

Supporting Information for:

In-Situ Transformation of Hydraulic Fracturing Surfactants from Well Injection to Produced Water

Brandon C. McAdams^{a,b,*}, Kimberly E. Carter^{a,b,c}, Jens Blotevogel^d, Thomas
Borch^{d,e,f}, J. Alexandra Hakala^{a,*}

^aNational Energy Technology Laboratory, United States Department of Energy, 626 Cochrans Mill Road, Pittsburgh, Pennsylvania 15236, United States, ^bOak Ridge Institute for Science and Education, 100 ORAU Way, Oak Ridge, Tennessee 37830, United States, ^cDepartment of Civil and Environmental Engineering, University of Tennessee, 325 John D. Tickle Building, Knoxville, Tennessee 37996, United States, ^dDepartment of Civil and Environmental Engineering, Colorado State University, 1320 Campus Delivery, Fort Collins, Colorado 80523, United States, ^eDepartment of Chemistry, Colorado State University, 1872 Campus Delivery, Fort Collins, Colorado 80523, United States, ^fDepartment of Soil and Crop Sciences, Colorado State University, 1170 Campus Delivery, Fort Collins, Colorado 80523, United States

*Corresponding Authors: Brandon C. McAdams, Phone: 412-386-5047, Email: Brandon.McAdams@netl.doe.gov; and J. Alexandra Hakala, Phone: 412-386-5487, Email: Alexandra.Hakala@netl.doe.gov

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Hydraulic Fracturing and Production Details

Hydraulic fracturing fluid (HFF) samples were collected for each stage from the blender during the pumping of each stage and contained hydraulic fracturing chemicals including friction reducer, biocide, scale and corrosion inhibitor, and iron control agent but no sand, gel, or breaker. A full accounting of HFF additives reported to fracfocus.org can including manufacturer, trade names, and mixture concentrations can be found in Table S1. The HFF samples contained source waters from fresh water, coal mine water, and recycled produced water from previous well completions. Wells 1 and 2 had 14 total fracturing stages, and well 3 had 10 total fracturing stages. With the exception of stages 1 and 3 from well 1 and stage 2 from well 3, all stages from the three wells were sampled. Where stages are not shown in figures or tables, no identifiable peaks were present in the QTOF-MS spectra. Stages were fractured separately using a plugging and perforation technique, and so fracturing fluids were not mixed among stages. Fracturing occurred over a week period from June 4th to June 11th, 2012 with a stage being fractured roughly every 12 hours. Production began the same day that the final stage was fractured for each well. Produced water samples were collected over a six day period and are labeled by both barrels of water produced and hours from collection of the first produced water sample (Figure 2).

Table S1. Additive trade names, purposes, manufacturers, and concentration ranges in hydraulic fracturing fluid (HFF) for the three wells studied as reported to fracfocus.org. Also included are components, component CAS numbers, and component concentration ranges in HFF additives. These include all possible additives used. *Actual additives used may vary per stage as discussed in the main text and shown in Tables S2-S4* (e.g. Polyethylene Glycols were observed in only 4 injection fluid samples).

Trade Name	Purpose	Manufacturer	Conc. in HFF (%)	Components	CAS#	Component Conc. (%)
Scale Hib A	Scale Inhibitor	NALCO	0.02–0.04	Triethanolamine Tri(Phosphate Ester)	68171-29-9	10–30
				Ethylene Glycol	107-21-1	10–30
I-7L	Iron Control	Weatherford	0.01–0.02	Ethylene Glycol	107-21-1	10–20
				Triethanolamine hydroxyacetate	68299-02-5	10–20
				Glycolic Acid	79-14-1	1–2.5
Unislik ST-50	Friction Reducer	Weatherford	0.07–0.08	Petroleum distillates	64742-47-8	10–30
				Alcohols, ethoxylated	68439-50-9	1–5
				Alcohols, ethoxylated	68551-12-1	1–5
				Alcohols, ethoxylated	68002-97-1	1–5
				Ammonium acetate	631-61-8	7–13
WGA-5	Dry Gellant	Franklin Well Services	0.02–0.03	Carboxymethylhydroxypropyl guar	N/A	N/A
Unihib G	Corrosion Inhibitor	GeoSafe Chemicals	0.0005	Short chained glycol ether	112-34-5	40–60
				Ethoxylated alcohol	68002-97-1	20–35
				Methanol	67-56-1	1–5
				Acetophenone	98-86-1	<1
				Formaldehyde	50-00-0	<1
				Thiourea	62-56-6	<1
LEB-10X	Enzymatic Breaker	Franklin Well Services	0.0007	Hemicellulase	N/A	N/A
				Ethylene Glycol	107-21-1	60
EC6116A	Biocide	NALCO	0.02–0.03	Dibromoacetone nitrile	3252-43-5	1–5
				2,2-Dibromo-3-nitrilopropionamide	10222-01-2	10–30
				Polyethylene Glycol	25322-68-3	30–60
15% HCl	Acid	Weatherford	0.6–0.9	Hydrochloric Acid	7647-01-0	15

Table S2. Summary of base peaks, base peak formulas, average observed m/z, average error, number of observations, and Kendrick mass defects for all surfactant species identified in injected hydraulic fracturing fluid and produced water from the three sampled wells.

	Surfactant Species	Base Peak	Base Peak Formula	Average Observed m/z	Theoretical m/z	Average Error (ppm)	Obs. (n)	Kendrick Mass	KMD
Injected Hydraulic Fracturing Fluid	C12-E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2636	341.2662	7.61	23	341.061	0.061
	C12-E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2893	385.2924	7.98	24	385.060	0.060
	C12-E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3151	429.3187	8.40	24	429.060	0.060
	C12-E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3410	473.3449	8.27	24	473.059	0.059
	C12-E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3668	517.3711	8.30	24	517.059	0.059
	C12-E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3923	561.3973	8.96	17	561.058	0.058
	C12-E09	[M+Na] ⁺	C ₃₀ H ₆₂ O ₁₀ Na ⁺	605.4186	605.4235	8.13	4	605.058	0.058
	C12-E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4382	556.4419	6.62	6	556.107	0.107
	C12-E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4643	600.4654	1.91	8	600.107	0.107
	C12-E010	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₁ ⁺	644.4903	644.4909	0.89	4	644.107	0.107
	C12-E011	[M+NH ₄] ⁺	C ₃₄ H ₇₄ NO ₁₂ ⁺	688.5156	688.5206	7.17	1	688.106	0.106
	C14-E03	[M+Na] ⁺	C ₂₀ H ₄₂ O ₄ Na ⁺	369.2949	369.2975	7.07	4	369.075	0.075
	C14-E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3205	413.3237	7.79	22	413.075	0.075
	C14-E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3465	457.3500	7.61	23	457.074	0.074
	C14-E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3724	501.3762	7.60	23	501.074	0.074
	C14-E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3982	545.4025	7.84	22	545.074	0.074
	C14-E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4244	589.4287	7.23	10	589.074	0.074
	C14-E09	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₀ ⁺	628.4949	628.4994	7.19	1	628.121	0.121
	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1024	217.1046	10.13	1	216.973	0.973
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1286	261.1309	8.63	4	260.973	0.973
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1547	305.1571	7.72	2	304.973	0.973
Produced Water	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1802	349.1833	8.88	1	348.972	0.972
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2062	393.2095	8.29	1	392.972	0.972
	C12-E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3187	429.3187	0.00	1	429.063	0.063
	C12-E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3712	517.3711	-0.19	1	517.063	0.063
	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1071	217.1046	-11.56	27	216.978	0.978
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1359	261.1309	-19.23	27	260.981	0.981
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1624	305.1571	-17.31	27	304.981	0.981
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.26	27	348.978	0.978
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2107	393.2095	-3.10	27	392.977	0.977

