Supporting Information

***Title*:** Aggregation in aqueous solutions of 2-(tetrafluoro(trifluoromethyl)-λ^6-sulfanyl-ethan-1-ol (CF_3SF_4-ethanol): A comparison with aqueous trifluoroethanol and hexafluoroisopropanol using molecular dynamics simulations and dynamic light scattering experiments.

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Table of Contents

Table S1: Parameters for bonds, angles and dihedrals for CF_3SF_4-ethanol

Parameter[a]	Gauche	Antiperiplanar
r(S-C)	1.85	1.85
r(S-F)	1.68	1.68
r(S-F1)	1.68	1.68
r(S-F2)	1.69	1.65
r(S-F3)	1.72	1.65
r(S-C2)	1.98	1.92
r(C-C1)	1.53	1.53
r(C-H3)	1.09	1.09
r(C-H4)	1.09	1.09
r(C1-O)	1.41	1.42
r(C1-H1)	1.10	1.10
r(C1-H2)	1.10	1.10
r(O-H)	0.96	0.97
r(C2-F4)	1.32	1.32
r(C2-F5)	1.31	1.32
r(C2-F6)	1.32	1.32
θ(S-C-C1)	115.1	115.5
θ(S-C-H1)	101.97	104.05
θ(S-C-H4)	104.16	104.8
θ(S-C2-F4)	108.88	108.4
θ(S-C2-F5)	109.51	109.9
θ(S-C2-F6)	108.19	109.9
θ(C-S-F)	92.64	92.30
θ(C-S-F1)	90.52	89.93
θ(C-S-F2)	90.48	90.23
θ(C-S-F3)	93.51	93.12
θ(C-S-C2)	177.58	177.19
θ(C-C1-O)	114.26	108.47
θ(C-C1-H1)	104.71	110.07
θ(C-C1-H2)	105.83	111.28
θ(C1-C-H3)	111.57	109.89
θ(C1-C-H4)	111.49	112.21
θ(C1-O-H)	108.17	108.12
θ(O-C1-H1)	106.09	112.06
θ(O-C1-H2)	112.78	106.65
θ(H1-C1-H2)	107.36	108.18

θ(H3-C-H4)	111.56	109.38
θ(F-S-F1)	176.86	176.65
θ(F-S-F2)	89.24	89.31
θ(F-S-F3)	89.50	90.59
θ(F-S-C2)	89.33	90.68
θ(F1-S-F2)	90.38	90.23
θ(F2-S-F3)	175.83	177.48
θ(F1-S-C2)	90.91	89.36
θ(F1-S-F3)	90.65	93.12
θ(F2-S-C2)	87.55	89.93
θ(F3-S-C2)	85.10	92.27
θ(F4-C2-F5)	110.39	109.3
θ(F5-C2-F6)	110.17	109.34
θ(F4-C2-F6)	109.66	109.7
ϕ(C-S-C2-F5)	-124.18	-165.71
ϕ(C-S-C2-F4)	-4.97	-46.11
ϕ(C-S-C2-F6)	115.01	73.40
ϕ(F3-S-C-C1)	108.51	-103.63
ϕ(F2-S-C-C1)	162.05	76.25
ϕ(F1-S-C-C1)	71.84	167.03
ϕ(F-S-C-C1)	-18.85	-14.35
ϕ(S-C-C1-O)	79.03	-172.43
ϕ(C-C1-O-H)	-72.58	-76.22
ϕ(C2-S-C-C1)	38.16	70.14
ϕ(F4-C2-S-F)	52.18	44.82
ϕ(F4-C2-S-F1)	-38.68	-45.95
ϕ(F4-C2-S-F3)	141.74	133.93
ϕ(F4-C2-S-F2)	-128.86	-136.68
ϕ(F5-C2-S-F)	-67.01	-74.68
ϕ(F5-C2-S-F1)	-157.9	-165.47
ϕ(F5-C2-S-F2)	111.93	14.43
ϕ(F5-C2-S-F3)	22.59	103.79
ϕ(F6-C2-S-F)	172.18	164.35
ϕ(F6-C2-S-F1)	81.03	73.57
ϕ(F6-C2-S-F2)	-8.87	-106.53
ϕ(F6-C2-S-F3)	-98.27	-17.16

a. All distances are reported in Angstroms (Å), and all angles and dihedrals are in degrees (°).

