Polymer Chemistry

Electronic Supplementary Information (ESI)

"Old" chemistry in a new context: photocleavable 2-oxoacetate-containing latex dispersions and core-shell microcapsules for the controlled release of volatile compounds

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Table S1. Amount of citral extracted from an emulsion of SDS in water containing profragrance **1**, latex nanoparticles **7** and microcapsules **A@1** to **D@1** after 3, 5.5 and 8 h of irradiation at 90'000 lux. Numerical data for the results depicted in Fig. 3a.

Sample	(*E*)- and (*Z*)-Citral released after irradiation for			
	3 h [ng μL^{-1}]	3 h [%]	5.5 h [ng μL^{-1}]	8 h [ng μL^{-1}]
1	14.7	1.2	9.5	6.0
7	27.7	2.3	18.7	10.2
A@1	8.4	0.7	6.7	3.0
B@1	6.5	0.5	7.6	n.d.
C@1	10.0	0.8	7.6	5.7
D@1	12.5	1.0	8.6	6.2

Table S2. Amount of 2-phenylacetaldehyde and (*Z*)-hex-3-enal extracted from an emulsion of SDS in water containing the corresponding profragrances, latex nanoparticles or microcapsules after 2 h of irradiation at 90'000 lux in the presence or absence of an organic layer. Numerical data for the results depicted in Fig. 4.

Sample	2-Phenylacetaldehyde released after irradiation for 2 h		
	with organic layer (continuous extraction)		no organic layer
	[ng μL^{-1}]	[%]	[ng μL^{-1}]
2	141.1	14.7	67.5
8	156.0	16.2	n.d.
A@2	39.7	4.1	n.d.
C@2	61.0	6.3	n.d.
D@2	95.0	9.9	79.2

Sample	(*Z*)-Hex-3-enal released after irradiation for 2 h		
	with organic layer (continuous extraction)		no organic layer
	[ng μL^{-1}]	[%]	[ng μL^{-1}]
3	65.1	8.3	10.6
9	96.5	12.3	n.d.
A@3	7.7	1.0	n.d.
C@3	15.4	2.0	n.d.
D@3	35.1	4.5	14.6

Table S3. Dynamic headspace concentrations (and standard deviations in parentheses) for the release of fragrance aldehydes from profragrances **1–3**, microcapsules of type **A–D**, latex nanoparticles **7–9** and the unmodified fragrance as the reference on cotton after photoirradiation with a xenon lamp. Numerical data for the results depicted in Fig. 5.

Time [min]	(*E*)- and (*Z*)-Citral released from [ng L^{-1}]						
	Reference	**1**	**7**	**A@1**	**B@1**	**C@1**	**D@1**
10	16.1 (±1.4)	124.5 (±97.2)	32.0 (±3.2)	78.4 (±4.4)	51.4 (±18.7)	61.8 (±2.0)	149.5 (±60.7)
25	16.0 (±0.7)	212.0 (±117.0)	41.2 (±14.0)	149.1 (±27.9)	94.3 (±47.0)	147.5 (±29.3)	250.3 (±101.2)
55	17.6 (±6.1)	228.5 (±93.7)	32.9 (±10.9)	152.3 (±16.4)	102.9 (±16.7)	153.9 (±33.1)	182.7 (±75.3)
85	16.3 (±0.6)	154.9 (±62.5)	20.2 (±3.5)	86.2 (±4.0)	76.5 (±11.4)	101.1 (±20.5)	113.5 (±64.2)
115	16.4 (±0.6)	104.8 (±60.9)	16.6 (±0.1)	49.6 (±9.2)	57.8 (±18.5)	66.8 (±3.4)	65.9 (±41.3)
145	16.1 (±0.4)			33.7 (±2.5)	43.2 (±9.5)	39.1	50.2 (±24.5)

