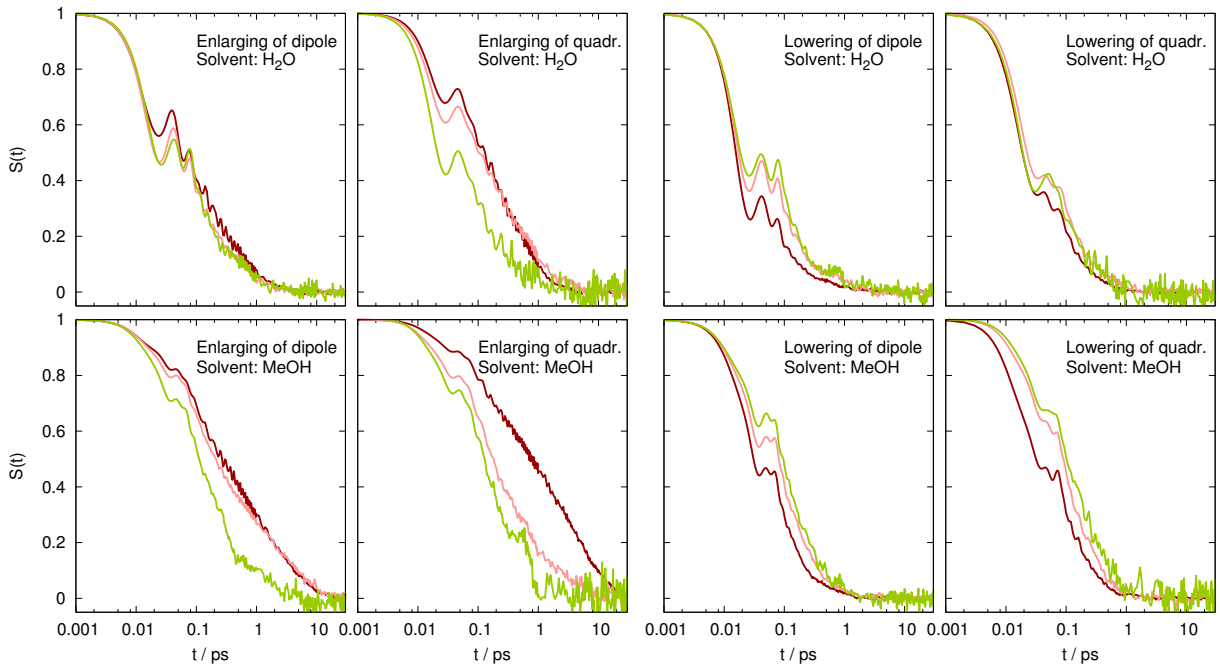

Figure S7: Solvation response of artificial benzene-like solute undergoing creation of dipole or quadrupole moments. Red curves correspond to large changes in Δq (here $\pm$ 1 e), pink curves to intermediate changes ($\pm$ 0.5 e) and green curves to small changes ($\pm$ 0.2 e). If a dipole or quadrupole is enlarged upon excitation, the relaxation around the largest change is slowest. If, on the other side, a dipole or quadrupole is decreased, the relaxation around the largest change is fastest.

8 Normal mode spectra

Table S2 lists the normal mode wavenumbers of MQ and 3tBu-MQ in the excited state, both from quantum mechanics calculations and molecular dynamics simulation. Most of the spectra is reproduced well using molecular dynamics simulation, although the force constants were not optimized. Table S3 lists which of the modes from Table S2 belong

Table S2: Normal modes frequencies [cm^{-1}] of MQ and 3tBu-MQ in the excited state obtained from quantum mechanics (QM) and molecular dynamics simulation (MD).

MQ (QM):											
83	269	475	694	793	947	1152	1304	1467	1535	3156	3217
112	347	511	710	847	1024	1199	1333	1481	1605	3200	3233
159	378	521	713	884	1074	1209	1346	1485	1640	3203	
217	434	590	741	936	1115	1233	1407	1499	3036	3205	
235	462	625	764	944	1139	1285	1433	1515	3086	3215	
MQ (MD):											
81	324	468	603	802	952	1052	1298	1453	2042	2902	2996
140	337	498	632	818	971	1153	1321	1480	2053	2947	2997
192	400	540	671	856	984	1186	1382	1522	2084	2949	
253	422	553	687	891	1009	1199	1380	1599	2797	2952	
298	428	577	789	944	1019	1231	1411	1640	2899	2996	
3tBu-MQ (QM):											
21	239	378	605	824	968	1212	1352	1484	1518	3081	3198
62	247	414	636	842	1037	1221	1390	1484	1537	3087	3200
86	267	430	641	885	1052	1223	1402	1486	1605	3089	3213
130	299	435	713	927	1054	1241	1406	1488	1635	3097	3232
149	313	476	729	930	1103	1265	1408	1491	3028	3097	3234
169	319	507	737	941	1141	1293	1430	1501	3030	3099	
213	333	546	770	944	1144	1302	1466	1505	3032	3101	
232	359	553	780	961	1164	1340	1479	1515	3038	3156	
3tBu-MQ (MD):											
28	255	399	574	830	936	1112	1351	1410	1604	2897	2946
90	297	403	596	837	854	1113	1388	1415	1643	2898	2949
106	300	448	647	849	959	1143	1390	1423	2082	2899	2951
148	317	471	665	867	987	1191	1393	1431	2126	2899	2995
151	321	485	707	884	1009	1217	1395	1445	2797	2900	2996
203	345	539	753	895	1012	1223	1397	1481	2799	2901	
236	351	557	769	900	1044	1287	1399	1498	2800	2901	
253	364	561	822	908	1056	1332	1406	1555	2801	2902	

to the same motion. Some of the assignments are difficult due to the change in motion

Table S3: The 20 lowest normal modes wavenumbers [cm^{-1}] of MQ compared to the normal mode wavenumbers of the corresponding movements in 3tBu-MQ, obtained from quantum mechanics (QM) and molecular dynamics simulation (MD).

QM		MD	
MQ	3tBu-MQ	MQ	3tBu-MQ
83	86	140	148
112	62	192	203
159	139	81	90
217	213	81	90
235	232	298	253
269	299	253	300
347	359	324	345
378	378	337	351
434	435	400	470
462	476	422	448
475	546	468	539
511	507	498	557
521	605	428	561
590	641	577	596
625	636	553	574
694	737	540	769
710	729	631	647
713	713	603	665
741	770	687	706
764	780	671	849

upon addition of the sidechain, so that the assignation should only be considered as approximate. Nevertheless, the quantum mechanical data clearly shows a rise in wavenumber of most modes between 250 and 800 cm^{-1} when a tertiary butyl group is added to MQ, and a decrease in wavenumber for modes below 250 cm^{-1}. Although molecular dynamics simulation does not reproduce all frequencies quantitatively, the qualitative behavior is conserved. Thus, molecular dynamics simulation is capable of depicting correctly the observed change in the normal mode spectra upon addition of sidechains to the studied chromophore.

References

[1] E. Heid, W. Moser, and C. Schröder. "On the Validity of Linear Response Approximations Regarding the Solvation Dynamics of Polyatomic Solutes." *Phys. Chem. Chem. Phys.*, **19**(2017), 10940.

[2] P. V. Kumar and M. Maroncelli. "Polar Solvation Dynamics of Polyatomic Solutes: Simulation Studies in Acetonitrile and Methanol." *J. Chem. Phys.*, **103**(1995), 3038.

