Electronic Supplementary Information for

Variations in bile salt surfactant structure allow tuning of the sorting of single-wall carbon nanotubes by aqueous two-phase extraction

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Section 1. Details of all systematic parameter variations

Table S1. Quantities of stock solutions used for the variation of the SDS concentration at a fixed DOC concentration. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 10% wt/V SDS, 20% wt/V SDS, all in D_2O. The SWCNT solution had a starting DOC concentration of 1.6% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1.6% DOC) (µL)	D_2O (µL)	SDS 10% (µL)	SDS 20% (µL)	total volume (µL)	DOC conc (% wt/V)	SDS conc (% wt/V)	SDS/DOC ratio
1	700	300	38	162	0	0	1200	0.0507	0	0
2	700	300	38	150	12	0	1200	0.0507	0.1	1.97
3	700	300	38	138	24	0	1200	0.0507	0.2	3.95
4	700	300	38	126	36	0	1200	0.0507	0.3	5.92
5	700	300	38	114	48	0	1200	0.0507	0.4	7.89
6	700	300	38	102	60	0	1200	0.0507	0.5	9.87
7	700	300	38	90	72	0	1200	0.0507	0.6	11.84
8	700	300	38	78	84	0	1200	0.0507	0.7	13.82
9	700	300	38	66	96	0	1200	0.0507	0.8	15.79
10	700	300	38	54	108	0	1200	0.0507	0.9	17.76
11	700	300	38	42	120	0	1200	0.0507	1.0	19.74
12	700	300	38	30	132	0	1200	0.0507	1.1	21.71
13	700	300	38	90	0	72	1200	0.0507	1.2	23.68
14	700	300	38	84	0	78	1200	0.0507	1.3	25.66
15	700	300	38	78	0	84	1200	0.0507	1.4	27.63
16	700	300	38	72	0	90	1200	0.0507	1.5	29.61
17	700	300	38	66	0	96	1200	0.0507	1.6	31.58
18	700	300	38	60	0	102	1200	0.0507	1.7	33.55
19	700	300	38	54	0	108	1200	0.0507	1.8	35.53
20	700	300	38	48	0	114	1200	0.0507	1.9	37.5
21	700	300	38	42	0	120	1200	0.0507	2.0	39.47
22	700	300	38	36	0	126	1200	0.0507	2.1	41.45

Table S2. Quantities of stock solutions used for the variation of the SDS concentration at a fixed SC concentration. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 5% wt/V SC, 0.1% wt/V SDS, 0.5% wt/V SDS, 1% wt/V SDS, 5% wt/V SDS, all in D_2O. The SWCNT solution had a starting SC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1% SC) (µL)	SC 5% (µL)	SDS 0.1% (µL)	SDS 0.5% (µL)	SDS 1% (µL)	SDS 5% (µL)	D_2O (µL)	total volume (µL)	SC conc. (% wt/V)	SDS conc. (% wt/V)	SDS/SC ratio
1	700	300	50	92	0	0	0	0	58	1200	0.425	0.0000	0.000
2	700	300	50	92	32	0	0	0	26	1200	0.425	0.0027	0.006
3	700	300	50	92	0	13	0	0	45	1200	0.425	0.0054	0.013
4	700	300	50	92	0	19	0	0	39	1200	0.425	0.0079	0.019
5	700	300	50	92	0	25	0	0	33	1200	0.425	0.0104	0.025
6	700	300	50	92	0	31	0	0	27	1200	0.425	0.0129	0.030
7	700	300	50	92	0	37	0	0	21	1200	0.425	0.0154	0.036
8	700	300	50	92	0	43	0	0	15	1200	0.425	0.0179	0.042
9	700	300	50	92	0	49	0	0	9	1200	0.425	0.0204	0.048
10	700	300	50	92	0	55	0	0	3	1200	0.425	0.0229	0.054
11	700	300	50	92	0	0	31	0	27	1200	0.425	0.0258	0.061
12	700	300	50	92	0	27	31	0	0	1200	0.425	0.0371	0.087
13	700	300	50	92	0	12	31	0	15	1200	0.425	0.0308	0.073
14	700	300	50	92	0	18	31	0	9	1200	0.425	0.0333	0.078
15	700	300	50	92	0	24	31	0	3	1200	0.425	0.0358	0.084
16	700	300	50	92	0	24	34	0	0	1200	0.425	0.0383	0.090
17	700	300	50	92	0	19	39	0	0	1200	0.425	0.0404	0.095
18	700	300	50	92	0	0	55	0	3	1200	0.425	0.0458	0.108
19	700	300	50	92	0	0	0	12	46	1200	0.425	0.0500	0.118
20	700	300	50	92	0	0	0	13	45	1200	0.425	0.0542	0.127
21	700	300	50	92	0	0	0	14	44	1200	0.425	0.0583	0.137
22	700	300	50	92	0	0	0	21	37	1200	0.425	0.0875	0.206
23	700	300	50	92	0	0	0	25.5	32.5	1200	0.425	0.1063	0.250
24	700	300	50	92	0	0	0	30.6	27.4	1200	0.425	0.1275	0.300
25	700	300	50	92	0	0	0	38	20	1200	0.425	0.1583	0.373
26	700	300	50	92	0	0	0	45	13	1200	0.425	0.1875	0.441

Table S3. Quantities of stock solutions used for the variation of the SDS concentration at a fixed CDOC concentration. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 5% wt/V CDOC, 10% wt/V SDS, 15% wt/V SDS, all in D_2O. The SWCNT solution had a starting CDOC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1% CDOC) (µL)	CDOC 5% (µL)	SDS 10% (µL)	SDS 15% (µL)	D_2O (µL)	total volume (µL)	CDOC conc. (% wt/V)	SDS conc. (% wt/V)	SDS/CDOC ratio
1	700	300	60	72	0	0	68	1200	0.35	0	0.000
2	700	300	60	72	21	0	47	1200	0.35	0.175	0.500
3	700	300	60	72	24	0	44	1200	0.35	0.2	0.571
4	700	300	60	72	27	0	41	1200	0.35	0.225	0.643
5	700	300	60	72	30	0	38	1200	0.35	0.25	0.714
6	700	300	60	72	33	0	35	1200	0.35	0.275	0.786
7	700	300	60	72	36	0	32	1200	0.35	0.3	0.857
8	700	300	60	72	39	0	29	1200	0.35	0.325	0.929
9	700	300	60	72	42	0	26	1200	0.35	0.35	1.000
10	700	300	60	72	45	0	23	1200	0.35	0.375	1.071
11	700	300	60	72	48	0	20	1200	0.35	0.4	1.143
12	700	300	60	72	51	0	17	1200	0.35	0.425	1.214
13	700	300	60	72	54	0	14	1200	0.35	0.45	1.286
14	700	300	60	72	57	0	11	1200	0.35	0.475	1.357
15	700	300	60	72	60	0	8	1200	0.35	0.5	1.429
16	700	300	60	72	63	0	5	1200	0.35	0.525	1.500
17	700	300	60	72	66	0	2	1200	0.35	0.55	1.571
18	700	300	60	72	0	46	22	1200	0.35	0.575	1.643
19	700	300	60	72	0	49.3	18.7	1200	0.35	0.61625	1.761
20	700	300	60	72	0	54	14	1200	0.35	0.675	1.929

Table S4. Quantities of stock solutions used for the variation of the DOC concentration without any cosurfactants. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 1% wt/V DOC, 5% wt/V DOC, all in D_2O. The SWCNT solution had a starting DOC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1% DOC) (µL)	D_2O (µL)	DOC 1% (µL)	DOC 5% (µL)	total volume (µL)	DOC conc. (% wt/V)
1	700	300	10	190	0	0	1200	0.00833
2	700	300	15	185	0	0	1200	0.0125
3	700	300	20	180	0	0	1200	0.01667
4	700	300	25	175	0	0	1200	0.0208
5	700	300	30	170	0	0	1200	0.025
6	700	300	30	160	10	0	1200	0.0333
7	700	300	30	150	20	0	1200	0.0417
8	700	300	30	140	30	0	1200	0.05
9	700	300	30	130	40	0	1200	0.0583
10	700	300	30	120	50	0	1200	0.0667
11	700	300	30	110	60	0	1200	0.075
12	700	300	30	100	70	0	1200	0.0833
13	700	300	30	90	80	0	1200	0.0917
14	700	300	30	80	90	0	1200	0.1
15	700	300	30	50	120	0	1200	0.125
16	700	300	30	30	140	0	1200	0.142
17	700	300	30	10	160	0	1200	0.158
18	700	300	30	35	120	15	1200	0.1875
19	700	300	30	20	120	30	1200	0.25

Table S5. Quantities of stock solutions used for the variation of the SC concentration without any cosurfactants. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 1% wt/V SC, 5% wt/V SC, all in D_2O. The SWCNT solution had a starting SC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1% SC) (µL)	SC 1% (µL)	SC 5% (µL)	D_2O (µL)	total volume (µL)	SC conc. (% wt/V)
1	700	300	60	60	0	80	1200	0.1
2	700	300	60	84	0	56	1200	0.12
3	700	300	60	58	10	72	1200	0.14
4	700	300	60	32	20	88	1200	0.16
5	700	300	60	56	20	64	1200	0.18
6	700	300	60	80	20	40	1200	0.2
7	700	300	60	54	30	56	1200	0.22
8	700	300	60	66	30	44	1200	0.23
9	700	300	60	28	40	72	1200	0.24
10	700	300	60	40	40	60	1200	0.25
11	700	300	60	52	40	48	1200	0.26
12	700	300	60	64	40	36	1200	0.27
13	700	300	60	76	40	24	1200	0.28
14	700	300	60	100	40	0	1200	0.3
15	700	300	60	74	50	16	1200	0.32
16	700	300	60	48	60	32	1200	0.34
17	700	300	60	72	60	8	1200	0.36
18	700	300	60	70	70	0	1200	0.4
19	700	300	60	40	100	0	1200	0.5

Table S6. Quantities of stock solutions used for the variation of the CDOC concentration without any cosurfactants. Stock solutions were prepared with following concentrations: 20% wt/V PEG, 20% wt/V dextran, 1% wt/V CDOC, 2% wt/V CDOC, 3% wt/V CDOC, all in D_2O. The SWCNT solution had a starting CDOC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 20% (µL)	Dextran 20% (µL)	SWCNT (1% CDOC) (µL)	CDOC 1% (µL)	CDOC 2% (µL)	CDOC 3% (µL)	D_2O (µL)	total volume (µL)	CDOC conc. (% wt/V)
1	700	300	40	0	0	0	160	1200	0.033
2	700	300	50	0	0	0	150	1200	0.042
3	700	300	60	0	0	0	140	1200	0.050
4	700	300	60	20	0	0	120	1200	0.067
5	700	300	60	40	0	0	100	1200	0.083
6	700	300	60	60	0	0	80	1200	0.100
7	700	300	60	80	0	0	60	1200	0.117
8	700	300	60	100	0	0	40	1200	0.133
9	700	300	60	120	0	0	20	1200	0.150
10	700	300	60	140	0	0	0	1200	0.167
11	700	300	60	60	50	0	30	1200	0.183
12	700	300	60	60	60	0	20	1200	0.200
13	700	300	60	60	70	0	10	1200	0.217
14	700	300	60	60	80	0	0	1200	0.233
15	700	300	60	0	45	50	45	1200	0.250
16	700	300	60	0	0	90	50	1200	0.275
17	700	300	60	0	0	100	40	1200	0.300
18	700	300	60	0	0	110	30	1200	0.325
19	700	300	60	0	0	120	20	1200	0.350

Table S7. Quantities of stock solutions used for the variation of the SC concentration at the fixed concentrations of DOC (0.1% wt/V) and SDBS (1.1% wt/V). Stock solutions were prepared with following concentrations: 25% wt/V PEG, 20% wt/V dextran, 20% wt/V SDBS, 40% wt/V SC, all in D_2O. The SWCNT solution had a starting DOC concentration of 1% wt/V, as verified by absorption spectroscopy. The total volume is kept constant, assuming no change upon mixing.

	PEG 25% (µL)	**Dextran 20% (µL)**	**SWCNT (1% DOC) (µL)**	**D_2O (µL)**	**SDBS 20% (µL)**	**SC 40% (µL)**	**total volume (µL)**	**SC conc. (% wt/V)**
1	560	300	120	154	66	0	1200	0.000
2	560	300	120	150	66	4	1200	0.133
3	560	300	120	146	66	8	1200	0.267
4	560	300	120	142	66	12	1200	0.400
5	560	300	120	138	66	16	1200	0.533
6	560	300	120	134	66	20	1200	0.667
7	560	300	120	130	66	24	1200	0.800
8	560	300	120	126	66	28	1200	0.933
9	560	300	120	122	66	32	1200	1.067
10	560	300	120	118	66	36	1200	1.200
11	560	300	120	114	66	40	1200	1.333
12	560	300	120	110	66	44	1200	1.467
13	560	300	120	106	66	48	1200	1.600

Section 2. 2D PLE maps for different surfactant and cosurfactant variations and examples of their fits to obtain the PL intensities for each chirality

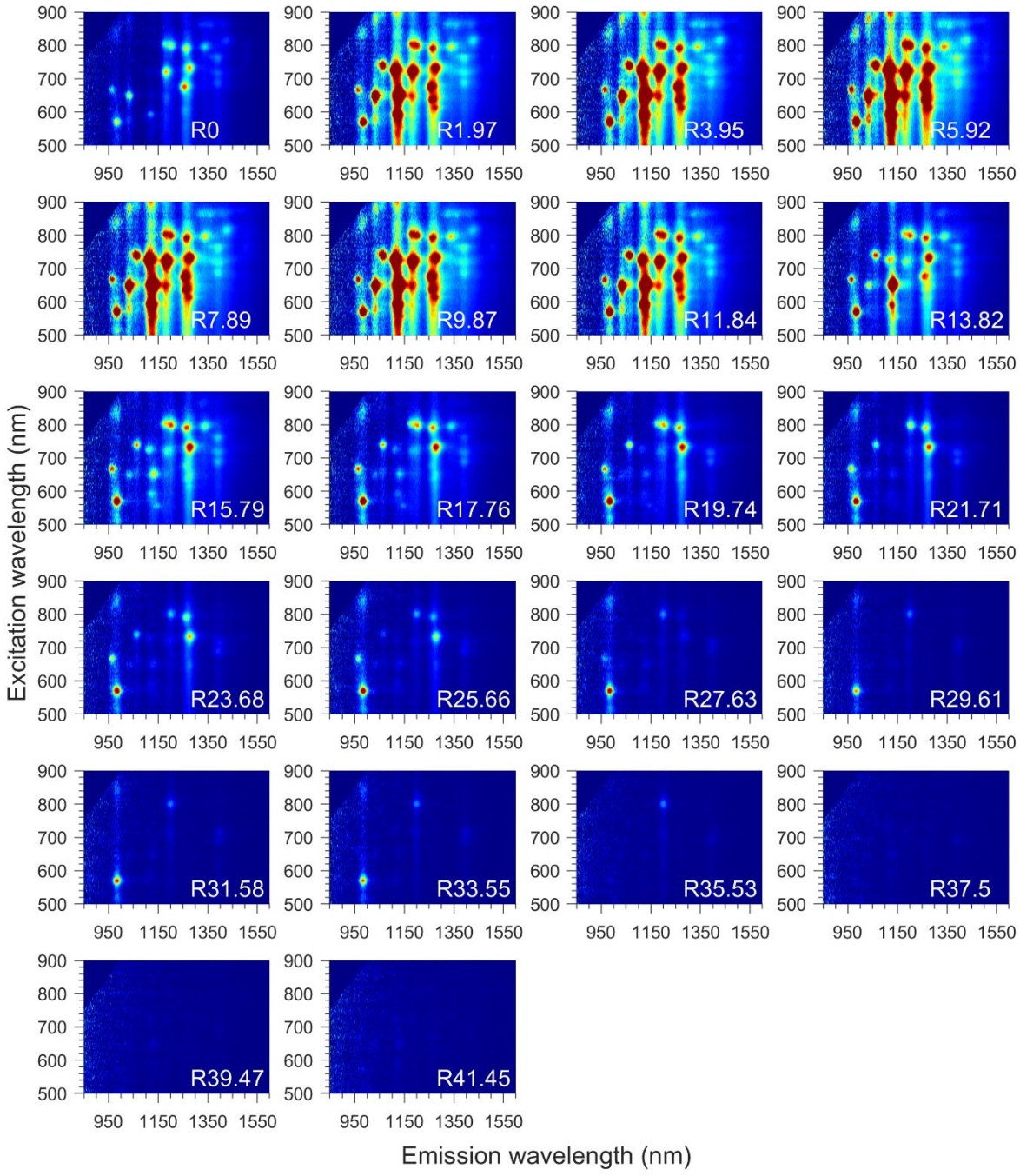

Figure S1.1: Overview of PLE maps of the bottom phases for the SDS/DOC variation. Intensities can be directly compared, and SDS/DOC ratios (R#) are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

