

Synthesis and assessment of new cationic Gemini surfactants as inhibitors for carbon steel corrosion in oilfield water

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Petrol-1 #83-1290 RT: 0.30-4.42 AV: 1208 NL: 1.00E5
T: {0,0} + c EI Full ms

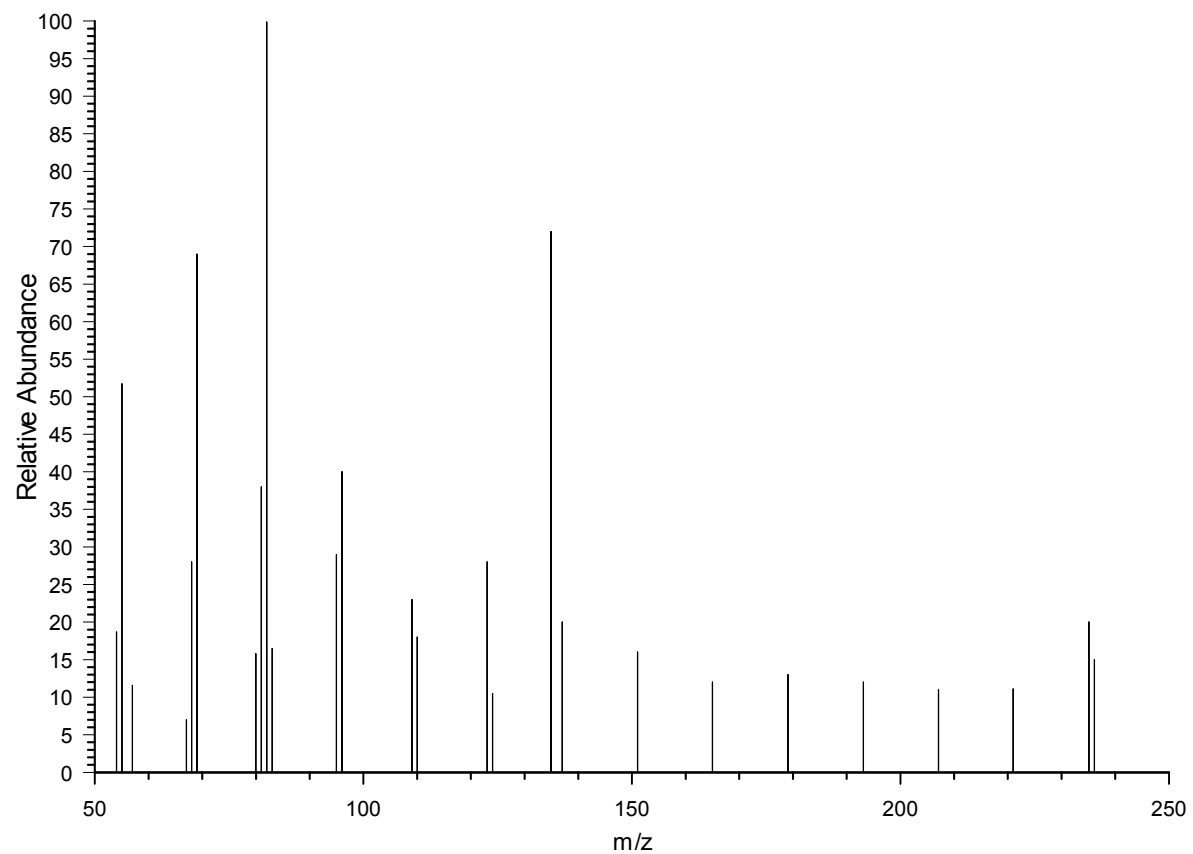


Fig. S 1: Mass spectrum of the intermediate compound.

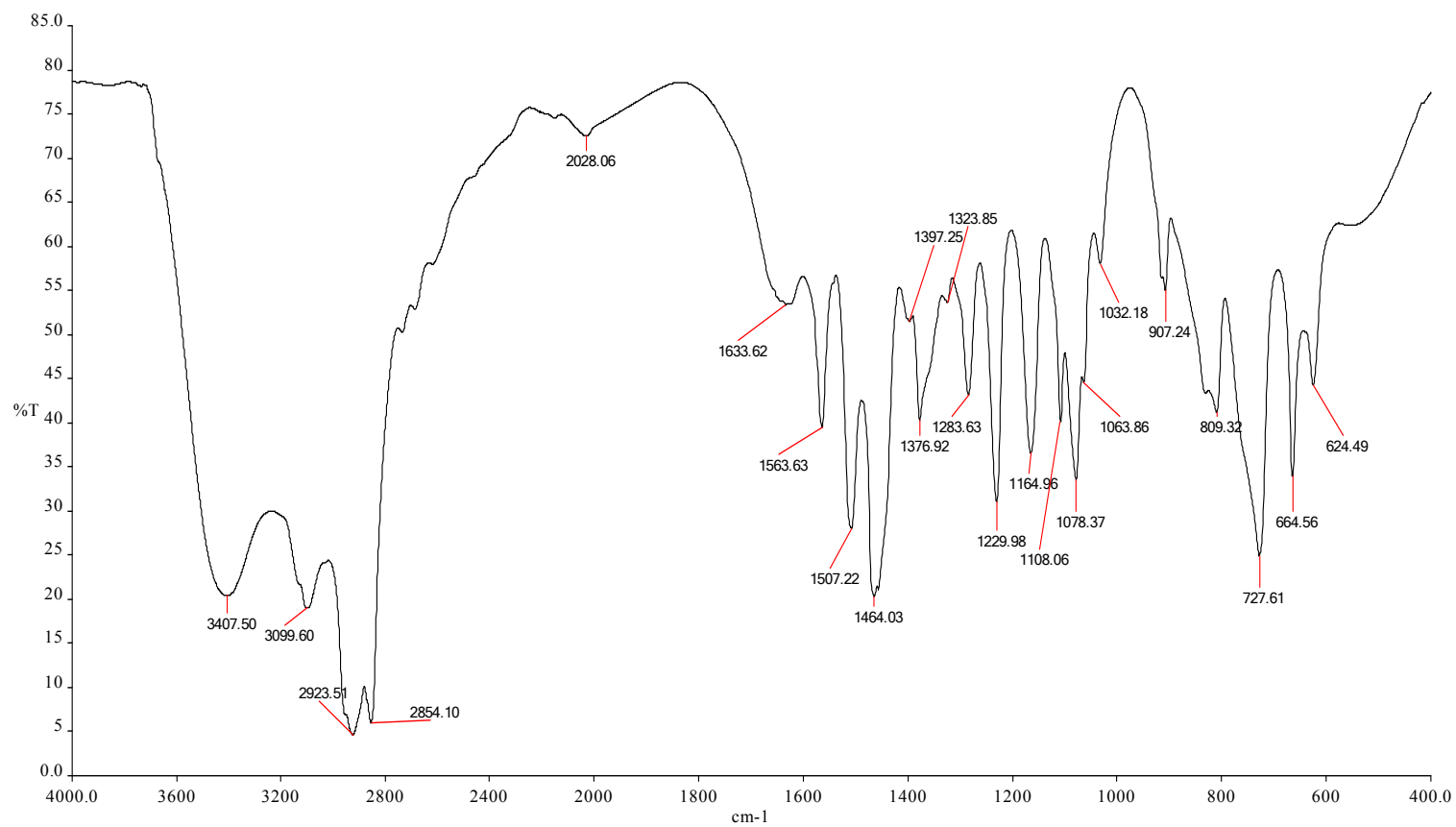


Fig. S 2: FT-IR spectrum of the intermediate compound.

