

Electronic Supplementary Information for

**Optimization of Analytical Method Greenness Scores:
A Case Study of Amino Acid Enantioseparations with
Carbonated Aqueous Systems**

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Table ESI-1: Chromatographic Figures of Merit for Carbonated H₂O Conditions

Compound Number	Amino Acid (D-/L-)	t_{r2} (min)	α	N_1	N_2	R_s
1	Alanine	1.55	1.18	18850	16900	1.86
2	Valine	1.71	1.11	14150	11000	1.19
3	Leucine	2.34	1.27	10450	5950	2.81
4	Isoleucine	2.24	1.23	10300	6750	2.44
5	Phenylalanine	2.58	1.11	8250	3850	1.18
6	Proline	2.73	2.08	12350	3250	7.01
7	Tryptophan	3.67	1.13	6400	2200	1.27
8	Serine	1.31	1.05	-	-	0.51
9	Threonine	1.35	1.04	-	-	0.54
10	Methionine	2.01	1.32	12800	8400	3.24
11	Cysteine	1.12	1.17	-	-	1.12
12	Asparagine	1.43	1.18	13650	13150	1.37
13	Glutamine	1.49	1.58	16900	14500	1.58
14	Aspartic Acid	1.02	1.00	-	-	0.00
15	Lysine	10.0	1.08	-	-	1.06
16	Tyrosine	1.94	1.08	9750	5250	0.79
17	Glutamic Acid	1.28	1.29	12900	13900	1.44
18	Arginine	13.6	1.12	-	-	2.32
19	Histidine	21.9	1.00	-	-	0.00
20	o-tyrosine	2.29	1.10	10150	5850	1.10
21	Norleucine	2.44	1.33	11450	5150	3.33
22	2-Fluorophenylalanine	2.70	1.12	7550	3400	1.22
23	3-Fluorophenylalanine	2.68	1.22	7800	3150	2.02
24	2-Phenylglycine	2.63	2.24	10800	1750	5.72
25	3,4-Dihydroxyphenylalanine	2.14	1.35	1850	850	1.26
26	6-Methyl-Tryptophan	5.39	1.06	2900	950	1.06
27	2-Fluorophenylglycine	2.06	1.67	10800	3500	4.28
28	Norvaline	1.95	1.35	15350	8900	3.58
29	Ethionine	2.45	1.33	10000	5400	3.33
30	α -methyl-m-tyrosine-methyl ester	2.26	1.25	7600	2300	1.82
31	2-aminobutyric acid	1.58	1.16	18300	15000	1.68
32	p-Bromo-phenylalanine	4.01	1.03	-	-	0.37
33	Pipecolic acid	2.91	1.38	8100	3050	3.33
34	5-Fluoro-Tryptophan	4.29	1.22	5250	1500	1.85
35	m-tyrosine	2.34	1.49	10650	2250	3.28
36	Homoserine	1.42	1.11	16850	15750	0.92
37	p-Nitro-phenylalanine	3.12	1.05	-	-	0.58
38	p-Fluoro-phenylalanine	2.69	1.14	6350	2450	1.18

Table ESI-2: Chromatographic Figures of Merit for Carbonated 80/20 H₂O/MeOH Conditions