Time [min]	2-Phenylacetaldehyde released from [ng L^{-1}]					
	Reference	**2**	**8**	**A@2**	**C@2**	**D@2**
10	1.3 (±2.7)	51.2 (±20.5)	781.9 (±420.8)	55.7 (±10.6)	105.9 (±20.3)	339.8 (±29.3)
25	2.1 (±3.9)	62.4 (±22.1)	675.5 (±331.5)	59.8 (±11.4)	113.7 (±18.3)	297.1 (±44.5)
55	5.2 (±9.0)	39.4 (±14.4)	368.6 (±142.3)	36.2 (±12.3)	69.8 (±11.9)	160.6 (±11.0)
85	6.2 (±8.8)	25.7 (±11.2)	193.1 (±53.5)	18.3 (±5.8)	42.6 (±8.7)	93.7 (±2.6)
115	8.7 (±13.4)	16.4 (±6.1)	111.9 (±27.8)	13.2 (±6.0)	26.9 (±5.4)	72.4 (±11.0)
145	9.4 (±10.3)	11.2 (±6.2)	66.5 (±8.0)	---	21.9 (±5.2)	53.7 (±10.0)

Time [min]	(*Z*)-Hex-3-enal released from [ng L^{-1}]					
	Reference	**3**	**9**	**A@3**	**C@3**	**D@3**
10	30.7 (±39.4)	343.5	465.4 (±120.4)	341.3 (±87.3)	663.4 (±468.2)	99.9 (±5.5)
25	25.6 (±20.7)	140.1	157.4 (±38.8)	134.0 (±37.7)	249.1 (±144.7)	51.9 (±15.1)
55	21.1 (±11.1)	81.9	36.6 (±10.2)	62.4 (±15.5)	100.9 (±77.0)	27.6 (±5.6)
85	18.8 (±7.8)	45.6	17.3 (±2.5)	31.5 (±9.7)	61.0 (±28.2)	18.2 (±2.7)
115	17.9 (±6.1)	343.5	13.3 (±0.5)	20.5 (±0.8)	34.0 (±16.5)	14.2 (±0.6)

Table S4. Dynamic headspace concentrations (and standard deviations in parentheses) for the release of 2-phenylacetaldehyde from profragrance **2**, microcapsule **D@2**, latex nanoparticle **8** and the unmodified fragrance as the reference on cotton after exposure to indoor daylight. Numerical data for the results depicted in Fig. 6.

Time [min]	2-Phenylacetaldehyde released from [ng L^{-1}]			
	Reference	**2**	**8**	**D@3**
30	0.3 (±0.0)	0.4 (±0.0)	5.2 (±1.2)	3.3 (±3.1)
90	0.4 (±0.0)	0.6 (±0.2)	10.8 (±3.2)	5.1 (±3.3)
150	0.4 (±0.0)	0.7 (±0.3)	13.0 (±4.5)	5.1 (±2.5)
210	0.4 (±0.1)	0.7 (±0.3)	14.4 (±4.2)	4.7 (±1.8)

Fig. S1 ^{1}H and ^{13}C NMR spectra of **4** in $CDCl_3$ with TMS as internal standard.

