

Supplementary Material

Quantitative profiling of endogenous fat-soluble vitamins and carotenoids in human plasma using an improved UHPSFC-ESI-MS interface

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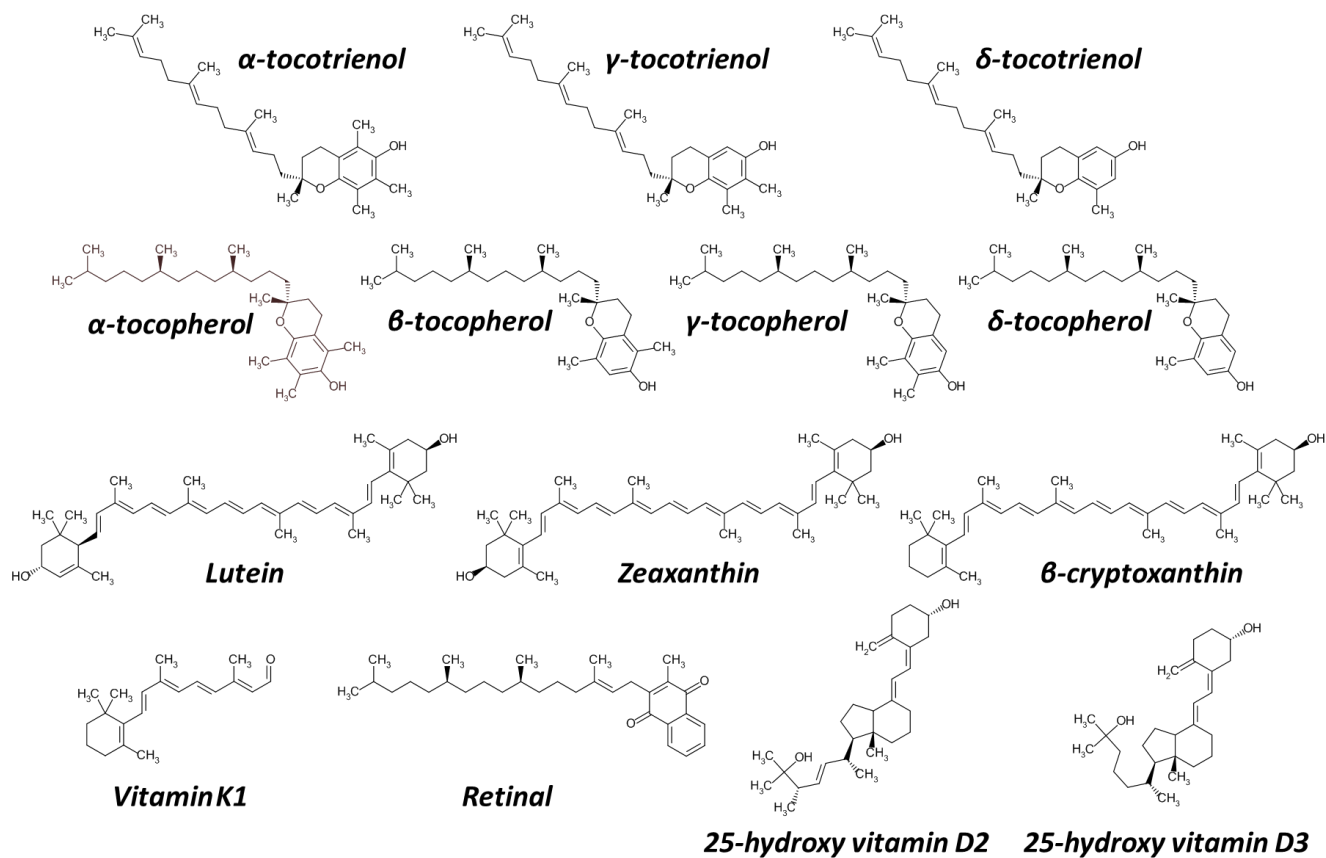
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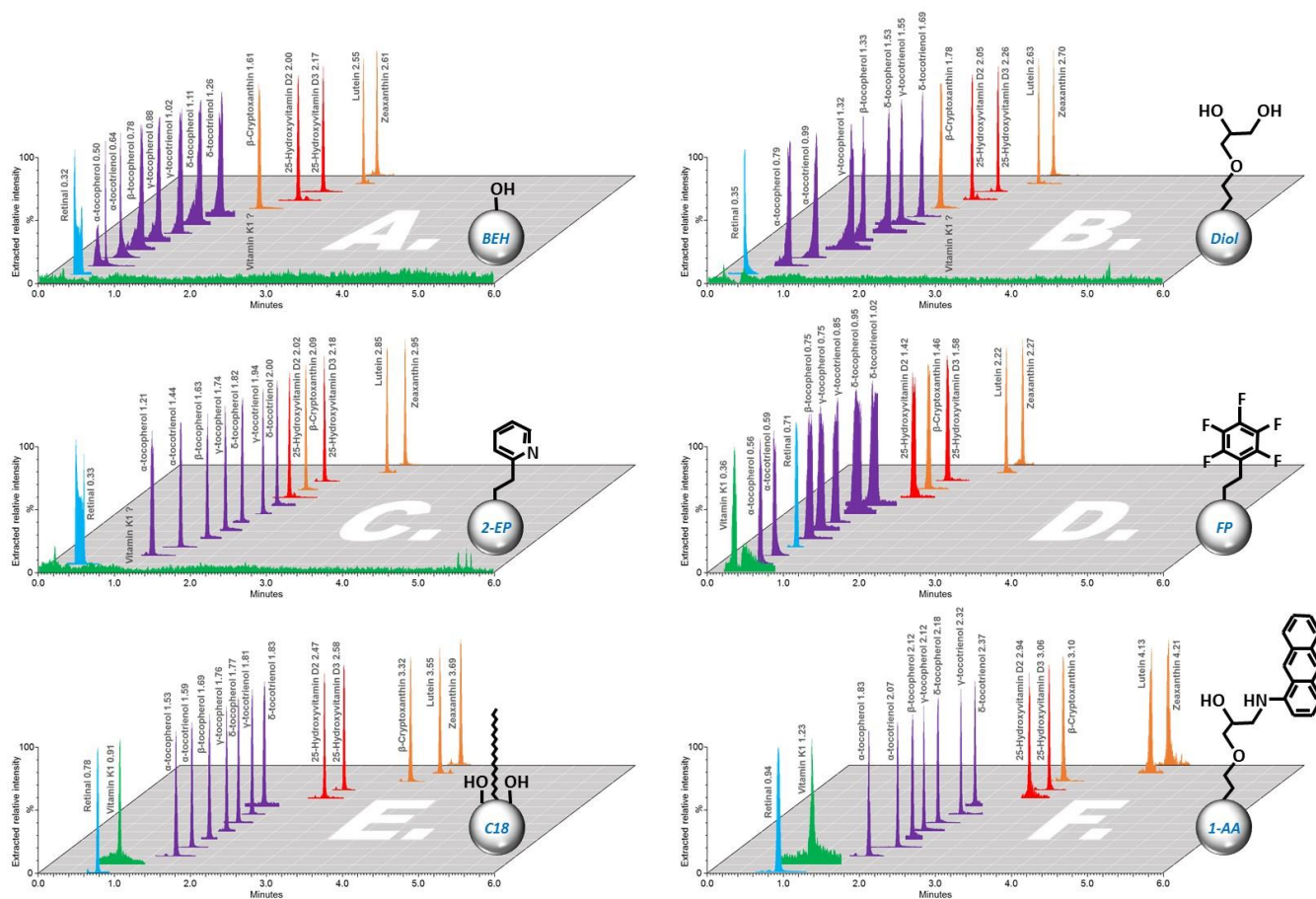
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Supplementary material content

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Supplementary Figure S-1: Detailed chemical structures of the investigated vitamins and carotenoids



Supplementary Figure S-2: UHPSFC-MS/MS separations of the 14 fat-soluble vitamins standards performed using a scouting gradient of MeOH + 20 mM AmF in CO₂ on six different stationary phases, i.e. BEH (A.), Diol (B.), 2-EP (C.), FP (D.), C18 (E.) and 1-AA (F.).