IsmaeelAbdulShafy-1-CDC13-H1
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 Sample directory: D05mm_test_12Mar2014-21:34:40
 Pulse Sequence: s2pu1
 Solvent: CDC13
 Temp. 30.0 C / 303.1 K
 File: IsmaeelAbdulShafy-1-CDC13-H1
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 12.0 degrees
 Acq. time 4.004 sec
 Width 6600.7 Hz
 32 repetitions
 OBSERVE H1, 300.0673634 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65536
 Total time 36 min, 56 sec
 Date: Sep 5 2017

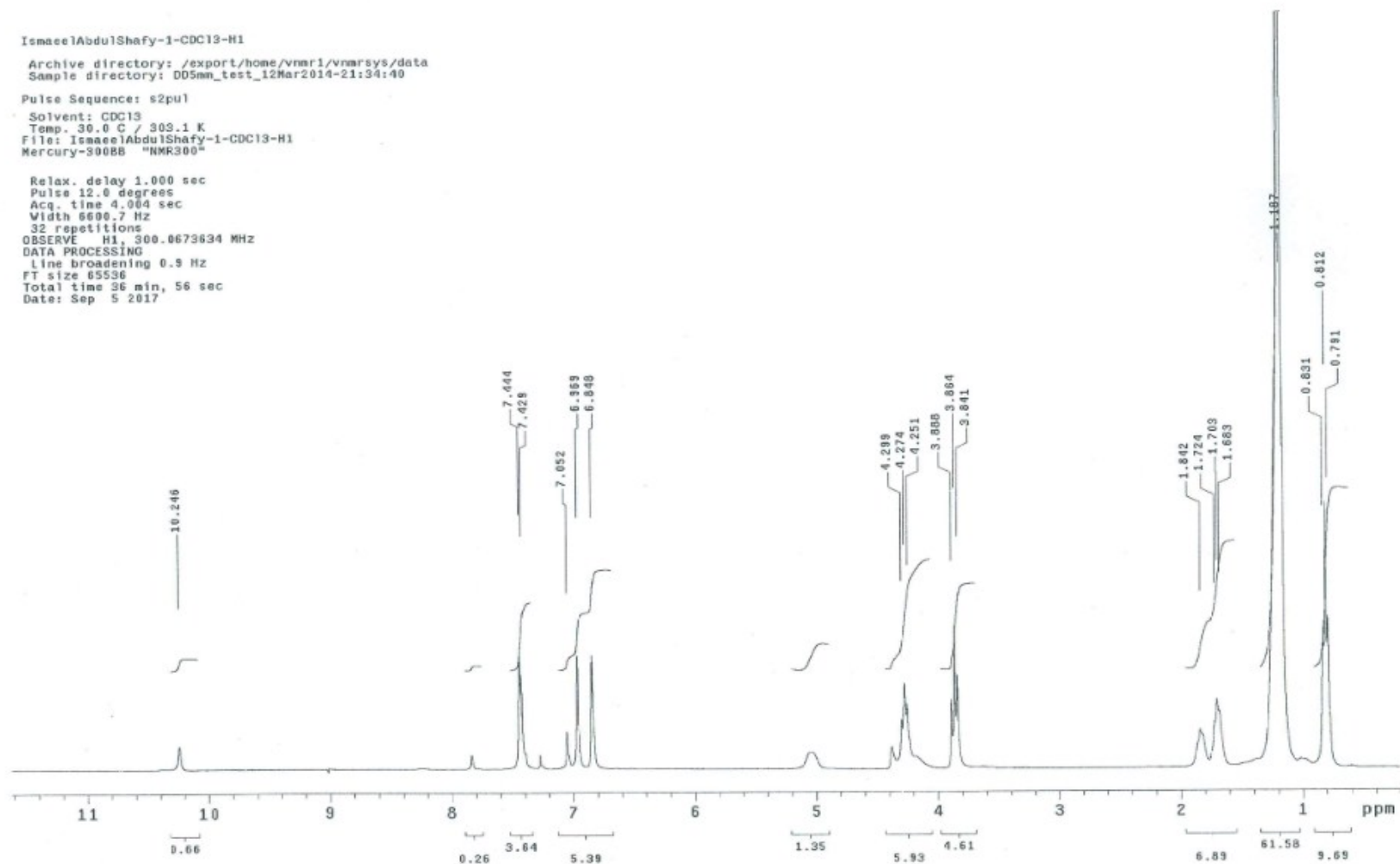


Fig. S 3: ¹H-NMR spectrum of the intermediate compound.

Petrol-2 #83-1290 RT: 0.31-4.42 AV: 1208 NL: 1.00E5
T: {0,0} + c EI Full ms

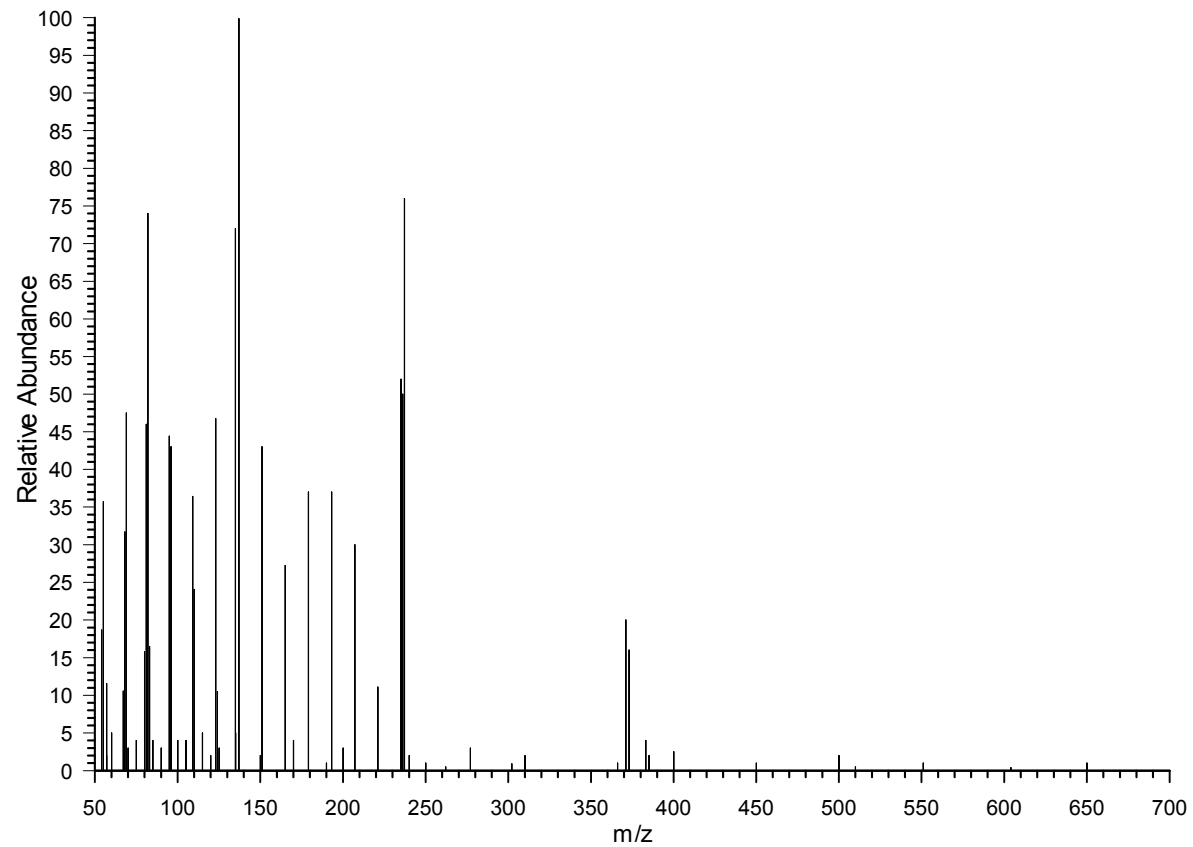


Fig. S 4: Mass spectrum of GS2.

