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Data Article

Data for molecular dynamic simulations in the OPLSAA force field: Partial charges of cholesterol, C7-hydroxycholesterol and C7-hydroperoxycholesterol, torsional parameters for the hydroperoxy group of C7-hydroperoxycholesterol

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ABSTRACT

This data article contains partial charges generated for cholesterol, C7-hydroxycholesterol and C7-hydroperoxycholesterol and torsional parameters for hydroperoxy of C7-hydroperoxycholesterol for molecular dynamics simulations in the OPLSAA force field [1] using the package Gromacs [2]. The hydroperoxy group remained unparameterized in the OPLSAA force field and the parameters obtained have the potential for re-use in similar simulations. The atom-centred point charges on each sterol molecule were derived using the restrained electrostatic potential (RESP) approach [3]. The parameters for the C7-O_{ET}-O_H-H_O and C8-C7-O_{ET}-O_H torsion angles were derived by fitting the parameters of the torsional term (Ryckaert-Bellemans function) of the OPLSAA potential energy function to the

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quantum mechanical rotational energy profile calculated at CCSD(T)/cc-pVQZ level of theory. This article presents data used in the research article "Chirality affects cholesterol-oxysterol association in water, a computational study" [4].

Specifications Table

Subject	Chemistry
Specific subject area	Molecular dynamic simulations
Type of data	Table Figure
How data were acquired	Quantum energy calculations were carried out using package Gaussian 09
Data format	Text format, raw, analyzed
Parameters for data collection	Quantum mechanical calculations at B3LYP/6-31++G(d,p), MP2/cc-pVQZ and CCSD(T)/cc-pVQZ levels of theory
Description of data collection	Data were obtained as a result of quantum mechanical calculations
Data source location	Department of Computational Biophysics and Bioinformatics, Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Krakow, Poland
Data accessibility	Data are supplied with this article and 10.5281/zenodo.5549934
Related research article	M. Markiewicz, R. Szczelina, B. Milanovic, W.K. Subczynski, M. Pasenkiewicz-Gierula, Chirality affects cholesterol-oxysterol association in water, a computational study. Comput. Struct. Biotechnol. J. 19, 4319–4335, 2021.

Value of the Data

- Parameters for hydroperoxy group in OPLSAA force field [1] are provided
- The force field parameters could be used in simulations of hydroperoxides, e.g. cholesterol hydroperoxides, which are key factors in the development of atherosclerotic plaque.
- The parameters, which have been missing in the OPLSAA force field so far, obtained in this work can be used in molecular dynamics simulations of biomolecular systems containing hydroperoxides especially lipid bilayers and lipoproteins using the package Gromacs [2].

1. Data Description

1. Sterol partial charges
2. Torsional parameters for the hydroperoxy group of 7-OOH-Chol in the OPLSAA force field

2. Experimental Design, Materials and Methods

1. Sterol partial charges

The atom-centred point monopole charges on each sterol molecule were derived using multi-conformation and multi-orientation restrained electrostatic potential (RESP) fitting [3] through the following steps:

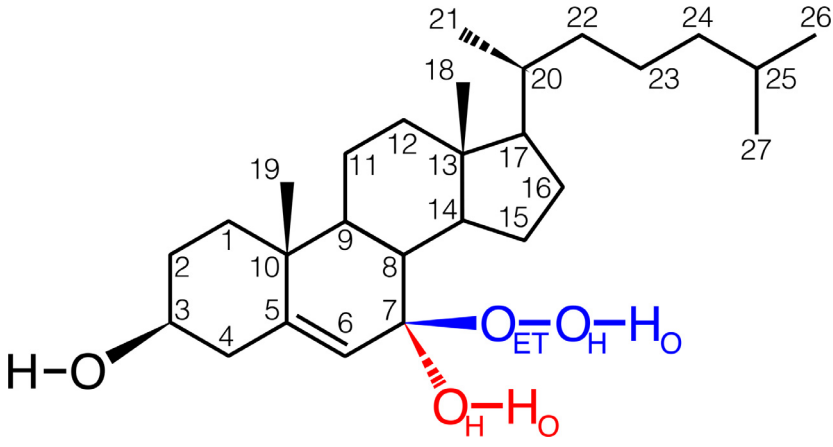

Fig. 1. Molecular structure of cholesterol (Chol, *black*), C7-hydroxycholesterol (*black* and *red*, 7-OH-Chol) and C7-hydroperoxycholesterol (*black* and *blue*, 7-OOH-Chol). The C7-OH group of 7β-OH-Chol is in *red*, and the C7-OOH group of 7α-OOH-Chol is in *blue*. The alpha stereoisomer has a substituent on the C7 atom which is oriented in the same direction as the OH group on the C3 atom, and that of the beta stereoisomer is oriented in the opposite direction. The Chol atoms are numbered according to the IUPAC convention [5]. The chemical symbol for carbon atoms, C, and the hydrogen atoms, H, are omitted except for the sterol polar groups, where the H atoms are explicitly included.

1a. For each sterol, 1000 conformations were generated by rotation around covalent bonds of the sterol hydrocarbon chain. From the generated conformations, 25 diverse conformations were selected on an RMSD basis (Fig. 2).

1b. The structures of the selected conformations were optimized at two levels of theory in QM calculations, first HF/6-31G* (Opt=Tight) and then B3LYP/6-31++G(d,p) (Opt=Tight, Int=UltraFine). All QM calculations were carried out using the package Gaussian 09 [6].

1c. For each of the optimized structures in four different orientations controlled by re-orientation algorithm incorporated into the R.E.D. program [7], the values of the electrostatic potential on a molecular surface were calculated at the HF/6-31G* level, in compliance with the OPLS force field. The partial charges were obtained by fitting the classical Coulomb electrostatic potential to the QM molecular electrostatic potential calculated at the grid points on the Connolly surface around the sterol molecule (A in Table 1) or using the CHELPG approach (B in Table 1) [8].

1d. For each sterol and the calculation method (A or B, above), the partial charges are averages over 100 sets of charges calculated for all optimized conformers in 4 different orientations (Table 1).

2. Torsional parameters for the hydroperoxy group of 7-OOH-Chol in the OPLSAA force field

2a. For the derived RESP charges and the optimized structure of the 7-OOH-Chol, torsions CT-OX-OH-HO (OPLS force field atom type names corresponding to C7-O_{ET}-O_H-H_O of the sterol, Fig. 1) and CT-CT-OX-OH (OPLSAA force field atom type names corresponding to C8-C7-O_{ET}-O_H of the sterol, Fig. 1) were rotated by increments of 10° about the O-O and the C-O bond, respectively; each rotation yielded 36 rotamers. The energy of each rotamer was calculated using methods at four levels of theory:

i. MP2/cc-pVDZ (marked below as MP2/SBS – small basis set)
ii. MP2/cc-pVQZ (marked below as MP2/LBS – large basis set)
iii. CCSD(T)/cc-pVDZ (marked below as CCSDT/SBS)
iv. CCSD(T)/cc-pVQZ (calculated using the HI-EM method [9] marked below as CCSDT/LBS)

2b. The parameters for the CT-OX-OH-HO and CT-CT-OX-OH torsion angles (Table 2) were obtained by fitting the parameters of the torsional term (Ryckaert-Bellemans function)

Table 1
Calculated partial atomic charges on sterol molecules. A and B refer to different ways of the grid calculations (cf. point 1c below). O_{ET} is the ether oxygen atom of the C7-OOH group, O_H is the hydroxy oxygen atom and H_O is the hydroxy hydrogen atom of the C7-OOH group; equivalent hydrogen atoms are omitted and the number assigned to the hydrogen atom corresponds to that assigned to the relevant carbon atom, e.g. H271 is bonded to C27; the numbers and names of atoms are such as in Fig. 1; colors of numbers in the Table correspond to the colors of groups in Fig. 1.

