



UNIwersytet
WARSAWSKI



WYDZIAŁOWE LABORATORIUM
POMIAROWE - SEKCJA MS

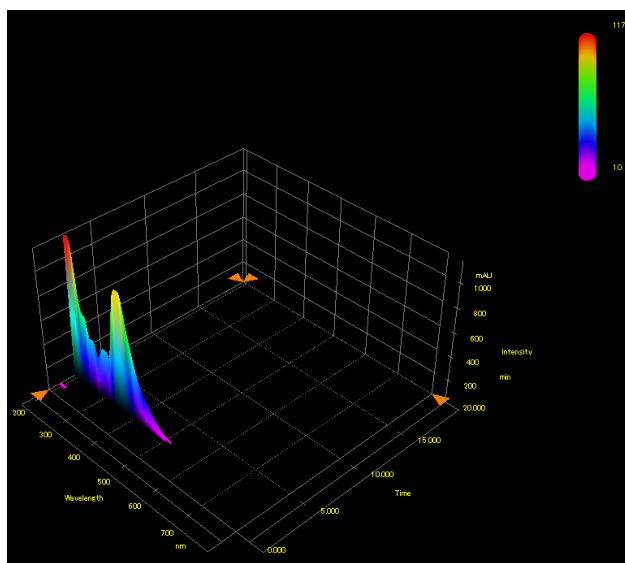
Metoda

Gradient 50%-97% B w 9.5 min

kolumna Kinetex C18 2.6 μ m 150 x 2.1 mm

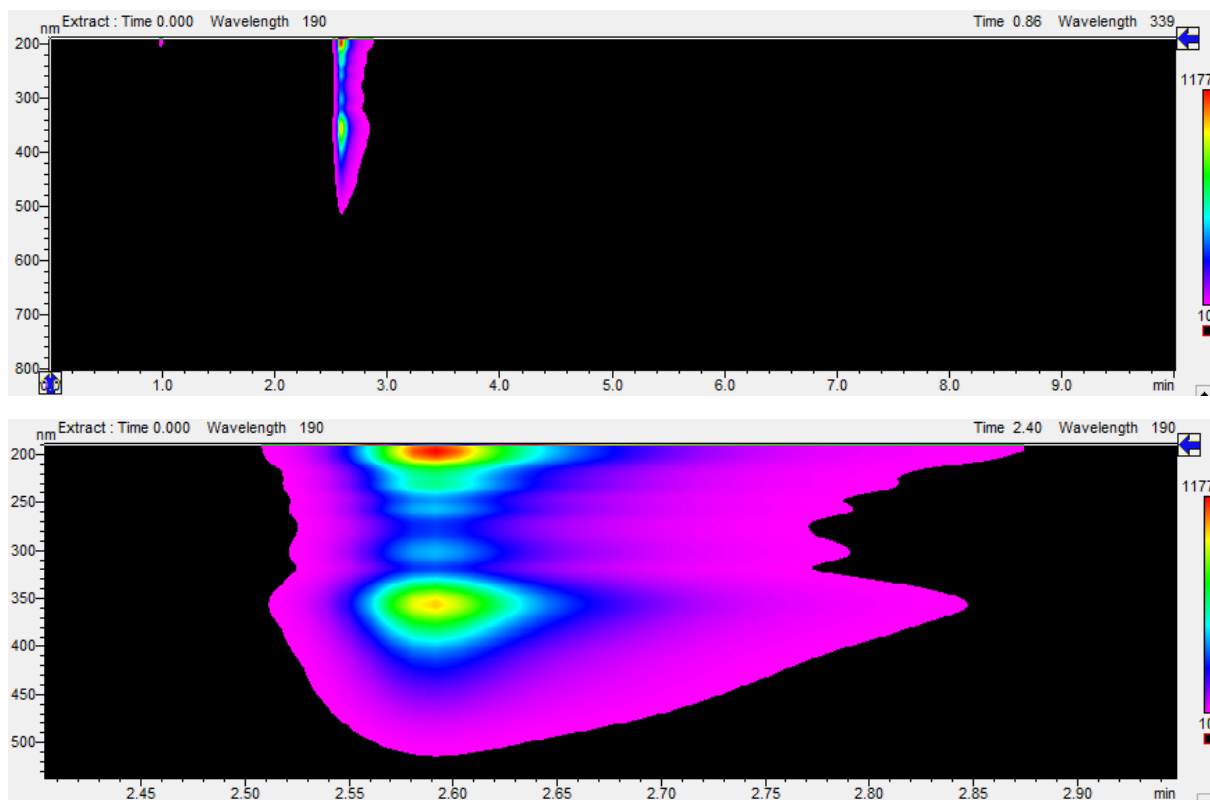
SB

3D Contour



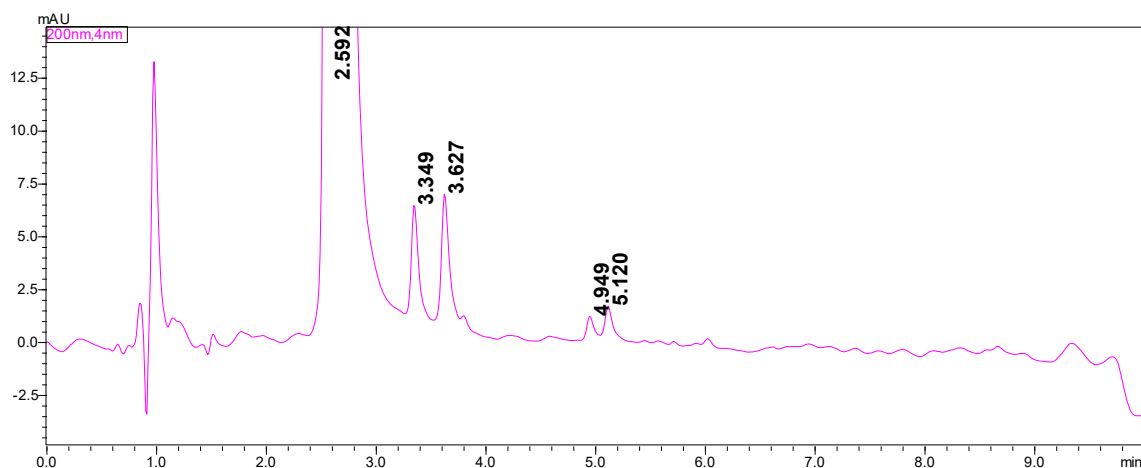
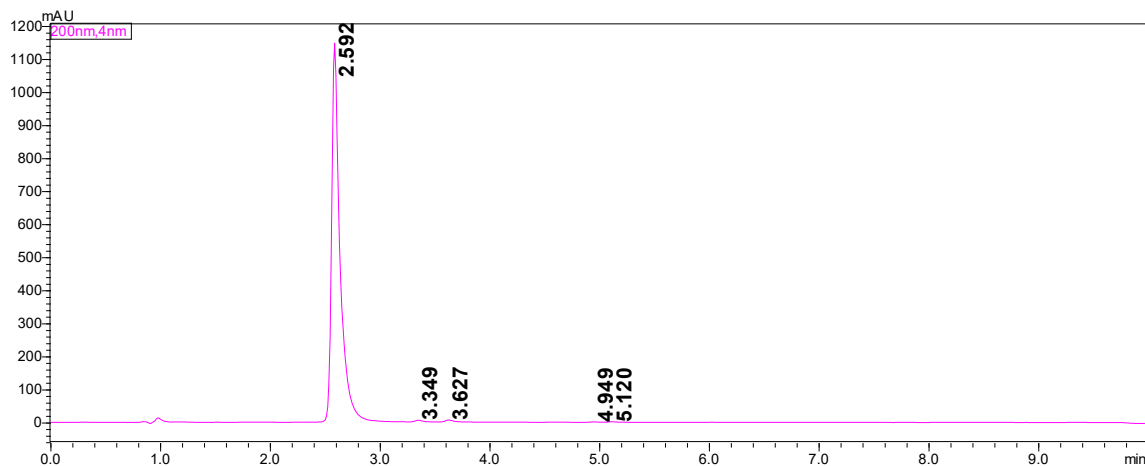