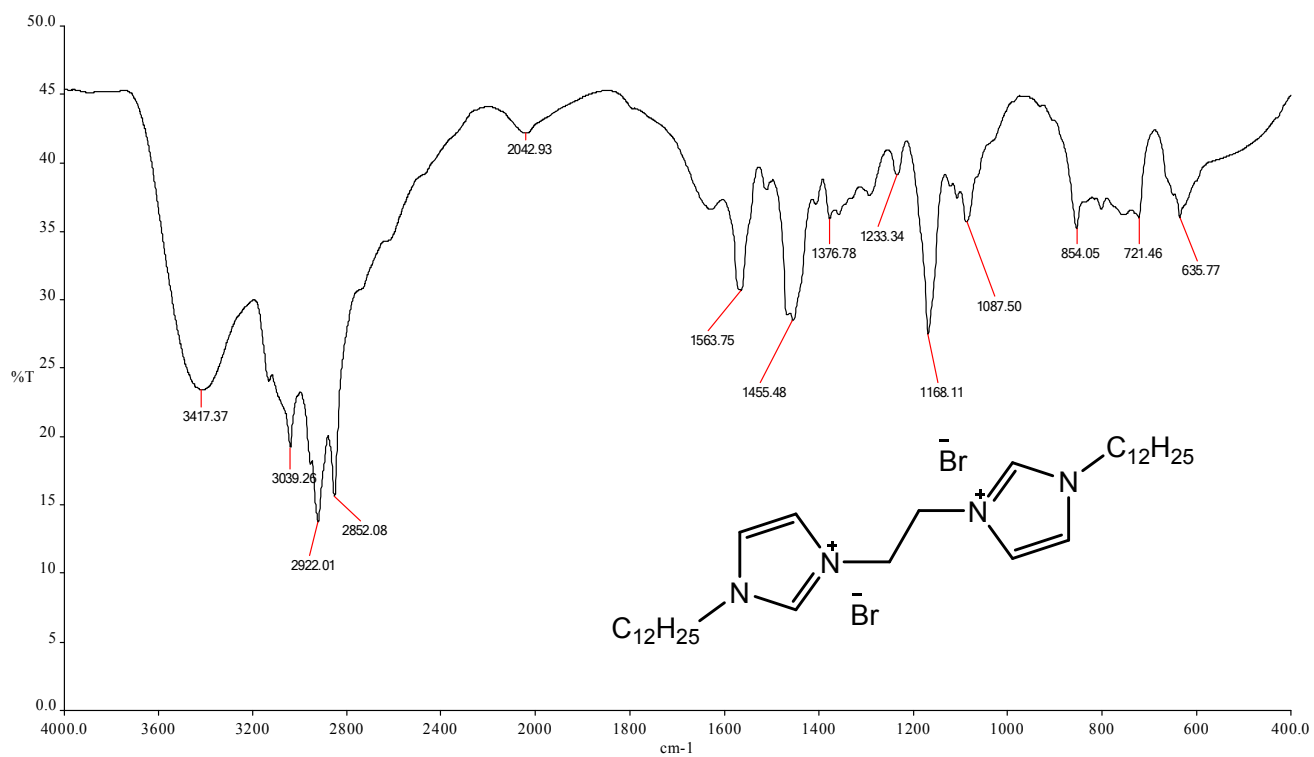


Fig. S 5: FT-IR spectrum of GS2.

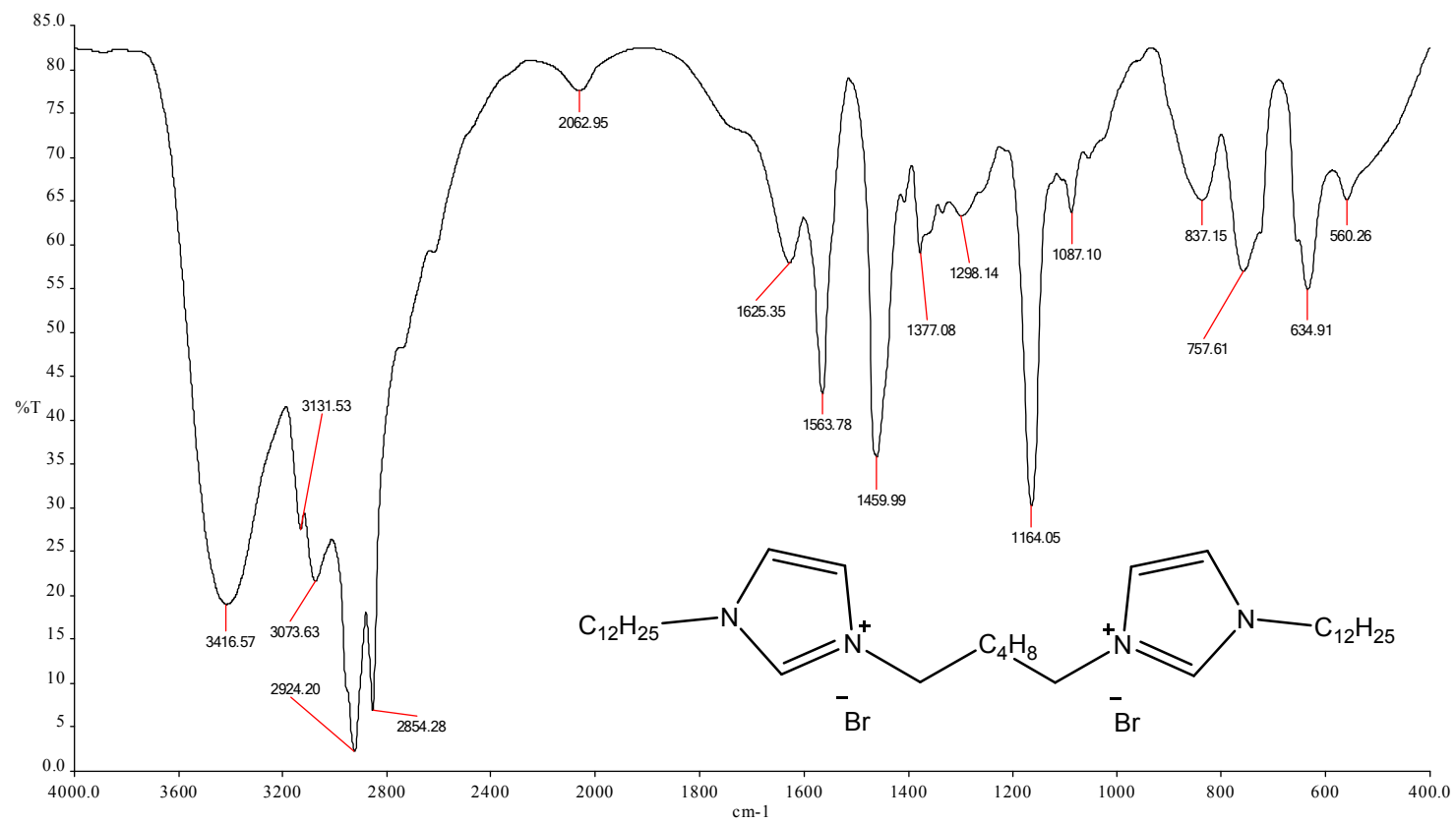


Fig. S 6: FT-IR spectrum of GS6.

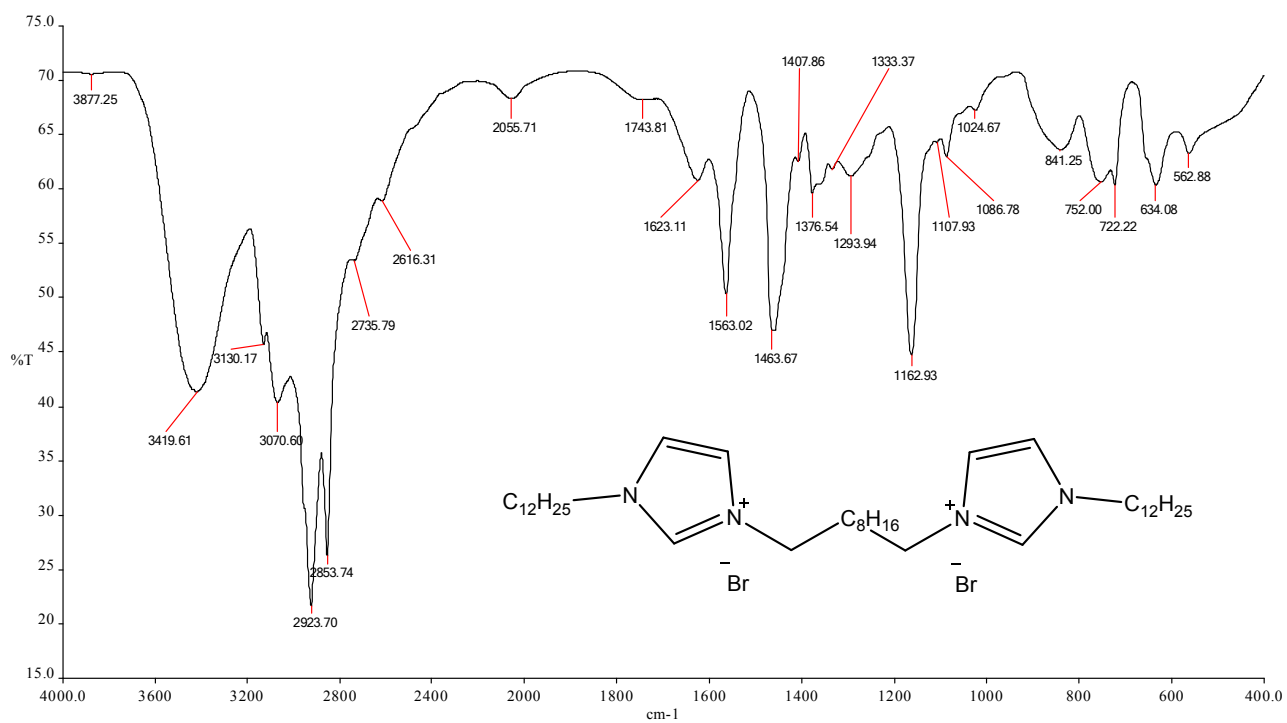


Fig. S 7: FT-IR spectrum of GS10.

