

Supporting Information

Impact of oil matrix on anionic and nonionic surfactants separation using Ultra-High-Performance-Liquid-Chromatography hyphenated to High-Resolution Mass Spectrometry

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Figure S1: (A) Brij mass spectrum in (+)HESI-HRMS; (B-C) Carboxylate mass spectra in respectively (-)HESI-HRMS and (+)HESI-HRMS conditions.

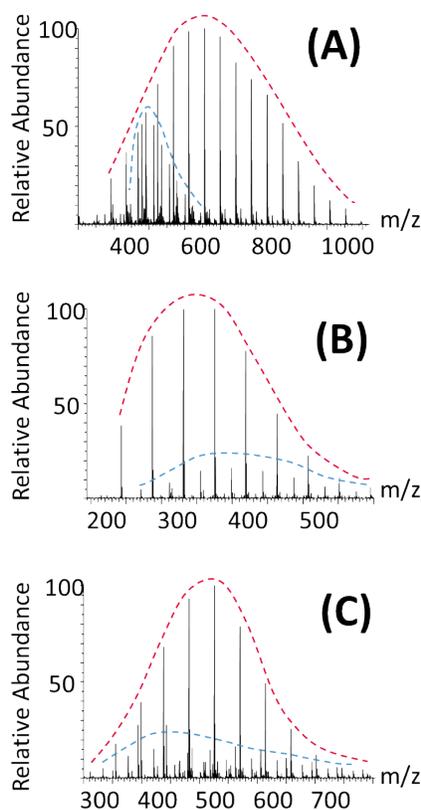


Figure S2: UHPLC-(+)HESI-HRMS EIC of BrijC10 homolog (m/z =744.5836): in 1 QC injection (blue color) and in 12 blanks injections (black color)

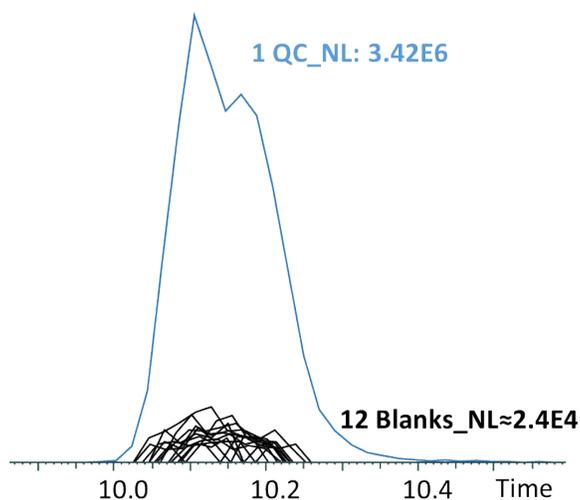


Table S1: Retention times, peak areas and their RSDs for the study of THF/Toluene impact on Brij separation

BrijC10 [M+NH ₄] ⁺		QCs				Surfactants + THF/Toluene			
m/z	Nb EO	tr	RSD (tr) (n=5)	Peak Area ×10 ⁶	RSD (Area) (n=5)	tr	RSD (tr) (n=5)	Peak Area ×10 ⁶	RSD (Area) (n=5)
392.374	3	11.70	0.26%	0.95	36.15%	11.64	0.10%	1.82	1.50%
436.400	4	11.40	0.19%	1.48	39.21%	11.33	0.13%	2.92	1.28%
480.426	5	11.15	0.16%	1.77	37.61%	11.08	0.13%	3.63	2.15%
524.453	6	10.93	0.21%	2.16	36.77%	10.85	0.11%	4.40	2.87%
568.479	7	10.74	0.20%	2.49	33.54%	10.68	0.09%	5.00	2.17%
612.505	8	10.57	0.17%	2.61	30.45%	10.50	0.10%	5.28	4.78%
656.531	9	10.41	0.20%	2.61	27.95%	10.35	0.13%	5.15	3.45%
700.557	10	10.27	0.14%	2.52	27.05%	10.21	0.10%	4.80	3.31%
744.584	11	10.14	0.24%	2.29	22.98%	10.09	0.07%	4.20	3.41%
788.610	12	10.02	0.23%	2.00	20.10%	9.97	0.15%	3.54	2.39%
832.636	13	9.91	0.23%	1.66	17.72%	9.86	0.18%	2.85	3.47%
876.662	14	9.80	0.16%	1.21	15.17%	9.76	0.07%	2.00	1.66%
920.688	15	9.71	0.15%	1.22	11.98%	9.66	0.09%	3.99	2.96%
964.715	16	9.62	0.23%	1.18	11.27%	9.58	0.06%	3.81	6.17%
1008.741	17	9.54	0.13%	0.99	10.74%	9.50	0.16%	3.11	3.19%
1052.767	18	9.46	0.18%	0.77	8.65%	9.42	0.06%	2.53	13.52%
1096.793	19	9.38	0.14%	0.57	8.12%	9.34	0.08%	1.75	2.85%