Table S3. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of *injected HFF* by stage for *well 1*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 5	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2644	341.2662	5.33	341.061	0.061	145883	4.89
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2904	385.2924	5.16	385.061	0.061	397562	13.33
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3161	429.3187	6.13	429.061	0.061	586593	19.67
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3420	473.3449	6.08	473.060	0.060	654723	21.95
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3680	517.3711	5.99	517.060	0.060	524408	17.58
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3212	413.3237	5.95	413.075	0.075	119945	4.02
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3474	457.3500	5.64	457.075	0.075	168928	5.66
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3735	501.3762	5.53	501.075	0.075	177214	5.94
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3992	545.4025	5.90	545.075	0.075	126511	4.24
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4251	589.4287	6.07	589.074	0.074	80560	2.70
Stage 7	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2644	341.2662	5.25	341.061	0.061	215834	4.74
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2901	385.2924	5.87	385.061	0.061	587217	12.90
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3161	429.3187	6.06	429.061	0.061	814021	17.89
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3421	473.3449	5.92	473.060	0.060	866360	19.04
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3680	517.3711	5.93	517.060	0.060	677839	14.89
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4386	556.4419	5.97	556.107	0.107	210126	4.62
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4651	600.4654	0.55	600.108	0.108	148848	3.27
	C ₁₂ -E010	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₁ ⁺	644.4912	644.4909	-0.50	644.108	0.108	82604	1.82
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3214	413.3237	5.61	413.075	0.075	176071	3.87
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3477	457.3500	5.01	457.076	0.076	237727	5.22
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3736	501.3762	5.30	501.075	0.075	241767	5.31
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3995	545.4025	5.39	545.075	0.075	174625	3.84
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4254	589.4287	5.62	589.075	0.075	117756	2.59

Table S3
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 8	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2643	341.2662	5.68	341.061	0.061	189626	4.10
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2902	385.2924	5.81	385.061	0.061	584065	12.63
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3160	429.3187	6.22	429.061	0.061	863506	18.67
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3421	473.3449	5.94	473.060	0.060	952515	20.59
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3680	517.3711	6.07	517.060	0.060	759889	16.43
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4385	556.4419	6.15	556.107	0.107	161686	3.50
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4648	600.4654	1.02	600.107	0.107	110290	2.38
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3213	413.3237	5.71	413.075	0.075	172294	3.72
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3475	457.3500	5.44	457.075	0.075	249744	5.40
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3735	501.3762	5.47	501.075	0.075	262044	5.67
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3994	545.4025	5.68	545.075	0.075	192340	4.16
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4252	589.4287	5.91	589.074	0.074	127565	2.76
Stage 10	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2639	341.2662	6.86	341.061	0.061	262426	5.23
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2895	385.2924	7.55	385.060	0.060	663882	13.24
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3154	429.3187	7.76	429.060	0.060	863722	17.22
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3413	473.3449	7.56	473.060	0.060	869136	17.33
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3671	517.3711	7.67	517.059	0.059	657745	13.12
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4377	556.4419	7.62	556.107	0.107	218332	4.35
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4639	600.4654	2.48	600.107	0.107	156642	3.12
	C ₁₂ -E010	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₁ ⁺	644.4900	644.4909	1.46	644.106	0.106	88792	1.77
	C ₁₄ -E03	[M+Na] ⁺	C ₂₀ H ₄₂ O ₄ Na ⁺	369.2947	369.2975	7.61	369.075	0.075	83697	1.67
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3209	413.3237	6.85	413.075	0.075	222665	4.44
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3468	457.3500	7.02	457.075	0.075	293095	5.84
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3728	501.3762	6.81	501.074	0.074	289406	5.77
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3986	545.4025	7.11	545.074	0.074	206264	4.11
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4244	589.4287	7.24	589.074	0.074	139386	2.78

Table S3
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 11	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2639	341.2662	6.65	341.061	0.061	215022	6.07
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2896	385.2924	7.32	385.060	0.060	511121	14.43
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3154	429.3187	7.66	429.060	0.060	660005	18.63
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3414	473.3449	7.44	473.060	0.060	663502	18.73
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3672	517.3711	7.58	517.059	0.059	489176	13.81
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4380	556.4419	7.01	556.107	0.107	127279	3.59
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4641	600.4654	2.13	600.107	0.107	82329	2.32
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3208	413.3237	7.02	413.075	0.075	165261	4.67
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3470	457.3500	6.67	457.075	0.075	209896	5.93
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3728	501.3762	6.77	501.074	0.074	199837	5.64
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3985	545.4025	7.32	545.074	0.074	135239	3.82
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4243	589.4287	7.35	589.074	0.074	83168	2.35
Stage 12	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2641	341.2662	6.04	341.061	0.061	218905	3.92
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2901	385.2924	5.94	385.061	0.061	645092	11.56
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3158	429.3187	6.69	429.060	0.060	985256	17.65
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3419	473.3449	6.44	473.060	0.060	1111063	19.90
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3677	517.3711	6.57	517.060	0.060	880831	15.78
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4386	556.4419	6.02	556.107	0.107	140553	2.52
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4648	600.4654	1.03	600.107	0.107	99501	1.78
	C ₁₄ -E03	[M+Na] ⁺	C ₂₀ H ₄₂ O ₄ Na ⁺	369.2952	369.2975	6.23	369.075	0.075	73341	1.31
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3212	413.3237	5.98	413.075	0.075	220737	3.95
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3474	457.3500	5.75	457.075	0.075	341375	6.11
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3733	501.3762	5.85	501.075	0.075	380741	6.82
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3993	545.4025	5.87	545.075	0.075	285986	5.12
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4251	589.4287	6.03	589.074	0.074	199361	3.57

Table S3
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 14	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2641	341.2662	6.12	341.061	0.061	299569	5.50
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2897	385.2924	6.90	385.060	0.060	741110	13.62
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3157	429.3187	7.06	429.060	0.060	950636	17.47
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3416	473.3449	6.89	473.060	0.060	954454	17.54
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3675	517.3711	7.05	517.060	0.060	710680	13.06
	C ₁₂ -E08	[M+NH ₄] ⁺	C ₂₈ H ₆₂ NO ₉ ⁺	556.4380	556.4419	6.95	556.107	0.107	224278	4.12
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4643	600.4654	1.90	600.107	0.107	154629	2.84
	C ₁₂ -E010	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₁ ⁺	644.4906	644.4909	0.47	644.107	0.107	83694	1.54
	C ₁₄ -E03	[M+Na] ⁺	C ₂₀ H ₄₂ O ₄ Na ⁺	369.2950	369.2975	6.85	369.075	0.075	92822	1.71
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3212	413.3237	6.15	413.075	0.075	241856	4.44
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3471	457.3500	6.38	457.075	0.075	313115	5.75
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3731	501.3762	6.27	501.075	0.075	309063	5.68
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3990	545.4025	6.38	545.074	0.074	218782	4.02
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4250	589.4287	6.32	589.074	0.074	147370	2.71

Table S4. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of *injected HFF* by stage for *well 2*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 1	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2638	341.2662	7.15	341.061	0.061	108134	4.65
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2894	385.2924	7.86	385.060	0.060	273049	11.73
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3150	429.3187	8.57	429.060	0.060	384224	16.51
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3408	473.3449	8.68	473.059	0.059	410864	17.66
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3667	517.3711	8.58	517.059	0.059	320454	13.77
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3926	561.3973	8.51	561.058	0.058	223978	9.63
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3202	413.3237	8.37	413.074	0.074	131850	5.67
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3464	457.3500	7.89	457.074	0.074	176499	7.59
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3723	501.3762	7.85	501.074	0.074	175126	7.53
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3980	545.4025	8.23	545.073	0.073	122653	5.27
Stage 2	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2636	341.2662	7.62	341.061	0.061	131812	3.31
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2895	385.2924	7.66	385.060	0.060	407149	10.22
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3149	429.3187	8.80	429.059	0.059	665792	16.71
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3407	473.3449	8.83	473.059	0.059	796644	20.00
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3665	517.3711	8.85	517.059	0.059	668222	16.77
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3923	561.3973	9.04	561.058	0.058	507042	12.73
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3202	413.3237	8.56	413.074	0.074	141823	3.56
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3463	457.3500	8.20	457.074	0.074	224452	5.63
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3722	501.3762	8.11	501.074	0.074	251491	6.31
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3979	545.4025	8.38	545.073	0.073	189510	4.76

