

Table S1 Concentrations of stock solutions, series of standard solution and calibration standard solutions of 10 analytes

No.	Analyte	Stock solution (mg/mL)	Series of standard solutions (µg/mL)							Series of calibration standard solutions (µg/mL)						
			1	2	3	4	5	6	7	1	2	3	4	5	6	7
1	PRM	12	30	60	120	240	600	900	1200	1.5	3	6	12	30	45	60
2	LTG	8	20	40	80	160	400	600	800	1	2	4	8	20	30	40
3	CBZE	1.2	3	6	12	24	60	90	120	0.15	0.3	0.6	1.2	3	4.5	6
4	MHD	10	2.5	5	10	20	50	75	100	1.25	2.5	5	10	25	37.5	50
5	PHB	20	50	100	200	400	1000	1500	2000	2.5	5	10	20	50	75	100
6	OXC	20	50	100	200	400	1000	1500	2000	2.5	5	10	20	50	75	100
7	ESLA	20	50	100	200	400	1000	1500	2000	2.5	5	10	20	50	75	100
8	CBZ	12	30	60	120	240	600	900	1200	1.5	3	6	12	30	45	60
9	CZP	4	10	20	40	80	200	300	400	0.5	1	2	4	10	15	20
10	DZP	4	10	20	40	80	200	300	400	0.5	1	2	4	10	15	20

Table S2 Influence of different solvents on the chromatographic parameters of analytes

Solvents	t_R (min)	n	f_s	R_s	k
PRM					
100% ethanol	16.988	52012	1.132	-	15.987
Ethanol-water (95:5, v/v)	17.337	50615	1.123	-	16.337
Ethanol-water (75:25, v/v)	16.815	59166	1.155	-	15.841
LTG					
100% ethanol	17.970	39375	0.937	2.998	16.969
Ethanol-water (95:5, v/v)	18.303	39647	0.957	2.861	17.303
Ethanol-water (75:25, v/v)	17.835	38356	0.955	3.201	16.834
CBZE					
100% ethanol	18.713	47445	1.088	2.131	17.713
Ethanol-water (95:5, v/v)	19.184	44872	1.093	2.398	18.184
Ethanol-water (75:25, v/v)	18.430	52533	1.152	1.743	17.429
MHD					
100% ethanol	19.580	50326	1.110	2.514	18.579
Ethanol-water (95:5, v/v)	20.081	47648	1.131	2.436	19.081
Ethanol-water (75:25, v/v)	19.306	52741	1.135	2.665	18.306
PHB					
100% ethanol	22.220	59113	1.087	7.436	21.221
Ethanol-water (95:5, v/v)	22.710	75873	1.089	7.517	21.711
Ethanol-water (75:25, v/v)	21.982	56608	1.092	7.651	20.981
OXC					
100% ethanol	22.933	91415	1.119	2.149	21.932
Ethanol-water (95:5, v/v)	23.366	119882	1.151	2.198	22.366
Ethanol-water (75:25, v/v)	22.696	82337	1.177	2.201	21.695
ESLA					
100% ethanol	25.500	251889	1.280	10.213	24.499
Ethanol-water (95:5, v/v)	25.754	280306	1.291	10.323	24.754
Ethanol-water (75:25, v/v)	25.419	253895	1.105	13.073	24.418
CBZ					
100% ethanol	26.735	298093	1.354	6.221	25.735
Ethanol-water (95:5, v/v)	26.974	296248	1.360	6.078	25.737
Ethanol-water (75:25, v/v)	26.692	271852	1.118	5.993	25.691
CZP					
100% ethanol	28.009	323619	1.408	2.155	27.009
Ethanol-water (95:5, v/v)	28.220	370712	1.421	2.169	27.221
Ethanol-water (75:25, v/v)	28.010	418827	1.131	2.459	27.009
DZP					
100% ethanol	31.550	211445	1.263	15.261	58.846
Ethanol-water (95:5, v/v)	31.847	238716	1.246	16.455	30.847
Ethanol-water (75:25, v/v)	31.561	256674	1.222	17.005	30.561

Note: t_R , retention time; n , theoretical plate number; f_s , symmetry factor; R_s : resolution (with previous peak); k , capacity factor; /, could not be obtained.

Table S3 Influence of different columns on the chromatographic parameters of analytes

Chromatographic column	t_R (min)	n	f_s	R_s	k
PRM					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	16.815	59166	1.155	/	15.841
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	17.742	61347	1.169	/	16.742
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	17.664	12899	1.475	/	16.663
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	16.479	21321	1.679	/	15.479
XDB C18 (150 mm × 4.6 mm, 5 μm)	16.714	36517	1.188	/	15.713
LTG					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	17.835	38356	0.855	3.201	16.834
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	19.704	95376	/	7.303	18.703
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	19.883	3614	1.199	2.363	18.883
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	18.541	/	/	/	17.541
XDB C18 (150 mm × 4.6 mm, 5 μm)	18.053	/	/	/	17.053
CBZE					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	18.430	52533	1.152	1.743	17.429
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	19.975	91747	/	1.031	39.026
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	/	/	/	/	/
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	/	/	/	/	/
XDB C18 (150 mm × 4.6 mm, 5 μm)	18.273	/	/	/	17.272
MHD					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	19.306	52741	1.135	2.665	18.306
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	/	/	/	/	/
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	/	/	/	/	/
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	/	/	/	/	/
XDB C18 (150 mm × 4.6 mm, 5 μm)	19.019	37586	1.174	/	18.018
PHB					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	21.982	56608	1.092	7.651	20.981
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	22.470	72818	1.091	6.901	21.496
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	22.337	19896	1.316	2.488	21.336
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	21.244	23081	1.706	3.282	20.243
XDB C18 (150 mm × 4.6 mm, 5 μm)	21.546	38621	1.108	6.134	20.545
OXC					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	22.696	82337	1.177	2.201	21.695
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	23.928	149282	1.339	5.087	22.927
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	23.827	26059	2.481	2.546	22.826
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	22.542	18579	1.615	2.224	21.541
XDB C18 (150 mm × 4.6 mm, 5 μm)	22.242	49363	1.183	1.675	21.242
ESLA					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	25.419	253895	1.305	13.073	24.418
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	26.256	340865	1.319	11.105	25.256
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	26.224	61175	/	5.073	25.224
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	25.364	103983	1.721	6.141	24.364
XDB C18 (150 mm × 4.6 mm, 5 μm)	25.097	166701	1.259	8.974	24.096
CBZ					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	26.692	271852	1.118	5.993	25.691
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	27.029	365985	1.342	4.396	26.028
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	27.025	64274	/	/	26.024
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	26.622	123581	/	4.274	25.622
XDB C18 (150 mm × 4.6 mm, 5 μm)	26.365	203232	1.283	5.361	25.364
CZP					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	28.010	418827	1.131	2.459	27.009
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	28.243	446963	1.359	4.822	27.243
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	28.221	92583	/	/	27.221
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	27.636	164369	/	1.855	26.636
XDB C18 (150 mm × 4.6 mm, 5 μm)	27.641	249015	1.297	1.869	26.664
DZP					
ZORBAX Eclipse C18 (150 mm × 4.6 mm, 3.5 μm)	31.561	256674	1.222	17.005	30.561
ZORBAX SB C8 (150 mm × 4.6 mm, 3.5 μm)	32.605	188959	1.301	18.859	31.605
ZORBAX SB C8 (150 mm × 4.6 mm, 5 μm)	32.400	56128	2.291	9.762	31.399
ZORBAX SB C18 (150 mm × 4.6 mm, 5 μm)	31.648	92396	1.687	12.151	30.647
XDB C18 (150 mm × 4.6 mm, 5 μm)	31.092	160808	1.210	13.177	30.092

Note: t_R , retention time; n , theoretical plate number; f_s , symmetry factor; R_s : resolution (with previous peak); k , capacity factor; /, could not be obtained.

Table S4 Influence of different mobile phase on the chromatographic parameters of analytes

