Supporting information for

Interaction of Amphiphilic Coumarin with DPPC/DPPS Lipid Bilayer: Effects of Concentration and Alkyl Tail Length

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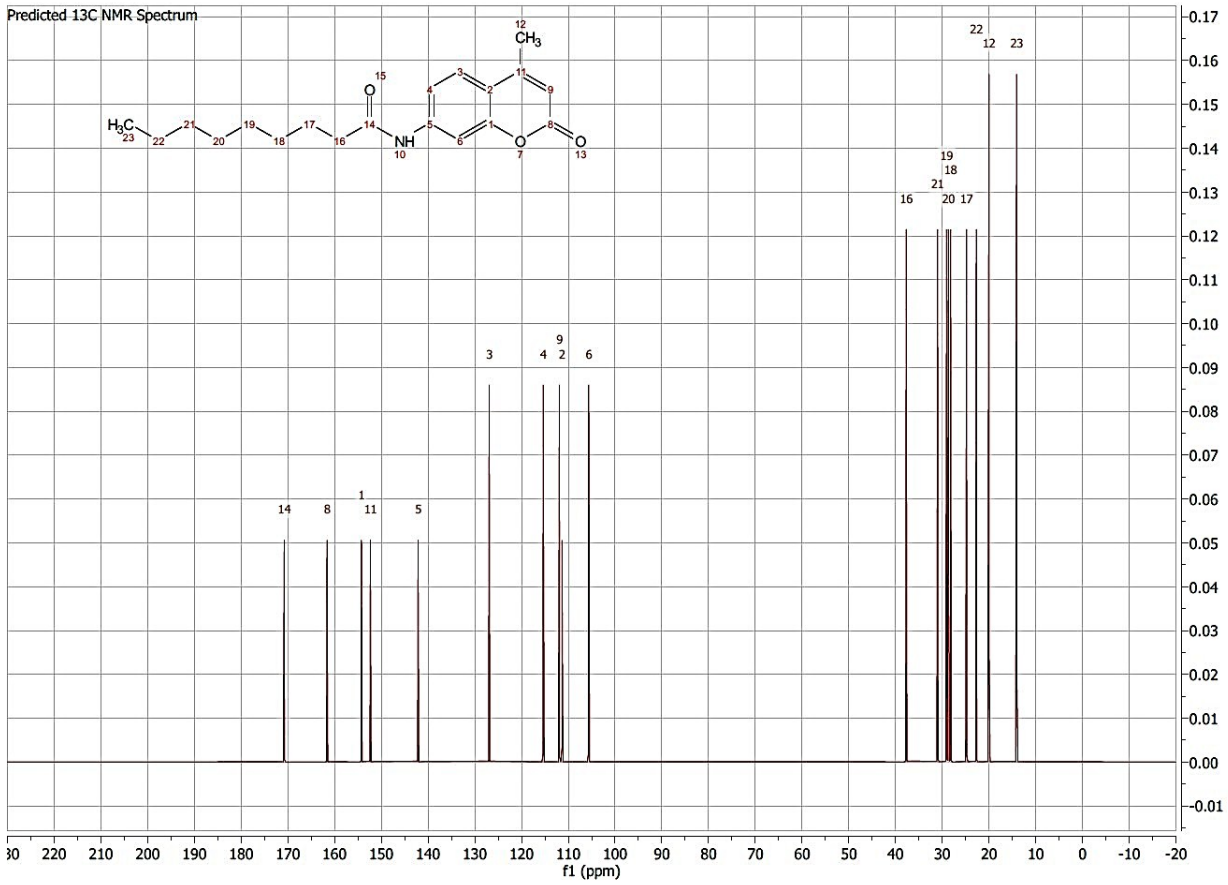


