Supplementary Information

Finding specific peaks (markers) using fuzzy divisive hierarchical associative-clustering based on the chromatographic profiles of medicinal plants extracts obtained at various detection wavelengths

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Table S1 Name and total radical scavenging capacity (RSC %) determined by DPPH• assay of the investigated hydroalcoholic medicinal plant extracts

No.	Name	Scientific name	RSC %	Antioxidant activity
1	Blueberry	*Vaccinium myrtillus*	46.71	**High**
2	Lingon berry	*Vaccinium vitis-idaea*	36.58	**High**
3	Rosemary	*Rosmarinus officinalis*	31.01	**High**
4	Hoary willowherb	*Epilobium parviflorum*	29.82	**High**
5	Lady's mantel	*Alchemilla vulgaris*	29.61	**High**
6	Quaking aspen	*Plopus nigra*	27.97	**High**
7	Lemon balm	*Melissa officinalis*	27.36	**High**
8	Sage	*Salvia officinalis*	27.36	**High**
9	Silver brich	*Betula pendula*	26.27	**High**
10	Saint John's wort	*Hypericum perforatum*	21.12	**Moderate**
11	Hawthorn	*Crataegus monogyma*	18.74	**Moderate**
12	Breckland thyme	*Thymus serpyllum*	15.48	**Moderate**
13	Burdock	*Arctium lappa*	13.98	**Moderate**
14	Great celandine	*Caelidonium majus*	12.86	**Moderate**
15	Lady's bedstraw	*Galium verum*	11.16	**Moderate**
16	Common juniper	*Juniperus communis*	10.13	**Moderate**
17	Yarrow	*Achillea millefolium*	9.45	**Moderate**
18	Spinycockle-bur	*Xanthium spinosum*	9.44	**Moderate**
19	Lavender	*Lavandula augustifolia*	8.93	**Moderate**
20	Artichoke	*Cynara scolymus*	7.42	**Moderate**
21	Liquorice	*Glycyrrhiza glabra*	4.93	**Low**
22	Gentian	*Gentiana asclepiadea*	4.46	**Low**
23	Echinacea	*Echinacea purpurea*	4.38	**Low**
24	Comfrey	*Symphytum officinale*	4.32	**Low**
25	Milk thistle	*Silybum marianum*	3.75	**Low**
26	Nettle	*Urtica dioica*	3.69	**Low**
27	Heart's ease	*Viola tricolor*	3.06	**Low**
28	Motherwort	*Leonurus cardiaca*	2.78	**Low**
29	Ginger	*Zingiber officinale*	2.26	**Low**
30	Valerian	*Valeriana officinalis*	2.09	**Low**
31	Shepherd's purse	*Capsella bursa-pastoris*	1.78	**Low**
32	Horsetail	*Equisetum arvense*	1.70	**Low**
33	Dill	*Anethum graveolens*	1.62	**Low**
34	Garlic	*Allium sativum*	1.45	**Low**
35	Mistletoe	*Viscum album*	1.20	**Low**
36	Elder	*Sambuctus nigra*	1.19	**Low**

37	Chili pepper	*Capsicum annuum*	1.05	**Low**
38	Sweet flag	*Acorus calamus*	1.00	**Low**
39	Hogweed	*Heracleum sphondylium*	0.68	**Low**
40	Wolf's-foot clubmoss	*Lycopodium clavatum*	0.37	**Low**
41	Celery	*Apium graveolens*	0.25	**Low**
42	Ramson	*Allium ursinum*	0.22	**Low**

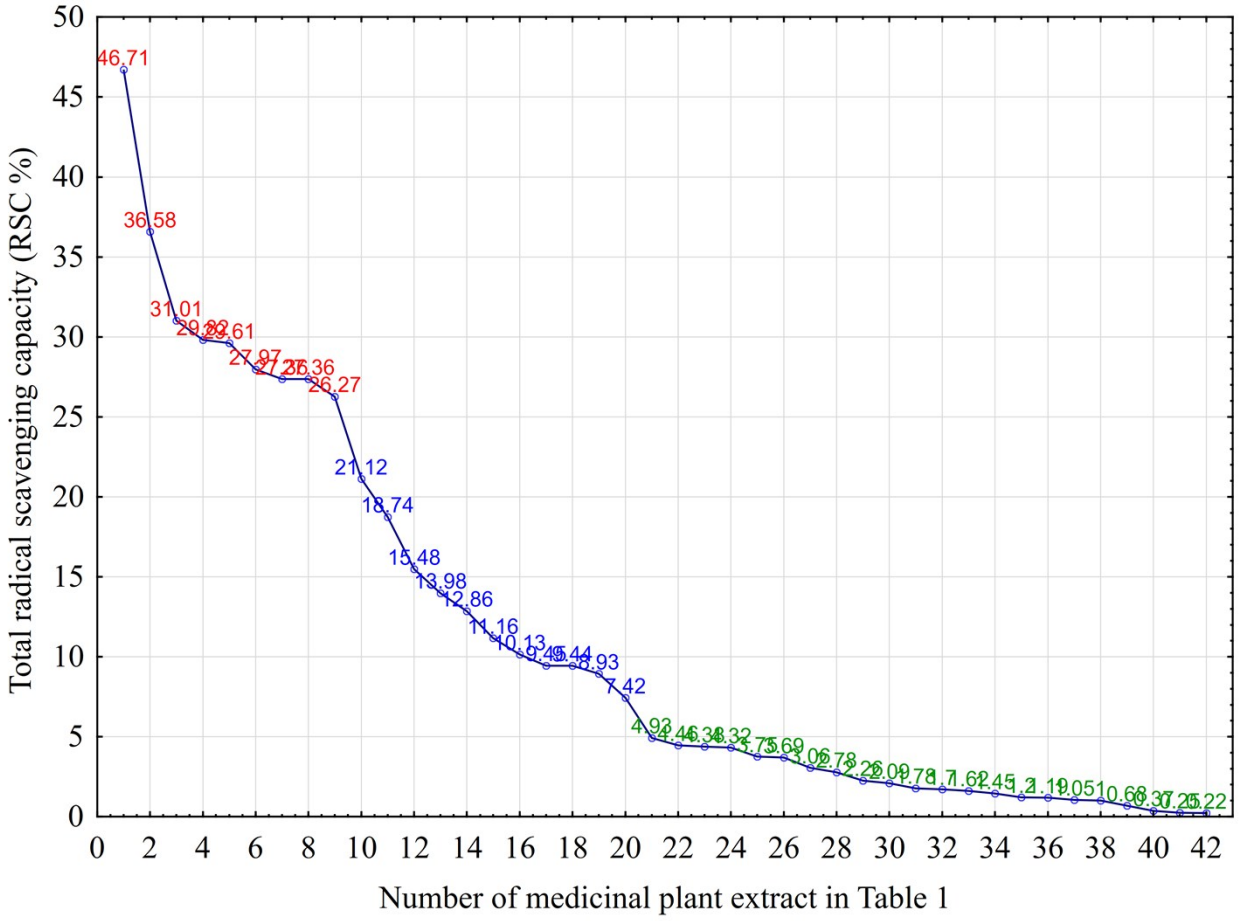


Fig. S1 The profile of antioxidant capacity of 42 medicinal plant extracts considered in this study (total radical scavenging capacity (RSC %) versus descending order of medicinal plant extract delineated in Table 1)