579.427	20	9.30	0.16%	0.77	6.61%	9.27	0.06%	1.18	4.10%
601.440	21	9.23	0.24%	0.52	8.74%	9.21	0.17%	0.77	3.51%
623.453	22	9.17	0.18%	0.33	6.11%	9.16	0.10%	0.47	4.64%
645.466	23	9.10	0.18%	0.20	8.05%	9.09	0.09%	0.29	4.26%
667.479	24	9.05	0.17%	0.12	5.82%	9.02	0.12%	0.17	6.73%
689.492	25	8.97	0.13%	0.07	3.50%	8.97	0.21%	0.09	7.59%
711.506	26	8.93	0.14%	0.04	7.25%	8.93	0.09%	0.05	3.71%
733.519	27	8.87	0.26%	0.02	16.90%	8.86	0.38%	0.02	5.71%
755.532	28	8.81	0.29%	0.00	37.76%	8.81	0.24%	0.01	17.82%
Min		/	0.13%	/	3.50%	/	0.06%	/	1.28%
Max		/	0.29%	/	39.21%	/	0.38%	/	17.82%

Table S2: Retention times, peak areas and their RSDs for the study of THF/Toluene impact on Carboxylate separation

Carboxylate (+/-)		QCs				Surfactants + THF/Toluene			
m/z	Nb EO	tr	RSD (tr) (n=5)	Peak Area ×10 ⁶	RSD (Area) (n=5)	tr	RSD (tr) (n=5)	Peak Area ×10 ⁶	RSD (Area) (n=5)
Carboxylate C11 and C13 (+) HESI									
350.291	3	15.00	0.16%	1.24	3.64%	14.92	0.14%	1.33	0.77%
394.317	4	14.20	0.18%	5.26	3.66%	14.12	0.05%	5.71	0.97%
438.343	5	13.58	0.18%	5.91	4.25%	13.50	0.09%	6.27	1.19%
482.369	6	13.04	0.20%	4.48	3.90%	12.98	0.05%	4.66	1.69%
526.395	7	12.58	0.24%	3.26	4.82%	12.52	0.08%	3.26	1.39%
570.422	8	12.19	0.14%	2.28	5.00%	12.14	0.08%	2.11	2.39%
614.448	9	11.84	0.22%	1.49	4.22%	11.79	0.08%	1.24	1.91%
658.474	10	11.53	0.25%	0.92	4.94%	11.47	0.18%	0.67	1.39%
702.500	11	11.25	0.16%	0.51	4.23%	11.20	0.19%	0.32	2.80%
746.527	12	11.00	0.17%	0.28	5.13%	10.95	0.23%	0.14	3.36%
378.322	3	17.15	0.14%	0.42	2.44%	17.06	0.11%	0.47	0.95%
422.348	4	16.29	0.18%	1.64	3.54%	16.18	0.10%	1.79	1.24%
466.374	5	15.60	0.14%	1.88	3.78%	15.52	0.16%	2.05	1.24%
510.401	6	15.02	0.14%	1.43	3.80%	14.96	0.05%	1.54	1.38%
554.427	7	14.54	0.20%	1.06	4.71%	14.46	0.12%	1.10	1.77%
598.453	8	14.10	0.16%	0.75	3.57%	14.03	0.09%	0.74	0.90%
642.479	9	13.71	0.25%	0.47	5.00%	13.65	0.12%	0.43	1.82%
686.505	10	13.39	0.22%	0.30	4.75%	13.33	0.16%	0.24	1.82%
730.532	11	13.08	0.18%	0.17	3.87%	13.01	0.17%	0.12	1.02%
774.558	12	12.79	0.19%	0.09	5.92%	12.73	0.18%	0.05	1.19%
Carboxylate C11 and C13 (-) HESI									
243.196	1	15.30	0.19%	0.02	6.28%	15.21	0.11%	0.02	12.42%
287.222	2	15.76	0.20%	0.13	1.52%	15.65	0.23%	0.13	2.46%
331.248	3	15.03	0.28%	0.19	1.94%	14.90	0.14%	0.20	3.06%
375.275	4	14.21	0.18%	0.18	2.64%	14.13	0.17%	0.19	1.12%
419.301	5	13.56	0.21%	0.14	3.57%	13.51	0.28%	0.15	1.53%
463.327	6	13.08	0.15%	0.10	4.12%	12.97	0.13%	0.10	3.03%
507.353	7	12.58	0.16%	0.07	3.79%	12.54	0.17%	0.07	4.32%
551.380	8	12.17	0.27%	0.05	4.85%	12.13	0.23%	0.05	3.30%
595.406	9	11.86	0.17%	0.03	12.02%	11.78	0.29%	0.03	5.42%
639.432	10	11.56	0.29%	0.02	8.84%	11.47	0.32%	0.01	18.97%
359.280	3	17.16	0.30%	0.09	3.87%	17.04	0.13%	0.09	2.25%
403.306	4	16.30	0.33%	0.07	2.56%	16.18	0.31%	0.07	1.08%