AymanEsmat-1-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05sm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
48 repetitions
OBSERVE M1, 300.0673638 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 36 min, 56 sec
Date: Oct 20 2016

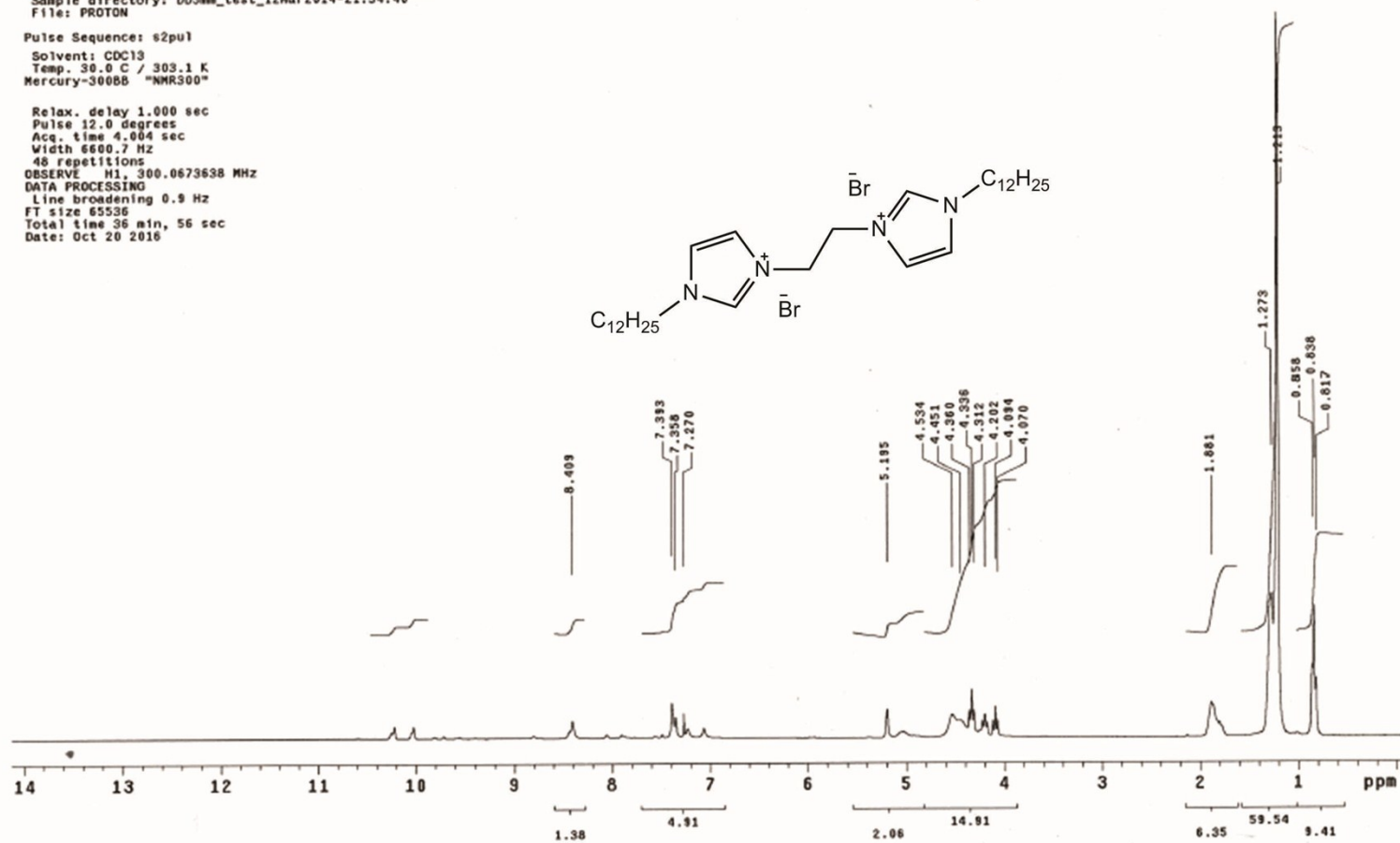


Fig. S 8: ¹H-NMR spectrum of GS2.

GS6

AymanEseat-2-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
56 repetitions
OBSERVE H1, 300.0673638 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 85536
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Date: Oct 20 2016

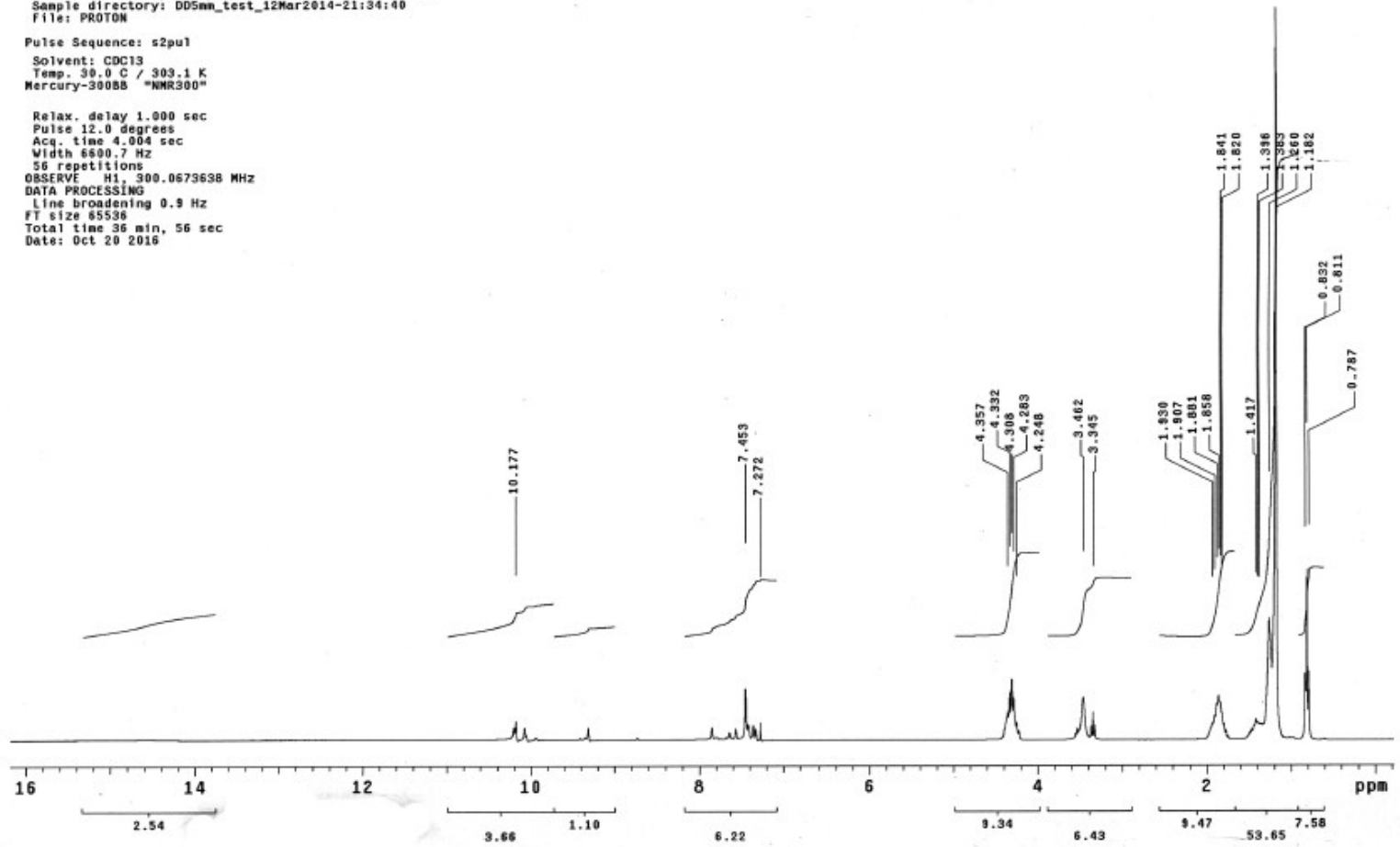


Fig. S 9: ^1H -NMR spectrum of GS6.