Appendix A

Force field MQ

```
* Toppar MQ
*

READ RTF CARD
*=============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using wB97XD - PCM
*=============================================================
*
99

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!      ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS    1  HGA3     1.008
MASS    2  HGR61    1.008
MASS    3  HGR63    1.008
MASS    4  CG2R61  12.011
MASS    5  CG2R62  12.011
MASS    6  CG334   12.011
MASS    7  NG2R61  14.007
MASS    8  OG312   16.000

AUTO ANGL DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State                              1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!          H2       H3
!            \     /
!   HN2      C2---C3
!       \   //    \\
! HN3--CN--N1(+)   C4--H4
!       /    \     /
!   HN1      C8A==C4A
!             /     \
!      H8--C8       C5--H5
!           \\     //
!            C7---C6
!           /      \
!          H7       O6(-)
!
RESI MQS0  0.00000
GROUP
ATOM     CN  CG334    -0.1027
ATOM    HN1   HGA3     0.0996
ATOM    HN2   HGA3     0.0996
ATOM    HN3   HGA3     0.0996
ATOM     N1 NG2R61     0.0273
ATOM     C2 CG2R62     0.0231
ATOM     H2  HGR63     0.1473
ATOM     C3 CG2R62    -0.1788
ATOM     H3  HGR63     0.1511
ATOM     C4 CG2R62    -0.0863
ATOM     H4  HGR63     0.1433
ATOM    C4A CG2R62     0.1894
ATOM     C5 CG2R61    -0.5888
ATOM     H5  HGR61     0.1746
ATOM     C6 CG2R61     0.7151
ATOM     O6  OG312    -0.8385
ATOM     C7 CG2R61    -0.2820
ATOM     H7  HGR61     0.1346
ATOM     C8 CG2R61    -0.1973
ATOM     H8  HGR61     0.1731
ATOM    C8A CG2R62     0.0967
BOND     CN    HN1
```

```
BOND     CN    HN2
BOND     CN    HN3
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     H3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited State                              1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI MQS1  0.00000
GROUP
ATOM     CN  CG334    -0.1790
ATOM    HN1   HGA3     0.1000
ATOM    HN2   HGA3     0.1000
ATOM    HN3   HGA3     0.1000
ATOM     N1 NG2R61     0.1388
ATOM     C2 CG2R62    -0.1851
ATOM     H2  HGR63     0.1580
ATOM     C3 CG2R62    -0.1201
ATOM     H3  HGR63     0.1266
ATOM     C4 CG2R62    -0.2404
ATOM     H4  HGR63     0.1277
ATOM    C4A CG2R62     0.1871
ATOM     C5 CG2R61    -0.3337
ATOM     H5  HGR61     0.1524
ATOM     C6 CG2R61     0.6980
ATOM     O6  OG312    -0.6610
ATOM     C7 CG2R61    -0.3645
ATOM     H7  HGR61     0.1342
ATOM     C8 CG2R61    -0.2041
ATOM     H8  HGR61     0.1902
ATOM    C8A CG2R62     0.0749
BOND     CN    HN1
BOND     CN    HN2
BOND     CN    HN3
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     H3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
```

```
PATCHING FIRST NONE LAST NONE

END

READ PARA CARD
*=============================================================
*.   P A R A M E T E R   O F   Q U I N O L O N E S
*=============================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       ID  NAME      MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS     1  HGA3      1.008
MASS     2  HGR61     1.008
MASS     3  HGR63     1.008
MASS     4  CG2R61   12.011
MASS     5  CG2R62   12.011
MASS     6  CG334    12.011
MASS     7  NG2R61   14.007
MASS     8  OG312    16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2     k [kcal/mol Angstroem^2]      r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG334      HGA3               322.0000                1.08428
CG334      NG2R61             400.0000                1.47636
CG2R61     HGR61              340.0000                1.08074
CG2R61     OG312              525.0000                1.24310
CG2R61     CG2R61             305.0000                1.42010
CG2R61     CG2R62             305.0000                1.40123
CG2R62     HGR63              350.0000                1.07940
CG2R62     CG2R62             420.0000                1.40974
CG2R62     NG2R61             302.0000                1.35950

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2     TYPE3      k [kcal/mol rad^2]      theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61     CG2R61     CG2R61           40.0000             119.101
CG2R61     CG2R61     CG2R62           40.0000             121.714
CG2R61     CG2R61     HGR61            30.0000             117.983
CG2R61     CG2R61     OG312            40.0000             122.942
CG2R61     CG2R62     CG2R62           40.0000             120.307
CG2R61     CG2R62     NG2R61           85.0000             123.357
CG2R62     CG2R61     HGR61            30.0000             120.942
CG2R62     CG2R62     CG2R62           40.0000             119.311
CG2R62     CG2R62     HGR63            80.0000             120.408
CG2R62     CG2R62     NG2R61           85.0000             119.765
CG2R62     NG2R61     CG2R62           30.0000             122.538
CG2R62     NG2R61     CG334            45.0000             118.731
HGA3       CG334      HGA3             35.5000             109.195
HGA3       CG334      NG2R61           33.4300             109.746
HGR63      CG2R62     NG2R61           80.0000             116.218

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2     TYPE3     TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61     CG2R61     CG2R61     CG2R61         3.1000       2       180.0000
```

```
CG2R61    CG2R61    CG2R61    CG2R62        3.1000      2      180.0000
CG2R61    CG2R61    CG2R61    HGR61         4.2000      2      180.0000
CG2R61    CG2R61    CG2R61    OG312         3.1000      2      180.0000
CG2R61    CG2R61    CG2R62    CG2R62        3.1000      2      180.0000
CG2R61    CG2R61    CG2R62    NG2R61        7.0000      2      180.0000
CG2R61    CG2R62    CG2R62    CG2R61        6.0000      2      180.0000
CG2R61    CG2R62    CG2R62    CG2R62        6.0000      2      180.0000
CG2R61    CG2R62    CG2R62    HGR63         1.0000      2      180.0000
CG2R61    CG2R62    CG2R62    NG2R61        7.0000      2      180.0000
CG2R61    CG2R62    NG2R61    CG2R62        4.0000      2      180.0000
CG2R61    CG2R62    NG2R61    CG334        11.0000      2      180.0000
CG2R62    CG2R61    CG2R61    HGR61         4.2000      2      180.0000
CG2R62    CG2R61    CG2R61    OG312         3.1000      2      180.0000
CG2R62    CG2R62    CG2R61    HGR61         4.2000      2      180.0000
CG2R62    CG2R62    CG2R62    CG2R62        6.0000      2      180.0000
CG2R62    CG2R62    CG2R62    HGR63         1.0000      2      180.0000
CG2R62    CG2R62    CG2R62    NG2R61        7.0000      2      180.0000
CG2R62    CG2R62    NG2R61    CG334        11.0000      2      180.0000
CG2R62    NG2R61    CG2R62    CG2R62        4.0000      2      180.0000
CG2R62    NG2R61    CG334     HGA3          0.0000      3        0.0000
CG334     NG2R61    CG2R62    HGR63         1.0000      2      180.0000
HGR61     CG2R61    CG2R61    HGR61         2.4000      2      180.0000
HGR61     CG2R61    CG2R61    OG312         2.4000      2      180.0000
HGR61     CG2R61    CG2R62    NG2R61        3.4000      2      180.0000
HGR63     CG2R62    CG2R62    HGR63         2.0000      2      180.0000
HGR63     CG2R62    CG2R62    NG2R61        7.0000      2      180.0000
HGR63     CG2R62    NG2R61    CG2R62        7.0000      2      180.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA3    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61   0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63   0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG334   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61  0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312   0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Force field EQ

```
* Toppar EQ
*

READ RTF CARD
*============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using wB97XD - PCM
*============================================================
*
99

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!      ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS    1  HGA3     1.008
MASS    2  HGA2     1.008
MASS    3  HGR61    1.008
MASS    4  HGR63    1.008
MASS    5  CG2R61  12.011
MASS    6  CG2R62  12.011
MASS    7  CG324   12.011
MASS    8  CG331   12.011
MASS    9  NG2R61  14.007
MASS    10 OG312   16.000

AUTO ANGL DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State                                1-ethyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!                H2       H3
!                  \     /
!    HA3  HN2      C2---C3
!       \    \    //    \\
!  HA2--CA1--CN--N1(+)   C4--H4
!       /    /    \      /
!    HA1  HN1      C8A==C4A
!                  /     \
!            H8--C8       C5--H5
!                 \\     //
!                  C7---C6
!                 /      \
!                H7       O6(-)
!
RESI EQS0  0.00000
GROUP
ATOM     CN  CG324    0.1781
ATOM    HN1   HGA2    0.0479
ATOM    HN2   HGA2    0.0479
ATOM    CA1  CG331   -0.2146
ATOM    HA1   HGA3    0.0771
ATOM    HA2   HGA3    0.0771
ATOM    HA3   HGA3    0.0771
ATOM     N1 NG2R61   -0.0890
ATOM     C2 CG2R62    0.0802
ATOM     H2  HGR63    0.1325
ATOM     C3 CG2R62   -0.1994
ATOM     H3  HGR63    0.1494
ATOM     C4 CG2R62   -0.0633
ATOM     H4  HGR63    0.1390
ATOM    C4A CG2R62    0.1614
ATOM     C5 CG2R61   -0.5586
ATOM     H5  HGR61    0.1700
ATOM     C6 CG2R61    0.6747
ATOM     O6  OG312   -0.8347
ATOM     C7 CG2R61   -0.2475
ATOM     H7  HGR61    0.1261
ATOM     C8 CG2R61   -0.2100
ATOM     H8  HGR61    0.1543
```

```
ATOM     C8A CG2R62     0.1243
BOND      CN     HN1
BOND      CN     HN2
BOND      CN     CA1
BOND     CA1    HA1
BOND     CA1    HA2
BOND     CA1    HA3
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      H3
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited State                              1-ethyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI EQS1   0.00000
GROUP
ATOM      CN   CG324      0.1713
ATOM     HN1    HGA2      0.0148
ATOM     HN2    HGA2      0.0148
ATOM      C9   CG331     -0.1664
ATOM     HN3    HGA3      0.0627
ATOM     HN4    HGA3      0.0627
ATOM     HN5    HGA3      0.0627
ATOM      N1  NG2R61      0.0164
ATOM      C2  CG2R62     -0.1270
ATOM      H2   HGR63      0.1402
ATOM      C3  CG2R62     -0.1454
ATOM      H3   HGR63      0.1260
ATOM      C4  CG2R62     -0.2287
ATOM      H4   HGR63      0.1259
ATOM     C4A  CG2R62      0.1712
ATOM      C5  CG2R61     -0.3194
ATOM      H5   HGR61      0.1494
ATOM      C6  CG2R61      0.6605
ATOM      O6   OG312     -0.6502
ATOM      C7  CG2R61     -0.3304
ATOM      H7   HGR61      0.1249
ATOM      C8  CG2R61     -0.2226
ATOM      H8   HGR61      0.1757
ATOM     C8A  CG2R62      0.1109
BOND      CN     HN1
BOND      CN     HN2
BOND      CN     CA1
BOND     CA1    HA1
BOND     CA1    HA2
BOND     CA1    HA3
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      H3
BOND      C3      C4
BOND      C4      H4
```

```
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
PATCHING FIRST NONE LAST NONE

END

READ PARA CARD
*=============================================================
*.   P A R A M E T E R   O F   Q U I N O L O N E S
*=============================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!      ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS    1  HGA3     1.008
MASS    2  HGA2     1.008
MASS    3  HGR61    1.008
MASS    4  HGR63    1.008
MASS    5  CG2R61  12.011
MASS    6  CG2R62  12.011
MASS    7  CG324   12.011
MASS    8  CG331   12.011
MASS    9  NG2R61  14.007
MASS    10 OG312   16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG324     HGA2              284.50                 1.08869
CG324     CG331             222.50                 1.51979
CG331     HGA3              322.00                 1.08941
CG324     NG2R61            400.0000               1.47636
CG2R61    HGR61             340.0000               1.08074
CG2R61    OG312             525.0000               1.24310
CG2R61    CG2R61            305.0000               1.42010
CG2R61    CG2R62            305.0000               1.40123
CG2R62    HGR63             350.0000               1.07940
CG2R62    CG2R62            420.0000               1.40974
CG2R62    NG2R61            302.0000               1.35950

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000            119.101
CG2R61    CG2R61    CG2R62          40.0000            121.714
CG2R61    CG2R61    HGR61           30.0000            117.983
CG2R61    CG2R61    OG312           40.0000            122.942
CG2R61    CG2R62    CG2R62          40.0000            120.307
CG2R61    CG2R62    NG2R61          85.0000            123.357
CG2R62    CG2R61    HGR61           30.0000            120.942
CG2R62    CG2R62    CG2R62          40.0000            119.311
CG2R62    CG2R62    HGR63           80.0000            120.408
```

```
CG2R62     CG2R62     NG2R61          85.0000            119.765
CG2R62     NG2R61     CG2R62          30.0000            122.538
CG2R62     NG2R61     CG324           45.0000            119.024
CG331      CG324      NG2R61          70.00              116.271
CG331      CG324      HGA2            34.60              109.621
NG2R61     CG324      HGA2            51.50              106.729
HGA2       CG324      HGA2            35.50              107.487
CG324      CG331      HGA3            34.60              110.873
HGA3       CG331      HGA3            35.50              107.984
HGR63      CG2R62     NG2R61          80.0000            116.218