Figure S1: ^{13}C-NMR spectra of C_9 amphiphile

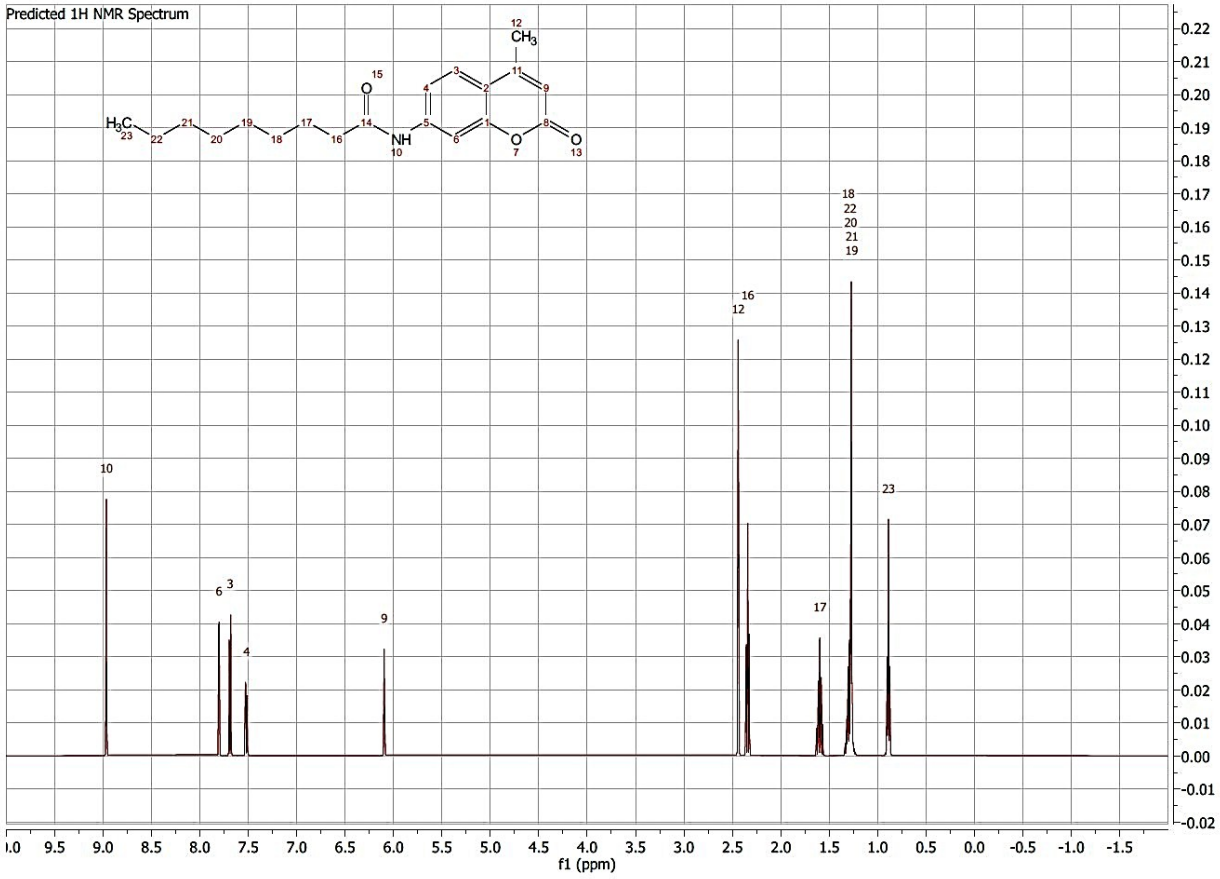