Table S4
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 3	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2635	341.2662	8.03	341.060	0.060	163391	4.22
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2893	385.2924	7.97	385.060	0.060	459542	11.86
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3150	429.3187	8.71	429.059	0.059	673351	17.38
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3409	473.3449	8.49	473.059	0.059	740010	19.10
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3666	517.3711	8.68	517.059	0.059	584108	15.08
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3925	561.3973	8.65	561.058	0.058	424884	10.97
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3203	413.3237	8.18	413.074	0.074	167530	4.33
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3465	457.3500	7.74	457.074	0.074	236941	6.12
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3723	501.3762	7.79	501.074	0.074	244693	6.32
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3980	545.4025	8.10	545.073	0.073	179019	4.62
Stage 4	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2638	341.2662	6.97	341.061	0.061	281949	5.64
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2893	385.2924	7.97	385.060	0.060	604377	12.08
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3152	429.3187	8.11	429.060	0.060	742466	14.84
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3411	473.3449	8.01	473.059	0.059	721919	14.43
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3670	517.3711	8.02	517.059	0.059	565164	11.30
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3928	561.3973	8.15	561.059	0.059	449730	8.99
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4634	600.4654	3.41	600.106	0.106	238074	4.76
	C ₁₂ -E010	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₁ ⁺	644.4895	644.4909	2.13	644.106	0.106	172423	3.45
	C ₁₂ -E011	[M+NH ₄] ⁺	C ₃₄ H ₇₄ NO ₁₂ ⁺	688.5156	688.5206	7.17	688.106	0.106	104730	2.09
	C ₁₄ -E03	[M+Na] ⁺	C ₂₀ H ₄₂ O ₄ Na ⁺	369.2947	369.2975	7.61	369.075	0.075	98125	1.96
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3207	413.3237	7.19	413.075	0.075	216442	4.33
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3465	457.3500	7.57	457.074	0.074	267141	5.34
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3725	501.3762	7.41	501.074	0.074	259132	5.18
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3985	545.4025	7.28	545.074	0.074	198085	3.96
	C ₁₄ -E09	[M+NH ₄] ⁺	C ₃₂ H ₇₀ NO ₁₀ ⁺	628.4949	628.4994	7.19	628.121	0.121	82843	1.66

Table S4
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 6	C12-E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2630	341.2662	9.41	341.060	0.060	152462	5.26
	C12-E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2888	385.2924	9.37	385.060	0.060	379947	13.12
	C12-E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3145	429.3187	9.81	429.059	0.059	516501	17.83
	C12-E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3404	473.3449	9.55	473.059	0.059	548996	18.95
	C12-E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3662	517.3711	9.49	517.058	0.058	426781	14.73
	C12-E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3921	561.3973	9.32	561.058	0.058	300317	10.37
	C14-E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3198	413.3237	9.41	413.074	0.074	128181	4.42
	C14-E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3460	457.3500	8.79	457.074	0.074	167903	5.80
	C14-E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3718	501.3762	8.89	501.073	0.073	163226	5.63
	C14-E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3973	545.4025	9.39	545.073	0.073	112708	3.89
Stage 7	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2888	385.2924	9.37	385.060	0.060	119803	1.53
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3149	429.3187	8.87	429.059	0.059	218730	2.79
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3408	473.3449	8.75	473.059	0.059	290862	3.71
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3666	517.3711	8.74	517.059	0.059	263750	3.36
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3923	561.3973	8.95	561.058	0.058	210607	2.68
	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1024	217.1046	10.36	216.973	0.973	1021397	13.01
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1285	261.1309	9.08	260.973	0.973	2136589	27.22
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1546	305.1571	8.36	304.973	0.973	2054833	26.18
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1802	349.1833	8.88	348.972	0.972	1082073	13.79
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2062	393.2095	8.29	392.972	0.972	449933	5.73
Stage 8	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1286	261.1309	8.92	260.973	0.973	115305	100.00

Table S4
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 9	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2635	341.2662	8.00	341.060	0.060	161213	5.05
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2892	385.2924	8.36	385.060	0.060	417342	13.08
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3150	429.3187	8.64	429.060	0.060	573973	17.99
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3408	473.3449	8.62	473.059	0.059	605276	18.97
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3667	517.3711	8.60	517.059	0.059	464127	14.55
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3925	561.3973	8.65	561.058	0.058	327622	10.27
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3203	413.3237	8.23	413.074	0.074	139804	4.38
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3464	457.3500	7.98	457.074	0.074	188384	5.91
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3723	501.3762	7.75	501.074	0.074	185041	5.80
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3980	545.4025	8.23	545.073	0.073	127206	3.99
Stage 10	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2636	341.2662	7.71	341.060	0.060	155311	5.01
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2894	385.2924	7.79	385.060	0.060	403279	13.01
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3152	429.3187	8.18	429.060	0.060	563395	18.18
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3411	473.3449	8.13	473.059	0.059	603554	19.48
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3669	517.3711	8.04	517.059	0.059	463546	14.96
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3929	561.3973	7.94	561.059	0.059	321413	10.37
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3204	413.3237	7.96	413.074	0.074	128640	4.15
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3465	457.3500	7.63	457.074	0.074	171301	5.53
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3725	501.3762	7.47	501.074	0.074	171513	5.53
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3982	545.4025	7.79	545.074	0.074	116766	3.77
Stage 11	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1289	261.1309	7.54	260.974	0.974	175012	57.99
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1549	305.1571	7.08	304.973	0.973	126789	42.01

Table S4
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 12	C12-E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2630	341.2662	9.46	341.060	0.060	109971	5.72
	C12-E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2890	385.2924	8.77	385.060	0.060	266051	13.84
	C12-E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3146	429.3187	9.57	429.059	0.059	374152	19.47
	C12-E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3403	473.3449	9.63	473.059	0.059	406529	21.15
	C12-E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3663	517.3711	9.35	517.058	0.058	315942	16.44
	C12-E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3923	561.3973	8.90	561.058	0.058	215948	11.24
	C14-E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3458	457.3500	9.21	457.074	0.074	118930	6.19
	C14-E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3716	501.3762	9.20	501.073	0.073	114224	5.94
Stage 14	C12-E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2633	341.2662	8.64	341.060	0.060	176275	4.34
	C12-E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2891	385.2924	8.62	385.060	0.060	492228	12.11
	C12-E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3147	429.3187	9.32	429.059	0.059	717153	17.64
	C12-E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3406	473.3449	9.13	473.059	0.059	774967	19.06
	C12-E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3663	517.3711	9.20	517.058	0.058	590613	14.53
	C12-E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3920	561.3973	9.47	561.058	0.058	407637	10.03
	C14-E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3201	413.3237	8.76	413.074	0.074	162240	3.99
	C14-E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3462	457.3500	8.40	457.074	0.074	235682	5.80
	C14-E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3719	501.3762	8.57	501.074	0.074	239217	5.88
	C14-E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3977	545.4025	8.71	545.073	0.073	166762	4.10
	C14-E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4233	589.4287	9.15	589.073	0.073	102326	2.52

Table S5. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of *injected HFF* by stage for *well 3*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 3	C ₁₂ -EO3	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2633	341.2662	8.59	341.060	0.060	181789	5.17
	C ₁₂ -EO4	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2889	385.2924	9.16	385.060	0.060	461707	13.13
	C ₁₂ -EO5	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3146	429.3187	9.53	429.059	0.059	614855	17.48
	C ₁₂ -EO6	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3405	473.3449	9.38	473.059	0.059	632333	17.98
	C ₁₂ -EO7	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3662	517.3711	9.51	517.058	0.058	477452	13.57
	C ₁₂ -EO8	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3919	561.3973	9.61	561.058	0.058	336688	9.57
	C ₁₂ -EO9	[M+Na] ⁺	C ₃₀ H ₆₂ O ₁₀ Na ⁺	605.4186	605.4235	8.13	605.058	0.058	179681	5.11
	C ₁₄ -EO4	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3200	413.3237	9.00	413.074	0.074	145625	4.14
	C ₁₄ -EO5	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3461	457.3500	8.64	457.074	0.074	186468	5.30
	C ₁₄ -EO6	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3718	501.3762	8.89	501.073	0.073	178456	5.07
	C ₁₄ -EO7	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3975	545.4025	9.17	545.073	0.073	122413	3.48
Stage 4	C ₁₂ -EO3	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2633	341.2662	8.41	341.060	0.060	178183	5.36
	C ₁₂ -EO4	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2888	385.2924	9.34	385.060	0.060	432647	13.02
	C ₁₂ -EO5	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3145	429.3187	9.74	429.059	0.059	573472	17.26
	C ₁₂ -EO6	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3404	473.3449	9.55	473.059	0.059	584456	17.59
	C ₁₂ -EO7	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3662	517.3711	9.53	517.058	0.058	434966	13.09
	C ₁₂ -EO8	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3921	561.3973	9.40	561.058	0.058	301749	9.08
	C ₁₂ -EO9	[M+Na] ⁺	C ₃₀ H ₆₂ O ₁₀ Na ⁺	605.4186	605.4235	8.13	605.058	0.058	159319	4.79
	C ₁₄ -EO4	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3200	413.3237	9.00	413.074	0.074	128079	3.85
	C ₁₄ -EO5	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3459	457.3500	8.90	457.074	0.074	163951	4.93
	C ₁₄ -EO6	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3718	501.3762	8.79	501.073	0.073	156484	4.71
	C ₁₄ -EO7	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3973	545.4025	9.42	545.073	0.073	104858	3.16
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1286	261.1309	8.96	260.973	0.973	104664	3.15