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2      TYPE3      TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61     CG2R61     CG2R61     CG2R61         3.1000       2       180.0000
CG2R61     CG2R61     CG2R61     CG2R62         3.1000       2       180.0000
CG2R61     CG2R61     CG2R61     HGR61          4.2000       2       180.0000
CG2R61     CG2R61     CG2R61     OG312          3.1000       2       180.0000
CG2R61     CG2R61     CG2R62     CG2R62         3.1000       2       180.0000
CG2R61     CG2R61     CG2R62     NG2R61         7.0000       2       180.0000
CG2R61     CG2R62     CG2R62     CG2R61         6.0000       2       180.0000
CG2R61     CG2R62     CG2R62     CG2R62         6.0000       2       180.0000
CG2R61     CG2R62     CG2R62     HGR63          1.0000       2       180.0000
CG2R61     CG2R62     CG2R62     NG2R61         7.0000       2       180.0000
CG2R61     CG2R62     NG2R61     CG2R62         4.0000       2       180.0000
CG2R62     CG2R61     CG2R61     HGR61          4.2000       2       180.0000
CG2R62     CG2R61     CG2R61     OG312          3.1000       2       180.0000
CG2R62     CG2R62     CG2R61     HGR61          4.2000       2       180.0000
CG2R62     CG2R62     CG2R62     CG2R62         6.0000       2       180.0000
CG2R62     CG2R62     CG2R62     HGR63          1.0000       2       180.0000
CG2R62     CG2R62     CG2R62     NG2R61         7.0000       2       180.0000
HGR61      CG2R61     CG2R61     HGR61          2.4000       2       180.0000
HGR61      CG2R61     CG2R61     OG312          2.4000       2       180.0000
HGR61      CG2R61     CG2R62     NG2R61         3.4000       2       180.0000
HGR63      CG2R62     CG2R62     HGR63          2.0000       2       180.0000
HGR63      CG2R62     CG2R62     NG2R61         7.0000       2       180.0000
CG2R62     NG2R61     CG2R62     CG2R62         4.0000       2       180.0000
HGR63      CG2R62     NG2R61     CG2R62         7.0000       2       180.0000
CG2R61     CG2R62     NG2R61     CG324         11.0000       2       180.0000
CG2R62     CG2R62     NG2R61     CG324         11.0000       2       180.0000
HGR63      CG2R62     NG2R61     CG324          1.0000       2       180.0000
NG2R61     CG324      CG331      HGA3           0.1950       3         0.0000
HGA2       CG324      CG331      HGA3           0.1600       3         0.0000
CG331      CG324      NG2R61     CG2R62         2.2087       1       180.0000
CG331      CG324      NG2R61     CG2R62         1.8892       2         0.0000
CG331      CG324      NG2R61     CG2R62         0.5201       3       180.0000
HGA2       CG324      NG2R61     CG2R62         0.0000       3         0.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1           epsilon    rmin/2       epsilon14   rmin14/2
!            [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA2     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGA3     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG324    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61   0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312    0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Force field iPrQ

```
* Toppar iPr-Q
*

READ RTF CARD
*============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using wB97xD-PCM
*============================================================
*
99

MASS     1  HGA1      1.008
MASS     2  HGA3      1.008
MASS     3  HGR61     1.008
MASS     4  HGR63     1.008
MASS     5  CG2R61   12.011
MASS     6  CG2R62   12.011
MASS     7  CG314    12.011
MASS     8  CG331    12.011
MASS     9  NG2R61   14.007
MASS    10  OG312    16.000

AUTO ANGLES DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State                          1-isoproyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       HA5       H2        H3
!         \         \      /
!     HA4-CA2-HA6   C2---C3
!           \      //    \\
!       HN1-CN----N1(+)    C4--H4
!           /       \      /
!     HA2-CA1-HA3   C8A==C4A
!         /         /      \
!       HA1   H8--C8        C5--H5
!                  \\      //
!                   C7---C6
!                  /       \
!                 H7        O6(-)
!
RESI IQS0   0.00000
GROUP
ATOM      CN   CG314     0.2638
ATOM     HN1    HGA1     0.0688
ATOM     CA1   CG331    -0.2118
ATOM     HA1    HGA3     0.0539
ATOM     HA2    HGA3     0.0539
ATOM     HA3    HGA3     0.0539
ATOM     CA2   CG331    -0.2118
ATOM     HA4    HGA3     0.0539
ATOM     HA5    HGA3     0.0539
ATOM     HA6    HGA3     0.0539
ATOM      N1  NG2R61    -0.1222
ATOM      C2  CG2R62     0.1464
ATOM      H2   HGR63     0.1066
ATOM      C3  CG2R62    -0.2415
ATOM      H3   HGR63     0.1429
ATOM      C4  CG2R62     0.0397
ATOM      H4   HGR63     0.1305
ATOM     C4A  CG2R62     0.0563
ATOM      C5  CG2R61    -0.4648
ATOM      H5   HGR61     0.1757
ATOM      C6  CG2R61     0.6896
ATOM      O6   OG312    -0.9088
ATOM      C7  CG2R61    -0.2955
ATOM      H7   HGR61     0.1204
ATOM      C8  CG2R61    -0.2204
ATOM      H8   HGR61     0.2196
```

```
ATOM     C8A CG2R62    0.1931
BOND      CN     CA1
BOND      CN     CA2
BOND      CN     HN1
BOND     CA1     HA1
BOND     CA1     HA2
BOND     CA1     HA3
BOND     CA2     HA4
BOND     CA2     HA5
BOND     CA2     HA6
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      H3
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited state                        1-isoproyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI IQS1  0.00000
GROUP
ATOM      CN  CG314    0.2257
ATOM     HN1   HGA1    0.0751
ATOM     CA1  CG331   -0.1992
ATOM     HA1   HGA3    0.0439
ATOM     HA2   HGA3    0.0439
ATOM     HA3   HGA3    0.0439
ATOM     CA2  CG331   -0.1992
ATOM     HA4   HGA3    0.0439
ATOM     HA5   HGA3    0.0439
ATOM     HA6   HGA3    0.0439
ATOM      N1 NG2R61   -0.0265
ATOM      C2 CG2R62   -0.0972
ATOM      H2  HGR63    0.1049
ATOM      C3 CG2R62   -0.1758
ATOM      H3  HGR63    0.1201
ATOM      C4 CG2R62   -0.1869
ATOM      H4  HGR63    0.1258
ATOM     C4A CG2R62    0.1291
ATOM      C5 CG2R61   -0.3026
ATOM      H5  HGR61    0.1604
ATOM      C6 CG2R61    0.6855
ATOM      O6  OG312   -0.6521
ATOM      C7 CG2R61   -0.4012
ATOM      H7  HGR61    0.1291
ATOM      C8 CG2R61   -0.1631
ATOM      H8  HGR61    0.2237
ATOM     C8A CG2R62    0.1610
BOND      CN     CA1
BOND      CN     CA2
BOND      CN     HN1
BOND     CA1     HA1
BOND     CA1     HA2
BOND     CA1     HA3
BOND     CA2     HA4
BOND     CA2     HA5
```

```
BOND    CA2    HA6
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     H3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
PATCHING FIRST NONE LAST NONE


END


READ PARA CARD
*============================================================
*.   P A R A M E T E R   O F   Q U I N O L O N E S
*============================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!      ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS    1  HGA1     1.008
MASS    2  HGA3     1.008
MASS    3  HGR61    1.008
MASS    4  HGR63    1.008
MASS    5  CG2R61  12.011
MASS    6  CG2R62  12.011
MASS    7  CG314   12.011
MASS    8  CG331   12.011
MASS    9  NG2R61  14.007
MASS   10  OG312   16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG314     HGA1              309.00                 1.08686
CG314     NG2R61            400.00                 1.50750
CG314     CG331             222.50                 1.53135
CG331     HGA3              322.00                 1.08858
CG2R61    HGR61             340.0000               1.08074
CG2R61    OG312             525.0000               1.24310
CG2R61    CG2R61            305.0000               1.42010
CG2R61    CG2R62            305.0000               1.40123
CG2R62    HGR63             350.0000               1.07940
CG2R62    CG2R62            420.0000               1.40974
CG2R62    NG2R61            302.0000               1.35950

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
```

```
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000             119.101
CG2R61    CG2R61    CG2R62          40.0000             121.714
CG2R61    CG2R61    HGR61           30.0000             117.983
CG2R61    CG2R61    OG312           40.0000             122.942
CG2R61    CG2R62    CG2R62          40.0000             120.307
CG2R61    CG2R62    NG2R61          85.0000             123.357
CG2R62    CG2R61    HGR61           30.0000             120.942
CG2R62    CG2R62    CG2R62          40.0000             119.311
CG2R62    CG2R62    HGR63           80.0000             120.408
CG2R62    CG2R62    NG2R61          85.0000             119.765
CG2R62    NG2R61    CG2R62          30.0000             122.538
CG2R62    NG2R61    CG314           45.0000             119.245
NG2R61    CG314     HGA1            48.00               102.686
CG331     CG314     CG331           53.35               115.134
CG331     CG314     NG2R61          70.00               112.753
CG331     CG314     HGA1            34.50               106.114
CG314     CG331     HGA3            33.43               110.891
HGA3      CG331     HGA3            35.50               107.996
HGR63     CG2R62    NG2R61          80.0000             116.575

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61    CG2R61          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    HGR61           4.2000       2       180.0000
CG2R61    CG2R61    CG2R61    OG312           3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R61          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R62          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    HGR63           1.0000       2       180.0000
CG2R61    CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG2R62          4.0000       2       180.0000
CG2R62    CG2R61    CG2R61    HGR61           4.2000       2       180.0000
CG2R62    CG2R61    CG2R61    OG312           3.1000       2       180.0000
CG2R62    CG2R62    CG2R61    HGR61           4.2000       2       180.0000
CG2R62    CG2R62    CG2R62    CG2R62          6.0000       2       180.0000
CG2R62    CG2R62    CG2R62    HGR63           1.0000       2       180.0000
CG2R62    CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R62    NG2R61    CG2R62    CG2R62          4.0000       2       180.0000
HGR61     CG2R61    CG2R61    HGR61           2.4000       2       180.0000
HGR61     CG2R61    CG2R61    OG312           2.4000       2       180.0000
HGR61     CG2R61    CG2R62    NG2R61          3.4000       2       180.0000
HGR63     CG2R62    CG2R62    HGR63           2.0000       2       180.0000
HGR63     CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG314          11.0000       2       180.0000
CG2R62    CG2R62    NG2R61    CG314          11.0000       2       180.0000
CG314     NG2R61    CG2R62    HGR63           1.0000       2       180.0000
CG2R62    NG2R61    CG314     HGA1            0.0000       3         0.0000
HGR63     CG2R62    NG2R61    CG2R62          7.0000       2       180.0000
CG331     CG314     CG331     HGA3            0.1950       3         0.0000
NG2R61    CG314     CG331     HGA3            0.2000       3         0.0000
HGA1      CG314     CG331     HGA3            0.1950       3         0.0000
CG331     CG314     NG2R61    CG2R62          4.9841       2         0.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA1    0.00  -0.02829   1.33203  0.00   -0.02829   1.33203
HGA3    0.00  -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61   0.00  -0.02829   1.33203  0.00   -0.02829   1.33203
```

```
HGR63   0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG314   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61  0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312   0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Force field 3iPr-MQ