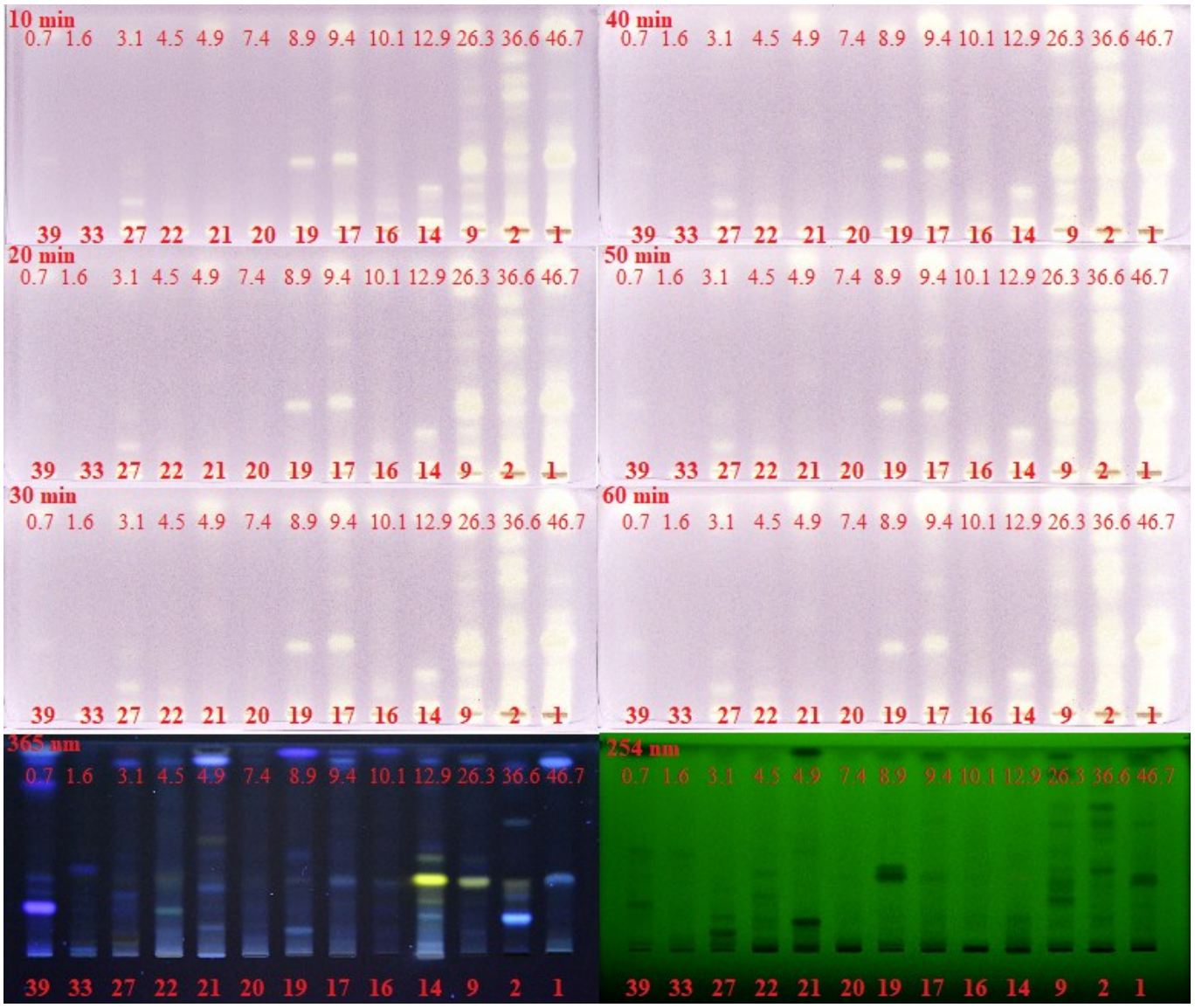
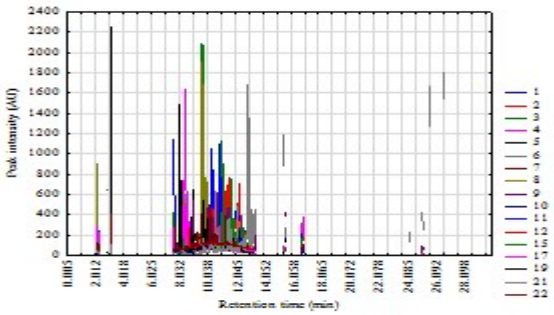
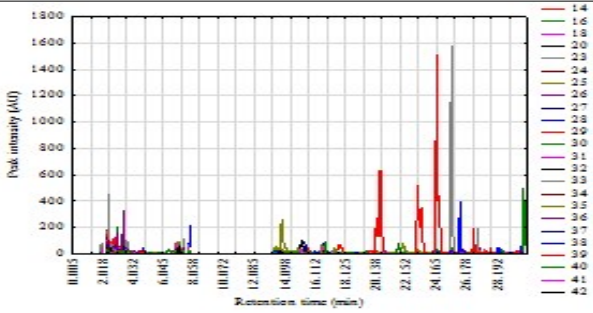
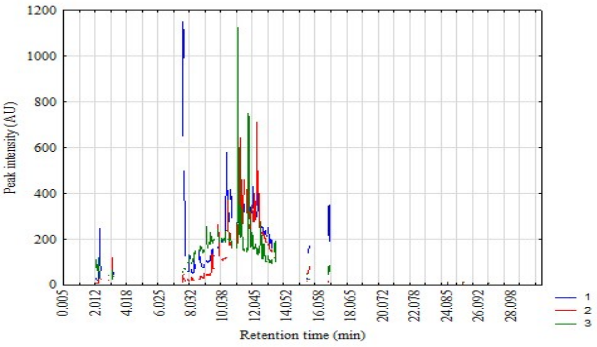


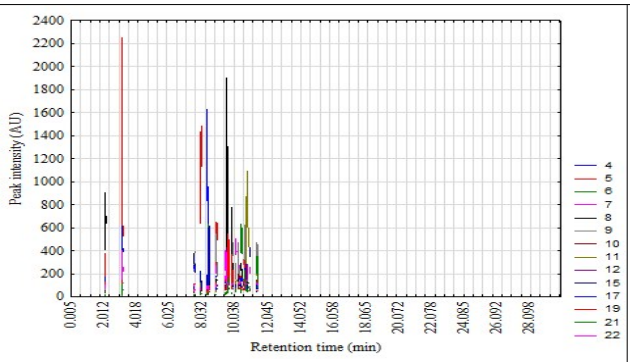
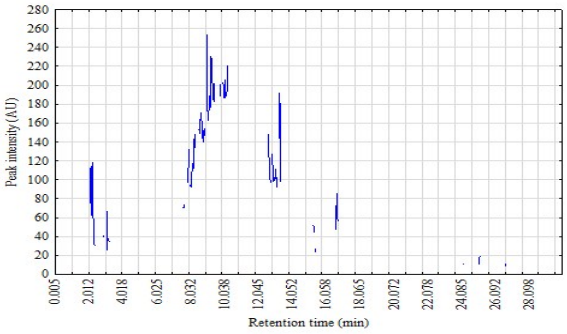
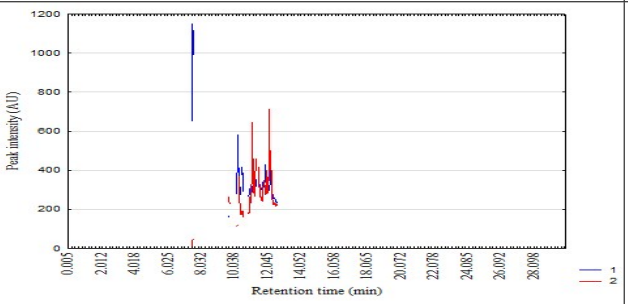
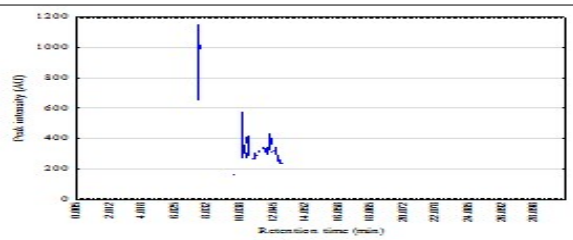
Fig. S2 The results of antioxidant capacity obtained using the DPPH· methodology by immersing the plate into the free radical solution (DPPH·). The number at the botom side of each TLC plate indicates the medicinal plant extract, and the value on the top represents the total radical scavenging capacity (RSC %) corresponding to the consdered medicinal plant extract according to Table 1.