Compound Number	Amino Acid (D-/L-)	t_{r2} (min)	α	N_1	N_2	R_s
1	Alanine	1.58	1.31	17750	14850	2.89
2	Valine	1.61	1.19	14650	12100	1.78
3	Leucine	1.94	1.46	13150	7400	3.99
4	Isoleucine	1.90	1.43	12050	7650	3.72
5	Phenylalanine	2.12	1.14	9650	5800	1.46
6	Proline	2.98	2.74	11950	3950	9.97
7	Tryptophan	2.86	1.17	7700	3650	1.73
8	Serine	1.34	1.10	-	-	0.79
9	Threonine	1.35	1.10	-	-	0.66
10	Methionine	1.96	1.54	12650	8500	4.74
11	Cysteine	1.48	1.27	9050	8400	1.69
12	Asparagine	1.51	1.27	11600	9850	1.93
13	Glutamine	1.53	2.01	14700	12700	2.01
14	Aspartic Acid	1.29	1.00	-	-	0.00
15	Lysine	8.70	1.12	-	-	1.28
16	Tyrosine	1.85	1.13	9400	6800	1.21
17	Glutamic Acid	1.37	1.35	12000	10750	1.95
18	Arginine	10.8	1.15	-	-	1.66
19	Histidine	11.6	1.00	-	-	0.00
20	o-tyrosine	2.07	1.13	10600	7350	1.41
21	Norleucine	2.08	1.56	13600	7000	4.97
22	2-Fluorophenylalanine	2.11	1.17	9650	5650	1.67
23	3-Fluorophenylalanine	2.24	1.34	9700	4800	3.01
24	2-Phenylglycine	2.78	2.96	11400	2400	8.19
25	3,4-Dihydroxyphenylalanine	2.12	1.51	2000	850	1.68
26	6-Methyl-Tryptophan	3.48	1.62	5600	2250	1.62
27	2-Fluorophenylglycine	2.03	2.13	11350	4400	6.14
28	Norvaline	1.88	1.60	15350	9100	5.15
29	Ethionine	2.07	1.50	12300	7950	4.59
30	α -methyl-m-tyrosine-methyl ester	2.08	1.35	9250	3250	2.55
31	2-aminobutyric acid	1.58	1.26	16550	13850	2.41
32	p-Bromo-phenylalanine	2.87	1.06	-	-	1.14
33	Pipecolic acid	2.39	1.66	11700	4500	5.27
34	5-Fluoro-Tryptophan	3.32	1.32	7000	2550	2.85
35	m-tyrosine	2.28	1.66	10550	3250	4.46
36	Homoserine	1.44	1.16	16350	15700	1.37
37	p-Nitro-phenylalanine	2.57	1.11	-	-	1.14
38	p-Fluoro-phenylalanine	2.05	1.11	10100	6550	1.14

Table ESI-3: Chromatographic Figures of Merit for Carbonated 60/40 H₂O/MeOH Conditions

Compound Number	Amino Acid (D-/L-)	t_{r2} (min)	α	N_1	N_2	R_s
1	Alanine	1.76	1.46	13950	11450	4.09
2	Valine	1.72	1.31	12800	10300	2.78
3	Leucine	2.08	1.61	11800	6150	4.83
4	Isoleucine	2.08	1.64	10400	6900	5.14
5	Phenylalanine	2.12	1.26	8500	5900	2.40
6	Proline	3.97	3.31	-	-	11.4
7	Tryptophan	2.55	1.27	7300	4300	2.55
8	Serine	1.43	1.16	-	-	1.21
9	Threonine	1.41	1.16	-	-	0.90
10	Methionine	2.12	1.74	9900	6950	5.68
11	Cysteine	1.64	1.41	-	-	2.29
12	Asparagine	1.66	1.39	4250	5150	2.01
13	Glutamine	1.62	2.50	11450	9750	2.50
14	Aspartic Acid	1.31	1.00	-	-	0.00
15	Lysine	-	-	-	-	-
16	Tyrosine	1.85	1.25	8150	6600	2.06
17	Glutamic Acid	1.53	1.48	8150	6650	2.53
18	Arginine	14.40	1.21	-	-	2.72
19	Histidine	14.23	1.00	-	-	0.00
20	o-tyrosine	2.04	1.20	9450	7150	2.05
21	Norleucine	2.22	1.82	12150	7600	6.78
22	2-Fluorophenylalanine	2.08	1.27	8550	5750	2.44
23	3-Fluorophenylalanine	2.20	1.46	8500	5150	3.74
24	2-Phenylglycine	3.43	3.86	10050	2700	11.0
25	3,4-Dihydroxyphenylalanine	2.13	1.53	1200	500	1.36
26	6-Methyl-Tryptophan	2.83	2.37	6100	3250	2.37
27	2-Fluorophenylglycine	2.32	2.64	9150	4300	8.06
28	Norvaline	2.11	1.92	13300	7950	7.10
29	Ethionine	2.11	1.64	10100	3500	5.22
30	α -methyl-m-tyrosine-methyl ester	1.98	1.38	9000	3800	2.70
31	2-aminobutyric acid	1.72	1.41	14050	11550	3.69
32	p-Bromo-phenylalanine	2.56	1.17	-	-	1.98
33	Pipecolic acid	2.63	1.88	9750	5150	6.91
34	5-Fluoro-Tryptophan	2.80	1.44	7100	3350	3.69
35	m-tyrosine	2.29	1.84	9200	3550	5.26
36	Homoserine	1.53	1.24	14700	12300	2.04
37	p-Nitro-phenylalanine	2.38	1.22	-	-	1.98
38	p-Fluoro-phenylalanine	2.03	1.06	9050	6700	2.14