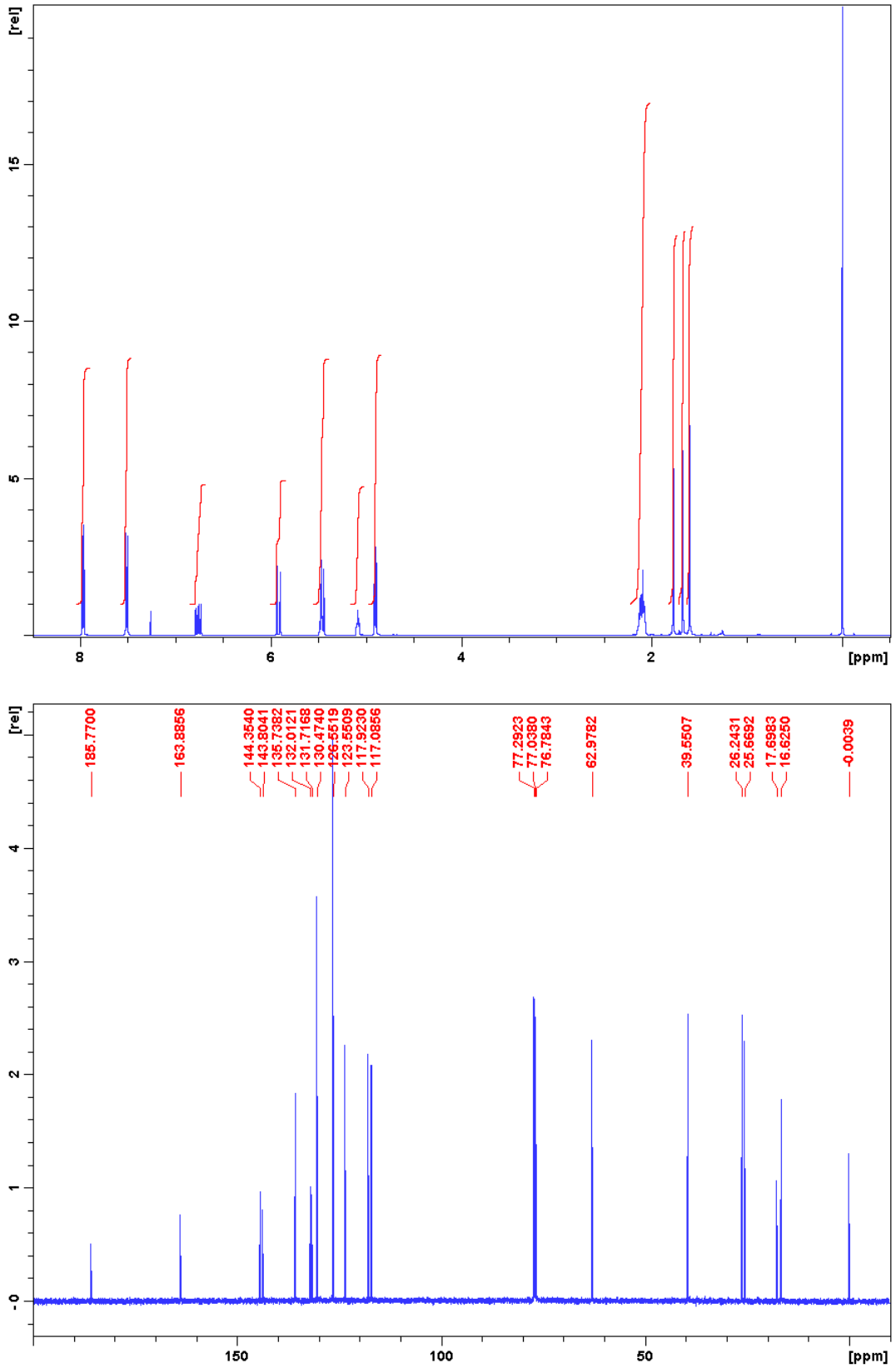

Fig. S2 ^{1}H and ^{13}C NMR spectra of **5** in $CDCl_3$ with TMS as internal standard.