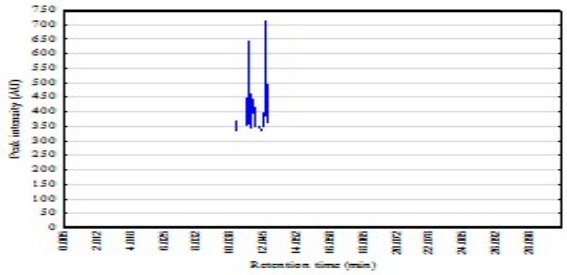
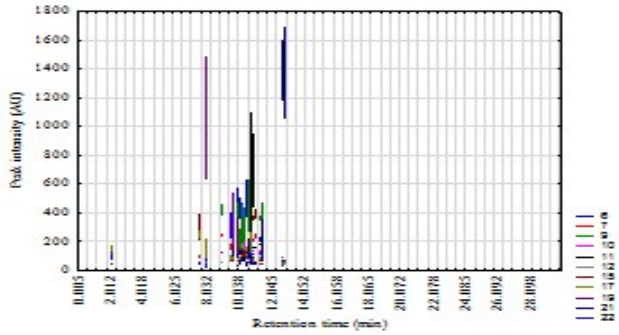
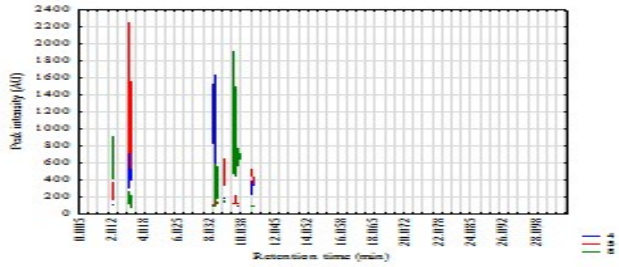
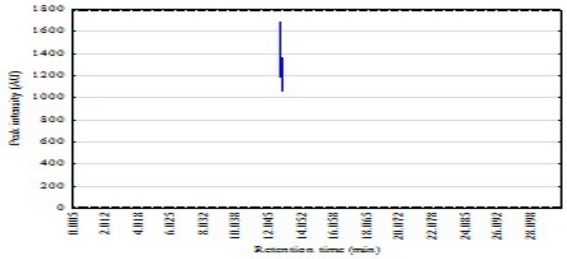
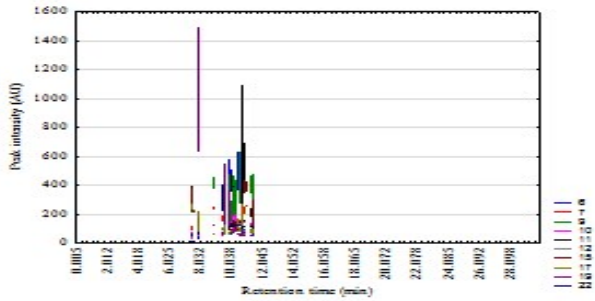
Table S2 The fuzzy clustering results obtained applying fuzzy divisive hierarchical clustering

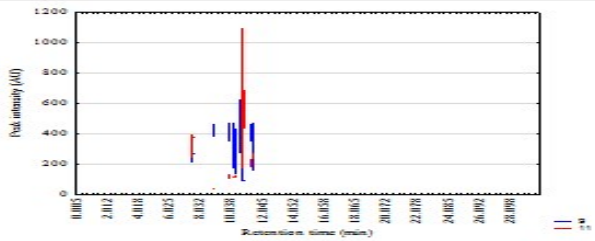
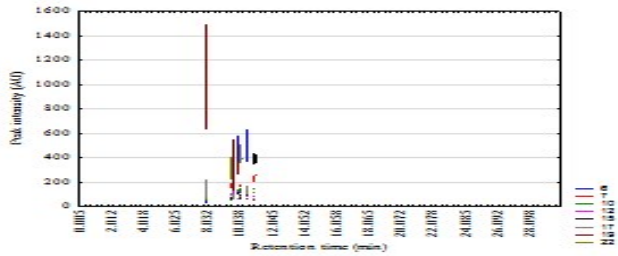
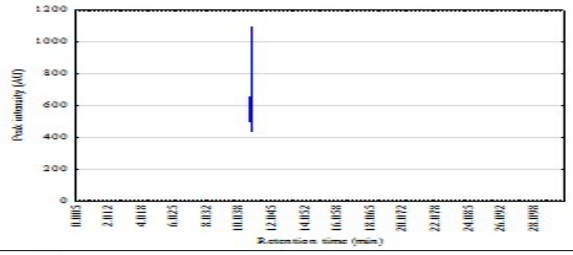
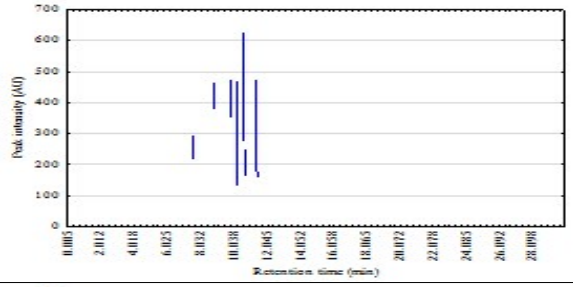
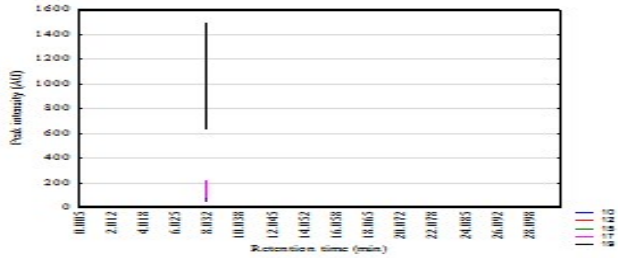
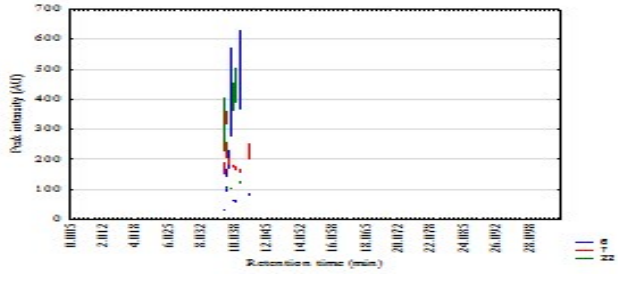
Fuzzy partition history	242 nm		260 nm		280 nm		320 nm		340 nm		380 nm	
	Sample	DOM (range)	Sample	DOM (range)	Sample	DOM (range)	Sample	DOM (range)	Sample	DOM (range)	Sample	DOM (range)
A1	13, 19, 21, 6, 17, 4, 10, 5, 15, 11, 8, 2, 3, 1, 22, 9, 12, 7	0.503 - 0.714	11, 27, 21,6, 19, 2, 15, 4, 9, 22, 5, 1, 8, 3, 12, 7	0.506 – 0.707	19, 6, 17, 13, 9, 4, 5, 1, 3, 8, 12, 7	0.524 – 0.740	15, 6, 1, 13, 17, 3, 8, 12, 7	0.509 – 0.745	11, 9, 27, 15, 6, 17, 1, 13, 3, 12, 8, 7	0.506 – 0.732	21, 3, 15, 2, 27, 1, 9, 5	0.514 – 0.663
A2	33, 39, 14, 27, 16, 24, 23, 35, 32, 38, 26, 25, 29, 18, 41, 42, 40, 34, 37, 36, 30, 20, 31, 28	0.510 – 0.943	14, 39, 17, 13, 24, 33, 38, 35, 23, 26, 16, 10, 25, 29, 41, 32, 42, 34, 36, 37, 18, 40, 30, 20, 31, 28	0.505 – 0.945	14, 11, 21, 15, 2, 27, 22, 39, 23, 24, 18, 25, 26, 16, 29, 41, 10, 42, 35, 34, 37, 38, 40, 36, 30, 20, 33, 32, 31, 28	0.519 – 0.970	11, 39, 27, 9, 19, 21, 2, 23, 24, 5, 18, 26, 22, 14, 20, 4, 40, 16, 29, 30, 41, 42, 38, 34, 25, 10, 37, 36, 35, 33, 28, 32, 31	0.526 – 0.981	39, 2, 21, 22, 19, 23, 24, 5, 26, 18, 16, 14, 20, 29, 33, 30, 40, 41, 42, 34, 25, 36, 10, 35, 38, 4, 37, 28, 32, 31	0.574 – 0.971	6, 11, 8, 16, 25, 22, 17, 19, 12, 7, 14, 35, 4, 33, 39, 30, 10, 36, 13, 29, 41, 42, 34, 24, 38, 23, 37, 40, 20, 32, 18, 31, 26, 28	0.503 – 0.986
A21	-	-	-	-	-	-	39, 11, 27, 9, 19, 21, 2, 23, 5, 18	0.273 – 0.500	-	-	6, 11, 8, 16, 4, 19, 10, 22, 17, 14, 12, 7	0.254 – 0.608
A22	-	-	-	-	-	-	22, 26, 24, 14, 20, 4, 40, 16, 28, 10, 25, 30, 35, 38, 29, 33, 41, 31, 42, 34, 36, 37, 32	0.411 – 0.912	-	-	25, 33, 35, 30, 28, 13, 39, 36, 18, 31, 20, 23, 29, 41, 42, 34, 24, 38, 37, 40, 32, 26	0.405 – 0.909
A221	-	-	-	-	-	-	26, 22, 14, 20, 4, 10, 35, 28, 31	0.229 – 0.581	-	-	35, 33, 30, 13, 20, 23, 28, 31, 18	0.266 – 0.526
A222	-	-	-	-	-	-	24, 16, 40, 25, 30, 33, 38, 29, 41, 42, 34, 32, 36, 37	0.224 – 0.801	-	-	25, 36, 39, 26, 32, 29, 4, 42, 24, 34, 37, 38, 40	0.203 – 0.849