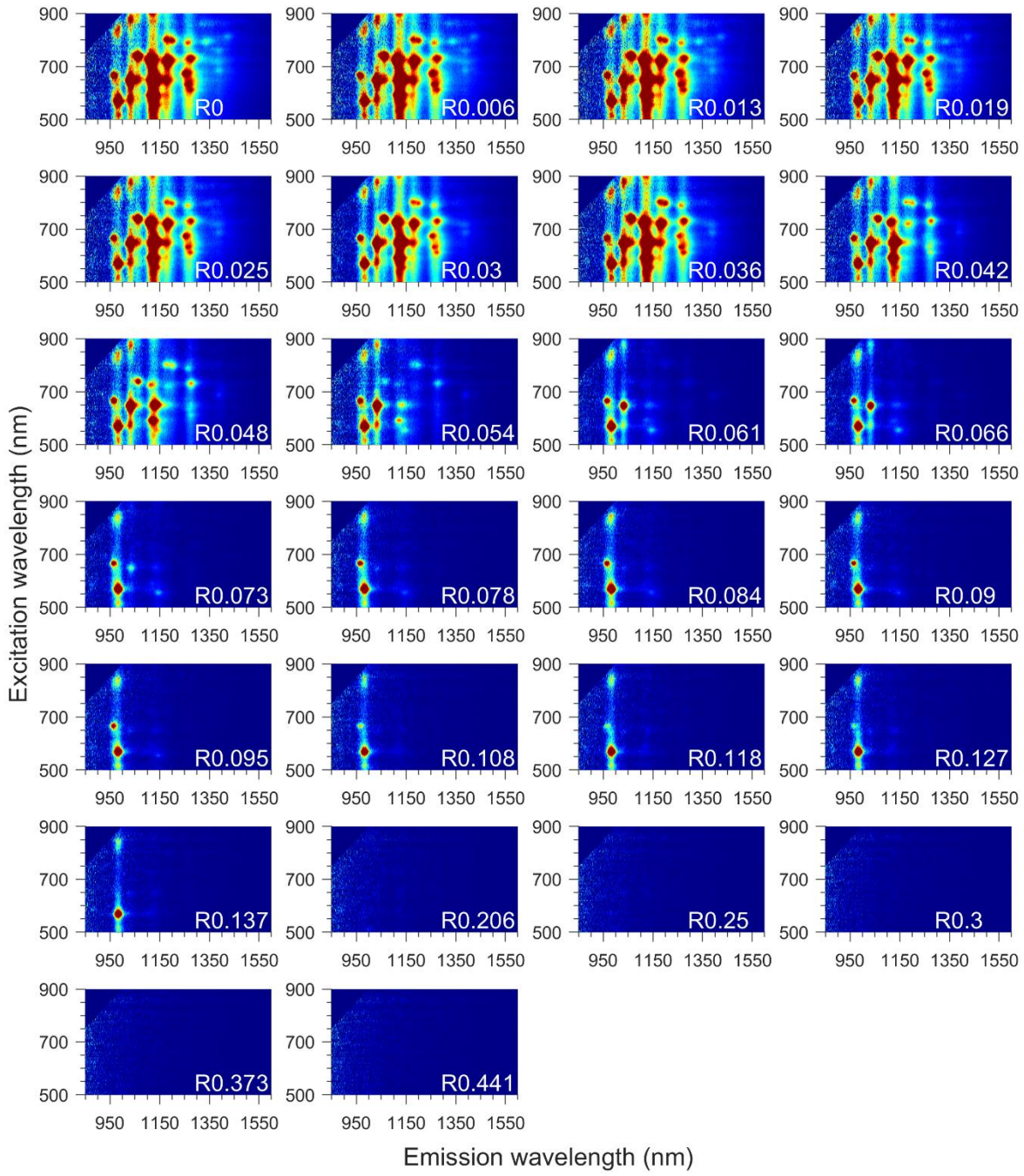

Figure S1.2: Overview of PLE maps of the bottom phases for the SDS/SC variation. Intensities can be directly compared, and SDS/SC ratios (R#) are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

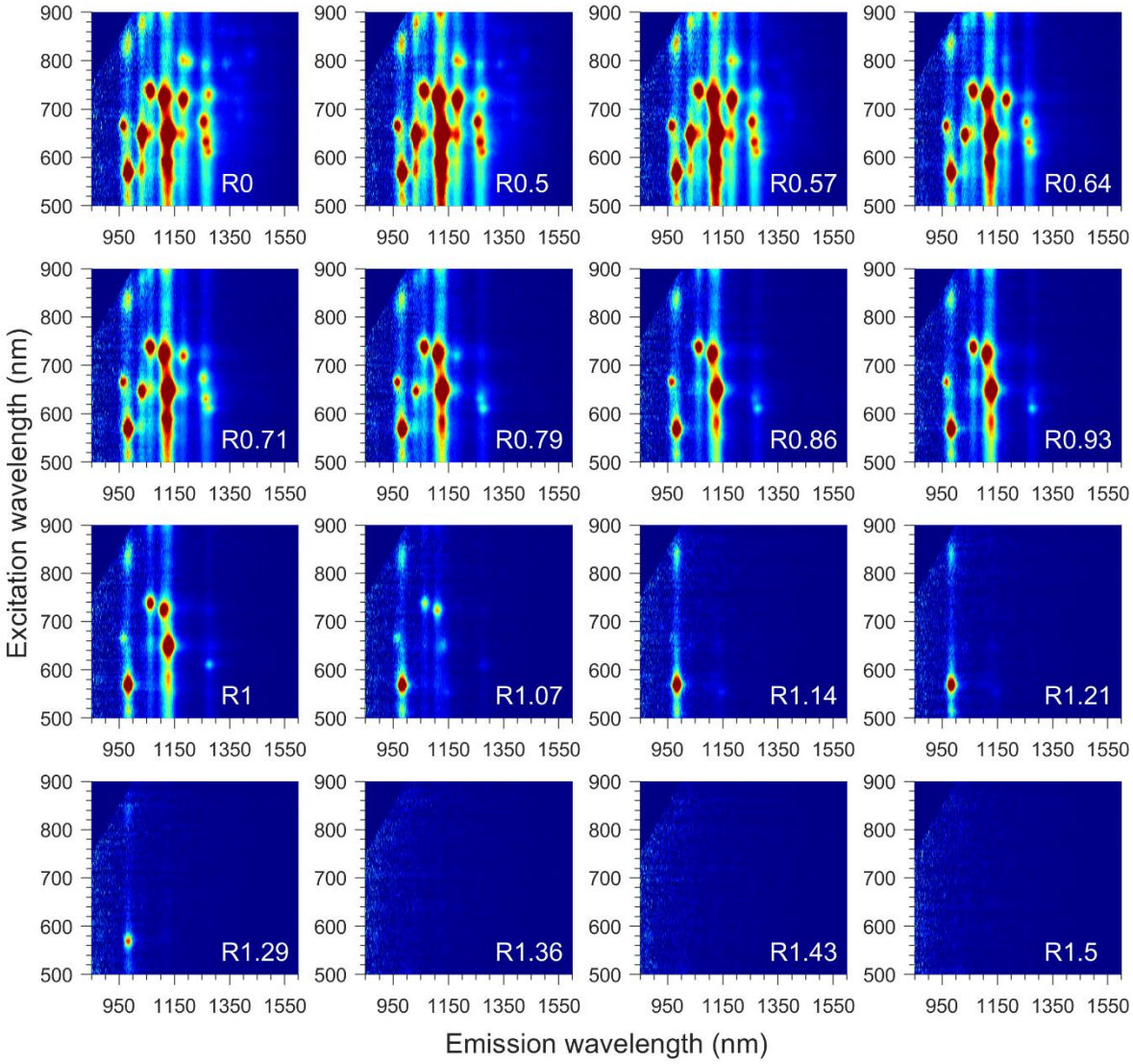

Figure S1.3: Overview of PLE maps of the bottom phases for the SDS/CDOC variation. Intensities can be directly compared, and SDS/CDOC ratios (R#) are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

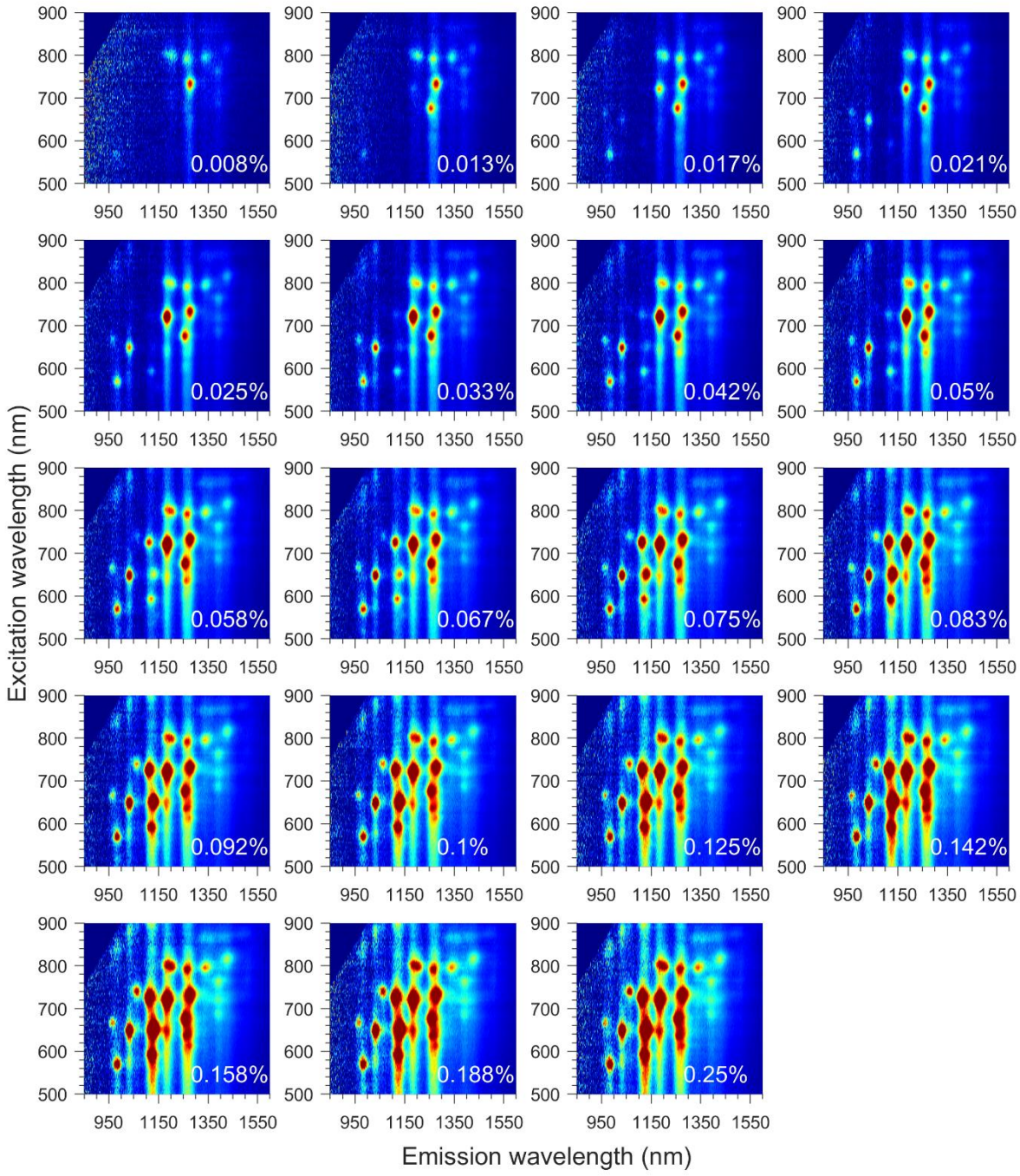

Figure S1.4: Overview of PLE maps of the bottom phases for the DOC alone experiment. Intensities can be directly compared, and DOC concentrations are written in white on the corresponding PLE maps. Note that even for the lowest DOC concentrations, some chiralities have not yet transitioned to the top phase. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

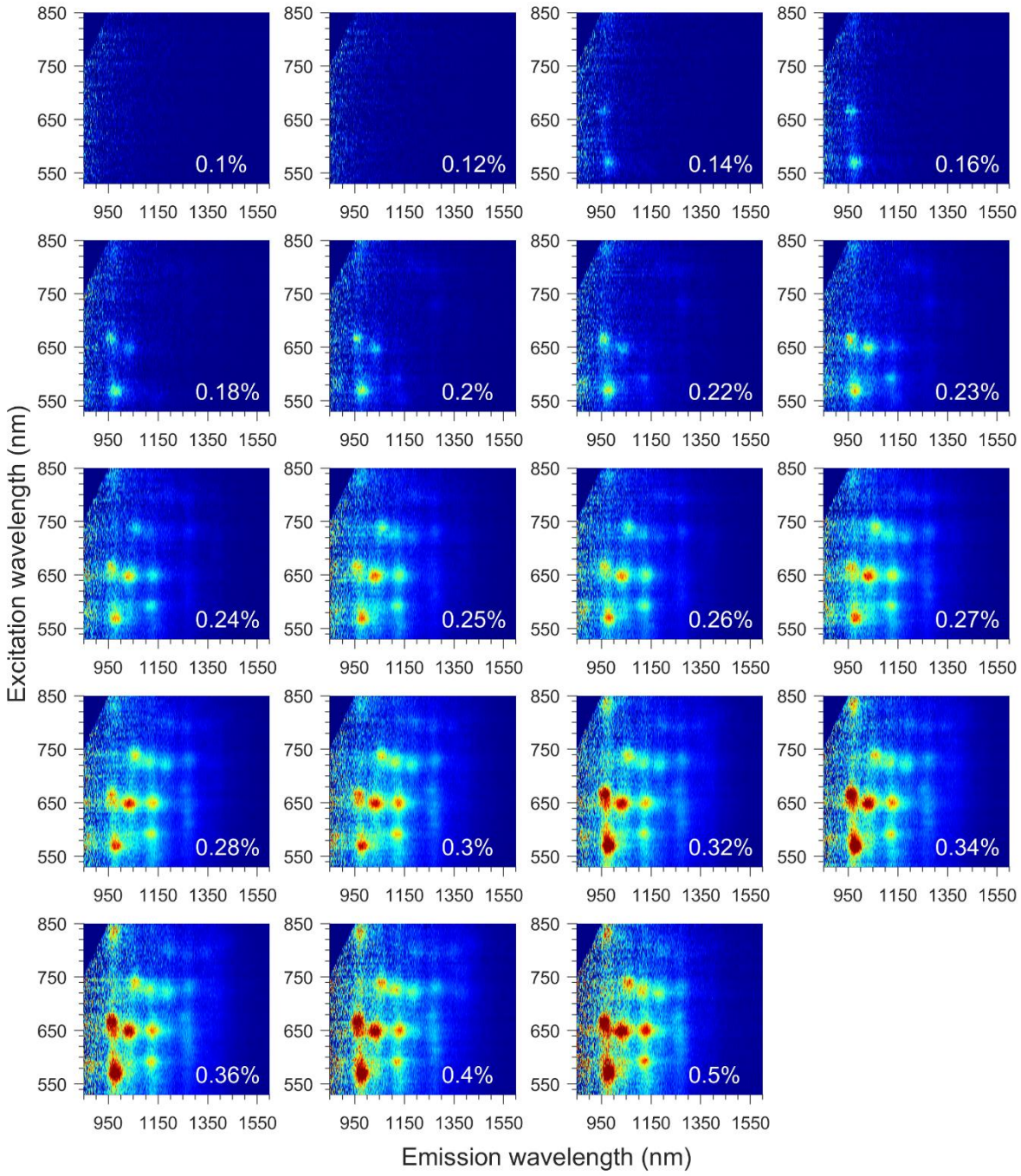

Figure S1.5: Overview of PLE maps of the bottom phases for the SC alone experiment. Intensities can be directly compared, and SC concentrations are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