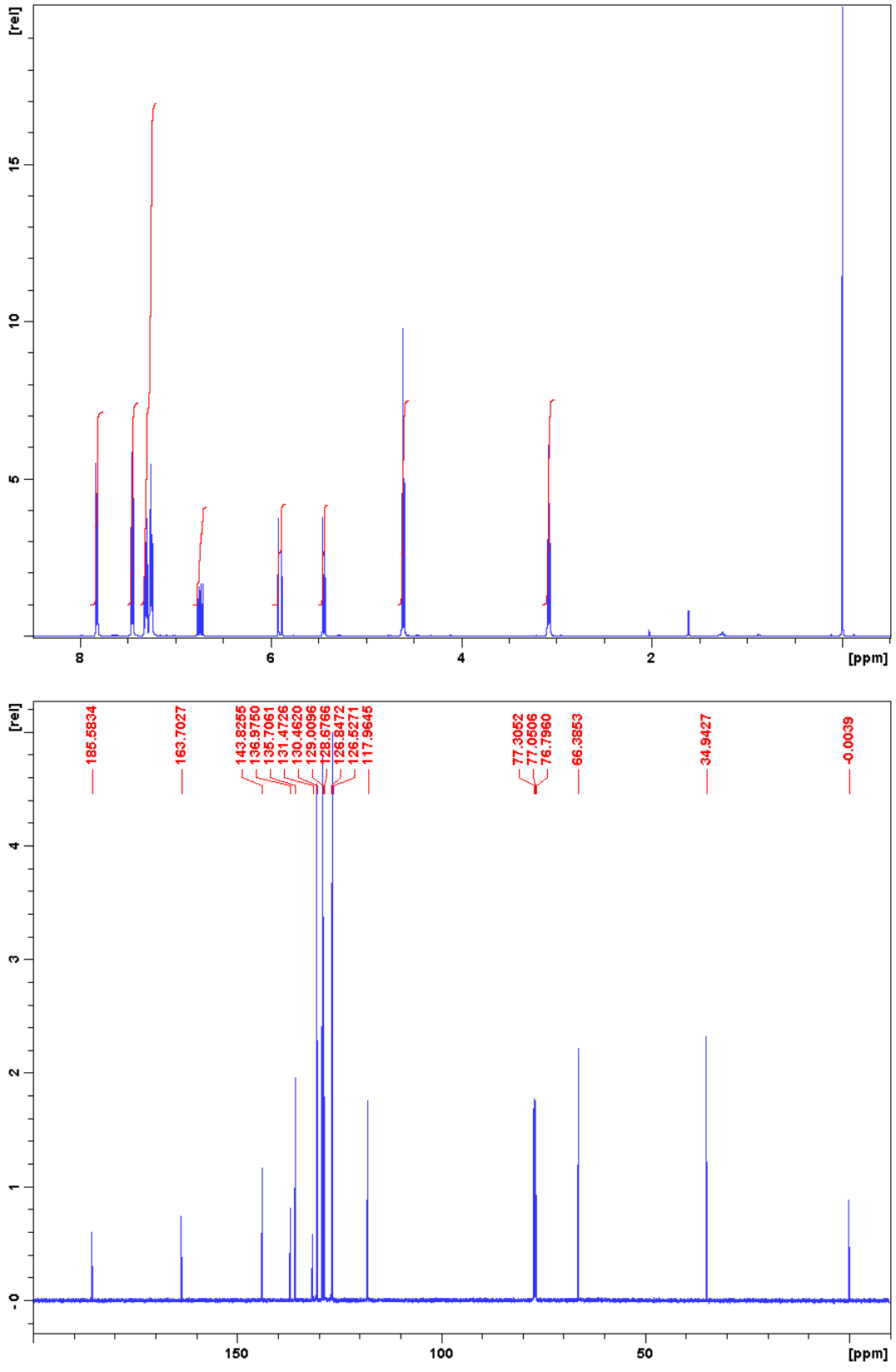

Fig. S3 ^{1}H and ^{13}C NMR spectra of **6** in $CDCl_3$ with TMS as internal standard.