Table S5
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 5	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2633	341.2662	8.64	341.060	0.060	180979	4.69
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2889	385.2924	9.01	385.060	0.060	486015	12.59
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3147	429.3187	9.43	429.059	0.059	672943	17.44
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3405	473.3449	9.34	473.059	0.059	714002	18.50
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3662	517.3711	9.39	517.058	0.058	548856	14.22
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3921	561.3973	9.31	561.058	0.058	388875	10.08
	C ₁₂ -E09	[M+Na] ⁺	C ₃₀ H ₆₂ O ₁₀ Na ⁺	605.4186	605.4235	8.13	605.058	0.058	202706	5.25
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3200	413.3237	8.93	413.074	0.074	145226	3.76
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3461	457.3500	8.55	457.074	0.074	194794	5.05
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3720	501.3762	8.49	501.074	0.074	190811	4.94
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3975	545.4025	9.13	545.073	0.073	134417	3.48
Stage 6	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2637	341.2662	7.38	341.061	0.061	193149	5.49
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2894	385.2924	7.86	385.060	0.060	465671	13.23
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3152	429.3187	8.08	429.060	0.060	620102	17.62
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3411	473.3449	7.96	473.059	0.059	644467	18.31
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3669	517.3711	8.10	517.059	0.059	493324	14.02
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3928	561.3973	8.01	561.059	0.059	357973	10.17
	C ₁₂ -E09	[M+NH ₄] ⁺	C ₃₀ H ₆₆ NO ₁₀ ⁺	600.4637	600.4654	2.78	600.106	0.106	108987	3.10
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3206	413.3237	7.60	413.075	0.075	145159	4.12
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3466	457.3500	7.37	457.074	0.074	185578	5.27
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3725	501.3762	7.43	501.074	0.074	180060	5.12
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3982	545.4025	7.85	545.074	0.074	125496	3.57

Table S5
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 7	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2635	341.2662	8.03	341.060	0.060	172177	4.13
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2892	385.2924	8.38	385.060	0.060	495532	11.88
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3150	429.3187	8.64	429.060	0.060	709766	17.01
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3409	473.3449	8.41	473.059	0.059	769084	18.43
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3668	517.3711	8.41	517.059	0.059	603032	14.45
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3926	561.3973	8.40	561.059	0.059	434489	10.41
	C ₁₂ -E09	[M+Na] ⁺	C ₃₀ H ₆₂ O ₁₀ Na ⁺	605.4186	605.4235	8.13	605.058	0.058	229349	5.50
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3203	413.3237	8.13	413.074	0.074	142126	3.41
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3464	457.3500	7.81	457.074	0.074	196233	4.70
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3724	501.3762	7.67	501.074	0.074	196671	4.71
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3980	545.4025	8.23	545.073	0.073	137646	3.30
	C ₁₄ -E08	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4236	589.4287	8.66	589.073	0.073	86231	2.07
Stage 9	C ₁₂ -E03	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2630	341.2662	9.38	341.060	0.060	176024	5.19
	C ₁₂ -E04	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2887	385.2924	9.68	385.059	0.059	452581	13.34
	C ₁₂ -E05	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3144	429.3187	9.97	429.059	0.059	617255	18.19
	C ₁₂ -E06	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3403	473.3449	9.80	473.059	0.059	645343	19.02
	C ₁₂ -E07	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3661	517.3711	9.76	517.058	0.058	486083	14.33
	C ₁₂ -E08	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3918	561.3973	9.91	561.058	0.058	337668	9.95
	C ₁₄ -E04	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3198	413.3237	9.34	413.074	0.074	151161	4.46
	C ₁₄ -E05	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3459	457.3500	9.01	457.074	0.074	200407	5.91
	C ₁₄ -E06	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3716	501.3762	9.22	501.073	0.073	194667	5.74
	C ₁₄ -E07	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3974	545.4025	9.28	545.073	0.073	131430	3.87

Table S5
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
Stage 10	C ₁₂ -EO3	[M+Na] ⁺	C ₁₈ H ₃₈ O ₄ Na ⁺	341.2629	341.2662	9.61	341.060	0.060	192354	4.48
	C ₁₂ -EO4	[M+Na] ⁺	C ₂₀ H ₄₂ O ₅ Na ⁺	385.2886	385.2924	9.84	385.059	0.059	555711	12.95
	C ₁₂ -EO5	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3143	429.3187	10.18	429.059	0.059	775594	18.08
	C ₁₂ -EO6	[M+Na] ⁺	C ₂₄ H ₅₀ O ₇ Na ⁺	473.3402	473.3449	10.01	473.058	0.058	815759	19.01
	C ₁₂ -EO7	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3659	517.3711	10.09	517.058	0.058	618794	14.42
	C ₁₂ -EO8	[M+Na] ⁺	C ₂₈ H ₅₈ O ₉ Na ⁺	561.3917	561.3973	10.11	561.058	0.058	433284	10.10
	C ₁₄ -EO4	[M+Na] ⁺	C ₂₂ H ₄₆ O ₅ Na ⁺	413.3198	413.3237	9.39	413.074	0.074	167181	3.90
	C ₁₄ -EO5	[M+Na] ⁺	C ₂₄ H ₅₀ O ₆ Na ⁺	457.3457	457.3500	9.36	457.074	0.074	232707	5.42
	C ₁₄ -EO6	[M+Na] ⁺	C ₂₆ H ₅₄ O ₇ Na ⁺	501.3716	501.3762	9.32	501.073	0.073	233139	5.43
	C ₁₄ -EO7	[M+Na] ⁺	C ₂₈ H ₅₈ O ₈ Na ⁺	545.3972	545.4025	9.61	545.073	0.073	163126	3.80
	C ₁₄ -EO8	[M+Na] ⁺	C ₃₀ H ₆₂ O ₉ Na ⁺	589.4228	589.4287	9.97	589.072	0.072	103141	2.40

Table S6. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of all *produced water* samples from *well 1*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
325 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1057	217.1046	-4.88	216.976	0.976	539837	19.82
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1355	261.1309	-17.65	260.980	0.980	820609	30.13
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1629	305.1571	-18.88	304.981	0.981	713875	26.21
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1866	349.1833	-9.34	348.979	0.979	464965	17.07
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2111	393.2095	-3.94	392.977	0.977	184168	6.76
1745 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1065	217.1046	-8.89	216.977	0.977	589186	23.56
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1360	261.1309	-19.53	260.981	0.981	738697	29.54
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1628	305.1571	-18.71	304.981	0.981	635352	25.41
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1861	349.1833	-7.96	348.978	0.978	396156	15.84
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2109	393.2095	-3.46	392.977	0.977	141325	5.65
8031 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1073	217.1046	-12.21	216.978	0.978	864488	28.96
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1356	261.1309	-17.88	260.980	0.980	837476	28.06
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1618	305.1571	-15.40	304.980	0.980	686384	22.99
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1855	349.1833	-6.24	348.978	0.978	451248	15.12
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.44	392.976	0.976	145420	4.87
13824 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1069	217.1046	-10.73	216.978	0.978	935096	27.80
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1356	261.1309	-17.88	260.980	0.980	930634	27.67
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1623	305.1571	-17.01	304.981	0.981	773028	22.98
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.16	348.978	0.978	525109	15.61
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.54	392.977	0.977	199848	5.94