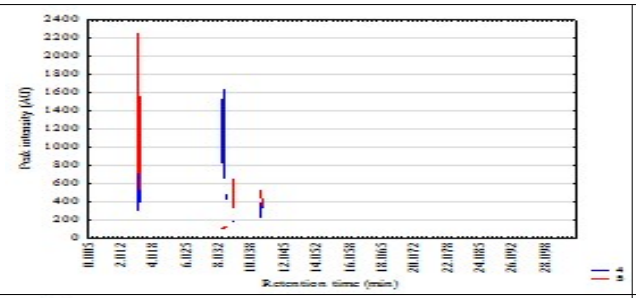
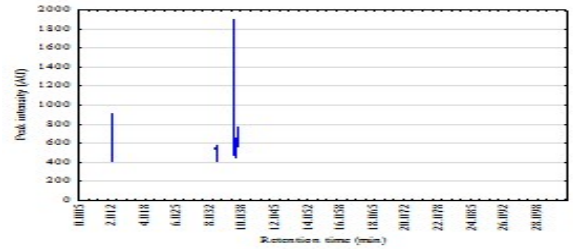
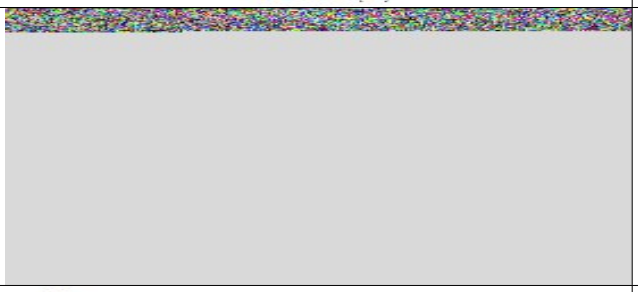
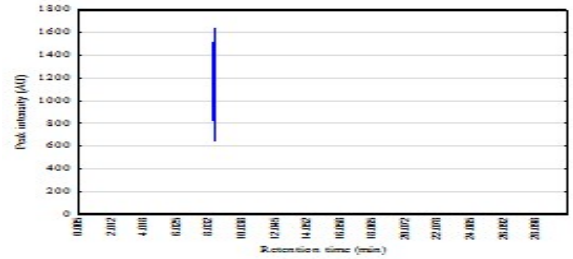
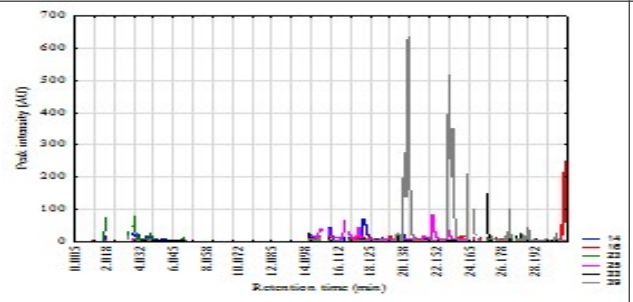
Table S3 Chromatographic specific markers (peaks) obtained applying FDHAC

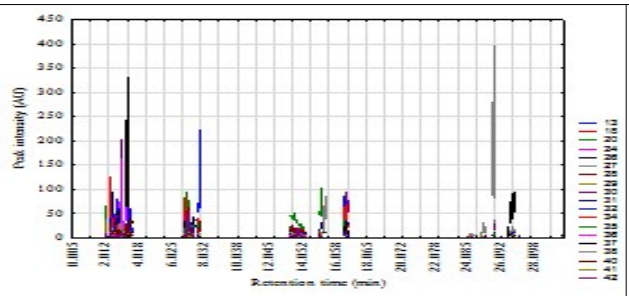
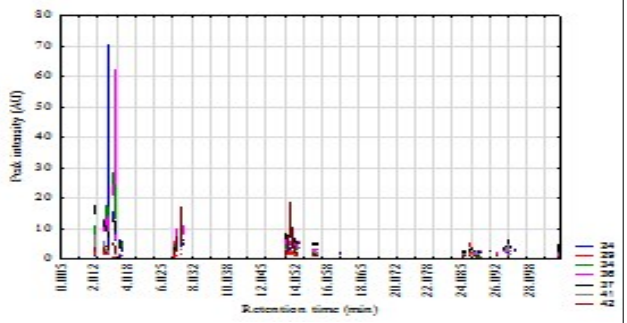
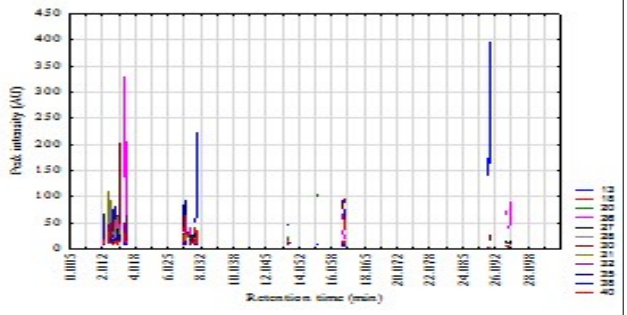
Partition	DOM range	Chromatographic specific markers	Retention time range
A1: 10; 17; 6; 19; 12; 1; 15; 11; 3; 21; 2; 22; 9; 4; 7; 8; 5	0.517-0.996		2.06-2.33 2.87 3.07-3.18 **7.83-13.25** 15.27-15.33 15.39-15.42 16.62-16.73 24.15-24.19 25.07-25.15 25.66-25.69 26.66-26.69
A2: 13; 39; 14; 29; 33; 41; 35; 42; 23; 34; 27; 37; 36; 16; 24; 25; 38; 18; 28; 30; 32; 40; 20; 31; 26	0.573-0.998		2.338-3.065 3.135-7.478 7.665-7.825 13.352-15.265 15.532-15.385 15.425-16.612 **16.732-24.138** 24.198-25.065 25.158-25.652 25.698-26.651 26.691-30.003
A1.1: 1; 2; 3	0.708-0.835		2.058-2.072 2.132-2.332 **2.865-2.872** 3.072-3.092 7.485-7.538 7.585-7.658 7.832-7.925 **7.998-8.278** 8.518-8.865 8.953-9.438 9.698-9.798 9.938-10.058 10.138-10.212 10.865-10.952 10.998-11.365 11.485-12.752 12.838-13.118 15.272-15.325