```
* Toppar 3iPr-MQ
*

READ RTF CARD
*============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using wB97xD
*============================================================
*
99

MASS     1  HGA1      1.008
MASS     2  HGA3      1.008
MASS     3  HGR61     1.008
MASS     4  HGR63     1.008
MASS     5  CG2R61   12.011
MASS     6  CG2R62   12.011
MASS     7  CG331    12.011
MASS     8  CG334    12.011
MASS     9  CG311    12.011
MASS    10  NG2R61   14.007
MASS    11  OG312    16.000

AUTO ANGLES DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State                3-isoproyl-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!                      HB2  HB3
!                        \ /
!                    HB1-CB1     HB4
!                          \     /
!                H2    HC1-CC--CB2-HB5
!                  \     /    \
!         HN3       C2---C3     HB6
!           \      //    \\
!       HN2-CN----N1(+)   C4--H4
!           /      \     /
!         HN1       C8A==C4A
!                   /     \
!             H8--C8       C5--H5
!                  \\     //
!                   C7---C6
!                  /      \
!                 H7       O6(-)
!
RESI LQS0  0.00000
GROUP
ATOM     CN  CG334    -0.1382
ATOM    HN1   HGA3     0.1109
ATOM    HN2   HGA3     0.1109
ATOM    HN3   HGA3     0.1109
ATOM     N1 NG2R61     0.0478
ATOM     C2 CG2R62    -0.0712
ATOM     H2  HGR63     0.1520
ATOM     C3 CG2R62     0.0130
ATOM     CC  CG311     0.2502
ATOM    HC1   HGA1     0.0027
ATOM    CB1  CG331    -0.2134
ATOM    HB1   HGA3     0.0472
ATOM    HB2   HGA3     0.0472
ATOM    HB3   HGA3     0.0472
ATOM    CB2  CG331    -0.2134
ATOM    HB4   HGA3     0.0472
ATOM    HB5   HGA3     0.0472
ATOM    HB6   HGA3     0.0472
ATOM     C4 CG2R62    -0.1758
ATOM     H4  HGR63     0.1785
ATOM    C4A CG2R62     0.1499
```

```
ATOM     C5 CG2R61    -0.5298
ATOM     H5  HGR61     0.1565
ATOM     C6 CG2R61     0.6584
ATOM     O6  OG312    -0.8280
ATOM     C7 CG2R61    -0.2524
ATOM     H7  HGR61     0.1241
ATOM     C8 CG2R61    -0.1732
ATOM     H8  HGR61     0.1520
ATOM    C8A CG2R62     0.0944
BOND     CN    HN1
BOND     CN    HN2
BOND     CN    HN3
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
BOND     CC    CB1
BOND     CC    CB2
BOND     CC    HC1
BOND     CB1   HB1
BOND     CB1   HB2
BOND     CB1   HB3
BOND     CB2   HB4
BOND     CB2   HB5
BOND     CB2   HB6
BOND     C3    CC
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited state               3-isoproyl-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI LQS1  0.00000
GROUP
ATOM     CN  CG334    -0.1544
ATOM    HN1   HGA3     0.0952
ATOM    HN2   HGA3     0.0952
ATOM    HN3   HGA3     0.0952
ATOM     N1 NG2R61     0.1406
ATOM     C2 CG2R62    -0.2628
ATOM     H2  HGR63     0.1521
ATOM     C3 CG2R62     0.1196
ATOM     CC  CG311     0.1460
ATOM    HC1   HGA1     0.0209
ATOM    CB1  CG331    -0.1585
ATOM    HB1   HGA3     0.0326
ATOM    HB2   HGA3     0.0326
ATOM    HB3   HGA3     0.0326
ATOM    CB2  CG331    -0.1585
ATOM    HB4   HGA3     0.0326
ATOM    HB5   HGA3     0.0326
ATOM    HB6   HGA3     0.0326
ATOM     C4 CG2R62    -0.3578
ATOM     H4  HGR63     0.1713
ATOM    C4A CG2R62     0.1617
ATOM     C5 CG2R61    -0.2694
ATOM     H5  HGR61     0.1342
ATOM     C6 CG2R61     0.6366
```

```
ATOM      O6  OG312     -0.6454
ATOM      C7 CG2R61     -0.3423
ATOM      H7  HGR61      0.1254
ATOM      C8 CG2R61     -0.1735
ATOM      H8  HGR61      0.1687
ATOM     C8A CG2R62      0.0643
BOND      CN     HN1
BOND      CN     HN2
BOND      CN     HN3
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
BOND      CC     CB1
BOND      CC     CB2
BOND      CC     HC1
BOND      CB1   HB1
BOND      CB1   HB2
BOND      CB1   HB3
BOND      CB2   HB4
BOND      CB2   HB5
BOND      CB2   HB6
BOND      C3     CC
PATCHING FIRST NONE LAST NONE

END


READ PARA CARD
*=================================================================
*.   P A R A M E T E R
*=================================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       ID  NAME      MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS     1  HGA1      1.008
MASS     2  HGA3      1.008
MASS     3  HGR61     1.008
MASS     4  HGR63     1.008
MASS     5  CG2R61   12.011
MASS     6  CG2R62   12.011
MASS     7  CG331    12.011
MASS     8  CG334    12.011
MASS     9  CG311    12.011
MASS    10  NG2R61   14.007
MASS    11  OG312    16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2    k [kcal/mol Angstroem^2]      r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
```

```
CG334     HGA3              322.0000              1.08428
CG334     NG2R61            400.0000              1.47636
CG2R61    HGR61             340.0000              1.08074
CG2R61    OG312             525.0000              1.24310
CG2R61    CG2R61            305.0000              1.42010
CG2R61    CG2R62            305.0000              1.40123
CG2R62    HGR63             350.0000              1.07940
CG2R62    CG2R62            420.0000              1.40974
CG2R62    NG2R61            302.0000              1.35950
CG311     CG331             222.50                1.53741
CG311     HGA1              309.00                1.09350
CG331     HGA3              322.00                1.09077
CG2R62    CG311             230.00                1.52130

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000             119.101
CG2R61    CG2R61    CG2R62          40.0000             121.714
CG2R61    CG2R61    HGR61           30.0000             117.983
CG2R61    CG2R61    OG312           40.0000             122.942
CG2R61    CG2R62    CG2R62          40.0000             120.307
CG2R61    CG2R62    NG2R61          85.0000             123.357
CG2R62    CG2R61    HGR61           30.0000             120.942
CG2R62    CG2R62    CG2R62          40.0000             119.311
CG2R62    CG2R62    HGR63           80.0000             120.408
CG2R62    CG2R62    NG2R61          85.0000             119.765
CG2R62    NG2R61    CG2R62          30.0000             122.538
CG2R62    NG2R61    CG334           45.0000             118.731
HGA3      CG334     HGA3            35.5000             109.195
HGA3      CG334     NG2R61          33.4300             109.746
HGR63     CG2R62    NG2R61          80.0000             116.218
CG2R62    CG2R62    CG311           40.00               121.079
CG2R62    CG311     CG331           51.80               111.779
CG2R62    CG311     HGA1            43.00               106.902
CG331     CG311     CG331           53.35               111.216
CG331     CG311     HGA1            34.50               107.437
CG311     CG331     HGA3            33.43               111.004
HGA3      CG331     HGA3            35.50               107.896

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61    CG2R61          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    HGR61           4.2000       2       180.0000
CG2R61    CG2R61    CG2R61    OG312           3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R61          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R62          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    HGR63           1.0000       2       180.0000
CG2R61    CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG2R62          4.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG334          11.0000       2       180.0000
CG2R62    CG2R61    CG2R61    HGR61           4.2000       2       180.0000
CG2R62    CG2R61    CG2R61    OG312           3.1000       2       180.0000
CG2R62    CG2R62    CG2R61    HGR61           4.2000       2       180.0000
CG2R62    CG2R62    CG2R62    CG2R62          6.0000       2       180.0000
CG2R62    CG2R62    CG2R62    HGR63           1.0000       2       180.0000
CG2R62    CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R62    CG2R62    NG2R61    CG334          11.0000       2       180.0000
CG2R62    NG2R61    CG2R62    CG2R62          4.0000       2       180.0000
```