GS10

AymanEsmat-10-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DDSmm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
80 repetitions
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DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 36 min, 56 sec
Date: Oct 20 2016

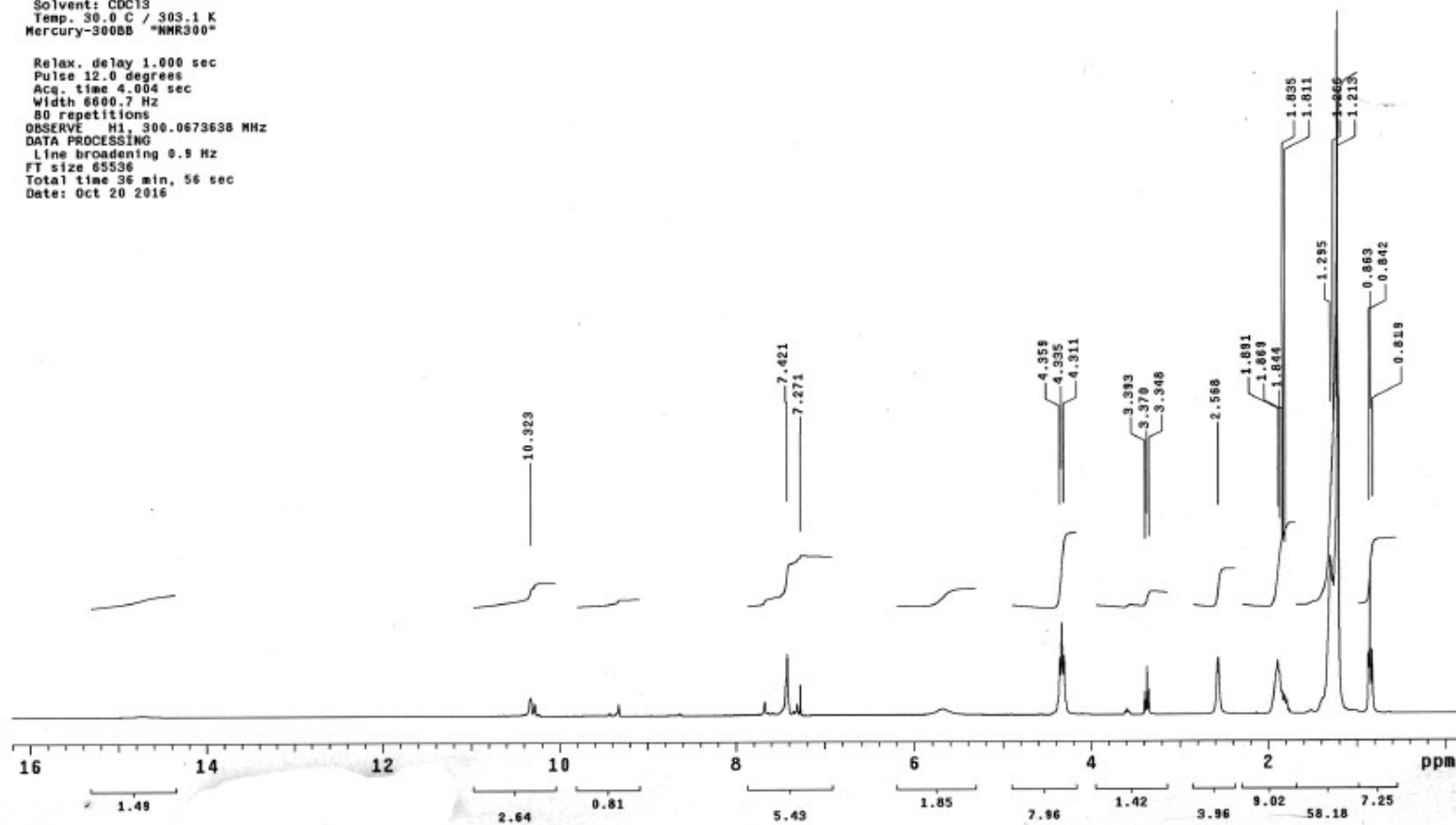


Fig. S 10: ^1H -NMR spectrum of GS10.

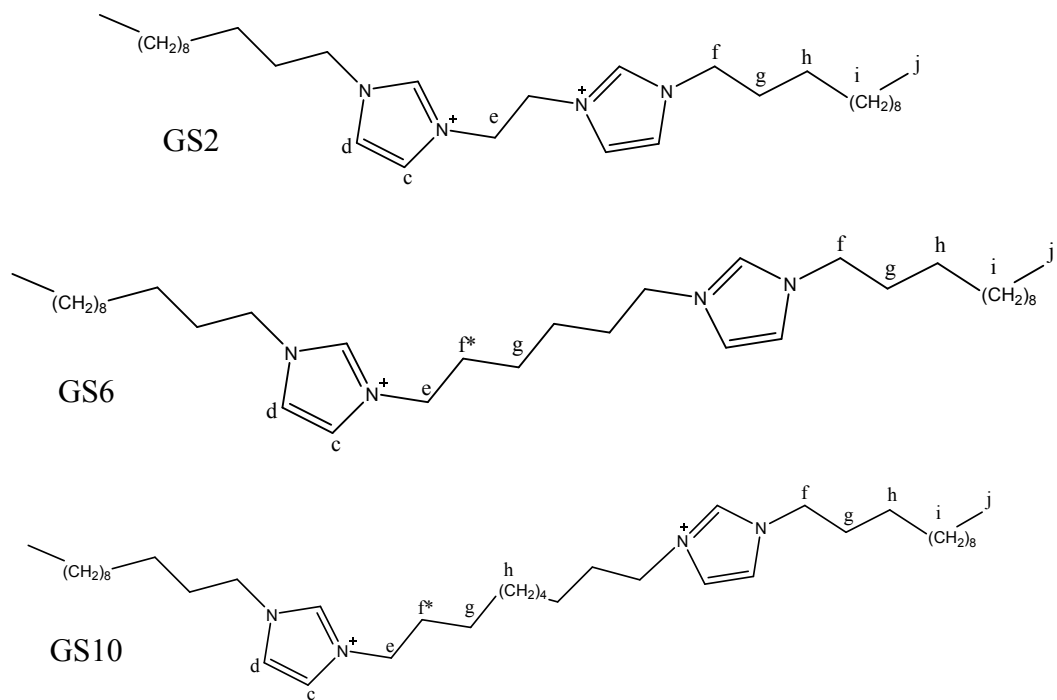
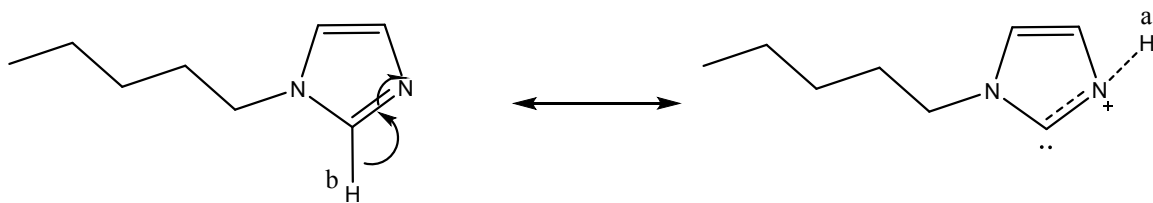
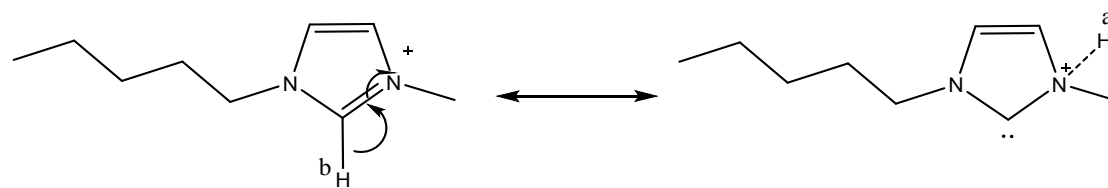


Fig. S 11: Different types of protons in Gemini surfactants.



Scheme S 1: Carbene proton and NH⁺ tautomerism for the intermediate compound.



Scheme S 2: Carbene proton and NH^+ tautomerism for the Gemini compounds.

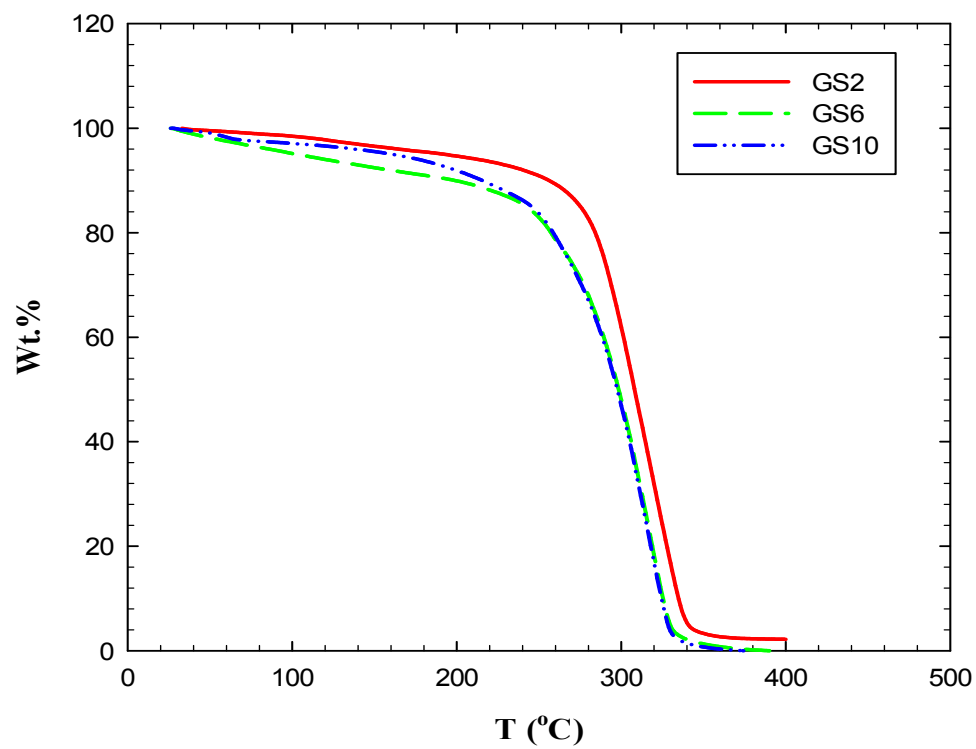


Fig. S 12: TGA curves for the synthesized Gemini surfactants.

