Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effective Computational Route to Vibrational Optical Activity Spectra of Chiral Molecules in Aqueous Solution

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S1 (L)-Methyl Lactate

S1.1 Force Field Parameters

Table S1: Methyl Lactate force field non bonded parameters.

atom index	atom	charge	σ (nm)	ϵ (kJ/mol)
1	CM	-0.242730	3.50000e-01	2.76144e-01
2	HM	0.098184	2.50000e-01	1.25520e-01
3	HM	0.096393	2.50000e-01	1.25520e-01
4	HM	0.100149	2.50000e-01	1.25520e-01
5	CT	0.012461	3.50000e-01	2.76144e-01
6	HT	0.121834	2.42000e-01	6.27600e-02
7	CO	0.286165	3.75000e-01	4.39320e-01
8	CS	-0.119458	3.50000e-01	2.76144e-01
9	HS	0.115533	2.42000e-01	6.27600e-02
10	HS	0.123079	2.42000e-01	6.27600e-02
11	HS	0.115729	2.42000e-01	6.27600e-02
12	OH	-0.471331	3.12000e-01	7.11280e-01
13	HO	0.317131	0.00000e+00	0.00000e+00
14	O	-0.348570	2.96000e-01	8.78640e-01
15	OS	-0.204570	3.00000e-01	7.11280e-01

Table S2: Methyl Lactate force field stetching parameters.

a_i	a_j	r_{eq} (nm)	k (kJ/mol)
7	14	1.2290e-01	4.7698e+05
7	15	1.3230e-01	3.7656e+05
7	5	1.5220e-01	2.6527e+05
15	8	1.4100e-01	2.6778e+05
6	5	1.0900e-01	2.8451e+05
5	1	1.5260e-01	2.5941e+05
5	12	1.4100e-01	2.6778e+05
1	4	1.0900e-01	2.8451e+05
1	3	1.0900e-01	2.8451e+05
1	2	1.0900e-01	2.8451e+05
12	13	9.6000e-02	4.6275e+05
8	9	1.0900e-01	2.8451e+05
8	10	1.0900e-01	2.8451e+05
8	11	1.0900e-01	2.8451e+05

Table S3: Methyl Lactate force field bending parameters.

a_i	a_j	a_k	r_{eq} (nm)	k (kJ/mol)
7	15	8	1.1700e+02	5.0208e+02
7	5	6	1.0950e+02	4.1840e+02
7	5	1	1.1110e+02	5.2718e+02
7	5	12	1.0870e+02	5.7446e+02
14	7	15	1.2500e+02	6.6944e+02
5	7	14	1.2040e+02	6.6944e+02
15	7	5	1.1500e+02	6.6944e+02
15	8	9	1.0950e+02	4.1840e+02
15	8	10	1.0950e+02	4.1840e+02
15	8	11	1.0950e+02	4.1840e+02
5	1	4	1.0950e+02	4.1840e+02
5	1	3	1.0950e+02	4.1840e+02
5	1	2	1.0950e+02	4.1840e+02
5	12	13	1.0850e+02	4.6024e+02
6	5	1	1.0950e+02	4.1840e+02
6	5	12	1.0950e+02	4.1840e+02
1	5	12	1.0950e+02	4.1840e+02
4	1	3	1.0950e+02	2.9288e+02
4	1	2	1.0950e+02	2.9288e+02
3	1	2	1.0950e+02	2.9288e+02
9	8	10	1.0950e+02	2.9288e+02
9	8	11	1.0950e+02	2.9288e+02
10	8	11	1.0950e+02	2.9288e+02

Table S4: Methyl Lactate force field dihedrals parameters.

a_i	a_j	a_k	a_l	r_{eq} (nm)	k (kJ/mol)	n
Improper						
7	5	14	15	0.0	647.193	
Proper						
12	5	7	14	180.00	2.020	1
12	5	7	14	180.00	3.776	2
12	5	7	14	180.00	1.067	3
14	7	15	8	180.00	11.500	1
14	7	15	8	180.00	20.026	2
2	1	5	12	15.00	6.252	3
9	8	15	7	0.00	2.187	3
6	5	12	13	300.00	5.324	1
6	5	12	13	60.00	1.580	2
6	5	12	13	180.00	-1.072	3

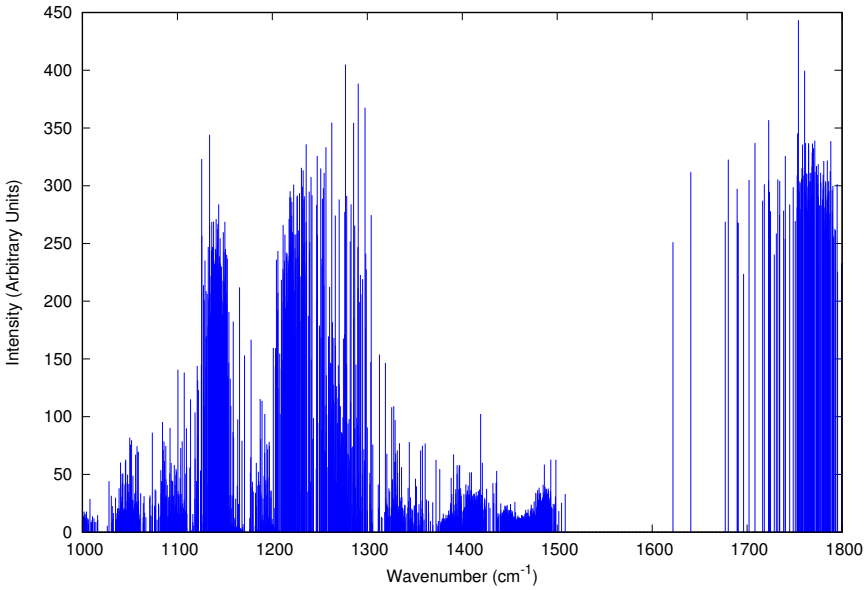

Figure S1: IR stick spectrum of ML in aqueous solution.