447.332	5	15.61	0.24%	0.05	2.96%	15.52	0.27%	0.06	2.71%
491.358	6	15.04	0.20%	0.03	5.69%	14.94	0.19%	0.04	5.15%
535.385	7	14.51	0.21%	0.03	9.09%	14.47	0.23%	0.03	6.77%
579.411	8	14.12	0.25%	0.02	10.35%	14.02	0.18%	0.01	9.69%
623.437	9	13.71	0.34%	0.01	8.82%	13.68	0.17%	0.01	11.51%
Min		/	0.14%	/	1.52%	/	0.05%	/	0.77%
Max		/	0.34%	/	12.02%	/	0.32%	/	18.97%

Table S3: Retention times, peak areas and their RSDs of Brij homologues injected in THF/Toluene containing 1% of Crude oil

BrijC10 [M+NH ₄] ⁺		QCs				Crude1%			
m/z	Nb EO	tr	RSD (tr) (n=3)	Peak Area ×10 ⁶	RSD (Area) (n=3)	tr	RSD (tr) (n=6)	Peak Area ×10 ⁶	RSD (Area) (n=6)
392.374	3	11.70	0.25%	0.25	18.51%	11.63	0.07%	1.95	1.82%
436.400	4	11.40	0.21%	0.38	14.65%	11.33	0.11%	2.80	2.88%
480.426	5	11.15	0.30%	0.51	16.81%	11.09	0.07%	3.88	1.68%
524.453	6	10.94	0.30%	0.68	17.07%	10.88	0.07%	4.77	1.33%
568.479	7	10.74	0.09%	0.89	14.50%	10.69	0.10%	5.18	1.89%
612.505	8	10.57	0.18%	1.08	14.07%	10.51	0.07%	5.38	1.67%
656.531	9	10.42	0.09%	1.22	12.97%	10.36	0.08%	5.16	1.73%
700.557	10	10.27	0.09%	1.29	10.68%	10.22	0.12%	4.74	1.96%
744.584	11	10.14	0.21%	1.31	13.43%	10.10	0.11%	4.14	2.08%
788.610	12	10.03	0.09%	1.24	9.05%	9.97	0.13%	3.48	1.88%
832.636	13	9.92	0.09%	1.09	11.34%	9.86	0.13%	2.79	1.94%
876.662	14	9.82	0.09%	0.84	10.76%	9.77	0.12%	1.94	1.73%
920.688	15	9.72	0.07%	0.89	9.86%	9.67	0.11%	4.29	1.49%
964.715	16	9.63	0.09%	0.89	9.20%	9.59	0.11%	3.98	1.40%
1008.741	17	9.55	0.15%	0.78	6.81%	9.50	0.04%	3.27	1.59%
1052.767	18	9.47	0.02%	0.61	8.31%	9.42	0.12%	2.49	1.59%
1096.793	19	9.38	0.14%	0.46	7.00%	9.34	0.09%	1.81	2.25%
579.427	20	9.32	0.09%	0.64	3.78%	9.27	0.14%	1.21	2.54%
601.440	21	9.24	0.09%	0.44	7.16%	9.20	0.09%	0.76	4.10%
623.453	22	9.18	0.30%	0.28	3.06%	9.14	0.08%	0.49	3.40%
645.466	23	9.12	0.09%	0.17	1.97%	9.09	0.23%	0.29	5.28%
667.479	24	9.06	0.02%	0.10	9.32%	9.03	0.25%	0.16	7.97%
689.492	25	9.01	0.17%	0.05	3.05%	8.97	0.24%	0.10	4.80%
711.506	26	8.94	0.28%	0.03	53.37%	8.92	0.28%	0.05	9.76%
733.519	27	8.90	0.29%	0.02	15.53%	8.86	0.16%	0.02	8.48%
755.532	28	8.85	0.09%	0.01	29.83%	8.80	0.49%	0.01	24.91%
Min		/	0.02%	/	1.97%	/	0.04%	/	1.33%
Max		/	0.30%	/	53.37%	/	0.49%	/	24.91%