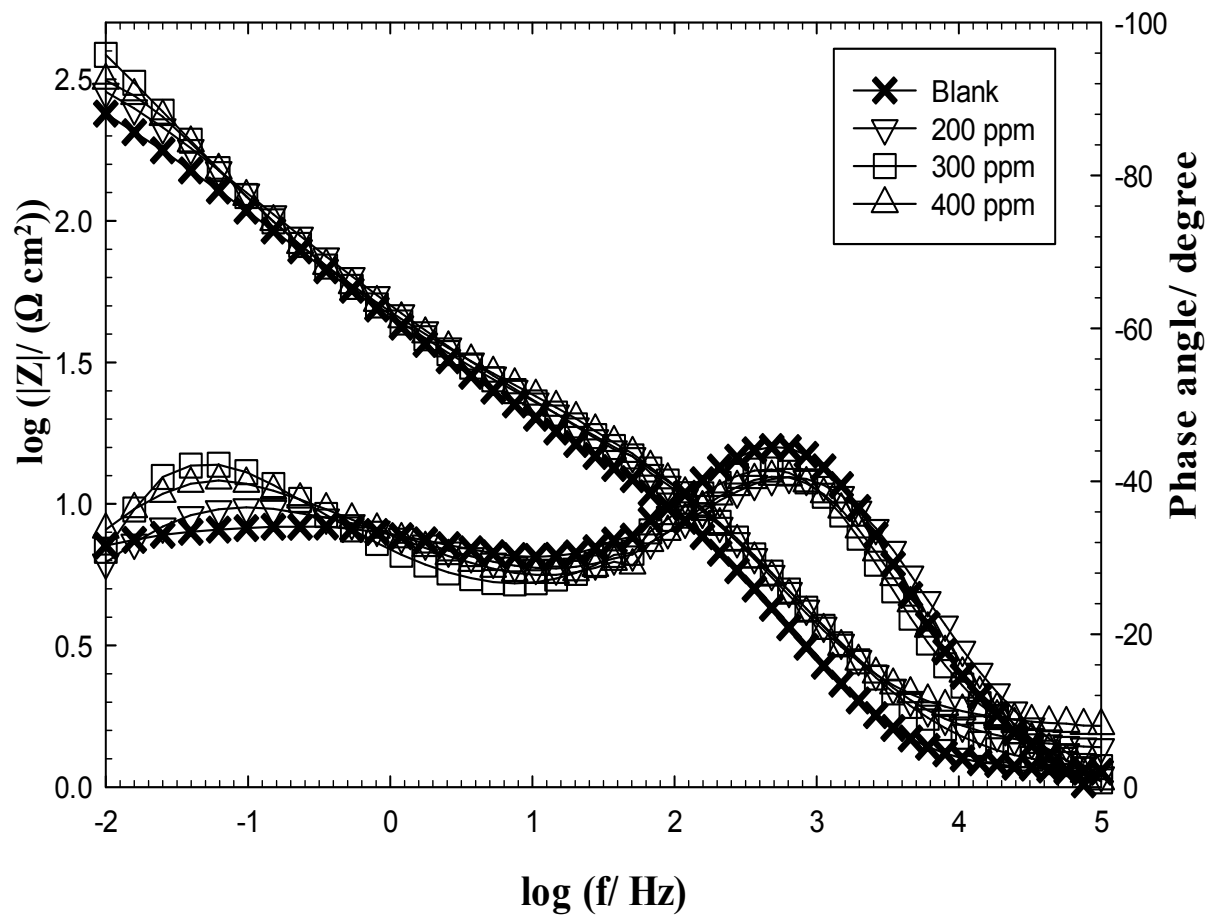


Fig. S 13: Bode plot for carbon steel in formation water as a function of GS6 concentration at 293 K.

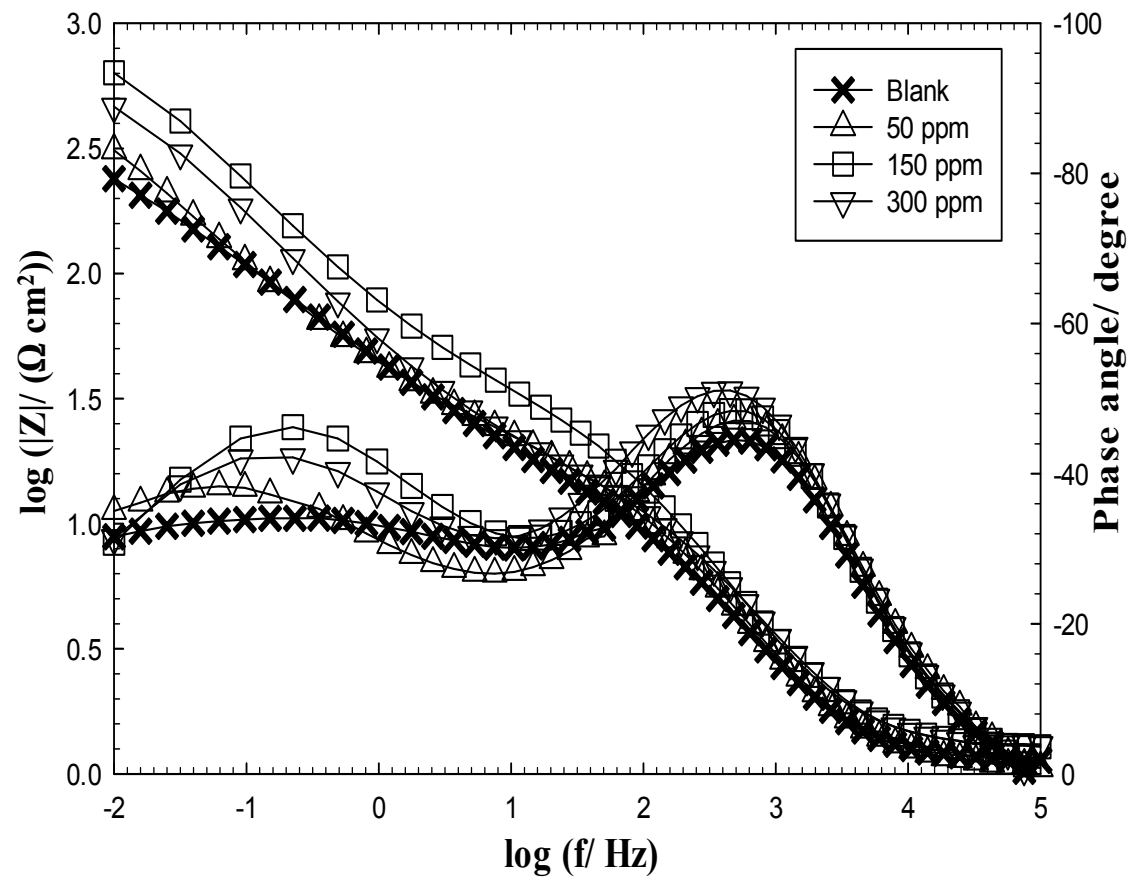


Fig. S 14: Bode plot for carbon steel in formation water as a function of GS10 concentration at 293 K.

