molecules

MDPI

Supplementary file

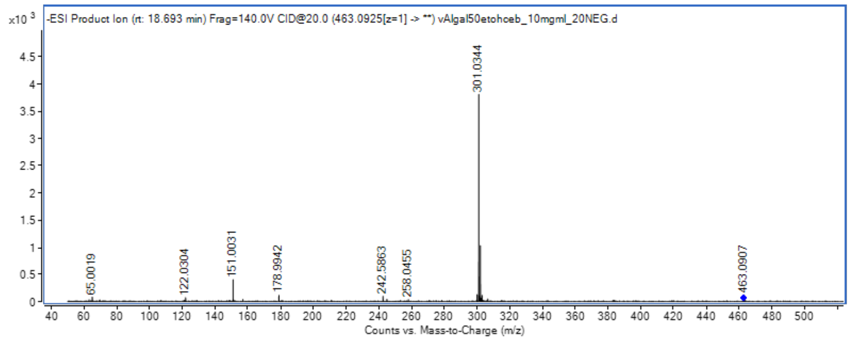
The phenolic compounds profile and cosmeceutical significance of two Kazakh species of onions: *Allium galanthum* and *A. turkestanicum*

Gulnara Kadyrbayeva [1], Justyna Zagórska [2], Agnieszka Grzegorczyk [3], Katarzyna Gaweł-Bęben [4], Marcelina Strzępek-Gomółka [4], Agnieszka Ludwiczuk [5], Karolina Czech [4], Manoj Kumar [6], Wojciech Koch [2], Anna Malm [3], Kazimierz Głowniak [4], Zuriyadda Sakipova [1] and Wirginia Kukula-Koch [7,*]

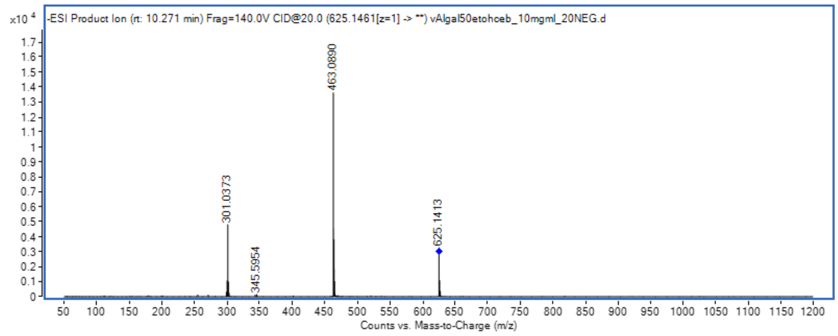
Figure S1. Mass chromatograms recorded for 50% ethanol extracts of Kazakhstani bulbs (top: *Allium galanthum* onion extract in negative ion mode, in positive ion mode, *Allium galanthum* chives extract in negative ion mode, in positive ion mode, *Allium turkestanicum* onion extract in positive ion mode, in negative ion mode).

Table S1. The MS/MS fragmentation spectra of the identified compounds.