Table S2: Parameters for bonds, angles and dihedrals for TFE

Parameter[a]	Gauche	Antiperiplanar
r(C1-F)	1.35	1.35
r(C1-F2)	1.34	1.34
r(C-C1)	1.51	1.51
r(C-H1)	1.10	1.10
r(C-H2)	1.09	1.09
r(C-O)	1.40	1.40
r(O-H)	0.97	0.97
θ(F-C1-F1)	107.9	107.5
θ(F1-C1-F2)	108.1	107.2
θ(F-C1-F2)	107.4	107.2
θ(F-C1-C)	109.95	110.9
θ(F1-C1-C)	110.75	110.4
θ(F2-C1-C)	112.53	112.7
θ(C1-C-H1)	107.38	107.3
θ(C1-C-H2)	108.42	107.85
θ(H1-C-O)	113.23	112.99
θ(H2-C-O)	107.6	107.5
θ(C-O-H)	107.5	109.4
θ(C1-C-O)	112.41	112.4
ϕ(F-C1-C-O)	58.67	180
ϕ(F1-C1-C-O)	-61.33	60.76
ϕ(F2-C1-C-O)	177.79	-60.76
ϕ(C2-C-O-H)	62.74	180

a. All distances are reported in Angstroms (Å), and all angles and dihedrals are in degrees (°).

Table S3: Parameters for bonds, angles and dihedrals for HFIP

Parameter[a]	Gauche	Antiperiplanar
*r(*O-C)	1.39	1.39
r(C-H1)	1.10	1.09
r(C-C1)	1.53	1.53
r(C-C2)	1.53	1.53
r(F-C1)	1.34	1.34
r(F1-C1)	1.33	1.33
r(F2-C1)	1.33	1.33
r(F3-C2)	1.33	1.33
r(F4-C2)	1.33	1.33
r(F5-C2)	1.33	1.33
θ(C-O-H)	109.14	107.5
θ(F-C1-C)	107.83	110.2
θ(H1-C-O)	113.11	107.6
θ(F1-C1-C)	113.4	109.7
θ(F2-C1-C)	111.6	112.3
θ(F-C1-F2)	107.5	108.3
θ(F-C1-F1)	107.6	107.8
θ(F1-C1-F2)	108.6	108.3
θ(C1-C-C2)	113.7	113.3
θ(C-C2-F3)	110.7	110.2
θ(C-C2-F4)	112.4	109.7
θ(C-C2-F5)	109.3	112.4
θ(F3-C2-F4)	108.4	107.8
θ(F3-C2-F5)	107.8	108.2
θ(F4-C2-F5)	108	108.2
ϕ(F-C1-C-O)	-53.42	-179.9
ϕ(F1-C1-C-O)	65.52	59.5
ϕ(F2-C1-C-O)	-171.67	-59.03
ϕ(F3-C2-C-O)	-177.76	58.53
ϕ(F4-C2-C-O)	-57.02	-60.02
ϕ(F5-C2-C-O)	63.32	179.4
ϕ(F-C1-C-C2)	-173.31	-55.9
ϕ(F1-C1-C-C2)	-54.37	-176.5
ϕ(F2-C1-C-C2)	68.43	64.9
ϕ(F3-C2-C-C1)	-55.68	-65.5
ϕ(F4-C2-C-C1)	65.06	175.9
ϕ(F5-C2-C-C1)	-174.59	55.4
ϕ(H-O-C-C1)	58.65	62.9
ϕ(H-O-C-C2)	-177.83	-62.9
ϕ(H1-C-O-H)	-57.09	179.99

a. All distances are reported in Angstroms (Å), and all angles and dihedrals are in degrees (°).

Table S4 : Summary of Charges for HFIP conformers

Atom ID	Charges[a](Gauche)	Charges[a](antiperiplanar)
C	-0.179624	-0.220327
C	0.485153	0.401674
F	-0.151961	-0.133323
F	-0.151961	-0.133323
F	-0.151961	-0.133323
C	0.485153	0.401674
F	-0.151961	-0.133323
F	-0.151961	-0.133323
F	-0.151961	-0.133323
O	-0.389807	-0.443433
H	0.354832	0.4016661
H	0.156059	0.258687

a. Values for partial Charge are presented in atomic units

Table S5 : Summary of charges for TFE conformers

Atom ID	Charges[a](Gauche)	Charges[a](Antiperiplanar)
C	0.543783	0.565457
C	-0.093684	-0.077413
O	-0.455792	-0.502283
H	0.350009	0.395821
H	0.119999	0.094675
H	0.119999	0.094675
F	-0.194771	-0.190311
F	-0.194771	-0.190311
F	-0.194771	-0.190311

a. Values for partial Charge are presented in atomic units

Table S6: Bonded parameters used for TFE

Bond stretching parameters for CF3SF4-ethanol used in simulation		
Bond	**r_{eq} (Å)**	**k_r (KJ/mol.nm^2)**
C-C	1.53	253632.1
C1-H1	1.10	281081.0
C1-O	1.40	262846.0
C-F	1.34	304431.0
O-H	0.96	309287.4
Bond angle parameters used in simulation		