Figure S2: ^{1}H-NMR spectra of C_9 amphiphile

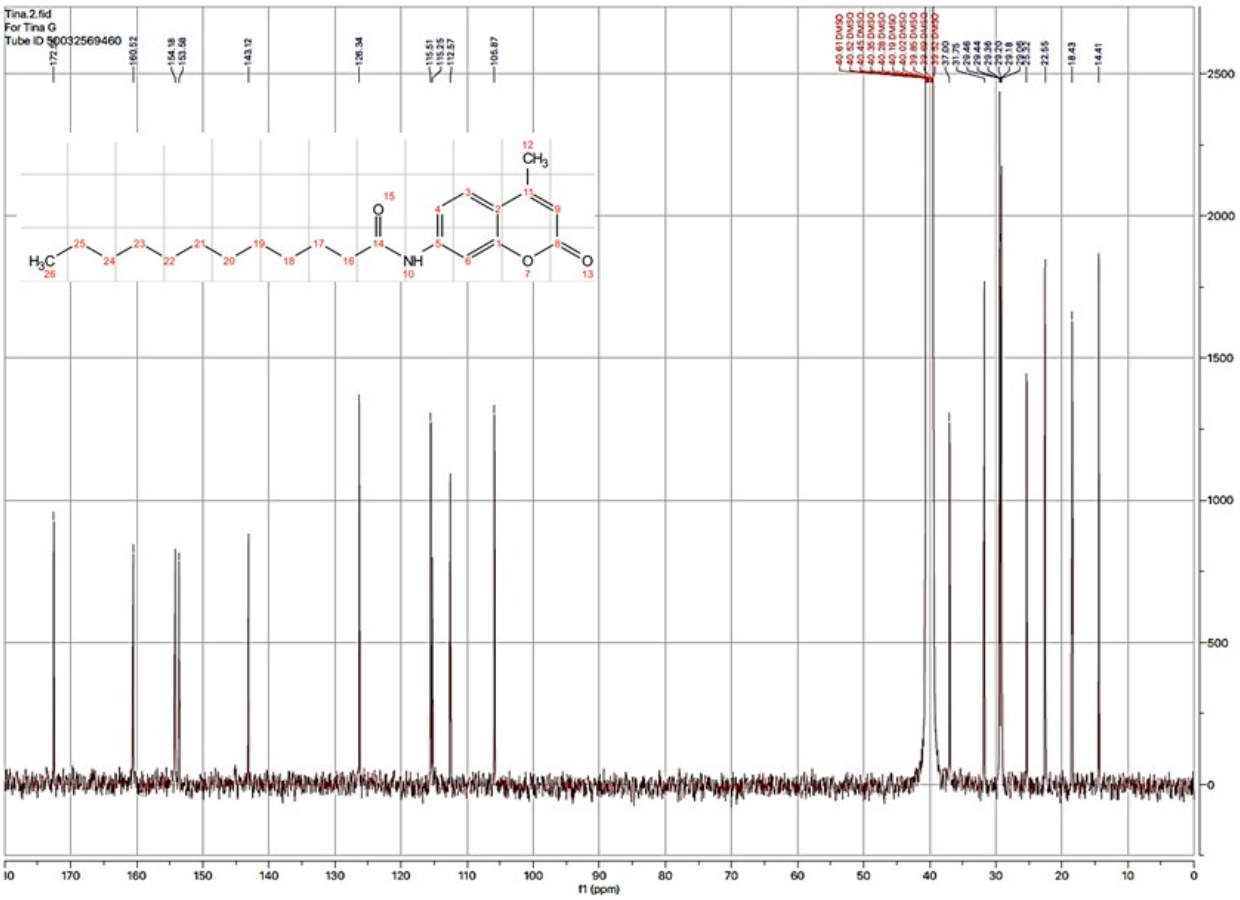


Figure S3: ^{13}C-NMR spectra