SciRad SCIENTIAE RADICES

SUPPLEMANTARY MATERIAL

Preliminary Phytochemical Characterization and Antibacterial Activity of Capparis spinosa L. Leaf Extract with LC-MS-Based Metabolite Profiling

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Table 1. Compounds detected in the hydro-ethanolic extract of *Capparis spinosa L.* using LC/MS analysis, with data analyzed through KNOWITALL software.

Compound Name	Symbol	Molecular formula	Molecular weight	Retention time (min)
Chorismic acid	C1	$C_{10}H_{10}O_6$	227	1.1040
Fraxetin	C2	$C_{10}H_8O_5$	209	1.4956
Fraxidinglucoside	C3	$C_{19}H_{24}O_7$	385	1.5815
1-(1-Hydroxybutyl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4,5,6,7-tetrol	C4	$C_{12}H_{20}O_6$	261	1.6411
6-Phosphogluconate	C5	$C_6H_{13}O_{10}P$	277	4.3266
Dehydrovariabilin	C6	$C_{17}H_{14}O_4$	283	25.512

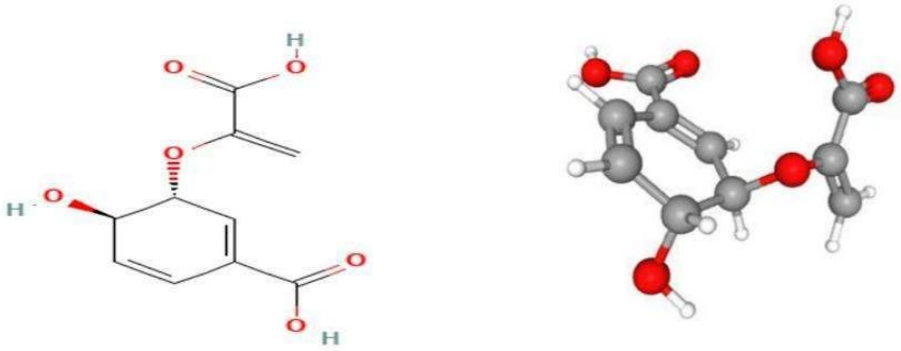


Figure 1 Chemical structure and 3D structure of C1 compound (Chorismic acid).

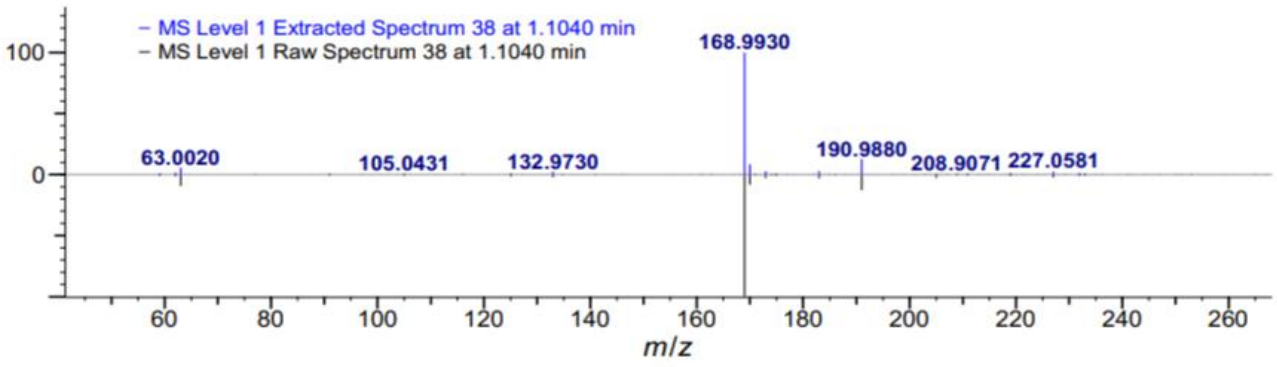


Figure 1.2 Mass spectra of Chorismic acid.