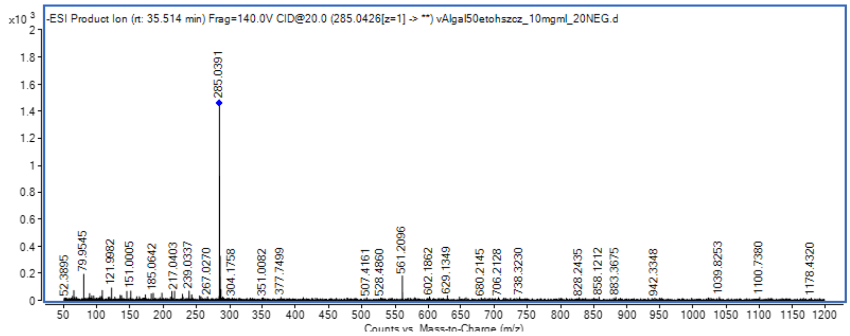
Isoquercetin



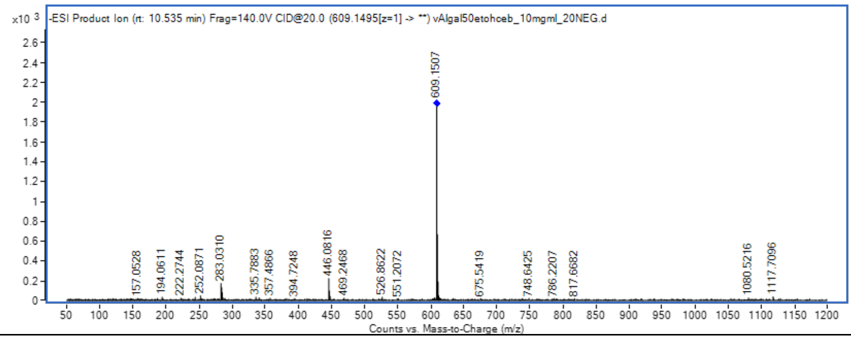
Quercetin dihexoside

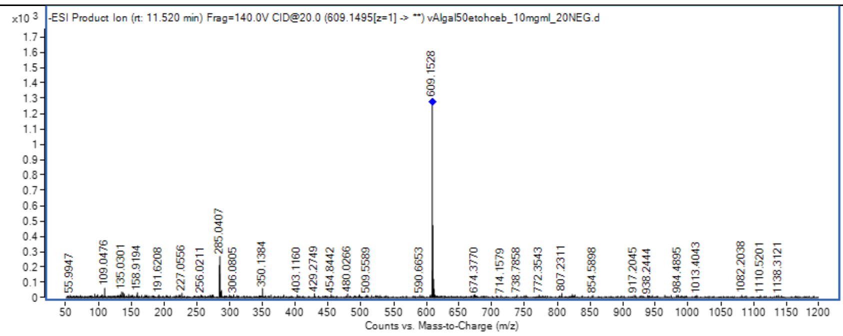


Kaempferol

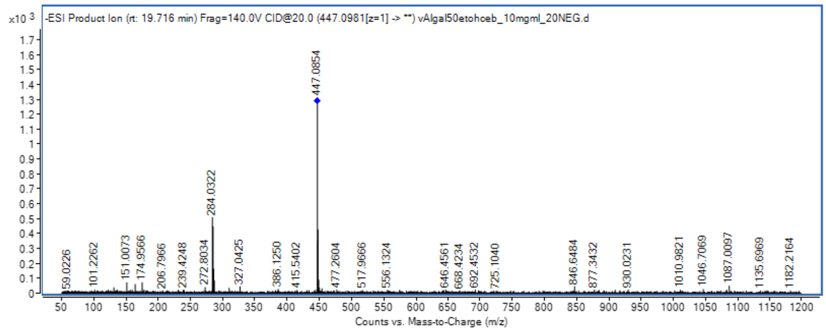


Kaempferol diglucosides

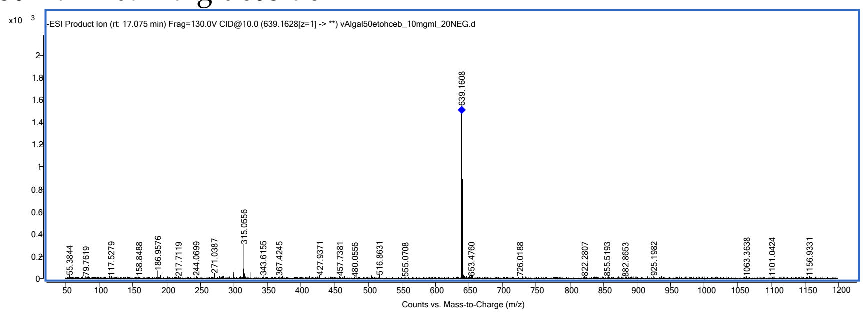


