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Crystal Structure, Molecular Packing, Intermolecular Interactions of *N*-Pentadecanoyltaurine and *N*-acyltaurine's Interaction with Cholesterol

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Table 1S: Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters of *N*-pentadecanoyltaurine

Atom	x	y	z	Ueq
S1c	0.6971(4)	0.58903(15)	0.46517(5)	0.0239
S1a	0.2778(4)	0.74717(16)	0.56804(6)	0.0267
S1b	0.1800(4)	0.89583(16)	0.45119(5)	0.0287
Na1	0.2046(5)	0.6576(2)	0.49733(8)	0.0278
O2c	0.8160(9)	0.4912(4)	0.46848(12)	0.0282
O3b	0.2644(9)	0.7926(4)	0.45906(13)	0.0299
O4c	0.7585(9)	0.6473(4)	0.49038(12)	0.0276
O2a	0.1606(10)	0.7522(4)	0.53789(13)	0.0316
O4a	0.5474(9)	0.7712(4)	0.56529(13)	0.0307
O3c	0.4261(8)	0.5811(4)	0.46077(13)	0.0274
O5c	1.1628(10)	0.5313(4)	0.37234(13)	0.034
O3a	0.2333(9)	0.6519(4)	0.58755(14)	0.0322
O4b	0.2551(10)	0.9574(4)	0.47470(13)	0.0375
O5b	0.6716(10)	0.8392(4)	0.35529(14)	0.0363
O2b	-0.0882(9)	0.9040(4)	0.44486(13)	0.0334
O5a	-0.1795(10)	0.8539(4)	0.65405(13)	0.0379
N3c	0.8735(11)	0.6551(5)	0.37500(15)	0.0245
H3c	0.819871	0.712272	0.366413	0.03
N3a	0.1695(11)	0.7727(5)	0.64240(15)	0.0258
H3a	0.265101	0.72133	0.64679	0.031
N3b	0.3584(12)	0.9486(5)	0.36094(16)	0.0306
H3b	0.282452	1.001948	0.352811	0.037
C2c	0.7451(14)	0.6082(6)	0.40230(18)	0.0239
C7b	0.6780(13)	0.9412(6)	0.29079(19)	0.0249
C4c	1.0726(15)	0.6142(6)	0.3623(2)	0.0249
C10c	0.6881(14)	0.5408(6)	0.24931(19)	0.0286
C10b	0.1849(14)	0.8525(6)	0.23450(19)	0.0304
C1c	0.8150(14)	0.6543(5)	0.43079(18)	0.0237
C8b	0.4236(14)	0.9192(6)	0.27748(19)	0.0271
C6b	0.6643(14)	0.9900(6)	0.32023(19)	0.0295
C8a	0.1154(14)	0.7581(6)	0.7282(2)	0.03
C4b	0.5675(15)	0.9200(7)	0.3468(2)	0.0322
C2a	0.2459(15)	0.8492(6)	0.6180(2)	0.0303
C10a	0.3403(15)	0.8221(6)	0.77267(19)	0.03
C12c	0.4572(14)	0.4755(6)	0.20473(19)	0.0304
C13c	0.4839(15)	0.4343(6)	0.1743(2)	0.0321
C8c	0.9304(14)	0.6044(6)	0.29302(19)	0.0284
C11c	0.7102(14)	0.4970(6)	0.21905(19)	0.0298
C14b	-0.2838(14)	0.7235(6)	0.14634(19)	0.0295
C1b	0.3338(15)	0.9448(6)	0.41708(19)	0.0294
C6a	-0.1081(14)	0.6936(6)	0.68316(19)	0.0278