atom↓			7-Oxysterol				7-Peroxysterol			
Form →	Cholesterol		alpha		beta		alpha		beta	
Grid →	A	B	A	B	A	B	A	B	A	B
HO3	.4224	.4258	.4158	.4092	.4112	.4076	.417	.4134	.4082	.4048
O3	−.711	−.7652	−.7096	.7383	−.6979	−.7391	−.718	−.7486	−.6944	−.732
C3	.2925	.4437	.3343	.4613	.2995	.4726	.3534	.4977	.3125	.4631
H3	.0149	-.0678	.0779	.012	.0872	.0069	.0756	.0113	.0833	.0087
C5	−.086	−.1976	−.0651	−.0692	−.0653	−.0414	−.0596	−.0362	−.1008	−.1086
C6	−.2429	−.3258	−.2962	−.4758	−.3319	−.5432	−.2397	−.4303	−.1968	−.3956
H6	.1334	.144	.1677	.1785	.1745	.1904	.1458	.1589	.1576	.1796
C7	−.0674	.1576	.1049	.5223	.1788	.6475	.0469	.4743	.064	.4623
H71	.0493	−.0209	.1183	−.0026	.1129	−.0227	.1216	.0016	.0883	−.0404
C8	−.021	.063	−.039	−.0531	−.0185	−.0726	−.0349	−.116	.0121	.1258
H8	.0704	−.0402	.0634	−.0475	.0964	−.0082	.0735	−.0269	.1167	−.0202
C9	.0271	.009	.0138	.0052	.0133	−.0434	.0219	.067	.0253	−.112
H9	.0345	−.0508	.0499	−.0359	.0165	−.054	.0477	−.0484	.0177	−.0458
C10	.0706	.4919	.085	.3688	.061	.3346	.0821	.3339	.0712	.3596
C19	−.0833	−.2356	−.0862	−.1547	−.0509	−.1549	−.1269	−.2007	−.0508	−.0948
H191	.0263	.037	.0249	.0192	.0125	.0175	.0335	.0307	.0158	.0041
C1	−.0669	−.2698	−.0286	−.1164	−.0395	−.0938	−.0257	−.073	−.0457	−.1159
H11	.0145	.0379	.0104	.0157	.0226	.0218	.0139	.0112	.0227	.0287
C2	−.0586	.054	−.1178	−.1352	−.1299	−.1584	−.112	−.1747	−.1274	−.1534
H21	.0577	.0162	.04	.0335	.0478	.0366	.0356	.0393	.0475	.0373
C11	−.072	.0246	−.1332	−.0248	−.0821	.1016	−.111	.0006	−.0836	.1199
H111	.034	−.006	.0567	.017	.0409	−.0147	.0486	.0052	.0379	−.0214
C12	−.0918	−.2028	−.083	−.1715	−.0952	−.2163	−.0871	−.171	−.0976	−.2187
H121	.015	.0183	.0128	.0087	.0192	.0164	.011	.0089	.0207	.021
C13	.1031	.449	.1189	.4346	.1021	.4651	.1736	.4392	.0951	.4137
C18	−.1187	−.3953	−.1369	−.4761	−.1676	−.4727	−.1948	−.4895	−.1398	−.4528