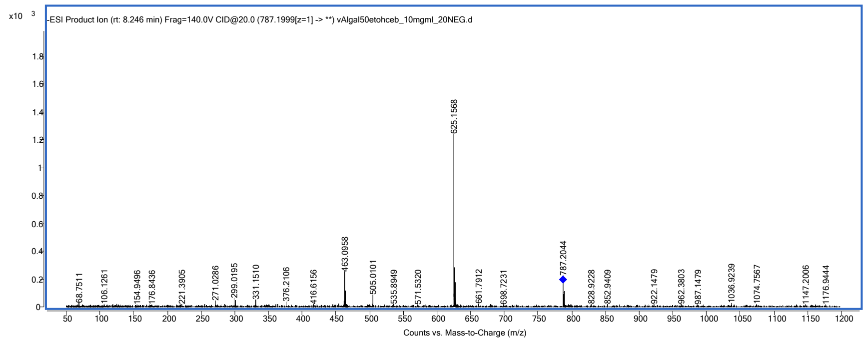


Kaempferol glucoside

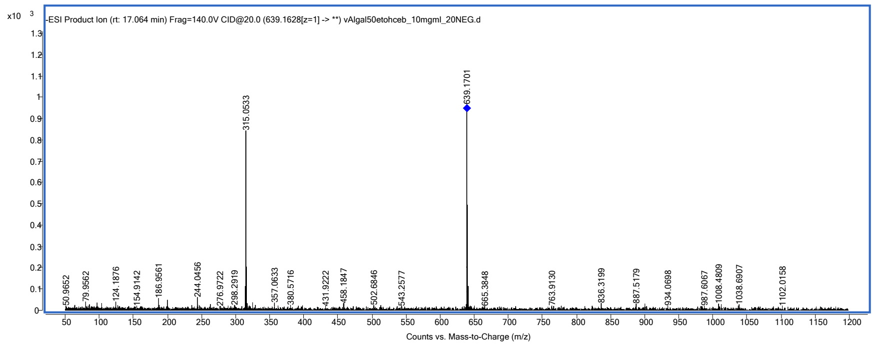


Isorhamnetin diglucoside

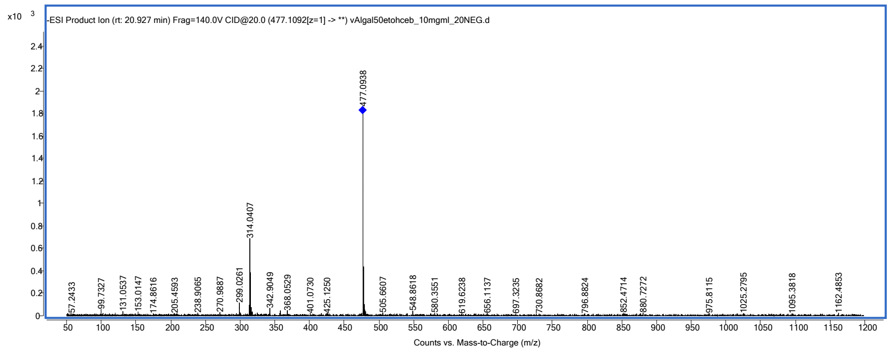




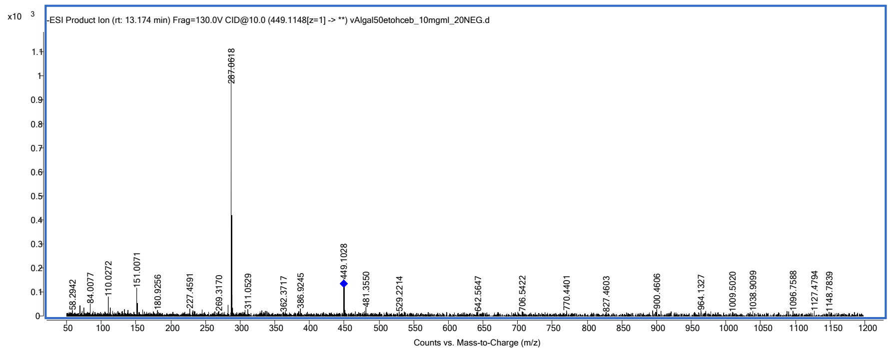
Quercetin triglycoside



