Supporting Information

Surface Modified Chitosan: An Adsorption Study of a "*Tweezer-Like*" Biopolymer with Fluorescein

Bahareh Vafakish and Lee D. Wilson *

Department of Chemistry, University of Saskatchewan, 110 Science Place, Saskatoon, Saskatchewan S7N 5C9, Canada

* Correspondence: lee.wilson@usask.ca, Tel.: +1-306-966-2961; Fax: +1-306-966-4730

Table S1: Literature Comparison of Q_m for FL with different adsorbents

Adsorbent	Adsorption capacity (mg g^{-1})	Limitations & Comments	Reference
Iron Oxide	16	Low cost/ Low adsorption capacity/ No regeneration reported	21, 22
Soil	-	Low cost Adsorbent/ Low adsorption Capacity	23
Copper–isonicotinate MOF	66.7	High adsorption Capacity/ Toxic Adsorbent/ No regeneration reported	24
Chitosan cross-linked with Epichlorohydrin	1.08 (predicted)	Low Cost Adsorbent/ Easy Synthetic Method/ Low Adsorption capacity/ No regeneration reported	25
Pillar[5]arene	2500	High Cost and Toxic Adsorbent/ Difficult Synthetic Method	26
Protein Crystal	26.5	High Cost/ Low adsorption capacity	27
Mango Seed based Activated Carbon	1.1	High Cost/ Low Adsorption capacity/ No regeneration reported	28
Zn-Al-Hydrotalcite	275	High Adsorption Capacity/ Difficult to Synthesis	29
Tweezers-like Adsorbent	**61.8**	Green and Sustainable Adsorbent/ Low cost/ Facile Synthetic Method	**This Study**

Degree of Substitution (DS): DS was calculated using ^{1}H-NMR spectra by eq. 1.