2D Contour





PDA 200 nm

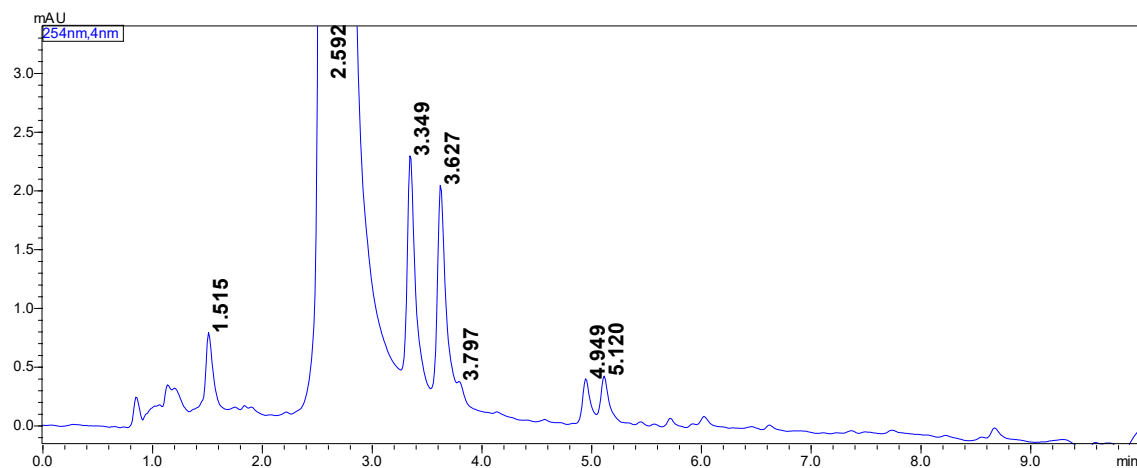
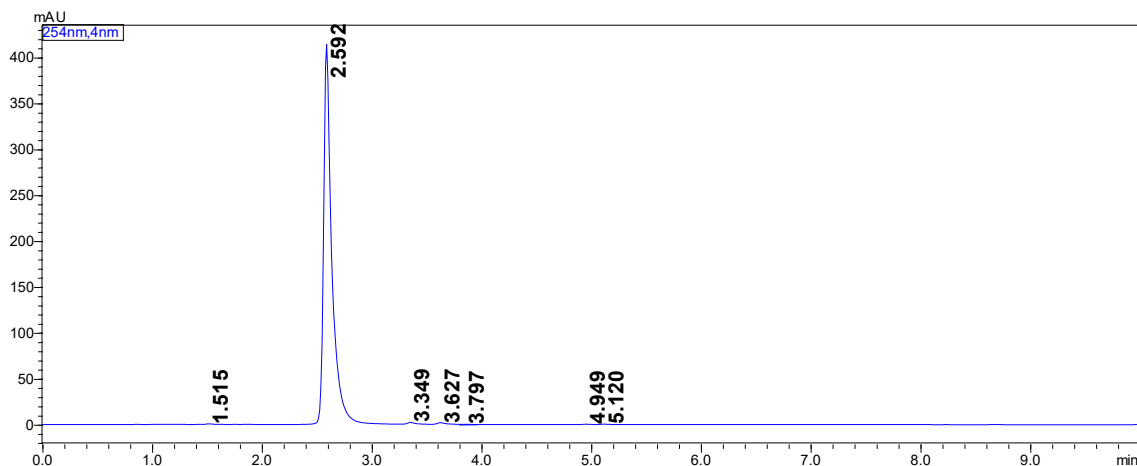


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.592	6120429	1147031	98.977
2	3.349	22518	5158	0.364
3	3.627	27119	5849	0.439
4	4.949	4706	1117	0.076
5	5.12	8936	1615	0.145
Total		6183707	1160771	100