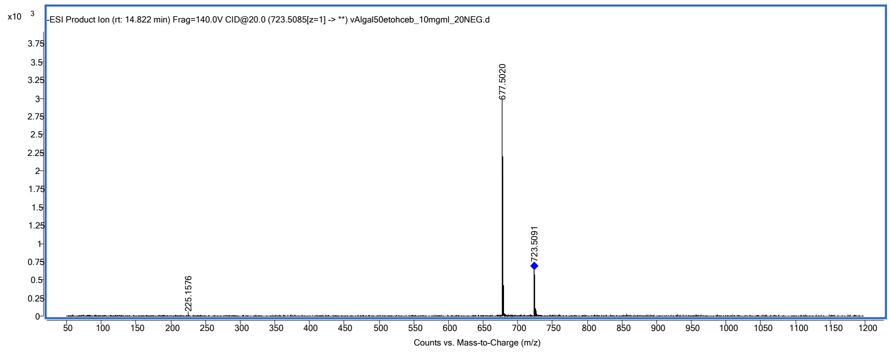
Isorhamnetin glucoside



Cyanidin glucoside



Unknown 1



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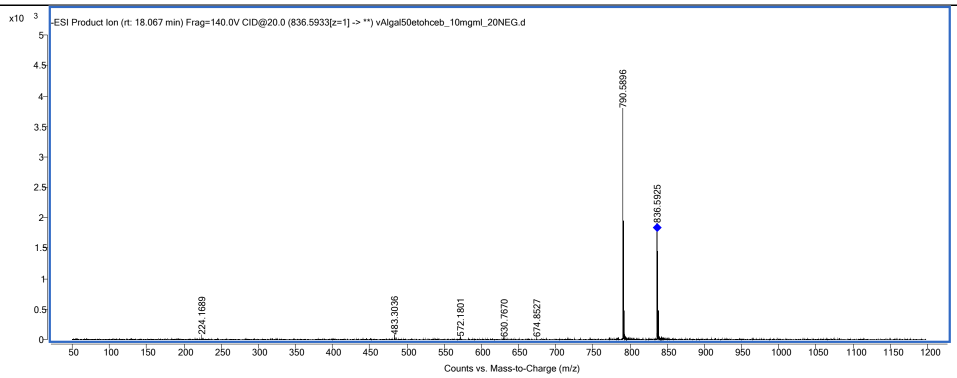
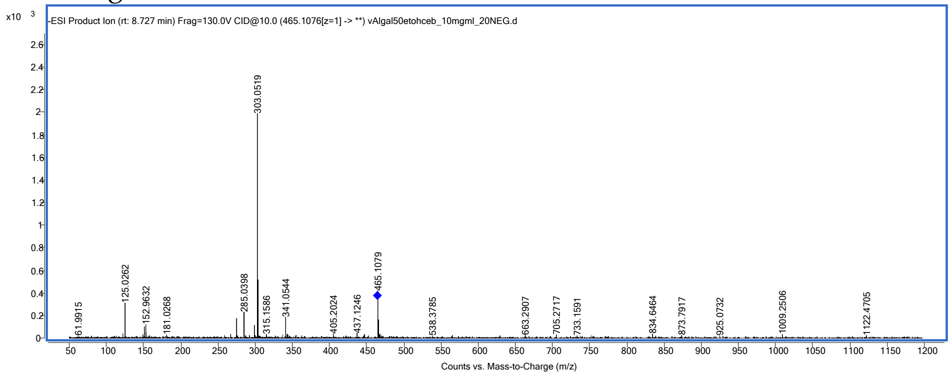
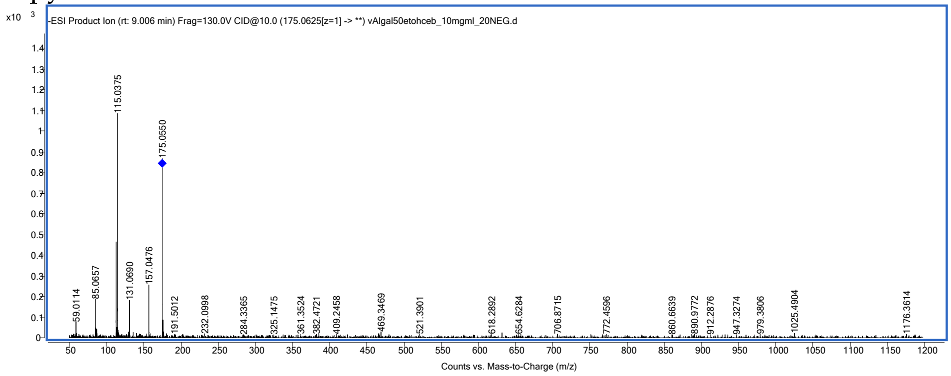