S1.2 Normal Modes (400 - 1800 cm^{-1})

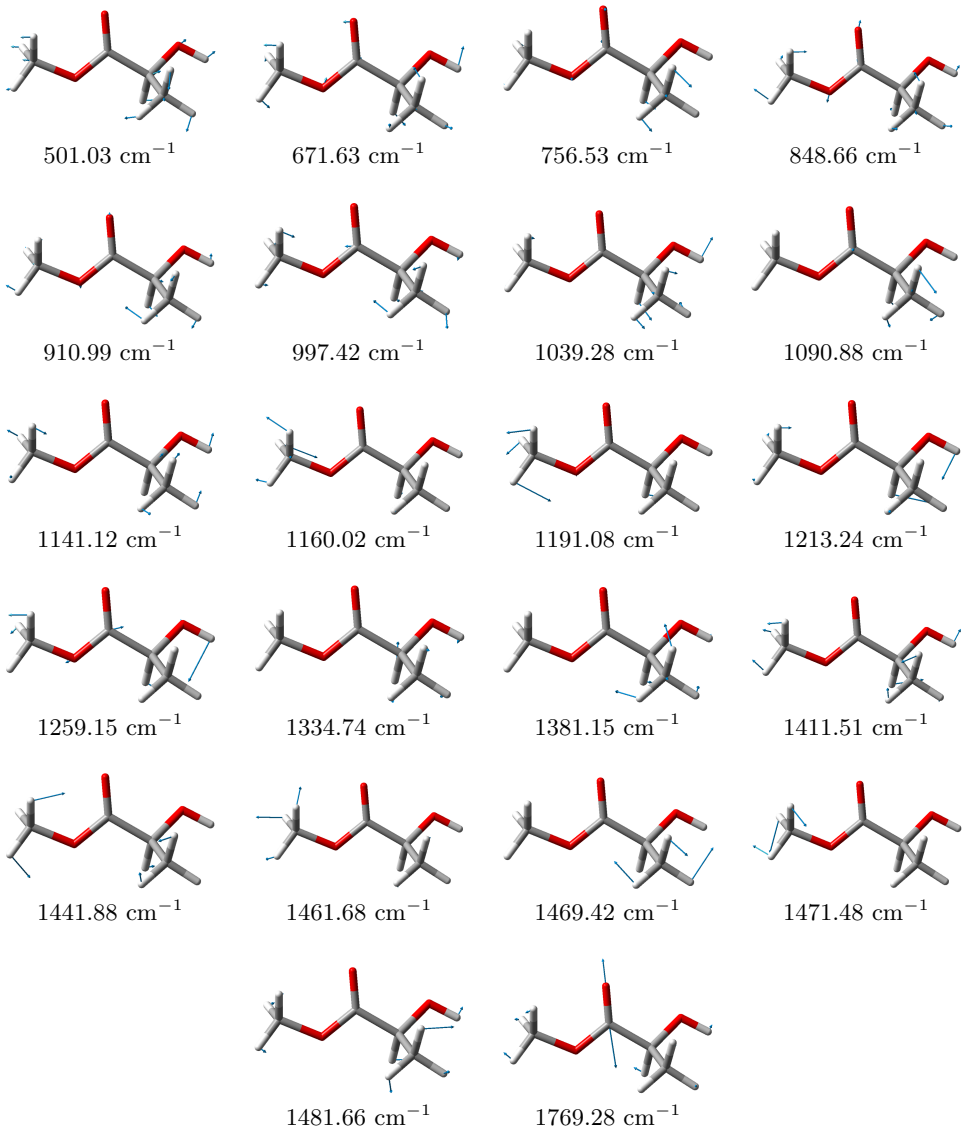

Figure S2: Normal modes of (L)-Methyl Lactate with QM/FQ model. The frequency of each mode is reported in parentheses. These modes are referred to one random snapshot (23)

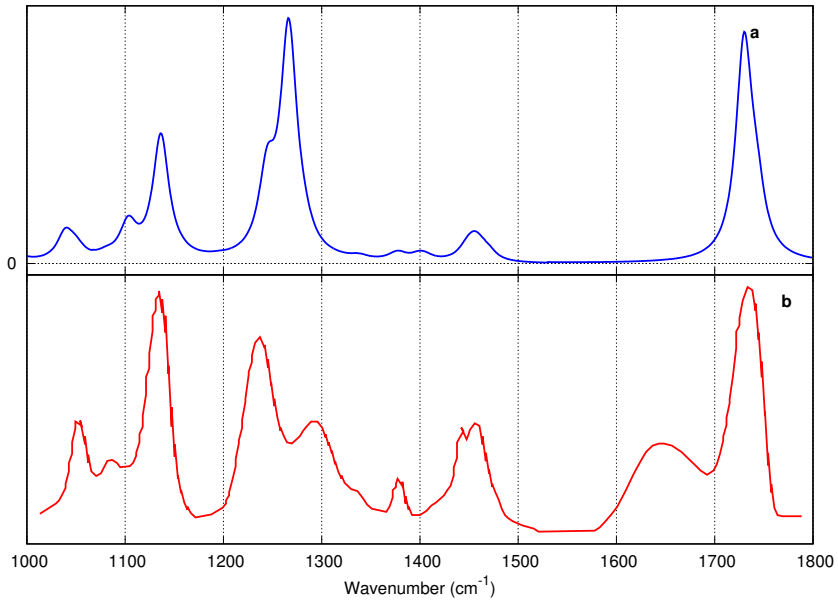

Figure S3: (**a**) QM/PCM IR spectrum of (L)-Methyl Lactate in aqueous solution. (**b**) Experimental spectrum taken from[1].