PDA 254 nm

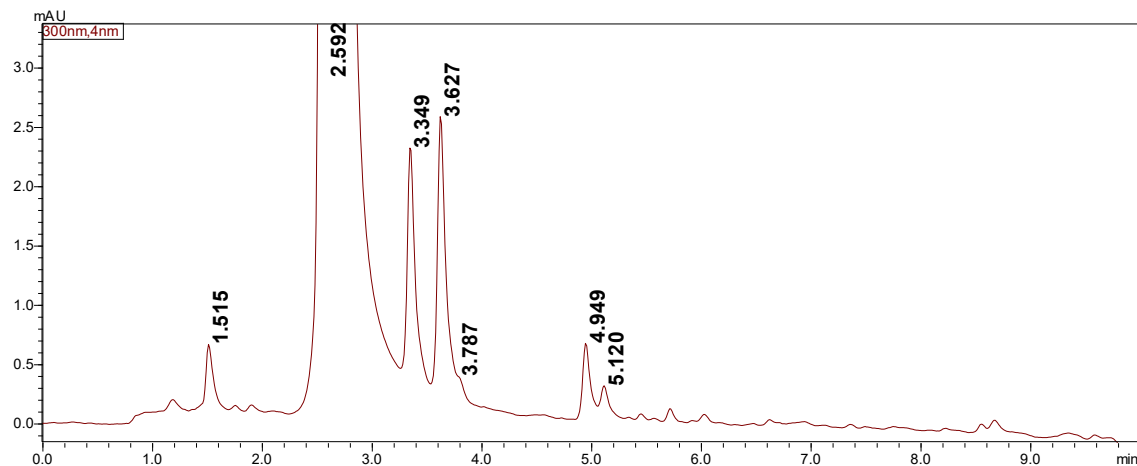
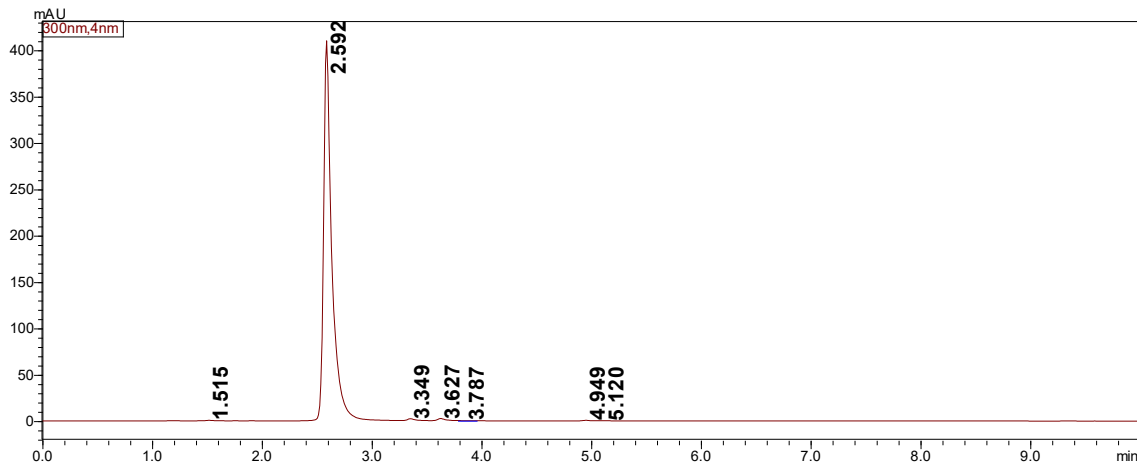


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	1.515	3166	661	0.145
2	2.592	2159149	413771	98.806
3	3.349	9102	1870	0.417
4	3.627	9233	1766	0.423
5	3.797	675	173	0.031
6	4.949	1835	375	0.084
7	5.12	2083	398	0.095
Total		2185243	419013	100