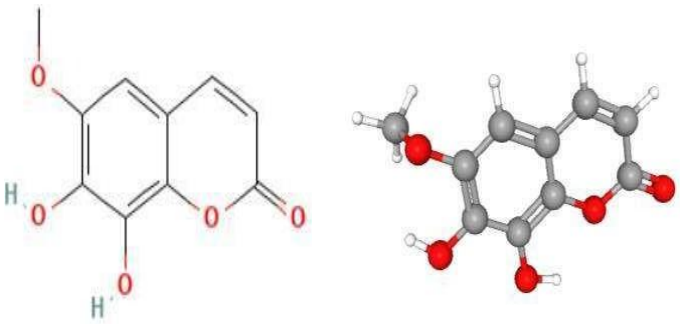


Figure 2 Chemical structure and 3D structure of C2 compound (Fraxetin).

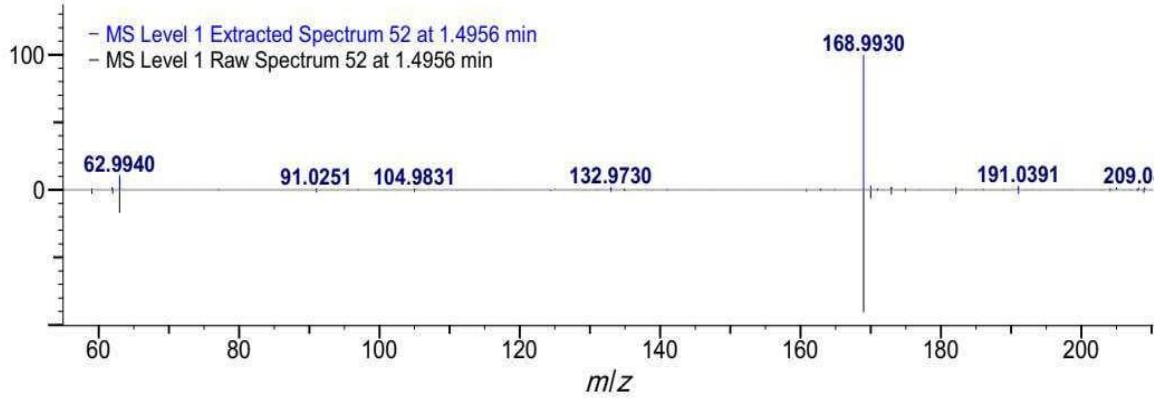


Figure 2..1Mass spectra of Fraxetin

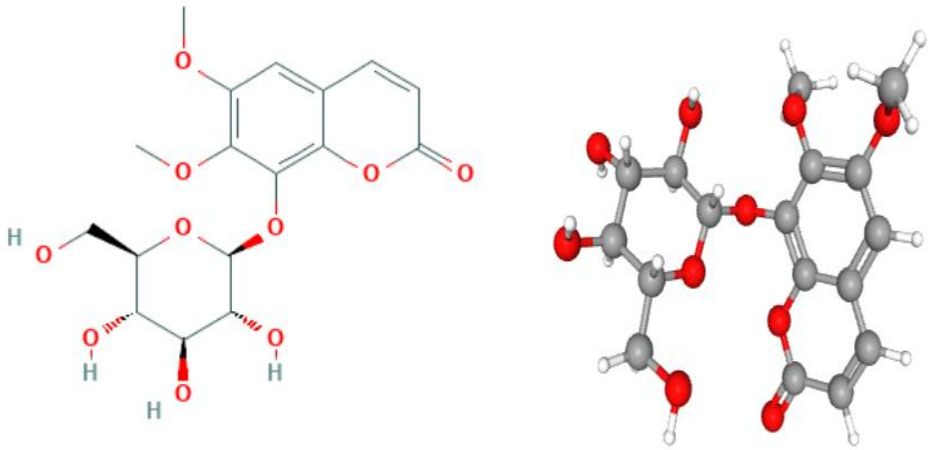
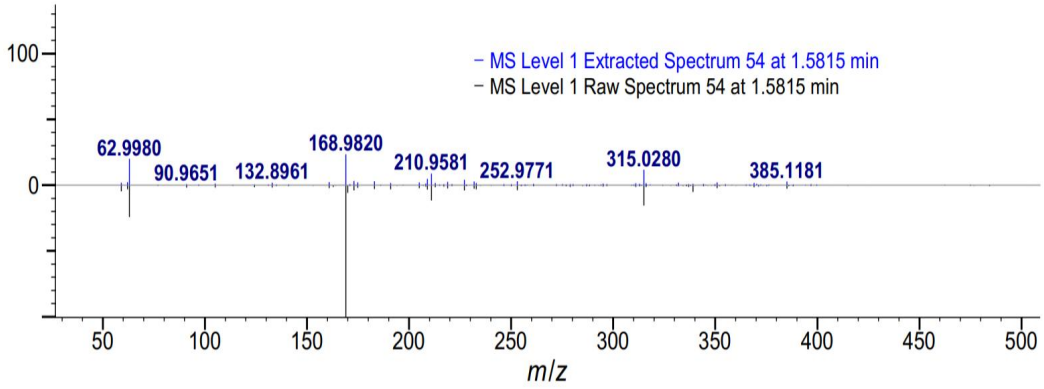