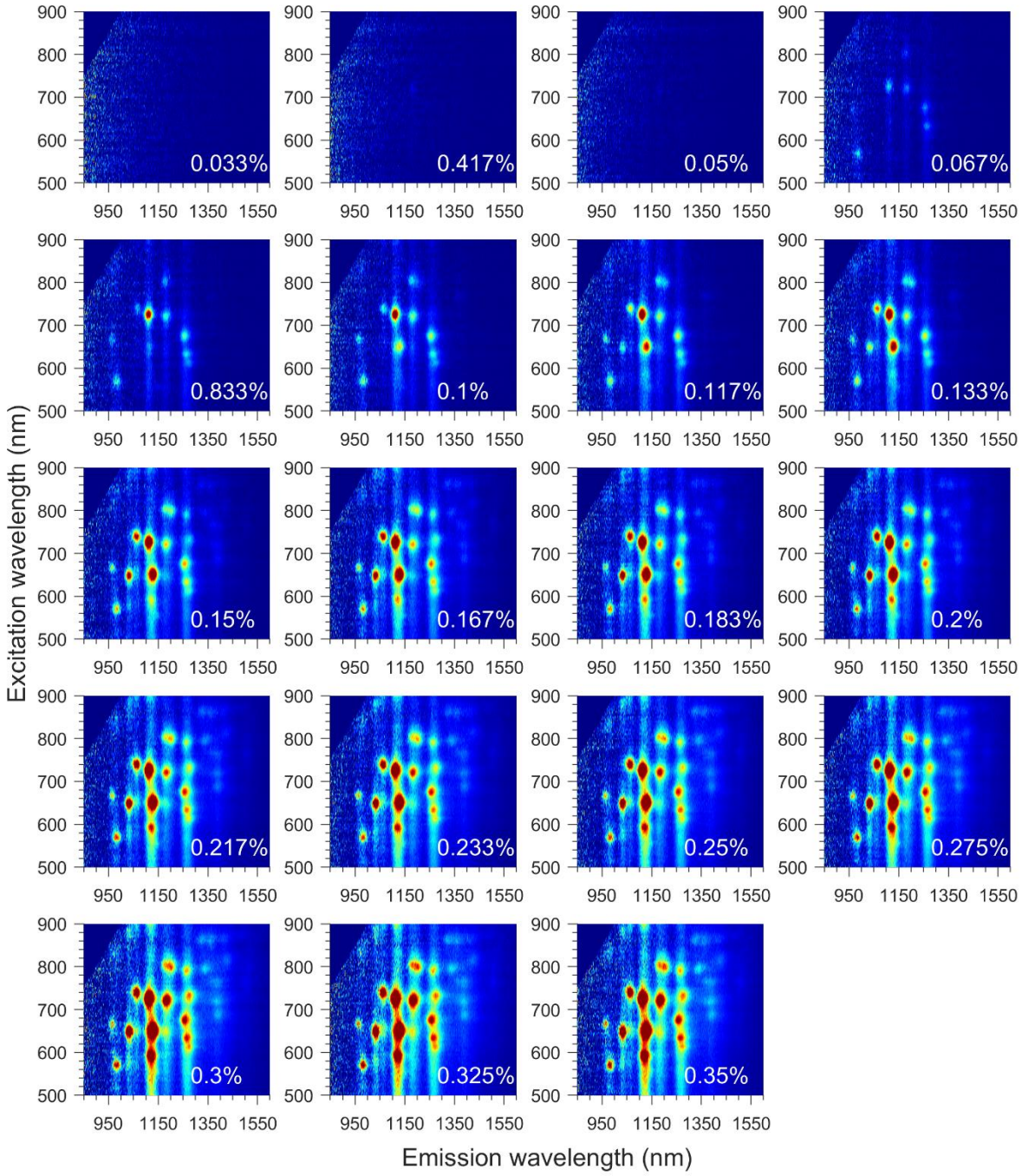

Figure S1.6: Overview of PLE maps of the bottom phases for the CDOC alone experiment. Intensities can be directly compared, and CDOC concentrations are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

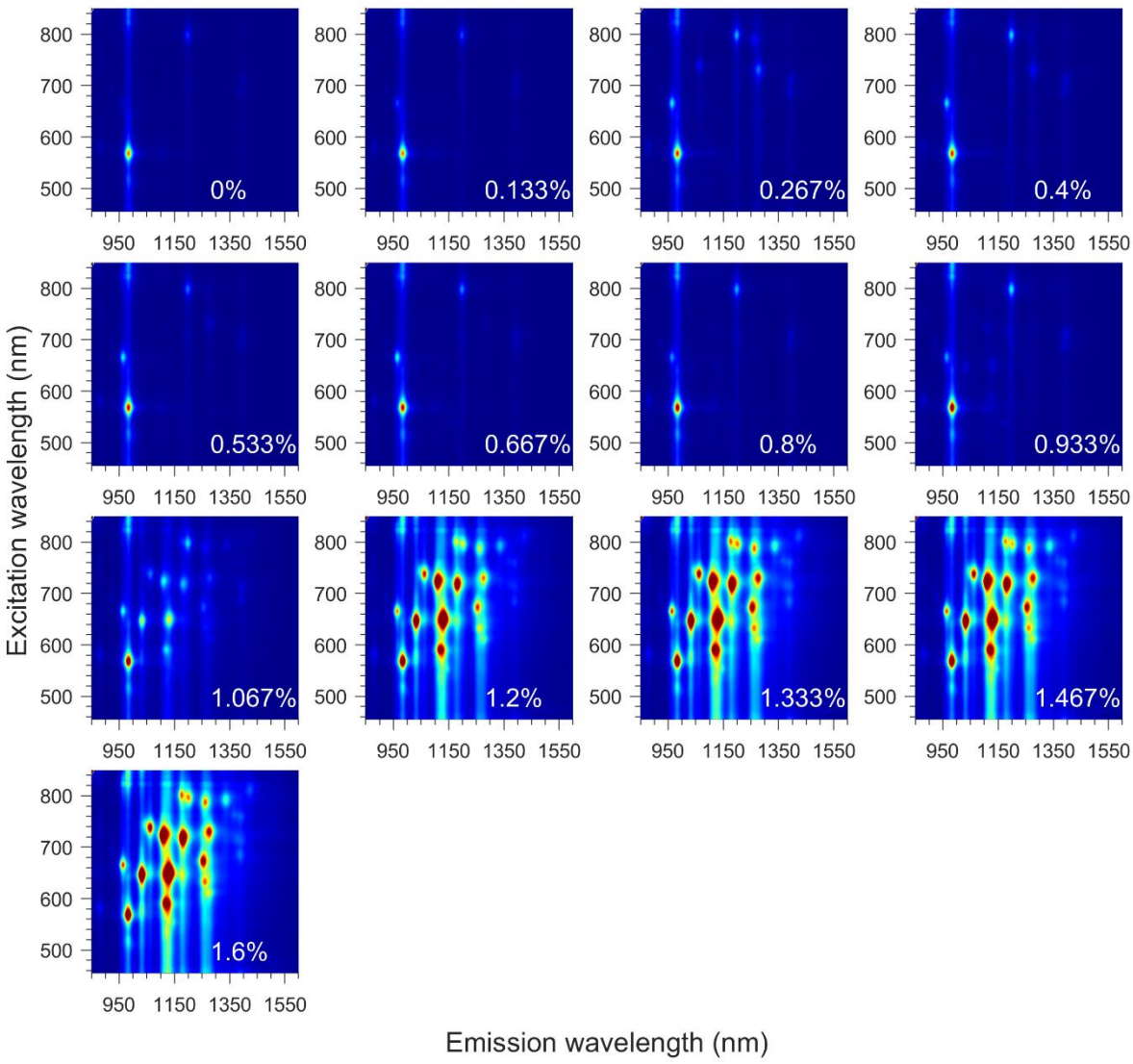

Figure S1.7: Overview of PLE maps of the bottom phases for the SDBS/DOC/SC variations. Intensities can be directly compared, and SC concentrations are written in white on the corresponding PLE maps. The colormaps are all plotted with the same minimum and maximum value, so that they can be directly compared, with blue corresponding to a zero intensity and red to maximum intensity.

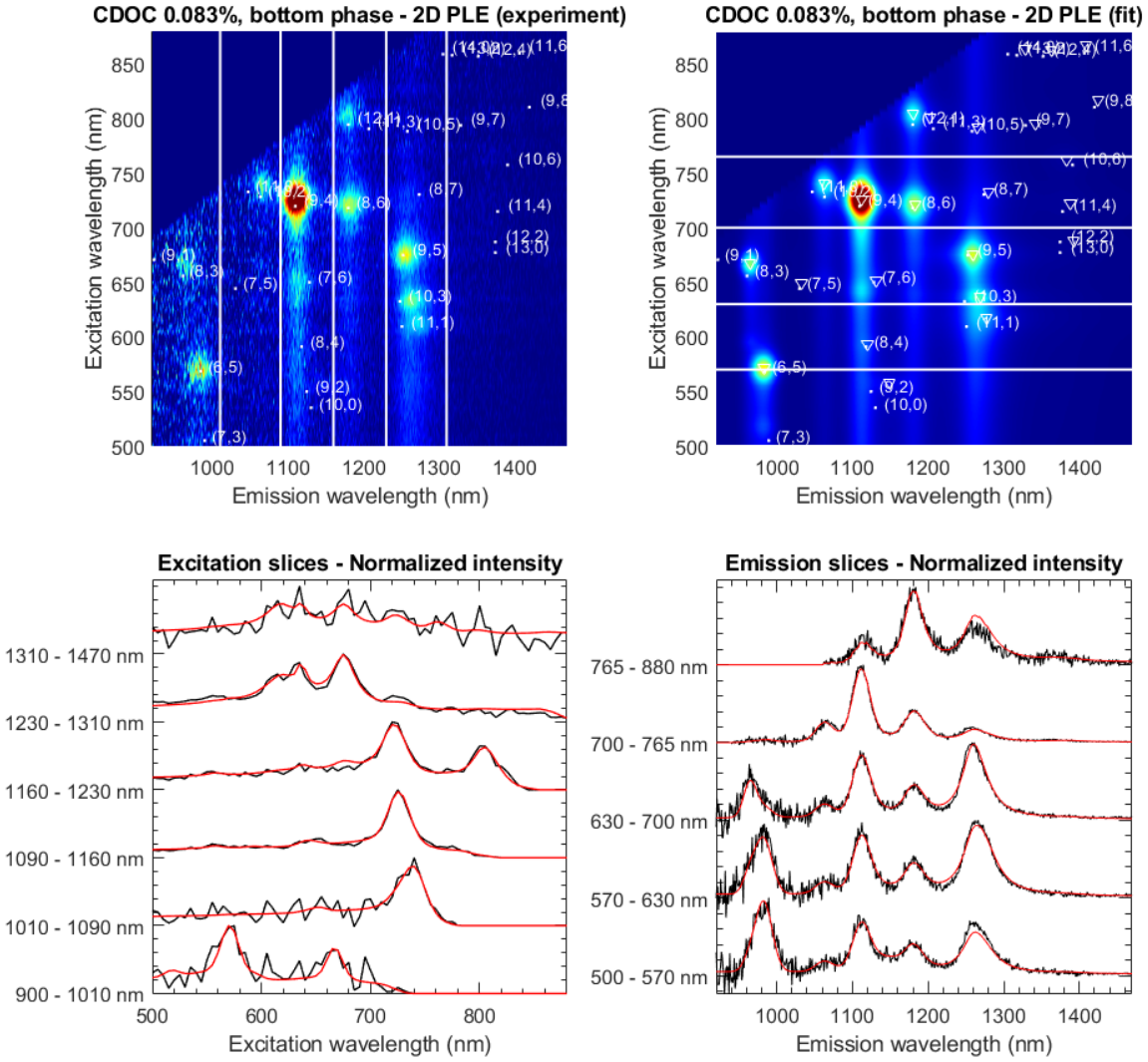

Figure S1.8: 2D PLE experimental data and fits for the bottom phase for CDOC concentration 0.083% wt/V (without any cosurfactants). The top left panel represents the experimental data, while the top right panel represents the 2D fit of the experimental data. The bottom two panels then represent excitation and emission slices of the experimental data (black) and fits (red), obtained by integrating over specific emission or excitation ranges, respectively, as indicated in the panels and also highlighted in the PLE maps by the white lines.

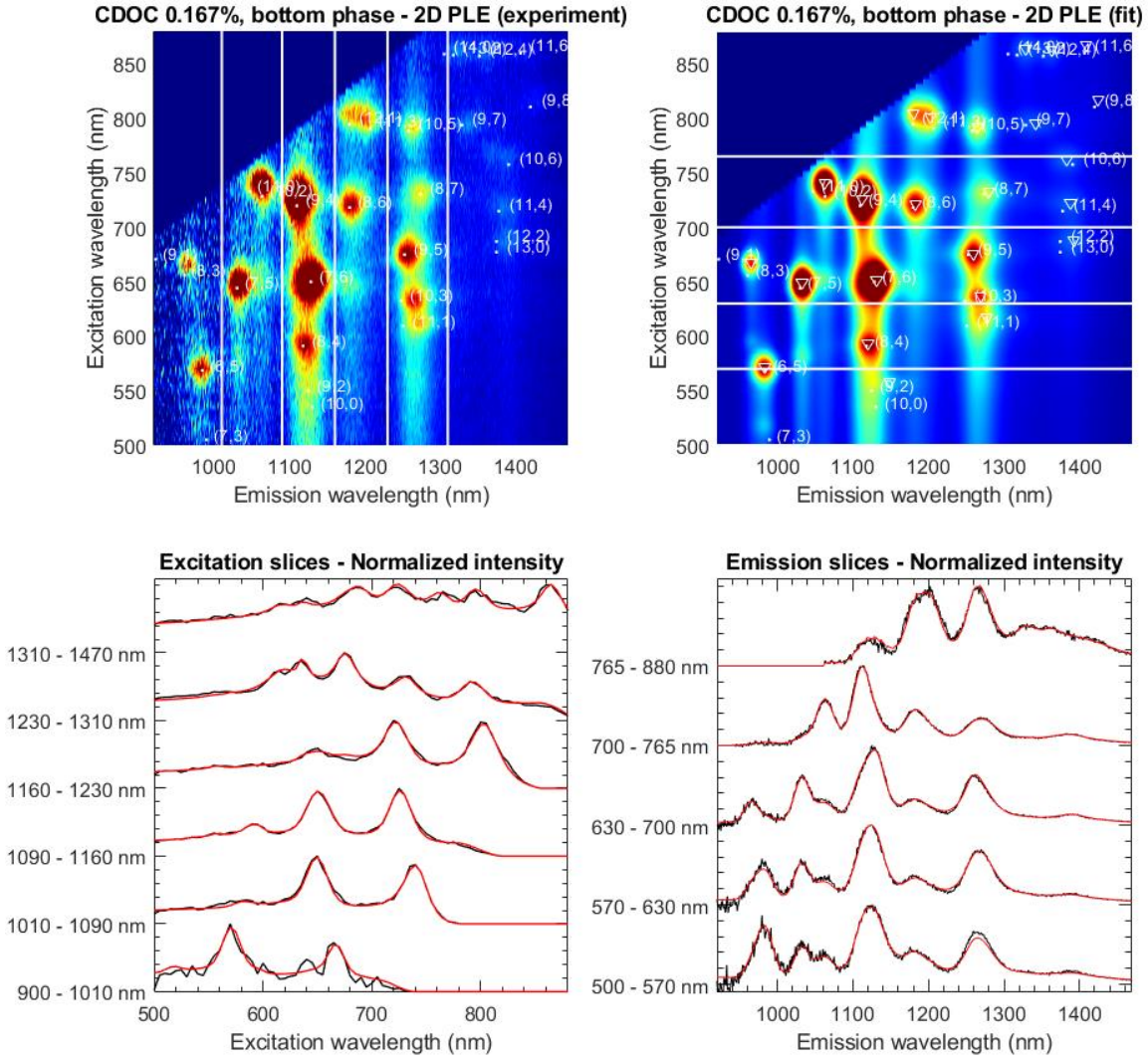

Figure S1.9: 2D PLE experimental data and fits for the bottom phase for CDOC concentration 0.167% wt/V (without any cosurfactants). Same color coding as in Figure S1.8.