Angle	θ_{eq} / degree	k_θ(KJ/mol.rad^2)
F-C-F	109.06	644.336
F-C-C1	109.24	418.400
C-C1-O	110.19	418.440
C-C1-H1	109.56	313.800
C1-O-H	109.5	460.250
O-C1-H1	110.26	292.880

Dihedral parameters used in simulations (Ryckaert-Bellemans type)

Dihedral	C_0	C_1	C_2	C_3
H3-C-C1-F	0.65689	1.97066	0.0	-2.62755
O-C1-C-H3	1.40600	-1.04600	0.0	0.0
H-O-C1-H2	0.995779	2.98736	0.0	-3.98316
C-C1-O-H	0.26778	-9.41032	9.10021	0.0

Table S7. Bonded parameters used for HFIP

Bond stretching parameters for CF3SF4-ethanol used in simulation

Bond	r_{eq} (Å)	k_r (KJ/mol.nm^2)
C-C1	1.53	253632.1
C-H1	1.09	281081.0
C-O	1.40	262846.0
C1-F	1.34	304431.0
O-H	0.96	309287.4

Bond angle parameters used in simulation

Angle	θ_{eq} / degree	k_θ(KJ/mol.rad^2)
F-C1-F1	109.06	644.336
F-C1-C	109.24	418.400
C1-C-O	109.50	418.440
C1-C-H1	109.56	313.800
C-O-H	109.50	460.250
O-C-H1	110.26	292.880

Dihedral parameters used in simulations (Ryckaert-Bellemans type)

Dihedral	C_0	C_1	C_2	C_3
H1-C-C1-F	0.79496	-0.79496	0.0	0.0
C1-C-C2-F3	0.65084	1.95253	0.0	-2.60338
H-O-C-H1	0.69733	2.09200	0.0	-2.78933
C2-C-O-H	0.26778	-9.41032	9.10021	0.0