H181	.025	.0739	.025	.0922	.0332	.0907	.035	.0945	.0296	.0908
C14	.0038	.0504	.0222	.2014	.0167	.1166	.0447	−.0902	.0328	−.0439
H14	.0229	−.0269	.0244	−.0588	−.0002	−.0541	.0016	−.0177	.0057	−.032
C15	−.0981	−.1183	−.0817	−.1189	−.0909	−.1078	−.0982	−.0022	−.1391	−.0597
H151	.029	.0145	.0291	.0133	.0355	.0187	.0303	.0032	.0442	.0146
C16	−.1212	−.0166	−.0887	−.0103	−.0982	−.0135	−.0975	−.1426	−.1079	−.0961
H161	.04	.0073	.0274	.0034	.0314	.0032	.0322	.0179	.0455	.0185
C17	.0292	−.0765	.0425	−.0764	.0393	−.0698	.0361	.2497	.0117	.085
H17	.0061	−.0274	.0066	−.0217	.0083	−.026	.0197	−.0658	.0131	−.046
C20	.0833	.285	.0838	.2783	.0812	.2665	.0934	.2735	.1104	.2865
H20	−.0116	−.0662	−.0154	−.0654	−.0137	−.0621	−.0195	−.0604	−.0189	−.0643
C21	−.121	−.316	−.1211	−.3123	−.1124	−.2971	−.1447	−.3002	−.1367	−.3027
H211	.0239	.0642	.0229	.0634	.0211	.0599	.0297	.0611	.0276	.0608
C22	−.0103	−.0716	−.0131	−.07	−.0053	−.0656	−.0294	−.1021	−.017	−.0941
H221	−.0043	−.0049	−.0043	−.0054	−.0058	−.0054	.0002	.0037	−.0031	.0023
C23	.0066	.1137	.0054	.1167	.0035	.1115	.0067	.1311	.0048	.1135
H231	.0022	−.0306	.0025	−.0313	.0025	−.0301	.0041	−.0319	.0019	−.0291
C24	−.065	−.1031	−.0691	−.1092	−.0683	−.1083	−.0783	−.1238	−.0779	−.1179
H241	.0039	−.0014	.0054	.0005	.0052	.0005	.0079	.0042	.0092	.0048
C25	.2607	.4183	.2595	.4198	.2615	.4195	.2677	.4248	.2618	.4176
H25	−.0405	−.0871	−.0402	−.0869	−.0409	−.0868	−.0407	−.0869	−.0417	−.087
C26	−.2078	−.2863	−.2138	−.291	−.2124	−.2911	−.2167	−.2911	−.2059	−.2899
H261	.0404	.0529	.0423	.0548	.0417	.0548	.0426	.0542	.0403	.0543
C27	−.2078	−.2858	−.2032	−.2895	−.2053	−.2897	−.2183	−.2951	−.217	−.2868
H271	.0404	.0531	.0393	.0537	.0398	.0539	.0433	.0557	.0433	.0541
H_O			.4072	.4037	.4139	.4126	.413	.4132	.3923	.39
O_H			−.6333	−.7276	−.6631	−.7559	−.4246	−.4339	−.3985	−.4042
O_{ET}							−.2308	−.3128	−.2568	−.3317