```
CG2R62     NG2R61     CG334      HGA3          0.0000       3         0.0000
CG334      NG2R61     CG2R62     HGR63         1.0000       2       180.0000
HGR61      CG2R61     CG2R61     HGR61         2.4000       2       180.0000
HGR61      CG2R61     CG2R61     OG312         2.4000       2       180.0000
HGR61      CG2R61     CG2R62     NG2R61        3.4000       2       180.0000
CG2R62     CG2R62     CG2R62     CG311         3.1000       2       180.0000
CG311      CG2R62     CG2R62     NG2R61        4.0000       2       180.0000
CG311      CG2R62     CG2R62     HGR63         4.0000       2       180.0000
CG2R62     CG2R62     CG311      CG331         0.2300       2       180.0000
CG2R62     CG2R62     CG311      HGA1          0.1000       6       180.0000
CG2R62     CG311      CG331      HGA3          0.0400       3         0.0000
CG331      CG311      CG331      HGA3          0.1950       3         0.0000
HGA1       CG311      CG331      HGA3          0.1950       3         0.0000
HGR63      G2R62      NG2R61     CG2R62        7.0000       2       180.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1           epsilon    rmin/2       epsilon14   rmin14/2
!            [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA1     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGA3     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG334    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG311    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61   0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312    0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Force field 3Am-MQ

```
* Toppar 3Am-1MQ
*

READ RTF CARD
*============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using wB97xD
*============================================================
*
99

MASS     1  HGA3      1.008
MASS     2  HGR61     1.008
MASS     3  HGR63     1.008
MASS     4  CG2R61   12.011
MASS     5  CG2R62   12.011
MASS     6  CG331    12.011
MASS     7  CG334    12.011
MASS     8  NG2R61   14.007
MASS     9  NG301    14.007
MASS    10  OG312    16.000

AUTO ANGLES DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State           3-dimethylamino-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!                      HB2  HB3
!                        \ /
!                    HB1-CB1     HB4
!                          \     /
!                H2         NC--CB2-HB5
!                  \      /    \
!         HN3       C2---C3     HB6
!           \      //    \\
!       HN2-CN----N1(+)   C4--H4
!           /       \     /
!         HN1       C8A==C4A
!                   /     \
!             H8--C8        C5--H5
!                  \\      //
!                   C7---C6
!                  /       \
!                 H7        O6(-)
!
RESI AQS0  0.00000
GROUP
ATOM      CN  CG334     -0.0835
ATOM     HN1   HGA3      0.0960
ATOM     HN2   HGA3      0.0960
ATOM     HN3   HGA3      0.0960
ATOM      N1 NG2R61      0.0834
ATOM      C2 CG2R62     -0.2270
ATOM      H2  HGR63      0.2165
ATOM      C3 CG2R62      0.3818
ATOM      NC  NG301     -0.4396
ATOM     CB1  CG331      0.0001
ATOM     HB1   HGA3      0.0574
ATOM     HB2   HGA3      0.0574
ATOM     HB3   HGA3      0.0574
ATOM     CB2  CG331      0.0001
ATOM     HB4   HGA3      0.0574
ATOM     HB5   HGA3      0.0574
ATOM     HB6   HGA3      0.0574
ATOM      C4 CG2R62     -0.2717
ATOM      H4  HGR63      0.1926
ATOM     C4A CG2R62      0.1540
ATOM      C5 CG2R61     -0.5286
ATOM      H5  HGR61      0.1539
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ATOM     C6 CG2R61     0.6728
ATOM     O6  OG312    -0.8351
ATOM     C7 CG2R61    -0.2698
ATOM     H7  HGR61     0.1249
ATOM     C8 CG2R61    -0.1760
ATOM     H8  HGR61     0.1551
ATOM    C8A CG2R62     0.0637
BOND     CN    HN1
BOND     CN    HN2
BOND     CN    HN3
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     NC
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
BOND     NC    CB1
BOND     NC    CB2
BOND     CB1   HB1
BOND     CB1   HB2
BOND     CB1   HB3
BOND     CB2   HB4
BOND     CB2   HB5
BOND     CB2   HB6
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited State          3-dimethylamino-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI AQS1  0.00000
GROUP
ATOM     CN  CG334    -0.0868
ATOM    HN1   HGA3     0.0758
ATOM    HN2   HGA3     0.0758
ATOM    HN3   HGA3     0.0758
ATOM     N1 NG2R61     0.1653
ATOM     C2 CG2R62    -0.4591
ATOM     H2  HGR63     0.2295
ATOM     C3 CG2R62     0.4863
ATOM     NC  NG301    -0.4924
ATOM    CB1  CG331     0.0305
ATOM    HB1   HGA3     0.0460
ATOM    HB2   HGA3     0.0460
ATOM    HB3   HGA3     0.0460
ATOM    CB2  CG331     0.0305
ATOM    HB4   HGA3     0.0460
ATOM    HB5   HGA3     0.0460
ATOM    HB6   HGA3     0.0460
ATOM     C4 CG2R62    -0.4161
ATOM     H4  HGR63     0.1777
ATOM    C4A CG2R62     0.1605
ATOM     C5 CG2R61    -0.2619
ATOM     H5  HGR61     0.1351
ATOM     C6 CG2R61     0.6533
ATOM     O6  OG312    -0.6627
ATOM     C7 CG2R61    -0.3574
ATOM     H7  HGR61     0.1295
ATOM     C8 CG2R61    -0.1819
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ATOM      H8  HGR61      0.1721
ATOM     C8A CG2R62      0.0446
BOND      CN     HN1
BOND      CN     HN2
BOND      CN     HN3
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      NC
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
BOND      NC     CB1
BOND      NC     CB2
BOND      CB1    HB1
BOND      CB1    HB2
BOND      CB1    HB3
BOND      CB2    HB4
BOND      CB2    HB5
BOND      CB2    HB6
PATCHING FIRST NONE LAST NONE

END


READ PARA CARD
*================================================================
*.   P A R A M E T E R
*================================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS    1  HGA3      1.008
MASS    2  HGR61     1.008
MASS    3  HGR63     1.008
MASS    4  CG2R61   12.011
MASS    5  CG2R62   12.011
MASS    6  CG331    12.011
MASS    7  CG334    12.011
MASS    8  NG2R61   14.007
MASS    9  NG301    14.007
MASS   10  OG312    16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG334     HGA3             322.0000              1.08428
CG334     NG2R61           400.0000              1.47636
CG2R61    HGR61            340.0000              1.08074
CG2R61    OG312            525.0000              1.24310
CG2R61    CG2R61           305.0000              1.42010
CG2R61    CG2R62           305.0000              1.40123
```

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CG2R62    HGR63             350.0000              1.07940
CG2R62    CG2R62            420.0000              1.40974
CG2R62    NG2R61            302.0000              1.35950
CG331     NG301             255.00                1.45869
CG331     HGA3              322.00                1.09174
CG2R62    NG301             330.00                1.40866

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000             119.101
CG2R61    CG2R61    CG2R62          40.0000             121.714
CG2R61    CG2R61    HGR61           30.0000             117.983
CG2R61    CG2R61    OG312           40.0000             122.942
CG2R61    CG2R62    CG2R62          40.0000             120.307
CG2R61    CG2R62    NG2R61          85.0000             123.357
CG2R62    CG2R61    HGR61           30.0000             120.942
CG2R62    CG2R62    CG2R62          40.0000             119.311
CG2R62    CG2R62    HGR63           80.0000             120.408
CG2R62    CG2R62    NG2R61          85.0000             119.765
CG2R62    NG2R61    CG2R62          30.0000             122.538
CG2R62    NG2R61    CG334           45.0000             118.731
HGA3      CG334     HGA3            35.5000             109.195
HGA3      CG334     NG2R61          33.4300             109.746
HGR63     CG2R62    NG2R61          80.0000             116.218
NG301     CG331     HGA3            30.50               110.725
HGA3      CG331     HGA3            35.50               108.177
CG2R62    CG2R62    NG301           40.00               121.136
CG2R62    NG301     CG331           55.00               114.652
CG331     NG301     CG331           53.00               112.339

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61    CG2R61         3.1000      2       180.0000
CG2R61    CG2R61    CG2R61    CG2R62         3.1000      2       180.0000
CG2R61    CG2R61    CG2R61    HGR61          4.2000      2       180.0000
CG2R61    CG2R61    CG2R61    OG312          3.1000      2       180.0000
CG2R61    CG2R61    CG2R62    CG2R62         3.1000      2       180.0000
CG2R61    CG2R61    CG2R62    NG2R61         7.0000      2       180.0000
CG2R61    CG2R62    CG2R62    CG2R61         6.0000      2       180.0000
CG2R61    CG2R62    CG2R62    CG2R62         6.0000      2       180.0000
CG2R61    CG2R62    CG2R62    HGR63          1.0000      2       180.0000
CG2R61    CG2R62    CG2R62    NG2R61         7.0000      2       180.0000
CG2R61    CG2R62    NG2R61    CG2R62         4.0000      2       180.0000
CG2R61    CG2R62    NG2R61    CG334         11.0000      2       180.0000
CG2R62    CG2R61    CG2R61    HGR61          4.2000      2       180.0000
CG2R62    CG2R61    CG2R61    OG312          3.1000      2       180.0000
CG2R62    CG2R62    CG2R61    HGR61          4.2000      2       180.0000
CG2R62    CG2R62    CG2R62    CG2R62         6.0000      2       180.0000
CG2R62    CG2R62    CG2R62    HGR63          1.0000      2       180.0000
CG2R62    CG2R62    CG2R62    NG2R61         7.0000      2       180.0000
CG2R62    CG2R62    NG2R61    CG334         11.0000      2       180.0000
CG2R62    NG2R61    CG2R62    CG2R62         4.0000      2       180.0000
CG2R62    NG2R61    CG334     HGA3           0.0000      3         0.0000
CG334     NG2R61    CG2R62    HGR63          1.0000      2       180.0000
HGR61     CG2R61    CG2R61    HGR61          2.4000      2       180.0000
HGR61     CG2R61    CG2R61    OG312          2.4000      2       180.0000
HGR61     CG2R61    CG2R62    NG2R61         3.4000      2       180.0000
HGA3      CG331     NG301     CG331          0.5848      1       180.0000
HGA3      CG331     NG301     CG331          0.6608      3       180.0000
HGA3      CG331     NG301     CG2R62         0.0000      3       180.0000
CG2R62    CG2R62    NG301     CG331          0.3000      4         0.0000
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CG2R62     CG2R62     NG301      CG331          1.2000       2       180.0000
NG301      CG2R62     CG2R62     HGR63          2.4000       2       180.0000
NG2R61     CG2R62     CG2R62     NG301          4.0000       2       180.0000
CG2R62     CG2R62     CG2R62     NG301          3.1000       2       180.0000
HGR63      CG2R62     NG2R61     CG2R62         7.0000       2       180.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA3     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG334    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61   0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
NG301    0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312    0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
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Force field 3tBu-MQ

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* Toppar 3tBu-MQ
*

READ RTF CARD
*============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using PBE0
*============================================================
*
99

MASS     1  HGA1      1.008
MASS     2  HGA3      1.008
MASS     3  HGR61     1.008
MASS     4  HGR63     1.008
MASS     5  CG2R61   12.011
MASS     6  CG2R62   12.011
MASS     7  CG331    12.011
MASS     8  CG334    12.011
MASS     9  CG301    12.011
MASS    10  NG2R61   14.007
MASS    11  OG312    16.000