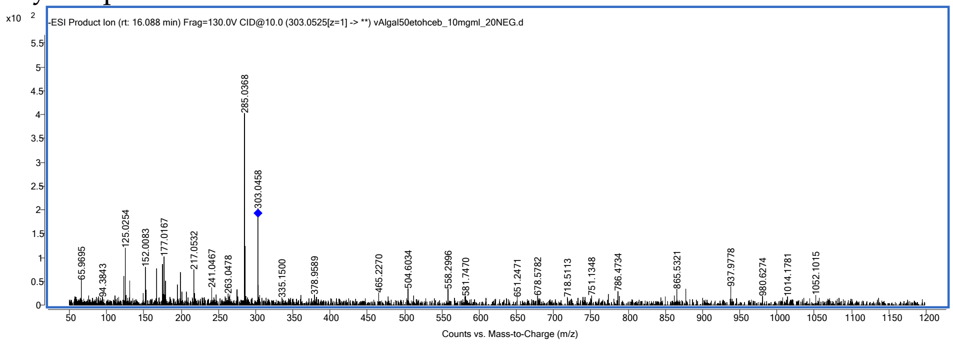
Taxifolin glucoside



Propylmalic acid



Dihydroquercetin



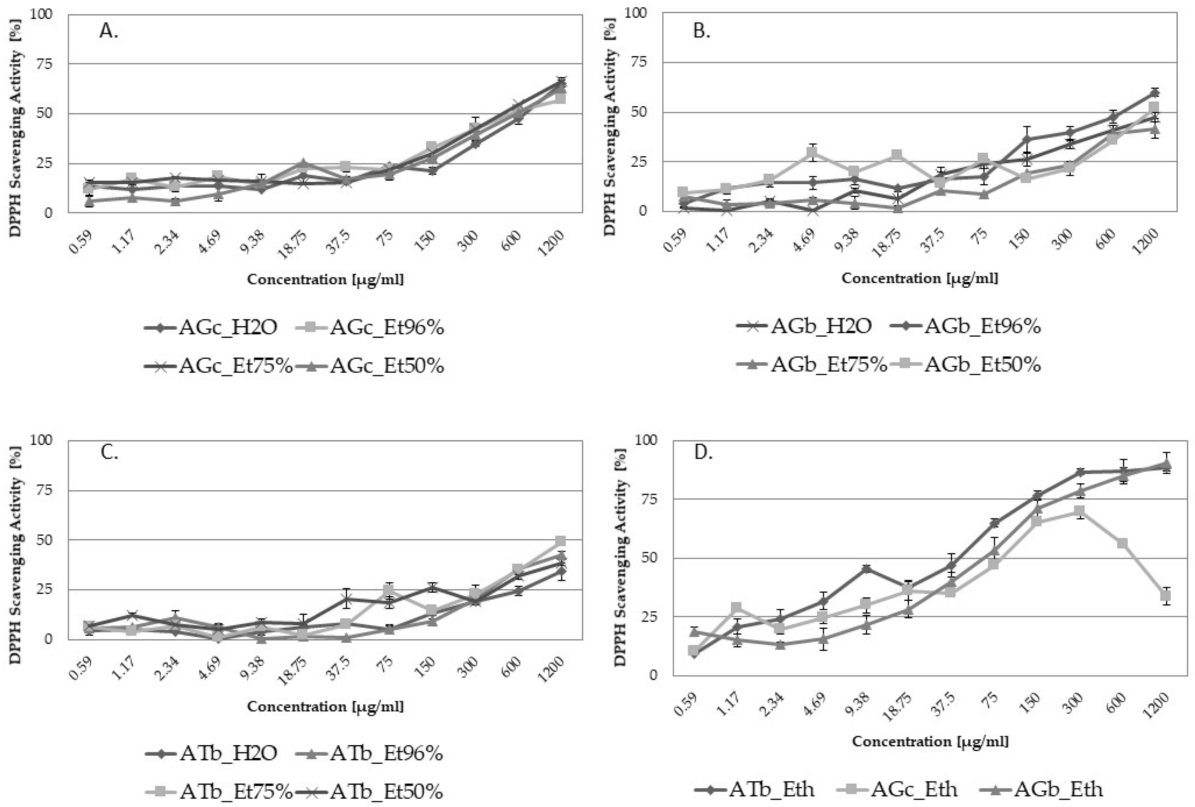


Figure S2. Scaveging of DPPH free radical by *A. galanthus* and *A. turkestanicum* extracts; graphs show mean ±SD (n = 3)