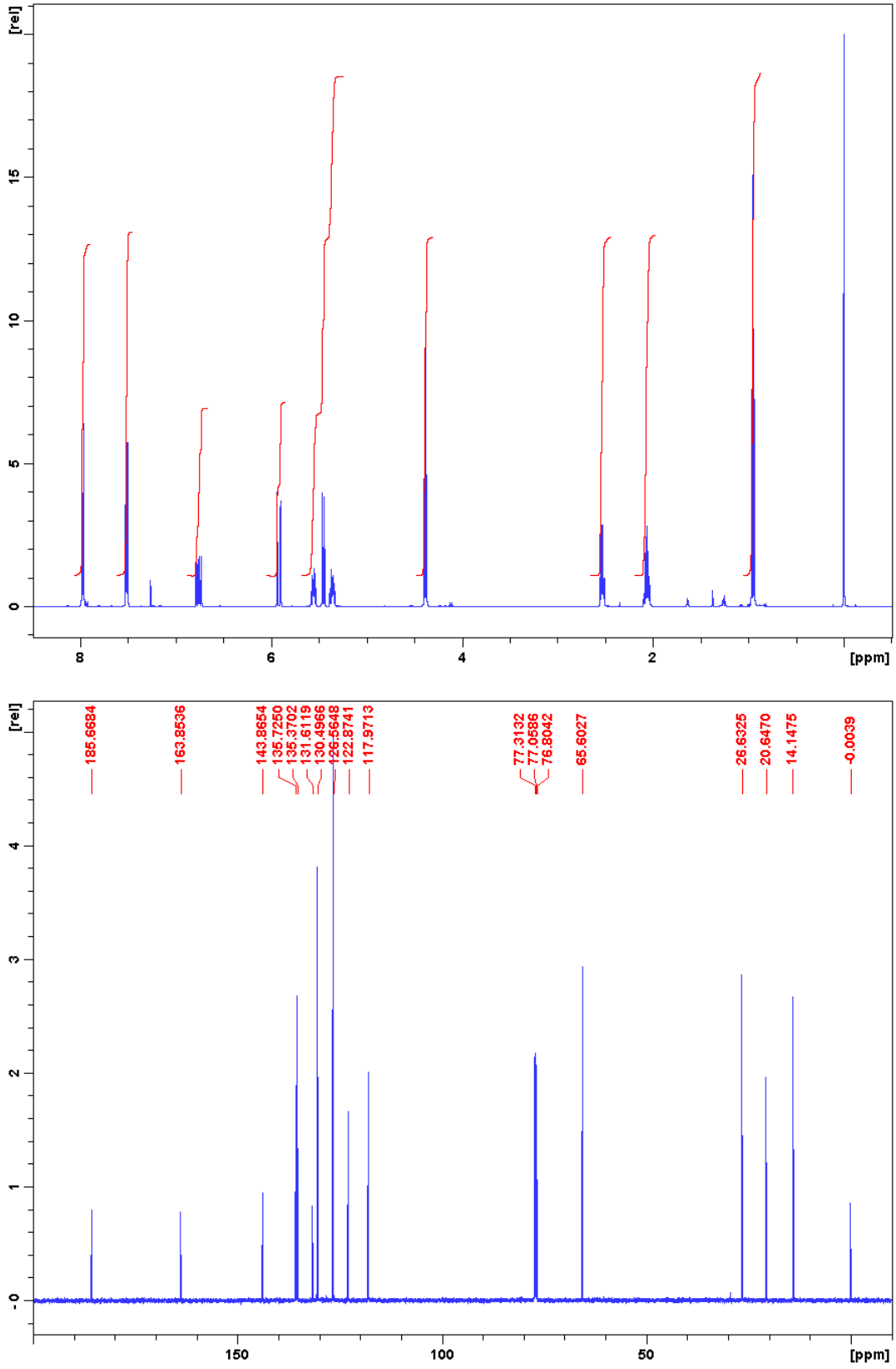

Fig. S4 Particle size distribution of microcapsules in water determined by FPIA.