Figure 3. Chemical structure and 3D structure of C3 compound Fraxidinglucoside



C3

Figure 3.1. Mass spectra of Fraxidinglucoside

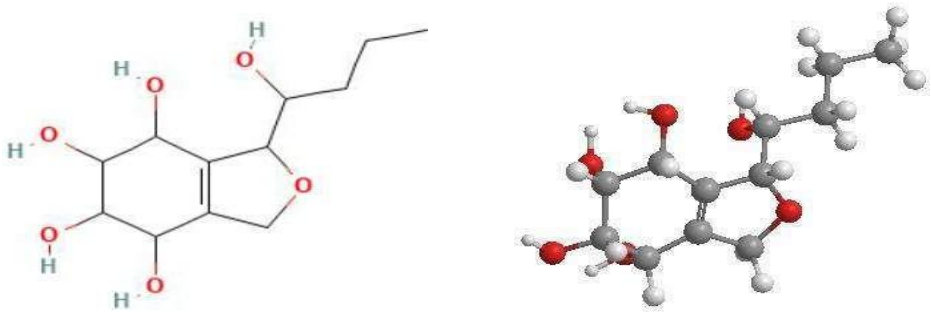


Figure 4. Chemical structure and 3D structure of C4 compound (1-(1-Hydroxybutyl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4,5,6,7-tetrol).

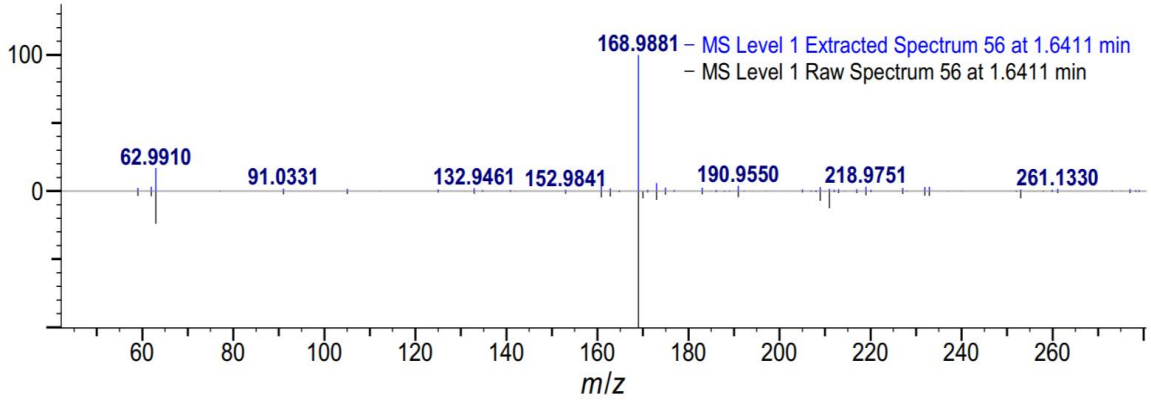


Figure 4..1Mass spectra of 1-(1-Hydroxybutyl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4,5,6,7-tetrol.