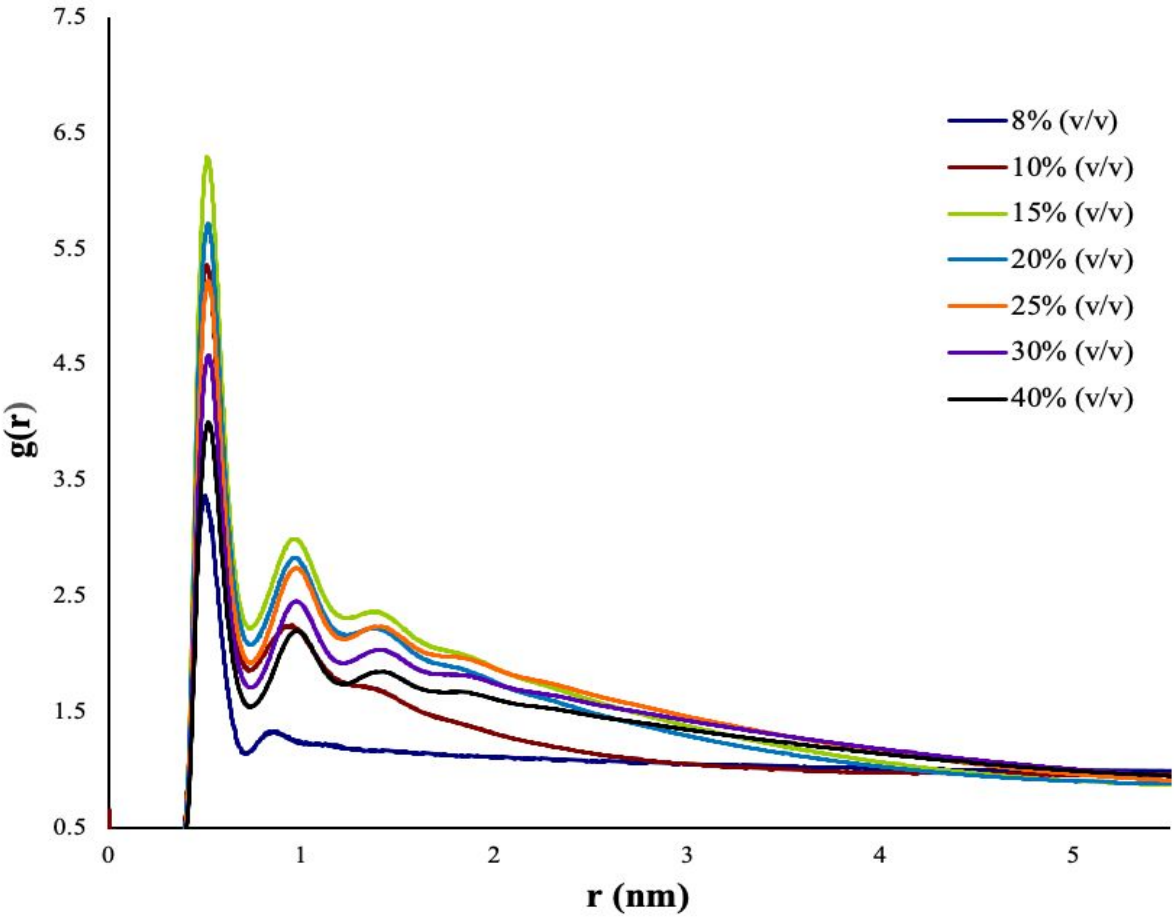

Figure S1: Radial Distribution Function g (r) for TFE-TFE

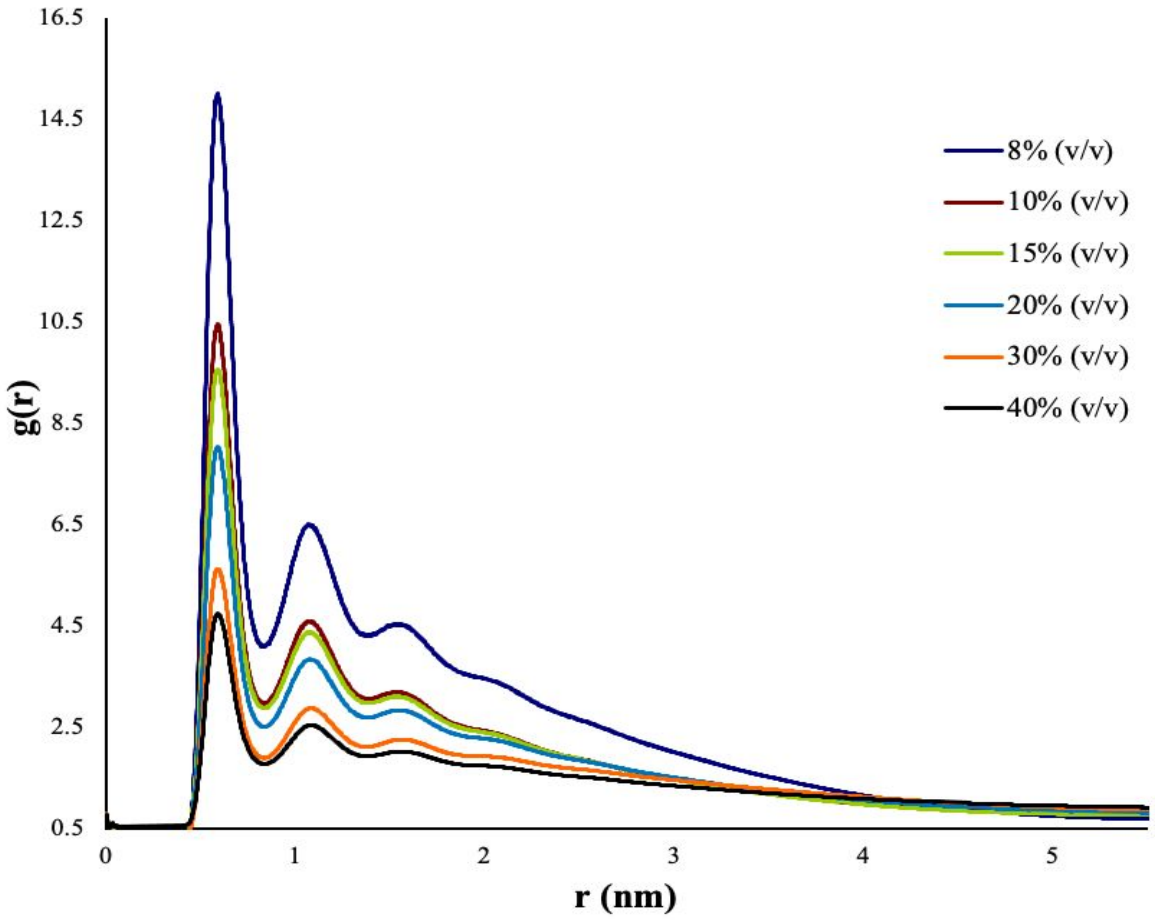