AUTO ANGLES DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State               3-tertbutyl-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!                 HB2   HB3  HB4 HB5
!                     \ /     | /
!                 HB1--CB1   CB2-HB6 HB7
!                        \  /       /
!               H2        CC------CB3--HB8
!                 \      /          \
!        HA1       C2---C3           HB0
!          \      //    \\
!     HA2--CN----N1(+)   C4--H4
!          /       \     /
!       HA3         C8A==C4A
!                   /     \
!            H8--C8        C5--H5
!                 \\      //
!                  C7---C6
!                 /       \
!                H7        O6(-)
!
RESI BQS0  0.00000
GROUP
ATOM     CN  CG334     -0.1425
ATOM    HN1   HGA3      0.1113
ATOM    HN2   HGA3      0.1113
ATOM    HN3   HGA3      0.1113
ATOM     N1 NG2R61      0.0188
ATOM     C2 CG2R62     -0.0634
ATOM     H2  HGR63      0.1781
ATOM     C3 CG2R62     -0.0740
ATOM     CC  CG301      0.4995
ATOM    CB1  CG331     -0.3048
ATOM    HB1   HGA3      0.0646
ATOM    HB2   HGA3      0.0646
ATOM    HB3   HGA3      0.0646
ATOM    CB2  CG331     -0.3048
ATOM    HB4   HGA3      0.0646
ATOM    HB5   HGA3      0.0646
ATOM    HB6   HGA3      0.0646
ATOM    CB3   CG331    -0.3048
ATOM    HB7   HGA3      0.0646
ATOM    HB8   HGA3      0.0646
ATOM    HB9   HGA3      0.0646
```

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ATOM     C4 CG2R62    -0.1508
ATOM     H4  HGR63     0.1491
ATOM    C4A CG2R62     0.1466
ATOM     C5 CG2R61    -0.5264
ATOM     H5  HGR61     0.1656
ATOM     C6 CG2R61     0.6507
ATOM     O6  OG312    -0.8104
ATOM     C7 CG2R61    -0.2553
ATOM     H7  HGR61     0.1271
ATOM     C8 CG2R61    -0.1924
ATOM     H8  HGR61     0.1573
ATOM    C8A CG2R62     0.1215
BOND     CN    HN1
BOND     CN    HN2
BOND     CN    HN3
BOND     CN     N1
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
BOND     CC    CB1
BOND     CC    CB2
BOND     CC    CB3
BOND     CB1   HB1
BOND     CB1   HB2
BOND     CB1   HB3
BOND     CB2   HB4
BOND     CB2   HB5
BOND     CB2   HB6
BOND     C3    CC
BOND     CB3   HB7
BOND     CB3   HB8
BOND     CB3   HB9
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited State              3-tertbutyl-1-methyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI BQS1  0.00000
GROUP
ATOM     CN  CG334    -0.1398
ATOM    HN1   HGA3     0.0897
ATOM    HN2   HGA3     0.0897
ATOM    HN3   HGA3     0.0897
ATOM     N1 NG2R61     0.1041
ATOM     C2 CG2R62    -0.2425
ATOM     H2  HGR63     0.1913
ATOM     C3 CG2R62     0.0381
ATOM     CC  CG301     0.4695
ATOM    CB1  CG331    -0.2957
ATOM    HB1   HGA3     0.0593
ATOM    HB2   HGA3     0.0593
ATOM    HB3   HGA3     0.0593
ATOM    CB2  CG331    -0.2957
ATOM    HB4   HGA3     0.0593
ATOM    HB5   HGA3     0.0593
ATOM    HB6   HGA3     0.0593
ATOM    CB3   CG331   -0.2957
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```
ATOM     HB7    HGA3      0.0593
ATOM     HB8    HGA3      0.0593
ATOM     HB9    HGA3      0.0593
ATOM      C4  CG2R62     -0.3360
ATOM      H4   HGR63      0.1368
ATOM     C4A  CG2R62      0.1870
ATOM      C5  CG2R61     -0.2665
ATOM      H5   HGR61      0.1429
ATOM      C6  CG2R61      0.6251
ATOM      O6   OG312     -0.6400
ATOM      C7  CG2R61     -0.3629
ATOM      H7   HGR61      0.1314
ATOM      C8  CG2R61     -0.1666
ATOM      H8   HGR61      0.1672
ATOM     C8A  CG2R62      0.0452
BOND      CN     HN1
BOND      CN     HN2
BOND      CN     HN3
BOND      CN      N1
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
BOND      CC     CB1
BOND      CC     CB2
BOND      CC     CB3
BOND     CB1    HB1
BOND     CB1    HB2
BOND     CB1    HB3
BOND     CB2    HB4
BOND     CB2    HB5
BOND     CB2    HB6
BOND      C3     CC
BOND     CB3    HB7
BOND     CB3    HB8
BOND     CB3    HB9
PATCHING FIRST NONE LAST NONE

END

READ PARA CARD
*=============================================================
*.   P A R A M E T E R
*=============================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       ID  NAME      MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS     1  HGA1      1.008
MASS     2  HGA3      1.008
MASS     3  HGR61     1.008
MASS     4  HGR63     1.008
MASS     5  CG2R61   12.011
MASS     6  CG2R62   12.011
MASS     7  CG331    12.011
MASS     8  CG334    12.011
```

```
MASS    9  CG301   12.011
MASS   10  NG2R61  14.007
MASS   11  OG312   16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG334     HGA3              322.0000               1.08428
CG334     NG2R61            400.0000               1.47636
CG2R61    HGR61             340.0000               1.08074
CG2R61    OG312             525.0000               1.24310
CG2R61    CG2R61            305.0000               1.42010
CG2R61    CG2R62            305.0000               1.40123
CG2R62    HGR63             350.0000               1.07940
CG2R62    CG2R62            420.0000               1.40974
CG2R62    NG2R61            302.0000               1.35950
CG301     CG331             222.5000               1.54245
CG331     HGA3              322.0000               1.09073
CG2R62    CG301             230.0000               1.53750

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000             119.101
CG2R61    CG2R61    CG2R62          40.0000             121.714
CG2R61    CG2R61    HGR61           30.0000             117.983
CG2R61    CG2R61    OG312           40.0000             122.942
CG2R61    CG2R62    CG2R62          40.0000             120.307
CG2R61    CG2R62    NG2R61          85.0000             123.357
CG2R62    CG2R61    HGR61           30.0000             120.942
CG2R62    CG2R62    CG2R62          40.0000             119.311
CG2R62    CG2R62    HGR63           80.0000             120.408
CG2R62    CG2R62    NG2R61          85.0000             119.765
CG2R62    NG2R61    CG2R62          30.0000             122.538
CG2R62    NG2R61    CG334           45.0000             118.731
HGA3      CG334     HGA3            35.5000             109.195
HGA3      CG334     NG2R61          33.4300             109.746
HGR63     CG2R62    NG2R61          80.0000             116.218
CG2R62    CG2R62    CG301           40.0000             121.448
CG2R62    CG301     CG331           51.8000             109.887
CG331     CG301     CG331           58.3500             108.647
CG301     CG331     HGA3            33.4300             111.059
HGA3      CG331     HGA3            35.5000             107.833

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61    CG2R61          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R61    HGR61           4.2000       2       180.0000
CG2R61    CG2R61    CG2R61    OG312           3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    CG2R62          3.1000       2       180.0000
CG2R61    CG2R61    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R61          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    CG2R62          6.0000       2       180.0000
CG2R61    CG2R62    CG2R62    HGR63           1.0000       2       180.0000
CG2R61    CG2R62    CG2R62    NG2R61          7.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG2R62          4.0000       2       180.0000
CG2R61    CG2R62    NG2R61    CG334          11.0000       2       180.0000
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CG2R62    CG2R61    CG2R61    HGR61         4.2000      2      180.0000
CG2R62    CG2R61    CG2R61    OG312         3.1000      2      180.0000
CG2R62    CG2R62    CG2R61    HGR61         4.2000      2      180.0000
CG2R62    CG2R62    CG2R62    CG2R62        6.0000      2      180.0000
CG2R62    CG2R62    CG2R62    HGR63         1.0000      2      180.0000
CG2R62    CG2R62    CG2R62    NG2R61        7.0000      2      180.0000
CG2R62    CG2R62    NG2R61    CG334        11.0000      2      180.0000
CG2R62    NG2R61    CG2R62    CG2R62        4.0000      2      180.0000
CG2R62    NG2R61    CG334     HGA3          0.0000      3        0.0000
CG334     NG2R61    CG2R62    HGR63         1.0000      2      180.0000
HGR61     CG2R61    CG2R61    HGR61         2.4000      2      180.0000
HGR61     CG2R61    CG2R61    OG312         2.4000      2      180.0000
HGR61     CG2R61    CG2R62    NG2R61        3.4000      2      180.0000
CG2R62    CG2R62    CG2R62    CG301         3.1000      2      180.0000
CG301     CG2R62    CG2R62    NG2R61        4.0000      2      180.0000
CG301     CG2R62    CG2R62    HGR63         4.0000      2      180.0000
CG2R62    CG2R62    CG301     CG331         0.2300      2      180.0000
CG2R62    CG301     CG331     HGA3          0.0400      3        0.0000
CG331     CG301     CG331     HGA3          0.1600      3        0.0000
HGR63     CG2R62    NG2R61    CG2R62        7.0000      2      180.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA1    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGA3    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61   0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63   0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62  0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG334   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG311   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG301   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61  0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312   0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Force field 3tBu-tBuQ

```
* Toppar 3tBu-tBuQ
*

READ RTF CARD
*=============================================================
*.   T O P O L O G Y   O F   Q U I N O L O N E S
*.
*. Partial charge distribution using PBE0
*=============================================================
*
99

MASS    1  HGA3     1.008
MASS    2  HGR61    1.008
MASS    3  HGR63    1.008
MASS    4  CG2R61  12.011
MASS    5  CG2R62  12.011
MASS    6  CG331   12.011
MASS    7  CG301   12.011
MASS    8  NG2R61  14.007
MASS    9  OG312   16.000

AUTO ANGLES DIHE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Ground State            3-tertbutyl-1-tertbutyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
!                     HB2   HB3  HB4 HB5
!                         \ /     | /
!                     HB1--CB1   CB2-HB6 HB7
!                            \  /       /
!          HA5       H2        CC------CB3--HB8
!            \         \      /          \
! HA7   HA4-CA2-HA6  C2---C3           HB0
!    \          \     //    \\
!HA8--CA3-----CN----N1(+)   C4--H4
!    /         /      \     /
! HA9   HA2-CA1-HA3  C8A==C4A
!           /         /     \
!         HA1  H8--C8        C5--H5
!                    \\     //
!                     C7---C6
!                    /      \
!                   H7       O6(-)
!
RESI BBS0  0.00000
GROUP
ATOM CN     CG301   0.4523
ATOM CA1    CG331  -0.2962
ATOM HA1    HGA3    0.0815
ATOM HA2    HGA3    0.0815
ATOM HA3    HGA3    0.0815
ATOM CA2    CG331  -0.2962
ATOM HA4    HGA3    0.0815
ATOM HA5    HGA3    0.0815
ATOM HA6    HGA3    0.0815
ATOM CA3    CG331  -0.2962
ATOM HA7    HGA3    0.0815
ATOM HA8    HGA3    0.0815
ATOM HA9    HGA3    0.0815
ATOM N1     NG2R61 -0.1291
ATOM C2     CG2R62  0.0288
ATOM H2     HGR63   0.1376
ATOM C3     CG2R62 -0.0897
ATOM CC     CG301   0.4704
ATOM CB1    CG331  -0.3053
ATOM HB1    HGA3    0.0675
ATOM HB2    HGA3    0.0675
ATOM HB3    HGA3    0.0675
```