of C_{12} amphiphile

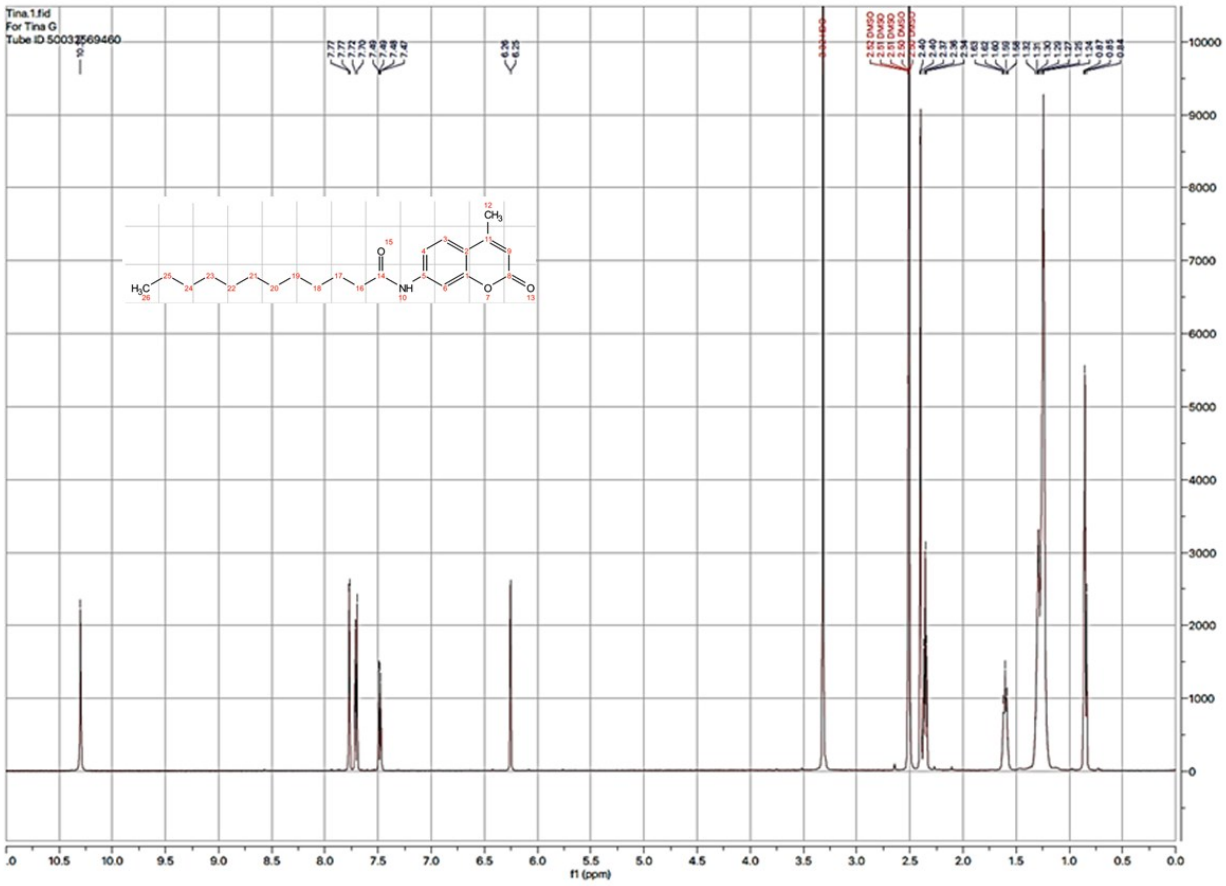
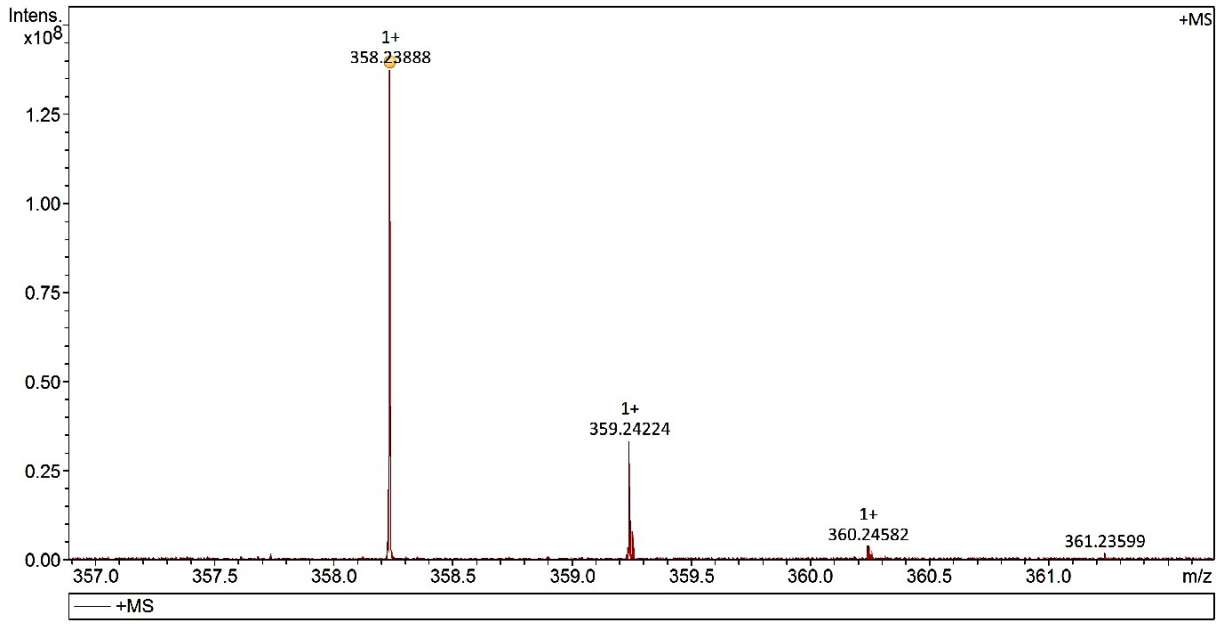


