



UNIwersYTET
WARSAWSKI



WYDZIAŁOWE LABORATORIUM
POMIAROWE - SEKCJA MS

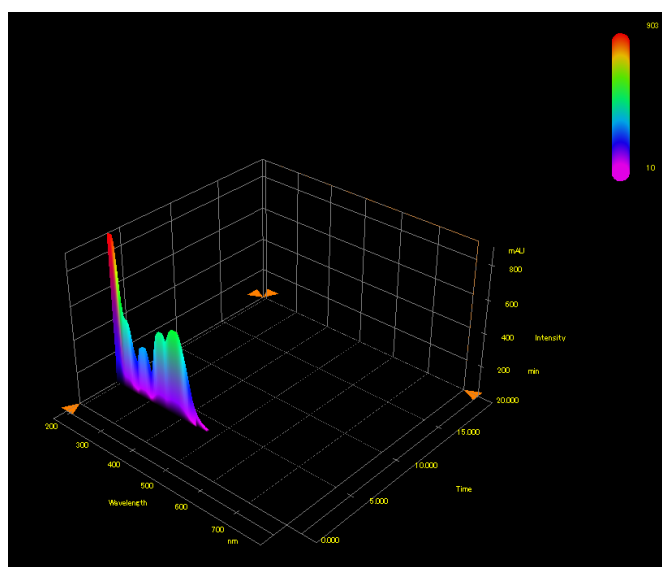
Metoda

Gradient 50%-97% B w 9.5 min