Mobile phase	t_R (min)	n	f_s	R_s	k
PRM					
100% ethanol-water	16.507	60843	1.158	/	15.507
100% ethanol-15 mM KDP water solution	16.655	60831	1.156	/	15.654
95% ethanol-15 mM KDP water solution	16.815	59166	1.155	/	15.841
85% ethanol-15 mM KDP water solution	19.260	55838	1.122	/	18.261
75% ethanol-15 mM KDP water solution	22.049	50473	1.095	/	21.049
CBZE					
100% ethanol-water	17.951	53904	1.156	3.865	16.951
100% ethanol-15 mM KDP water solution	18.132	26742	0.778	4.300	17.131
95% ethanol-15 mM KDP water solution	17.835	38356	0.855	3.201	16.834
85% ethanol-15 mM KDP water solution	21.513	21341	0.789	5.005	20.513
75% ethanol-15 mM KDP water solution	24.448	70403	0.799	6.383	23.488
MHD					
100% ethanol-water	18.791	54841	1.152	2.694	17.791
100% ethanol-15 mM KDP water solution	/	/	/	/	/
95% ethanol-15 mM KDP water solution	18.430	52533	1.152	1.743	17.429
85% ethanol-15 mM KDP water solution	22.166	58904	1.067	1.391	21.166
75% ethanol-15 mM KDP water solution	25.256	216456	1.166	2.778	24.255
LTG					
100% ethanol-water	19.761	10948	1.682	1.835	18.761
100% ethanol-15 mM KDP water solution	19.088	54819	1.130	2.359	18.008
95% ethanol-15 mM KDP water solution	19.306	52741	1.135	2.665	18.306
85% ethanol-15 mM KDP water solution	22.984	94111	1.112	2.481	21.984
75% ethanol-15 mM KDP water solution	25.69	225381	1.237	1.980	24.691
PHB					
100% ethanol-water	21.032	14383	0.850	1.747	20.032
100% ethanol-15 mM KDP water solution	21.641	55926	1.107	7.662	20.640
95% ethanol-15 mM KDP water solution	21.982	56608	1.092	7.651	20.981
85% ethanol-15 mM KDP water solution	24.692	175112	1.161	6.437	23.691
75% ethanol-15 mM KDP water solution	26.863	254101	1.201	5.453	25.863
OXC					
100% ethanol-water	22.060	59537	1.209	1.914	21.061
100% ethanol-15 mM KDP water solution	22.339	69224	1.142	1.991	21.338
95% ethanol-15 mM KDP water solution	22.696	82337	1.177	2.201	21.695
85% ethanol-15 mM KDP water solution	25.276	252712	1.246	2.710	24.275
75% ethanol-15 mM KDP water solution	27.498	333612	1.389	3.171	26.497
ESLA					
100% ethanol-water	25.039	247644	1.294	10.740	24.039
100% ethanol-15 mM KDP water solution	25.181	267588	1.244	10.682	24.180
95% ethanol-15 mM KDP water solution	25.419	253895	1.305	13.073	24.418
85% ethanol-15 mM KDP water solution	27.203	348756	1.303	10.131	26.203
75% ethanol-15 mM KDP water solution	29.382	356447	1.322	9.683	28.382
CBZ					
100% ethanol-water	26.338	289805	1.274	6.441	25.337
100% ethanol-15 mM KDP water solution	26.450	307694	1.301	5.271	25.451
95% ethanol-15 mM KDP water solution	26.692	271852	1.118	5.993	25.691
85% ethanol-15 mM KDP water solution	28.344	346807	1.347	6.025	27.344
75% ethanol-15 mM KDP water solution	30.882	258582	1.261	6.698	29.882
CZP					
100% ethanol-water	27.641	391921	1.387	2.243	26.641
100% ethanol-15 mM KDP water solution	27.740	442192	1.369	2.452	26.739
95% ethanol-15 mM KDP water solution	28.010	418827	1.131	2.459	27.009
85% ethanol-15 mM KDP water solution	29.644	350324	1.343	2.357	28.643
75% ethanol-15 mM KDP water solution	32.081	185552	1.182	4.392	31.081
DZP					
100% ethanol-water	30.867	268379	1.271	15.914	29.866
100% ethanol-15 mM KDP water solution	31.000	280599	1.259	16.594	30.000
95% ethanol-15 mM KDP water solution	31.561	256674	1.222	17.005	30.561
85% ethanol-15 mM KDP water solution	/	/	/	/	/
75% ethanol-15 mM KDP water solution	/	/	/	/	/

Note: t_R , retention time; n , theoretical plate number; f_s , symmetry factor; R_s : resolution (with previous peak); k , capacity factor; /, could not be obtained.

Table S5 Influence of KDP concentration on the chromatographic parameters of analytes

KDP concentration in water phase	t_R (min)	n	f_s	R_s	k
PRM					
10 mM KDP	17.048	62254	1.159	/	16.047
15 mM KDP	16.815	59166	1.155	/	15.841
25 mM KDP	16.915	63068	1.162	/	15.914
LTG					
10 mM KDP	18.389	28881	0.789	3.916	17.389
15 mM KDP	17.835	38356	0.855	3.201	16.834
25 mM KDP	17.562	49958	1.148	2.138	16.562
CBZE					
10 mM KDP	18.799	54551	/	1.116	17.799
15 mM KDP	18.430	52533	1.152	1.743	17.429
25 mM KDP	18.504	54897	1.118	2.891	17.504
MHD					
10 mM KDP	19.682	55541	1.144	2.693	18.681
15 mM KDP	19.306	52741	1.135	2.665	18.306
25 mM KDP	19.396	54241	1.169	2.756	18.396
PHB					
10 mM KDP	22.342	68539	1.111	7.914	21.342
15 mM KDP	21.982	56608	1.092	7.651	20.981
25 mM KDP	22.126	64211	1.097	8.024	21.125
OXC					
10 mM KDP	23.055	111109	1.144	2.321	22.055
15 mM KDP	22.696	82337	1.177	2.201	21.695
25 mM KDP	22.763	92098	1.196	1.974	21.763
ESLA					
10 mM KDP	25.546	283548	1.333	10.576	24.545
15 mM KDP	25.419	253895	1.305	13.073	24.418
25 mM KDP	25.415	264161	1.275	10.596	24.414
CBZ					
10 mM KDP	26.772	293991	1.331	5.981	25.771
15 mM KDP	26.692	271852	1.118	5.993	25.691
25 mM KDP	26.674	283364	1.266	5.927	25.673
CZP					
10 mM KDP	28.058	397209	1.397	2.381	27.058
15 mM KDP	28.010	418827	1.131	2.459	27.009
25 mM KDP	27.959	408720	1.392	2.392	26.959
DZP					
10 mM KDP	31.679	228377	1.267	16.615	30.679
15 mM KDP	31.561	256674	1.222	17.005	30.561
25 mM KDP	31.489	243444	1.235	16.559	30.489

Note: t_R , retention time; n , theoretical plate number; f_s , symmetry factor; R_s : resolution (with previous peak); k , capacity factor; /, could not be obtained.

Table S6 Influence of column temperature on the chromatographic parameters of analytes

Column temperature	t_R (min)	n	f_s	R_s	k
PRM					
30 °C	16.815	59166	1.155	/	15.841
32 °C	17.157	60099	1.151	/	16.156
35 °C	16.625	64401	1.130	/	15.625
38 °C	16.191	63956	1.135	/	15.190
40 °C	15.885	68989	1.141	/	14.885
LTG					
30 °C	17.835	38356	0.855	3.201	16.834
32 °C	18.337	36865	0.821	3.623	17.336
35 °C	17.125	51346	1.163	1.679	16.125
38 °C	17.392	25492	0.731	3.582	16.391
40 °C	17.048	26669	0.737	3.638	16.048
CBZE					
30 °C	18.430	52533	1.152	1.743	17.429
32 °C	19.098	55287	1.113	2.178	18.097
35 °C	18.349	58700	1.119	4.105	17.438
38 °C	18.114	58158	1.114	2.015	17.113
40 °C	17.779	62060	1.131	2.137	16.779
MHD					
30 °C	19.306	52741	1.135	2.665	18.306
32 °C	19.921	55308	1.146	2.477	18.921
35 °C	19.170	58222	1.134	2.326	18.171
38 °C	18.713	57186	1.118	1.948	17.713
40 °C	18.309	61828	1.129	1.821	17.309
PHB					
30 °C	21.982	56608	1.092	7.651	20.981
32 °C	22.460	70725	1.103	7.532	21.459
35 °C	21.566	58631	1.091	7.091	20.566
38 °C	20.802	58718	1.105	6.365	19.802
40 °C	20.248	61035	1.095	6.231	19.247
OXC					
30 °C	22.696	82337	1.177	2.201	21.695
32 °C	23.277	1187113	1.183	2.703	22.276
35 °C	22.500	73022	1.353	2.728	21.501
38 °C	21.971	60057	1.147	3.343	20.971
40 °C	21.043	57906	1.163	3.395	20.401
ESLA					
30 °C	25.419	253895	1.105	13.073	24.418
32 °C	25.762	291826	1.102	10.757	24.762
35 °C	25.400	287102	1.263	10.962	24.399
38 °C	25.190	264109	1.202	11.532	24.190
40 °C	24.948	254547	1.199	12.795	23.947
CBZ					
30 °C	26.692	271852	1.118	5.993	25.691
32 °C	26.969	301961	1.361	5.064	25.969
35 °C	26.653	306381	1.143	6.014	25.653
38 °C	26.464	297321	1.207	6.101	25.464
40 °C	26.256	299616	1.181	6.426	25.255
CZP					
30 °C	28.010	418827	1.131	2.459	27.009
32 °C	28.208	430841	1.386	2.741	27.207
35 °C	27.896	498321	1.265	3.611	26.896
38 °C	27.726	473620	1.253	4.370	26.725
40 °C	27.529	477954	1.266	5.009	26.528
DZP					
30 °C	31.561	256674	1.222	17.005	30.561
32 °C	31.906	232427	1.269	17.296	30.905
35 °C	31.543	281824	1.188	7.864	30.543
38 °C	31.38	291194	1.151	18.103	30.386
40 °C	31.181	307763	1.173	19.127	30.181

Note: t_R , retention time; n , theoretical plate number; f_s , symmetry factor; R_s : resolution (with previous peak); k , capacity factor; /, could not be obtained.

Table S7 Influences of different solvents on the extraction recoveries of 10 analytes in human serum (n=3, mean $\pm$ SD)

