

Single and double chain surfactant–cobalt(III) complexes: The impact of hydrophobicity on the interaction with calf thymus DNA, and their biological activities

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Table S1. Selected bond distances (Å) and angles (°) for optimized complexes **1–4** in the ground state geometry at B3LYB/LAN2DZ (Co)/6-31g (d,p) level.

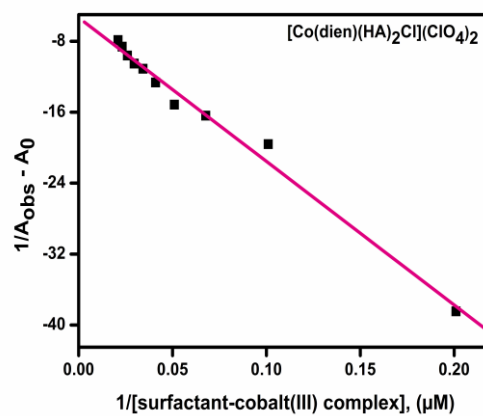
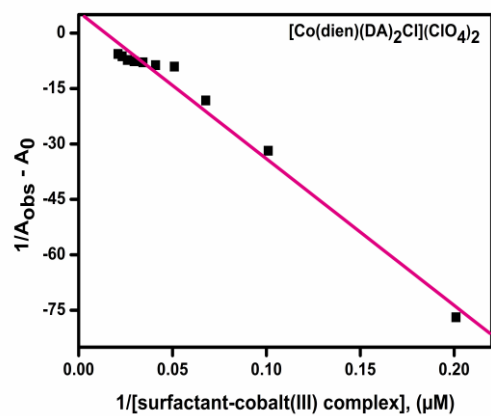
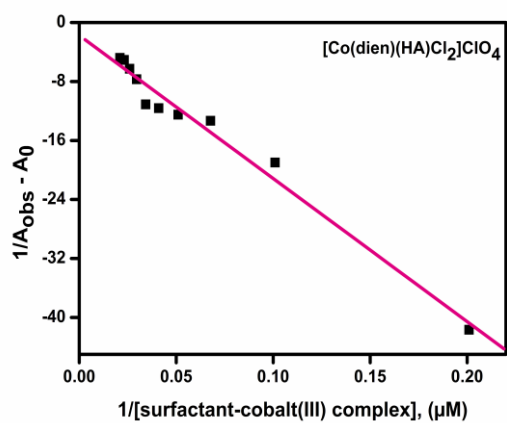
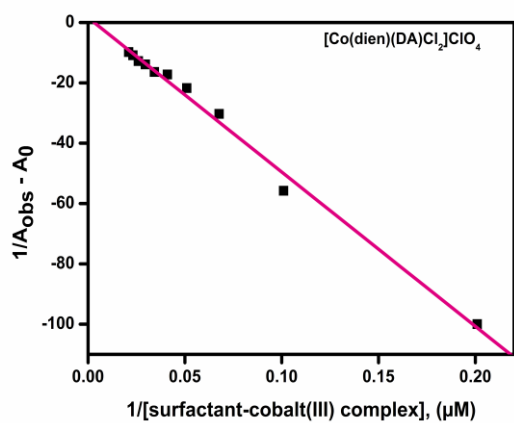


Figure S1. Benesi-Hildebrand plot of $1/A_{\text{obs}} - A_0$ on the reciprocal of [surfactant–cobalt(III) complex] 1–4

Results

	Size (d.nm):	% Intensity	Width (d.n...
Z-Average (d.nm): 436.3	Peak 1: 354.1	100.0	91.77
Pdl: 0.499	Peak 2: 0.000	0.0	0.000
Intercept: 0.998	Peak 3: 0.000	0.0	0.000