kolumna Kinetex C18 2.6 μ m 150 x 2.1 mm

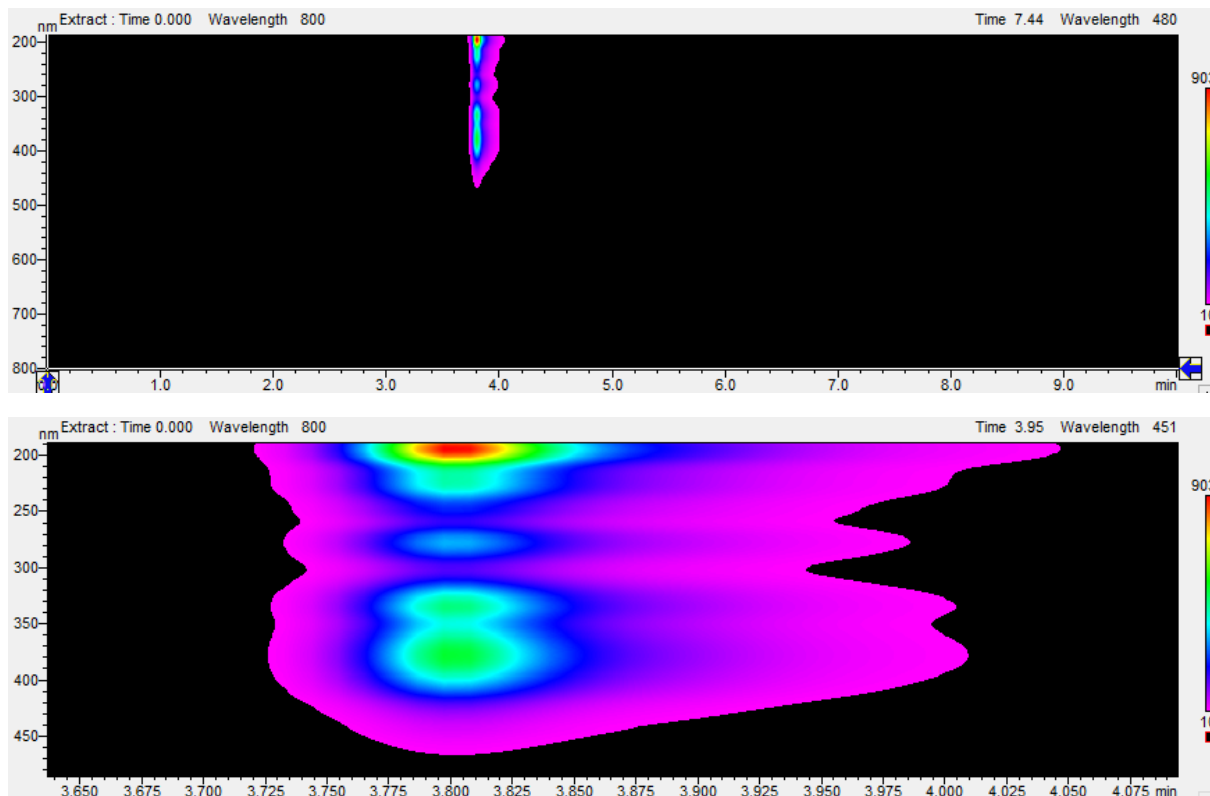
SCh_1

3D Contour



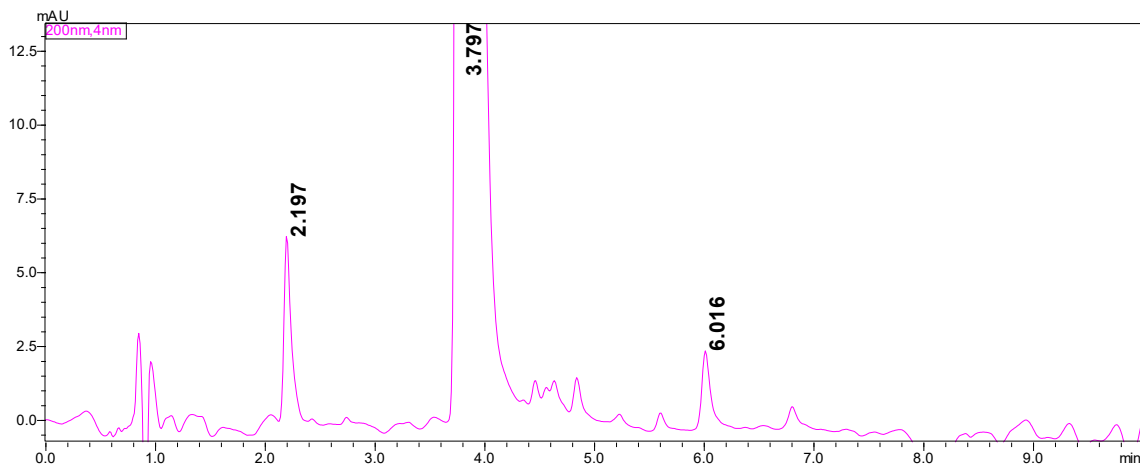
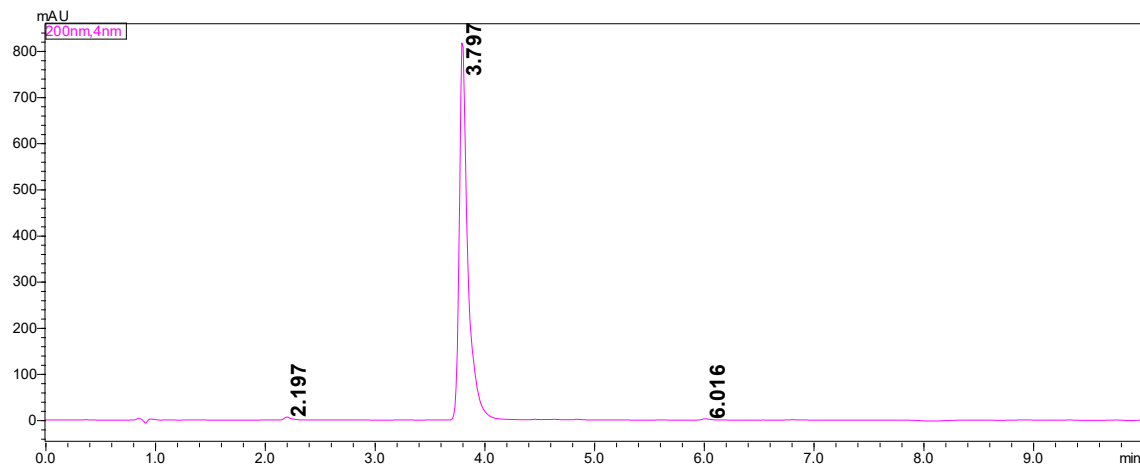