No.	Analyte	Concentration ($\mu\text{g/mL}$)	Extraction recovery (%)				
			100% ethanol	100% ethanol with 0.05% formic acid	100 % acetonitrile	100% acetonitrile with 0.05% formic acid	Ethyl acetate
1	PRM	3	97.88 $\pm$ 1.75	91.39 $\pm$ 0.92**	93.82 $\pm$ 0.91*	95.45 $\pm$ 0.81	98.28 $\pm$ 1.50
		45	96.29 $\pm$ 1.67	95.52 $\pm$ 3.42	94.72 $\pm$ 1.03	95.12 $\pm$ 3.55	97.20 $\pm$ 1.53
2	LTG	2	98.31 $\pm$ 1.54	96.83 $\pm$ 2.79	96.53 $\pm$ 0.21	97.11 $\pm$ 2.02	98.71 $\pm$ 0.40
		30	95.65 $\pm$ 3.36	94.69 $\pm$ 1.42	93.94 $\pm$ 3.08	98.71 $\pm$ 0.60	96.29 $\pm$ 2.44
3	CBZE	0.3	96.22 $\pm$ 3.03	98.06 $\pm$ 2.26	96.71 $\pm$ 0.47	96.62 $\pm$ 2.93	98.39 $\pm$ 0.55
		4.5	96.60 $\pm$ 1.49	97.23 $\pm$ 2.36	96.90 $\pm$ 1.76	97.03 $\pm$ 0.42	95.05 $\pm$ 4.16
4	MHD	2.5	97.54 $\pm$ 3.16	97.00 $\pm$ 1.02	98.42 $\pm$ 1.71	98.33 $\pm$ 1.13	99.16 $\pm$ 0.69
		37.5	96.29 $\pm$ 3.75	95.22 $\pm$ 1.46	95.83 $\pm$ 2.27	96.64 $\pm$ 1.31	95.92 $\pm$ 2.85
5	PHB	5	97.84 $\pm$ 0.82	97.64 $\pm$ 1.83	97.39 $\pm$ 0.52	96.70 $\pm$ 2.84	96.05 $\pm$ 2.79
		75	96.77 $\pm$ 3.80	95.47 $\pm$ 1.98	96.73 $\pm$ 1.07	95.87 $\pm$ 1.24	93.37 $\pm$ 3.24
6	OXC	5	96.28 $\pm$ 3.18	94.55 $\pm$ 1.15	95.84 $\pm$ 2.18	93.05 $\pm$ 2.34	92.95 $\pm$ 2.21
		75	97.10 $\pm$ 2.07	93.04 $\pm$ 2.71	93.07 $\pm$ 1.34	94.89 $\pm$ 3.80	96.27 $\pm$ 4.26
7	ELSA	5	96.95 $\pm$ 2.69	96.86 $\pm$ 2.52	92.42 $\pm$ 0.31*	97.59 $\pm$ 2.36	99.06 $\pm$ 0.65
		75	98.85 $\pm$ 0.80	99.02 $\pm$ 1.11	99.20 $\pm$ 0.49	97.77 $\pm$ 1.32	98.99 $\pm$ 0.66
8	CBZ	3	98.65 $\pm$ 1.35	96.42 $\pm$ 0.47	96.21 $\pm$ 0.58*	94.73 $\pm$ 1.07*	97.33 $\pm$ 1.71
		45	97.65 $\pm$ 2.83	97.78 $\pm$ 0.62	97.99 $\pm$ 1.33	97.36 $\pm$ 2.32	98.97 $\pm$ 0.98
9	CZP	1	95.79 $\pm$ 4.80	93.40 $\pm$ 1.07	93.16 $\pm$ 2.36	92.56 $\pm$ 3.31	97.90 $\pm$ 1.88
		15	94.32 $\pm$ 3.08	96.36 $\pm$ 3.36	95.33 $\pm$ 1.01	95.77 $\pm$ 2.37	95.16 $\pm$ 1.84
10	DZP	1	95.85 $\pm$ 2.41	97.03 $\pm$ 2.01	93.97 $\pm$ 3.20	96.09 $\pm$ 3.15	92.81 $\pm$ 1.10
		15	98.23 $\pm$ 0.69	96.99 $\pm$ 3.81	93.87 $\pm$ 0.84**	95.60 $\pm$ 4.80	97.20 $\pm$ 0.79

*P<0.05 or **P<0.01 vs 100 % ethanol.

Table S8 Dilution integrity of 10 analytes in human serum (Mean $\pm$ SD, n=5)

Analyte	Nominal concentration after dilution ($\mu\text{g/mL}$)	Found ($\mu\text{g/mL}$)	Accuracy (%)	Precision (RSD%)
PRM	3	2.74 $\pm$ 0.04	91.41 $\pm$ 1.25	1.4
	45	42.87 $\pm$ 0.49	95.28 $\pm$ 1.10	1.2
LTG	2	1.83 $\pm$ 0.06	91.69 $\pm$ 3.04	3.3
	30	29.01 $\pm$ 0.67	96.69 $\pm$ 2.23	2.3
CBZE	0.3	0.27 $\pm$ 0.01	90.69 $\pm$ 4.77	5.3
	4.5	4.38 $\pm$ 0.03	97.34 $\pm$ 0.74	0.8
MHD	2.5	2.40 $\pm$ 0.06	95.83 $\pm$ 2.26	2.4
	37.5	37.24 $\pm$ 0.12	99.32 $\pm$ 0.33	0.3
PHB	5	4.81 $\pm$ 0.05	96.3 $\pm$ 0.91	0.9
	75	73.52 $\pm$ 0.22	98.03 $\pm$ 0.29	0.3
OXC	5	4.79 $\pm$ 0.12	95.87 $\pm$ 2.31	2.4
	75	74.08 $\pm$ 0.25	98.77 $\pm$ 0.33	0.3
ESLA	5	4.89 $\pm$ 0.03	97.74 $\pm$ 0.57	0.6
	75	74.27 $\pm$ 0.39	99.02 $\pm$ 0.52	0.5
CBZ	3	2.77 $\pm$ 0.06	92.38 $\pm$ 1.88	2.0
	45	43.84 $\pm$ 0.49	97.42 $\pm$ 1.09	1.1
CZP	1	0.95 $\pm$ 0.03	95.11 $\pm$ 3.12	3.3
	15	14.47 $\pm$ 0.11	96.46 $\pm$ 0.75	0.8
DZP	1	0.95 $\pm$ 0.05	94.79 $\pm$ 4.69	4.9
	15	14.51 $\pm$ 0.14	96.76 $\pm$ 0.94	1.0

Table S9 Incurred sample analysis of real serum containing PHB

Original detected concentration (mg/L)	Re-detected concentration (mg/L)	Difference	Mean	Difference %
6.33	5.78	-0.55	6.06	-9.08
15.19	14.30	-0.89	14.75	-6.04
3.98	3.66	-0.32	3.82	-8.38
3.26	3.58	0.32	3.42	9.36
3.44	3.03	-0.41	3.24	-12.67
2.09	2.17	0.08	2.13	3.76
4.35	4.12	-0.23	4.24	-5.43
22.14	20.32	-1.82	21.23	-8.57
2.79	2.67	-0.12	2.73	-4.40
3.79	3.45	-0.34	3.62	-9.39

Table S10 Detailed parameters used in AGREEprep tool

Sample preparation	Hazardous materials	Materials renewability	Waste volume (mL)	Sample volume (μL)	Prepared samples	Steps	Automation	Energy consumption	Instrument	Safety	Reference*
ex situ	without	unsustainable or non-renewable	30.55	900	40/h	≤2	Semi-automation	≤0.1KW/h	HPLC	1	23
ex situ	without	unsustainable or non-renewable	12	100	20/h	5	Semi-automation	≤0.1KW/h	HPLC	3	24
ex situ	without	unsustainable or non-renewable	15	200	40/h	≤2	Semi-automation	≤0.1KW/h	HPLC	2	25
ex situ	without	unsustainable or non-renewable	20	200	40/h	≤2	Semi-automation	≤0.1KW/h	HPLC	2	26
ex situ	without	unsustainable or non-renewable	18	2000	20/h	4	Semi-automation	≤0.1KWh/	HPLC	10	27
ex situ	without	unsustainable or non-renewable	17.5	100	40/h	3	Semi-automation	≤0.1KW/h	HPLC	0	This study

*The reference numbers presented in this table are identical with that in main text (manuscript).

Table S11 Detailed parameters used in AGREE tool

Sample	Flow (mL/min)	Run time (min)	Sample preparation	Sample volume (μL)	Instrumental position	Number of steps	Automation	Derivatization	Waste (mL)	Analyte numbers/h	Sample numbers /h	Energy consumption	Hazardous material	Toxic reagents	Threats	Reference*
Serum	1.3	23.5	Off-line	900	Off-line	≤3	Semi-automation	No	30.55	11	2	≤0.1KW/h	Non-bio-based sources	Yes	Flammable	23
Plasma	1.0	12	Off-line	100	Off-line	5	Semi-automation	No	12	2	5	≤0.1KW/h	Non-bio-based sources	Yes	Flammable	24
Plasma	1.0	15	Off-line	200	Off-line	≤3	Semi-automation	No	15	3	4	≤0.1KW/h	Non-bio-based sources	Yes	Flammable	25
Plasma	1.0	20	Off-line	200	Off-line	≤3	Semi-automation	No	20	2	3	≤0.1KW/h	Non-bio-based sources	Yes	Flammable	26
Plasma	1.0	18	Off-line	2000	Off-line	4	Semi-automation	No	18	3	3	≤0.1KW/h	Non-bio-based sources	Yes	Flammable	27
Serum	0.5	35	Off-line	100	Off-line	≤3	Semi-automation	No	17.5	10	2	≤0.1KW/h	Bio-based source	No	Flammable	This study

*The reference numbers presented in this table are identical with that in main text (manuscript).

Table S12 Detailed parameters used in GAPI tool

Method type	Sample							Solvents/reagents					Instrument			Reference*
	Collection	Preservation	Transportation	Storage	Preparation	Preparation scale	Solvents used	Additional treatment	Amount (mL)	Toxicity (NFPA score)	Safety (NFPA score)	Energy consumption	Occupational hazard	Waste volume (mL)	Waste recycling	
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Simple step	micro	Non-green	No	10-100	2	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	23
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Extraction step	micro	Non-green	No	10-100	2	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	24
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Simple step	micro	Non-green	No	10-100	1	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	25
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Simple step	micro	Non-green	No	10-100	1	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	26
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Extraction step	micro	Non-green	No	10-100	2	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	27
Quantification	On-line	No physical or chemical preservation	No	Normal condition	Simple step	micro	Green	No	10-100	2	3	≤0.1KW/h	Hermetic sealing	> 10	Recycling	This study

*The reference numbers presented in this table are identical with that in main text (manuscript).