Result quality : Refer to quality report

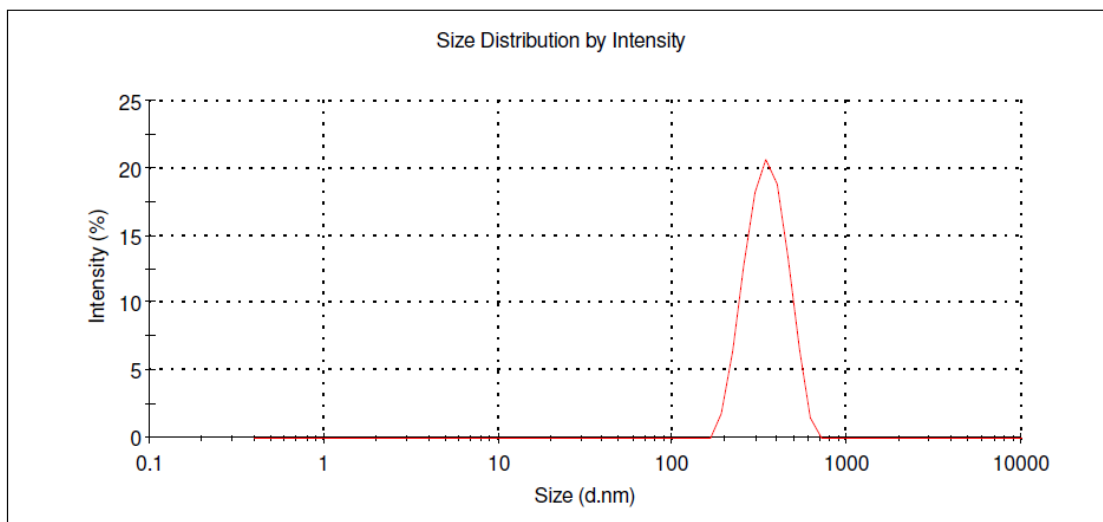


Figure S2(a). DLS measurements for the average hydrodynamic size distributions of DNA

Results

	Size (d.nm):	% Intensity	Width (d.nm)
Z-Average (d.nm): 588.2	Peak 1: 1322	75.3	715.3
Pdl: 0.477	Peak 2: 327.7	24.7	86.35
Intercept: 1.01	Peak 3: 0.000	0.0	0.000

Result quality : Refer to quality report

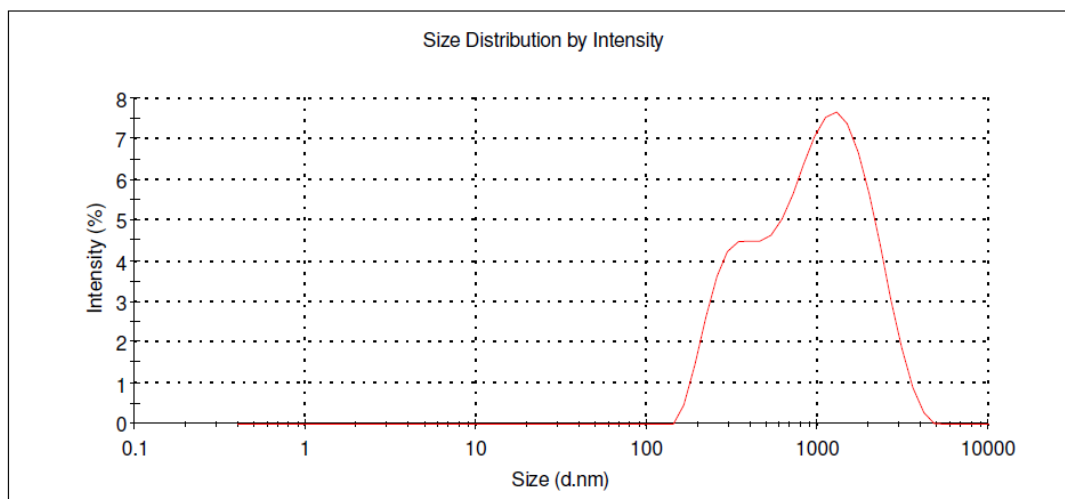


Figure S2 (b). DLS measurements for the average hydrodynamic size distributions of DNA+ complex 1