Table S4: Retention times, peak areas and their RSDs of Carboxylate homologues injected in THF/Toluene containing 1% of Crude oil

Carboxylate (+/-)		QCs				Crude1%			
m/z	Nb EO	tr	RSD (tr) (n=3)	Peak Area ×10 ⁶	RSD (Area) (n=3)	tr	RSD (tr) (n=6)	Peak Area ×10 ⁶	RSD (Area) (n=6)
Carboxylate C11 and C13 (+) HESI									
350.291	3	15.01	0.10%	1.30	0.89%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
394.317	4	14.18	0.10%	5.57	0.36%	14.12	0.11%	4.86	2.67%
438.343	5	13.55	0.08%	6.26	1.05%	13.50	0.09%	4.76	2.76%
482.369	6	13.03	0.10%	4.73	1.04%	12.98	0.08%	2.70	3.36%
526.395	7	12.59	0.30%	3.41	1.45%	12.53	0.17%	2.12	3.73%
570.422	8	12.19	0.17%	2.37	1.11%	12.14	0.12%	1.21	4.50%
614.448	9	11.82	0.08%	1.53	2.13%	11.79	0.13%	0.76	4.16%
658.474	10	11.51	0.21%	0.95	0.42%	11.49	0.19%	0.42	4.39%
702.500	11	11.23	0.16%	0.55	2.12%	11.20	0.26%	0.23	5.88%
746.527	12	10.99	0.19%	0.29	1.06%	10.96	0.16%	0.09	6.68%
378.322	3	17.18	0.08%	0.45	1.93%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
422.348	4	16.27	0.17%	1.72	1.64%	16.19	0.09%	1.73	2.47%
466.374	5	15.61	0.13%	1.97	1.75%	15.51	0.04%	1.64	3.13%
510.401	6	15.01	0.07%	1.50	1.31%	14.95	0.15%	0.59	11.54%
554.427	7	14.53	0.19%	1.10	0.19%	14.45	0.15%	0.70	3.89%
598.453	8	14.11	0.32%	0.79	1.11%	14.03	0.18%	0.39	5.90%
642.479	9	13.72	0.15%	0.50	1.41%	13.67	0.21%	0.25	4.39%
686.505	10	13.39	0.24%	0.32	1.56%	13.33	0.13%	0.17	4.45%
730.532	11	13.05	0.22%	0.19	0.61%	13.02	0.29%	0.09	6.25%
774.558	12	12.82	0.02%	0.10	2.18%	12.74	0.33%	0.02	25.27%
Carboxylate C11 and C13 (-) HESI									
243.196	1	15.27	0.15%	0.02	7.14%	15.14	0.28%	0.05	9.72%
287.222	2	15.69	0.28%	0.13	3.25%	15.65	0.19%	0.30	3.45%
331.248	3	15.01	0.12%	0.19	2.46%	14.91	0.16%	0.21	3.31%
375.275	4	14.18	0.15%	0.19	1.01%	14.11	0.16%	0.16	4.56%
419.301	5	13.58	0.21%	0.15	2.11%	13.52	0.17%	0.11	3.24%
463.327	6	13.05	0.23%	0.11	1.73%	13.00	0.16%	0.07	7.30%
507.353	7	12.61	0.09%	0.08	1.83%	12.50	0.23%	0.05	5.09%
551.380	8	12.24	0.08%	0.05	5.50%	12.13	0.27%	0.03	6.93%
595.406	9	11.87	0.20%	0.03	5.48%	11.77	0.30%	0.02	13.63%
639.432	10	11.52	0.41%	0.02	1.37%	11.51	0.23%	0.00	38.39%
359.280	3	17.17	0.34%	0.09	6.10%	17.06	0.13%	0.65	5.53%
403.306	4	16.27	0.31%	0.07	1.16%	16.19	0.11%	0.44	3.68%