2D Contour





PDA 200 nm

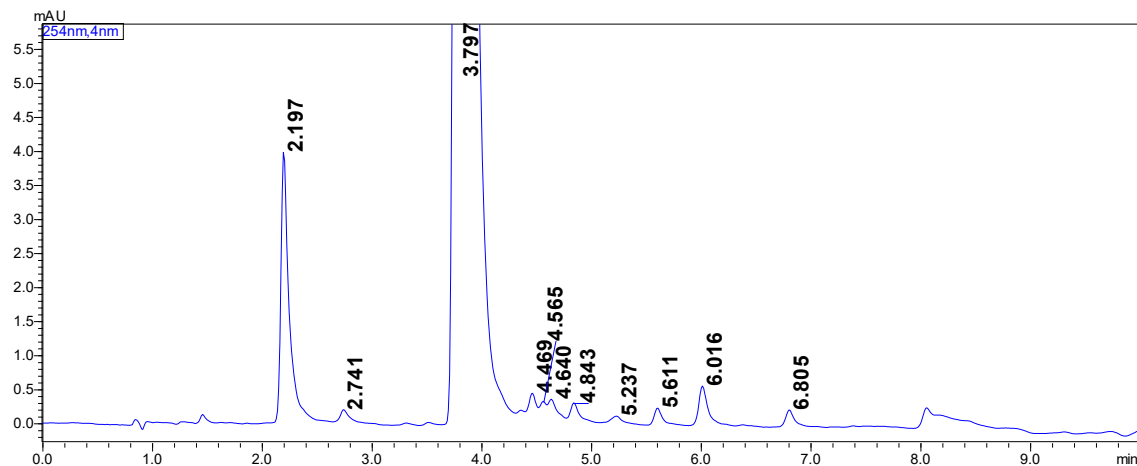
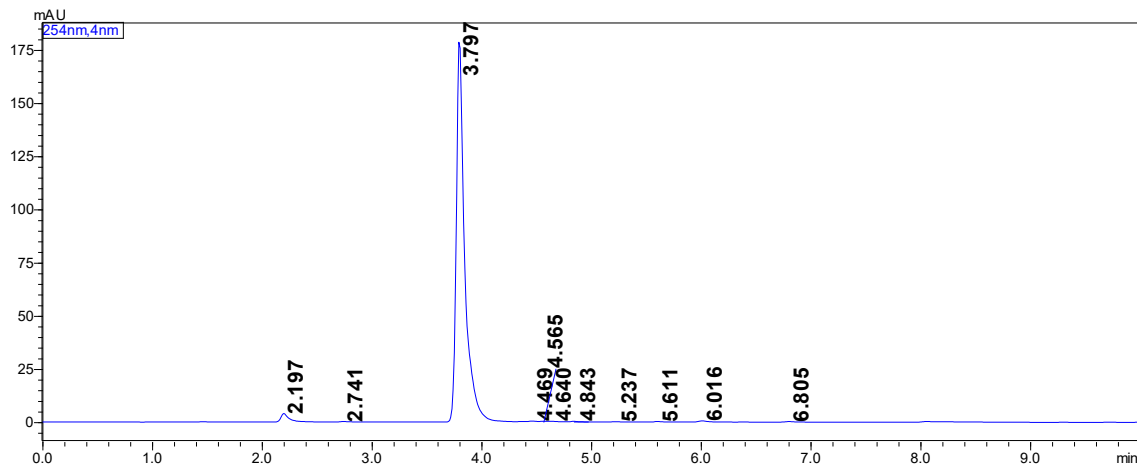


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.197	26988	6105	0.606
2	3.797	4419693	816733	99.171
3	6.016	9947	2224	0.223
Total		4456628	825061	100



PDA 254 nm

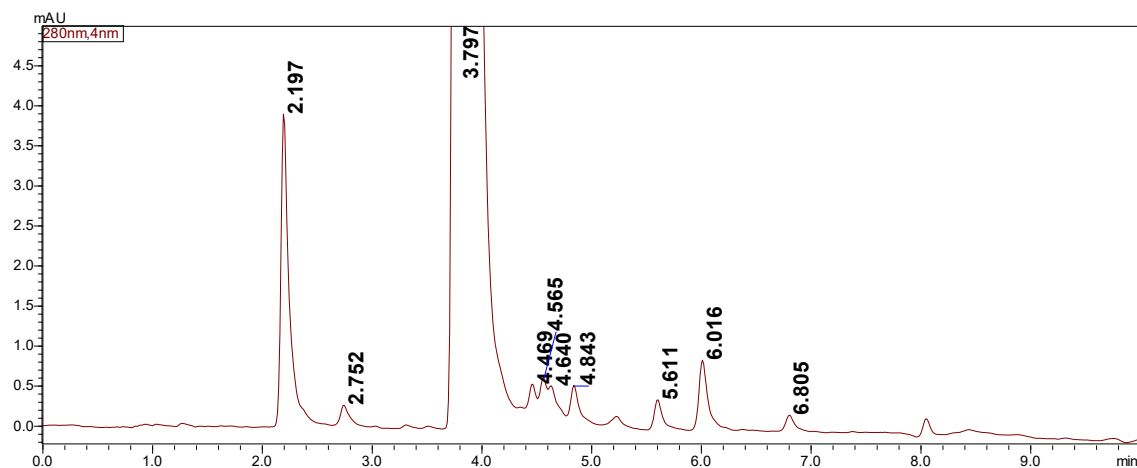
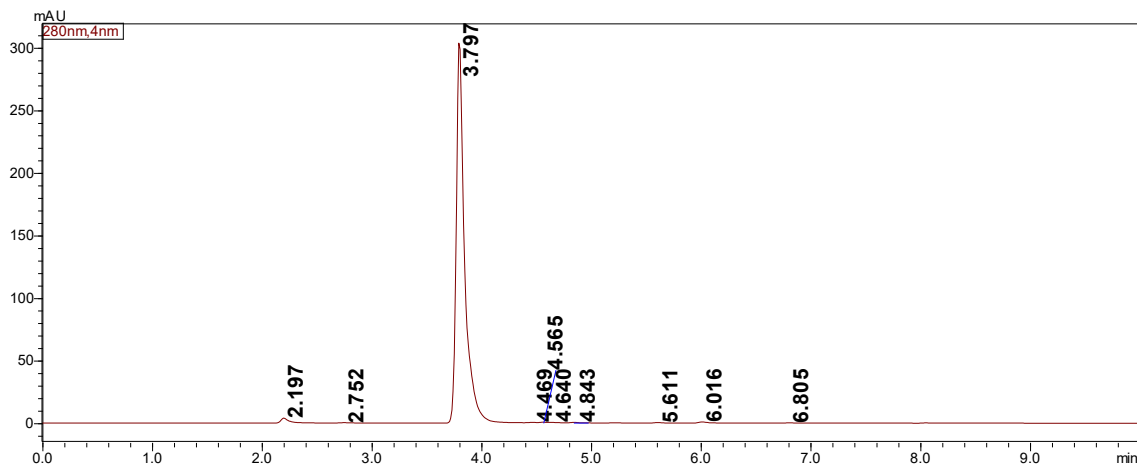