Figure S4: ^{1}H-NMR spectra of C_{12} amphiphile



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
358.238880	1	C22H32NO3	100.00	358.237670	-3.4	-3.7	4.1	7.5	even	ok

Figure S5: HR-MS spectra of C_{12} amphiphile

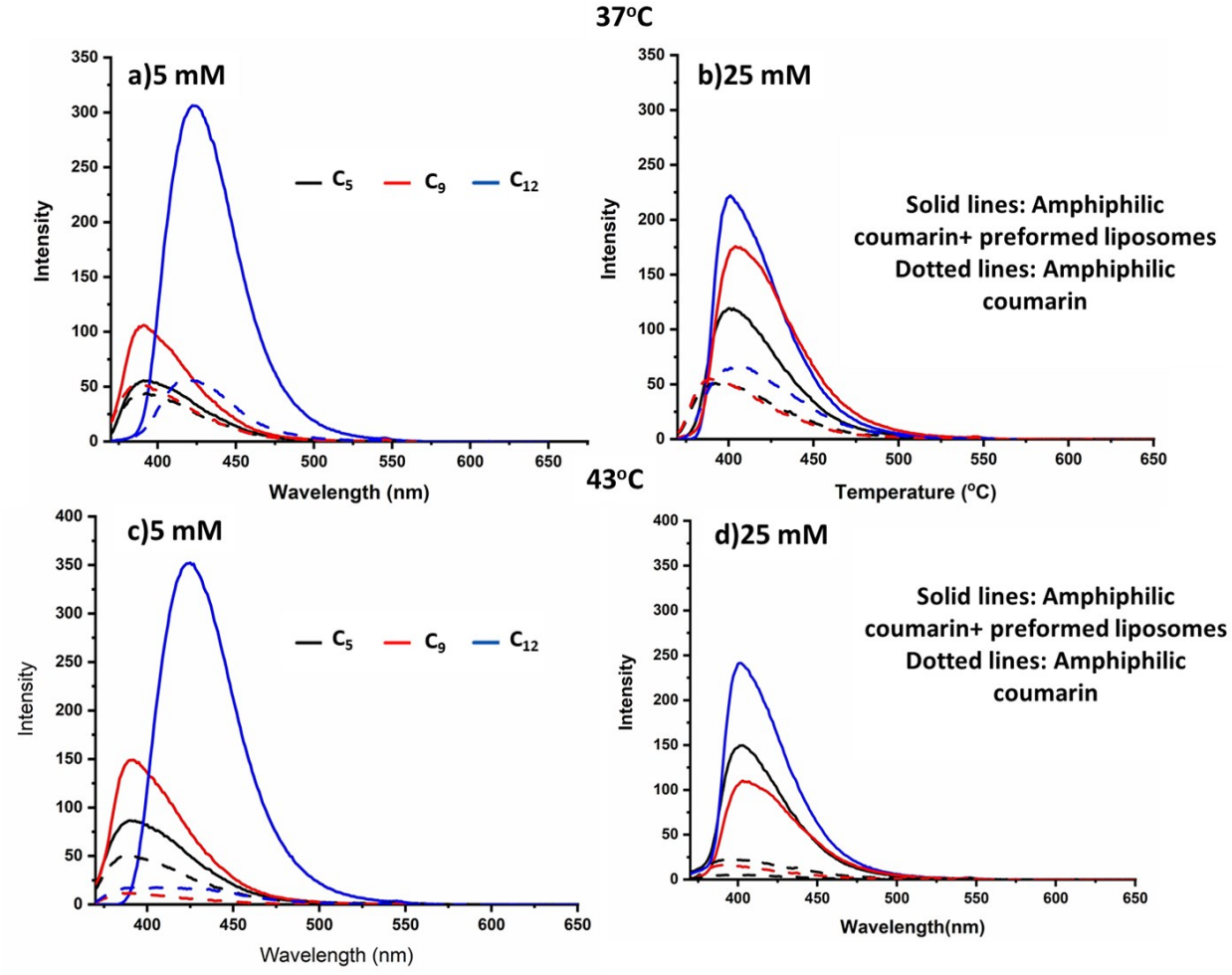


Figure S6: Fluorescence spectroscopy of amphiphilic fluorometric probes at 37°C & 43°C