Table S13 Detailed parameters used in BAGI tool

Analysis type	Analyte numbers	Instrumentation	Sample numbers	Sample preparation scale	Analyzed samples/h	Reagents and materials	Pre-concentration	Automation	Sample amount (μL)	Reference*
Quantitative and confirmatory	6-15 (same chemical class)	HPLC-DAD	13-95	Protein precipitation in one-step	2	Common commercially available	Yes	Semi-automation	900	23
Quantitative and confirmatory	2-5 (same chemical class)	HPLC-DAD	13-95	Liquid-liquid extraction in more steps	5	Common commercially available	Yes	Semi-automation	100	24
Quantitative and confirmatory	2-5 (same chemical class)	HPLC-DAD	13-95	Protein precipitation in one-step	4	Common commercially available	No	Semi-automation	200	25
Quantitative and confirmatory	2-5 (same chemical class)	HPLC-DAD	13-95	Protein precipitation in one-step	3	Common commercially available	No	Semi-automation	200	26
Quantitative and confirmatory	2-5 (same chemical class)	HPLC-DAD	13-95	Solid-phase micro-extraction in more step	3	Non-common commercially available	Yes	Semi-automation	2000	27
Quantitative and confirmatory	6-15 (same chemical class)	HPLC-DAD	13-95	Protein precipitation in one-step	2	Common commercially available	Yes	Semi-automation	100	This study

*The reference numbers presented in this table are identical with that in main text (manuscript).

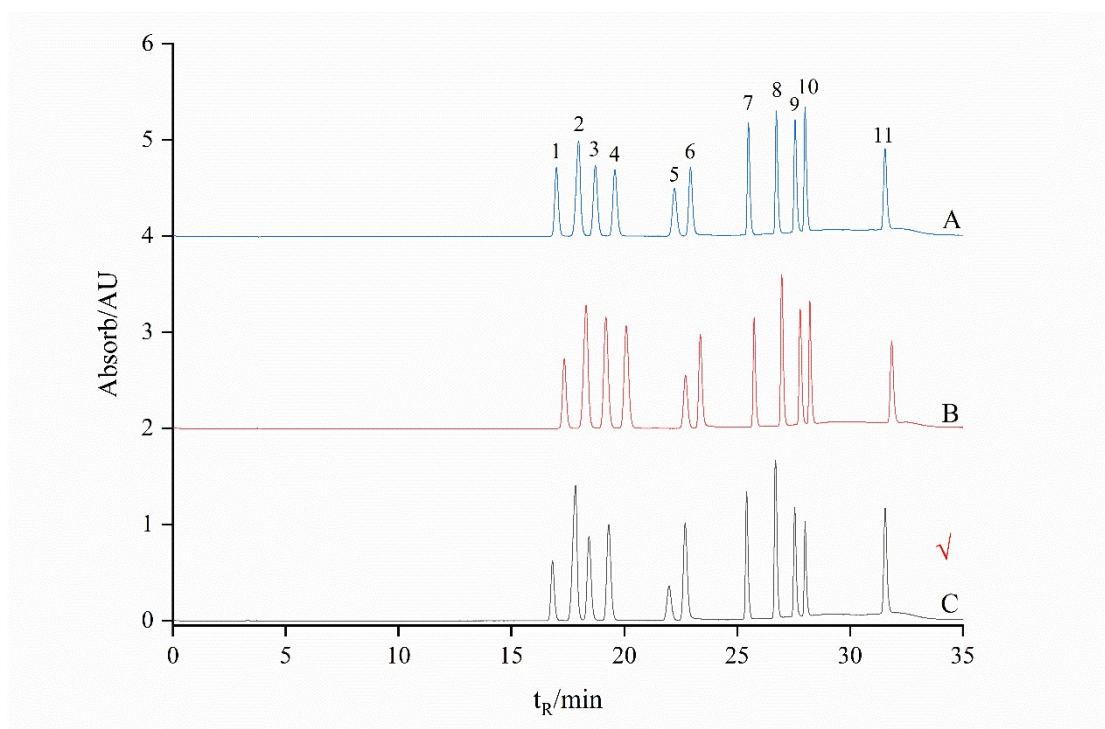


Fig. S1 Representative chromatogram of 10 analytes and IS dissolved in 100 % ethanol (A), ethanol-water (95:5, v/v) (B), and ethanol-water (75:25, v/v) (C). 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.

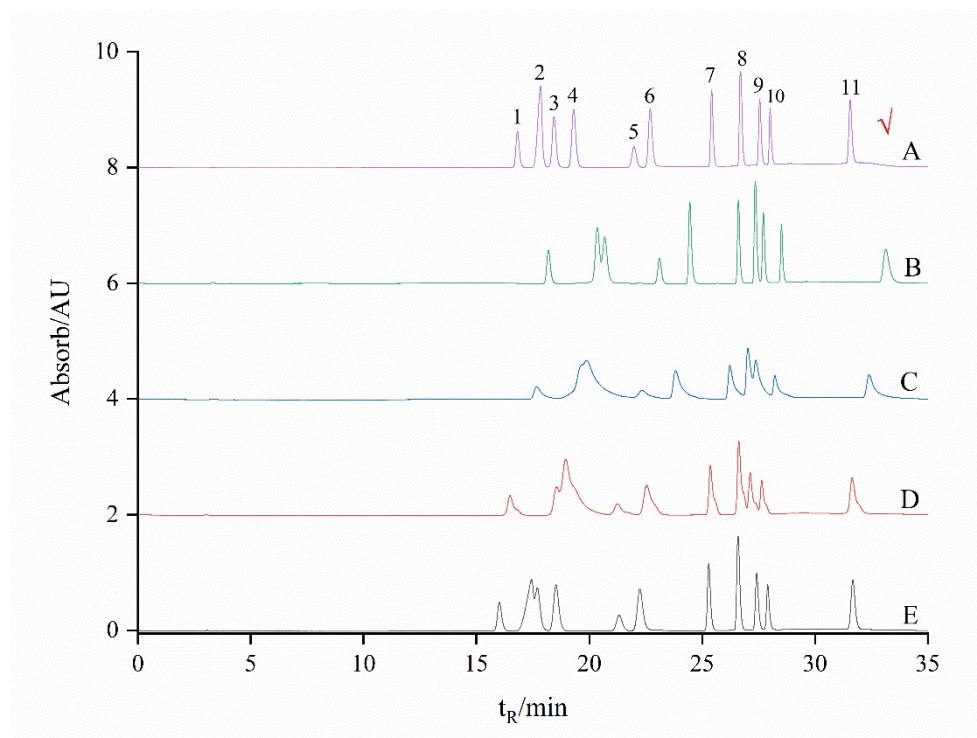


Fig. S2 Representative chromatogram of 10 analytes and IS separated on Agilent ZORBAX Eclipse C₁₈ (150 mm × 4.6 mm, 3.5 μm) (A), ZORBAX SB C₈ (150 mm × 4.6 mm, 3.5 μm) (B), ZORBAX SB C₈ (150 mm × 4.6 mm, 5 μm) (C), ZORBAX SB C₁₈ (150 mm × 4.6 mm, 5 μm) (D), and XDB C₁₈ (150 mm × 4.6 mm, 5 μm) (E). 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ; 10. CZP (IS); 11. DZP.

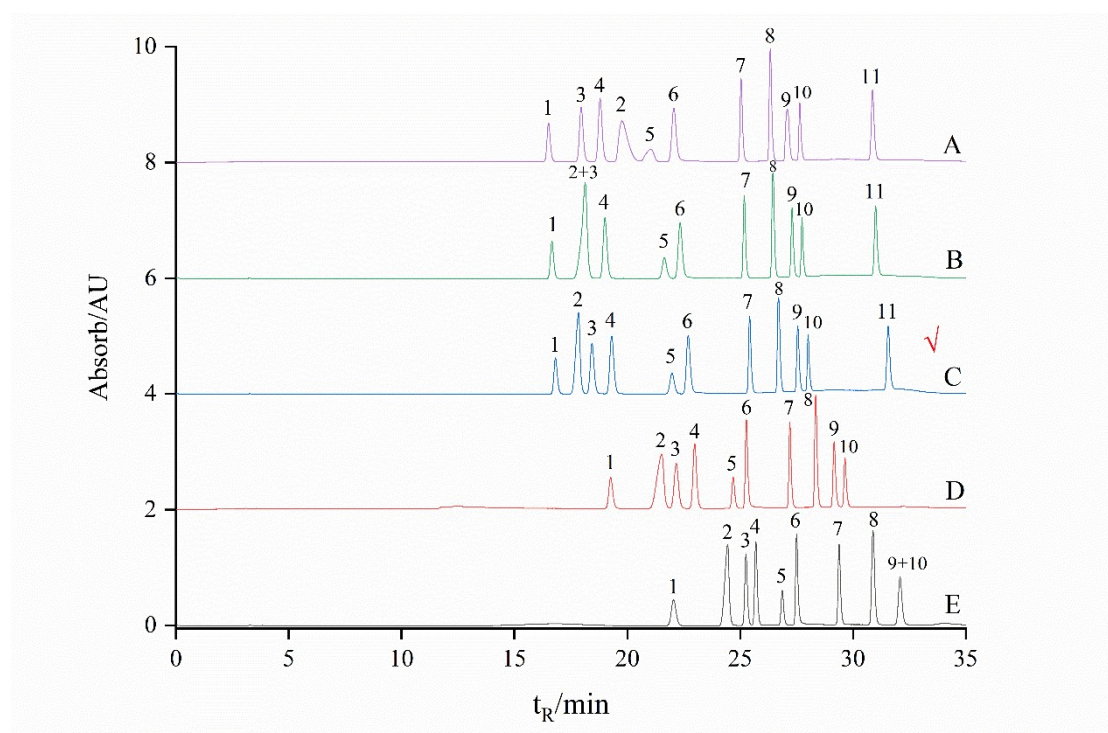


Fig. S3 Representative chromatogram of 10 analytes and IS separated with 100% ethanol-water (A), 100% ethanol-15 mM potassium dihydrogen phosphate (KDP) water solution (B), 95% ethanol-15 mM KDP water solution (C), 85% ethanol-15 mM KDP water solution (D), and 75% ethanol-15 mM KDP water solution (E) as mobile phase, respectively. 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.