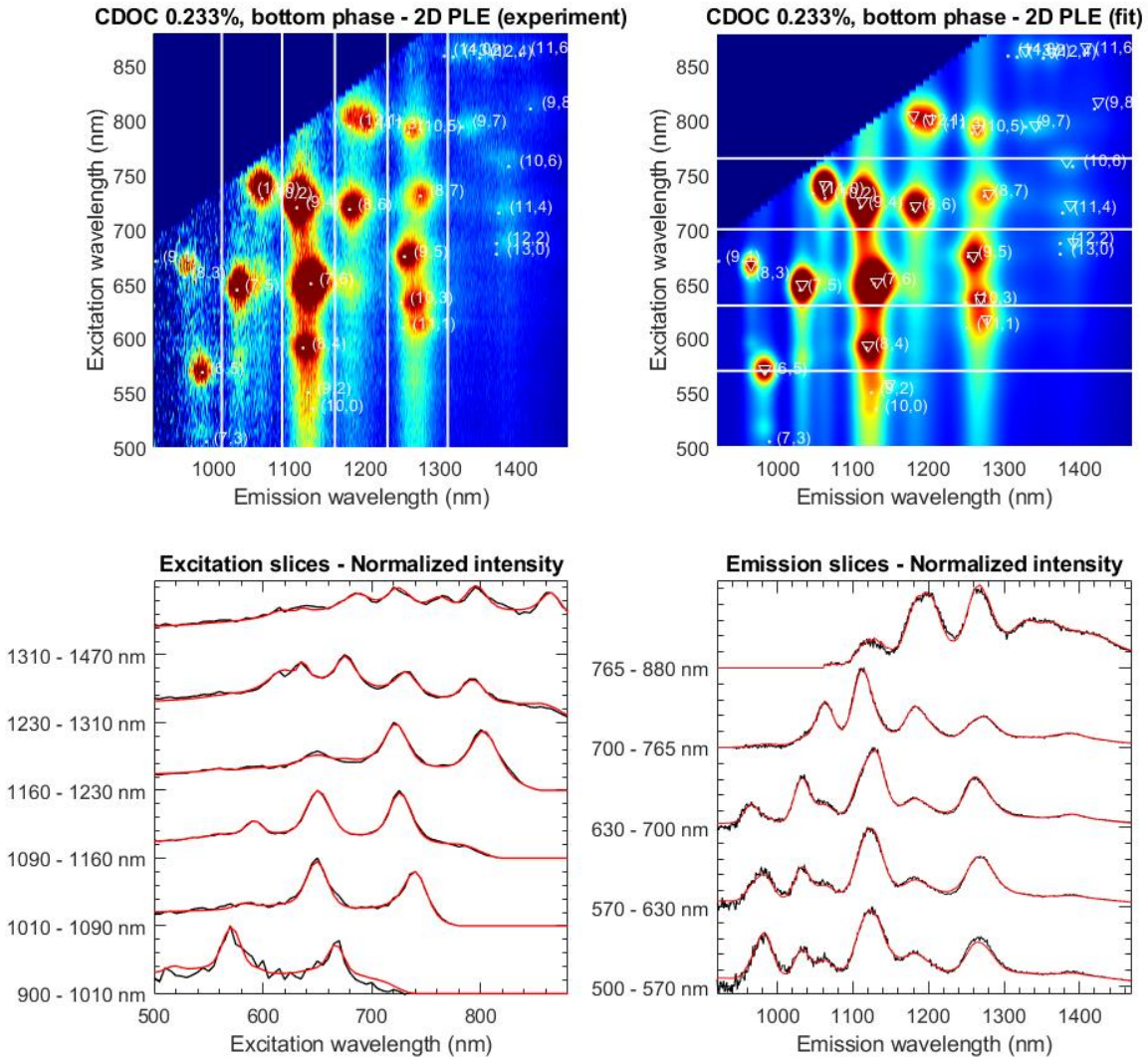

Figure S1.10: 2D PLE experimental data and fits for the bottom phase for CDOC concentration 0.233% wt/V (without any cosurfactants). Same color coding as in Figure S1.8.

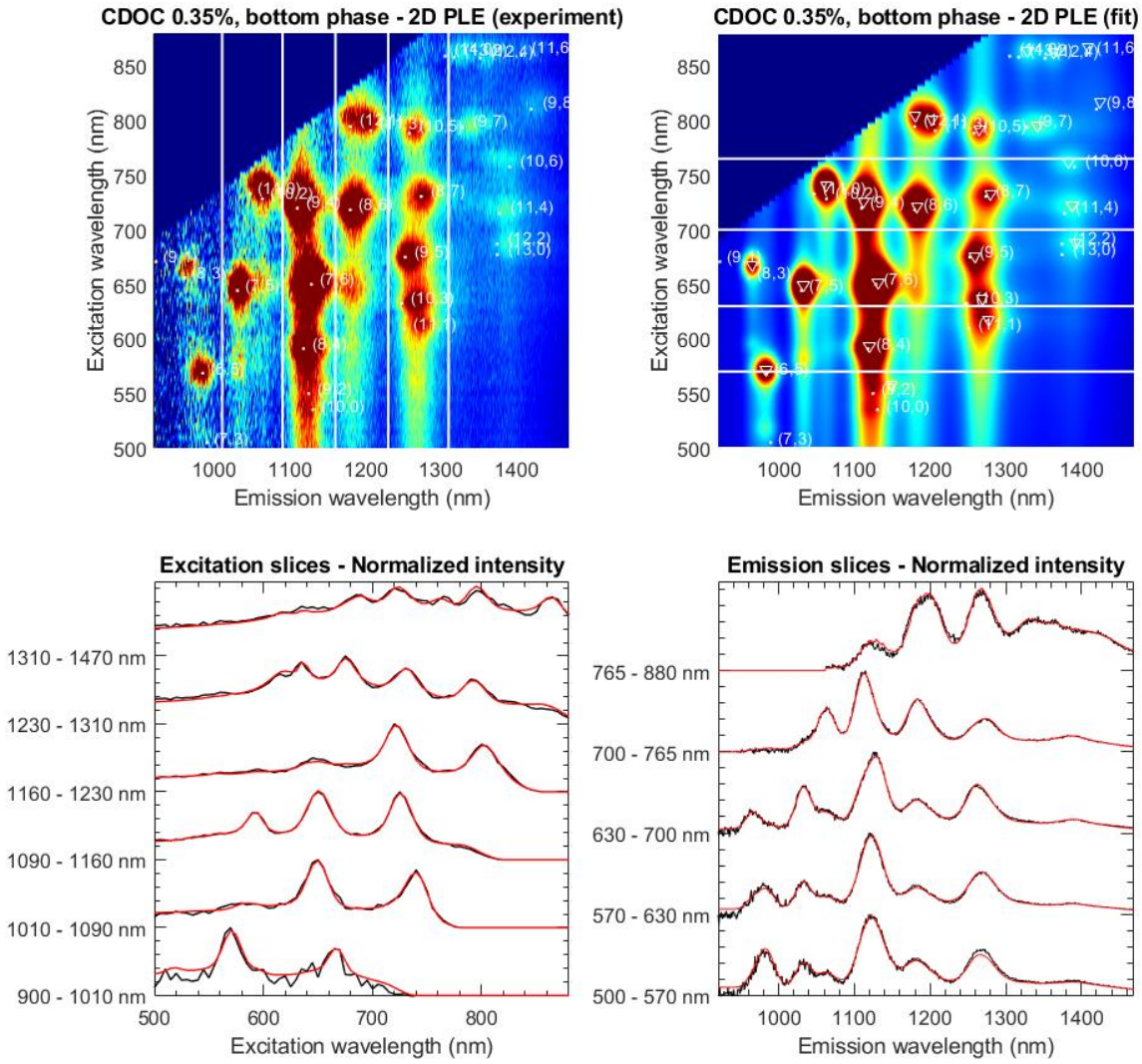

Figure S1.11: 2D PLE experimental data and fits for the bottom phase for CDOC concentration 0.35% wt/V (without any cosurfactants). Same color coding as in Figure S1.8.

Table S8: SWCNT chiralities probed with PLE in different systematic ATPE experiments.

Chirality	A systematic ATPE experiment						
	DOC	**SC**	**CDOC**	**SDS/DOC**	**SDS/SC**	**SDS/CDOC**	**SC/DOC-SDBS**
(6,4)	–	–	–	–	–	–	+
(6,5)	+	+	+	+	+	+	+
(7,5)	+	+	+	+	+	+	+
(7,6)	+	+	+	+	+	+	+
(8,3)	+	+	+	+	+	+	+
(8,4)	+	+	+	+	+	+	+
(8,6)	+	+	+	+	+	+	+
(8,7)	+	+	+	+	+	+	+
(9,2)	+	+	+	+	+	+	+
(9,4)	+	+	+	+	+	+	+
(9,5)	+	+	+	+	+	+	+
(9,7)	+	+	+	+	+	+	+
(9,8)	+	+	+	+	+	+	+
(10,0)	–	–	–	–	–	–	+
(10,2)	+	+	+	+	+	+	+
(10,3)	+	+	+	+	+	+	+
(10,5)	+	+	+	+	+	+	+
(10,6)	+	+	+	+	+	+	+
(11,1)	+	+	+	+	+	+	+
(11,3)	+	+	+	+	+	+	+
(11,4)	+	+	+	+	+	+	+
(11,6)	+	–	+	+	+	+	–
(12,1)	+	+	+	+	+	+	+
(12,2)	+	+	+	+	+	+	+
(12,4)	+	–	+	+	+	+	–
(13,2)	+	–	+	+	+	+	–
Total number of chiralities	**24**	**21**	**24**	**24**	**24**	**24**	**23**

Section 3. Examples of resonant Raman spectra and their fits at different excitation wavelengths

Table S9: Excitation wavelengths and corresponding measured SWCNT chiralities in RRS in different systematic ATPE experiments.

Laser	Excitation wavelength	Chiralities in each systematic ATPE experiment			
		DOC CDOC SDS/DOC SDS/SC	**SC**	**SDS/CDOC**	**SC/DOC-SDBS**
Ti:Sapphire	824 nm	(5,4)			–
	785 nm	(9,7), (10,5), (11,3), (12,1)			
	725 nm	(11,4), (8,7), (8,6), (9,4), (10,2)	(8,7), (8,6), (9,4), (10,2)	(11,4), (8,7), (8,6), (9,4), (10,2)	
	710 nm	(5,3), (9,1)	(9,1)	(5,3), (9,1)	–
Ar^+	502 nm	(7,7), (8,5), (9,3)			–
	457 nm	(12,2), (6,6), (7,4)			–
Kr^+	647 nm	(10,3), (7,6), (7,5), (8,3), (14,2), (13,4), (12,6), (16,1)			–
Rh6G Dye Laser	570 nm	(10,4), (11,2), (6,5), (6,4), (7,2)		(11,2), (6,5), (6,4), (7,2)	(10,4), (11,2), (6,5), (6,4), (7,2)
Total number of chiralities		**31**	**29**	**30**	**14**

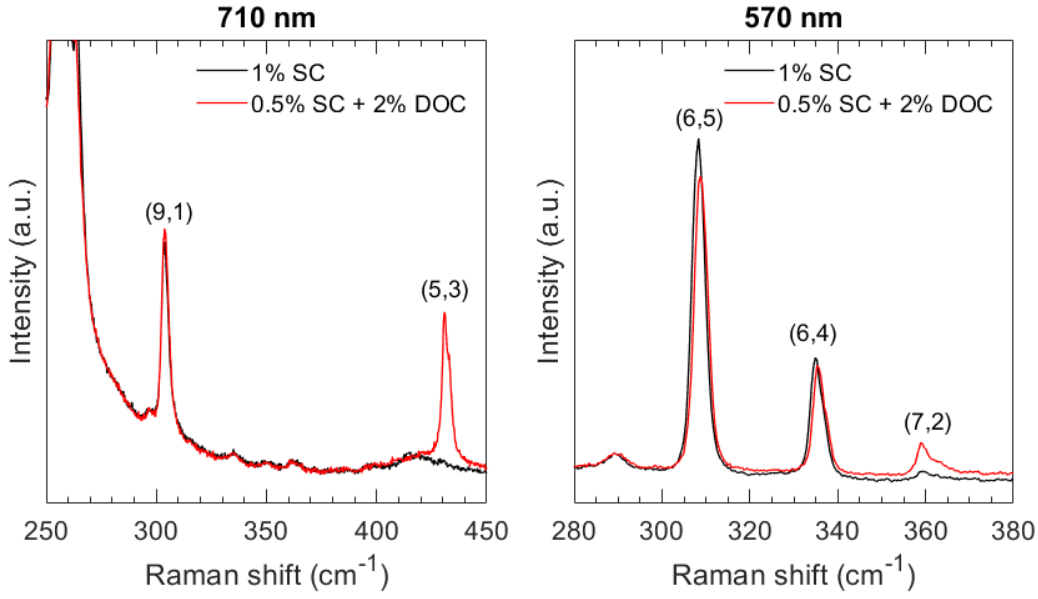

Figure S2.1: Raman spectra obtained at 710 nm (in resonance with the (5,3) chirality) and 570 nm (in resonance with the (6,5), (6,4) and (7,2) chiralities) for a 1% SC SWCNT solution (in black) and the same solution after the dilution to 2 wt/V% DOC (in red), showing that the Raman cross-sections of the (5,3) and (7,2) SWCNTs are strongly suppressed in SC compared to DOC.

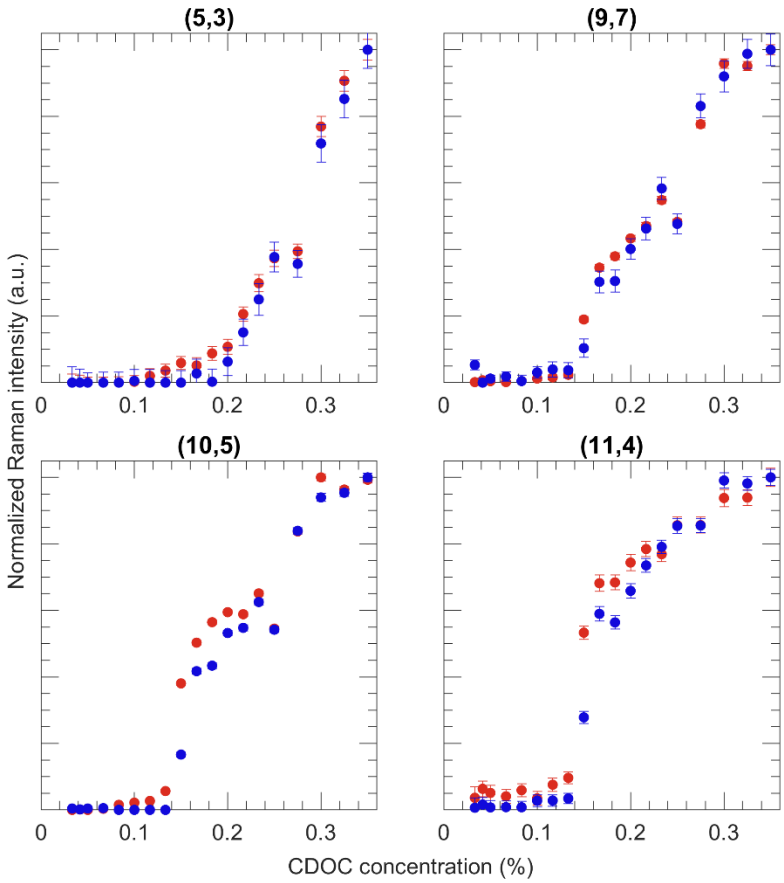

Figure S2.2: Normalized Raman intensities for a selection of SWCNT chiralities as a function of increasing CDOC concentration: transition curves for empty and water-filled SWCNTs are shown with red and blue circles, respectively. While relative intensities of left- or right-handed empty or water-filled SWCNTs may be different, there are not differences observed in the transition points, thus in these cases the empty and water-filled intensities were added together to fit the transition points. If two-step enantiomer transitions are present, they are observed for both the empty and the water-filled SWCNTs. The fitted error bars are plotted, but often smaller than the marker size.