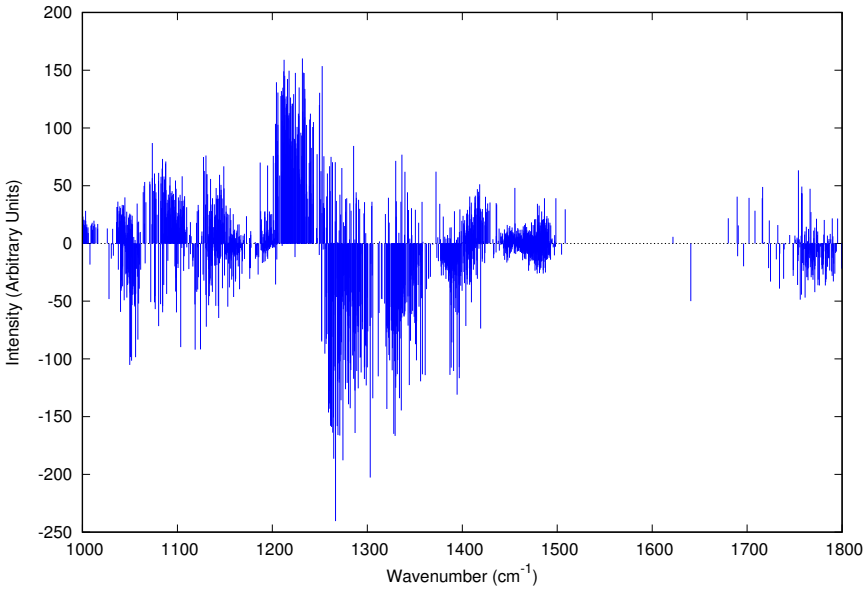

Figure S4: VCD stick spectrum of ML in aqueous solution.

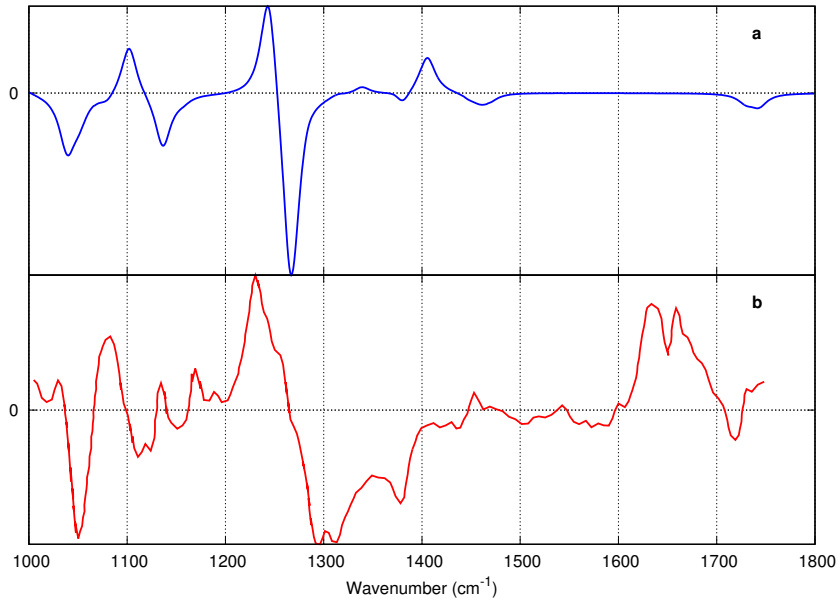

Figure S5: (**a**) QM/PCM VCD spectrum of (L)-Methyl Lactate in aqueous solution. (**b**) Experimental spectrum taken from[1].

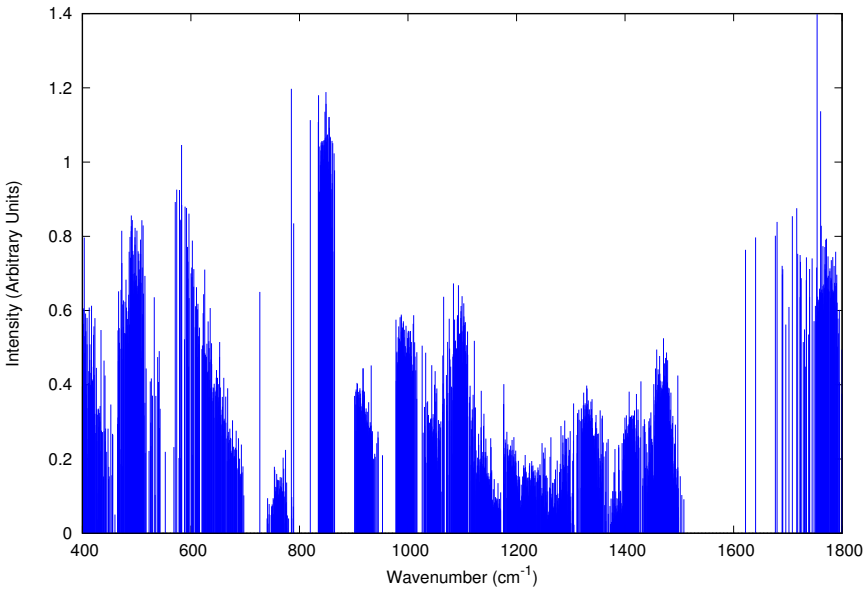

Figure S6: Raman stick spectrum of ML in aqueous solution. Excitation wavelength: 488 nm