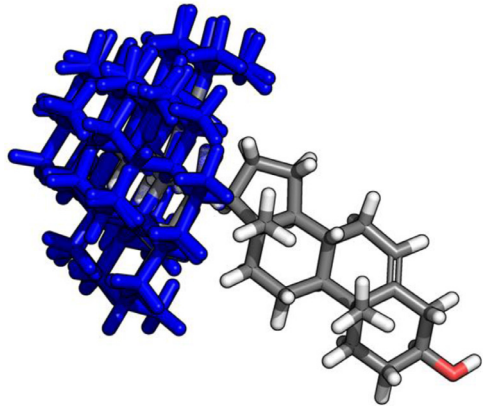

Fig. 2. Conformations of Chol selected for calculation of partial charges.

Table 2
Torsional parameters for the C7-O_{ET}-O_H-H_O and C8-C7-O_{ET}-O_H torsion angles (Fig. 1) obtained from fitting the Ryckaert-Bellemans dihedral function to the CCSD(T)/cc-pVQZ energy profile.

Torsion	C_0	C_1	C_2	C_3	C_4	C_5
C7-O_{ET}-O_H-H_O	−3.65214	−0.35069	9.99453	−4.5091		
C8-C7-O_{ET}-O_H	−1.3566	4.42684	9.6062	−18.5349	−0.64	4.42

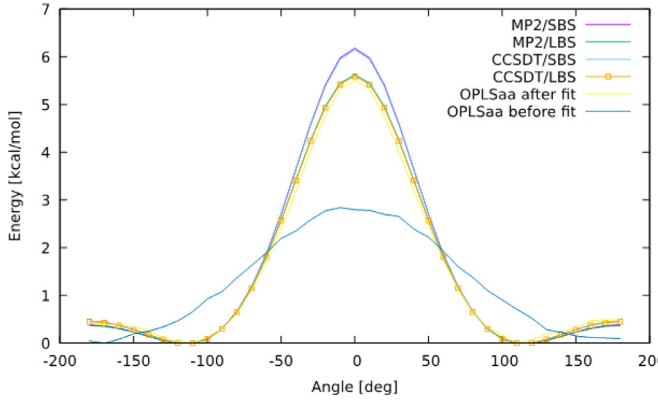

Fig. 3. 2D potential energy surfaces for rotation about the O-O bond in the C7-O_{ET}-O_H-H_O isolated moiety calculated at four levels of theory in QM calculations (see below) together with the energy profile, calculated on the basis of the original OPLSAA parameters (*blue*) and those obtained in the fitting procedure (*yellow*).

of the OPLSAA potential energy function (Eq. (1)) to the CCSD(T)/cc-pVQZ energy profile for rotation (Figs. 3 and 4), each based on the 36 energy values calculated in point 2a above.

$$V_{rb}(\phi) = \sum_{n=0}^{5} C_n(\cos(\psi))^n, \text{ where } \psi = \phi - 180^0 \quad (1)$$

Eq. (1). Ryckaert-Bellemans dihedral potential.

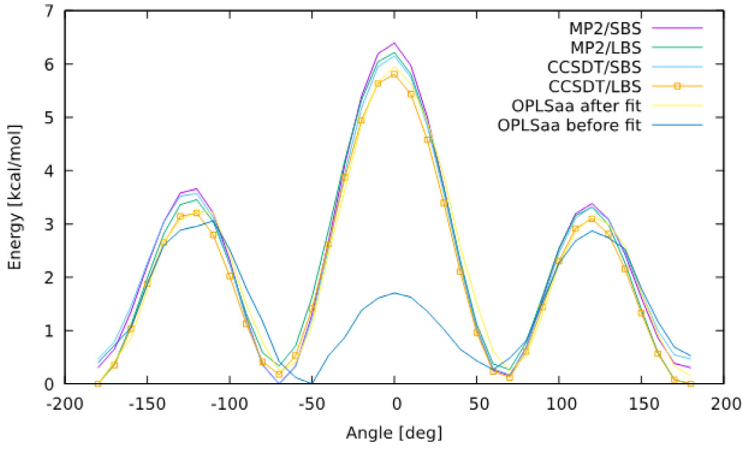

Fig. 4. 2D potential energy surfaces for rotation about the C-O bond in the C8-C7-O_{ET}-O_H isolated moiety calculated at four levels of theory in QM calculations (see below) together with the energy profile, calculated on the basis of the original OPLSAA parameters (*blue*) and those obtained in the fitting procedure (*yellow*).

2.1. Files description

Provided datasets include (1) partial atomic charges of cholesterol, C7-hydroxycholesterol and C7-hydroperoxycholesterol. The names and order of atoms in the molecules are according to the IUPAC convention [5]; (2) torsional parameters for the C7-O_{ET}-O_H-H_O and C8-C7-O_{ET}-O_H torsion angles. The data file format is Excel(.xlsx).

Ethics Statement

The studies described in the manuscript are computational, therefore were not conducted on humans or animals.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Author Statement

Michal Markiewicz: Methodology, Validation, Formal analysis, Investigation, Writing – original draft; **Robert Szczelina:** Methodology, Software, Validation, Formal analysis, Investigation, Writing – review & editing; **Marta Pasenkiewicz-Gierula:** Conceptualization, Validation, Writing – review & editing, Supervision, Project administration, Funding acquisition.

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