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AQbD-Based UPLC-ELSD Method for Quantifying Medium Chain Triglycerides in Labrafac™ WL 1349 for Nanoemulsion Applications

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Table S1. Chromatographic DoE results evaluation. (1) Tricaprylin. (2) 1,2-caprate-3-caprylate. (3) 1,2-caprylate-3-caprate. (4) Tricaprin.

Chromatographic DoE Evaluation							
Solution 1 of 100 Response	**Predicted Mean**	**Std Dev**	**n**	**SE Pred**	**95% PI low**	**Data Mean**	**95% PI high**
K prime (1)	2.71044	0.777196	6	N/A	2.0391	2.4	3.3291
Height (1)	1.47825E+06	263335	6	128161	1.22371E+06	1.91214E+06	1.73279E+06
Tailing (1)	1.25336	0.109543	6	N/A	1.11181	1.2	1.38108
Resolution (2)	5.44306	1.11716	6	N/A	4.44834	5.39939	6.41202
K prime (2)	4.02276	1.18739	6	N/A	3.0004	3.5	4.96123
Height (2)	1.59498E+06	290058	6	127359	1.34236E+06	1.91253E+06	1.84759E+06
Tailing (2)	1.37087	0.35705	6	N/A	1.04915	1.28571	1.65248
Resolution (3)	6.86837	1.26698	6	0.558607	5.75924	7.2	7.9775
K prime (3)	5.75815	1.65939	6	N/A	4.24986	5.11647	7.11923
Height (3)	843231	350038	6	N/A	532991	1.32887E+06	1.13547E+06
Tailing (3)	1.19441	0.0915907	6	N/A	1.08406	1.2	1.2948
Resolution (4)	9.4186	1.95305	6	N/A	7.68369	10.8317	11.0693
K prime (4)	8.61785	3.00025	6	N/A	5.87177	7.63312	11.0838
Height (4)	34158.7	13351.9	6	N/A	21881.6	65326.5	45233.4
Tailing (4)	1.02965	0.176655	6	N/A	0.876305	0.968157	1.18521

Table S2. Robustness results for Tricaprylin, K prime correlation.

Dependent Variable: K prime Tricaprylin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.033[1]	6	0.006	0.589	0.736
Intercept	114.266	1	114.266	12056.707	<0.001
Drift Tube Temperature	0.017	2	0.009	0.916	0.412
Nebulizer Power	0.003	2	0.002	0.175	0.841
Gas Pressure	0.012	2	0.006	0.634	0.538
Error	0.265	28	0.009		
Total	191.010	35			
Corrected Total	0.299	34			

[1]R Squared = 0.112 (Adjusted R Squared = -0.078).

Table S3. Robustness results for Tricaprylin, height correlation.

Dependent Variable: Height Tricaprylin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	257606868825.801[1]	6	42934478137.634	0.904	0.506
Intercept	5232360501817.071	1	5232360501817.071	110.111	<0.001
Drift Tube Temperature	43076688505.197	2	21538344252.599	0.453	0.640
Nebulizer Power	104399287492.296	2	52199643746.148	1.099	0.347
Gas Pressure	73763967076.222	2	36881983538.111	0.776	0.470
Error	1330527676208.884	28	47518845578.889		
Total	9826247407869.000	35			
Corrected Total	1588134545034.686	34			

[1]R Squared = 0.162 (Adjusted R Squared = -0.017).

Table S4. Robustness results for Tricaprylin, tailing correlation.

Dependent Variable: Tailing Tricaprylin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.015[1]	6	0.002	1.999	0.100
Intercept	28.881	1	28.881	23233.700	<0.001
Drift Tube Temperature	0.012	2	0.006	4.919	0.015
Nebulizer Power	0.004	2	0.002	1.538	0.232
Gas Pressure	0.003	2	0.002	1.371	0.270
Error	0.035	28	0.001		
Total	49.020	35			
Corrected Total	0.050	34			

[1]R Squared = 0.300 (Adjusted R Squared = 0.150).