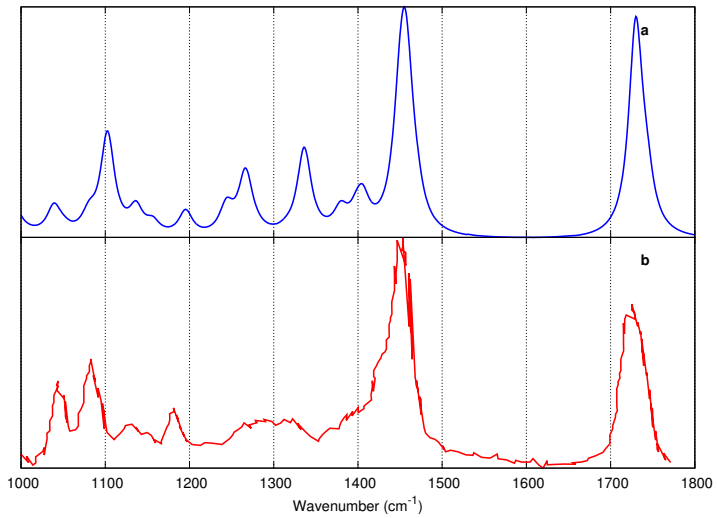

Figure S7: (**a**) QM/PCM Raman spectrum of (L)-Methyl Lactate in aqueous solution. (**b**) Experimental spectrum taken from[2]. Excitation wavelength: 488 nm

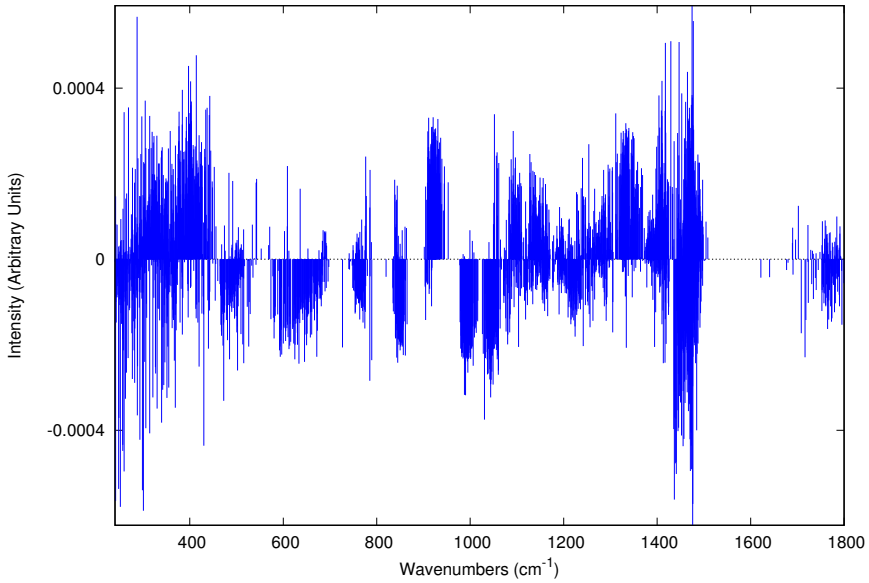

Figure S8: ROA stick spectrum of ML in aqueous solution. Excitation wavelength: 532 nm

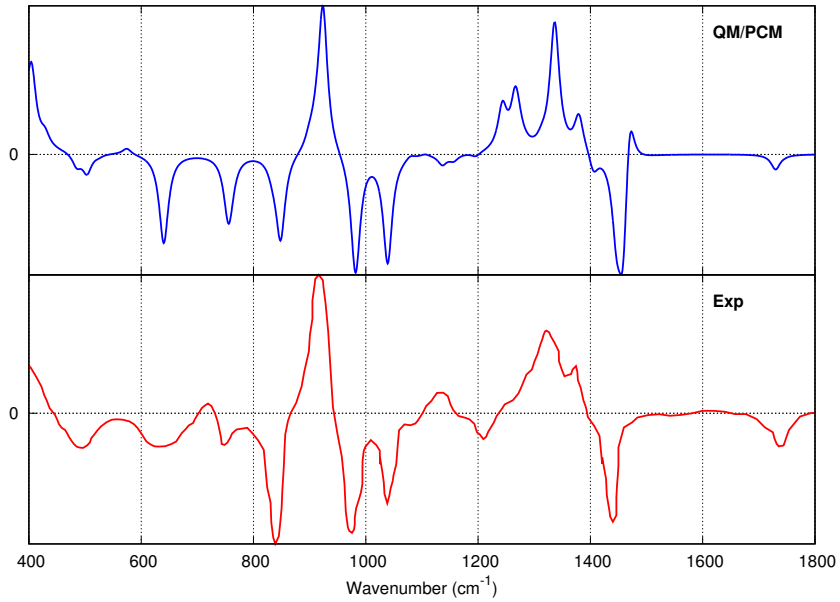

Figure S9: QM/PCM ROA spectrum of ML in aqueous solution. Excitation wavelength: 532 nm

S2 (S)-Glycidol

S2.1 Force Field Parameters

Table S5: Glycidol force field non bonded parameters.

atom index	atom	charge	σ (nm)	ϵ (kJ/mol)
1	CT	-0.157485	3.39967e-01	4.57730e-01
2	H1	0.154879	2.47135e-01	6.56888e-02
3	H1	0.157478	2.47135e-01	6.56888e-02
4	CT	-0.128325	3.39967e-01	4.57730e-01
5	H1	0.176500	2.47135e-01	6.56888e-02
6	OS	-0.314449	3.00001e-01	7.11280e-01
7	CT	0.255371	3.39967e-01	4.57730e-01
8	H1	0.035359	2.47135e-01	6.56888e-02
9	H1	0.072470	2.47135e-01	6.56888e-02
10	OH	-0.683740	3.06647e-01	8.80314e-01
11	HO	0.431942	0.00000e+00	0.00000e+00