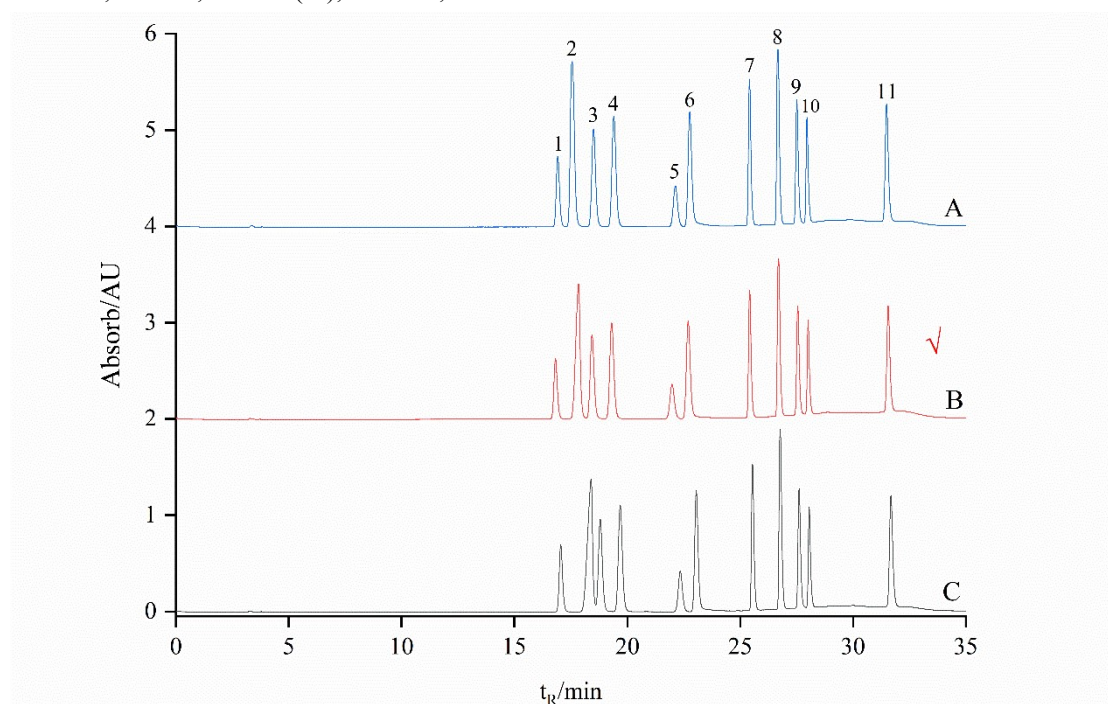


Fig. S4 Representative chromatogram of 10 analytes and IS separated with 95% ethanol-10 mM KDP water solution (A), 95% ethanol-15 mM KDP water solution (B), 95% ethanol-20 mM KDP water solution (C) as mobile phase, respectively. 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.

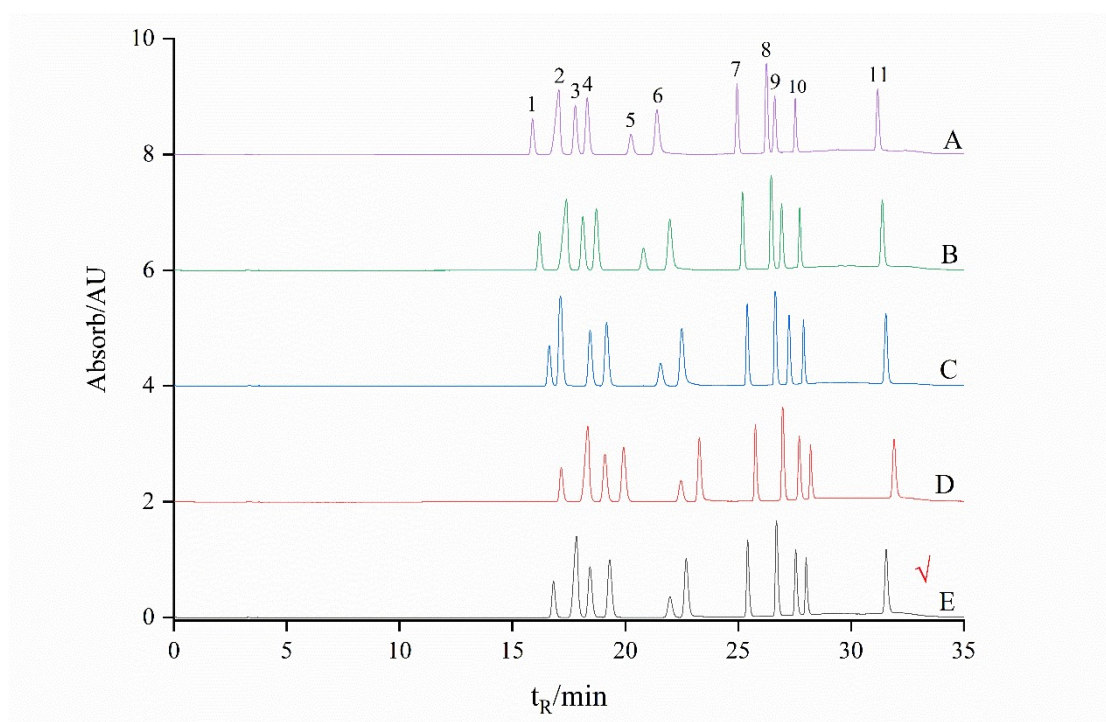


Fig. S5 Representative chromatogram of 10 analytes and IS separated under column temperature 30 °C (A), 32 °C (B), 35 °C (C), 38 °C (D) and 40 °C (E). 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.