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.197	20442	3961	2.062
2	2.741	1022	182	0.103
3	3.797	959577	178522	96.803
4	4.469	1092	284	0.11
5	4.565	681	191	0.069
6	4.64	1140	240	0.115
7	4.843	1126	240	0.114
8	5.237	495	91	0.05
9	5.611	1225	243	0.124
10	6.016	3159	575	0.319
11	6.805	1310	244	0.132
Total		991269	184773	100



PDA 280nm

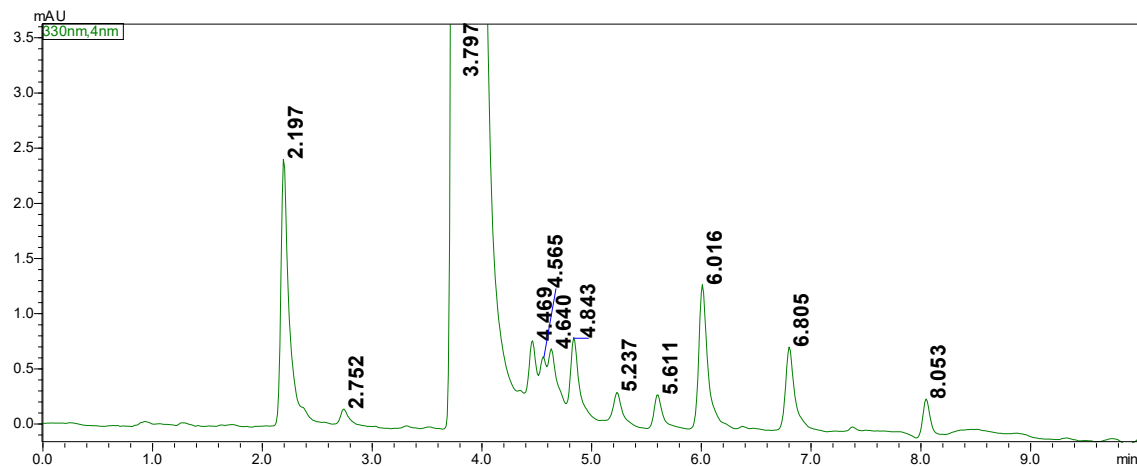
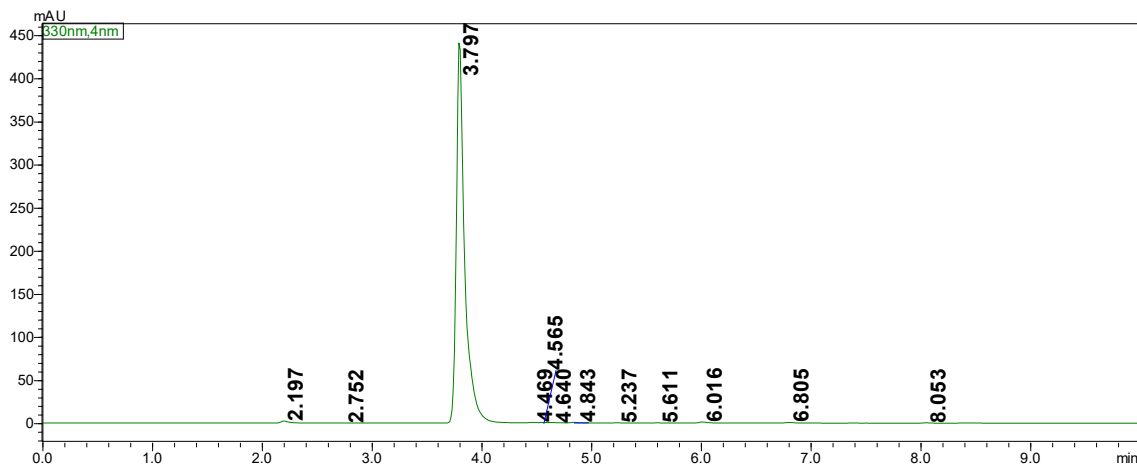