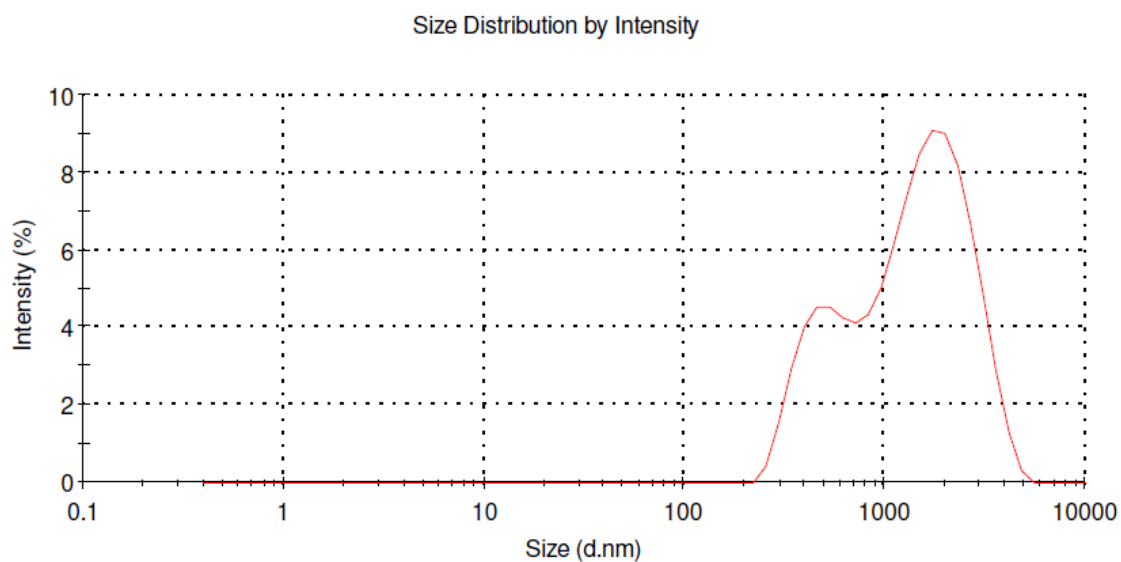


Figure S2 (c). DLS measurements for the average hydrodynamic size distributions of DNA+ complex 2

Results

	Size (d.nm):	% Intensity	Width (d.n...
Z-Average (d.nm): 977.2	Peak 1: 1833	74.6	825.7
Pdl: 0.342	Peak 2: 500.3	25.4	132.4
Intercept: 0.946	Peak 3: 0.000	0.0	0.000