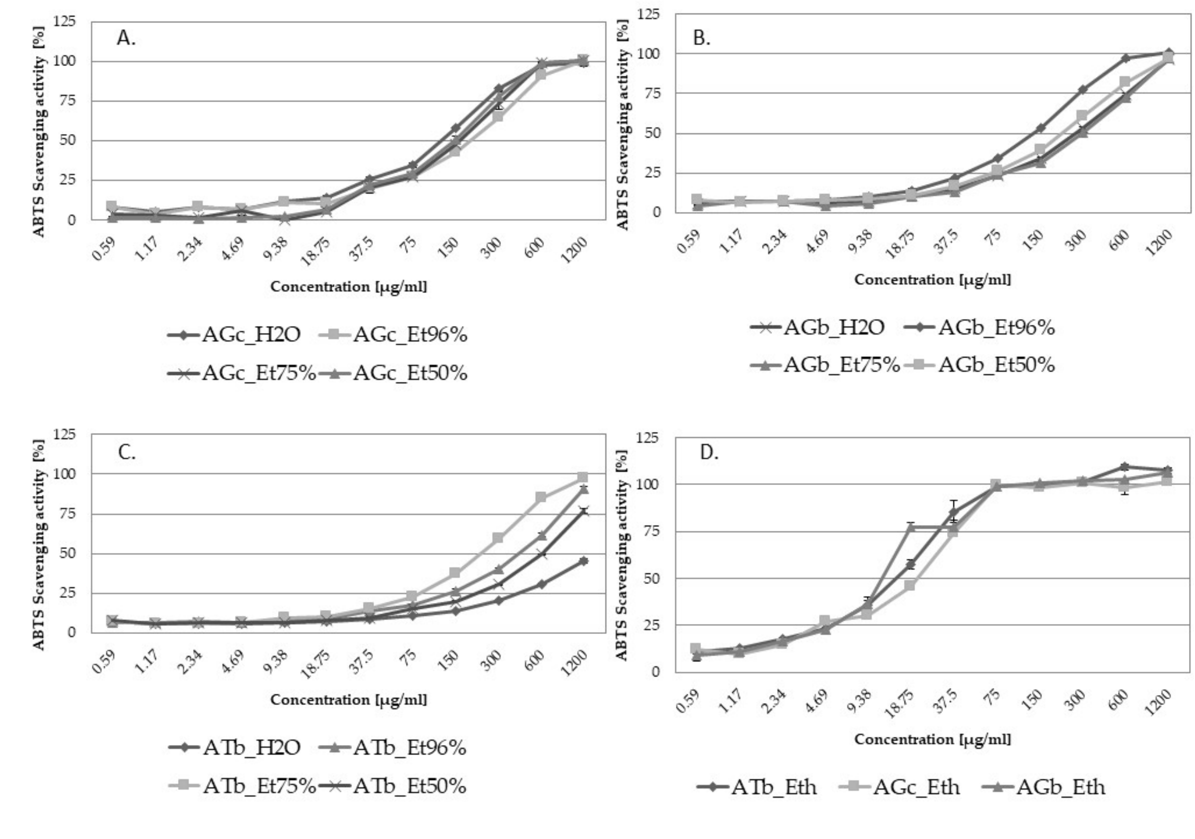


Figure S3. Scaveging of ABTS free radical by *A. galanthus* and *A. turkestanicum* extracts; graphs show mean ±SD (n = 3)

Table S2. The list of screened compounds during the compositional studies

			m/z calculated		
	Ferulic acid		194.057910 193.050085 195.065735		

			224.068475 223.060650 225.076300		

			286.047740 285.039915 287.055565		
	Kaempferol		286.047740 285.039915 287.055565		

		$[M+H]^+$ $C_{15}H_{11}O_6$			
			270.052825 269.052825 271.060650		

			177.045966 176.038141 178.053791		

			162.017309 161.009484 163.025133		
		$C_{29}H_{50}O$	414.386165 413.378340 415.393990		

			380.214015 379.206190 381.221840		

			124,052430 123.044605 125.060255		
			72.021130 71.013305 73.028955		

			892.535316 891.527491 893.543141		

		$C55H70O6N4Mg$ [M-H]- $C55H69O6N4Mg$ [M+H]+ $C55H71O6N4Mg$	906,514581 905.506756 907,522406		
		$C_6H_8O_6$ [M-H]- $C_6H_7O_6$	176,032090 175.024265 177,039915		
			177.045966 176.038141 178.053791		