**Table S6
cont.**

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
15484 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1072	217.1046	-11.79	216.978	0.978	885192	27.23
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1358	261.1309	-18.57	260.980	0.980	898143	27.63
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1624	305.1571	-17.34	304.981	0.981	755453	23.24
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.25	348.978	0.978	521309	16.04
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2106	393.2095	-2.85	392.977	0.977	190720	5.87
16506 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1073	217.1046	-12.53	216.978	0.978	909418	28.20
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1356	261.1309	-18.04	260.980	0.980	891818	27.66
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1620	305.1571	-16.16	304.980	0.980	742349	23.02
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1855	349.1833	-6.19	348.978	0.978	504718	15.65
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2103	393.2095	-2.11	392.976	0.976	176347	5.47
16526 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1075	217.1046	-13.13	216.978	0.978	901845	29.19
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1356	261.1309	-18.08	260.980	0.980	868274	28.11
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1619	305.1571	-15.57	304.980	0.980	715519	23.16
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1854	349.1833	-6.01	348.978	0.978	466057	15.09
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2104	393.2095	-2.31	392.976	0.976	137359	4.45
17533 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1073	217.1046	-12.44	216.978	0.978	873685	30.36
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1350	261.1309	-15.85	260.980	0.980	822575	28.58
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1610	305.1571	-12.65	304.979	0.979	673078	23.39
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1848	349.1833	-4.32	348.977	0.977	402785	14.00
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2101	393.2095	-1.60	392.976	0.976	105679	3.67

Table S7. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of all *produced water* samples from *well 2*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
279 BBL	C ₁₂ -EO5	[M+Na] ⁺	C ₂₂ H ₄₆ O ₆ Na ⁺	429.3187	429.3187	0.00	429.063	0.063	55589	1.63
	C ₁₂ -EO7	[M+Na] ⁺	C ₂₆ H ₅₄ O ₈ Na ⁺	517.3712	517.3711	-0.19	517.063	0.063	100557	2.95
	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1049	217.1046	-1.24	216.976	0.976	470807	13.82
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1336	261.1309	-10.26	260.978	0.978	961696	28.23
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1613	305.1571	-13.67	304.980	0.980	916425	26.90
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1860	349.1833	-7.76	348.978	0.978	601448	17.66
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2111	393.2095	-3.94	392.977	0.977	299778	8.80
1693 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1066	217.1046	-9.12	216.977	0.977	834143	24.25
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1365	261.1309	-21.33	260.981	0.981	1022714	29.73
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1634	305.1571	-20.55	304.982	0.982	861283	25.04
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1865	349.1833	-9.16	348.979	0.979	532982	15.50
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2110	393.2095	-3.76	392.977	0.977	188358	5.48
2548 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1071	217.1046	-11.52	216.978	0.978	827345	25.16
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1361	261.1309	-19.91	260.981	0.981	960086	29.20
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1626	305.1571	-17.89	304.981	0.981	820860	24.97
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1860	349.1833	-7.85	348.978	0.978	497040	15.12
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2112	393.2095	-4.22	392.977	0.977	182400	5.55
2977 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1073	217.1046	-12.57	216.978	0.978	851794	25.41
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1366	261.1309	-21.94	260.981	0.981	955688	28.51
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1633	305.1571	-20.22	304.982	0.982	815805	24.34
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1866	349.1833	-9.36	348.979	0.979	528825	15.78
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2112	393.2095	-4.20	392.977	0.977	199960	5.97

Table S7
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
3341 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1067	217.1046	-9.63	216.977	0.977	762957	24.54
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1363	261.1309	-20.64	260.981	0.981	921627	29.65
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1629	305.1571	-18.97	304.981	0.981	772475	24.85
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1861	349.1833	-8.08	348.978	0.978	475198	15.29
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2109	393.2095	-3.59	392.977	0.977	176427	5.68
3450 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1072	217.1046	-12.02	216.978	0.978	814281	26.61
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1364	261.1309	-20.99	260.981	0.981	899383	29.39
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1627	305.1571	-18.45	304.981	0.981	747506	24.43
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1860	349.1833	-7.76	348.978	0.978	439635	14.37
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2110	393.2095	-3.74	392.977	0.977	158998	5.20
9861 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1077	217.1046	-14.05	216.978	0.978	1118480	28.91
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1359	261.1309	-19.22	260.981	0.981	1088203	28.13
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1620	305.1571	-16.02	304.980	0.980	892833	23.08
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1855	349.1833	-6.24	348.978	0.978	587571	15.19
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.64	392.977	0.977	181400	4.69
11112 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1080	217.1046	-15.57	216.979	0.979	1194783	29.70
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1360	261.1309	-19.49	260.981	0.981	1105277	27.48
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1621	305.1571	-16.45	304.981	0.981	903574	22.46
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1856	349.1833	-6.50	348.978	0.978	610496	15.18
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.54	392.977	0.977	208182	5.18

**Table S7
cont.**

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
11991 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1079	217.1046	-15.11	216.979	0.979	1182820	28.60
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1365	261.1309	-21.48	260.981	0.981	1154857	27.92
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1628	305.1571	-18.68	304.981	0.981	940441	22.74
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1860	349.1833	-7.85	348.978	0.978	637211	15.41
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2107	393.2095	-3.10	392.977	0.977	220967	5.34
12303 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1078	217.1046	-14.69	216.979	0.979	1104962	29.55
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1361	261.1309	-19.76	260.981	0.981	1047120	28.00
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1622	305.1571	-16.71	304.981	0.981	849265	22.71
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1857	349.1833	-6.76	348.978	0.978	559814	14.97
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2106	393.2095	-2.85	392.977	0.977	177915	4.76
12360 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1068	217.1046	-10.23	216.978	0.978	1158212	27.47
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1358	261.1309	-18.76	260.980	0.980	1155445	27.40
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1627	305.1571	-18.42	304.981	0.981	957341	22.70
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1862	349.1833	-8.36	348.978	0.978	662144	15.70
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2106	393.2095	-2.72	392.977	0.977	283665	6.73

Table S8. Base peak, base peak formula, observed m/z , theoretical m/z , mass errors, Kendrick masses, Kendrick mass defects (KMD), and abundances of surfactants identified in QTOF-MS spectra of all *produced water* samples from *well 3*.

	Surfactant Species	Base Peak	Base Peak Formula	Observed m/z	Theoretical m/z	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
377 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1074	217.1046	-12.71	216.978	0.978	761990	29.07
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1366	261.1309	-21.75	260.981	0.981	809950	30.90
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1625	305.1571	-17.60	304.981	0.981	647408	24.70
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1853	349.1833	-5.76	348.978	0.978	312876	11.94
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2107	393.2095	-3.13	392.977	0.977	88843	3.39
5052 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1072	217.1046	-12.16	216.978	0.978	737674	26.44
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1365	261.1309	-21.60	260.981	0.981	808608	28.98
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1632	305.1571	-19.86	304.982	0.982	678354	24.31
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1862	349.1833	-8.36	348.978	0.978	419497	15.04
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2109	393.2095	-3.61	392.977	0.977	145867	5.23
6230 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1069	217.1046	-10.78	216.978	0.978	675790	26.56
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1363	261.1309	-20.79	260.981	0.981	759417	29.85
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1627	305.1571	-18.48	304.981	0.981	628678	24.71
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.22	348.978	0.978	362108	14.23
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2107	393.2095	-3.05	392.977	0.977	117965	4.64
6924 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1072	217.1046	-12.16	216.978	0.978	707717	27.72
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1362	261.1309	-20.30	260.981	0.981	774466	30.33
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1623	305.1571	-16.91	304.981	0.981	636965	24.95
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.07	348.978	0.978	331275	12.97
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2111	393.2095	-4.12	392.977	0.977	102854	4.03

**Table S8
cont.**

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
7253 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1075	217.1046	-13.36	216.978	0.978	924545	29.80
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1359	261.1309	-19.11	260.980	0.980	878016	28.30
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1621	305.1571	-16.35	304.980	0.980	705736	22.75
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1855	349.1833	-6.39	348.978	0.978	452844	14.60
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.64	392.977	0.977	141488	4.56
7606 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1078	217.1046	-14.60	216.979	0.979	886362	31.23
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1358	261.1309	-18.69	260.980	0.980	809753	28.54
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1616	305.1571	-14.62	304.980	0.980	644325	22.71
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1849	349.1833	-4.70	348.977	0.977	391781	13.81
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2102	393.2095	-1.65	392.976	0.976	105508	3.72
7730 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1081	217.1046	-16.26	216.979	0.979	920879	32.04
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1358	261.1309	-18.88	260.980	0.980	819963	28.53
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1615	305.1571	-14.35	304.980	0.980	647664	22.53
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1852	349.1833	-5.33	348.977	0.977	385582	13.41
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2104	393.2095	-2.31	392.976	0.976	100433	3.49
7877 BBL	PEG-EO4	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1079	217.1046	-15.38	216.979	0.979	908240	31.80
	PEG-EO5	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1358	261.1309	-18.65	260.980	0.980	819219	28.68
	PEG-EO6	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1614	305.1571	-14.06	304.980	0.980	648250	22.70
	PEG-EO7	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1850	349.1833	-4.73	348.977	0.977	382270	13.38
	PEG-EO8	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2102	393.2095	-1.83	392.976	0.976	98050	3.43

Table S8
cont.