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.197	21206	3905	1.279
2	2.752	1467	254	0.088
3	3.797	1620357	303613	97.726
4	4.469	1255	327	0.076
5	4.565	1849	437	0.111
6	4.64	1783	354	0.108
7	4.843	2079	422	0.125
8	5.611	1912	369	0.115
9	6.016	5019	871	0.303
10	6.805	1138	202	0.069
Total		1658065	310755	100



PDA 330 nm

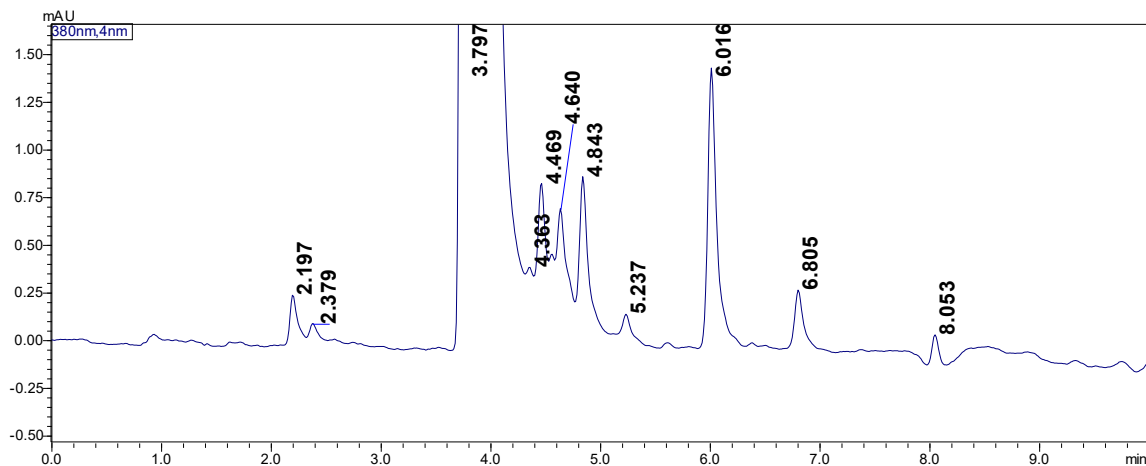
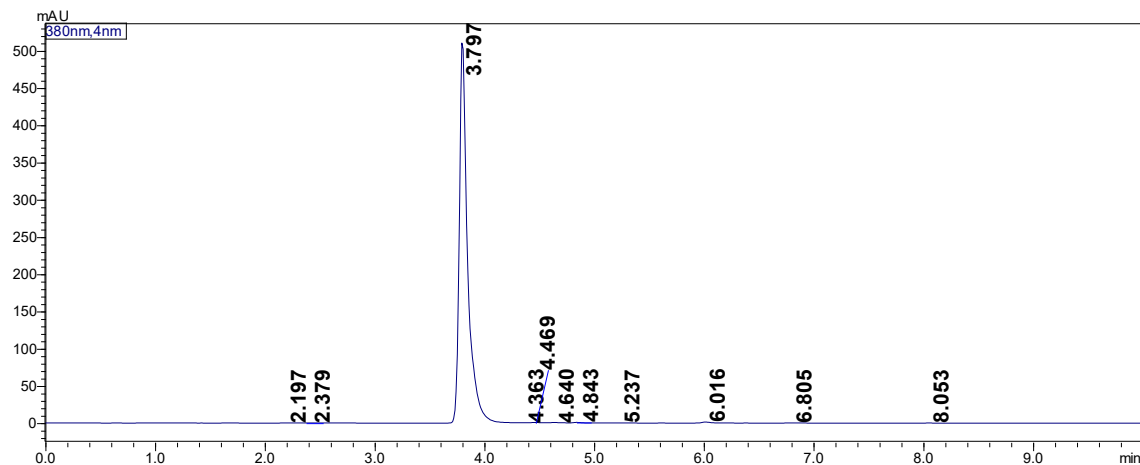


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.197	12634	2408	0.532
2	2.752	754	141	0.032
3	3.797	2337366	440816	98.333
4	4.469	2066	503	0.087
5	4.565	1449	392	0.061
6	4.64	2665	492	0.112
7	4.843	3359	668	0.141
8	5.237	1320	261	0.056
9	5.611	1641	304	0.069
10	6.016	7556	1307	0.318
11	6.805	4408	752	0.185
12	8.053	1771	349	0.075
Total		2376989	448392	100