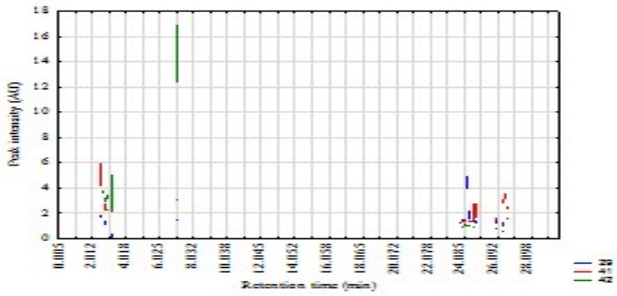
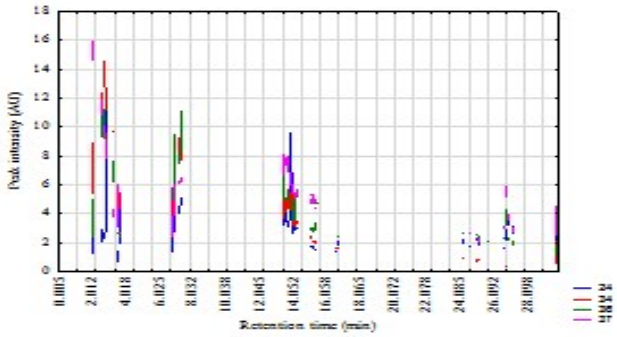
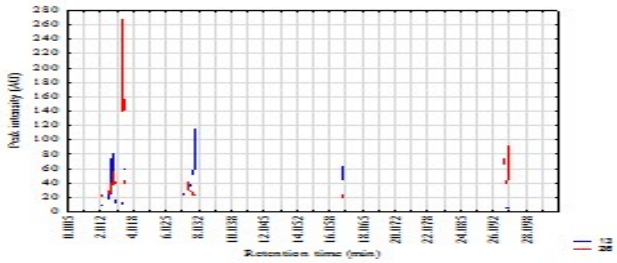
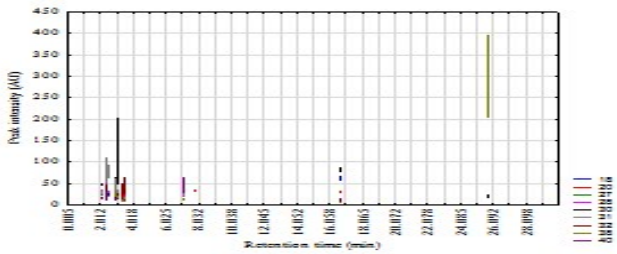
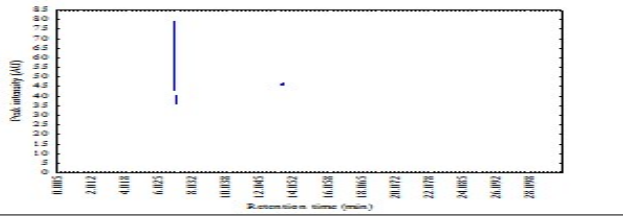
A1.2: 10; 6; 17; 19; 12; 15; 11; 7; 21; 22; 4; 5; 8; 9	0.490 – 0.955		2.078-2.125 3.105-3.165 8.285-8.512 8,872-8.945 9.445-9.698 9.805-9.932 10.065-10.132 10.218-10.318 10.605-10.865 11.365-11.472
A1.1.1: 3	0.834		2.058-2.072 2.132-2.332 3.072-3.105 7.598-7.658 7.832-7.925 7.998-8.278 8.525-8.865 8.958-9.438 9.738-9.805 9.958-10.058 10.138-10.185 12.065-12.752 12.838-13.118
A1.1.2: 1; 2	0.539 – 0.688		7.485-7.538 9.698-9.732 10.192-10.212 10.325-10.405 10.478-10.598 10.865-10.952 10.998-11.365 11.485-12.612
A1.1.2.1: 1	0.539		11.972-11.178 11.292-11.365 11.485-11.506 11.825-11.852 11.972-12.018 12.092-12.258

A1.1.2.2: 2	0.688		10.325-10.332 11.072-11.178 11.292-11.365 11.485-11.505 11.825-11.852 11.972-12.018 12.092-12.258
A1.2.1: 17; 7; 10; 6; 12; 11; 19; 15; 9; 21; 22	0.432 – 0.916		7.932-7.992 9.445-9.492 9.618-9.692 9.858-9.932 10.065-10.132 10.218-10.318 10.412-10.472 10.075-10.865 11.372-11.485 12.772-12.836
A1.2.2: 4; 5; 8	0.833 – 0.924		2.078-2.125 3.105-3.164 8.285-8.512 8.892-8.945 9.505-9.618 9.812-9.852 10.658-10.698
A1.2.1.1: 21	0.847		12.758-12.832
A1.2.1.2: 17; 10; 7; 12; 6; 11; 15; 9; 19; 22	0.333 – 0.915		7.545-7.578 7.958-7.992 9.445-9.492 9.618-9.692 9.858-9.932 10.065-10.132 10.218-10.318 10.418-10.472 10.605-10.645 1. 767-10.858 11.372-11.478

A1.2.1.2.1: 11; 9	0.519 – 0.652		7.545-7.587 9.905-9.932 10.212-10.318 10.605-10.652 10.705-10.865 11.378-11,478
A1.2.1.2.2: 17; 10; 7; 12; 6; 15; 19; 22	0.296 – 0.899		7.932-7.998 9.445-9.492 9.618-9.690 9.858-9.885 10.065-10.132 10.412-10.478 10.958-10.992
A1.2.1.2.1.1: 11	0.519		10.745-1.858
A1.2.1.2.1.2: 9	0.652		7.545-7.578 9.892-9.932 10.218-10.318 10.605-10.645 10.705-10.738 11.372-11.478
A1.2.1.2.2.1: 10; 17; 12; 19; 15	0.256 – 0.554		7.932-7.992
A1.2.1.2.2.2: 7; 6; 22	0.325 – 0.898		9.445-9.492 9.618-9.692 9.858-9.885 10.065-10.123 10.412-10.472

A1.2.2.1: 4; 5	0.778 – 0.826		3.105-3.165 8.285-8.425 8.472-8.512 8.885-8.945 10.645-10.698
A1.2.2.2: 8	0.919		2.078-2.125 8.432-8.465 9.505-9.612 9.812-9.852
A1.2.2.1.1: 5	0.825		3.105-3.165 8.472-8.512 10.645-10.698
A1.2.2.1.2: 4	0.778		8.285-8.425 8.885-8.945
A2.1: 39; 23; 25; 14; 16; 33	0.434 – 0.868		0.005-1.985 3.258-3.298 3.952-3.632 3.698-6.778 14.292-15.132 15.498-16.585 16.825-24.092 24.432-24.518 24.572-24.598 24.738-24.885 25.252-25.625 25.765-26.185 26.225-26.632 26.745-26.818 26.978-30.000

A2.2: 13; 26; 18; 29; 35; 41; 42; 27; 34; 37; 24; 36; 30; 28; 20; 38; 31; 40; 32	0.460 – 0.975		1.992-2.052 2.358-3.065 3.185-3.258 3.305-3.585 3.638-3.692 6.785-7.478 7.665-7.852 13.352-14.285 15.138-15.265 15.332-15.492 16.732-16.818 24.098-24.132 24.198-24.425 24.525-24.558 24.605-24.725 24.892-25.065 25.158-25.252 25.698-25.805 26.693-26.978 29.885-29.972
A2.2.1: 29; 41; 42; 34; 24; 37; 36	0.741 – 0.912		1.992-2.052 2.565-2.664 3.218-3.252 3.305-3.325 3.512-3.585 3.638-3.692 6.785-6.478 7.665-7.852 13.352-14.285 15.332-15.492 24.198-24.425 24.525-24.558 24.605-24.725 24.892-25.065 25.158-25.252 26.285-26.218 29.885-29.972
A2.2.2: 13; 26; 40; 18; 38; 32; 30; 35; 27; 28; 20; 31	0.391 – 0.947		2.032-2.052 2.338-2.558 2.665-2.772 2.912-3.065 3.338-3.505 7.065-7.205 7.385-7.478 7.665-7.825 13.393-13.432 25.698-25.732 26.878-26.932

A2.2.1.1: 29; 41; 42	0.670 – 0.811		2.572-2.585 2.825-2.852 2.885-2.905 3.198-3.252 7.172-7.198 24.205-24.238 24.312-24.205 24.532-24.552 24.612-24.712 24.898-25.065
A2.2.1.2: 24; 34; 37; 36	0.724 – 0.907		2.592-2.645 2.785-2.818 3.305-3.332 3.512-3.585 3.638-3.692 6.785-6.972 7.205-7.378 13.438-14.285 15.332-15.385 15.432-15.492 24.245-24.305 25.192-25.245 26.812-26.852 29.892-29.965
A2.2.2.1: 13; 26; 35	0.332 – 0.731		2.465-2.558 2.665-2.765 7.112-7.172 7.405-7.478 7.685-7.825 13.352-13.432 26.878-26.932
A2.2.2.2: 18; 40; 38; 32; 30; 28; 31; 27; 20	0.462 – 0.925		2.338-2.458 2.938-3.065 3.365-3.485 7.018-7.105 25.698-25.718
A2.2.2.1.1: 35	0.730		6.985-7.012 7.112-7.132 13.325-13.438