3.1: Raman spectra at 824 nm: (5,4)

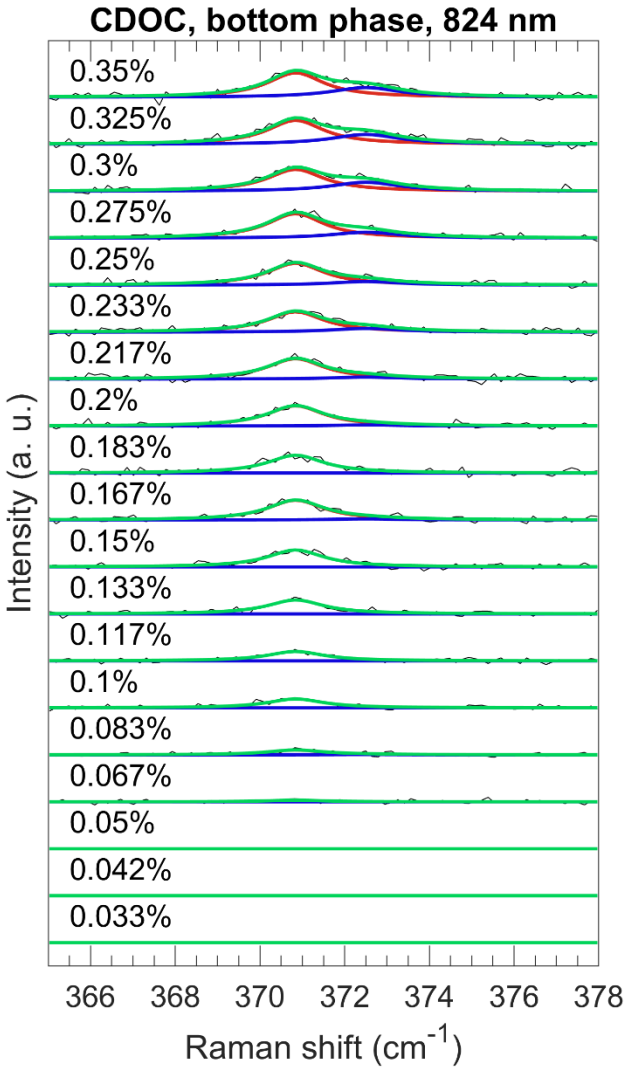

Figure S3.1: Individual Raman spectra at 824 nm of the different bottom phases (black) and fits (green) composed out of RBMs of both empty and water-filled (5,4) SWCNTs (individual Lorentzians are shown in red and blue, respectively). The values on the left in black denote the CDOC concentration.

3.2: Raman spectra at 785 nm: (9,7), (10,5), (11,3) and (12,1)

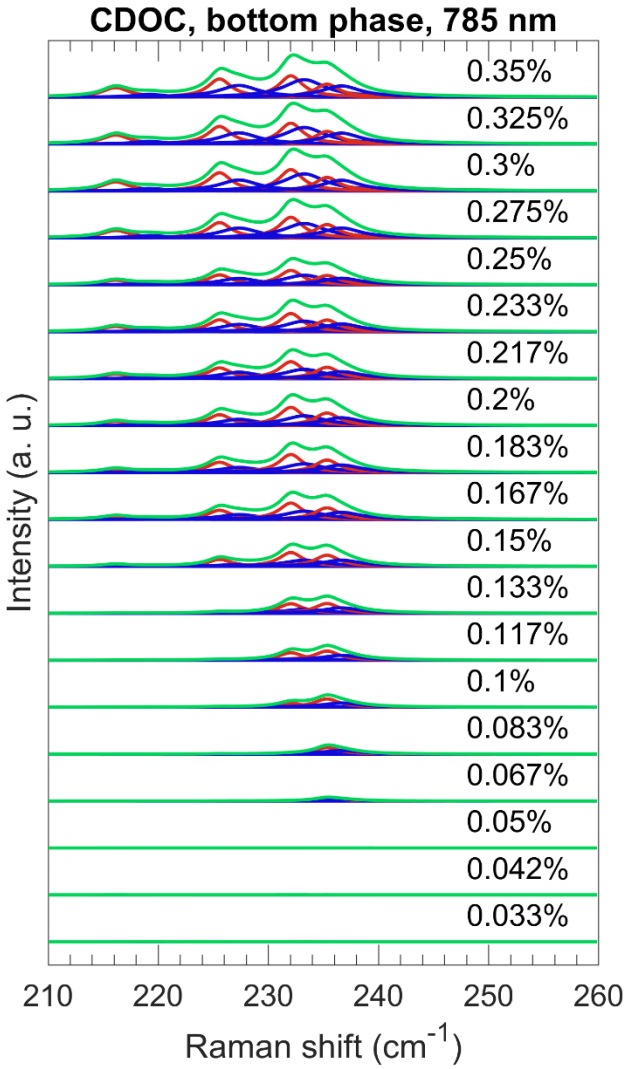

Figure S3.2: RRS spectra (black) and fits (green) obtained at 785 nm composed out of individual Lorentzians corresponding to the RBMs of both empty (red) and water-filled (blue) (9,7), (10,5), (11,3) and (12,1) SWCNTs (assigned from lower to higher Raman frequency, respectively). The values on the right in black denote the CDOC concentration.

3.3: Raman spectra at 725 nm: (11,4), (8,7), (8,6), (9,4) and (10,2)

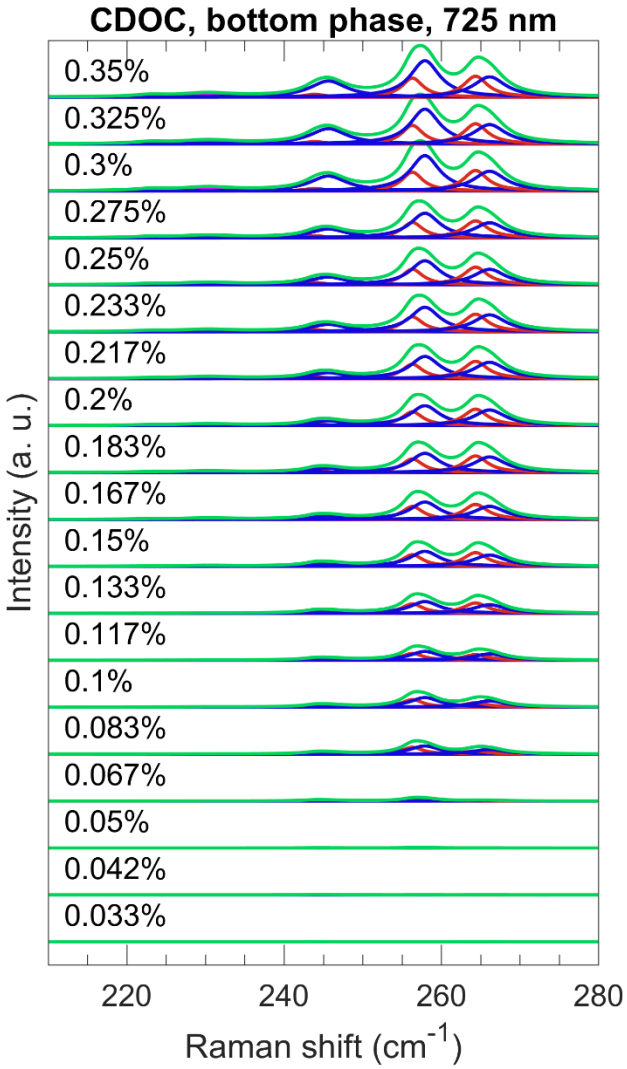

Figure S3.3: RRS spectra (black) and fits (green) obtained at 725 nm composed out of individual Lorentzians corresponding to the RBMs of both empty (red) and water-filled (blue) (11,4), (8,7), (8,6), (9,4) and (10,2) SWCNTs (assigned from lower to higher Raman frequency respectively). The values on the left in black denote the CDOC concentration.

3.4: Raman spectra at 710 nm: (5,3) and (9,1)

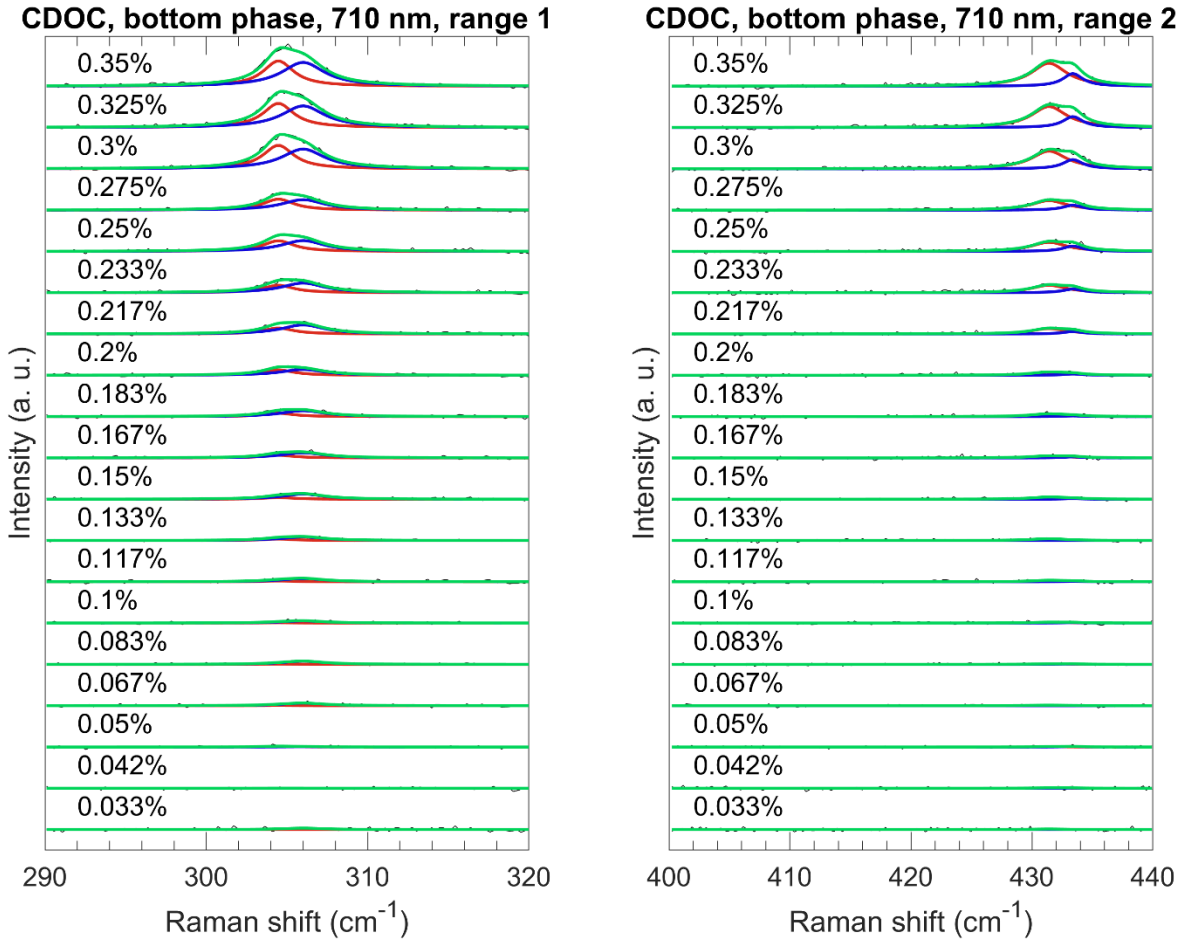

Figure S3.4: RRS spectra (black) and fits (green) obtained at 710 nm composed of individual Lorentzians corresponding to the RBMs of empty (red) and water-filled (blue) (9,1) (the left panel) and (5,3) (the right panel) SWCNTs. The values on the left of each panel in blue denote the CDOC concentration.

3.5: Raman spectra at 502 nm: (7,7), (8,5) and (9,3)

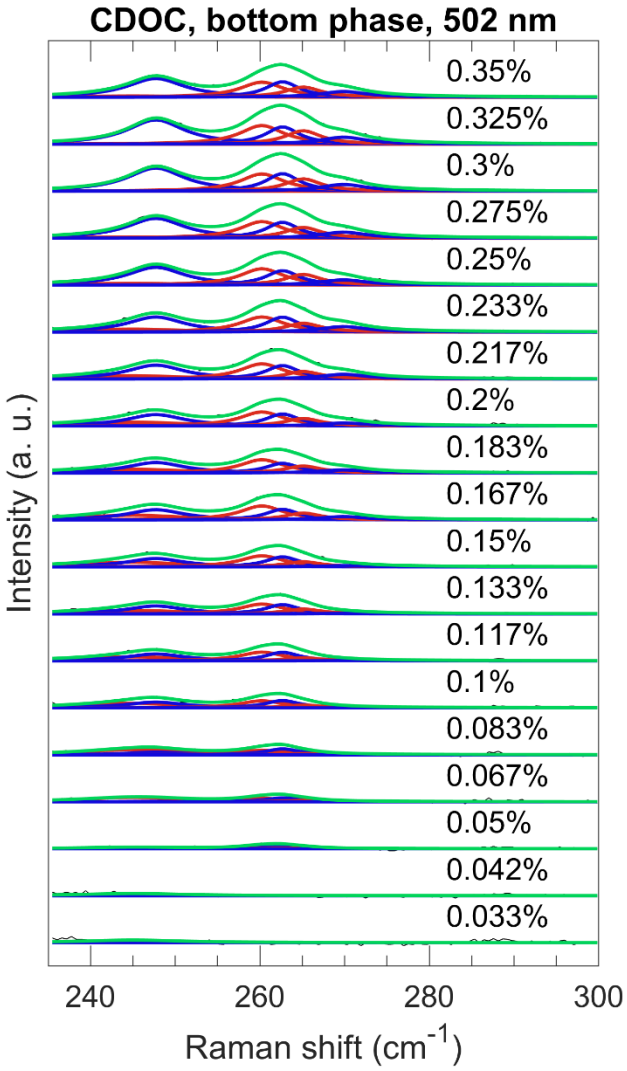

Figure S3.5: RRS spectra (black) and fits (green) obtained at 502 nm composed out of individual Lorentzians corresponding to the RBMs of empty (red) and water-filled (blue) (7,7), (8,5) and (9,3) SWCNTs (assigned from lower to higher Raman frequency respectively). The values on the right in black denote the CDOC concentration.