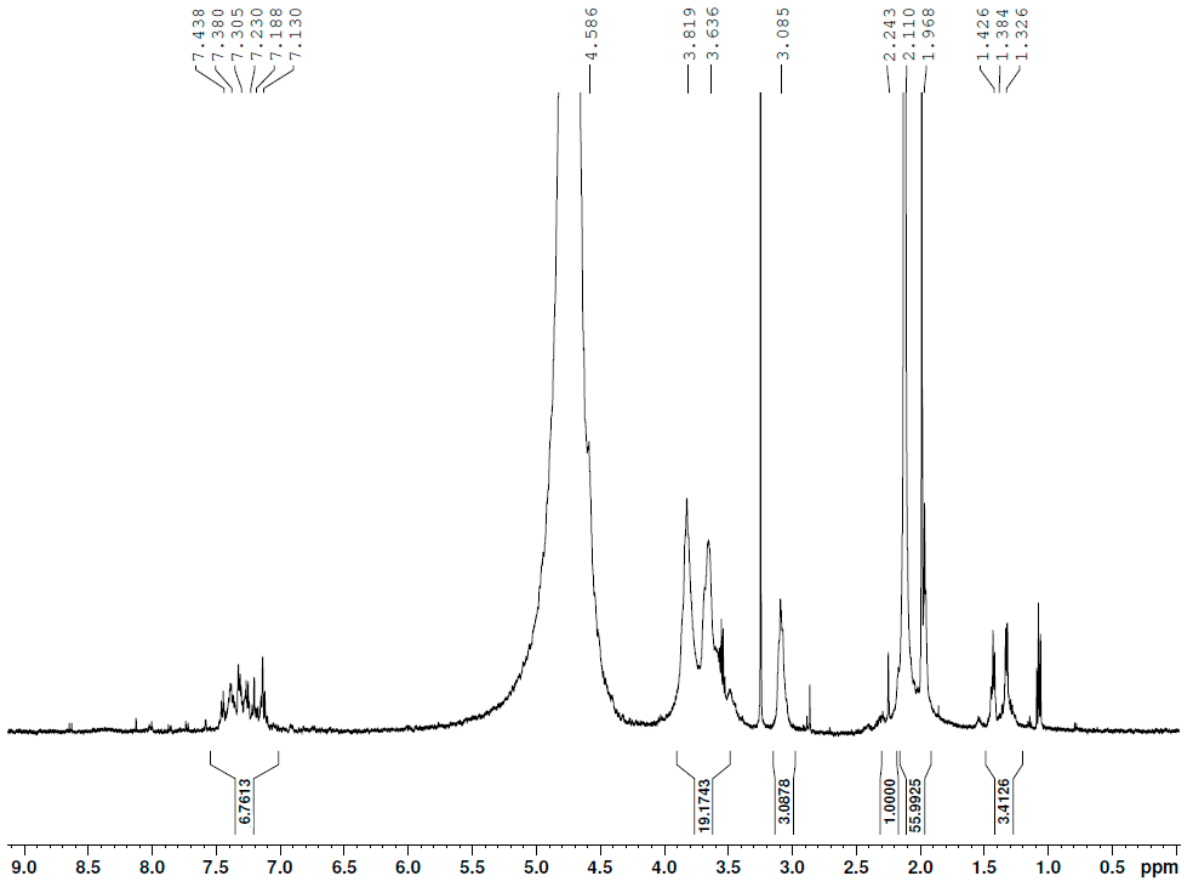


Figure S1: ^{1}H-NMR of CS-Ac-An with integration

^{13}C-NMR Spectroscopy:

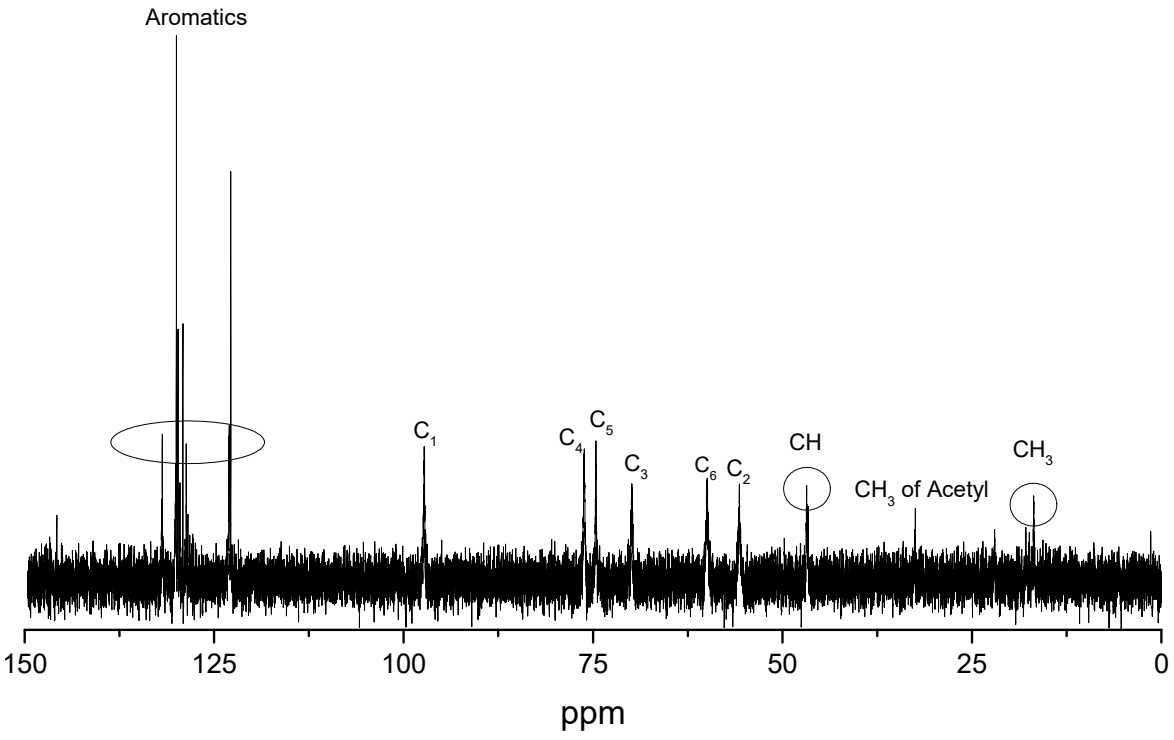


Figure S2: ^{13}C-NMR Spectra of CS-Ac-An

Table S2: Equilibrium adsorption parameters for the FL Uptake with CS-Ac-An according to Sips models.

Sips Parameters				
Q_m (mg g^{-1})	K_s (L mg^{-1})	n_s	Chi-Square	Adj-R^2
58.3	152.6	1.85	3.68	0.985