PDA 300 nm

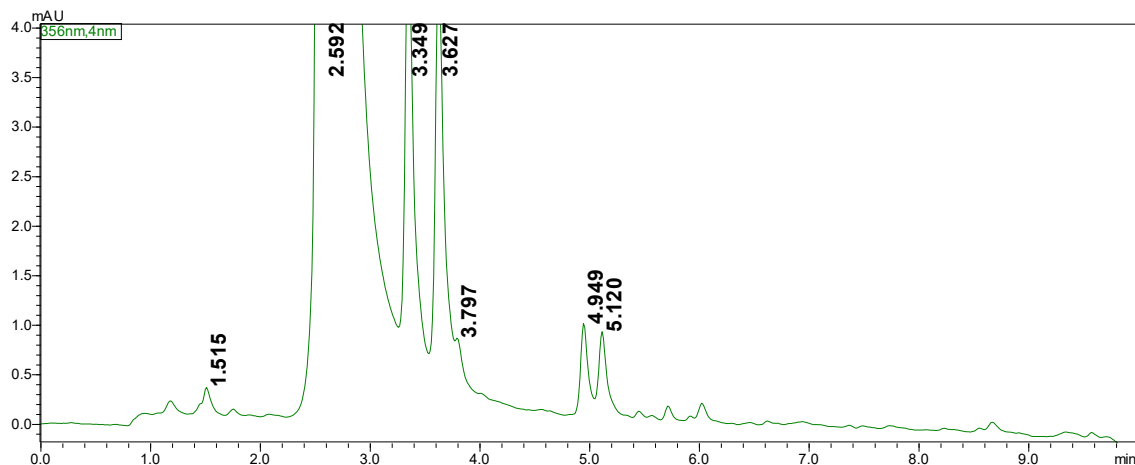
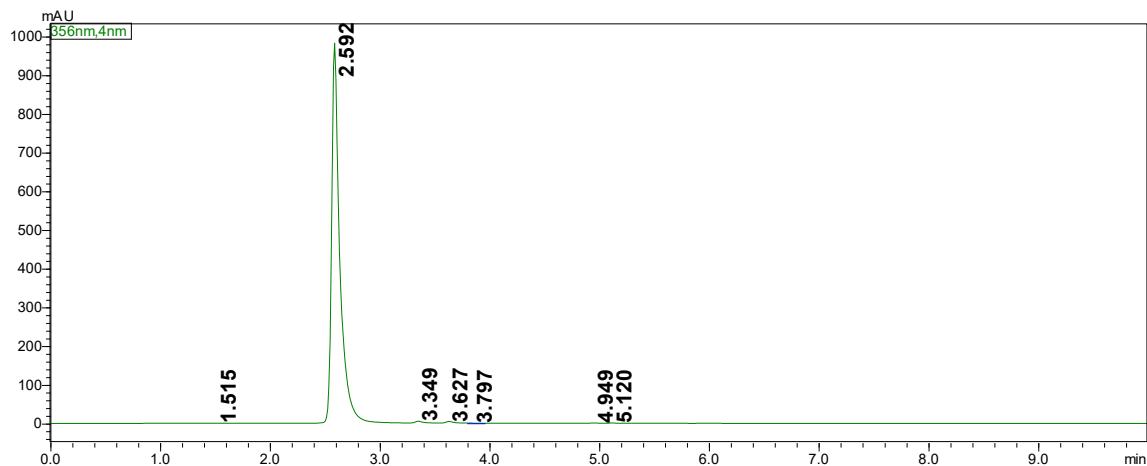


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	1.515	4940	653	0.227
2	2.592	2142645	409891	98.549
3	3.349	9299	1899	0.428
4	3.627	12120	2292	0.557
5	3.787	575	175	0.026
6	4.949	3190	637	0.147
7	5.12	1418	274	0.065
Total		2174187	415822	100