	Surfactant Species	Base Peak	Base Peak Formula	Observed <i>m/z</i>	Theoretical <i>m/z</i>	Error (ppm)	Kendrick Mass	KMD	Abundance (counts)	Relative Abundance (%)
8305 BBL	PEG-E04	[M+Na] ⁺	C ₈ H ₁₈ O ₅ Na ⁺	217.1077	217.1046	-14.05	216.978	0.978	1013491	30.21
	PEG-E05	[M+Na] ⁺	C ₁₀ H ₂₂ O ₆ Na ⁺	261.1362	261.1309	-20.22	260.981	0.981	937116	27.93
	PEG-E06	[M+Na] ⁺	C ₁₂ H ₂₆ O ₇ Na ⁺	305.1625	305.1571	-17.63	304.981	0.981	748055	22.29
	PEG-E07	[M+Na] ⁺	C ₁₄ H ₃₀ O ₈ Na ⁺	349.1858	349.1833	-7.02	348.978	0.978	490730	14.63
	PEG-E08	[M+Na] ⁺	C ₁₆ H ₃₄ O ₉ Na ⁺	393.2105	393.2095	-2.54	392.977	0.977	165899	4.94

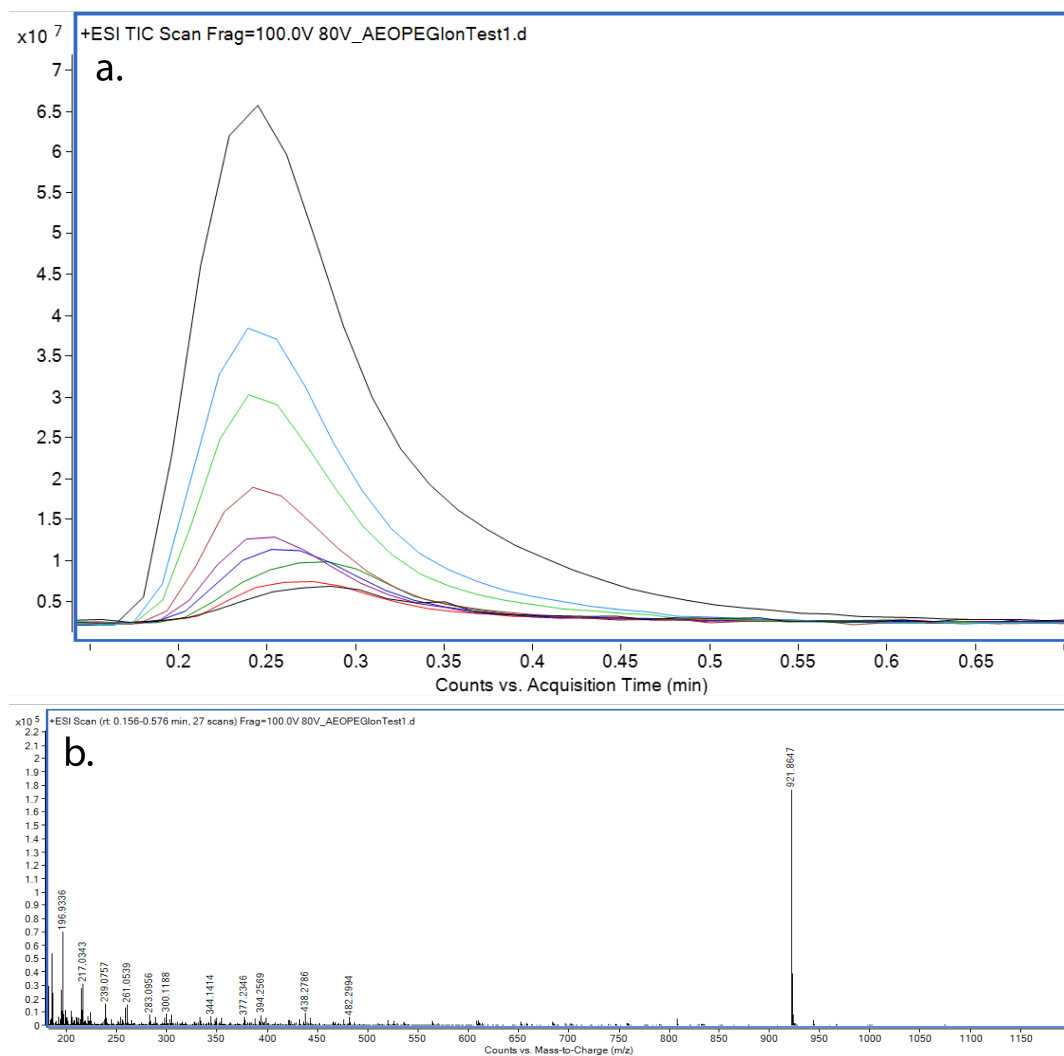


Figure S1. Mass spectra of serial dilutions of a PEG/AEO mixture showing no preferential ionization or ion suppression with changes in concentration indicating that our observations are not a result of analytical artifacts. a. Total ion signal increasing with increasing concentrations and b-j. shows spectra with increasing concentrations (from b to j) of the PEG/AEO mixture.

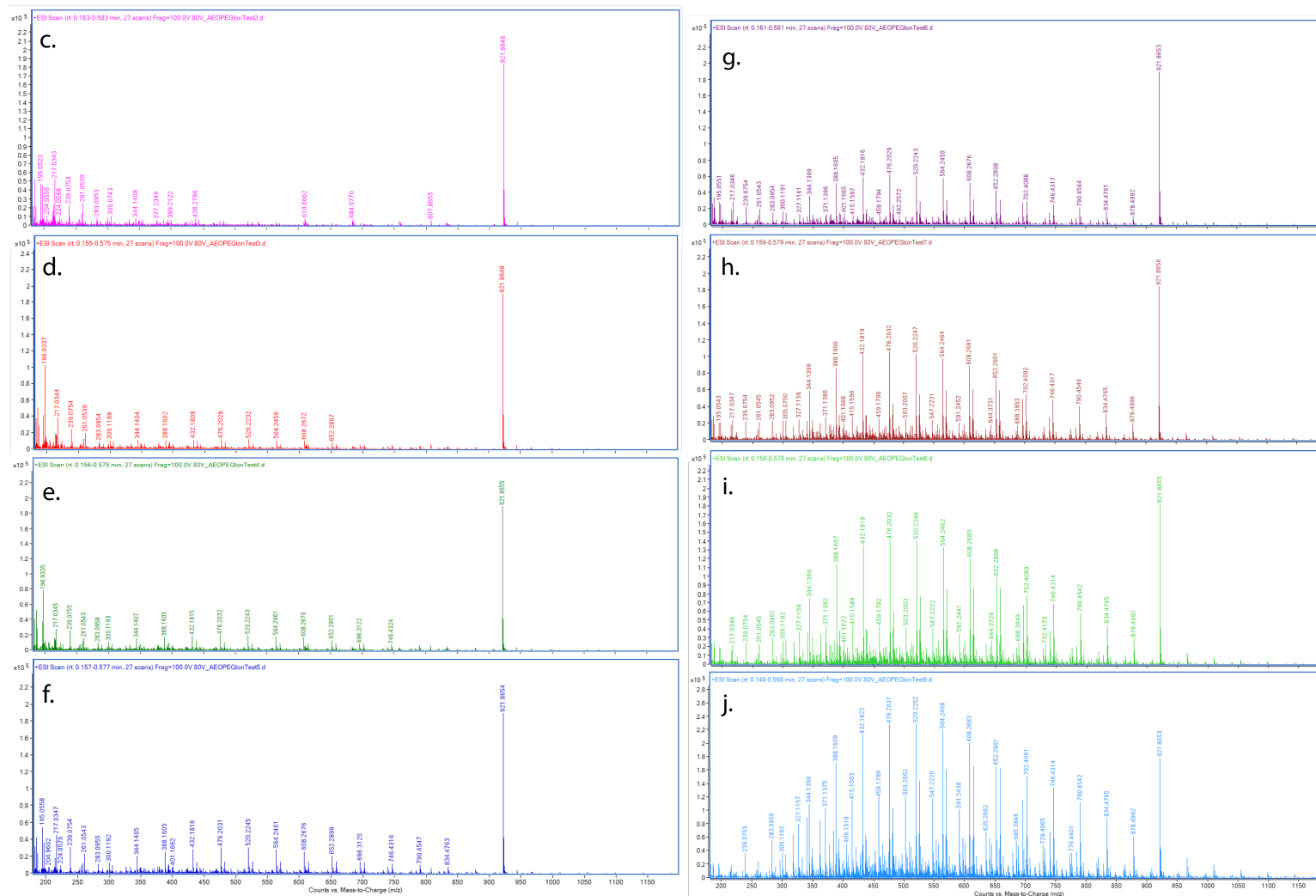


Figure S1 cont. Mass spectra of serial dilutions of a PEG/AEO mixture showing no preferential ionization or ion suppression with changes in concentration indicating that our observations are not a result of analytical artifacts. a. Total ion signal increasing with increasing concentrations and b-j. shows spectra with increasing concentrations (from b to j) of the PEG/AEO mixture.