3.6: Raman spectra at 457 nm: (12,2), (9,3), (6,6) and (7,4)

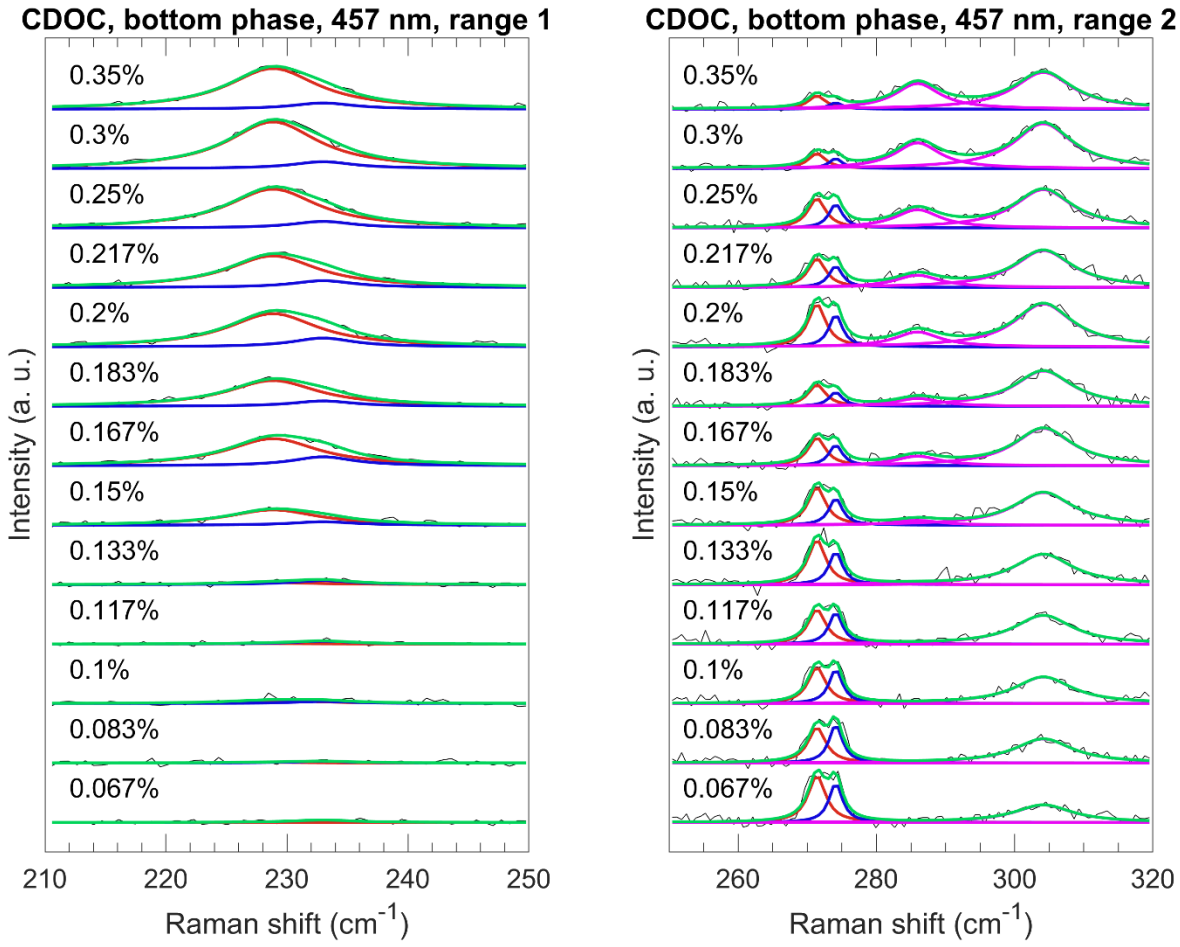

Figure S3.6: RRS spectra (black) and fits (green) obtained at 457 nm composed of individual Lorentzians corresponding to the RBMs of empty (red) and water-filled (blue) (12,2) (the left panel) and (9,3), (6,6) and (7,4) (the right panel) SWCNTs (assigned from lower to higher Raman frequency respectively). The Lorentzians shown in magenta correspond to the cases when empty and water-filled contributions of a certain chirality are not resolved. The values on the left of each panel in blue denote the CDOC concentration.

3.7: Raman spectra at 647 nm: (10,3), (7,6), (7,5), (8,3), (14,2), (13,4), (12,6) and (16,1)

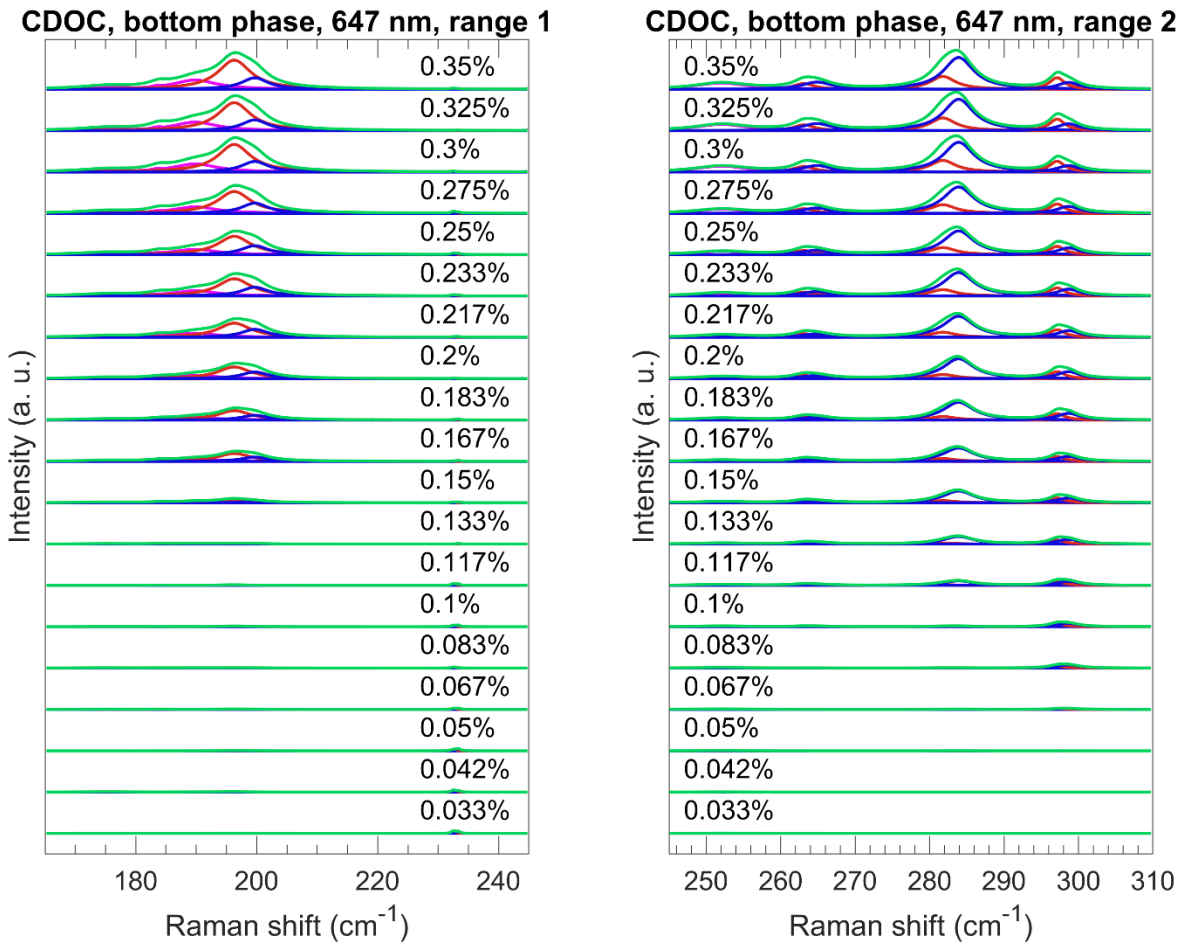

Figure S3.7: RRS spectra (black) and fits (green) obtained at 647 nm composed out of individual Lorentzians corresponding to the RBMs of empty (red) and water-filled (blue) (16,1), (14,2), (13,4), (12,6) (the left panel), and (10,3), (7,6), (7,5) and (8,3) SWCNTs (the right panel, assigned from lower to higher Raman frequency respectively). The Lorentzians shown in magenta correspond to the cases when empty and water-filled contributions of a certain chirality are not resolved. The values in black denote the CDOC concentration.

3.8: Raman spectra at 570 nm: (10,4), (11,2), (6,5), (6,4) and (7,2)

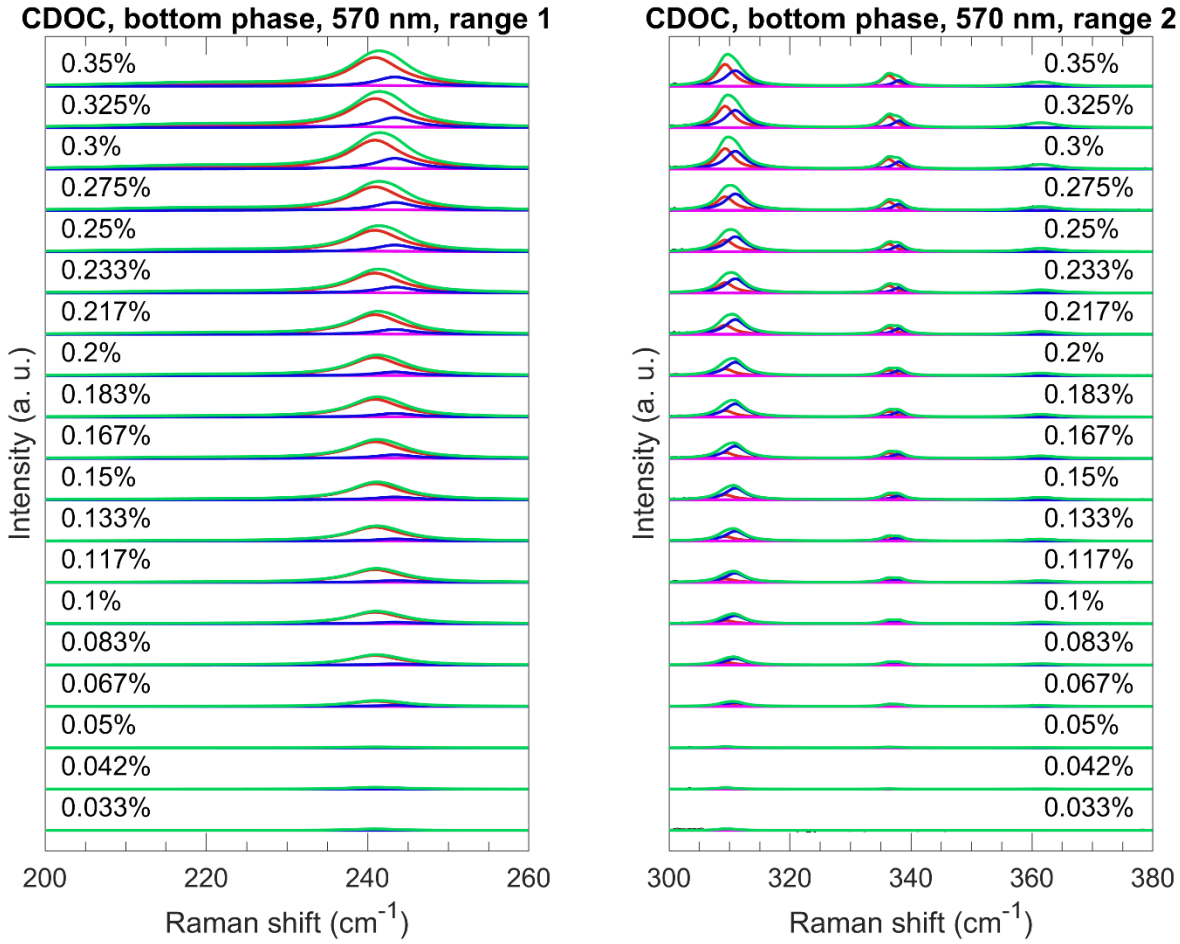

Figure S3.8: RRS spectra (black) and fits (green) obtained at 570 nm composed out of individual Lorentzians corresponding to the RBMs of empty (red) and water-filled (blue) (10,4) and (11,2) (the left panel) and (6,5), (6,4) and (7,2) SWCNT (the right panel, assigned from lower to higher Raman frequency respectively). The Lorentzians shown in magenta correspond to the cases when empty and water-filled contributions of a certain chirality are not resolved. The values in black denote the CDOC concentration.