PDA 356 nm

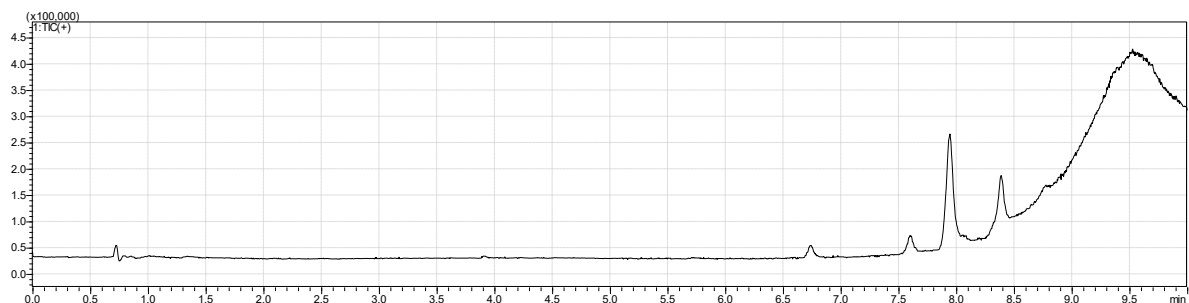


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	1.515	1353	257	0.026
2	2.592	5107592	982259	98.931
3	3.349	21676	4441	0.42
4	3.627	21611	4198	0.419
5	3.797	1648	392	0.032
6	4.949	4356	918	0.084
7	5.12	4524	838	0.088
Total		5162760	993303	100