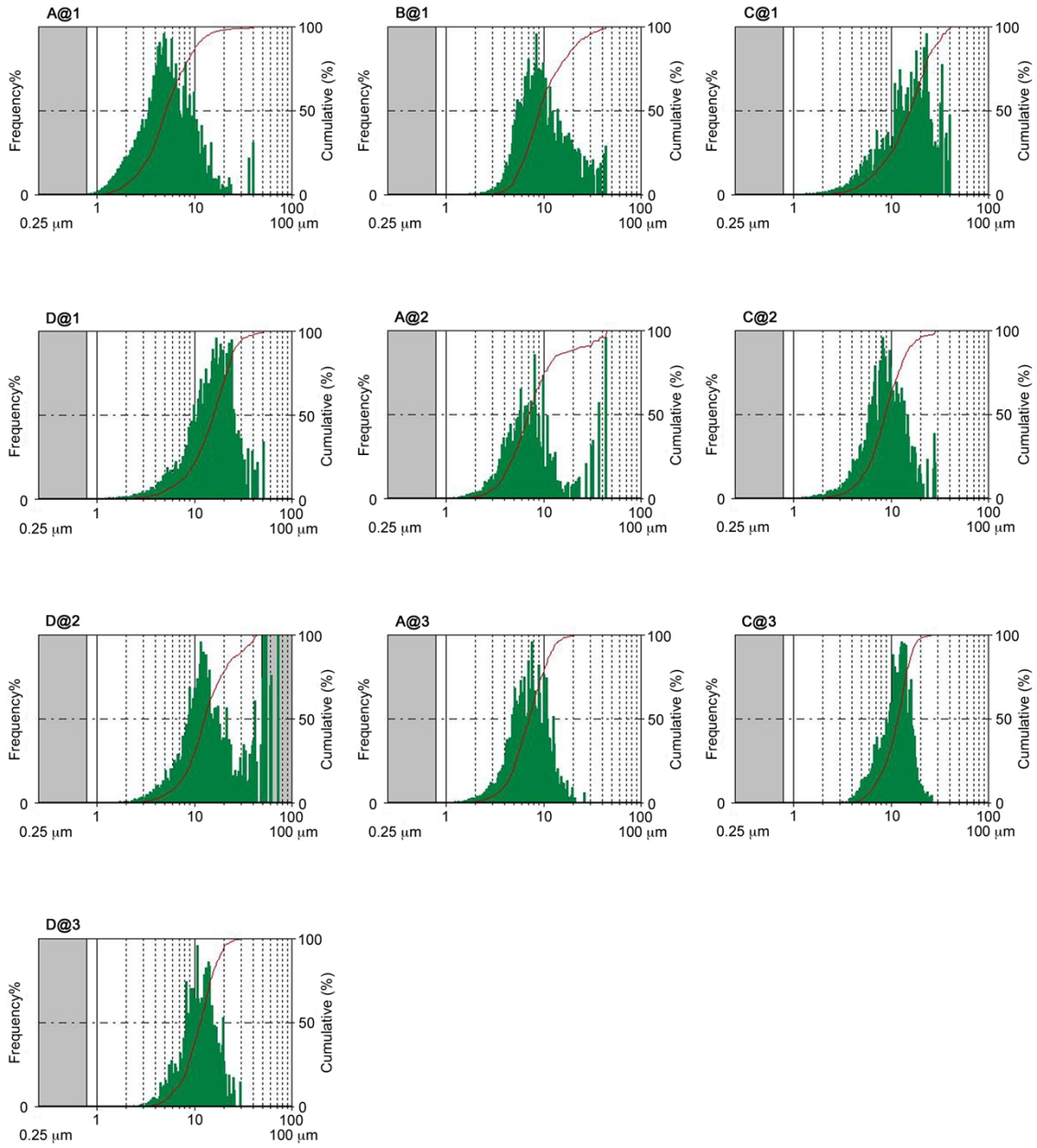

Fig. S5 Particle size distribution of latex nanoparticles **7** (*a*), **8** (*b*) and **9** (*c*) in water determined by dynamic light scattering.