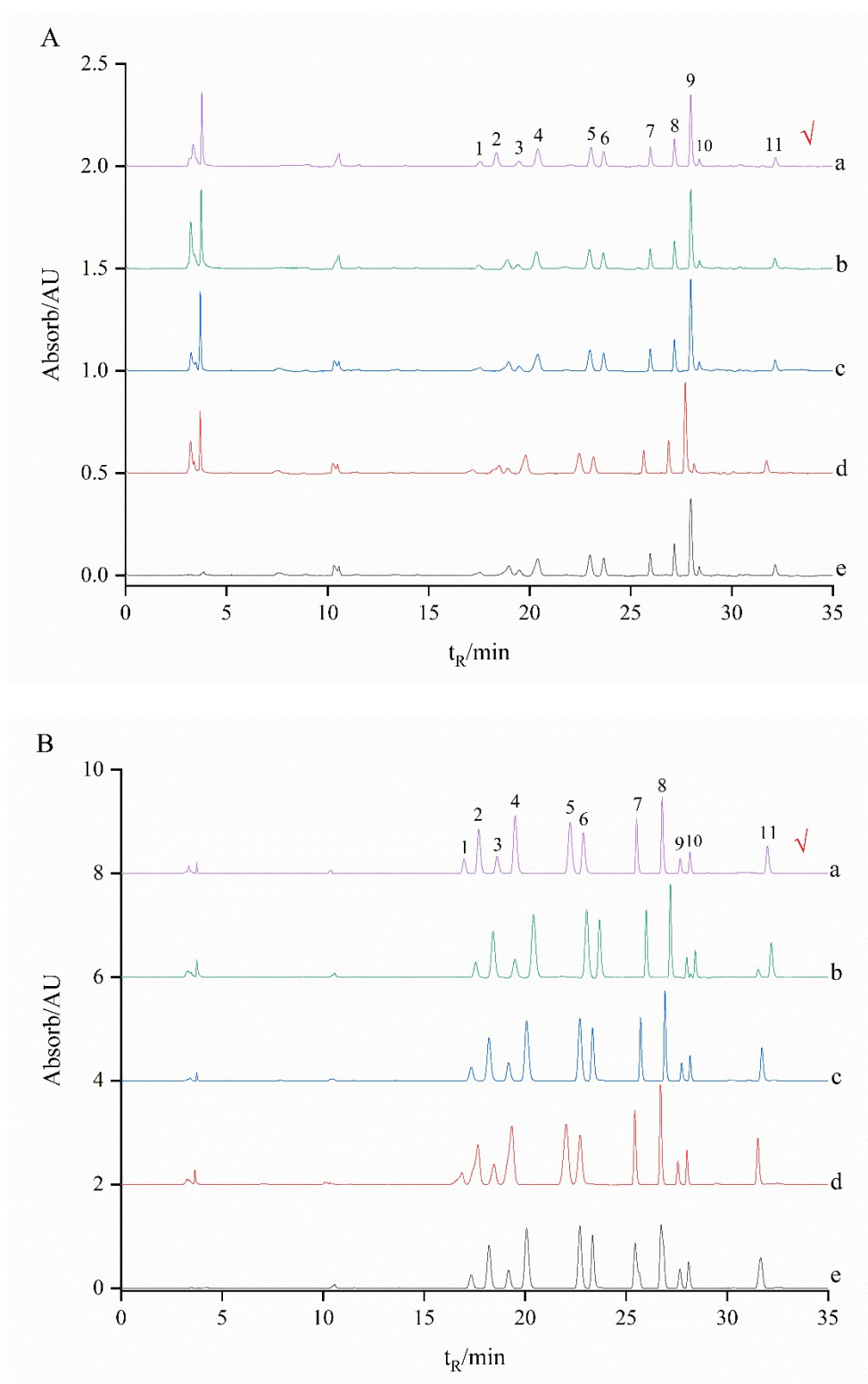
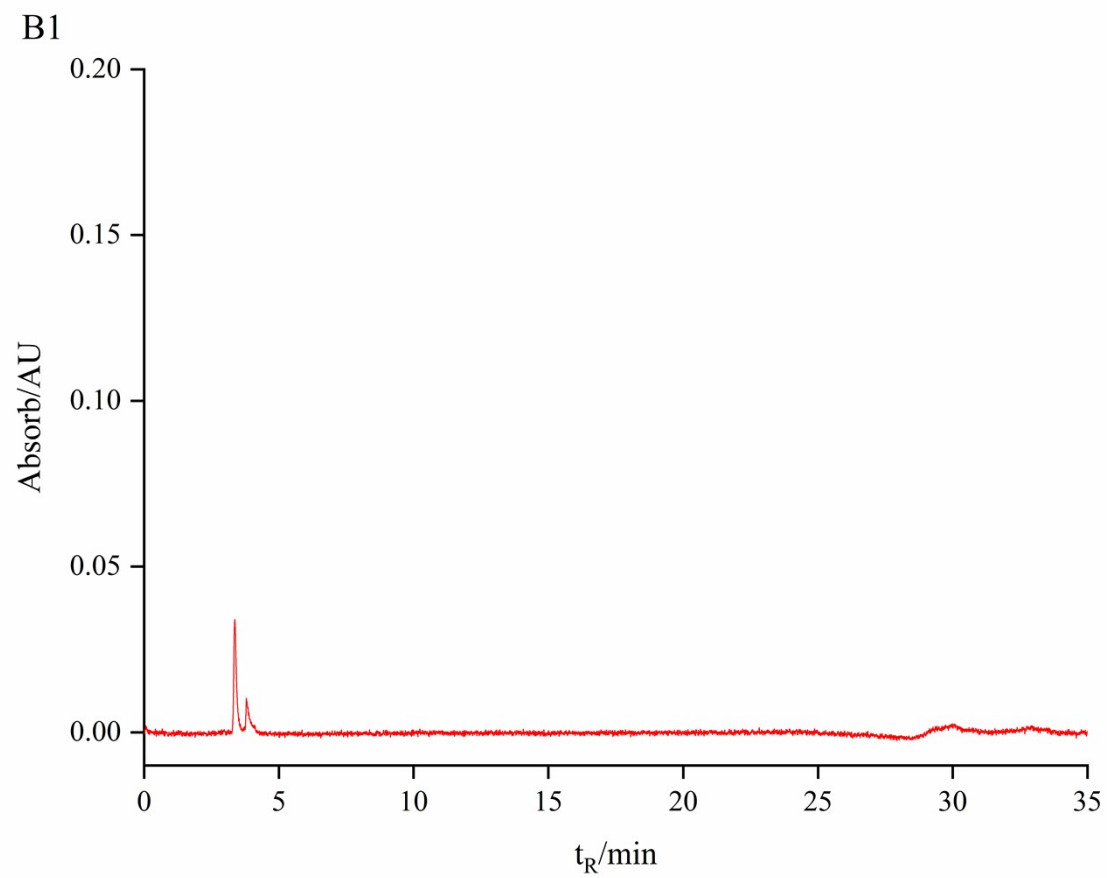
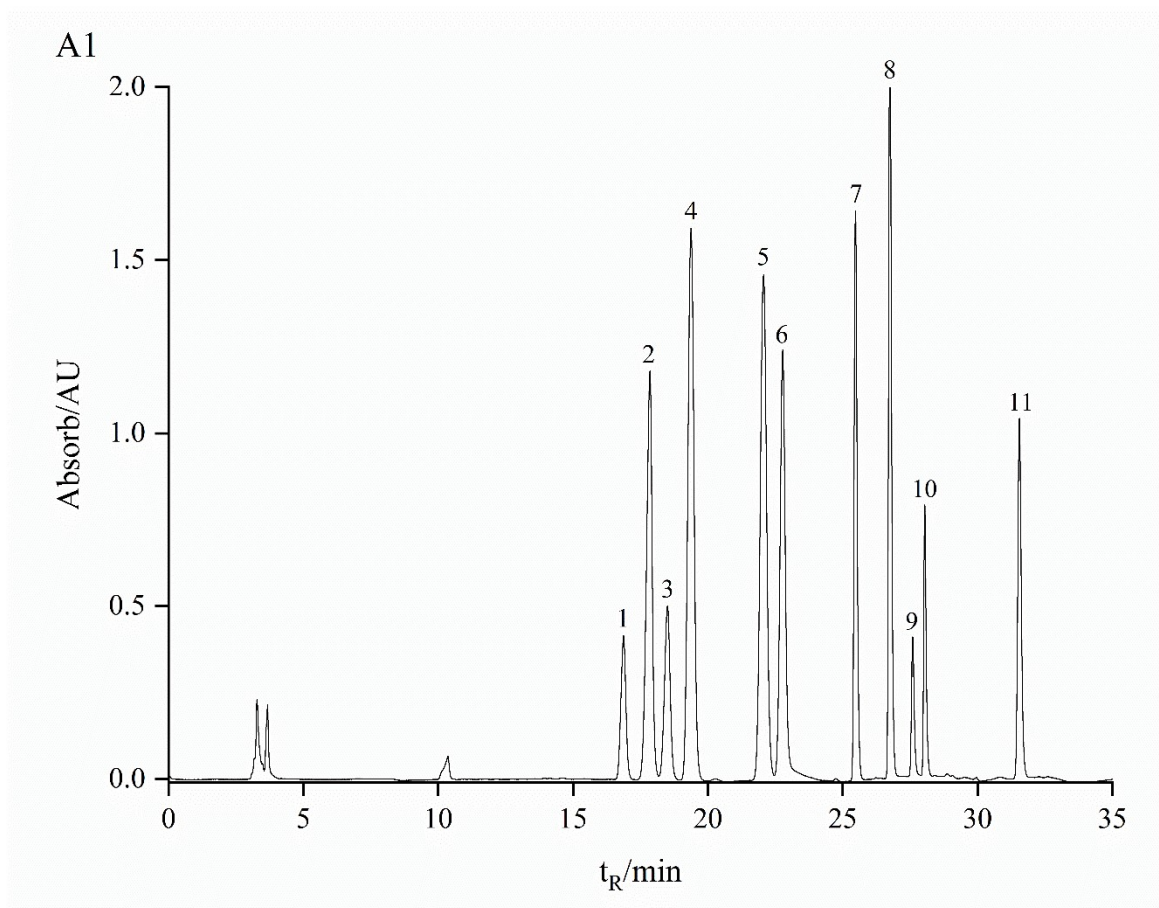
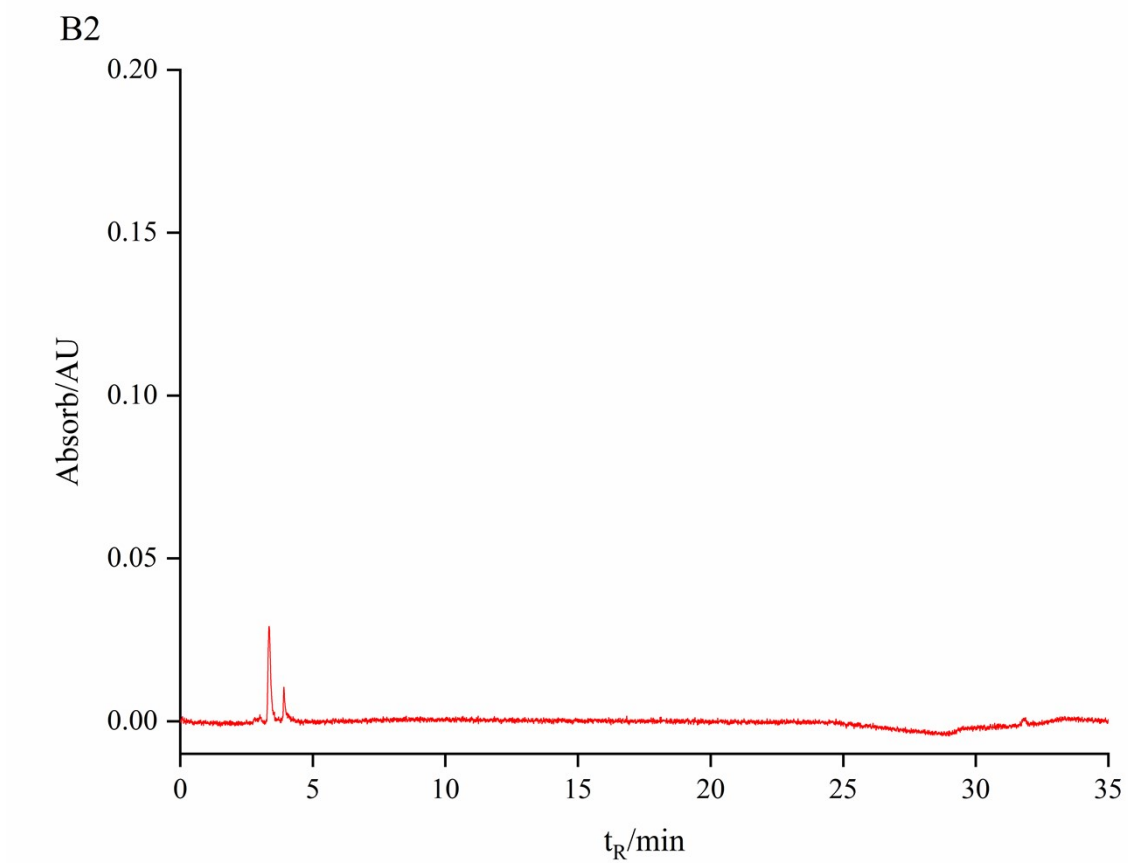
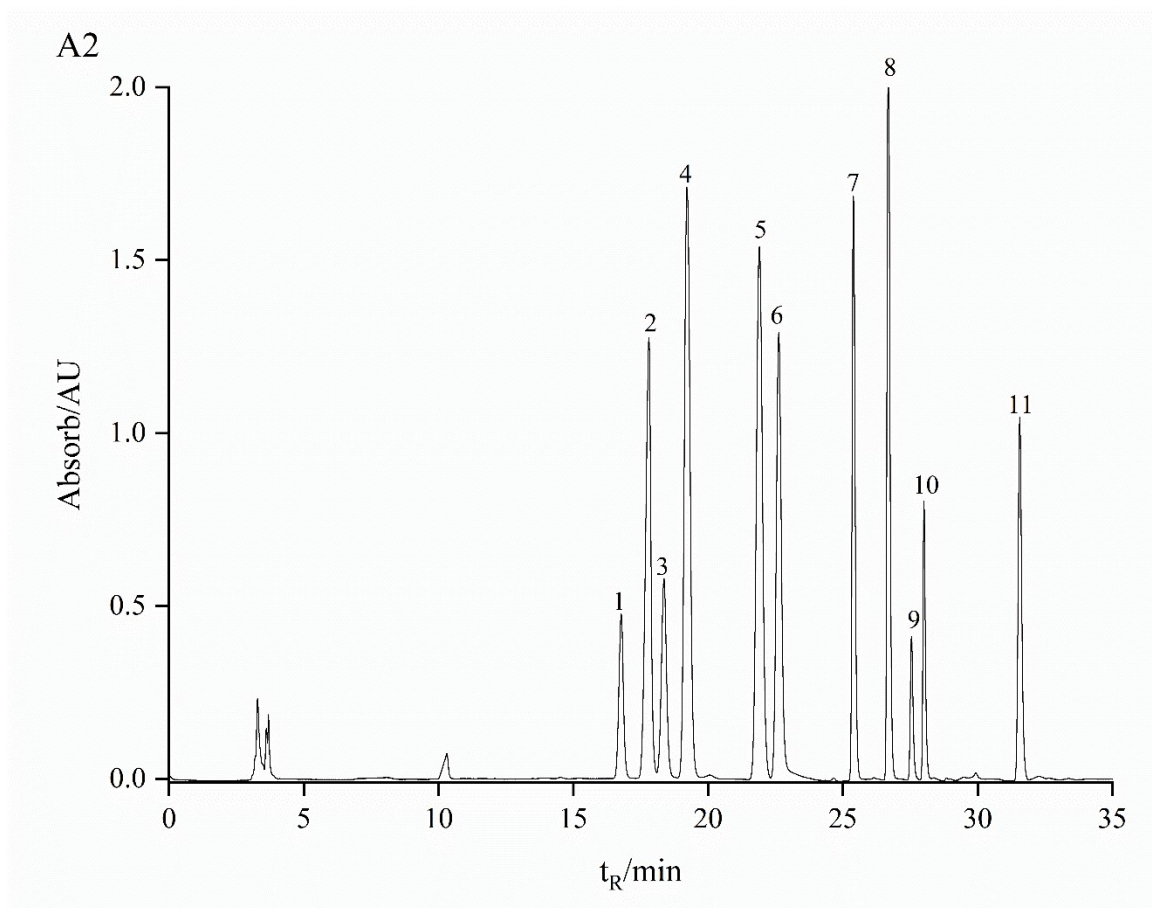