		$C_5H_{11}NO_2S$ [M+H]+ $C_5H_{12}NO_2S$	149.051051 148,043226 150,058876		
		$C_9H_{14}OS_3$ [M-H]- $C_9H_{13}OS_3$ [M+H]+ $C_9H_{15}OS_3$	234.020681 233.012856 235.028506		
		$C_9H_{14}OS_3$ [M-H]- $C_9H_{13}OS_3$ [M+H]+ $C_9H_{15}OS_3$	234.020681 233.012856 235.028506		

		$C_6H_8S_2$ [M-H]- $C_6H_7S_2$ [M+H]+ $C_6H_9S_2$	144.006744 142.998919 145.014569		
		$C_6H_{10}S$ [M-H]- C_6H_9S [M+H]+ $C_6H_{11}S$	114.050322 113.042497 115.058146		
		$C_6H_{10}S_2$ [M-H]- $C_6H_9S_2$ [M+H]+ $C_6H_{11}S_2$	146.022394 145.014569 147.030219		
		$C_6H_{10}S_3$ [M-H]- $C_6H_9S_3$	177.994466 176.986641		

		[M+H]+ $C_6H_{11}S_3$	179.002291		
		C_4H_8S [M-H]- C_4H_7S [M+H]+ C_4H_9S	88.034672 87.026847 89.042497		
		$C_{69}H_{114}O_{39}$ [M-H]- $C_{69}H_{113}O_{39}$ [M+H]+ $C_{69}H_{115}0_{39}$	1566.693735 1565.685910 1567.701560		5
		$C_{62}H_{100}O_{34}$ [M-H]- $C_{62}H_{99}O_{34}$ [M+H]+ $C_{62}H_{101}O_{34}$	1388.609610 1387.601785 1389.617435		

		$C_{62}H_{102}O_{36}$ [M-H]- $C_{62}H_{101}O_{36}$ [M+H]+ $C_{62}H_{103}O_{36}$	1422.615090 1421.607265 1423.622915		
		$C_{56}H_{94}0_{27}$ [M-H]- $C_{56}H_{93}0_{27}$ [M+H]+ $C_{56}H_{95}0_{27}$	1198.598254 1197.590430 1199.606080		

		$C_{62}H_{104}O_{32}$ [M-H]- $C_{62}H_{103}O_{32}$ [M+H]+ $C_{62}H_{105}O_{32}$	1360.651080 1359.643255 1361.658905		
		-	-		
		$C_5H_{11}NO_3S_2$ [M-H]- $C_5H_{10}NO_3S_2$ [M+H]+ $C_5H_{12}NO_3S_2$	197.018038 196.010213 198.025863		

		$C_{10}H_{18}N_2O_6S_2$ [M-H]- $C_{10}H_{17}N_2O_6S_2$ [M+H]+ $C_{10}H_{19}N_2O_6S_2$	326.060632 325.052807 327.068456		
		$C_4H_9NO_3S$ [M-H]- $C_4H_8NO_3S$ [M+H]+ $C_4H_{10}NO_3S$	151.030316 150.022491 152.038141		

		$C_6H_{13}NO_3S$ [M-H]- $C_6H_{12}NO_3S$ [M+H]+ $C_6H_{14}NO_3S$	179.061616 178.053791 180.069440		
		$C_7H_{10}N_20_3S$ [M-H]- $C_7H_9N_20_3S$ [M+H]+ $C_7H_{11}N_20_3S$	202.041215 201.033390 203.049040		

		$C_8H_{10}N_2O_3S$ [M-H]- $C_8H_9N_2O_3S$ [M+H]+ $C_8H_{11}N_2O_3S$	214.041215 213.033390 215.049040		
		$C_8H_{10}N_2O_3S$ [M-H]- $C_8H_9N_2O_3S$ [M+H]+ $C_8H_{11}N_2O_3S$	214.041215 213.033390 215.049040		

		$C_{18}H_{36}O$ [M-H]- $C_{18}H_{35}O$ [M+H]+ $C_{18}H_{37}O$	268.276615 267.268789 269.284440		
		C_2H_6O [M-H]- C_2H_5O [M+H]+ C_2H_7O	46.041865 45.034040 47.049690		
		$C_{29}H_{50}O$ [M-H]- $C_{29}H_{49}O$ [M+H]+ $C_{29}H_{51}O$	414.386165 413.378340 415.393990		