Table S6: Glycidol force field stetching parameters.

a_i	a_j	r_{eq} (nm)	k (kJ/mol)
1	2	1.0900e-01	2.8451e+05
1	3	1.0900e-01	2.8451e+05
1	4	1.5260e-01	2.5941e+05
1	6	1.4100e-01	2.6778e+05
4	5	1.0900e-01	2.8451e+05
4	6	1.4100e-01	2.6778e+05
4	7	1.5260e-01	2.5941e+05
7	8	1.0900e-01	2.8451e+05
7	9	1.0900e-01	2.8451e+05
7	10	1.4100e-01	2.6778e+05
10	11	9.6000e-02	4.6275e+05

Table S7: Glycidol force field bending parameters.

a_i	a_j	a_k	r_{eq} (nm)	k (kJ/mol)
1	4	5	1.0950e+02	4.1840e+02
1	4	6	1.0950e+02	4.1840e+02
1	4	7	1.0950e+02	3.3472e+02
1	6	4	1.0950e+02	5.0208e+02
2	1	3	1.0950e+02	2.9288e+02
2	1	4	1.0950e+02	4.1840e+02
2	1	6	1.0950e+02	4.1840e+02
3	1	4	1.0950e+02	4.1840e+02
3	1	6	1.0950e+02	4.1840e+02
4	1	6	1.0950e+02	4.1840e+02
4	7	8	1.0950e+02	4.1840e+02
4	7	9	1.0950e+02	4.1840e+02
4	7	10	1.0950e+02	4.1840e+02
5	4	6	1.0950e+02	4.1840e+02
5	4	7	1.0950e+02	4.1840e+02
6	4	7	1.0950e+02	4.1840e+02
7	10	11	1.0850e+02	4.6024e+02
8	7	9	1.0950e+02	2.9288e+02
8	7	10	1.0950e+02	4.1840e+02
9	7	10	1.0950e+02	4.1840e+02

Table S8: Glycidol force field dihedrals parameters.

a_i	a_j	a_k	a_l	r_{eq} (nm)	k (kJ/mol)	n
1	6	4	5	0.00	1.60387	3
1	6	4	7	0.00	1.60247	3
1	6	4	7	180.00	0.41840	2
2	1	4	5	0.00	0.65084	3
2	1	4	6	0.00	0.00000	0
2	1	4	6	0.00	1.04600	1
2	1	4	7	0.00	0.65084	3
2	1	6	4	0.00	1.60387	3
3	1	4	5	0.00	0.65084	3
3	1	4	6	0.00	0.00000	0
3	1	4	6	0.00	1.04600	1
3	1	4	7	0.00	0.65084	3
3	1	6	4	0.00	1.60387	3
6	1	4	5	0.00	0.00000	0
6	1	4	5	0.00	1.04600	1
6	1	4	7	0.00	0.65084	3
4	7	10	11	0.00	0.66944	3
4	7	10	11	0.00	1.04600	1
8	7	10	11	0.00	0.69733	3
9	7	10	11	0.00	0.69733	3
6	4	7	10	101.25	1.873	1
6	4	7	10	22.51	2.225	2
6	4	7	10	303.76	4.989	3
6	4	7	10	225.02	-0.526	4