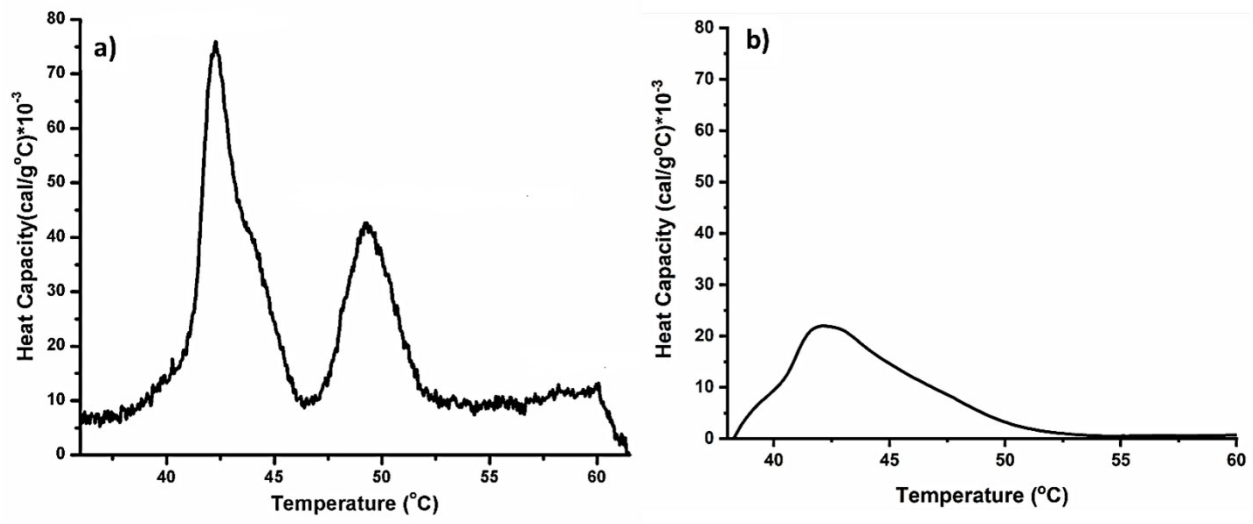


Figure S7: DSC Thermogram of a) pure DPPC/DPPS(85/15mol%) b) effect of DMSO on DPPC/DPPS (85/15 mol%)

Figure S8: Flip-flop modes for 20 randomly selected molecules (each in a unique color) in system (a) C_5-42, (b) C_5-166, (c) C_5-166, and (d) C_5-209. Trajectory of the coumarin ring for each molecule is shown in a unique color.