447.332	5	15.60	0.09%	0.06	3.98%	15.52	0.24%	0.12	2.71%
491.358	6	15.01	0.15%	0.04	6.91%	14.95	0.19%	0.04	7.77%
535.385	7	14.56	0.15%	0.02	9.20%	14.48	0.25%	0.02	12.76%
579.411	8	14.10	0.30%	0.02	1.81%	14.06	0.39%	0.01	21.31%
623.437	9	13.75	0.11%	0.01	15.20%	13.66	0.29%	0.00	33.49%
Min		/	0.02%	/	0.19%	/	0.04%	/	2.47%
Max		/	0.41%	/	15.20%	/	0.39%	/	38.39%

Table S5: Retention times, peak areas and their RSDs of Brij homologues injected in THF/Toluene containing 10% of Crude oil

BrijC10 [M+NH ₄] ⁺		QCs				Crude10%			
m/z	Nb EO	tr	RSD (tr) (n=3)	Peak Area ×10 ⁶	RSD (Area) (n=3)	tr	RSD (tr) (n=6)	Peak Area ×10 ⁶	RSD (Area) (n=6)
392.374	3	11.73	0.04%	0.12	59.50%	11.65	0.13%	1.66	6.93%
436.400	4	11.42	0.03%	0.23	20.13%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
480.426	5	11.17	0.08%	0.31	18.27%	11.09	0.07%	3.59	5.46%
524.453	6	10.95	0.03%	0.43	18.77%	10.88	0.07%	4.42	6.05%
568.479	7	10.75	0.12%	0.58	17.49%	10.69	0.10%	4.69	6.04%
612.505	8	10.58	0.14%	0.71	16.91%	10.52	0.15%	5.49	4.07%
656.531	9	10.44	0.11%	0.80	14.31%	10.37	0.07%	4.97	4.33%
700.557	10	10.29	0.03%	0.87	15.04%	10.22	0.14%	4.85	4.96%
744.584	11	10.16	0.03%	0.89	14.60%	10.10	0.07%	4.19	5.23%
788.610	12	10.03	0.14%	0.85	13.23%	9.98	0.08%	3.50	5.57%
832.636	13	9.93	0.09%	0.76	12.68%	9.87	0.22%	2.96	3.85%
876.662	14	9.83	0.03%	0.60	11.53%	9.78	0.14%	2.05	4.41%
920.688	15	9.73	0.03%	0.66	10.84%	9.68	0.06%	4.33	3.65%
964.715	16	9.64	0.15%	0.68	12.79%	9.59	0.06%	3.77	5.24%
1008.741	17	9.55	0.08%	0.60	9.73%	9.51	0.13%	2.97	3.32%
1052.767	18	9.47	0.13%	0.49	8.73%	9.44	0.17%	2.21	5.02%
1096.793	19	9.39	0.03%	0.36	8.82%	9.36	0.19%	1.61	7.90%
579.427	20	9.32	0.23%	0.49	7.28%	9.29	0.15%	1.14	5.73%
601.440	21	9.26	0.04%	0.34	4.21%	9.24	0.37%	0.62	11.14%
623.453	22	9.18	0.17%	0.22	5.07%	9.17	0.29%	0.45	12.38%
645.466	23	9.13	0.16%	0.15	6.85%	9.09	0.12%	0.38	15.79%
667.479	24	9.06	0.17%	0.08	10.57%	9.06	0.41%	0.12	29.06%
689.492	25	8.99	0.13%	0.05	9.94%	9.00	0.29%	0.08	25.27%
711.506	26	8.96	0.16%	0.03	18.85%	8.95	0.22%	0.02	60.75%
733.519	27	8.91	0.05%	0.01	7.57%	8.88	0.67%	0.01	7.49%
755.532	28	8.84	0.24%	0.00	20.06%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
Min		/	0.03%	/	4.21%	/	0.06%	/	3.32%
Max		/	0.24%	/	59.50%	/	0.67%	/	60.75%

Table S6: Retention times, peak areas and their RSDs of Carboxylate homologues injected in THF/Toluene containing 10% of Crude oil