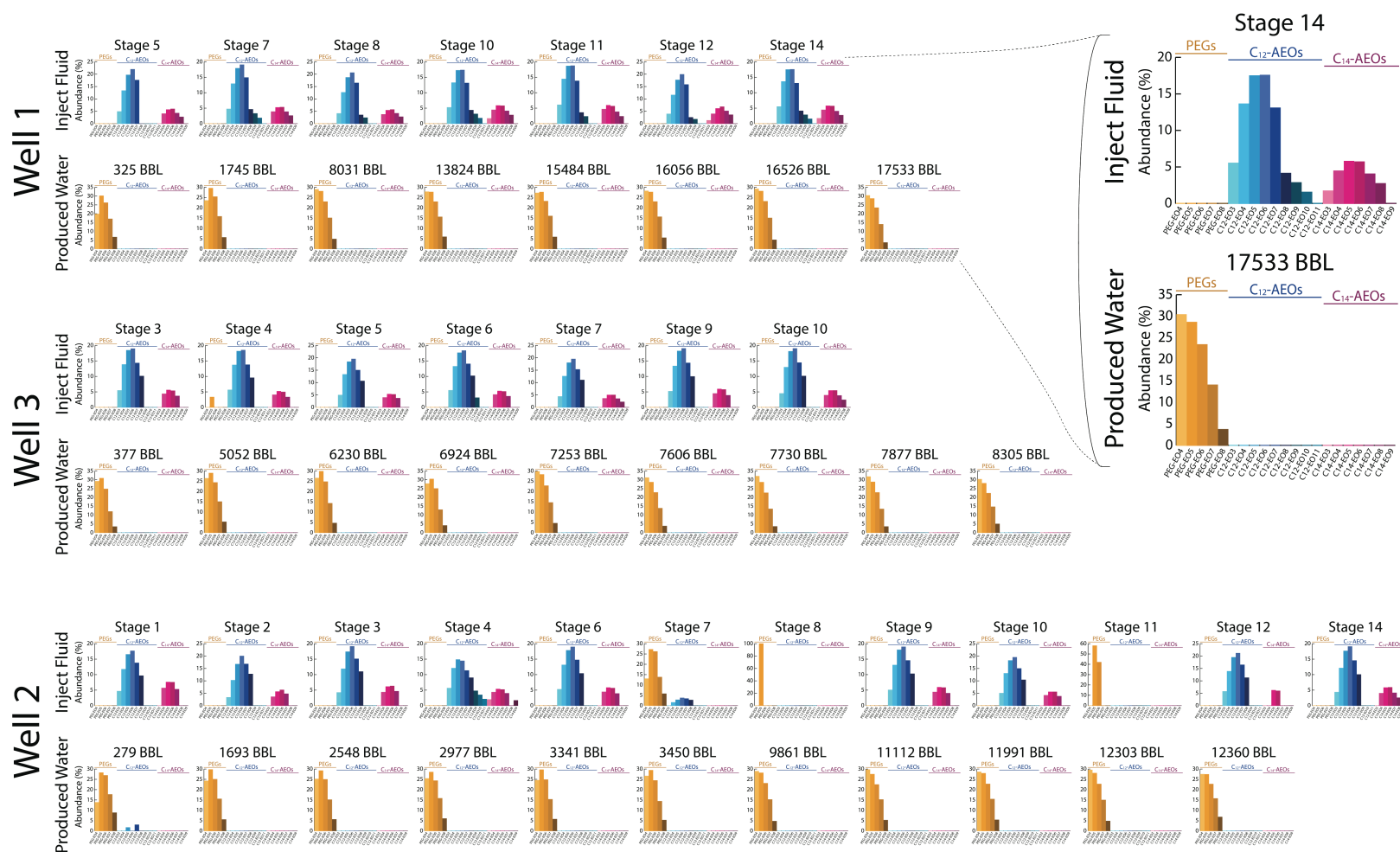


Figure S2. Relative abundance (as %) of PEG-EOs (yellow), C₁₂-AEOs (blue), and C₁₄-AEOs (red) in injected fluid and produced water (labelled as barrels of water produced, BBL) from wells 1, 2, and 3 showing a transition from AEO dominance in the injected to PEG dominance in the produced water. Produced waters also show a shift to lower EO number PEGs over the course of production. Injected fluids are presented above the produced water for each respective well. Well 1 stage 14 inject fluid and 17533 BBL produced water have been expanded to better show the compounds presented: PEG-E04 to PEG-E08, C₁₂-E03 to C₁₂-E011, and C₁₄-E03 to C₁₄-E09.

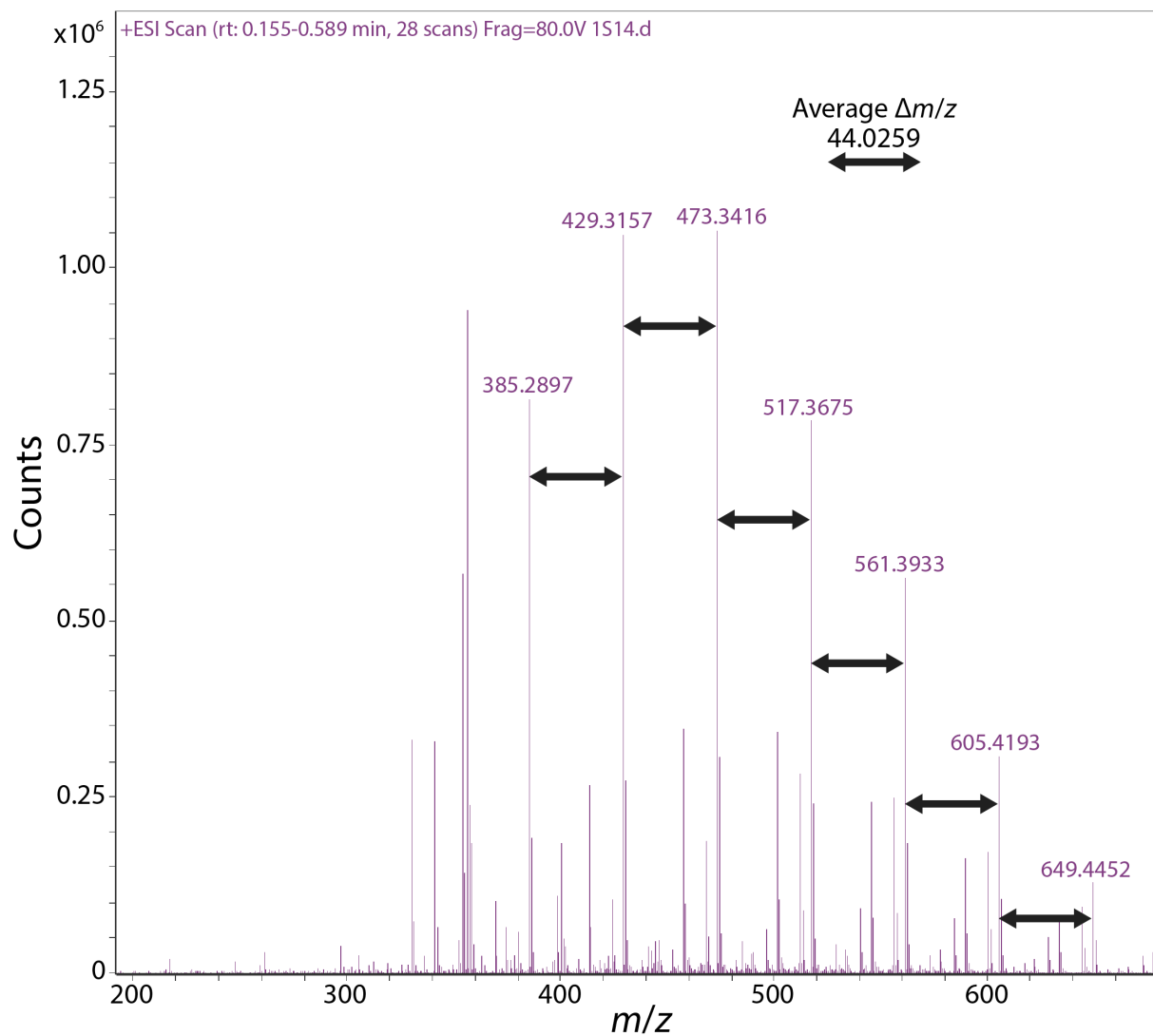


Figure S3. Representative mass spectra of *injected HFF* (from well 1, stage 14) showing identified AEOs with an average $\Delta m/z$ of 44.026, but an absence of PEGs.