PDA 380 nm

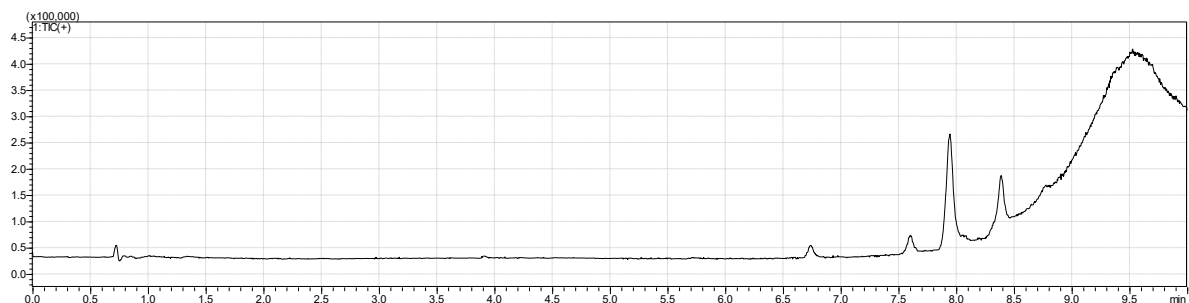


Purity (% peak area)

Peak#	Ret. Time	Area	Height	Area%
1	2.197	1298	258	0.048
2	2.379	786	108	0.029
3	3.797	2700013	510327	99.286
4	4.363	97	42	0.004
5	4.469	1496	436	0.055
6	4.64	1380	333	0.051
7	4.843	3221	692	0.118
8	5.237	478	113	0.018
9	6.016	8317	1459	0.306
10	6.805	1834	311	0.067
11	8.053	521	144	0.019
Total		2719440	514225	100



TIC (+) blank

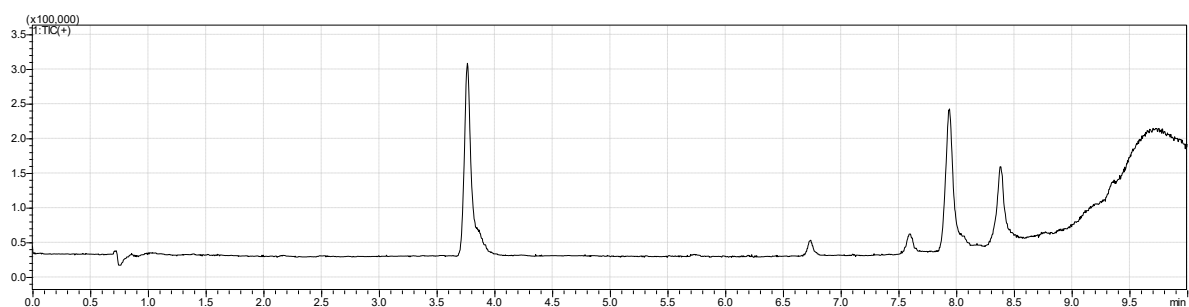


SCh1_1

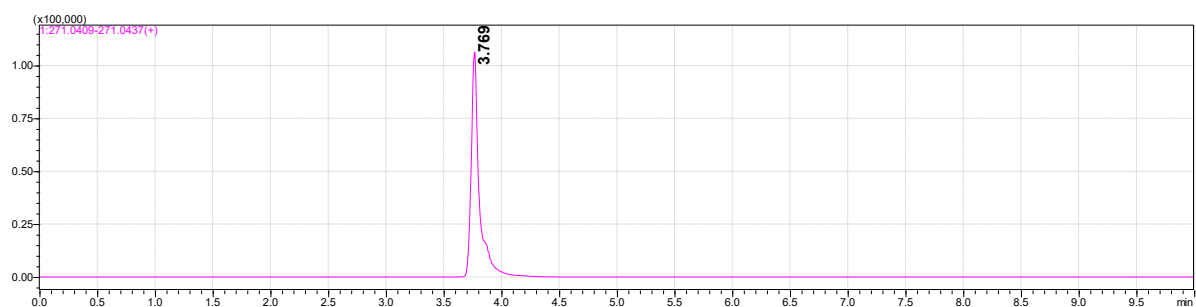
C₁₅H₁₀O₃S

$[M+H]^+_{\text{theo}} = 271.0423 \text{ m/z}$

TIC (+)