```
ATOM CB2    CG331  -0.3053
ATOM HB4    HGA3    0.0675
ATOM HB5    HGA3    0.0675
ATOM HB6    HGA3    0.0675
ATOM CB3    CG331  -0.3053
ATOM HB7    HGA3    0.0675
ATOM HB8    HGA3    0.0675
ATOM HB9    HGA3    0.0675
ATOM C4     CG2R62 -0.1349
ATOM H4     HGR63   0.1458
ATOM C4A    CG2R62  0.1769
ATOM C5     CG2R61 -0.5572
ATOM H5     HGR61   0.1632
ATOM C6     CG2R61  0.6802
ATOM O6     OG312  -0.8380
ATOM C7     CG2R61 -0.2911
ATOM H7     HGR61   0.1227
ATOM C8     CG2R61 -0.1551
ATOM H8     HGR61   0.1902
ATOM C8A    CG2R62  0.0905
BOND     N1    CN
BOND     CN    CA1
BOND     CN    CA2
BOND     CN    CA3
BOND     CA1   HA1
BOND     CA1   HA2
BOND     CA1   HA3
BOND     CA2   HA4
BOND     CA2   HA5
BOND     CA2   HA5
BOND     CA3   HA7
BOND     CA3   HA8
BOND     CA3   HA9
BOND     N1     C2
BOND     N1    C8A
BOND     C2     H2
BOND     C2     C3
BOND     C3     C4
BOND     C4     H4
BOND     C4    C4A
BOND    C4A     C5
BOND    C4A    C8A
BOND     C5     H5
BOND     C5     C6
BOND     C6     O6
BOND     C6     C7
BOND     C7     H7
BOND     C7     C8
BOND     C8     H8
BOND     C8    C8A
BOND     CC    CB1
BOND     CC    CB2
BOND     CC    CB3
BOND     CB1   HB1
BOND     CB1   HB2
BOND     CB1   HB3
BOND     CB2   HB4
BOND     CB2   HB5
BOND     CB2   HB6
BOND     C3    CC
BOND     CB3   HB7
BOND     CB3   HB8
BOND     CB3   HB9
PATCHING FIRST NONE LAST NONE

!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
! Excited State           3-tertbutyl-1-tertbutyl-6-quinolone
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
RESI BBS1  0.00000
GROUP
ATOM CN     CG301   0.4002
```

```
ATOM CA1     CG331   -0.2848
ATOM HA1     HGA3     0.0736
ATOM HA2     HGA3     0.0736
ATOM HA3     HGA3     0.0736
ATOM CA2     CG331   -0.2848
ATOM HA4     HGA3     0.0736
ATOM HA5     HGA3     0.0736
ATOM HA6     HGA3     0.0736
ATOM CA3     CG331   -0.2848
ATOM HA7     HGA3     0.0736
ATOM HA8     HGA3     0.0736
ATOM HA8     HGA3     0.0736
ATOM N1      NG2R61  -0.0030
ATOM C2      CG2R62  -0.1950
ATOM H2      HGR63    0.1569
ATOM C3      CG2R62   0.0144
ATOM CC      CG301    0.4474
ATOM CB1     CG331   -0.2968
ATOM HB1     HGA3     0.0615
ATOM HB2     HGA3     0.0615
ATOM HB3     HGA3     0.0615
ATOM CB2     CG331   -0.2968
ATOM HB4     HGA3     0.0615
ATOM HB5     HGA3     0.0615
ATOM HB6     HGA3     0.0615
ATOM CB3     CG331   -0.2968
ATOM HB7     HGA3     0.0615
ATOM HB8     HGA3     0.0615
ATOM HB9     HGA3     0.0615
ATOM C4      CG2R62  -0.3340
ATOM H4      HGR63    0.1330
ATOM C4A     CG2R62   0.2051
ATOM C5      CG2R61  -0.3169
ATOM H5      HGR61    0.1459
ATOM C6      CG2R61   0.6671
ATOM O6      OG312   -0.6527
ATOM C7      CG2R61  -0.3871
ATOM H7      HGR61    0.1256
ATOM C8      CG2R61  -0.1402
ATOM H8      HGR61    0.2100
ATOM C8A     CG2R62   0.0522
BOND      N1     CN
BOND      CN     CA1
BOND      CN     CA2
BOND      CN     CA3
BOND      CA1    HA1
BOND      CA1    HA2
BOND      CA1    HA3
BOND      CA2    HA4
BOND      CA2    HA5
BOND      CA2    HA5
BOND      CA3    HA7
BOND      CA3    HA8
BOND      CA3    HA9
BOND      N1      C2
BOND      N1     C8A
BOND      C2      H2
BOND      C2      C3
BOND      C3      C4
BOND      C4      H4
BOND      C4     C4A
BOND     C4A      C5
BOND     C4A     C8A
BOND      C5      H5
BOND      C5      C6
BOND      C6      O6
BOND      C6      C7
BOND      C7      H7
BOND      C7      C8
BOND      C8      H8
BOND      C8     C8A
```

```
BOND      CC    CB1
BOND      CC    CB2
BOND      CC    CB3
BOND      CB1   HB1
BOND      CB1   HB2
BOND      CB1   HB3
BOND      CB2   HB4
BOND      CB2   HB5
BOND      CB2   HB6
BOND      C3    CC
BOND      CB3   HB7
BOND      CB3   HB8
BOND      CB3   HB9
PATCHING FIRST NONE LAST NONE

END

READ PARA CARD
*==============================================================
*.   P A R A M E T E R
*==============================================================
*

ATOMS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!       ID  NAME     MASS
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
MASS     1  HGA3      1.008
MASS     2  HGR61     1.008
MASS     3  HGR63     1.008
MASS     4  CG2R61   12.011
MASS     5  CG2R62   12.011
MASS     6  CG331    12.011
MASS     7  CG301    12.011
MASS     8  NG2R61   14.007
MASS     9  OG312    16.000

BONDS
!
! U_bond = k ( r - r0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2    k [kcal/mol Angstroem^2]     r0 [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    HGR61             340.0000               1.07930
CG2R61    OG312             525.0000               1.24515
CG2R61    CG2R61            305.0000               1.41484
CG2R61    CG2R62            305.0000               1.40382
CG2R62    HGR63             350.0000               1.07417
CG2R62    CG2R62            420.0000               1.41104
CG2R62    NG2R61            302.0000               1.36557
CG301     CG331             222.5000               1.54107
CG331     HGA3              322.0000               1.08904
CG2R62    CG301             230.0000               1.53687
CG301     NG2R61            400.0000               1.54051

ANGLES
!
! U_angle = k ( theta - theta0 )^2
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1    TYPE2     TYPE3     k [kcal/mol rad^2]     theta0 [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61    CG2R61    CG2R61          40.0000             118.871
CG2R61    CG2R61    CG2R62          40.0000             122.278
CG2R61    CG2R61    HGR61           30.0000             117.684
CG2R61    CG2R61    OG312           40.0000             123.269
CG2R61    CG2R62    CG2R62          40.0000             119.520
CG2R61    CG2R62    NG2R61          85.0000             125.030
CG2R62    CG2R61    HGR61           30.0000             120.216
CG2R62    CG2R62    CG2R62          40.0000             119.028
```

```
CG2R62     CG2R62     HGR63           80.0000            119.186
CG2R62     CG2R62     NG2R61          85.0000            121.195
CG2R62     NG2R61     CG2R62          30.0000            120.528
HGR63      CG2R62     NG2R61          80.0000            116.447
CG2R62     CG2R62     CG301           40.0000            121.467
CG2R62     CG301      CG331           51.8000            110.310
CG331      CG301      CG331           58.3500            108.753
CG301      CG331      HGA3            33.4300            111.000
HGA3       CG331      HGA3            35.5000            107.880
CG2R62     NG2R61     CG301           70.0000            119.736
CG331      CG301      NG2R61          70.0000            110.060

DIHEDRALS
!
! U_dihedral = k ( 1 + Cos[n phi - delta] )
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1     TYPE2      TYPE3      TYPE4     k [kcal/mol]     n      delta [deg]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
CG2R61     CG2R61     CG2R61     CG2R61         3.1000       2       180.0000
CG2R61     CG2R61     CG2R61     CG2R62         3.1000       2       180.0000
CG2R61     CG2R61     CG2R61     HGR61          4.2000       2       180.0000
CG2R61     CG2R61     CG2R61     OG312          3.1000       2       180.0000
CG2R61     CG2R61     CG2R62     CG2R62         3.1000       2       180.0000
CG2R61     CG2R61     CG2R62     NG2R61         7.0000       2       180.0000
CG2R61     CG2R62     CG2R62     CG2R61         6.0000       2       180.0000
CG2R61     CG2R62     CG2R62     CG2R62         6.0000       2       180.0000
CG2R61     CG2R62     CG2R62     HGR63          1.0000       2       180.0000
CG2R61     CG2R62     CG2R62     NG2R61         7.0000       2       180.0000
CG2R61     CG2R62     NG2R61     CG2R62         4.0000       2       180.0000
CG2R62     CG2R61     CG2R61     HGR61          4.2000       2       180.0000
CG2R62     CG2R61     CG2R61     OG312          3.1000       2       180.0000
CG2R62     CG2R62     CG2R61     HGR61          4.2000       2       180.0000
CG2R62     CG2R62     CG2R62     CG2R62         6.0000       2       180.0000
CG2R62     CG2R62     CG2R62     HGR63          1.0000       2       180.0000
CG2R62     CG2R62     CG2R62     NG2R61         7.0000       2       180.0000
CG2R62     NG2R61     CG2R62     CG2R62         4.0000       2       180.0000
HGR61      CG2R61     CG2R61     HGR61          2.4000       2       180.0000
HGR61      CG2R61     CG2R61     OG312          2.4000       2       180.0000
HGR61      CG2R61     CG2R62     NG2R61         3.4000       2       180.0000
CG2R62     CG2R62     CG2R62     CG301          3.1000       2       180.0000
CG301      CG2R62     CG2R62     NG2R61         4.0000       2       180.0000
CG301      CG2R62     CG2R62     HGR63          4.0000       2       180.0000
CG2R62     CG2R62     CG301      CG331          0.2300       2       180.0000
CG2R62     CG301      CG331      HGA3           0.0400       3         0.0000
CG331      CG301      CG331      HGA3           0.1600       3         0.0000
HGR63      CG2R62     NG2R61     CG2R62         7.0000       2       180.0000
NG2R61     CG301      CG331      HGA3           0.2000       3         0.0000
CG2R61     CG2R62     NG2R61     CG301         11.0000       2       180.0000
CG2R62     CG2R62     NG2R61     CG301         11.0000       2       180.0000
HGR63      CG2R62     NG2R61     CG301          0.3000       2       180.0000
CG331      CG301      NG2R61     CG2R62         1.8000       1         0.0000