Carboxylate (+/-)		QCs				Crude10%			
m/z	Nb EO	tr	RSD (tr) (n=3)	Peak Area ×10 ⁶	RSD (Area) (n=3)	TR	RSD (tr) (n=6)	Peak Area ×10 ⁶	RSD (Area) (n=6)
Carboxylate C11 and C13 (+) HESI									
350.291	3	15.02	0.22%	1.27	2.50%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
394.317	4	14.20	0.10%	5.45	0.54%	14.13	0.10%	3.39	5.93%
438.343	5	13.57	0.12%	6.19	0.37%	13.51	0.08%	5.17	3.05%
482.369	6	13.03	0.13%	4.66	0.37%	12.99	0.11%	1.31	2.83%
526.395	7	12.59	0.27%	3.40	1.25%	12.54	0.20%	2.91	3.02%
570.422	8	12.19	0.18%	2.37	0.56%	12.14	0.18%	1.63	5.66%
614.448	9	11.87	0.20%	1.54	2.13%	11.80	0.25%	1.27	4.65%
658.474	10	11.54	0.21%	0.96	1.83%	11.49	0.09%	0.94	4.93%
702.500	11	11.25	0.19%	0.55	0.97%	11.23	0.18%	0.55	8.88%
746.527	12	11.00	0.21%	0.29	0.85%	10.99	0.47%	0.20	20.91%
378.322	3	17.16	0.26%	0.42	6.98%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
422.348	4	16.28	0.16%	1.63	1.99%	16.19	0.13%	0.40	31.13%
466.374	5	15.61	0.18%	1.90	0.11%	15.53	0.17%	1.40	5.84%
510.401	6	15.01	0.12%	1.45	1.93%	<i>nd</i>	<i>nd</i>	<i>nd</i>	<i>nd</i>
554.427	7	14.55	0.29%	1.07	0.58%	14.47	0.17%	0.71	8.98%
598.453	8	14.13	0.16%	0.77	1.50%	14.06	0.20%	0.16	43.53%
642.479	9	13.71	0.08%	0.49	0.85%	13.66	0.16%	0.36	5.33%
686.505	10	13.37	0.12%	0.31	1.92%	13.35	0.17%	0.42	13.76%
730.532	11	13.12	0.08%	0.18	1.71%	13.06	0.32%	0.19	22.07%
774.558	12	12.81	0.22%	0.10	2.03%	12.80	0.43%	0.11	23.78%
Carboxylate C11 and C13 (-) HESI									
243.196	1	15.26	0.30%	0.02	5.24%	15.17	0.34%	0.17	10.07%
287.222	2	15.74	0.56%	0.13	2.66%	15.63	0.12%	1.03	4.21%
331.248	3	15.00	0.25%	0.19	2.90%	14.95	0.17%	1.59	3.03%
375.275	4	14.21	0.14%	0.18	2.47%	14.14	0.07%	0.80	1.55%
419.301	5	13.60	0.19%	0.15	1.47%	13.53	0.13%	0.47	3.47%
463.327	6	13.02	0.08%	0.10	1.55%	13.03	0.22%	0.25	5.75%
507.353	7	12.59	0.36%	0.07	2.99%	12.54	0.17%	0.12	4.14%
551.380	8	12.21	0.29%	0.05	5.93%	12.15	0.22%	0.05	7.36%
595.406	9	11.83	0.12%	0.03	2.53%	11.81	0.29%	0.03	3.39%
639.432	10	11.57	0.43%	0.02	4.44%	11.50	0.33%	0.01	10.27%
359.280	3	17.17	0.21%	0.09	5.63%	17.09	0.65%	0.68	31.15%
403.306	4	16.28	0.17%	0.07	2.31%	16.16	0.14%	0.67	5.16%

447.332	5	15.64	0.15%	0.05	2.98%	15.53	0.14%	0.37	14.12%
491.358	6	15.00	0.12%	0.03	7.35%	14.97	0.27%	0.42	5.00%
535.385	7	14.52	0.18%	0.03	2.92%	14.49	0.31%	0.20	5.05%
579.411	8	14.12	0.19%	0.02	15.23%	14.05	0.30%	0.07	5.64%
623.437	9	13.74	0.13%	0.01	16.83%	13.67	0.16%	0.05	14.18%
Min		/	0.08%	/	0.11%	/	0.07%	/	1.55%
Max		/	0.56%	/	16.83%	/	0.65%	/	43.53%