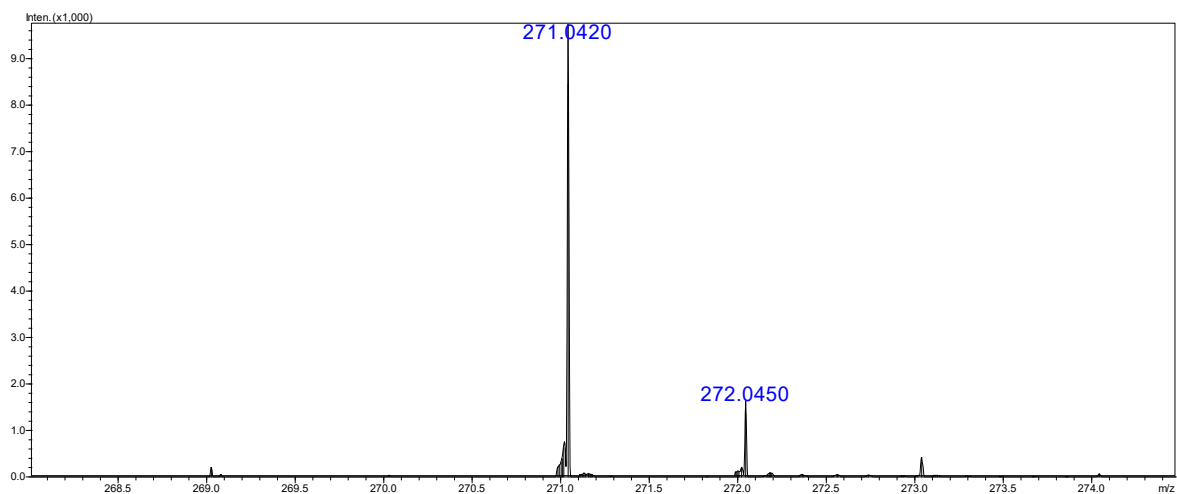
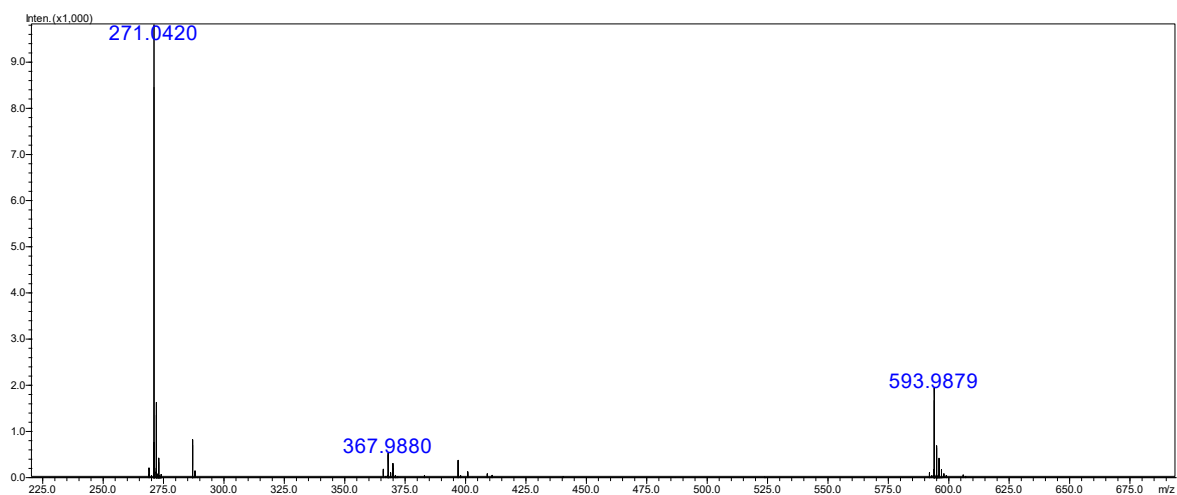
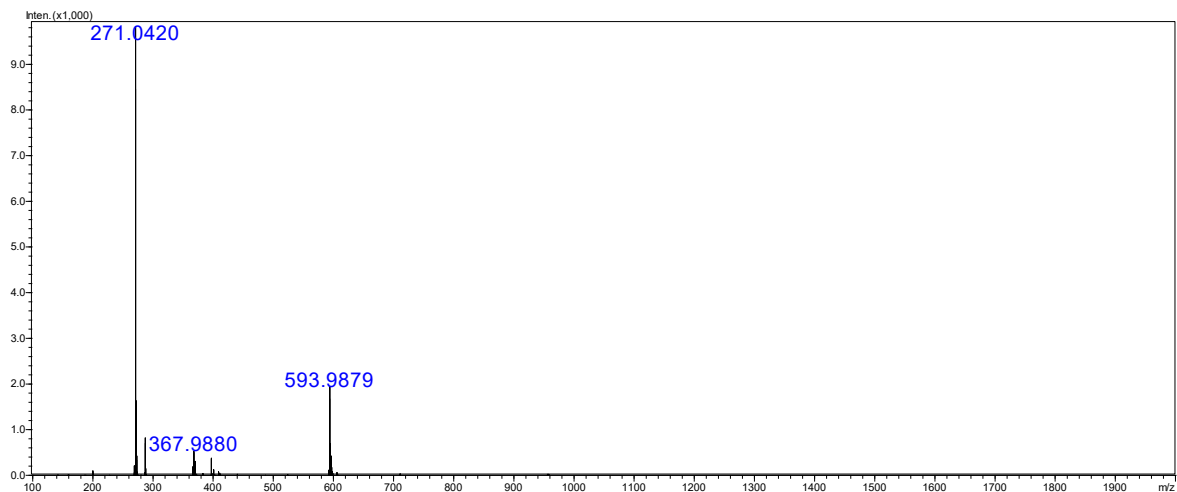