		$C_{29}H_{46}$ [M-H]- $C_{29}H_{45}$ [M+H]+ $C_{29}H_{47}$	394.359950 393.352125 395.367775		
		$C_{19}H_{40}O$ [M-H]- $C_{19}H_{39}O$ [M+H]+ $C_{19}H_{41}O$	284.307915 283.300090 285.315740		
		$C_{15}H_{32}O$ [M-H]- $C_{15}H_{31}O$ [M+H]+ $C_{15}H_{33}O$	228.245315 227.237490 229.253140		

		$C_6H_8S_2$ [M-H]- $C_6H_7S_2$ [M+H]+ $C_6H_9S_2$	144.006744 142.998919 145.014569		
		$C_{21}H_{20}O_{11}$ [M-H]- $C_{21}H_{19}O_{11}$ [M+H]+ $C_{21}H_{21}O_{11}$	448.100564 447.092740 449.108390		

		$C_{21}H_{20}O_{12}$ [M-H]- $C_{21}H_{19}O_{12}$ [M+H]+ $C_{21}H_{21}O_{12}$	464.095480 463.087655 465.103305		

		Kaempferol 3-O-glucoside-7-O-glucuronide $C_{27}H_{28}O_{17}$ [M-H]- $C_{27}H_{27}O_{17}$ [M+H]+ $C_{27}H_{29}O_{17}$	624.132655 623.124830 625.140480		

		Kaempferol 3-neohesperidoside $C_{27}H_{30}O_{15}$ [M-H]- $C_{27}H_{29}O_{15}$ [M+H]+ $C_{27}H_{31}O_{15}$	594.158475 593.150650 595.166300		
		$C_{27}H_{30}O_{16}$ [M-H]- $C_{27}H_{29}O_{16}$ [M+H]+ $C_{27}H_{31}O_{16}$	610.153390 609.145565 611.161215		

		Quercetin 3-glucoside-7-glucuronide $C_{27}H_{28}O_{18}$ [M-H]- $C_{27}H_{27}O_{18}$ [M+H]+ $C_{27}H_{29}O_{18}$	640.127570 639.119745 641.135395		
		quercetin 3,7-di-O-β-D-glucoside Quercetin 3,7-diglucoside $C_{27}H_{30}O_{17}$ [M-H]- $C_{27}H_{29}O_{17}$ [M+H]+ $C_{27}H_{31}O_{17}$	626.148305 625.140480 627.156130		

		$C_9H_8O_3$ [M-H]- $C_9H_7O_3$ [M+H]+ $C_9H_9O_3$	164.047345 163.039520 165.055170		
		$C_{27}H_{30}O_{16}$ [M-H]- $C_{27}H_{29}O_{16}$ [M+H]+ $C_{27}H_{31}O_{16}$	610.153390 609.145565 611.161215		

([1] Laurian Vlase, Marcel Parvu, Elena Alina Parvu, and Anca Toiu. Chemical Constituents of Three Allium Species from Romania, 2012; [2] D.I.Stajner, A.Kapor, Exploring Allium species as a Source of Potential Medicinal Agents, 2006; [3] Kusterer, J., Fritsch, R. M., & Keusgen, M. (2011). Allium Species from Central and Southwest Asia Are Rich Sources of Marasmin. Journal of Agricultural and Food Chemistry, 59(15), 8289–8297.; [4] Modern state of the study of some plants of the genus Allium L.: a review article [5] Kuroda, M., Ori, K., Takayama, H., Sakagami, H., & Mimaki, Y. (2015). Karataviosides G–K, five new bisdesmosidic steroidal glycosides from the bulbs of Allium karataviense. Steroids, 93, 96–104. doi:10.1016/j.steroids.2014.09.010; [6] de Guzman Alvindia, D., Mangoba, M.A.A. Bioactivities of *Allium longicuspis* Regel against anthracnose of mango caused by *Colletotrichum gloeosporioides* (Penz.). Scientific Reports volume 10, Article number: 11367 (2020), [7] D. N. Olennikov. Flavonol glycosides from leaves of Allium microdictyon. Chemistry of Natural Compounds, Vol. 56, No. 6, November, 2020. 56(6):1035-1039)