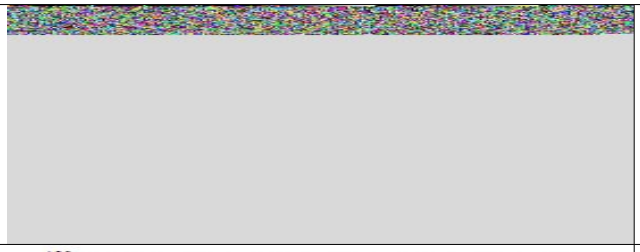
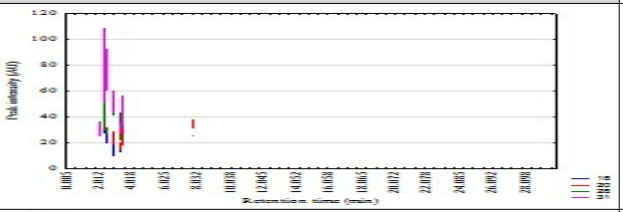
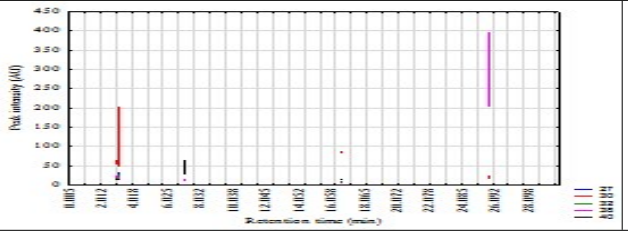
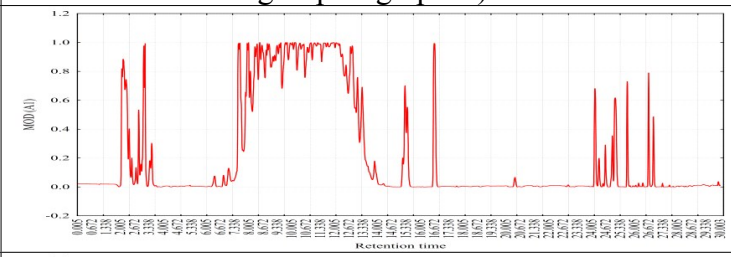
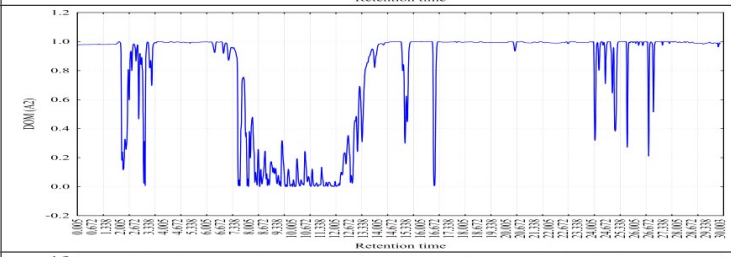
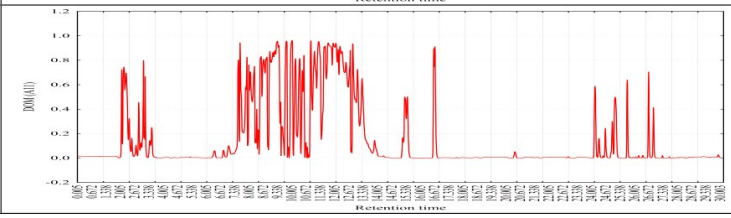
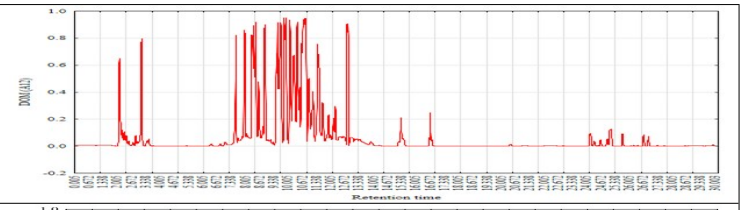
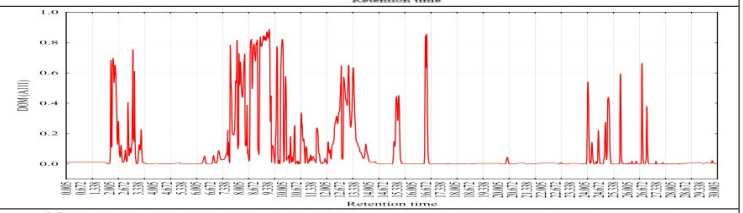
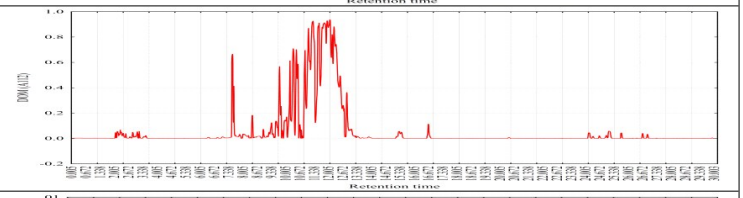
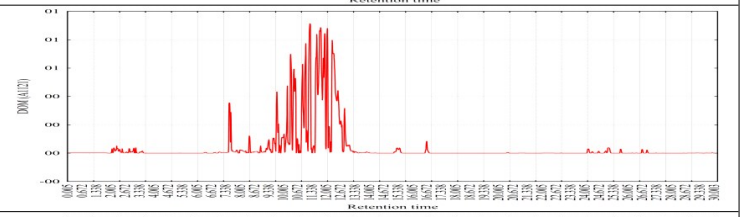
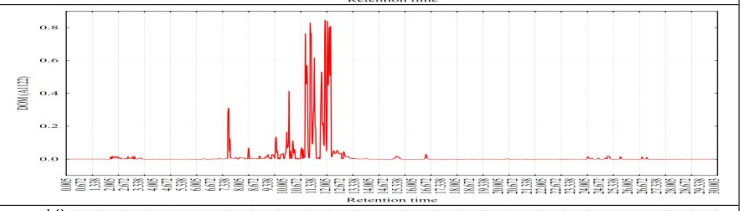
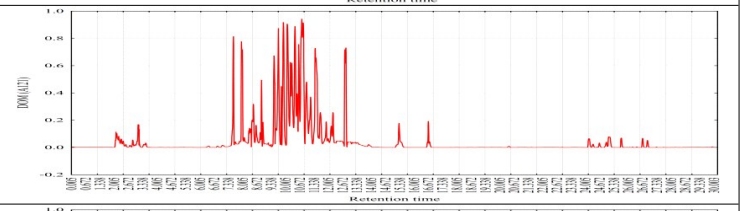
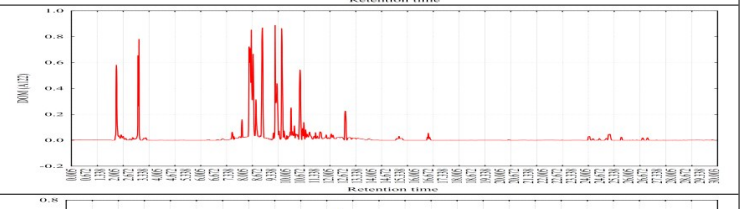
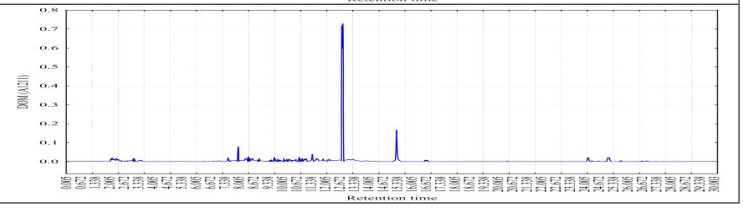
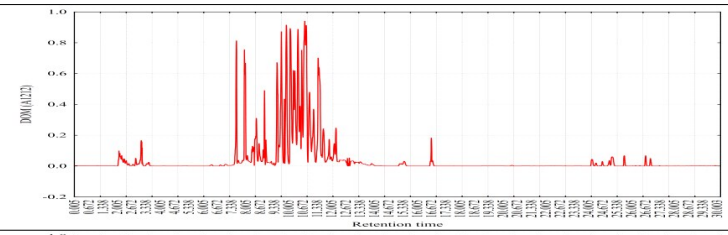
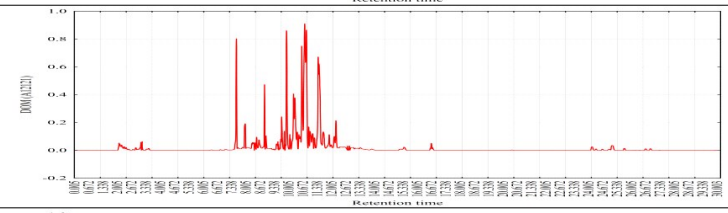
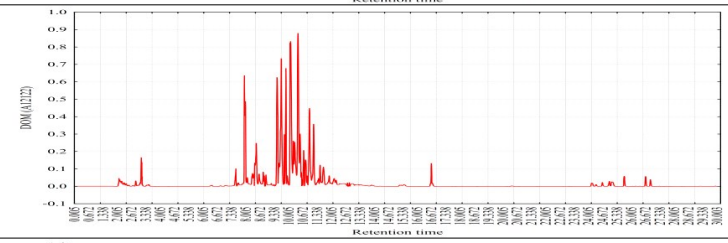
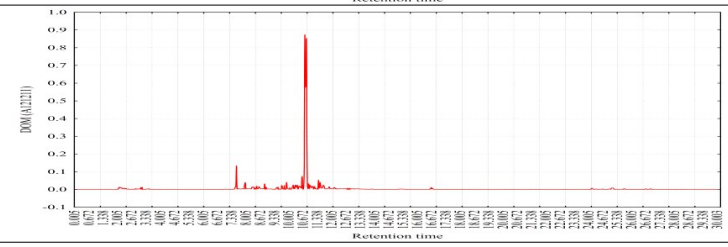
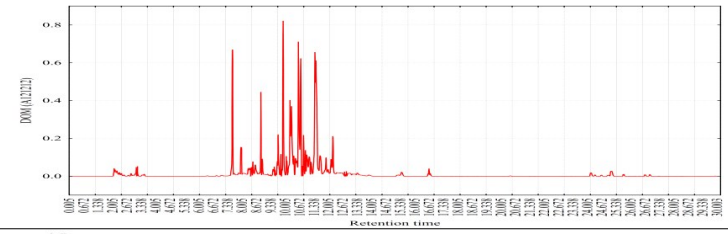
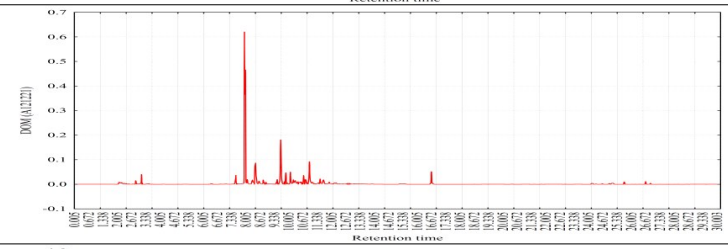
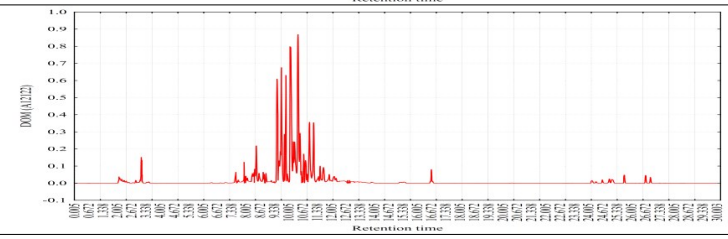
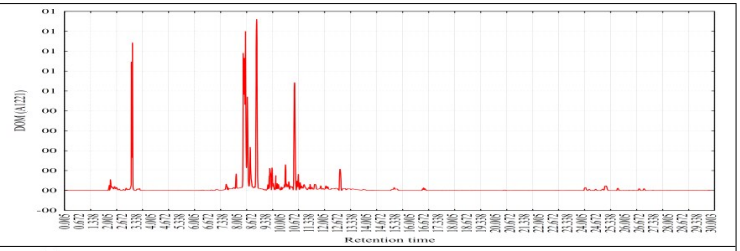
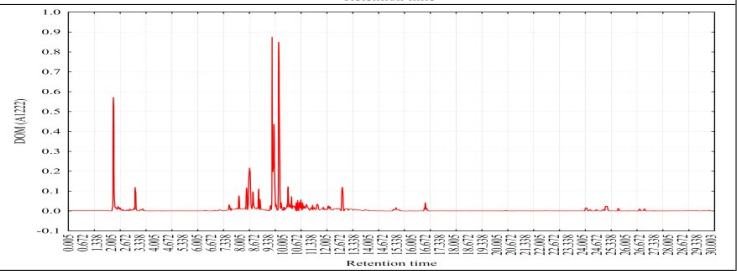
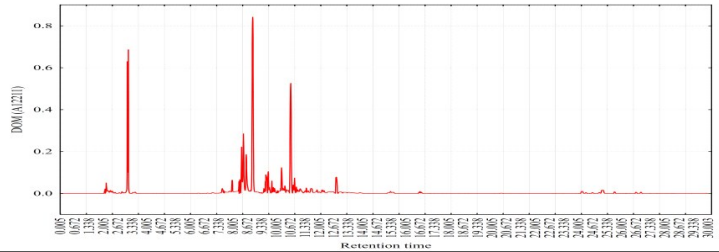
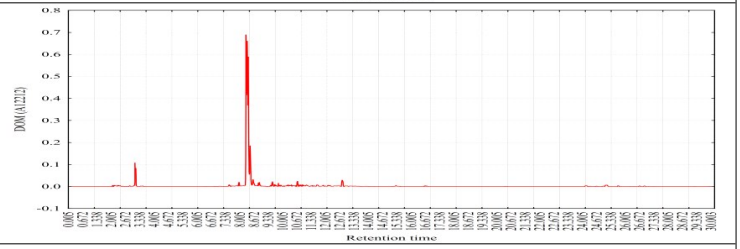
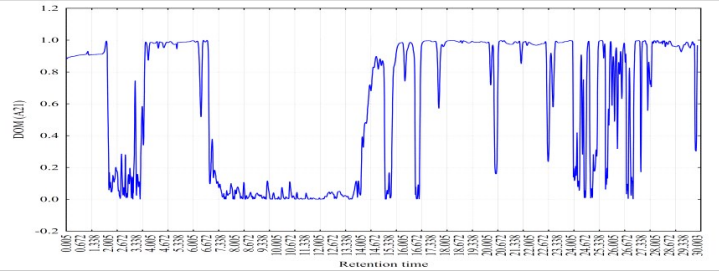
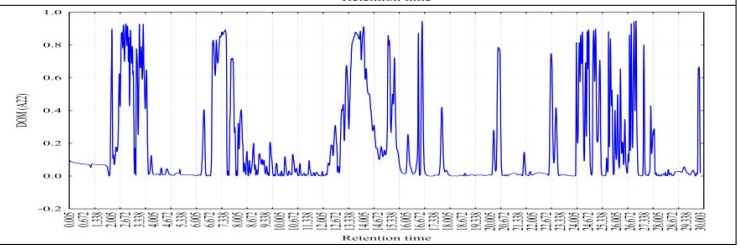
A2.2.2.1.2: 13; 26	0.328 – 0.544		2.465-2.558 2.665-2.765 7.405-7.478 7.685-7.825 26.878-26.932
A2.2.2.2.1: 18; 31; 28; 20	0.453 – 0.832		2.338-2.458 2.938-2.972 3.365-3.485
A2.2.2.2.2: 40; 38; 32; 30; 27	0.579 – 0.813		3.005-3.065 25.698-25.718