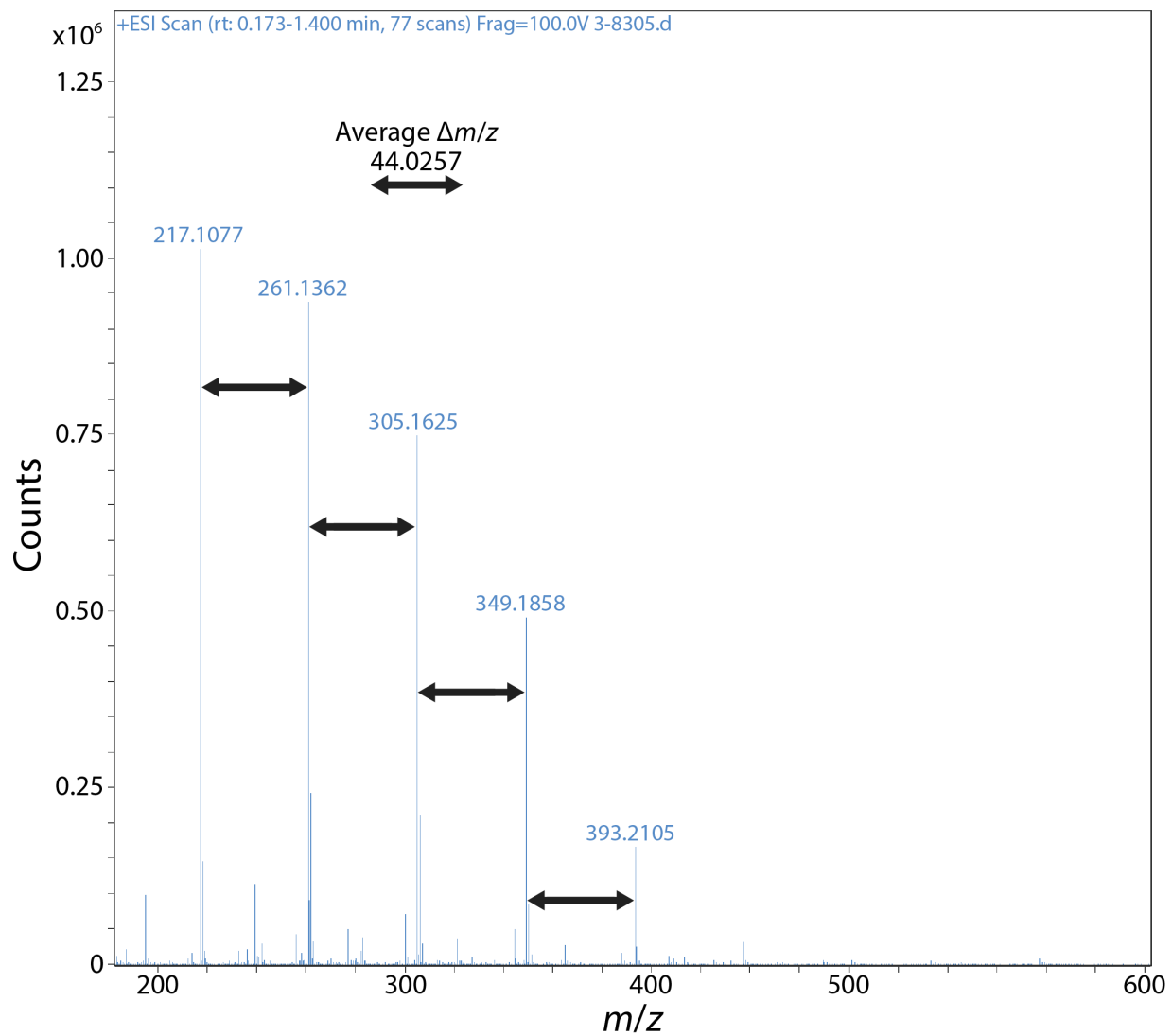


Figure S4. Representative mass spectra of *produced water* (from well 3, 8305 BBL) showing identified PEGs with an average $\Delta m/z$ of 44.026, but an absence of AEOs.

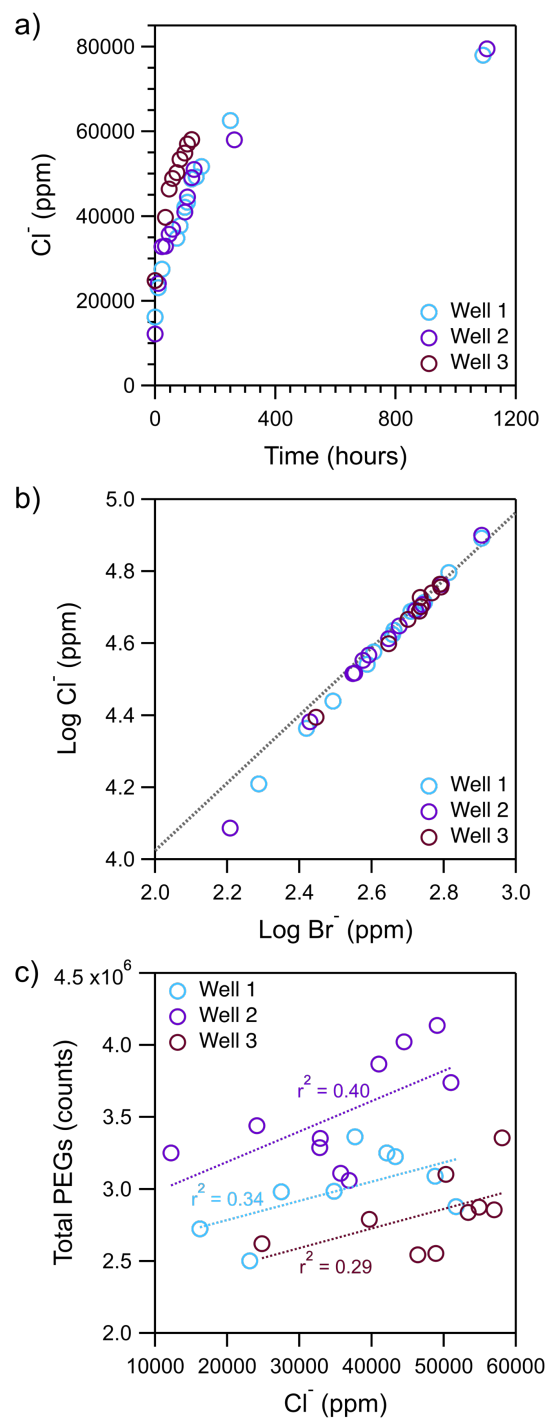


Figure S5. Produced water chemistry a) Chloride concentrations over production time showing a typical asymptotic increase in Chloride that indicates mixing with subsurface brine; b) Log Chloride concentrations over Log Bromide concentrations showing a trend towards a mixing line (gray dashed line) developed for southwestern Pennsylvania shale reservoirs from Barbot *et al.*¹; c) total PEG counts over Chloride concentrations showing no dilution of PEGs during production as PEG counts stay consistently similar while Chloride increases during production.

References

- (1) Barbot, E.; Vidic, N. S.; Gregory, K. B.; Vidic, R. D. Spatial and Temporal Correlation of Water Quality Parameters of Produced Waters from Devonian-Age Shale following Hydraulic Fracturing. *Environ. Sci. Technol.* **2013**, *47* (6), 2562-2569, DOI: 10.1021/es304638h.