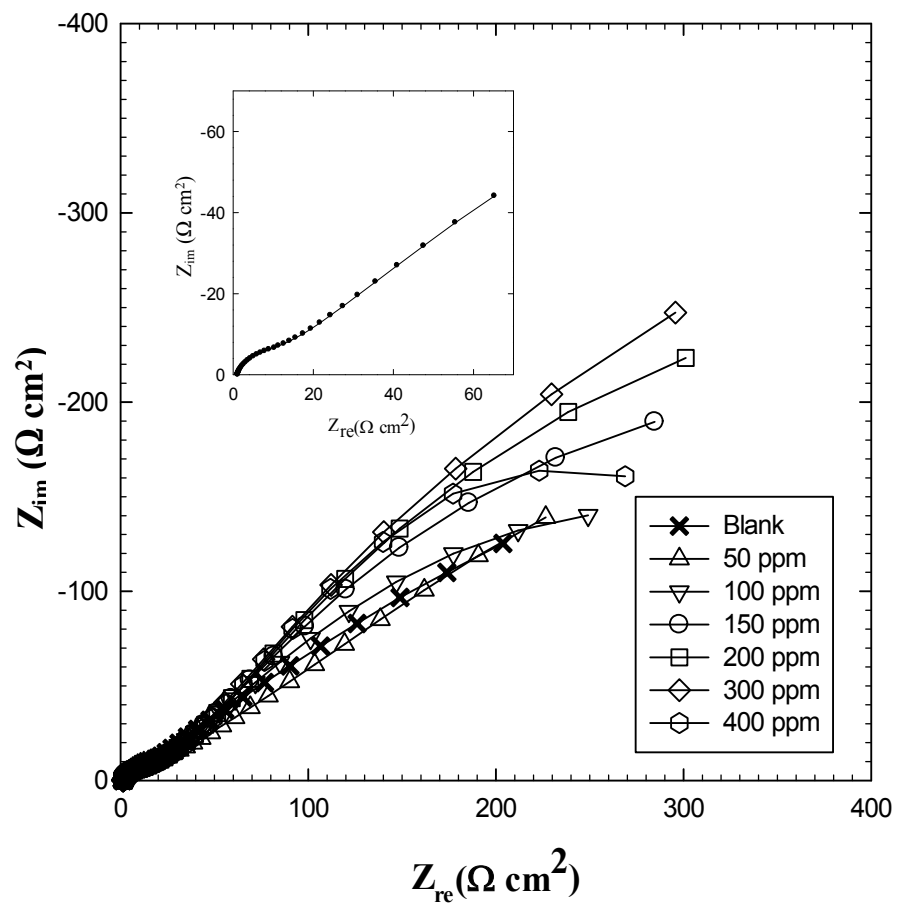


Fig. S 15: Nyquist plot for carbon steel in formation water as a function of GS6 concentration at 293 K. Inset: the Nyquist plot for CS in blank formation water.

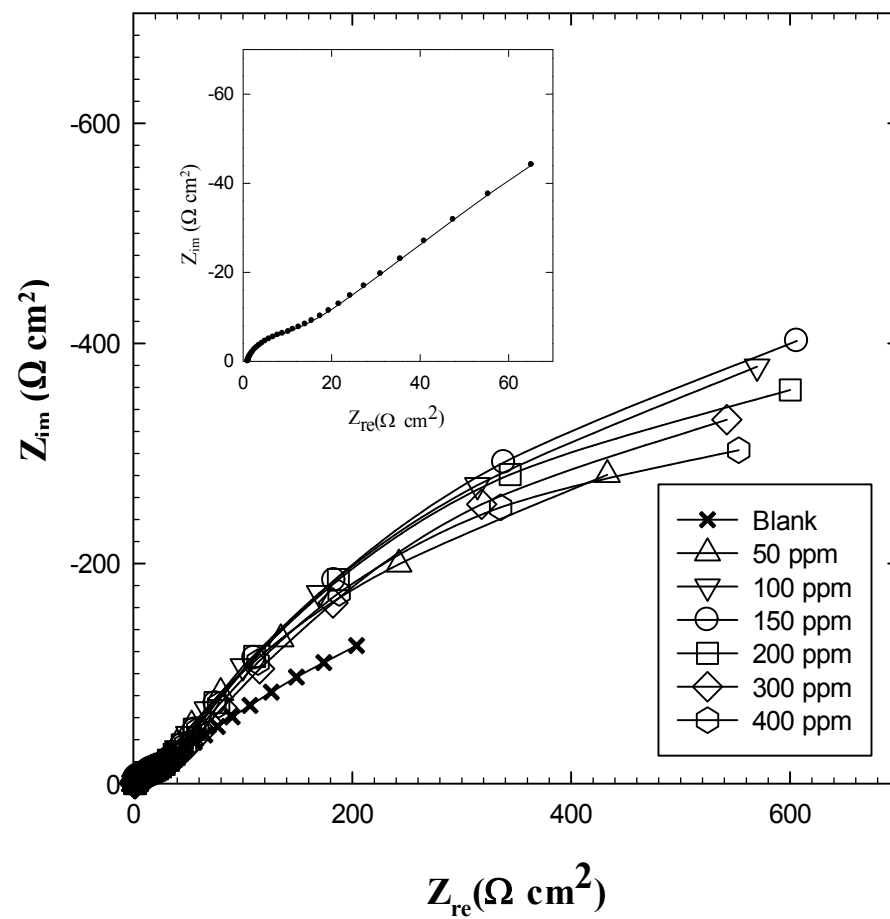


Fig. S 16: Nyquist plot for carbon steel in formation water as a function of GS10 concentration at 293 K. Inset: the Nyquist plot for CS in blank formation water.

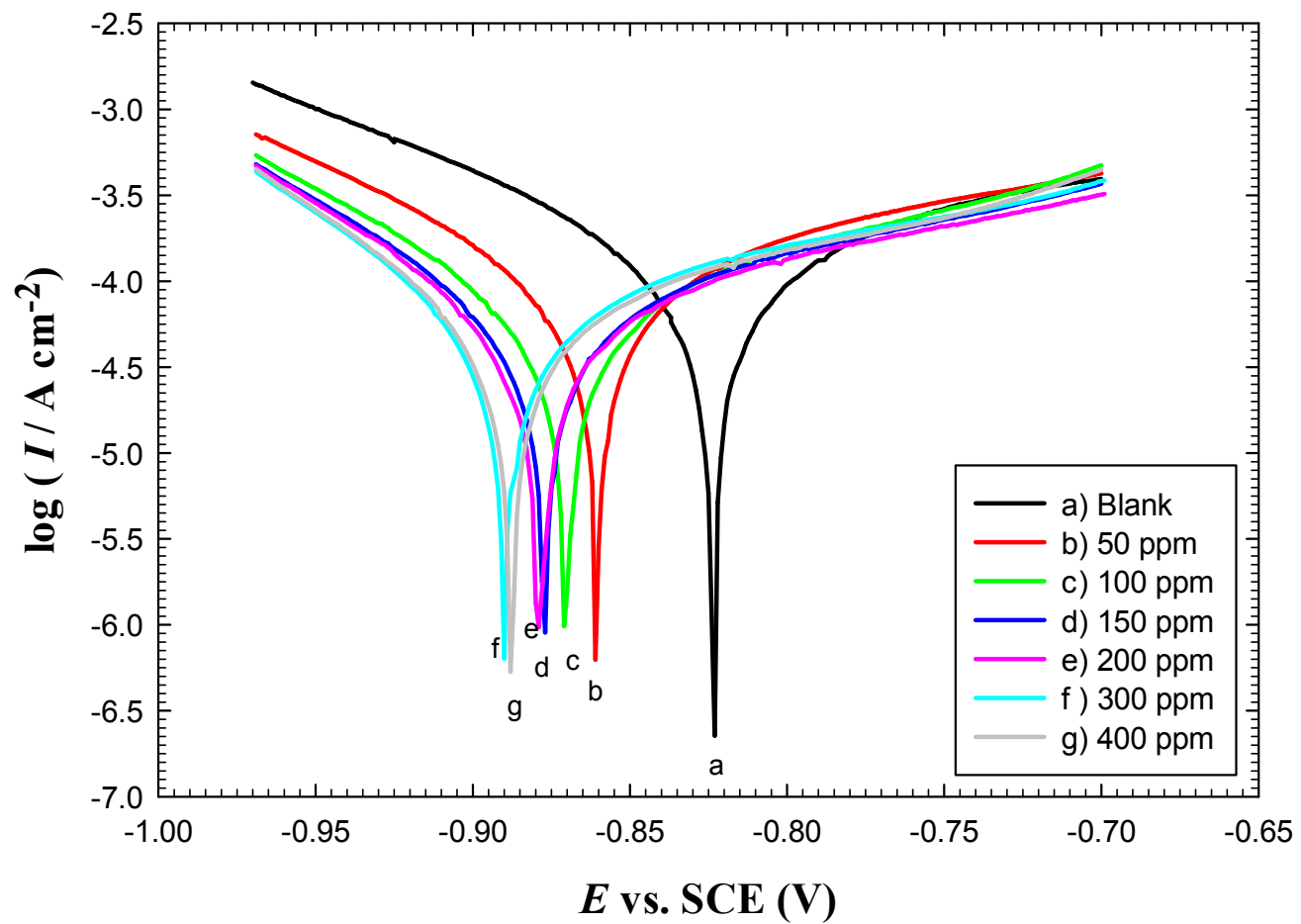


Fig. S 17: Polarization curves for carbon steel in formation water as a function of GS6 concentration at 293 K.