Table S5. Robustness results for 1,2-caprate-3-caprylate, resolution correlation.

Dependent Variable: Resolution 1,2-caprate-3-caprylate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.578[1]	6	0.096	1.562	0.195
Intercept	695.362	1	695.362	11271.576	<0.001
Drift Tube Temperature	0.088	2	0.044	0.710	0.500
Nebulizer Power	0.041	2	0.021	0.336	0.717
Gas Pressure	0.401	2	0.201	3.254	0.054
Error	1.727	28	0.062		
Total	1156.620	35			
Corrected Total	2.306	34			

[1]R Squared = 0.251 (Adjusted R Squared = 0.090)

Table S6. Robustness results for 1,2-caprate-3-caprylate, K prime correlation.

Dependent Variable: K prime 1,2-caprate-3-caprylate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.089[1]	6	0.015	0.864	0.533
Intercept	244.123	1	244.123	14220.012	<0.001
Drift Tube Temperature	0.037	2	0.018	1.074	0.355
Nebulizer Power	0.012	2	0.006	0.337	0.716
Gas Pressure	0.047	2	0.024	1.371	0.270
Error	0.481	28	0.017		
Total	409.260	35			
Corrected Total	0.570	34			

[1]R Squared = 0.156 (Adjusted R Squared = -0.025).

Table S7. Robustness results for 1,2-caprate-3-caprylate, height correlation.

Dependent Variable: Height 1,2-caprate-3-caprylate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	360428126521.016[1]	6	60071354420.169	0.995	0.448
Intercept	13956237398580.740	1	13956237398580.740	231.280	<0.001
Drift Tube Temperature	136695564890.440	2	68347782445.220	1.133	0.336
Nebulizer Power	87801661766.209	2	43900830883.105	0.728	0.492
Gas Pressure	116506180505.659	2	58253090252.829	0.965	0.393
Error	1689618804579.384	28	60343528734.978		
Total	24779769843814.000	35			
Corrected Total	2050046931100.400	34			

[1]R Squared = 0.176 (Adjusted R Squared = -0.001).

Table S8. Robustness results for 1,2-caprate-3-caprylate, tailing correlation.

Dependent Variable: Tailing 1,2-caprate-3-caprylate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.009[1]	6	0.001	0.863	0.534
Intercept	33.533	1	33.533	19866.852	<0.001
Drift Tube Temperature	0.006	2	0.003	1.728	0.196
Nebulizer Power	0.001	2	0.001	0.411	0.667
Gas Pressure	0.001	2	0.000	0.220	0.804
Error	0.047	28	0.002		
Total	57.400	35			
Corrected Total	0.056	34			

[1]R Squared = 0.156 (Adjusted R Squared = -0.025).

Table S9. Robustness results for 1,2-caprylate-3-caprate, resolution correlation.

Dependent Variable: Resolution 1,2-caprylate-3-caprate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	1.126[1]	6	0.188	0.664	0.679
Intercept	986.936	1	986.936	3491.029	<0.001
Drift Tube Temperature	0.290	2	0.145	0.513	0.604
Nebulizer Power	0.041	2	0.021	0.073	0.930
Gas Pressure	0.681	2	0.340	1.204	0.315
Error	7.916	28	0.283		
Total	1638.340	35			
Corrected Total	9.042	34			

[1]R Squared = 0.125 (Adjusted R Squared = -0.063).

Table S10. Robustness results for 1,2-caprylate-3-caprate, height correlation.

Dependent Variable: Height 1,2-caprylate-3-caprate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	101487041315.400[1]	6	16914506885.900	1.066	0.406
Intercept	1515690641980.627	1	1515690641980.627	95.557	<0.001
Drift Tube Temperature	4800113063.841	2	2400056531.920	0.151	0.860
Nebulizer Power	12165030529.844	2	6082515264.922	0.383	0.685
Gas Pressure	67123798811.942	2	33561899405.971	2.116	0.139
Error	444125988701.171	28	15861642453.613		
Total	2904821510728.000	35			
Corrected Total	545613030016.571	34			

[1]R Squared = 0.186 (Adjusted R Squared = 0.012).