Figure S2: Radial Distribution Function g (r) for HFIP-HFIP

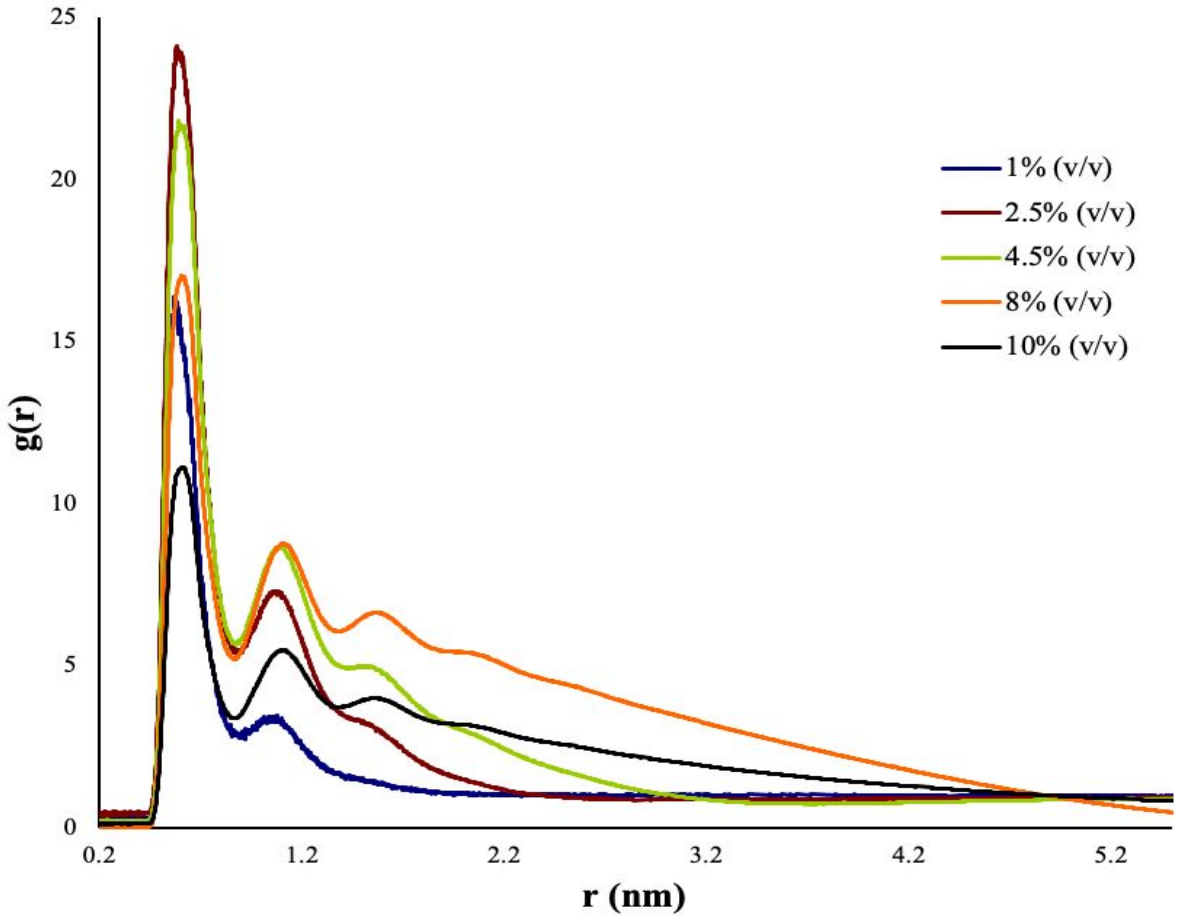

Figure S3: Radial Distribution Function g (r) for CF_3SF_4-ethanol-CF_3SF_4-ethanol