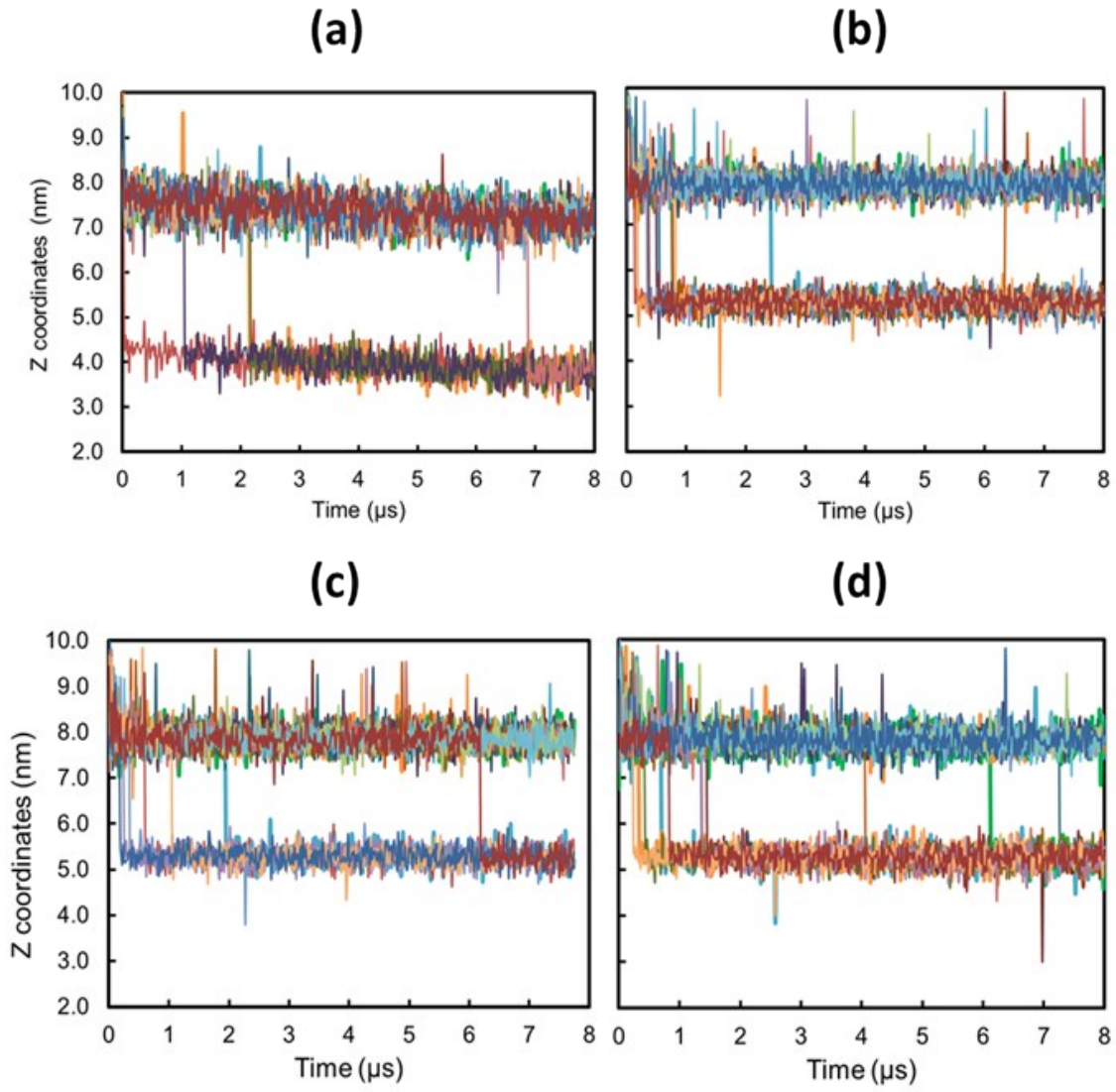


Figure S8: Flip-flop modes for 20 randomly selected molecules (each in a unique color) in system (a) C_5-42, (b) C_5-166, (c) C_5-166, and (d) C_5-209. Trajectory of the coumarin ring for each molecule is shown in a unique color.