Table S11. Robustness results for 1,2-caprylate-3-caprate, K prime correlation.

Dependent Variable: K prime 1,2-caprylate-3-caprate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.151[1]	6	0.025	00.523	0.786
Intercept	522.653	1	522.653	10858.771	<0.001
Drift Tube Temperature	0.067	2	0.033	0.691	0.509
Nebulizer Power	0.018	2	0.009	0.190	0.828
Gas Pressure	0.068	2	0.034	0.705	0.503
Error	1.348	28	00.048		
Total	874.500	35			
Corrected Total	1.499	34			

[1]R Squared = 0.101 (Adjusted R Squared = -0.092).

Table S12. Robustness results for 1,2-caprylate-3-caprate, tailing correlation.

Dependent Variable: Tailing 1,2-caprylate-3-caprate					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.013[1]	6	0.002	0.520	0.788
Intercept	36.421	1	36.421	8624.573	<0.001
Drift Tube Temperature	0.003	2	0.001	0.303	0.741
Nebulizer Power	0.009	2	0.005	1.101	0.346
Gas Pressure	0.001	2	0.001	0.165	0.849
Error	0.118	28	0.004		
Total	61.910	35			
Corrected Total	0.131	34			

[1]R Squared = 0.100 (Adjusted R Squared = -0.092).

Table S13. Robustness results for Tricaprin, resolution correlation.

Dependent Variable: Resolution Tricaprin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	1.341[1]	6	0.223	0.211	0.970
Intercept	1552.478	1	1552.478	1467.657	<0.001
Drift Tube Temperature	0.179	2	0.089	0.084	0.919
Nebulizer Power	0.774	2	0.387	0.366	0.697
Gas Pressure	0.028	2	0.014	0.013	0.987
Error	29.618	28	1.058		
Total	2580.150	35			
Corrected Total	30.959	34			

[1]R Squared = 0.043 (Adjusted R Squared = -0.162).

Table S14. Robustness results for Tricaprin, height correlation.

Dependent Variable: Height Tricaprin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	318118337.745[1]	6	53019722.957	1.178	0.346
Intercept	3489657082.481	1	3489657082.481	77.559	<0.001
Drift Tube Temperature	62689792.368	2	31344896.184	0.697	0.507
Nebulizer Power	110220782.058	2	55110391.029	1.225	0.309
Gas Pressure	108814084.973	2	54407042.487	1.209	0.314
Error	1259828180.427	28	44993863.587		
Total	7151998600.000	35			
Corrected Total	1577946518.171	34			

[1]R Squared = 0.202 (Adjusted R Squared = 0.031).

Table S15. Robustness results for Tricaprin, K prime correlation.

Dependent Variable: K prime Tricaprin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.450[1]	6	0.075	0.649	0.690
Intercept	1157.722	1	1157.722	10029.645	<0.001
Drift Tube Temperature	0.190	2	0.095	0.823	0.449
Nebulizer Power	0.065	2	0.033	0.283	0.756
Gas Pressure	0.193	2	0.097	0.837	0.444
Error	3.232	28	0.115		
Total	1932.140	35			
Corrected Total	3.682	34			

[1]R Squared = 0.122 (Adjusted R Squared = -0.066).

Table S16. Robustness results for Tricaprin, Tailing correlation.

Dependent Variable: Tailing Tricaprin					
Source	**Type III Sum of Squares**	**df**	**Mean Square**	**F**	**Significance**
Corrected Model	0.062[1]	6	0.010	0.198	0.975
Intercept	33.843	1	33.843	654.341	<0.001
Drift Tube Temperature	0.005	2	0.002	0.048	0.953
Nebulizer Power	0.037	2	0.019	0.358	0.702
Gas Pressure	0.018	2	0.009	0.169	0.845
Error	1.448	28	0.052		
Total	60.920	35			
Corrected Total	1.510	34			

[1]R Squared = 0.041 (Adjusted R Squared = -0.165).