Freundlich fitting of the experimental data

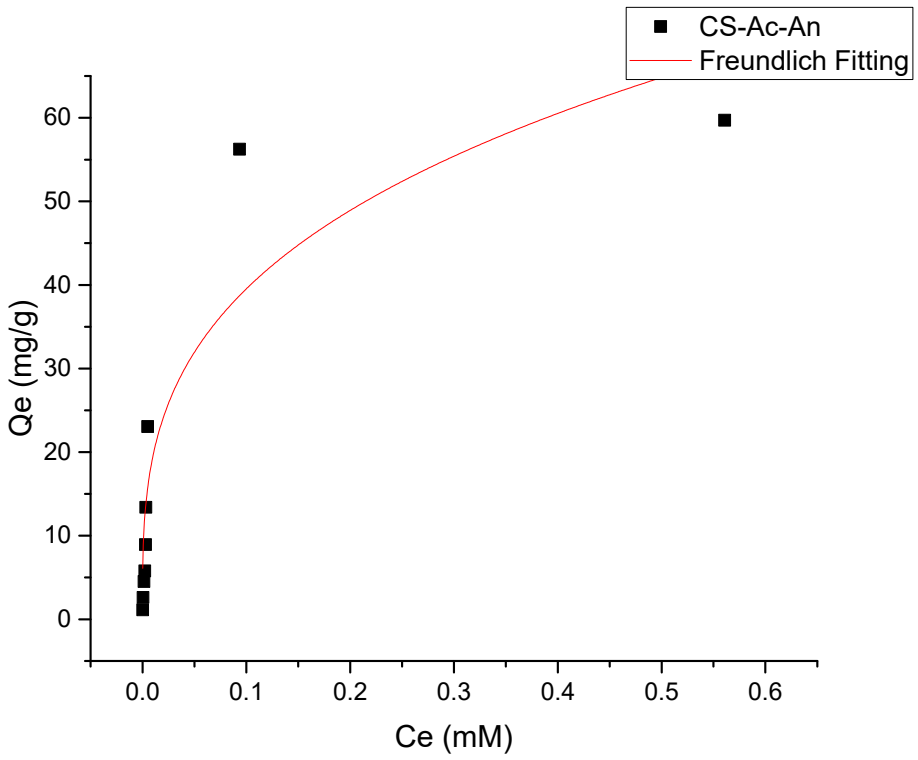


Figure S3: Isotherm Sorption for FL uptake with CS and CS-Ac-An, where the solid line represents the best-fit line by the Freundlich model with chi-square = 82.0 and adjusted R^2 = 0.842

Effect of pH on the adsorption process

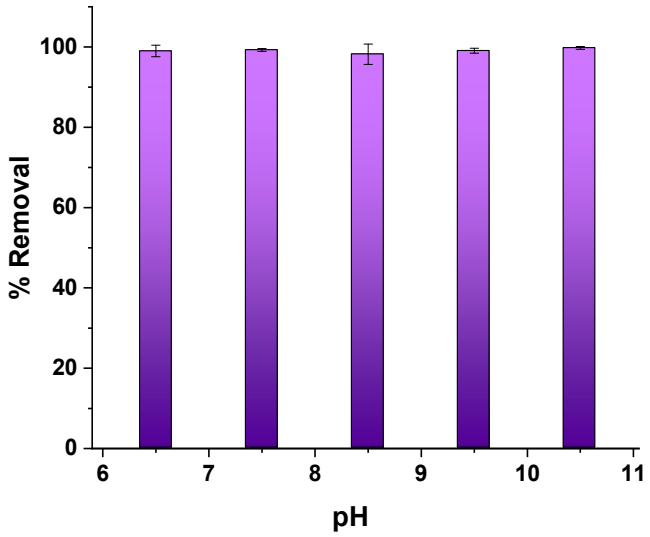


Fig S4: Effect of pH on the removal efficiency of FL by CS-Ac-An. (Initial concentration of FL= 30 μM, contact time 24 h, adsorbent dosage 10 mg, Volume: 5mL). Error bars show the standard deviations of two replicates.