S2.2 Hydration Patter

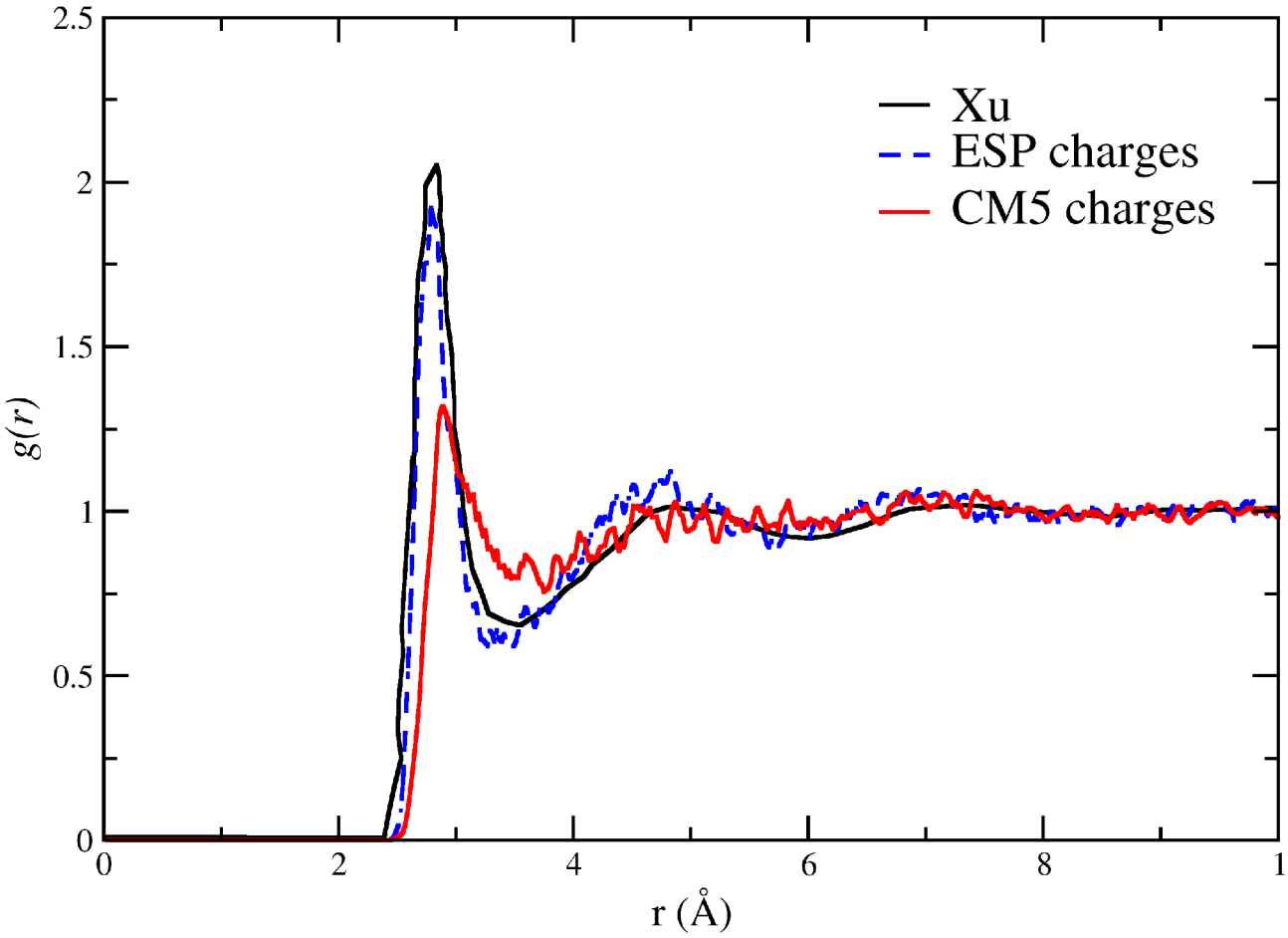

Figure S10: CM5, RESP $g(r)$ functions obtained from the 50 ns MD. Literature data are also reported.[3]

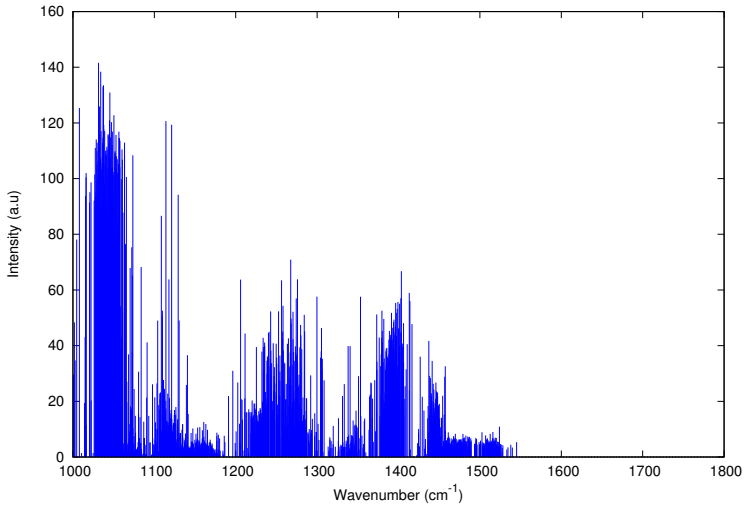

Figure S11: IR stick spectrum of GL in aqeuous solution

S2.3 Normal Modes (700 - 1800 cm^{-1})

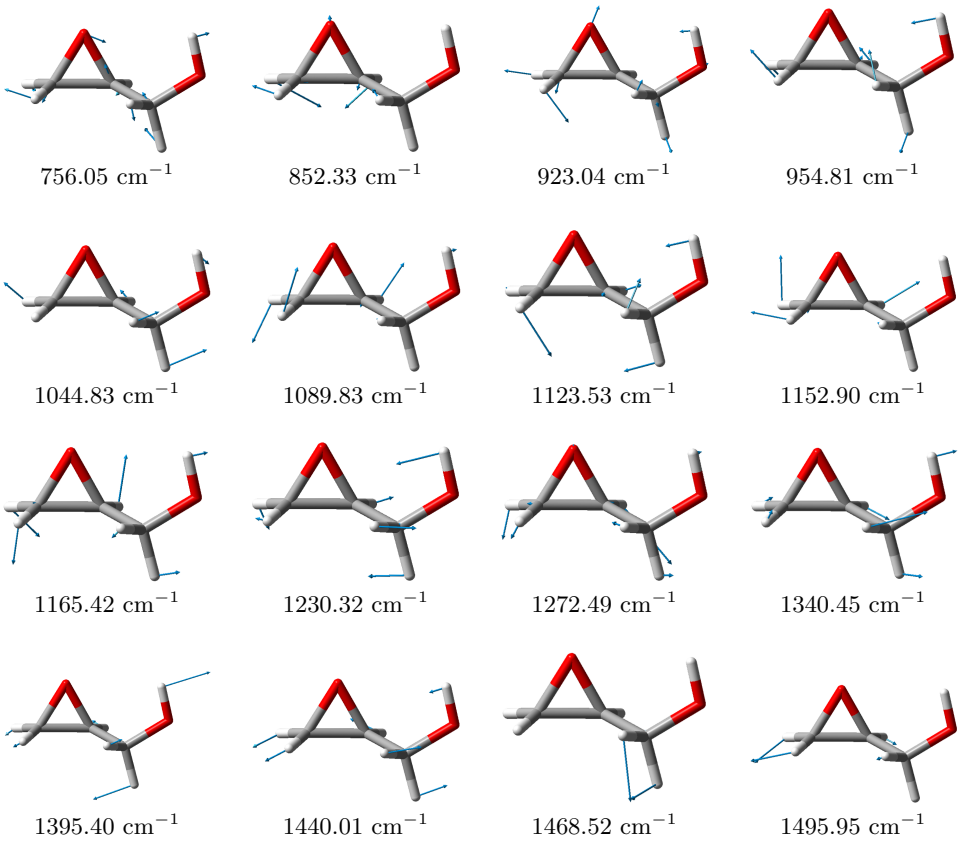

Figure S12: Normal modes of (S)-Glycidol with QM/FQ model. The frequency of each mode is reported in parentheses. These modes are referred to one random snapshot (137)