Section 4. Examples of the fits of the partition coefficient curves

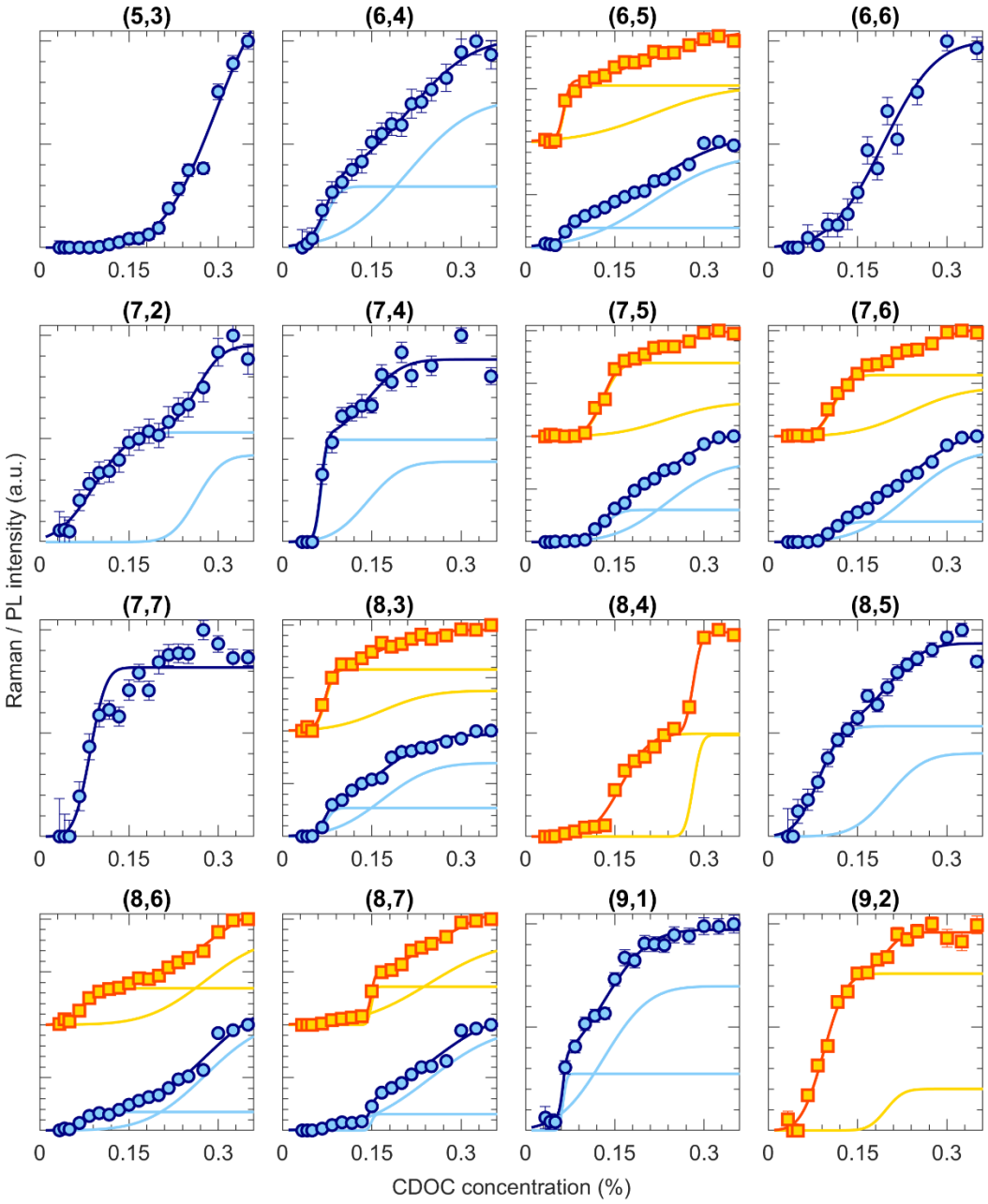

Figure S4 continues on next page

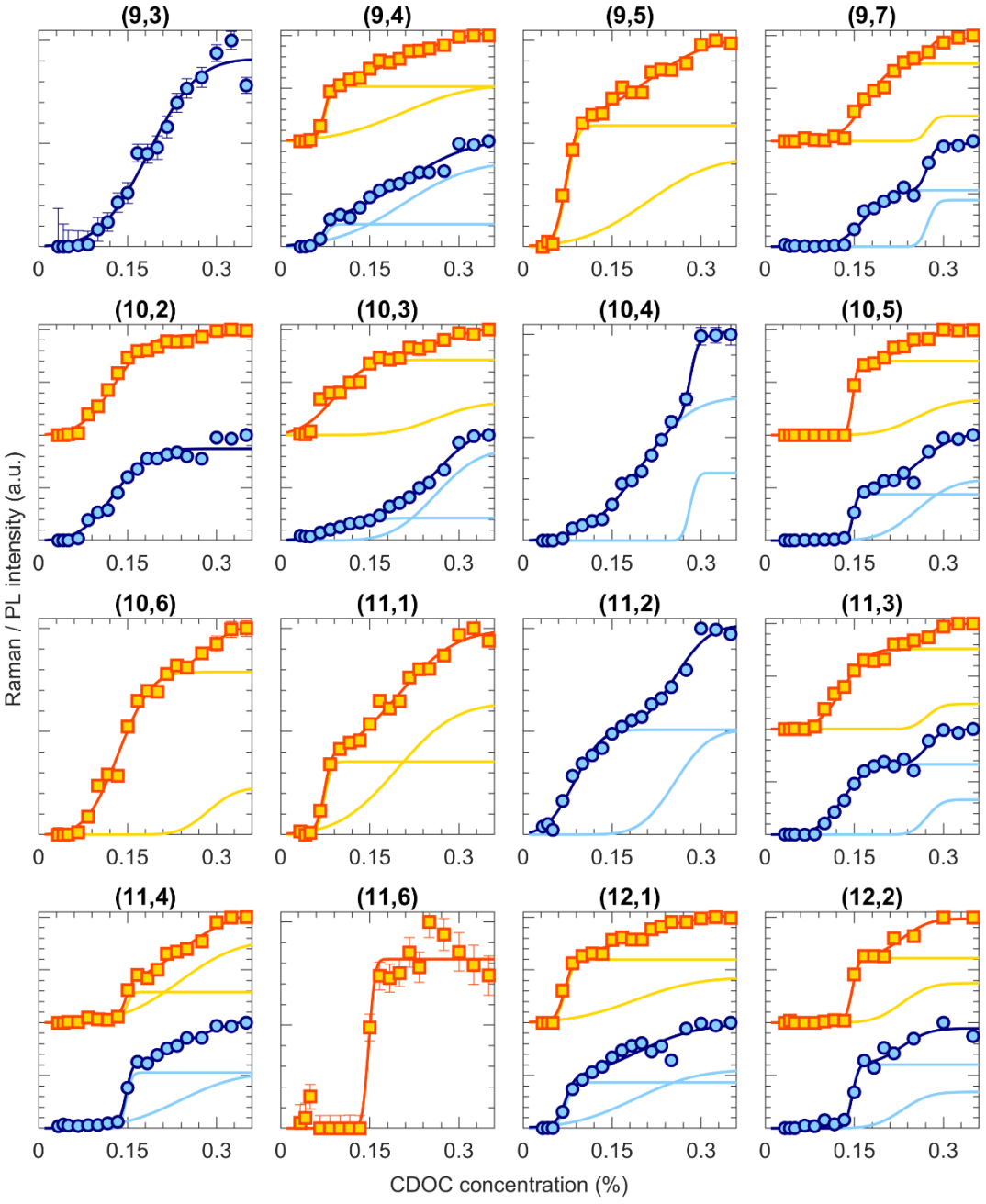

Figure S4 continues on next page

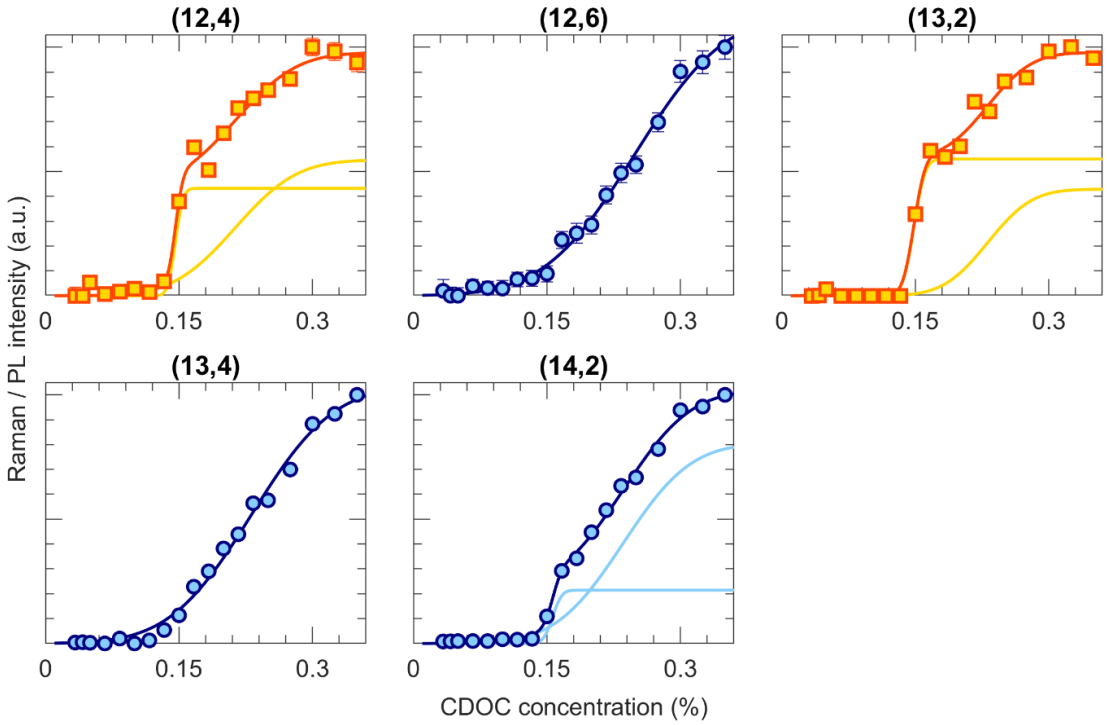

Figure S4.1: Normalized PL (yellow squares) and Raman (blue circles) intensities for SWCNT chiralities as a function of increasing CDOC concentration. The fit components are shown with yellow and blue solid lines, their sums are shown in orange and darker blue.

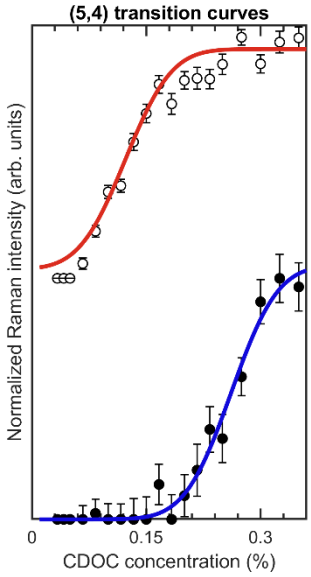

Figure S4.2: Raman transition curves for empty (open circles) and water-filled (filled circles) (5,4) SWCNTs as a function of increasing CDOC concentration and their fit with an error function shown with the red and blue lines, respectively.

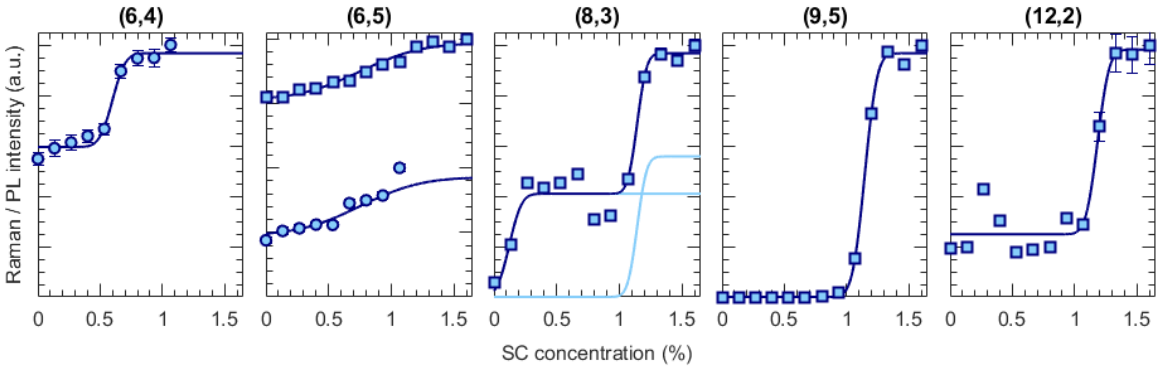

Figure S5: Normalized PL (squares) and Raman (circles) intensities in the bottom phase for a selected set of SWCNT chiralities in the SC/DOC/SDBS systematic experiment, plotted as a function of added SC concentration while the concentrations of DOC and SDBS are kept constant at 0.1 and 1.1 % wt/V, respectively. The fit components are shown with blue solid lines, their sums are shown in dark blue.

Section 5. Tables of transition points for all surfactant combinations

Table S10: Transitions points from **bottom to top phase** with increasing SDS concentration, as determined from the **bottom phase data** for SWCNTs in SDS/DOC (at a fixed concentration of 0.0507% wt/V DOC). The cells with white and grey background correspond to the transitions shown in black and dark gray in Figure 4 of the main text, respectively. Here and further, the 'ratio' stands for the mass ratio of the used surfactants.

Chirality	Diameter, nm	First transition (position), SDS/DOC ratio	First transition (position error), SDS/DOC ratio	First transition (width), SDS/DOC ratio	First transition (width error), SDS/DOC ratio	Second transition (position), SDS/DOC ratio	Second transition (position error), SDS/DOC ratio	Second transition (width), SDS/DOC ratio	Second transition (width error), SDS/DOC ratio
(5,4)	0.611	25.772	0.503	4.339	0.728				
(6,4)	0.683	34.214	0.511	1.899	0.686				
(6,6)	0.814	17.005	0.448	6.486	0.595				
(7,4)	0.755	28.558	0.895	6.459	1.499				
(7,5)	0.817	12.926	0.134	0.706	0.103				
(7,6)	0.882	14.473	0.146	1.027	0.181				
(7,7)	0.949	15.763	0.573	6.069	0.764				
(8,5)	0.889	15.700	0.578	3.979	0.774				
(8,6)	0.952	12.510	0.094	0.818	0.097				
(8,7)	1.018	24.405	0.358	3.544	0.483				
(9,1)	0.747	20.509	0.603	6.119	0.843				
(9,4)	0.903	11.932	0.081	0.797	0.450				
(9,5)	0.962	13.722	0.054	1.505	0.077				
(9,7)	1.088	18.122	0.180	2.146	0.245				
(10,3)	0.923	17.209	0.379	2.998	0.495				
(10,4)	0.978	18.185	0.259	4.699	0.349				
(10,5)	1.036	24.496	0.186	2.685	0.253				
(10,6)	1.096	17.283	0.207	2.318	0.280				
(11,2)	0.949	16.103	0.481	5.347	0.645				
(11,4)	1.053	20.787	0.365	3.983	0.506				
(11,6)	1.169	12.006	0.360	3.016	0.445				
(12,2)	1.027	23.739	0.280	3.583	0.378				
(13,2)	1.104	15.729	0.205	2.331	0.278				
(14,2)	1.182	15.513	0.299	5.945	0.421				
(7,2)	0.641	9.868…11.96		<2.092		18.056	1.062	4.702	0.897
(11,1)	0.903	11.84…13.82		<0.99		23.286	2.583	5.429	3.030
(6,5)	0.747	23.563	2.890	9.182	3.232	33.5…35.53		<1.015	
(12,1)	0.981	12.999	0.421	0.916	0.386	19.76…21.71		<0.975	
(5,3)	0.548	12.473	0.374	0.436	0.389	16.148	1.012	7.629	0.910
(8,3)	0.771	19.889	2.344	4.047	2.173	27.305	0.262	1.509	0.352
(8,4)	0.829	12.887	0.059	0.757	0.052	17.810	2.606	6.754	1.843
(9,3)	0.847	14.935	0.521	1.698	0.774	21.744	5.249	4.328	3.563
(10,2)	0.872	13.367	0.228	0.658	0.316	23.343	0.194	3.259	0.256
(11,3)	1.000	22.556	0.381	1.715	0.521	36.478	0.582	0.879	0.507
(12,4)	1.129	12.018	0.127	0.796	0.420	18.756	0.808	3.452	0.664
(12,6)	1.243	6.108	1.583	0.487	4.411	16.663	0.182	2.361	0.185
(13,4)	1.205	7.410	0.143	0.982	0.192	16.571	0.149	2.572	0.212

Table S11: Transitions points from **bottom to top phase** with increasing SDS concentration, as determined from the **bottom phase data** for SWCNTs in SDS/SC (at a fixed concentration of 0.425% wt/V SC). The cells with white, grey, red and blue background correspond to the transitions shown in black, dark gray, red and blue in Figure 4 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), SDS/SC ratio	First transition (position error), SDS/SC ratio	First transition (width), SDS/SC ratio	First transition (width error), SDS/SC ratio	Second transition (position), SDS/SC ratio	Second transition (position error), SDS/SC ratio	Second transition (width), SDS/SC ratio	Second transition (width error), SDS/SC ratio
(6,4)	0.683	0.269	0.008	0.084	0.013				
(6,6)	0.814	0.066	0.001	0.012	0.002				
(7,2)	0.641	0.046	0.000	0.006	0.000				
(7,6)	0.882	0.049	0.001	0.006	0.001				
(7,7)	0.949	0.041	0.001	0.008	0.002				
(8,3)	0.771	0.113	0.005	0.016	0.006				
(8,4)	0.829	0.050	0.001	0.007	0.002				
(8,5)	0.889	0.049	0.001	0.009	0.001				
(8,7)	1.018	0.052	0.001	0.009	0.002				
(9,2)	0.795	0.068	0.005	0.032	0.009				
(9,3)	0.847	0.072	0.002	0.014	0.002				
(9,5)	0.962	0.034	0.001	0.009	0.001				
(9,8)	1.153	0.023	0.001	0.009	0.001				
(10,3)	0.923	0.042	0.002	0.010	0.002				
(10,4)	0.978	0.045	0.001	0.010	0.001				
(10,6)	1.096	0.024	0.002	0.012	0.002				
(11,2)	0.949	0.045	0.000	0.007	0.001				
(11,3)	1.000	0.053	0.001	0.006	0.001				
(11,4)	1.053	0.048	0.001	0.010	0.001				
(11,6)	1.169	0.024	0.001	0.006	0.002				
(12,4)	1.129	0.024	0.001	0.011	0.002				
(12,6)	1.243	0.036	0.001	0.011	0.002				
(13,4)	1.205	0.049	0.002	0.024	0.002				
(9,1)	0.747	0.049	0.002	0.022	0.003	0.192	0.082	0.019	0.111

Chirality	Diameter, nm	Transition (position) of **empty** SWCNTs, SDS/SC ratio	Transition (position error) of **empty** SWCNTs, SDS/SC ratio	Transition (width) of **empty** SWCNTs, SDS/SC ratio	Transition (width error) of **empty** SWCNTs, SDS/SC ratio	Transition (position) of **water-filled** SWCNTs, SDS/SC ratio	Transition (position error) of **water-filled** SWCNTs, SDS/SC ratio	Transition (width) of **water-filled** SWCNTs, SDS/SC ratio	Transition (width error) of **water-filled** SWCNTs, SDS/SC ratio
(5,3)	0.548	0.042	0.001	0.004	0.001	0.051	0.005	0.004	0.006
(5,4)	0.611	0.158	0.017	0.088	0.021	0.058	0.007	0.031	0.008
(6,5)	0.747	0.117	0.007	0.060	0.013	0.170	0.007	0.024	0.005
(7,4)	0.755	0.218	0.005	0.025	0.006	0.240	0.010	0.023	0.014
(7,5)	0.817	0.054	0.001	0.011	0.002	0.067	0.008	0.009	0.012
(8,6)	0.952	0.038	0.000	0.002	0.000	0.044	0.009	0.009	0.012
(9,4)	0.903	0.043	0.000	0.007	0.000	0.046	0.001	0.008	0.002
(9,7)	1.088	0.016	0.006	0.021	0.004	0.041	0.011	0.010	0.015
(10,2)	0.872	0.047	0.000	0.006	0.000	0.053	0.005	0.003	0.012
(10,5)	1.036	0.048	0.000	0.006	0.000	0.059	0.005	0.007	0.007
(12,1)	0.981	0.052	0.001	0.002	0.001	0.056	0.005	0.009	0.007
(12,2)	1.027	0.058	0.001	0.012	0.002	0.078	0.009	0.006	0.012
(14,2)	1.182	0.051	0.001	0.012	0.002	0.068	0.012	0.007	0.016