Point of Zero Charge of CS-Ac-An

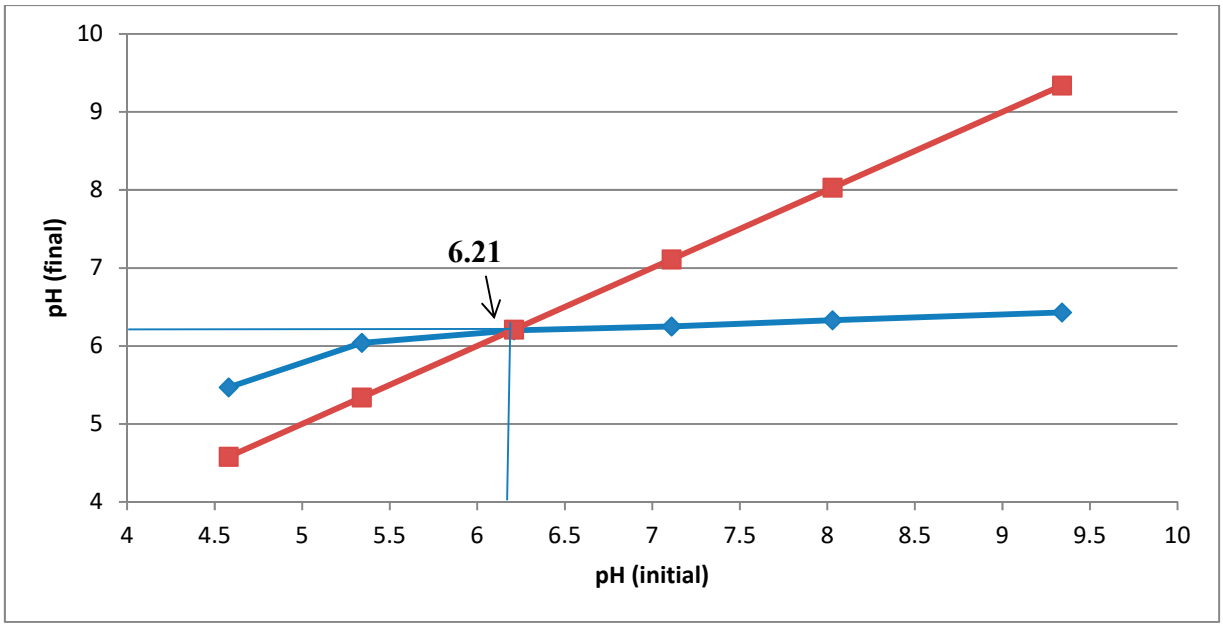
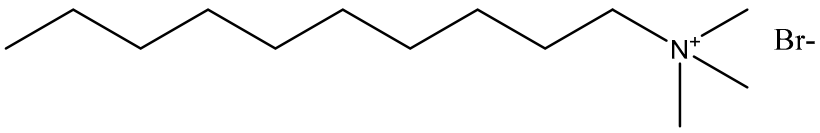


Figure S5: Determination of pH_{PZC} of CS-Ac-An.

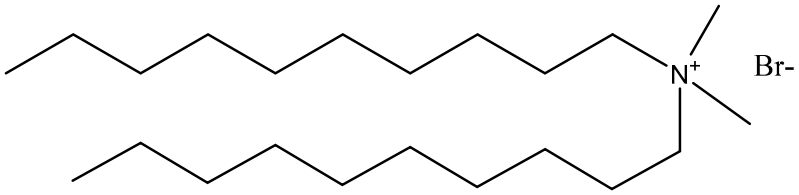
Table S3: Monomeric and Dimeric Cationic Surfactant Properties

	Chemical Formula	MW (g mol^{-1})	CMC (mmol L^{-1})
DTAB[a]	$C_{15}H_{35}NBr$	308	14
DDAB[b]	C26H56NBr	462	1