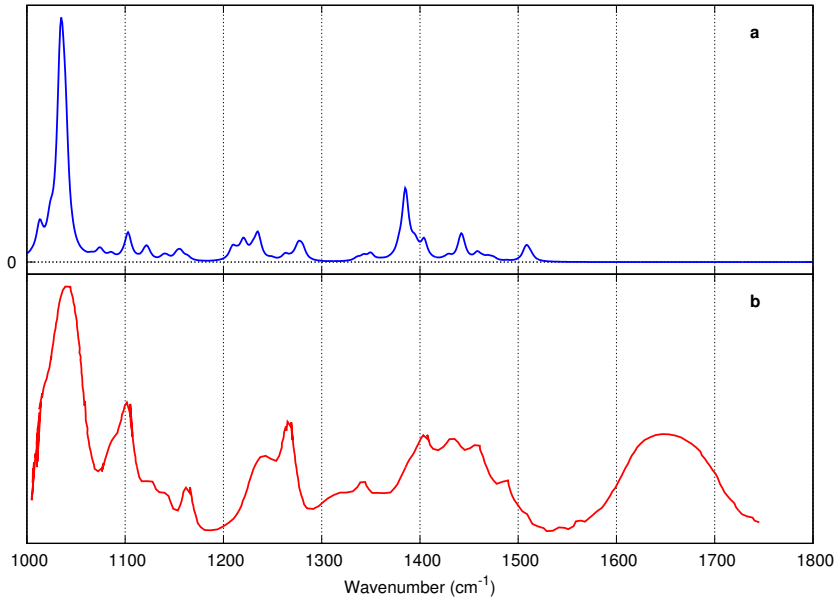

Figure S13: (**a**) QM/PCM IR spectrum of (S)-Glycidol in aqueous solution. (**b**) Experimental spectrum taken from[3].

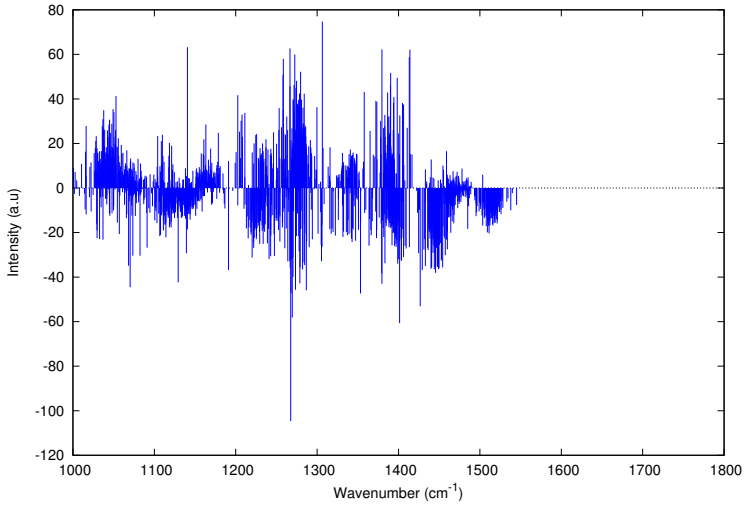

Figure S14: VCD stick spectrum of GL in aqueous solution

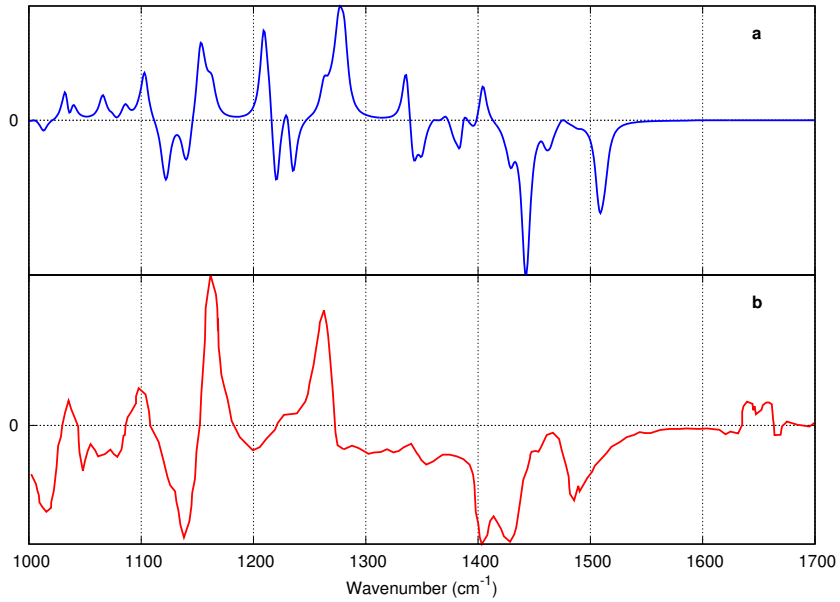

Figure S15: (**a**) QM/PCM VCD spectrum of (S)-Glycidol in aqueous solution. (**b**) Experimental spectrum taken from[3].