C1a	0.1383(14)	0.8410(5)	0.58617(19)	0.0253
C9b	0.4421(14)	0.8715(6)	0.24811(19)	0.0292
C7c	1.1887(15)	0.6246(6)	0.30577(19)	0.0311
C9c	0.9426(14)	0.5613(7)	0.26310(19)	0.0327
C15b	-0.2638(15)	0.6767(6)	0.1170(2)	0.0327
C7a	-0.1320(15)	0.7287(6)	0.7152(2)	0.0349
C4a	-0.0449(15)	0.7779(6)	0.6588(2)	0.0326
C15c	0.2608(15)	0.3670(7)	0.1297(2)	0.0372
C12b	-0.0522(14)	0.7875(6)	0.1906(2)	0.0318
C13a	0.5497(14)	0.9314(7)	0.8466(2)	0.0364
C11a	0.3194(15)	0.8650(6)	0.8028(2)	0.034
C6c	1.1855(15)	0.6759(6)	0.33455(19)	0.0308
C13b	-0.0334(14)	0.7406(7)	0.1613(2)	0.0347
C14a	0.7995(14)	0.9536(6)	0.86049(19)	0.0314
C14c	0.2347(15)	0.4100(6)	0.1599(2)	0.038
C11b	0.2020(14)	0.8051(6)	0.20487(19)	0.0313
C2b	0.2553(16)	0.8948(7)	0.3889(2)	0.0396
C17b	-0.4980(15)	0.6144(7)	0.0719(2)	0.0389
C17a	1.0150(15)	1.0608(7)	0.9355(2)	0.0392
C9a	0.0889(14)	0.7950(6)	0.7590(2)	0.032
C16b	-0.5195(14)	0.6610(7)	0.1016(2)	0.037
C18a	1.2700(16)	1.0784(7)	0.9498(2)	0.0488
C12a	0.5714(15)	0.8879(6)	0.81674(19)	0.0328
C15a	0.7812(15)	0.9969(6)	0.8909(2)	0.0391
C16a	1.0332(15)	1.0189(7)	0.9050(2)	0.0396
C16c	0.0116(15)	0.3453(7)	0.1152(2)	0.0383
C18c	-0.2107(16)	0.2810(7)	0.0701(2)	0.0497
C17c	0.0374(16)	0.3013(7)	0.0851(2)	0.0421
C19a	1.2486(18)	1.1221(8)	0.9799(2)	0.0646
C19b	-0.7258(18)	0.5504(8)	0.0276(2)	0.0613
C18b	-0.7483(16)	0.5987(7)	0.0570(2)	0.0484
C19c	-0.178(2)	0.2359(8)	0.0399(2)	0.0677
Na1	1.2046(5)	0.6576(2)	0.49733(8)	0.0278
Na1	0.7954(5)	0.3424(2)	0.50267(8)	0.0278
O2c	0.1840(9)	0.5088(4)	0.53152(12)	0.0282
O4c	-0.2415(9)	0.6473(4)	0.49038(12)	0.0276
O1aa	-0.3122(12)	0.8577(5)	0.50473(17)	0.0553
H1ac	-0.168(9)	0.893(5)	0.503(2)	0.083
H1ad	-0.395(14)	0.843(6)	0.5228(10)	0.083
O1c	0.2232(12)	0.4254(6)	0.43184(17)	0.063
H1cc	0.323707	0.458153	0.441738	0.094
H1cd	0.100509	0.411342	0.444151	0.094
O20a	0.4097(12)	0.5729(5)	0.64620(15)	0.0434
H20a	0.426681	0.559208	0.665629	0.065
H20b	0.510367	0.533281	0.638759	0.065

Table 2S: Bond Distances (Å) and Bond Angles (degree) of *N*-pentadecanoyltaurine

Bond Distances (Å)