TIC (+) blank

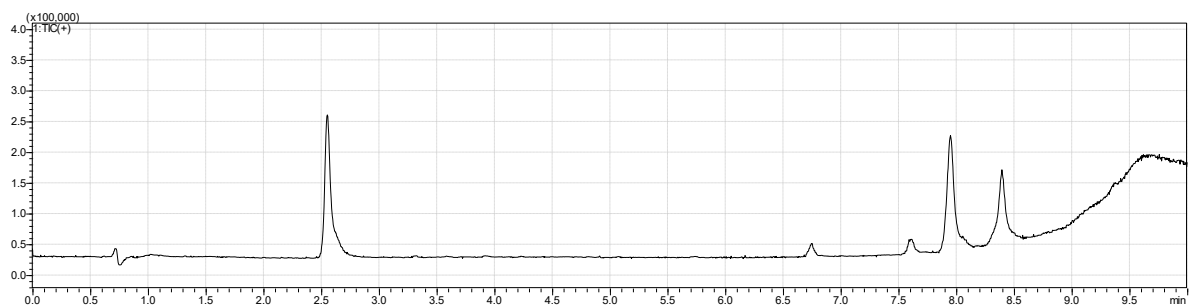


SB

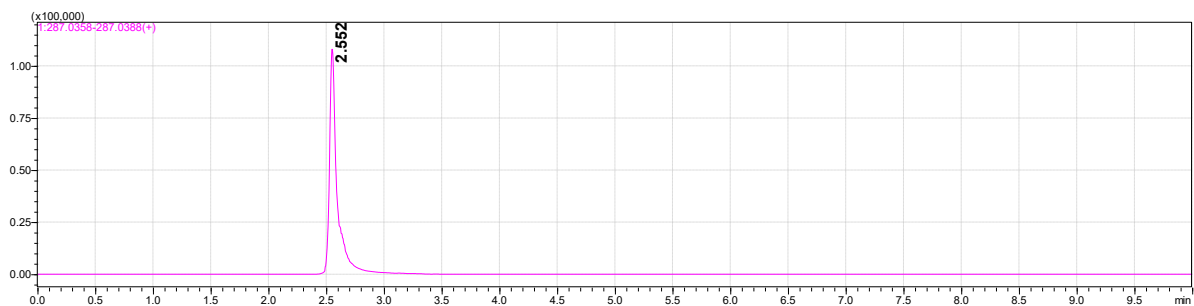
C₁₅H₁₀O₄S

$[M+H]^+_{\text{theo}} = 287.0373 \text{ m/z}$