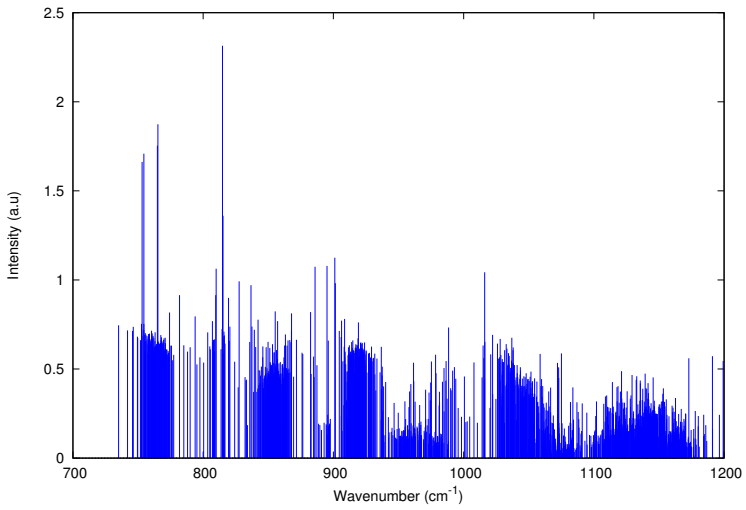

Figure S16: Stick Raman spectrum of GL in aqueous solution. Excitation energy: 1064 nm

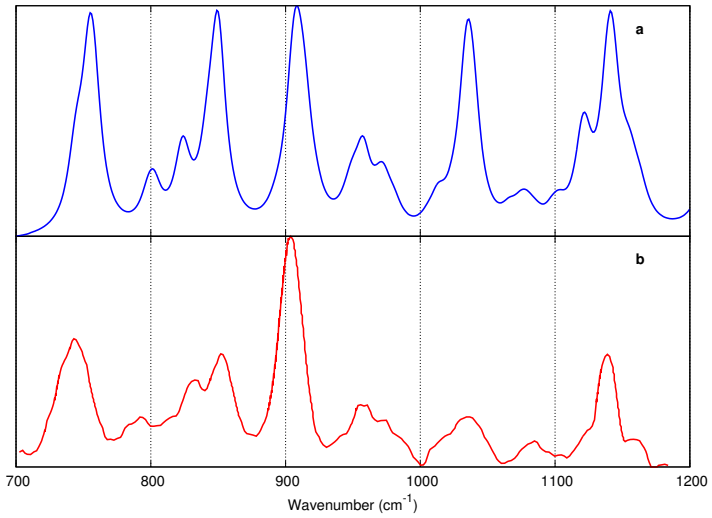

Figure S17: (**a**) QM/PCM Raman spectrum of (S)-Glycidol in aqueous solution. (**b**) Experimental spectrum taken from[4]. Excitation wavelength: 1064 nm

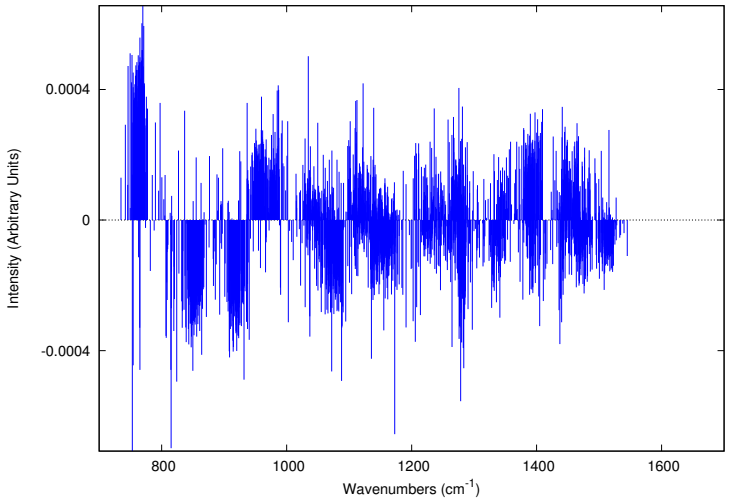

Figure S18: Stick ROA spectrum of GL in aqueous solution. Excitation energy: 514 nm

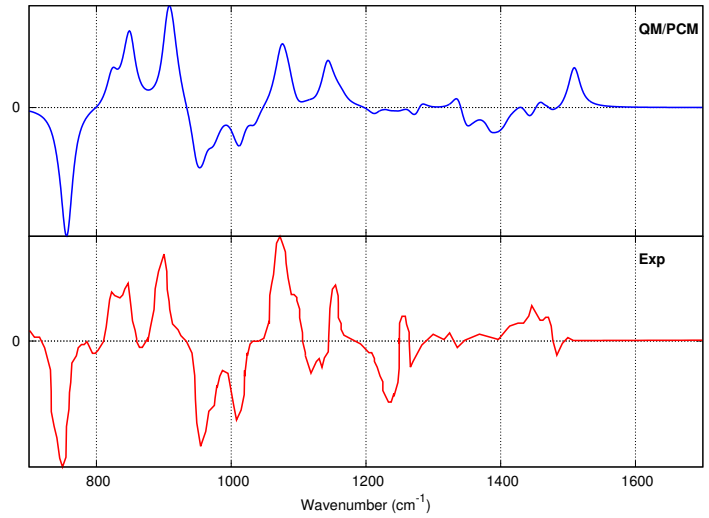

Figure S19: (**a**) QM/PCM ROA spectrum of (S)-Glycidol in aqueous solution. (**b**) Experimental spectrum taken from[4]. Excitation wavelength: 514 nm

References

(1) Losada, M.; Xu, Y. *Phys. Chem. Chem. Phys.* **2007**, *9*, 3127–3135.

(2) Cassanas, G.; Morssli, M.; Fabregue, E.; Bardet, L. *J. Raman Spectrosc.* **1991**, *22*, 409–413.

(3) Yang, G.; Xu, Y. *J. Chem. Phys.* **2009**, *130*, 164506–164506.

(4) Badawi, H. M.; Ali, S. A. *Spectrochim. Acta A* **2009**, *74*, 558–562.