Atom groups	Molecule A	Molecule B	Molecule C
C19–C18	1.527(11)	1.524(12)	1.538(12)
C18–C17	1.518(11)	1.509(11)	1.519(11)
C17–C16	1.521(11)	1.521(11)	1.525(10)
C16–C15	1.522(11)	1.544(10)	1.512(10)
C15–C14	1.525(10)	1.508(10)	1.518(10)
C14–C13	1.514(10)	1.512(10)	1.517(10)
C13–C12	1.505(10)	1.509(10)	1.509(10)
C12–C11	1.525(10)	1.521(10)	1.532(10)
C11–C10	1.505(10)	1.528(10)	1.530(10)
C10–C9	1.535(10)	1.529(10)	1.530(10)
C9–C8	1.499(10)	1.510(10)	1.506(10)
C8–C7	1.506(10)	1.522(10)	1.526(10)
C7–C6	1.532(10)	1.523(10)	1.521(10)
C6–C4	1.486(11)	1.481(10)	1.504(11)
C4–N3	1.343(9)	1.343(9)	1.344(9)
N3–C2	1.435(9)	1.438(9)	1.435(9)
C2–C1	1.517(10)	1.532(11)	1.498(10)
C1–S1	1.750(7)	1.758(8)	1.755(7)
S1–O2	1.455(6)	1.458(5)	1.457(5)
O2–Na1	2.328(6)	2.326(6)	2.337(6)
S1–O4	1.477(5)	1.462(6)	1.472(5)
S1–O3	1.470(5)	1.461(5)	1.464(5)

Bond Angles (degree)

Atom groups	Molecule A	Molecule B	Molecule C
C19–C18–C17	112.8(7)	113.6(7)	113.4(8)
C18–C17–C16	113.8(7)	113.4(7)	114.6(7)
C17–C16–C15	115.0(7)	113.4(6)	113.8(7)
C16–C15–C14	114.5(7)	113.6(7)	113.8(7)
C15–C14–C13	114.4(7)	114.1(6)	114.5(7)
C14–C13–C12	114.0(7)	114.8(6)	114.4(7)
C13–C12–C11	114.5(6)	113.9(6)	113.5(6)
C12–C11–C10	114.2(6)	113.9(6)	114.0(6)
C11–C10–C9	114.4(6)	113.5(6)	112.7(6)
C10–C9–C8	113.8(6)	113.6(6)	114.9(6)
C9–C8–C7	114.0(6)	113.8(6)	113.2(6)
C8–C7–C6	114.0(7)	114.6(6)	115.0(6)
C7–C6–C4	112.1(7)	112.2(7)	113.6(7)
C6–C4–O5	121.1(7)	121.3(8)	120.2(7)
C6–C4–N3	118.7(7)	117.4(8)	115.4(7)
C4–N3–C2	123.5(7)	123.9(7)	122.9(7)
N3–C2–C1	116.0(7)	110.2(7)	112.5(6)
C2–C1–S1	113.7(5)	113.7(6)	114.3(6)
C1–S1–O3	107.7(4)	107.4(3)	105.8(4)
C1–S1–O4	105.9(3)	106.8(4)	108.1(3)
C1–S1–O2	106.9(4)	106.1(4)	106.2(3)
S1–O2–Na1	133.5(3)	139.4(3)	137.5(3)
O2–S1–O4	111.3(3)	111.8(3)	113.1(3)
O2–S1–O3	112.9(3)	112.9(3)	110.9(3)
O3–S1–O4	111.8(3)	111.3(3)	112.3(3)

Table 3S: Hydrogen bond distances (Å) and bond Angles (degree) of *N*-pentadecanoyltaurine

	$d_{H\cdots O}$	$d_{D\cdots O}$	$\angle$D–H···O
N3c–H3c···O5b	1.867	2.735(8)	168.7
N3a–H3a···O20a	2.142	2.977(9)	158.0
N3b–H3b···O5a	1.987	2.822(9)	158.2
O1aa–H1ad···O4a	2.039	2.852(8)	159.8
O20a–H20b···O5c	2.018	2.839(8)	162.0
O1c–H1cc···O4a	2.101	2.942(8)	170.2
O1c–H1cd···O2c	2.195	2.875(9)	136.9