TIC (+) SB



XIC (+) 287.0373 m/z



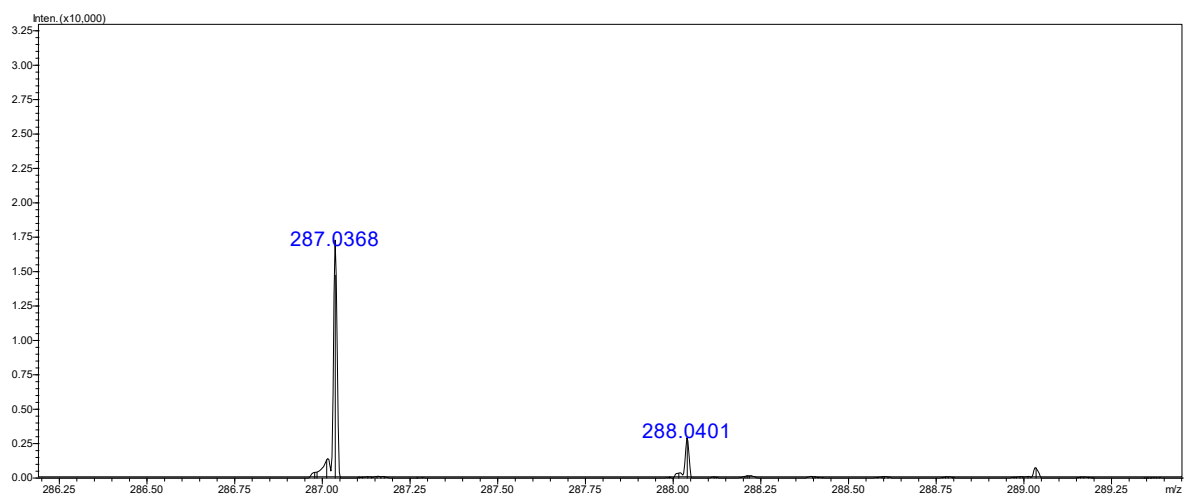
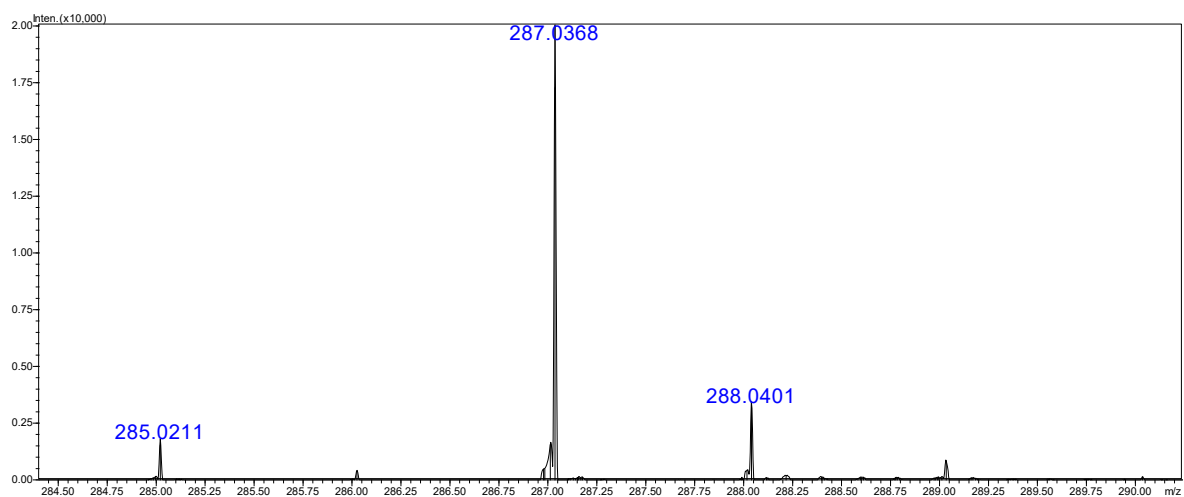
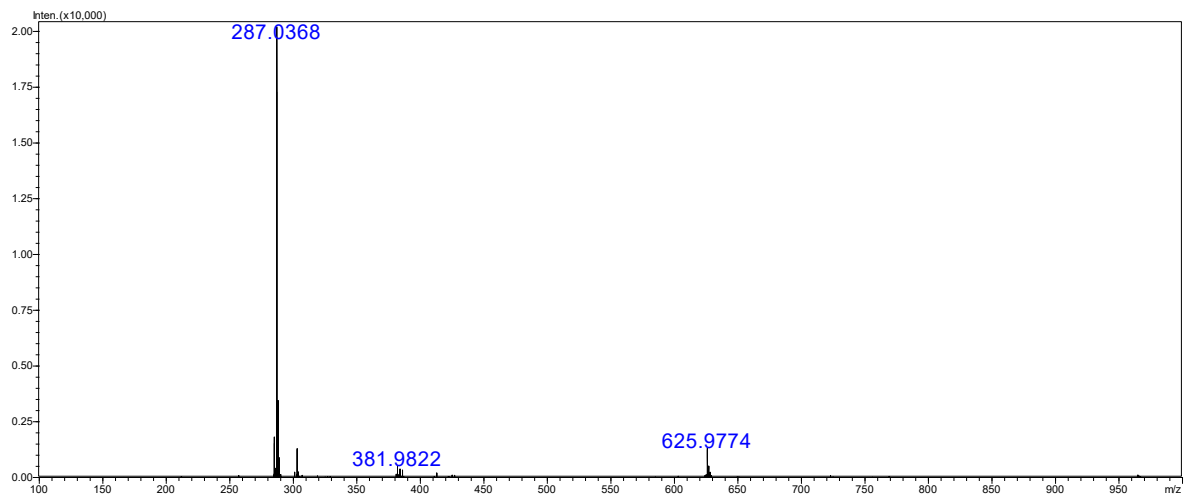