Table S12: Transitions points from **bottom to top phase** with increasing SDS concentration, as determined from the **bottom phase data** for SWCNTs in SDS/CDOC (at a fixed concentration of 0.35% wt/V CDOC). The cells with white and grey background correspond to the transitions shown in black and dark gray in Figure 4 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), SDS/ CDOC ratio	First transition (position error), SDS/ CDOC ratio	First transition (width), SDS/ CDOC ratio	First transition (width error), SDS/ CDOC ratio	Second transition (position), SDS/ CDOC ratio	Second transition (position error), SDS/ CDOC ratio	Second transition (width), SDS/ CDOC ratio	Second transition (width error), SDS/ CDOC ratio
(5,3)	0.548	0.669	0.010	0.079	0.013				
(6,6)	0.814	0.5…0.642		<0.142					
(7,2)	0.641	0.733	0.024	0.136	0.029				
(7,5)	0.817	0.699	0.013	0.141	0.015				
(7,7)	0.949	0.618	0.012	0.103	0.014				
(8,3)	0.771	0.969	0.012	0.182	0.015				
(8,4)	0.829	0.650	0.024	0.110	0.025				
(8,6)	0.952	0.708	0.020	0.074	0.024				
(9,1)	0.747	1.336	0.031	0.135	0.040				
(9,2)	0.795	0.937	0.070	0.321	0.076				
(9,3)	0.847	0.620	0.096	0.161	0.067				
(9,4)	0.903	1.005	0.008	0.102	0.011				
(9,5)	0.962	0.715	0.010	0.067	0.014				
(9,7)	1.088	0.542	0.005	0.070	0.007				
(9,8)	1.153	0.521	0.003	0.066	0.004				
(10,2)	0.872	1.033	0.010	0.090	0.013				
(10,3)	0.923	0.777	0.014	0.161	0.018				
(10,5)	1.036	0.559	0.004	0.056	0.006				
(10,6)	1.096	0.590	0.006	0.058	0.007				
(11,2)	0.949	0.700	0.010	0.129	0.012				
(11,3)	1.000	0.582	0.006	0.052	0.008				
(11,4)	1.053	0.584	0.006	0.045	0.008				
(11,6)	1.169	0.517	0.002	0.045	0.003				
(12,1)	0.981	0.615	0.006	0.059	0.007				
(12,2)	1.027	0.609	0.026	0.104	0.032				
(12,4)	1.129	0.550	0.003	0.083	0.004				
(13,2)	1.104	0.570	0.005	0.047	0.008				
(13,4)	1.205	0.462	0.021	0.193	0.028				
(14,2)	1.182	0.472	0.009	0.149	0.013				
(11,1)	0.903	1…1.144		<0.144					
(5,4)	0.611	0.704	0.093	0.131	0.126	1.231	0.314	0.338	0.206
(6,5)	0.747	0.893	0.066	0.310	0.050	1.269	0.006	0.051	0.009
(7,6)	0.882	0.710	0.037	0.101	0.050	1.028	0.006	0.035	0.006
(8,7)	1.018	0.541	0.021	0.110	0.034	1.053	0.078	0.081	0.102
(6,4)	0.683	1.191	0.071	0.357	0.087	1.754…1.93		<0.176	
(7,4)	0.755	1.047	0.052	0.186	0.053	1.357…1.501		<0.144	
(8,5)	0.889	0.938	0.048	0.255	0.066	1.643…1.929		<0.286	

Table S13: Transitions from **top to bottom phase** with increasing DOC concentration as obtained from the **bottom phase data** for the SWCNTs in DOC alone. The cells with white and grey background correspond to the transitions shown in black and dark gray in Figure 6 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), % DOC	First transition (position error), % DOC	First transition (width), % DOC	First transition (width error), % DOC	Second transition (position), % DOC	Second transition (position error), % DOC	Second transition (width), % DOC	Second transition (width error), % DOC
(5,3)	0.548	0.02497	0.00071	0.00517	0.00110				
(6,6)	0.814	0.02374	0.00070	0.00265	0.00103				
(7,6)	0.882	0.07312	0.00327	0.02629	0.00409				
(7,7)	0.949	0.01838	0.00099	0.00578	0.00127				
(8,5)	0.889	0.07337	0.00199	0.02775	0.00296				
(9,3)	0.847	0.07177	0.00126	0.02591	0.00147				
(9,4)	0.903	0.06257	0.00268	0.02087	0.00330				
(10,2)	0.872	0.07606	0.00464	0.02993	0.00556				
(8,7)	1.018	<0.14		<0.07					
(9,7)	1.088	<0.125		<0.0625					
(10,5)	1.036	<0.125		<0.0625					
(10,6)	1.096	<0.14		<0.07					
(11,3)	1.000	<0.125		<0.0625					
(11,4)	1.053	<0.1		<0.05					
(11,6)	1.169	<0.125		<0.0625					
(12,1)	0.981	<0.14		<0.07					
(12,2)	1.027	<0.14		<0.07					
(12,4)	1.129	<0.09		<0.045					
(13,2)	1.104	<0.14		<0.07					
(9,5)	0.962	<0.013		<0.0065		0.05244	0.02001	0.03894	0.02004
(5,4)	0.611	0.02066	0.00222	0.00651	0.00438	0.07074	0.02026	0.04218	0.01883
(6,4)	0.683	0.02164	0.00083	0.00551	0.00167	0.07605	0.00868	0.03778	0.00989
(6,5)	0.747	0.01894	0.00090	0.00599	0.00132	0.05724	0.00626	0.06619	0.00577
(7,2)	0.641	0.02423	0.00046	0.00282	0.00079	0.07225	0.00597	0.03793	0.00568
(7,4)	0.755	0.01984	0.00189	0.00466	0.00263	0.05073	0.01842	0.08073	0.02206
(7,5)	0.817	0.02130	0.00097	0.00436	0.00177	0.06437	0.00655	0.03046	0.00577
(8,3)	0.771	0.01983	0.00193	0.00719	0.00320	0.06400	0.01879	0.05786	0.01416
(8,4)	0.829	0.02193	0.00091	0.00465	0.00172	0.07518	0.00354	0.03271	0.00425
(8,6)	0.952	0.02053	0.00070	0.00586	0.00150	0.05723	0.00880	0.02791	0.00653
(9,1)	0.747	0.05959	0.00391	0.02347	0.00665	0.11427	0.02338	0.08163	0.01648
(10,3)	0.923	0.02928	0.00205	0.00494	0.00240	0.05943	0.00285	0.02765	0.00194
(10,4)	0.978	0.02401	0.00184	0.00394	0.00397	0.04870	0.04224	0.05151	0.02983
(11,2)	0.949	0.02237	0.00087	0.00504	0.00142	0.04873	0.00503	0.04474	0.00491
(12,6)	1.243	0.02473	0.00081	0.00474	0.00158	0.05362	0.00379	0.02504	0.00239
(13,4)	1.205	0.02560	0.00121	0.00302	0.00281	0.05209	0.00217	0.02807	0.00159
(14,2)	1.182	0.02206	0.00176	0.01059	0.00170	0.06234	0.00455	0.01243	0.00477

Table S14: Transitions from **top to bottom phase** with increasing SC concentration as obtained from the **bottom phase data** for the SWCNTs in SC alone. The cells with white, grey, red and blue background correspond to the transitions shown in black, dark gray, red and blue in Figure 6 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), % SC	First transition (position error), % SC	First transition (width), % SC	First transition (width error), % SC	Second transition (position), % SC	Second transition (position error), % SC	Second transition (width), % SC	Second transition (width error), % SC
(6,4)	0.683	0.200	0.005	0.070	0.007				
(6,5)	0.747	0.209	0.005	0.074	0.007				
(6,6)	0.814	0.234	0.002	0.037	0.004				
(7,2)	0.641	0.261	0.002	0.029	0.003				
(7,4)	0.755	0.195	0.006	0.072	0.008				
(7,5)	0.817	0.232	0.002	0.046	0.003				
(7,6)	0.882	0.250	0.003	0.031	0.004				
(7,7)	0.949	0.275	0.002	0.027	0.002				
(8,3)	0.771	0.198	0.005	0.058	0.006				
(8,4)	0.829	0.221	0.002	0.031	0.003				
(8,5)	0.889	0.263	0.002	0.032	0.004				
(8,6)	0.952	0.270	0.002	0.031	0.003				
(8,7)	1.018	0.246	0.002	0.050	0.004				
(9,3)	0.847	0.251	0.002	0.040	0.003				
(9,4)	0.903	0.261	0.003	0.027	0.004				
(9,5)	0.962	0.268	0.003	0.026	0.005				
(9,7)	1.088	0.283	0.004	0.036	0.005				
(9,8)	1.153	0.324	0.006	0.047	0.005				
(10,2)	0.872	0.248	0.002	0.024	0.003				
(10,3)	0.923	0.266	0.004	0.042	0.005				
(10,4)	0.978	0.272	0.002	0.041	0.002				
(10,6)	1.096	0.319	0.031	0.067	0.024				
(11,1)	0.903	0.247	0.003	0.029	0.004				
(11,2)	0.949	0.265	0.002	0.027	0.003				
(11,3)	1.000	0.215	0.007	0.046	0.009				
(11,4)	1.053	0.316	0.005	0.026	0.005				
(12,6)	1.243	0.253	0.005	0.046	0.008				
(13,4)	1.205	0.237	0.005	0.058	0.007				
(14,2)	1.182	0.230	0.003	0.047	0.005				
(9,1)	0.747	0.137	0.024	0.025	0.027	0.250	0.009	0.036	0.010
(10,5)	1.036	0.181	0.002	0.012	0.004	0.271	0.004	0.013	0.006
(12,1)	0.981	0.182	0.004	0.009	0.013	0.250	0.016	0.043	0.015
(12,2)	1.027	0.158	0.006	0.013	0.009	0.245	0.006	0.033	0.008
Chirality	Diameter, nm	Transition (position) of **empty** SWCNTs, % SC	Transition (position error) of **empty** SWCNTs, % SC	Transition (width) of **empty** SWCNTs, % SC	Transition (width error) of **empty** SWCNTs, % SC	Transition (position) of **water-filled** SWCNTs, % SC	Transition (position error) of **water-filled** SWCNTs, % SC	Transition (width) of **water-filled** SWCNTs, % SC	Transition (width error) of **water-filled** SWCNTs, % SC
(5,4)	0.611	0.207	0.006	0.034	0.008	0.275	0.016	0.033	0.021

Table S15: Transitions from **top to bottom phase** with increasing CDOC concentration as obtained from the **bottom phase data** for the SWCNTs in CDOC alone. The cells with white, grey, red and blue background correspond to the transitions shown in black, dark gray, red and blue in Figure 6 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), % CDOC	First transition (position error), % CDOC	First transition (width), % CDOC	First transition (width error), % CDOC	Second transition (position), % CDOC	Second transition (position error), % CDOC	Second transition (width), % CDOC	Second transition (width error), % CDOC
(5,3)	0.548	0.295	0.019	0.071	0.012				
(6,6)	0.814	0.193	0.007	0.069	0.008				
(7,7)	0.949	0.085	0.006	0.021	0.007				
(9,3)	0.847	0.185	0.006	0.065	0.008				
(10,2)	0.872	0.127	0.004	0.046	0.005				
(11,6)	1.169	0.148	0.003	0.009	0.006				
(12,6)	1.243	0.248	0.006	0.080	0.005				
(13,4)	1.205	0.231	0.007	0.072	0.007				
(6,4)	0.683	0.072	0.005	0.019	0.011	0.209	0.020	0.086	0.030
(7,5)	0.817	0.130	0.002	0.022	0.003	0.239	0.011	0.070	0.013
(7,6)	0.882	0.110	0.002	0.022	0.003	0.237	0.008	0.072	0.014
(8,3)	0.771	0.072	0.002	0.012	0.003	0.168	0.010	0.065	0.009
(8,5)	0.889	0.083	0.012	0.032	0.009	0.202	0.028	0.048	0.028
(8,6)	0.952	0.073	0.004	0.022	0.005	0.278	0.012	0.078	0.013
(9,4)	0.903	0.075	0.003	0.009	0.003	0.205	0.014	0.089	0.015
(9,5)	0.962	0.073	0.002	0.015	0.003	0.209	0.019	0.086	0.026
(10,3)	0.923	0.091	0.007	0.044	0.008	0.260	0.012	0.058	0.017
(10,5)	1.036	0.148	0.002	0.007	0.004	0.255	0.009	0.049	0.016
(11,1)	0.903	0.074	0.003	0.010	0.003	0.196	0.011	0.077	0.013
(11,2)	0.949	0.086	0.007	0.036	0.008	0.256	0.010	0.046	0.015
(12,1)	0.981	0.071	0.003	0.012	0.005	0.188	0.029	0.083	0.029
(12,2)	1.027	0.146	0.001	0.009	0.002	0.230	0.010	0.037	0.015
(12,4)	1.129	0.146	0.003	0.007	0.005	0.213	0.014	0.055	0.011
(14,2)	1.182	0.156	0.003	0.008	0.004	0.236	0.006	0.060	0.005
(7,2)	0.641	0.090	0.007	0.048	0.008	0.264	0.008	0.034	0.011
(8,4)	0.829	0.161	0.004	0.038	0.005	0.282	0.003	0.011	0.003
(9,2)	0.795	0.093	0.003	0.030	0.003	0.198	0.009	0.023	0.011
(10,6)	1.096	0.135	0.006	0.043	0.006	0.286	0.021	0.037	0.033
(6,5)	0.747	0.05…0.084		<0.034		0.214	0.014	0.096	0.017
(7,4)	0.755	0.05…0.084		<0.034		0.142	0.025	0.046	0.024
(8,7)	1.018	0.133…0.167		<0.034		0.247	0.013	0.091	0.008
(9,1)	0.747	0.05…0.084		<0.034		0.131	0.007	0.060	0.006
(11,4)	1.053	0.133…0.167		<0.034		0.238	0.009	0.077	0.007
(13,2)	1.104	0.133…0.167		<0.034		0.231	0.011	0.039	0.014
(9,7)	1.088	0.168	0.004	0.034	0.004	0.25…0.3		<0.05	
(10,4)	0.978	0.196	0.014	0.069	0.009	0.275…0.301		<0.026	
(11,3)	1.000	0.130	0.003	0.034	0.003	0.233…0.301		<0.068	
Chirality	Diameter, nm	Transition (position) of **empty** SWCNTs, % CDOC	Transition (position error) of **empty** SWCNTs, % CDOC	Transition (width) of **empty** SWCNTs, % CDOC	Transition (width error) of **empty** SWCNTs, % CDOC	Transition (position) of **water-filled** SWCNTs, % CDOC	Transition (position error) of **water-filled** SWCNTs, % CDOC	Transition (width) of **water-filled** SWCNTs, % CDOC	Transition (width error) of **water-filled** SWCNTs, % CDOC
(5,4)	0.611	0.123	0.005	0.048	0.006	0.262	0.021	0.048	0.022

Table S16: Transitions from **top to bottom phase** with increasing SC concentration as obtained from the **bottom phase data** for the SWCNTs in SC/DOC/SDBS (at fixed concentrations of 0.1% wt/V DOC and 1.1% wt/V SDBS). The cells with white and grey background correspond to the transitions shown in black and dark gray in Figure 7 of the main text, respectively.

Chirality	Diameter, nm	First transition (position), % SC	First transition (position error), % SC	First transition (width), % SC	First transition (width error), % SC	Second transition (position), % SC	Second transition (position error), % SC	Second transition (width), % SC	Second transition (width error), % SC
(6,4)	0.683	0.599	0.017	0.082	0.020				
(7,2)	0.641	1.089	0.032	0.079	0.050				
(7,5)	0.817	1.103	0.006	0.082	0.008				
(7,6)	0.882	1.109	0.005	0.073	0.006				
(8,4)	0.829	1.113	0.008	0.079	0.010				
(8,6)	0.952	1.086	0.014	0.080	0.023				
(8,7)	1.018	1.098	0.035	0.089	0.049				
(9,4)	0.903	1.087	0.014	0.072	0.025				
(9,5)	0.962	1.146	0.005	0.078	0.005				
(9,7)	1.088	1.121	0.009	0.089	0.012				
(9,8)	1.153	1.145	0.002	0.083	0.003				
(10,2)	0.872	1.090	0.015	0.074	0.025				
(10,3)	0.923	1.123	0.001	0.074	0.002				
(10,4)	0.978	1.129	0.019	0.119	0.025				
(10,5)	1.036	1.121	0.017	0.085	0.021				
(10,6)	1.096	1.155	0.001	0.079	0.002				
(11,1)	0.903	1.131	0.006	0.054	0.005				
(11,2)	0.949	1.085	0.008	0.099	0.011				
(12,1)	0.981	1.120	0.010	0.082	0.013				
(6,5)	0.747					0.751	0.116	0.385	0.169
(11,3)	1.000					1.098	0.026	0.118	0.034
(11,4)	1.053					1.068	0.020	0.126	0.027
(12,2)	1.027					1.184	0.019	0.074	0.034
(8,3)	0.771	0.122	0.031	0.078	0.055	1.143	0.026	0.060	0.023