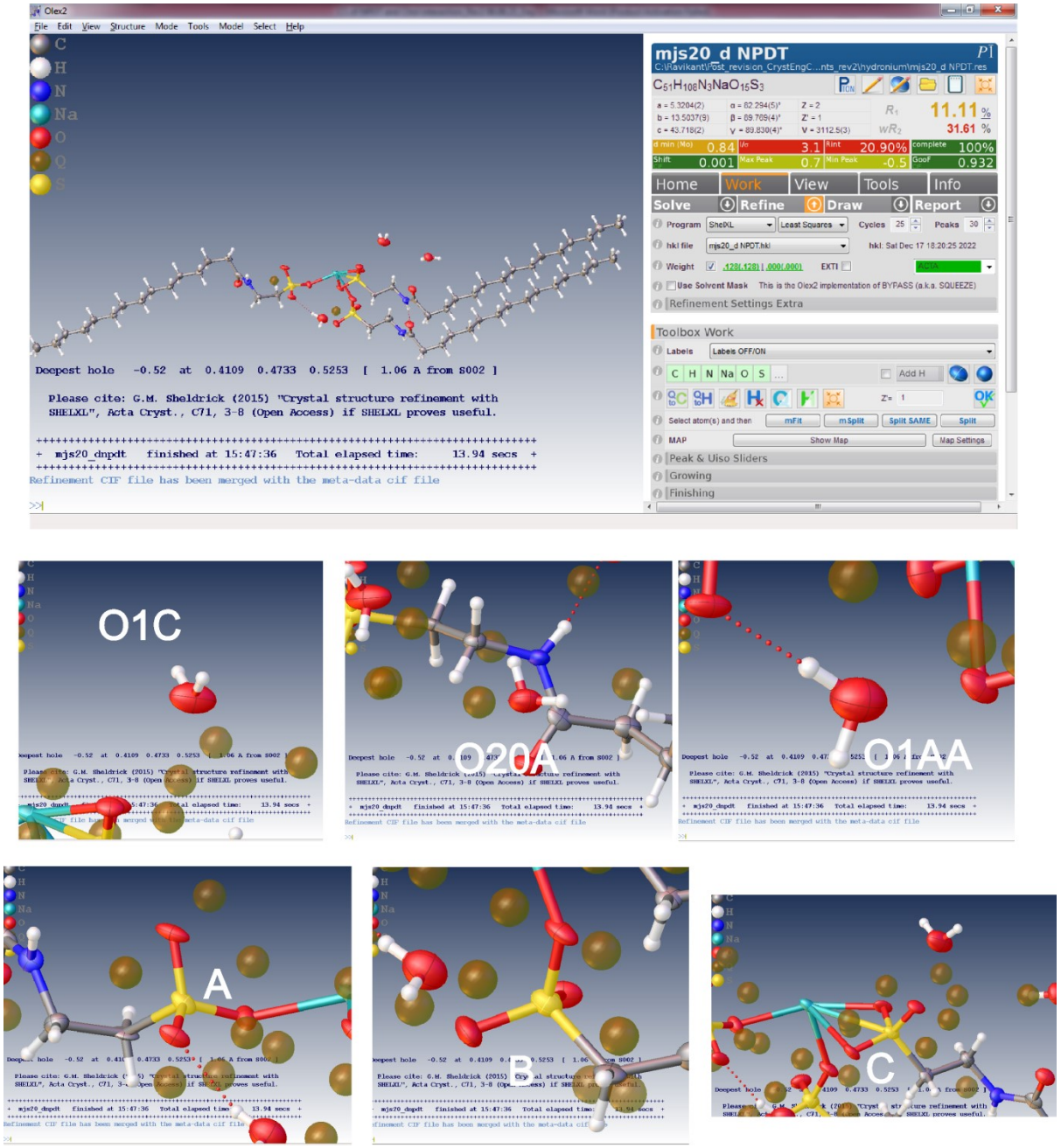

Figure S1. Snapshots of crystal structure refinement in Olex2 (top panel) showing the Q-peaks near the water molecules (middle panel) that could be suggestive of hydronium ions. Q-peaks close to O1C and O20A are about ~ 1.2 Å from the oxygens respectively while that is at 2.3 Å from O1AA. The bottom panel shows Q-peaks around the SO_3 groups.