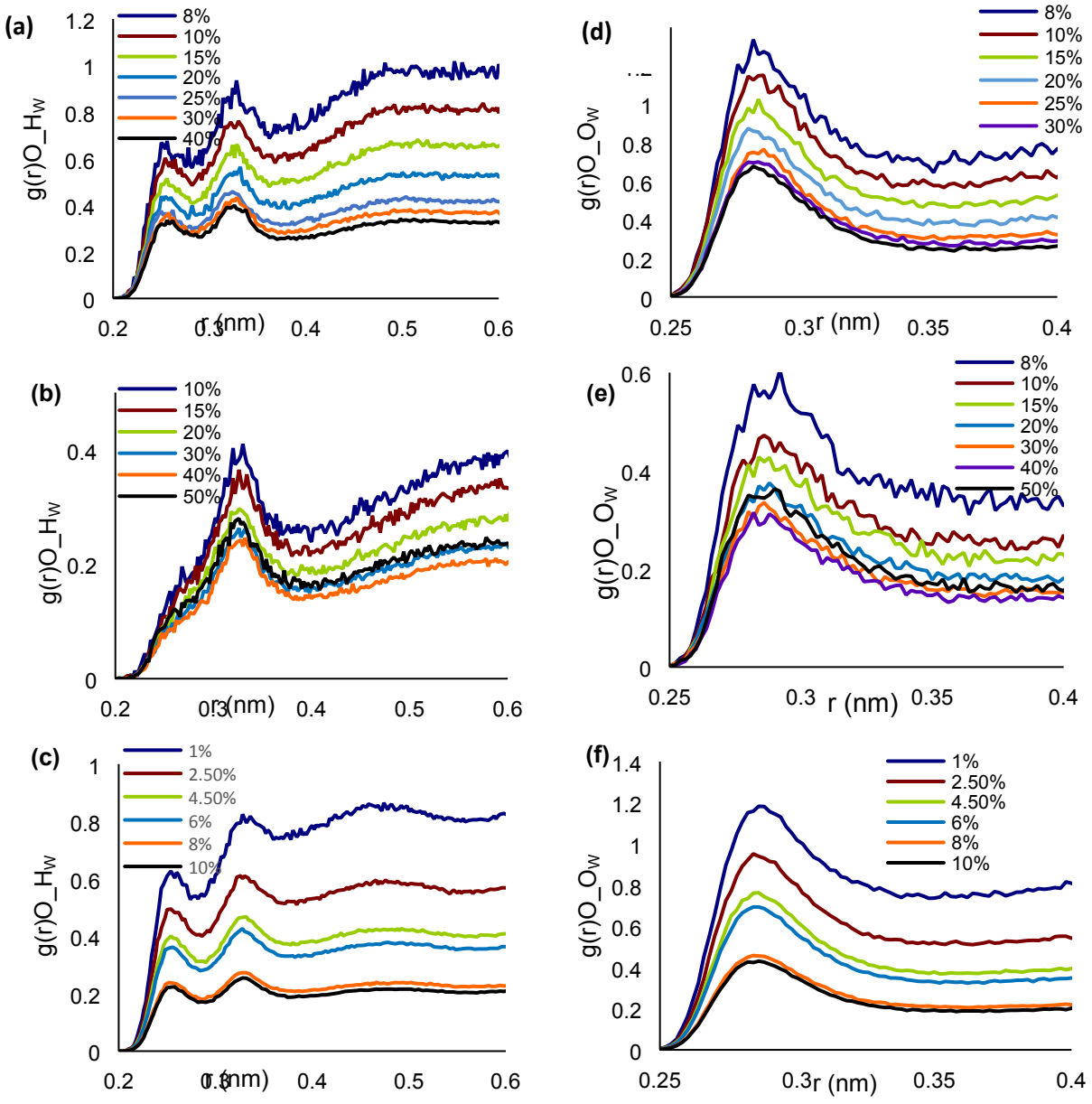

Figure S4. RDFs for aqueous mixtures of fluorinated alcohols. Presented above are the RDFs for the O_{TFE}-H_{Water} distribution in TFE (a), HFIP (b) and CF_3SF_4-ethanol (c) and for the O_{TFE}-O_{Water} distribution in TFE (d) HFIP, (e) and CF_3SF_4-ethanol (f).