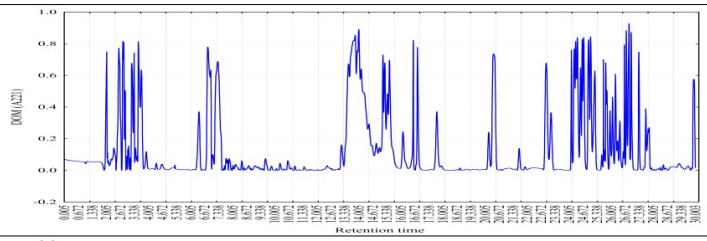
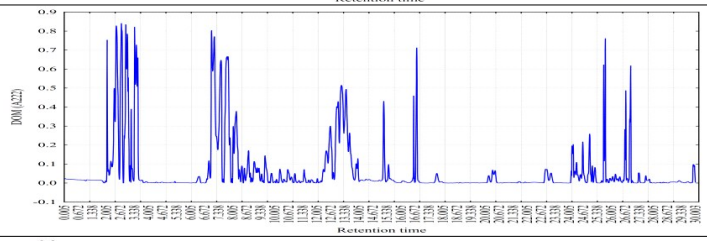
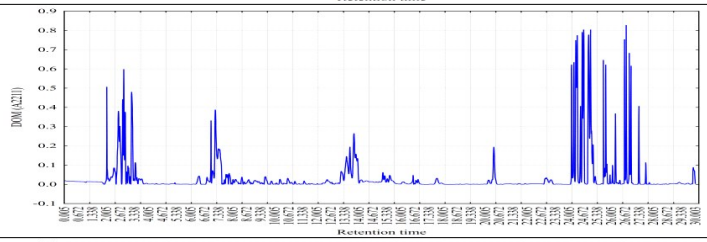
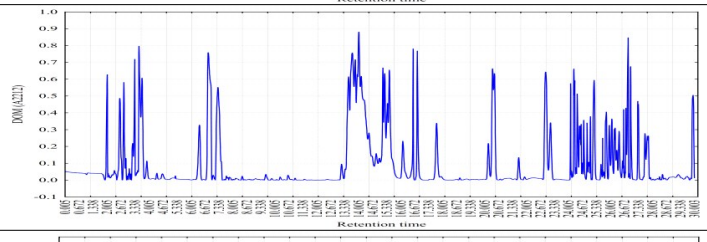
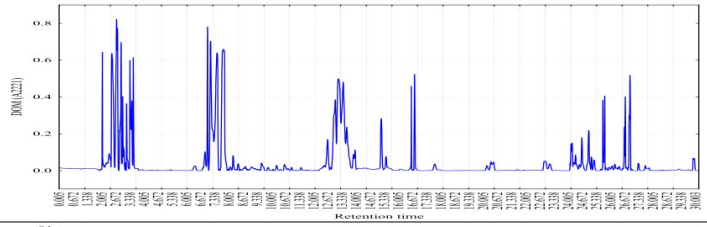
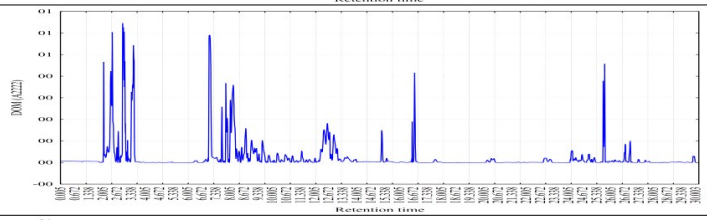
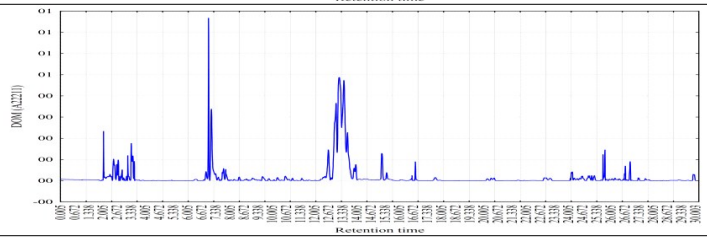
Table S4 Fuzzy DOMs markers obtained applying FDHAC