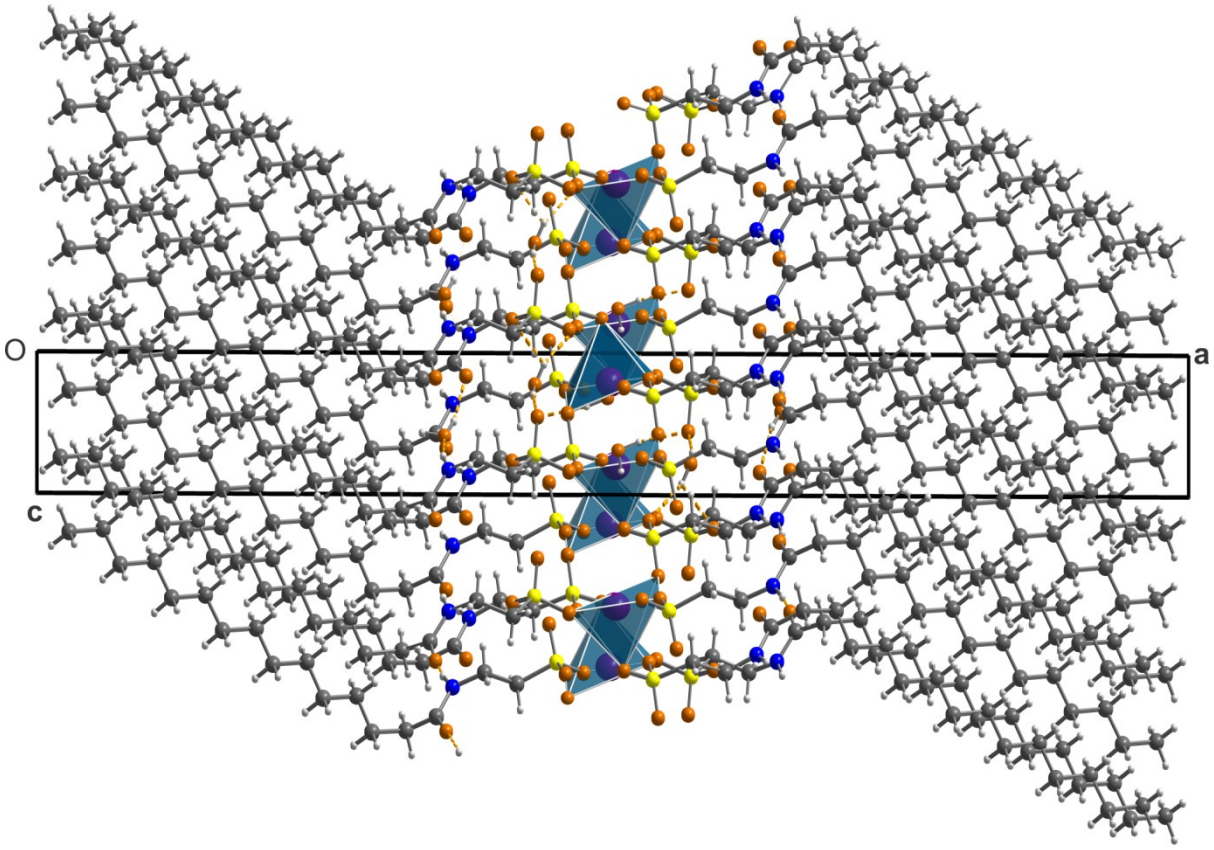

Figure S2. View along [010] of part of crystal packing emphasizing the Na–O polyhedra. The adjacent distorted square pyramids displaced along [010] are antiparallel and shifted away from the adjacent ones along [100].