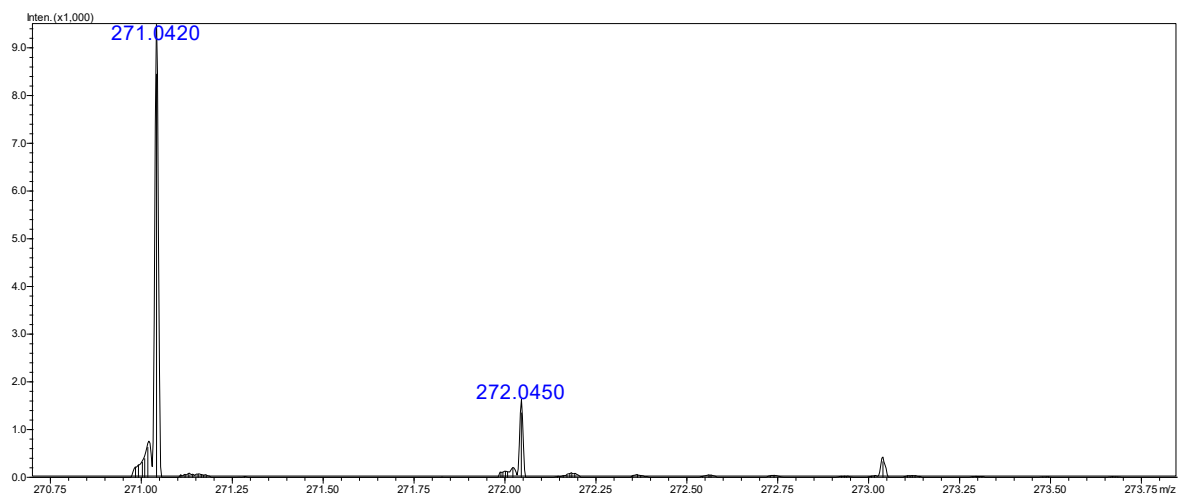
XIC (+) 271.0423 m/z



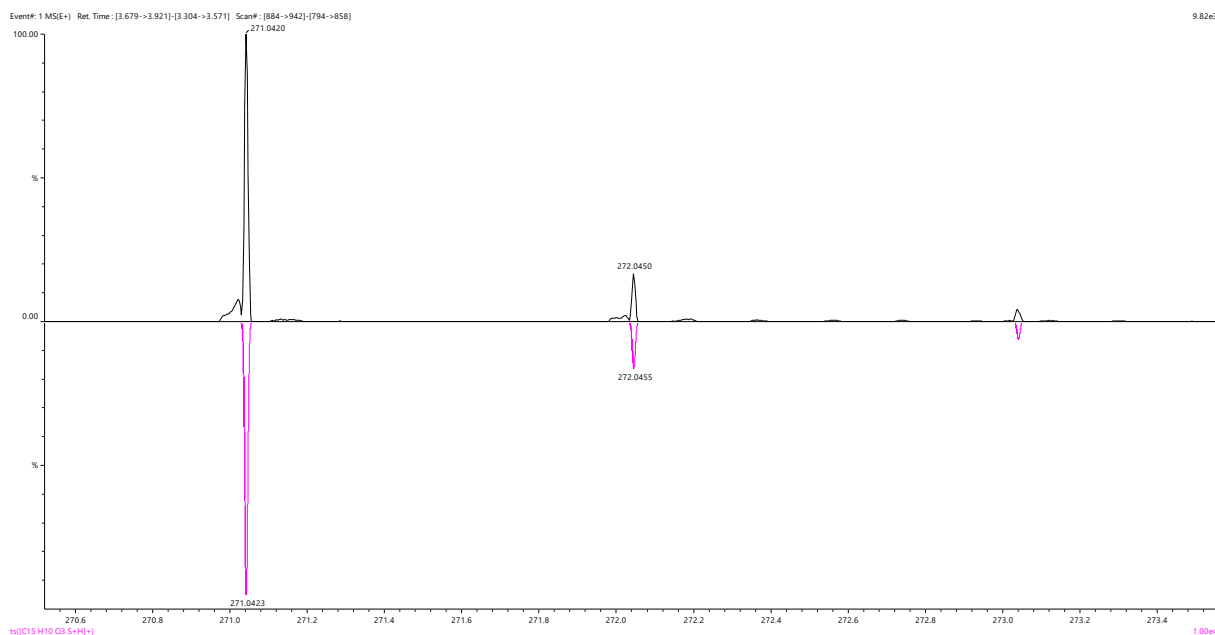


MS @ RT 3.77 min





Isotopic Distribution 271.0420 m/z



Formula Predictor

#	Score	Pred. (M)	Pred. m/z	Meas. m/z	Diff. (mDa)	Formula (M)	Ion	Diff. (ppm)	Iso Score	DBE
1	74.11	270.03507	271.04234	271.04197	-0.37	C15 H10 O3 S	[M+H] ⁺	-1.372	71.23	11.0