Supplementary Table S-1: UHPSFC optimized mobile phase gradient program.

Time [min]	Flow rate [mL/min]	%A (CO ₂)	%B (Cosolvent)	Make-up flow rate [mL/min]
0.0	2.0	98	2	0.1
0.6	2.0	98	2	0.1
1.2	2.0	97	3	0.1
1.8	2.0	95	5	0.1
2.4	2.0	95	5	0.1
3.0	2.0	92	8	0.1
3.6	2.0	90	10	0.1
4.2	2.0	88	12	0.1
4.8	2.0	88	12	0.1
6.0	2.0	80	20	0.1
6.6	2.0	80	20	0.1
6.7	2.0	98	2	0.1
8.0	2.0	98	2	0.1

Supplementary Table S-2: MS/MS transitions and energies.

Compound	Retention time [min]	SRM transition [m/z]	Collision energy [V]	Cone voltage [V]
Retinal	0.83	285.26>161.06	8	4
Vitamin K1	0.94	451.37>128.14	62	70
² H ₄ -vitamin K1 (IS)	0.94	458.45>193.99	24	2
α-tocopherol	1.74	432.50>97.07	16	60
² H ₉ -α-tocopherol (IS)	1.74	437.52>171.02	22	2
α-tocotrienol	1.83	425.31>165.07	22	46
β-tocopherol	2.02	417.38>123.07	42	28
γ-tocopherol	2.14	417.38>95.05	22	44
δ-tocopherol	2.17	403.38 > 136.90	18	36
γ-tocotrienol	2.22	411.31 > 191.10	14	20
δ-tocotrienol	2.26	397.25 > 136.99	24	46
25-Hydroxyvitamin D2	3.53	395.39 > 107.13	28	20
25-Hydroxyvitamin D3	3.77	383.33 > 257.18	14	10
² H ₆ -25-Hydroxyvitamin D3 (IS)	3.77	389.39 > 263.23	18	48
β-cryptoxanthin	4.78	553.45 > 119.04	38	30
Tomatidine (IS)	5.33	416.57 > 105.06	56	8
Lutein	5.51	551.51 > 119.05	40	54
Zeaxanthin	5.76	569.51 > 119.1	48	58

Supplementary Table S-3: Linearity and limits of detection/quantification

Compound	Determination coefficient (R ²)	Calibration curve equation	LOD [ng/mL]	LOQ [ng/mL]
Retinal	0.9964	0.1757x + 0.3358	0.4	2
Vitamin K1	0.9963	0.2415x - 0.0096	0.004	0.02
α-tocopherol	0.9924	0.0005x + 0.5253	3200	16000
α-tocotrienol	0.9901	0.0682x - 6.0943	0.04	0.2
β-tocopherol	0.9922	0.0053x - 0.0362	0.04	0.2
γ-tocopherol	0.9916	0.0053x - 0.1346	0.04	0.2
δ-tocopherol	0.9905	0.0246x - 1.3157	0.04	0.2
γ-tocotrienol	0.9942	0.0067x - 0.2241	0.02	2
δ-tocotrienol	0.9926	0.0355x - 0.7466	0.04	2
25-Hydroxyvitamin D2	0.9949	0.0205x + 0.4821	0.4	2
25-Hydroxyvitamin D3	0.9909	0.027x + 0.7272	0.4	0.2
β-cryptoxanthin	0.9922	0.0124x - 0.3326	0.04	0.2
Lutein	0.9928	0.0168x - 0.8674	0.2	0.4
Zeaxanthin	0.9939	0.0258x - 0.7173	0.2	0.4