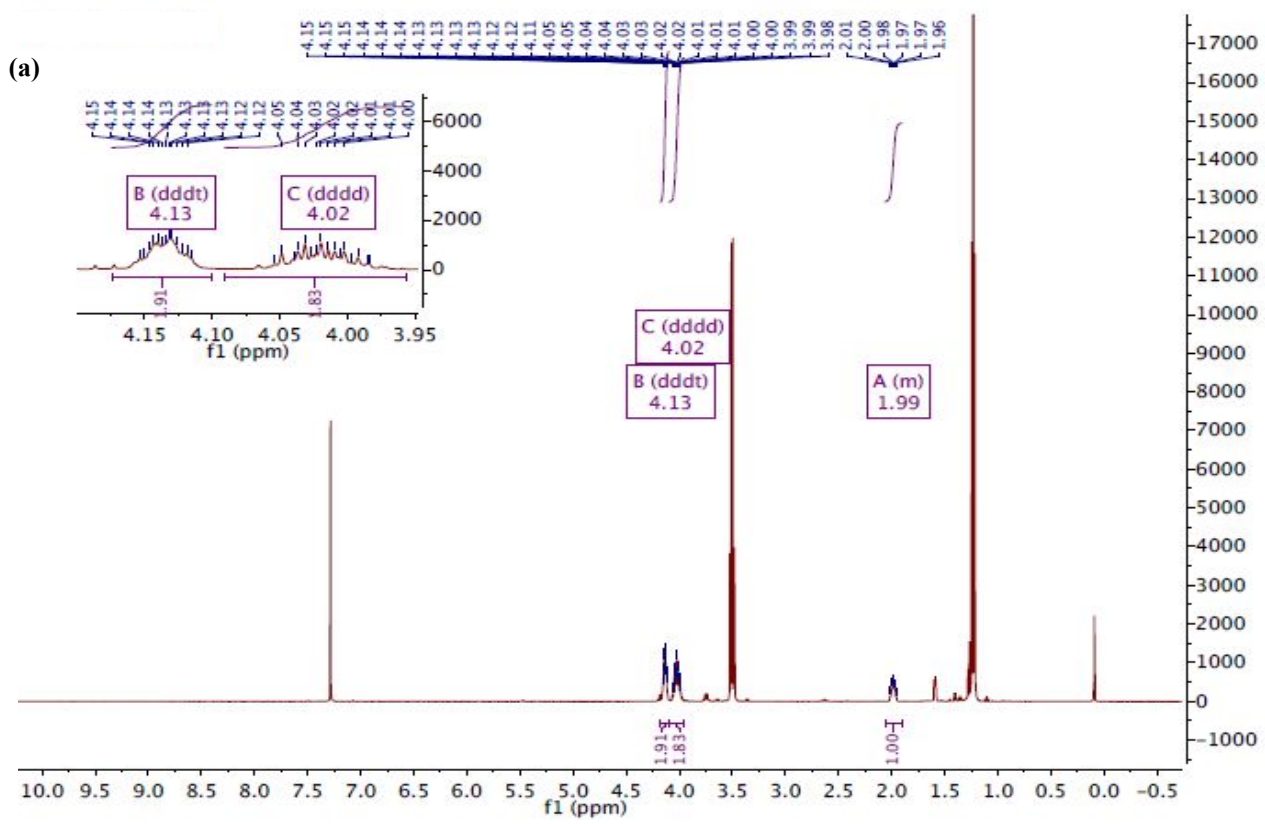

Figure S5 : (a) ^{1}H Nmr spectrum of 2-(tetrafluoro(trifluoromethyl)-λ^{6}-sulfanyl)ethan-1-ol