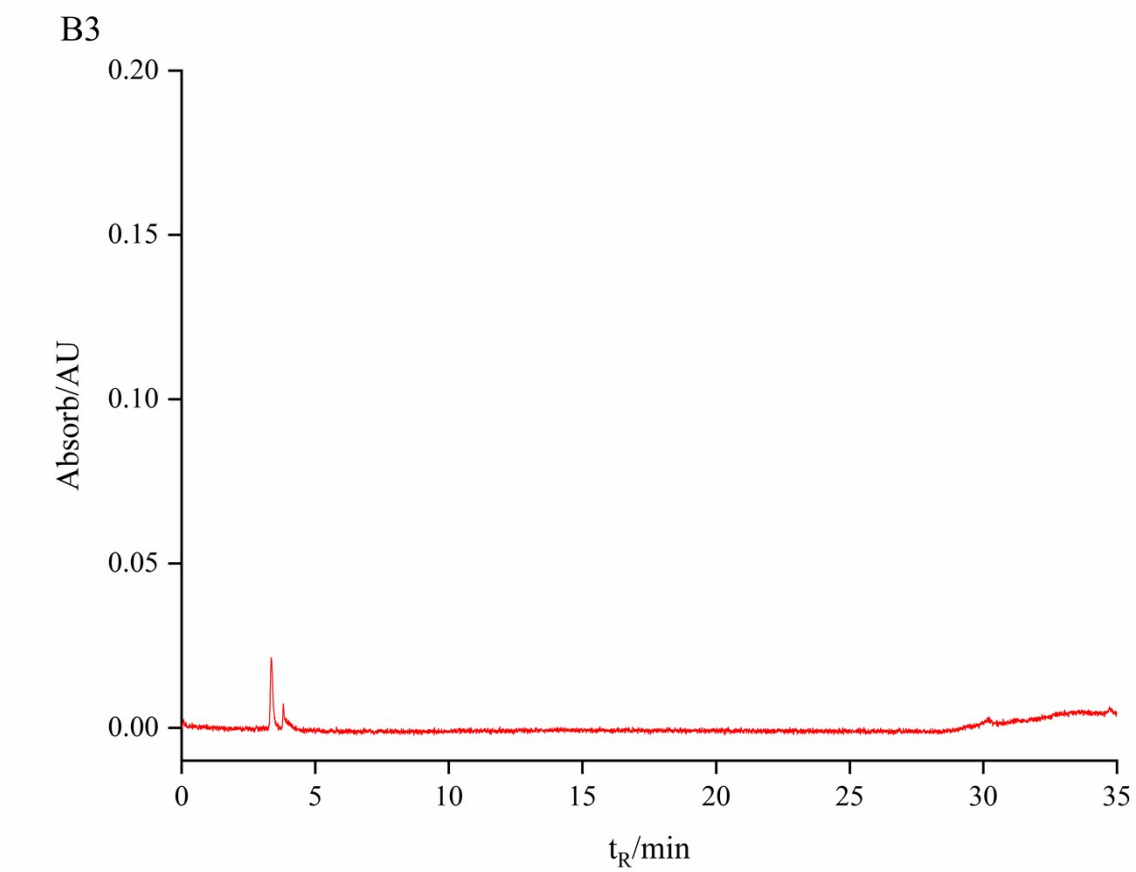
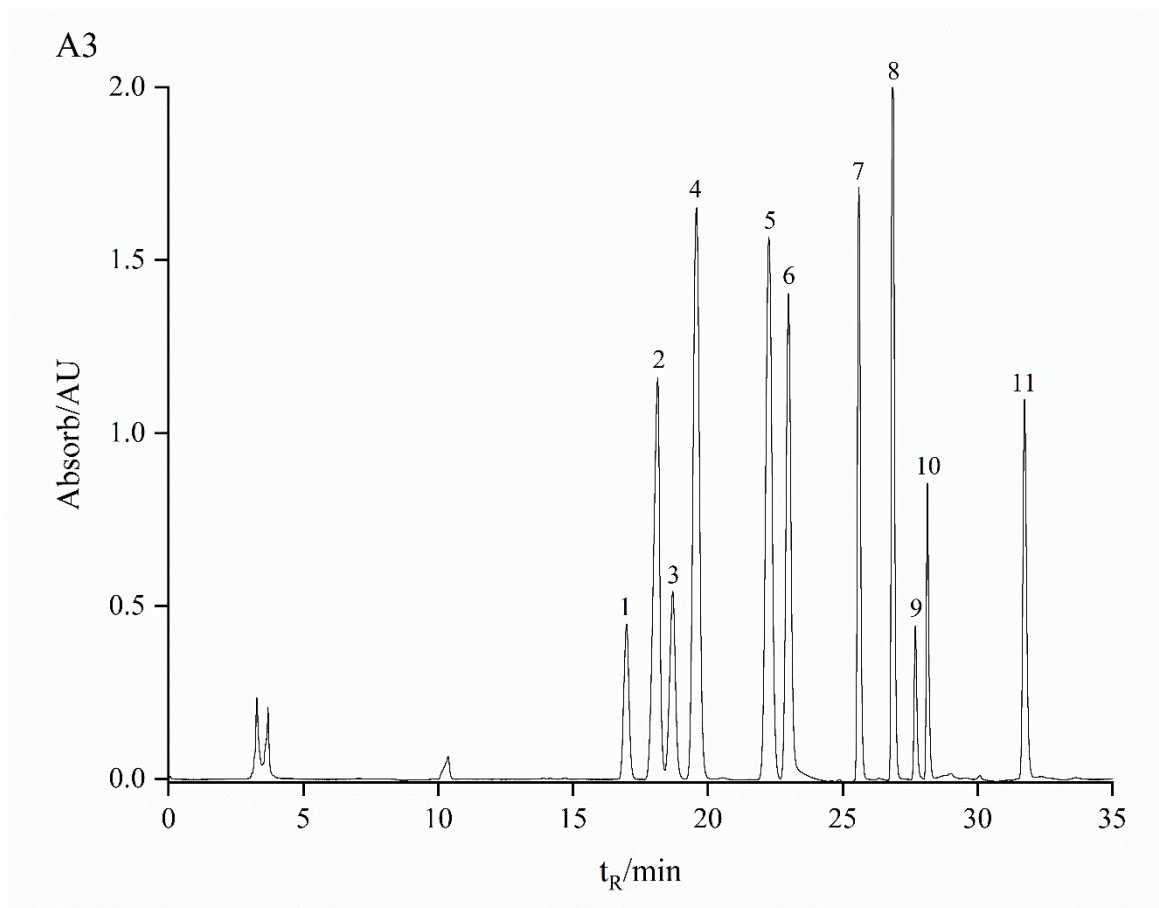
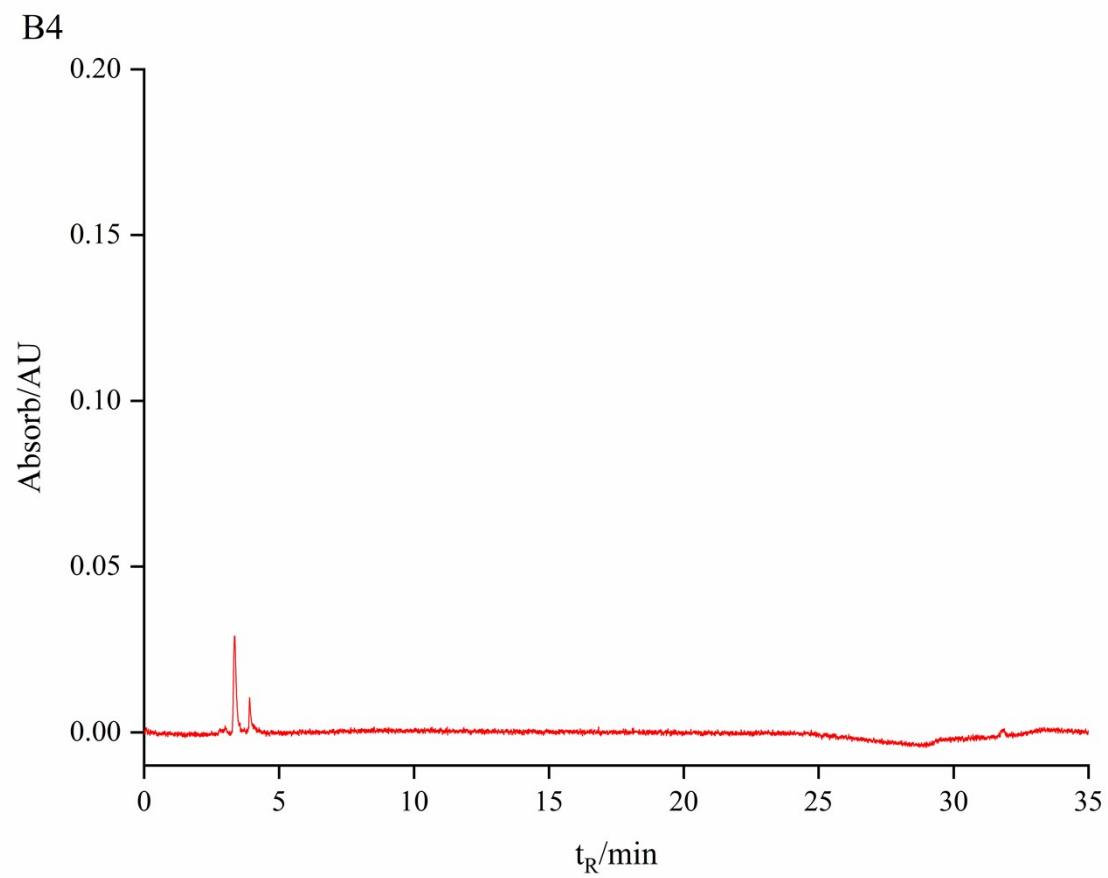
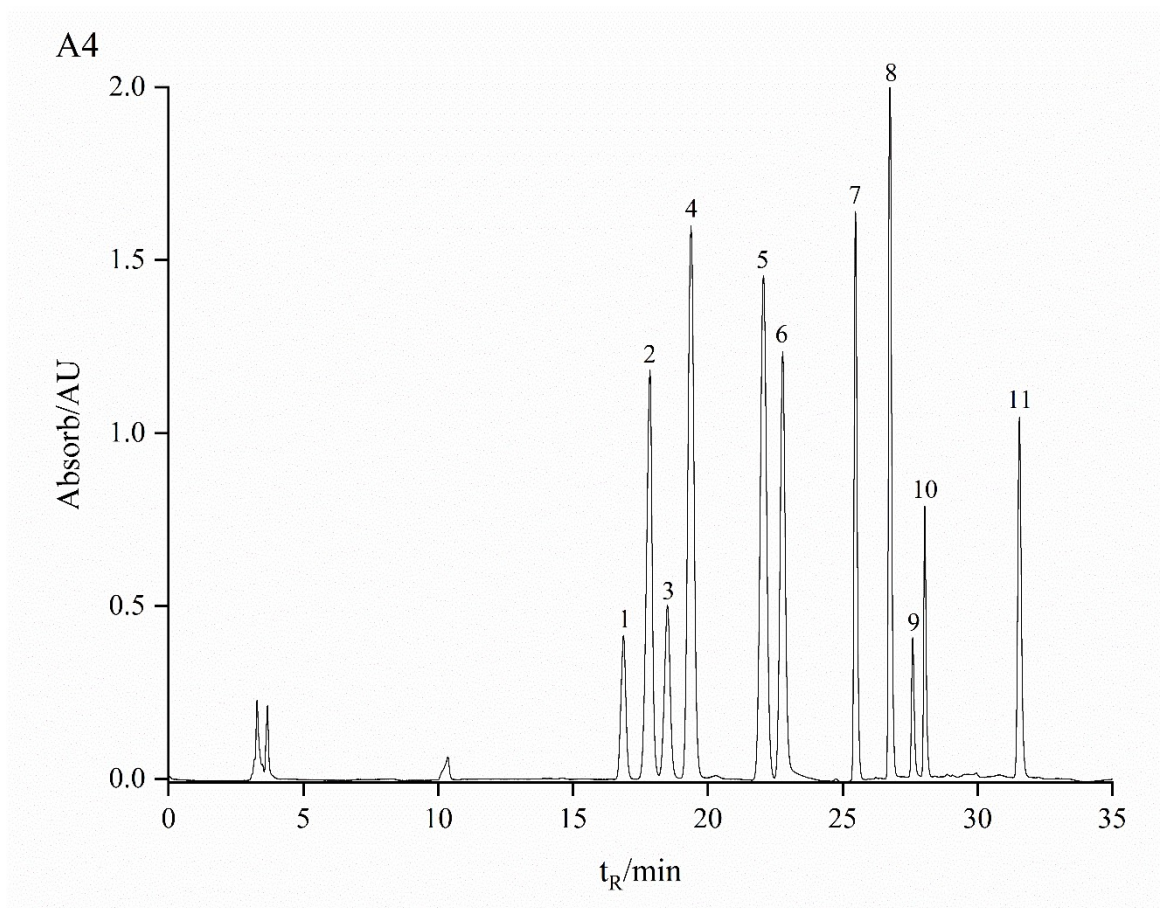