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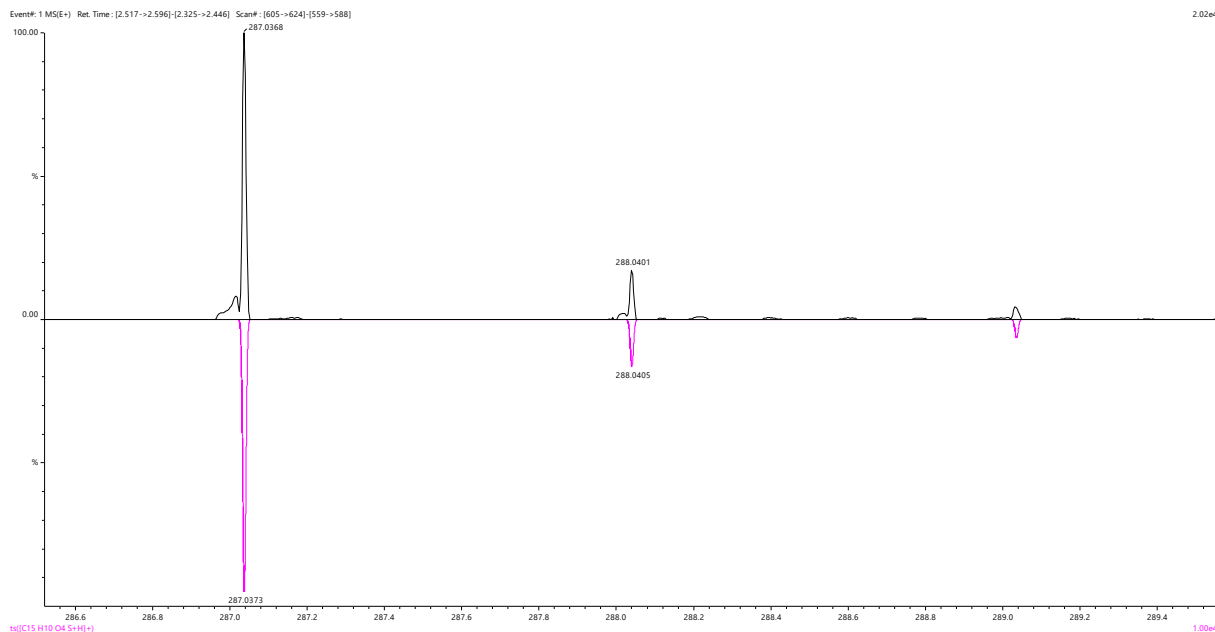
WYDZIAŁOWE LABORATORIUM
POMIAROWE - SEKCJA MS

MS @ RT 2.55





Isotopic Distribution 287.0368 m/z



Formula Predictor

#	Score	Pred. (M)	Pred. m/z	Meas. m/z	Diff. (mDa)	Formula (M)	Ion	Diff. (ppm)	Iso Score	DBE
1	74.57	286.02998	287.03726	287.03684	-0.42	C15 H10 O4 S	[M+H] ⁺	-1.451	71.74	11.0