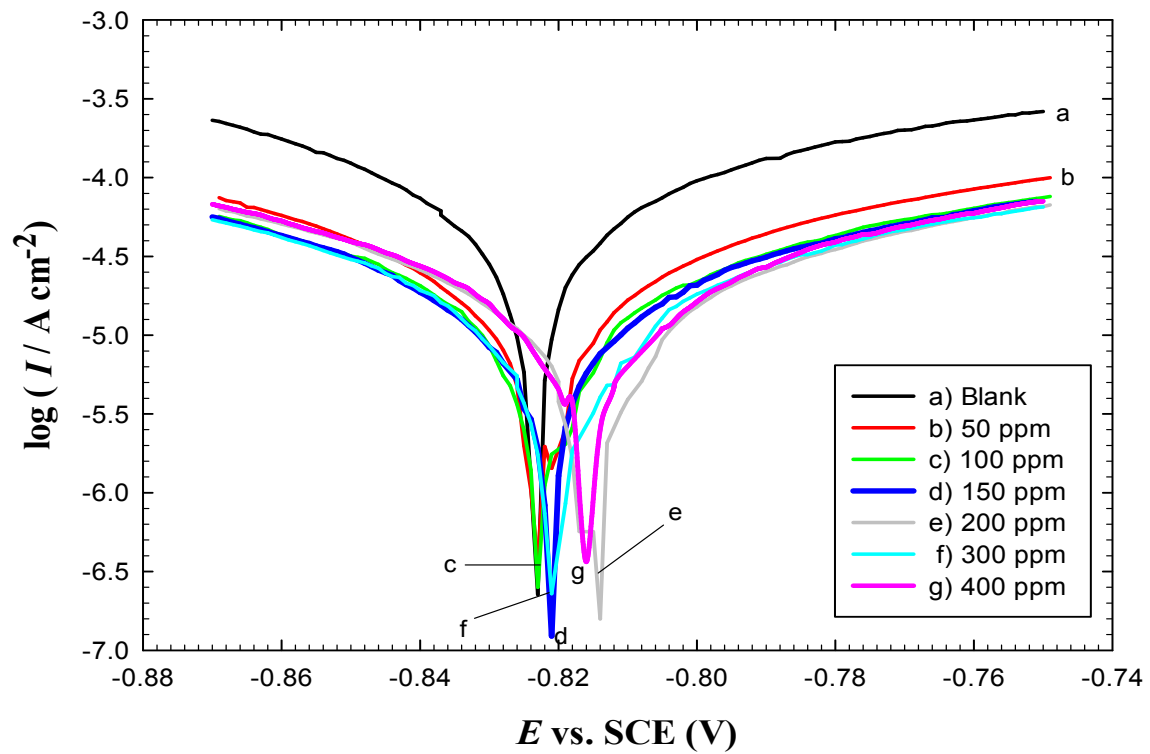


Fig. S 18: Polarization curves for carbon steel in formation water as a function of GS10 concentration at 293 K.

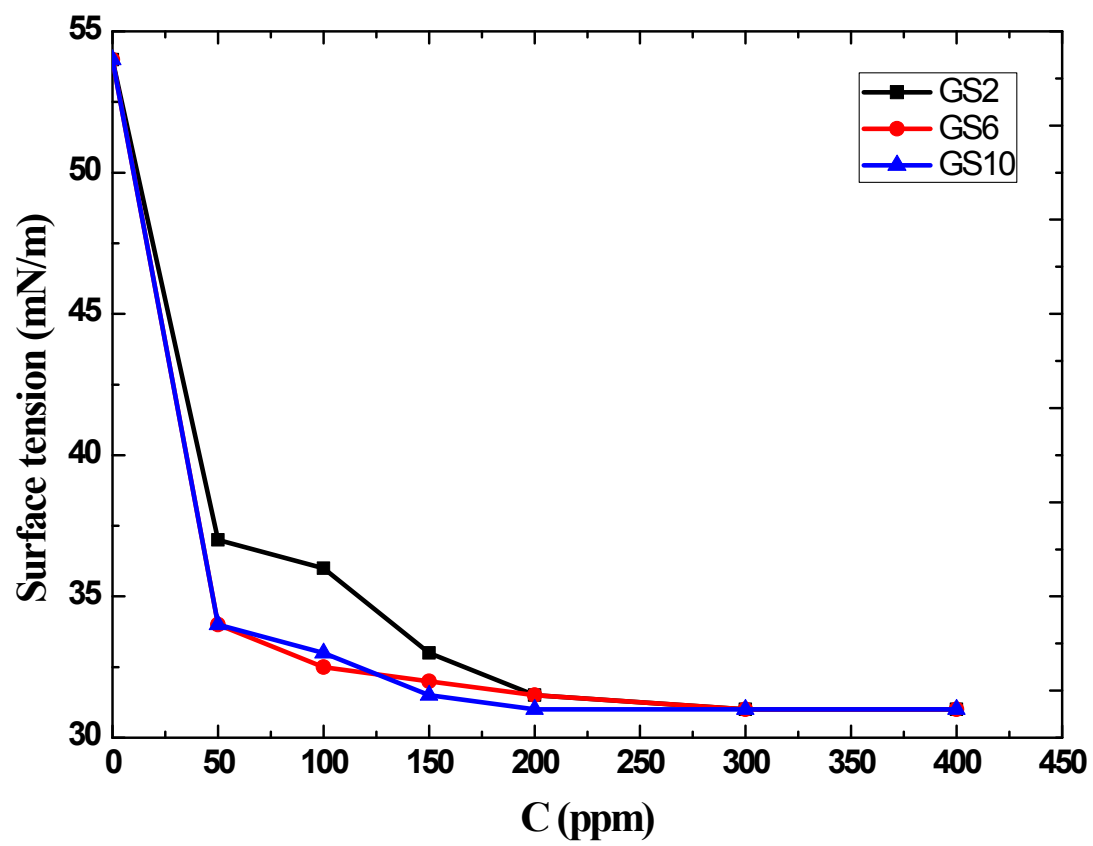


Fig. S 19: Variation of the surface tension with concentrations of GS2, GS6 and GS10.

Table S 1: FT-IR absorption bands (ν/cm^{-1}) for the intermediate, GS2, GS6 and GS10.

Assignment ⁷⁸	N-H	Aromatic C - H	Aliphatic C - H	Combination	Aromatic	C - Br	
				N-H	C=C or C=N		
Intermediate	3407	3099	2923 - 2854	2028	1564	
Absorption bands (cm^{-1})	GS2	3417	3039	2922 - 2852	2042	1563	636
	GS6	3416	3073	2924 - 2854	2062	1625	635
	GS10	3419	3070	2923 - 2853	2055	1623	635

Table S 2: Chemical shifts (δ/ppm) for the intermediate. Notes: spin multiplicity; s = singlet, d = Doublet, t = Triplet, m = Multiplet.

Protons	a	b	c	d	e	f, f'	g	h	i
Signals	10.246	7.436	6.969	6.843	4.274	3.864	1.703	1.187	0.812
	(s)	(d)	(d)	(d)	(t)	(m)	(m)	(m)	(t)

Table S 3: Chemical shifts (δ/ppm) for GS2, GS6 and GS10. Notes: spin multiplicity; s = singlet, d = Doublet, t = Triplet, m = Multiplet.

Compound	a	b	c	d	e	f, f'	g	h	i	J
GS2	10.168	8.409	7.376	7.270	4.534	4.202	4.094	1.881	1.273	0.838
	(s)	(s)	(d)	(d)	(t)	(t)	(m)	(m)	(m)	(t)
GS6	10.177	9.375	7.453	7.272	4.308	4.248 (t)	3.462	1.858	1.383	0.811
	(s)	(s)	(d)	(d)	(t)	4.283 (m)	(m)	(m)	(m)	(t)
GS10	10.323	9.274	7.421	7.271	4.335	3.370 (t)	2.568	1.844	1.235	0.842
	(s)	(s)	(d)	(d)	(t)	3.393 (m)	(m)	(m)	(m)	(t)

Table S 4: Elemental analysis of compounds GS2, GS6 and GS10.

Compound	Element							
	C%		H%		N%		Br%	
	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.
GS2	58.18	57.98	9.15	9.24	8.48	8.37	24.19	24.41
GS6	60.33	60.57	9.56	9.47	7.82	7.67	22.30	22.44
GS10	62.16	61.79	9.91	9.99	7.25	7.49	20.68	20.73