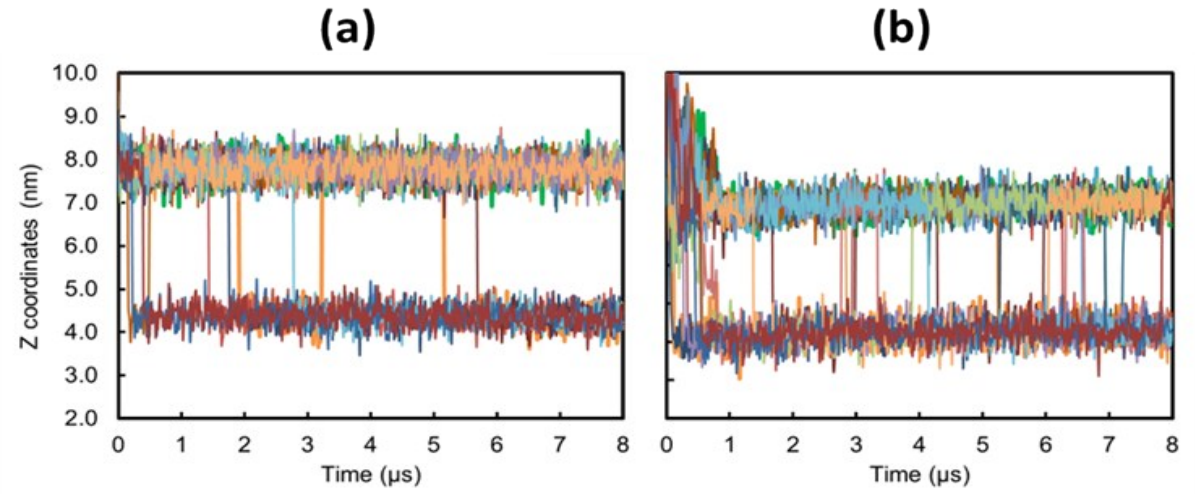


Figure S9: Flip-flop modes for 20 randomly selected molecules (each in a unique color) in system (a) C_{12}-42 and (b) C_{12}-166. Trajectory of the coumarin ring for each molecule is shown in a unique color.

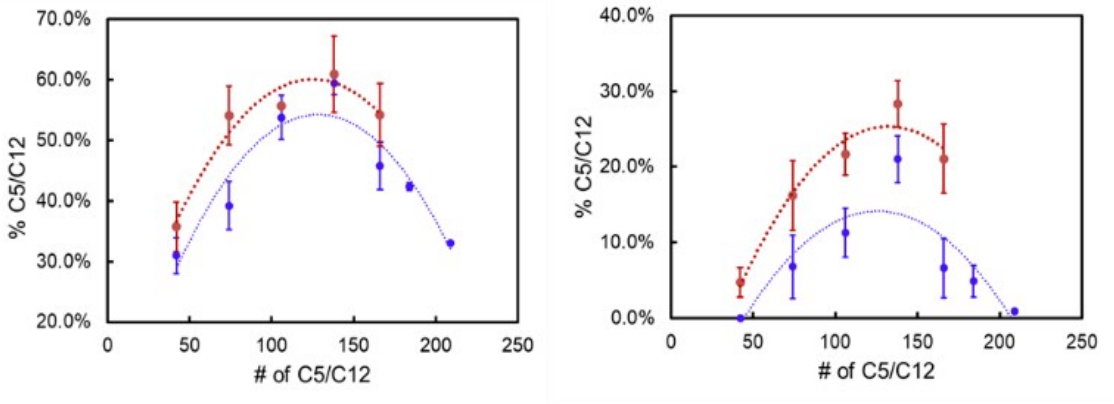


Figure S10: Comparison of flip-flop (%) for C_5 (blue) and C_{12} (red) molecules over a range of concentrations. with (a) ≥1 flip-flop (b) ≥2 flip-flops

Bond	r_{eq}(nm)	k_{bond} (kJ mol^{-1} nm^{-2})	Angle	θ_{eq}(deg)	k_{angle} (kJ mol^{-1})
1-2	0.295	Constrained	1-2-4	87	50
1-3	0.288	Constrained	2-1-3	75	50
2-4	0.303	Constrained	1-3-4	112	50
3-4	0.206	Constrained	1-3-5	155	50
3-5	0.330	5000	2-4-3	86	50
4-5	0.393	5000	2-4-5	142	50
5-6	0.347	5000	3-5-6	92	50
			4-5-6	108	50

Table S1: Equilibrium bond length (req), angle (θeq), and respective force constant for C_5 model.

Bond	r_{eq}(nm)	k_{bond} (kJ mol^{-1} nm^{-2})	Angle	θ_{eq}(deg)	k_{angle} (kJ mol^{-1})
1-2	0.295	Constrained	1-2-4	87	50
1-3	0.288	Constrained	2-1-3	75	50
2-4	0.303	20000	1-3-4	112	50
3-4	0.206	Constrained	1-3-5	171	50
3-5	0.348	5000	2-4-3	86	50
4-5	0.341	5000	2-4-5	158	50
5-6	0.339	5000	3-5-6	122	50
6-7	0.398	5000	4-5-6	144	50
7-8	0.413	5000	5-6-7	120	50
			6-7-8	143	50

Table S2: Equilibrium bond length (req), angle (θeq), and respective force constant for C_{12} model.