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 0.5 wmin 1.5
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!TYPE1          epsilon    rmin/2       epsilon14   rmin14/2
!           [kcal/mol] [Angstroem]    [kcal/mol] [Angstroem]
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
HGA3     0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR61    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
HGR63    0.00   -0.02829   1.33203  0.00   -0.02829   1.33203
CG2R61   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG2R62   0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG331    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
CG301    0.00   -0.06630   2.00987  0.00   -0.06630   2.00987
NG2R61   0.00   -0.10465   1.87514  0.00   -0.10465   1.87514
OG312    0.00   -0.30571   1.54903  0.00   -0.30571   1.54903

END
RETURN
```

Appendix B

Geometry MQ

CN	2.453080	0.000000	4.254897
HN1	2.227729	0.000000	5.314507
HN2	3.025203	0.889939	4.007828
HN3	3.025203	-0.889939	4.007828
N1	1.193172	0.000000	3.503663
C2	0.049483	0.000000	4.176774
H2	0.119204	0.000000	5.252383
C3	-1.173003	0.000000	3.515834
H3	-2.079712	0.000000	4.099804
C4	-1.197665	0.000000	2.149961
H4	-2.142155	0.000000	1.622457
C4A	0.002691	0.000000	1.403449
C5	0.015012	0.000000	0.006777
H5	-0.931618	0.000000	-0.519076
C6	1.210883	0.000000	-0.741190
O6	1.263841	0.000000	-2.004712
C7	2.425559	0.000000	0.054681
H7	3.364285	0.000000	-0.485697
C8	2.440438	0.000000	1.414005
H8	3.387904	0.000000	1.930841
C8A	1.225477	0.000000	2.132251

Geometry EQ

CN	16.072167	1.052947	9.548346
HN1	15.841381	2.036039	9.954767
HN2	16.389221	0.422115	10.377208
CA1	17.200213	1.170647	8.536649
HA1	18.058731	1.599821	9.052898
HA2	17.508596	0.204484	8.139370
HA3	16.952079	1.833861	7.709047
N1	14.788830	0.485701	9.042994
C2	14.680266	0.112498	7.755078
H2	15.543635	0.241222	7.130307
C3	13.487197	-0.417760	7.265808
H3	13.439545	-0.707837	6.226851
C4	12.408103	-0.561259	8.098577
H4	11.480047	-0.972526	7.724598
C4A	12.478794	-0.178326	9.466647
C5	11.409796	-0.308303	10.338274
H5	10.476507	-0.717702	9.975250
C6	11.479417	0.075652	11.717506
O6	10.545240	-0.025698	12.532591
C7	12.779317	0.618793	12.123163
H7	12.865135	0.920896	13.159001
C8	13.846549	0.754201	11.284447
H8	14.764400	1.165849	11.674412
C8A	13.742497	0.364349	9.926242

Geometry iPrQ

CN	16.199660	0.832120	9.659165
HN1	16.791754	0.789706	8.748727
CA1	16.226468	2.293122	10.116537
HA1	17.266601	2.606040	10.211386
HA2	15.748043	2.934855	9.377352
HA3	15.740677	2.458849	11.073384
CA2	16.840395	-0.165019	10.629091
HA4	17.891182	0.100052	10.749306
HA5	16.383151	-0.172584	11.613491
HA6	16.794076	-1.176259	10.224863
N1	14.836337	0.393869	9.188161
C2	14.750766	0.102939	7.872980
H2	15.652984	0.212013	7.295920
C3	13.553858	-0.318282	7.299287
H3	13.535248	-0.539430	6.242526

C4	12.435347	-0.445846	8.079460
H4	11.499778	-0.773744	7.646870
C4A	12.473502	-0.153281	9.470635
C5	11.356717	-0.274657	10.281312
H5	10.422353	-0.604656	9.846769
C6	11.373642	0.020346	11.682619
O6	10.394102	-0.073660	12.443506
C7	12.678521	0.462887	12.181216
H7	12.729127	0.698680	13.236533
C8	13.790917	0.588859	11.404827
H8	14.702326	0.925898	11.865381
C8A	13.747275	0.287563	10.019701

Geometry 3iPr-MQ

CN	16.255566	0.192522	9.931840
HN1	16.406278	1.199768	10.313597
HN2	16.352189	-0.520687	10.747139
HN3	17.004377	-0.020871	9.177398
N1	14.922839	0.080259	9.318851
C2	14.855660	-0.229526	8.007806
H2	15.797161	-0.376842	7.504578
C3	13.630641	-0.353076	7.346999
CC	13.619058	-0.707510	5.867648
HC1	14.662255	-0.818655	5.559152
CB1	13.005038	0.415958	5.016199
HB1	13.067585	0.167613	3.955419
HB2	11.952119	0.565849	5.259835
HB3	13.521797	1.363017	5.174597
CB2	12.915814	-2.049608	5.608476
HB4	12.973798	-2.312797	4.551258
HB5	13.371406	-2.854829	6.185085
HB6	11.860718	-1.999371	5.880534
C4	12.481998	-0.145526	8.077605
H4	11.513553	-0.232886	7.601828
C4A	12.505768	0.184974	9.461014
C5	11.359124	0.398054	10.209579
H5	10.390171	0.314173	9.735448
C6	11.392347	0.729370	11.603969
O6	10.388638	0.929852	12.311105
C7	12.742353	0.822987	12.173103
H7	12.797317	1.072342	13.224851
C8	13.884640	0.618118	11.458359
H8	14.841444	0.706755	11.951340
C8A	13.809132	0.293685	10.081145

Geometry 3Am-MQ

CN	16.132627	0.771352	9.687569
HN1	16.088156	1.796837	10.046326
HN2	16.453247	0.119570	10.496737
HN3	16.841476	0.707319	8.869731
N1	14.807580	0.352116	9.201068
C2	14.707780	-0.010631	7.909621
H2	15.620135	-0.002741	7.340693
C3	13.477733	-0.425427	7.359610
NC	13.457538	-0.836795	6.012482
CB1	12.240703	-1.481401	5.542823
HB1	12.432207	-1.904709	4.558045
HB2	11.963264	-2.292693	6.213082
HB3	11.388999	-0.791995	5.455815
CB2	14.010587	0.091690	5.027187
HB4	14.164183	-0.437110	4.087380
HB5	13.342510	0.943939	4.841281
HB6	14.972200	0.480168	5.349494
C4	12.382606	-0.465607	8.198110
H4	11.418207	-0.772236	7.822638
C4A	12.466086	-0.108314	9.575134
C5	11.377423	-0.142556	10.430091
H5	10.416542	-0.471791	10.057517

C6	11.457244	0.247016	11.808040
O6	10.501742	0.229512	12.604766
C7	12.788387	0.689072	12.242679
H7	12.874965	0.991950	13.277892
C8	13.873763	0.728620	11.422485
H8	14.822391	1.065237	11.814024
C8A	13.752155	0.332558	10.065485

Geometry 3tBu-MQ

CN	2.473333	0.004499	4.233460
HN1	3.053035	-0.884092	3.995215
HN2	3.052487	0.890357	3.983540
HN3	2.244139	0.012538	5.293238
N1	1.211176	-0.001079	3.476214
C2	0.059280	-0.008336	4.173035
H2	0.165860	-0.011409	5.243921
C3	-1.191729	-0.010401	3.536583
CC	-2.463280	-0.030698	4.400673
CB1	-2.473237	1.193069	5.342943
HB1	-3.379078	1.190785	5.951687
HB2	-1.621920	1.194095	6.024573
HB3	-2.449220	2.123580	4.774754
CB2	-2.492642	-1.327490	5.240328
HB4	-3.398536	-1.363009	5.847746
HB5	-2.479982	-2.208886	4.597755
HB6	-1.640214	-1.394812	5.917393
CB3	-3.736747	0.016368	3.540184
HB7	-4.612023	0.008600	4.190073
HB8	-3.783144	0.921420	2.933492
HB9	-3.812161	-0.845401	2.876164
C4	-1.195069	-0.003239	2.160954
H4	-2.129397	-0.004468	1.619601
C4A	0.000000	0.000000	1.384928
C5	0.000000	0.000000	0.000000
H5	-0.941340	0.001134	-0.533236
C6	1.206248	-0.002643	-0.776683
O6	1.248478	-0.003550	-2.020015
C7	2.439705	-0.004501	0.018575
H7	3.365906	-0.008994	-0.541063
C8	2.463990	-0.000758	1.381310
H8	3.414389	-0.002563	1.894482
C8A	1.249023	0.000000	2.109923

Geometry 3tBu-tBuQ

CN	2.473333	0.004499	4.233460
HN1	3.053035	-0.884092	3.995215
HN2	3.052487	0.890357	3.983540
HN3	2.244139	0.012538	5.293238
N1	1.211176	-0.001079	3.476214
C2	0.059280	-0.008336	4.173035
H2	0.165860	-0.011409	5.243921
C3	-1.191729	-0.010401	3.536583
CC	-2.463280	-0.030698	4.400673
CB1	-2.473237	1.193069	5.342943
HB1	-3.379078	1.190785	5.951687
HB2	-1.621920	1.194095	6.024573
HB3	-2.449220	2.123580	4.774754
CB2	-2.492642	-1.327490	5.240328
HB4	-3.398536	-1.363009	5.847746
HB5	-2.479982	-2.208886	4.597755
HB6	-1.640214	-1.394812	5.917393
CB3	-3.736747	0.016368	3.540184
HB7	-4.612023	0.008600	4.190073
HB8	-3.783144	0.921420	2.933492
HB9	-3.812161	-0.845401	2.876164
C4	-1.195069	-0.003239	2.160954
H4	-2.129397	-0.004468	1.619601
C4A	0.000000	0.000000	1.384928

C5	0.000000	0.000000	0.000000
H5	-0.941340	0.001134	-0.533236
C6	1.206248	-0.002643	-0.776683
O6	1.248478	-0.003550	-2.020015
C7	2.439705	-0.004501	0.018575
H7	3.365906	-0.008994	-0.541063
C8	2.463990	-0.000758	1.381310
H8	3.414389	-0.002563	1.894482
C8A	1.249023	0.000000	2.109923