Result quality : Good

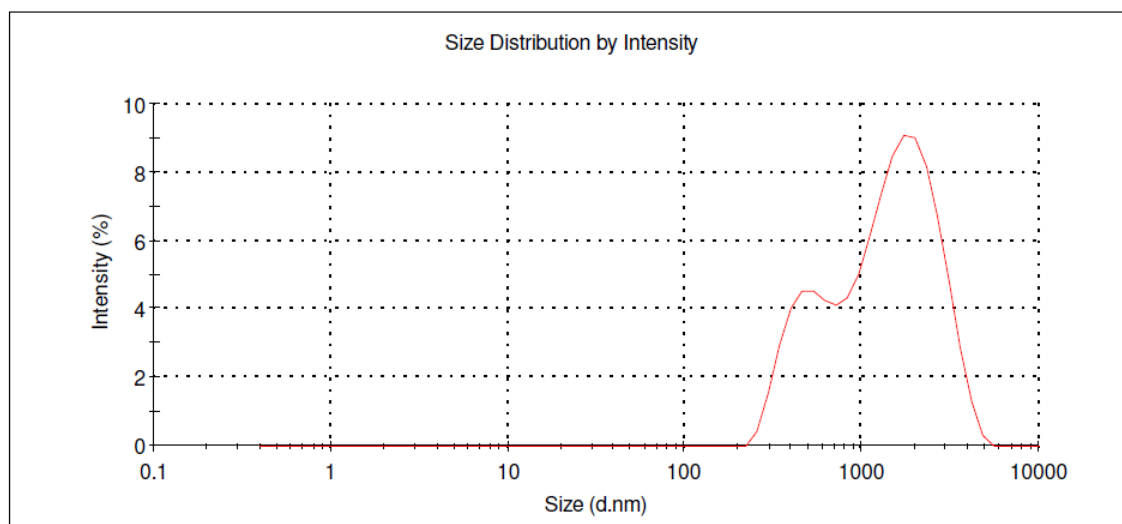


Figure S2 (d). DLS measurements for the average hydrodynamic size distributions of DNA+ complex 3

Results

	Size (d.nm):	% Intensity	Width (d.nm)
Z-Average (d.nm): 1081	Peak 1: 2257	79.6	1207
PdI: 0.499	Peak 2: 388.2	20.4	107.6
Intercept: 0.946	Peak 3: 0.000	0.0	0.000

Result quality : Refer to quality report

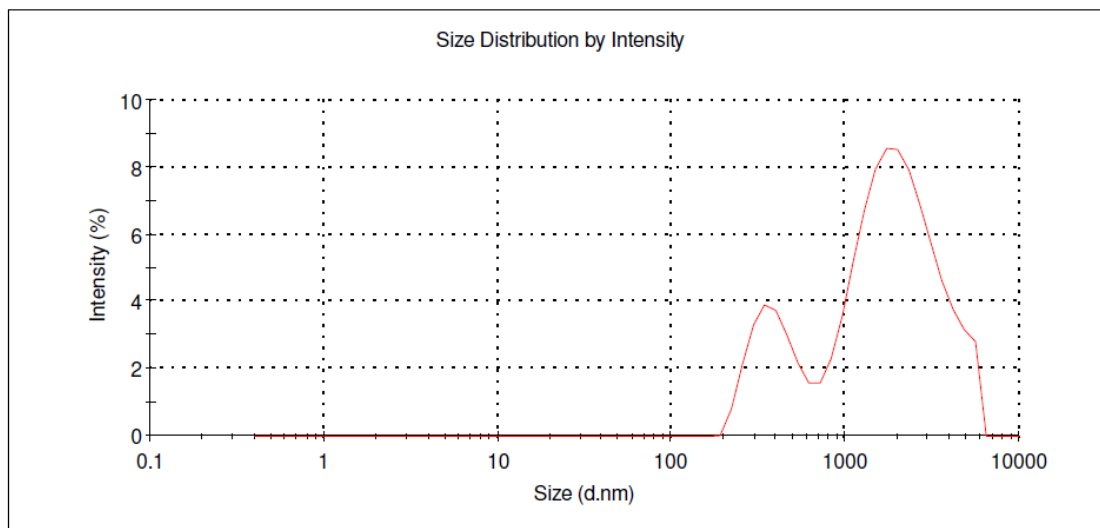


Figure S2 (e). DLS measurements for the average hydrodynamic size distributions of DNA+ complex 4