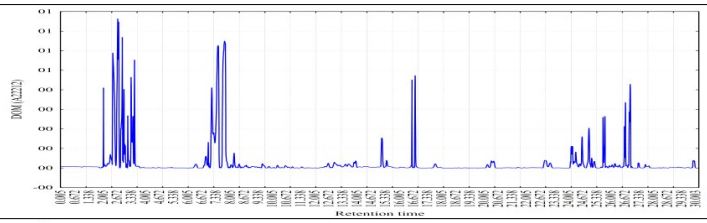
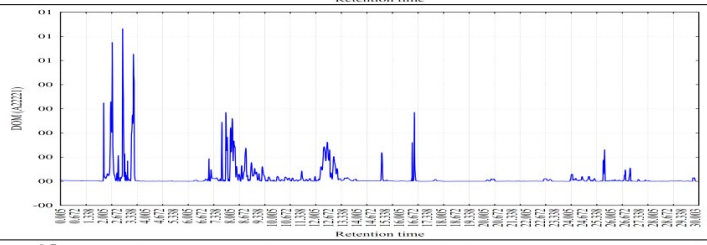
Fuzzy partition	DOM (range)	Chromatographic region fingerprint (chromatographic group fingerprint)
A1: 10; 17; 6; 19; 12; 1; 15; 11; 3; 21; 2; 22; 9; 4; 7; 8; 5	• - 0.996	
A2: 13; 39; 14; 29; 33; 41; 35; 42; 23; 34; 27; 37; 36; 16; 24; 25; 38; 18; 28; 30; 32; 40; 20; 31; 26	• - 0.998	
A1.1: 1; 2; 3	0.708- 0.835	

A1.2: 10; 6; 17; 19; 12; 15; 11; 7; 21; 22; 4; 5; 8; 9	0.490 - 0.955	
A1.1.1: 3	0.834	
A1.1.2: 1; 2	0.539 – 0.688	
A1.1.2.1: 1	0.539	
A1.1.2.2: 2	0.688	
A1.2.1: 17; 7; 10; 6; 12; 11; 19; 15; 9; 21; 22	0.432 - 0.916	
A1.2.2: 4; 5; 8	0.833 – 0.924	
A1.2.1.1: 21	0.847	

A1.2.1.2: 17; 10; 7; 12; 6; 11; 15; 9; 19; 22	0.333 - 0.915	
A1.2.1.2.1: 11; 9	0.519 – 0.652	
A1.2.1.2.2: 17; 10; 7; 12; 6; 15; 19; 22	0.296 - 0.899	
A1.2.1.2.1.1: 11	0.519	
A1.2.1.2.1.2: 9	0.652	
A1.2.1.2.2.1: 10; 17; 12; 19; 15	0.256 – 0.554	
A1.2.1.2.2.2: 7; 6; 22	0.325 – 0.898	

A1.2.2.1: 4; 5	0.778 – 0.826	
A1.2.2.2: 8	0.919	
A1.2.2.1.1: 5	0.825	
A1.2.2.1.2: 4	0.778	
A2.1: 39; 23; 25; 14; 16; 33	0.434 - 0.868	
A2.2: 13; 26; 18; 29; 35; 41; 42; 27; 34; 37; 24; 36; 30; 28; 20; 38; 31; 40; 32	0.460 - 0.975	

A2.2.1: 29; 41; 42; 34; 24; 37; 36	0.741 - 0.912	
A2.2.2: 13; 26; 40; 18; 38; 32; 30; 35; 27; 28; 20; 31	0.391 - 0.947	
A2.2.1.1: 29; 41; 42	0.670 – 0.811	
A2.2.1.2: 24; 34; 37; 36	0.724 – 0.907	
A2.2.2.1: 13; 26; 35	0.332 – 0.731	
A2.2.2.2: 18; 40; 38; 32; 30; 28; 31; 27; 20	0.462 – 0.925	
A2.2.2.1.1: 35	0.730	

A2.2.2.1.2: 13; 26	0.328 – 0.544	
A2.2.2.2.1: 18; 31; 28; 20	0.453 – 0.832	
A2.2.2.2.2: 40; 38; 32; 30; 27	0.579 – 0.813