Fig. S6. Representative chromatogram of blank serum spiked with 10 analytes and IS at low (A) or high (B) concentration levels treated with 100 % ethanol (a), 100 % ethanol with 0.05% formic acid (b), 100 % acetonitrile (c), 100 % acetonitrile with 0.05 % formic acid (d), and ethyl acetate (e), respectively. 1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.









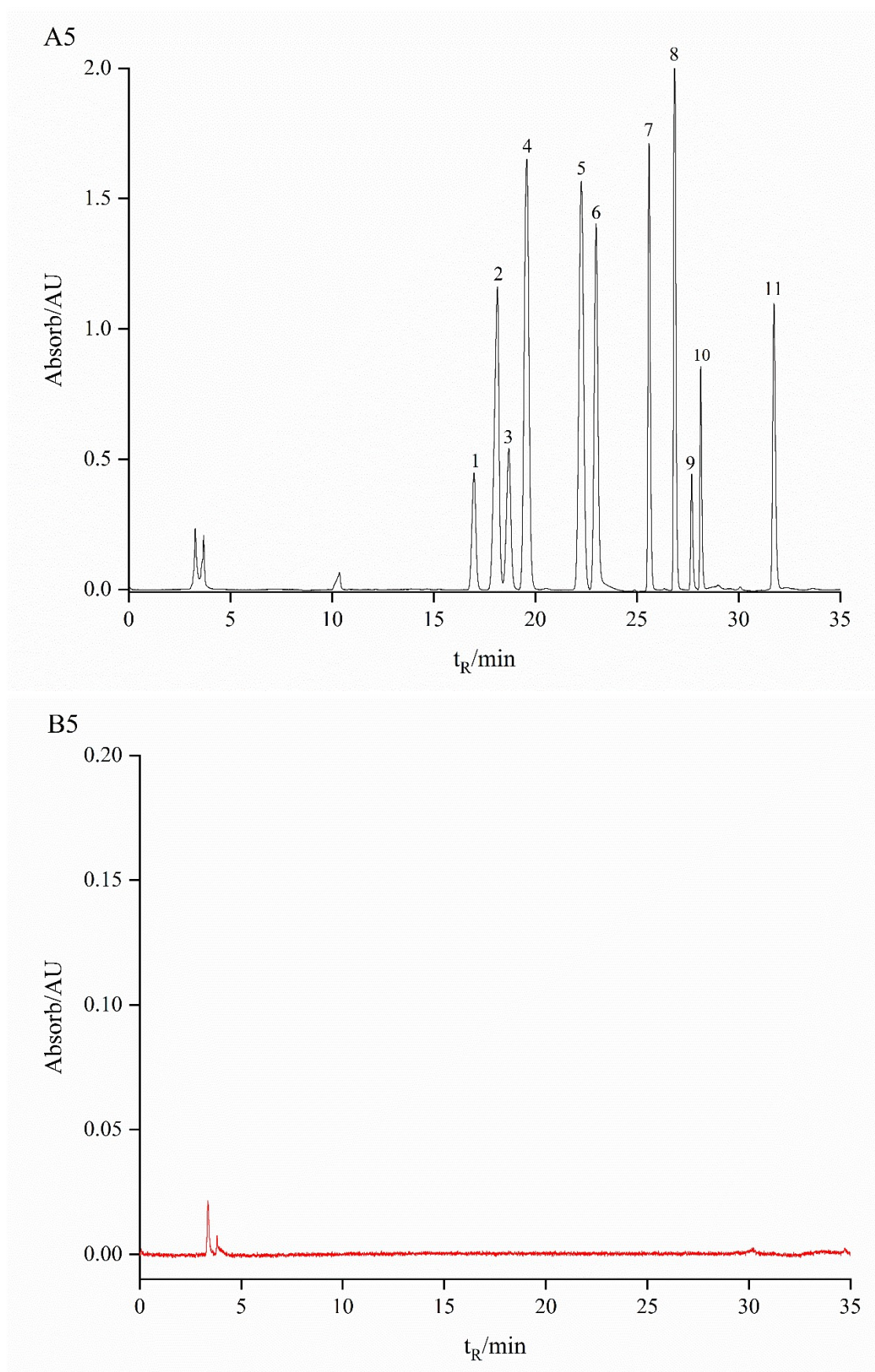


Fig. S7. Chromatograms of five replicates of blank serum (B) sequentially after injecting an ULOQ sample (A).
1. PRM; 2. LTG; 3. CBZE; 4. MHD; 5. PHB; 6. OXC; 7. ESLA; 8. CBZ; 9. CLZ (IS); 10. CZP; 11. DZP.