a) DTAB Structure



b) DDAB Structure



PSO Fitting of Experimental Data

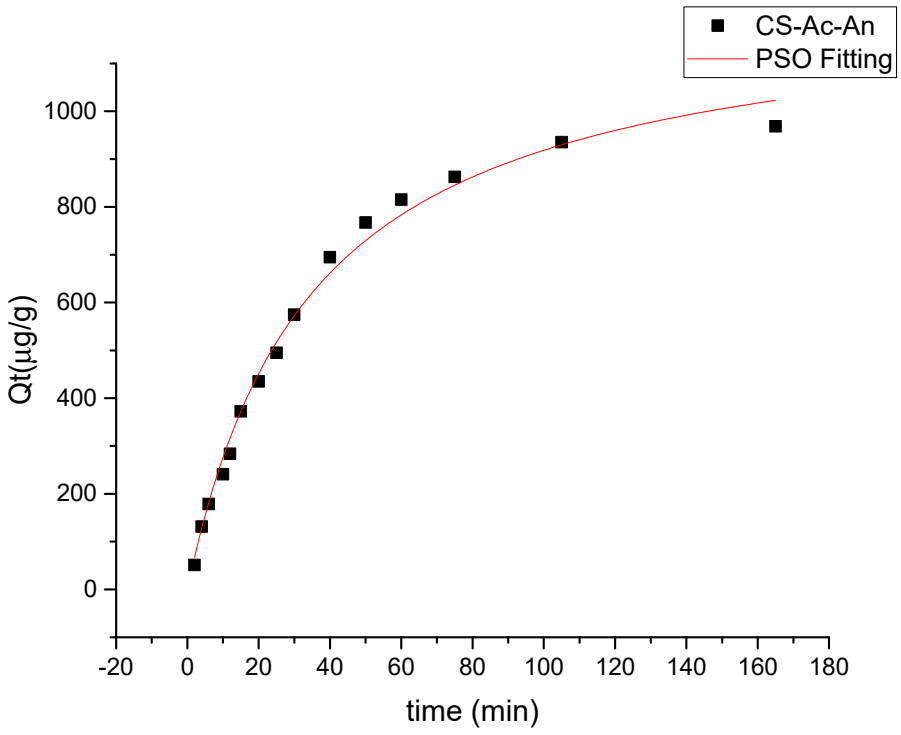
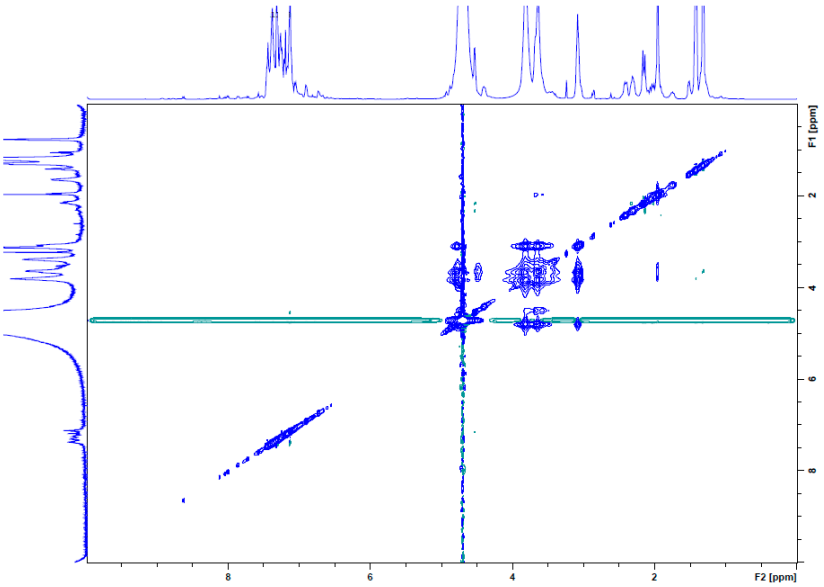


Figure S6: Kinetic Adsorption Profile for FL uptake with CS-Ac-An at ambient pH with 20 mg of CS-Ac-An while the initial concentration of FL solution was 20 µM and volume of 200 ml. The solid line shows the PSO fit to the experimental data

2D-NOESY spectra of FL/CS-Ac-An in D_2O/HCl (5% v/v)

a)



b)

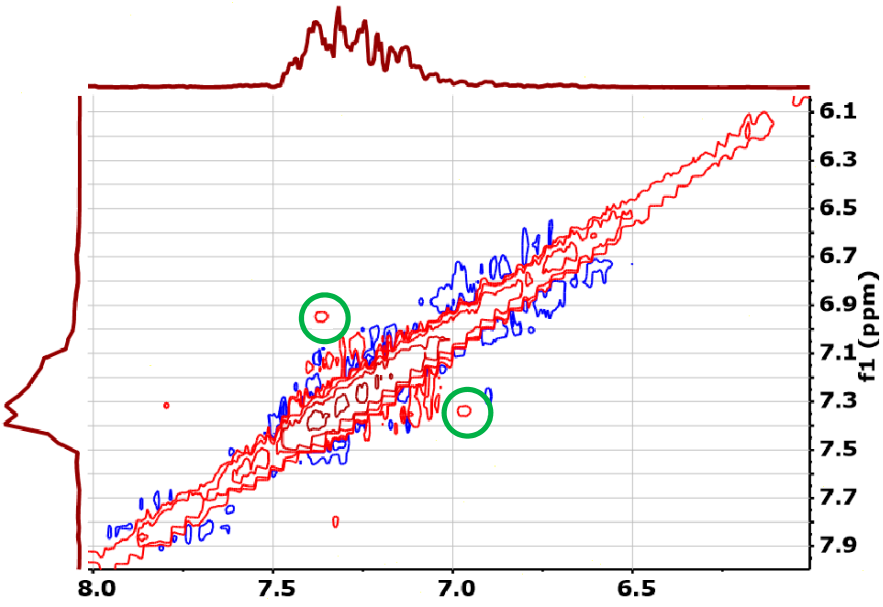


Figure S7: (a) 2D-NOESY spectra of FL/CS-Ac-An in D_2O/HCl (5% v/v) and (b) Expansion of aromatic spectral region. Red circles show the mentioned cross peaks.