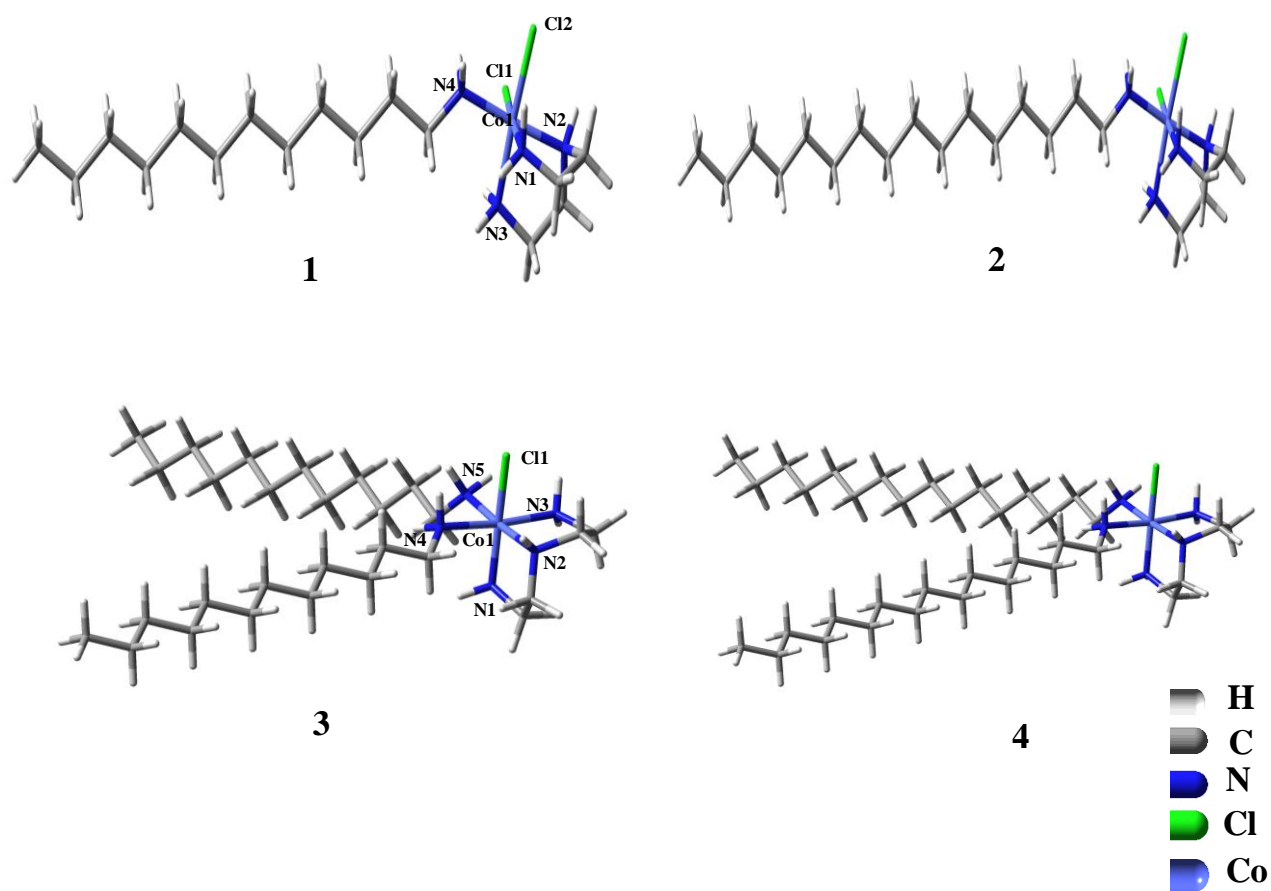


Figure S2. Ground state optimized molecular structures of complexes 1-4 calculated at B3LYB/LAN2DZ (Co)/6-31g(d,p) level.

Table S1. Selected bond distances (Å) and angles (°) for optimized complexes **1-4** in the ground state geometry at B3LYB/LAN2DZ (Co)/6-31g (d,p) level.

Bond Parameters	Complex 1	Complex 2	Complex 3	Complex 4
Co-Cl1	2.278	2.278	2.272	2.275
Co-Cl2	2.277	2.277	-	-
Co-N1	1.997	2.021	2.020	2.023
Co-N2	1.984	1.983	2.009	2.010
Co-N3	2.024	2.024	2.023	2.025
Co-N4	1.997	1.996	2.026	2.026
Co-N5	-	-	2.033	2.035
N1-Co-Cl1	176.5	176.5	176.3	176.2
N2-Co-N4	177.0	176.9	175.4	175.4
N3-Co-Cl2	176.0	176.0	-	-
N3-Co-N5	-	-	173.4	173.4