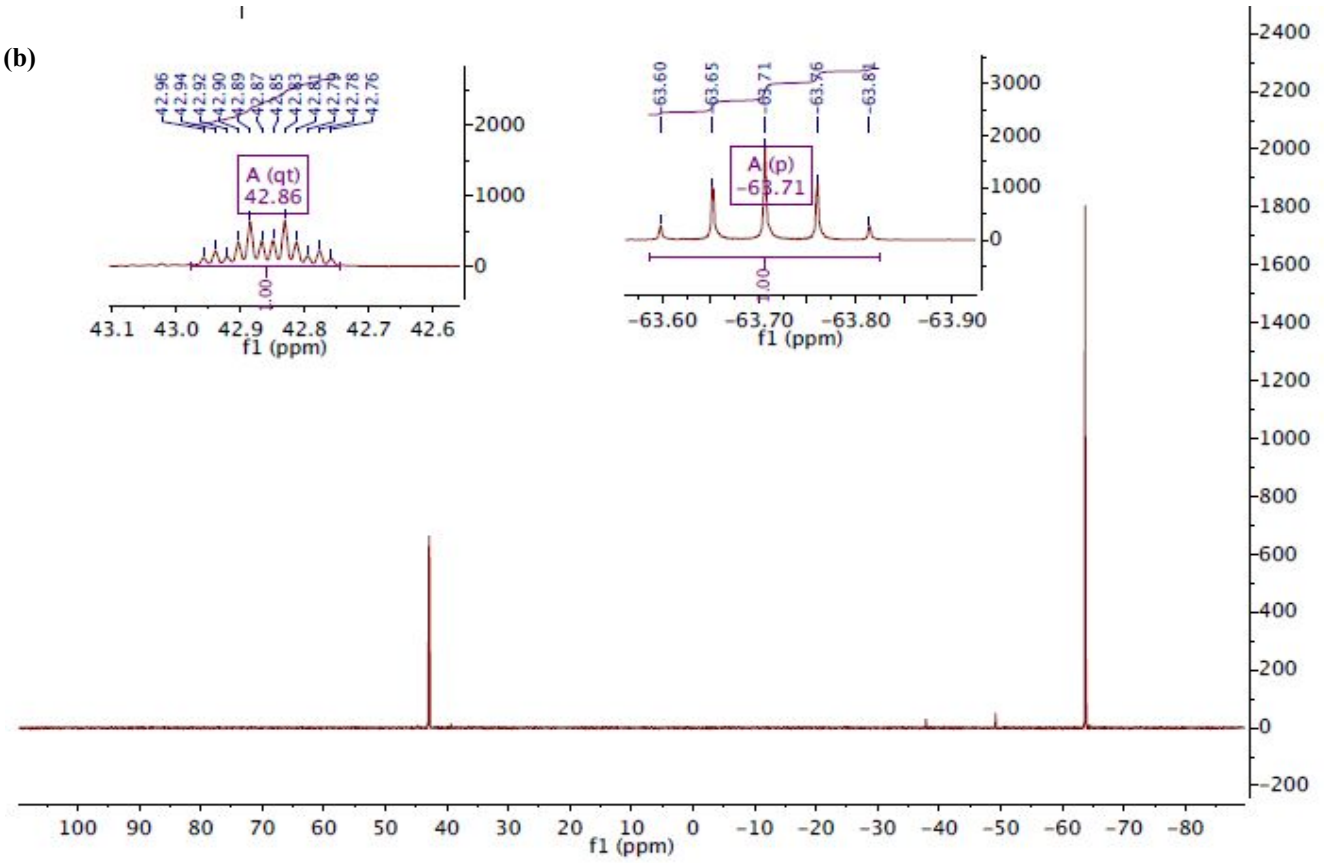

Figure S5 : (b) ^{19}F Nmr spectra of 2-(tetrafluoro(trifluoromethyl)-λ^{6}-sulfanyl)ethan-1-ol

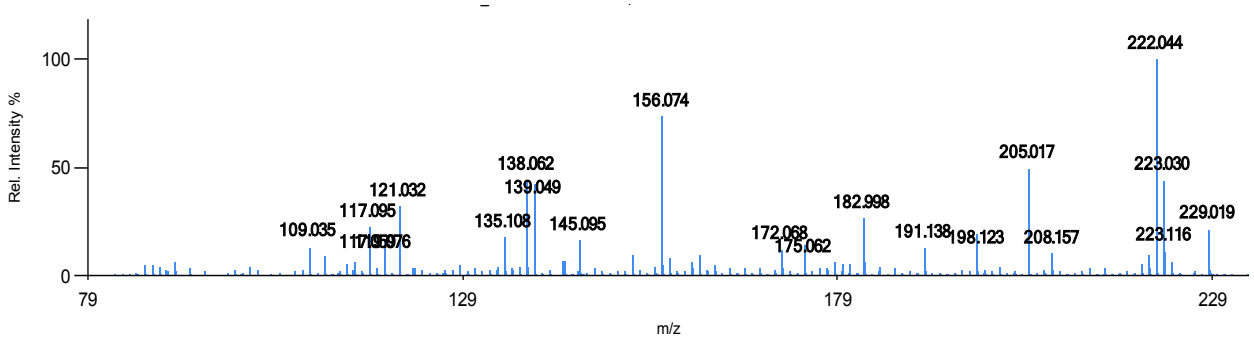

Figure S5 : (c) HRMS (DART-ESI, m/z, positive) spectrum of 2-(tetrafluoro(trifluoromethyl)-λ^6-sulfanyl)ethan-1-ol