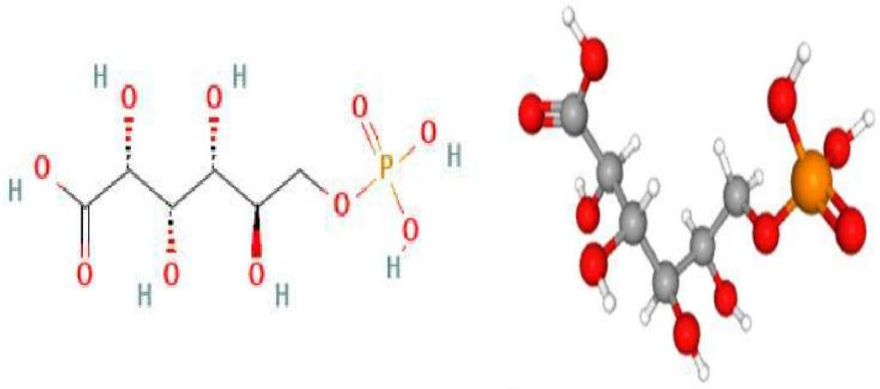


Figure 5. Chemical structure and 3D structure of C5 compound (6-Phosphogluconate).

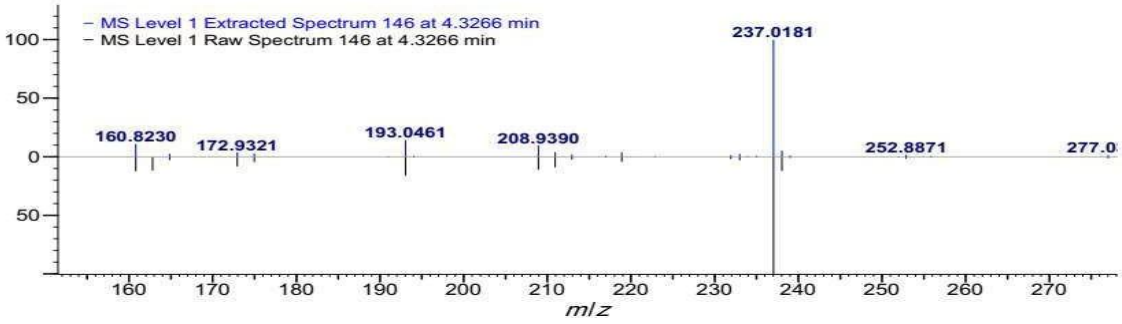


Figure 5..1 Mass spectra of 6-Phosphogluconate.

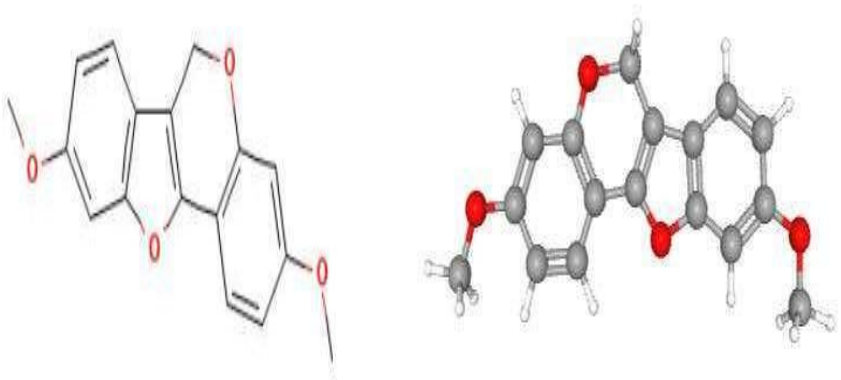


Figure 6. Chemical structure and 3D structure of C6 compound (Dehydrovariabilin).

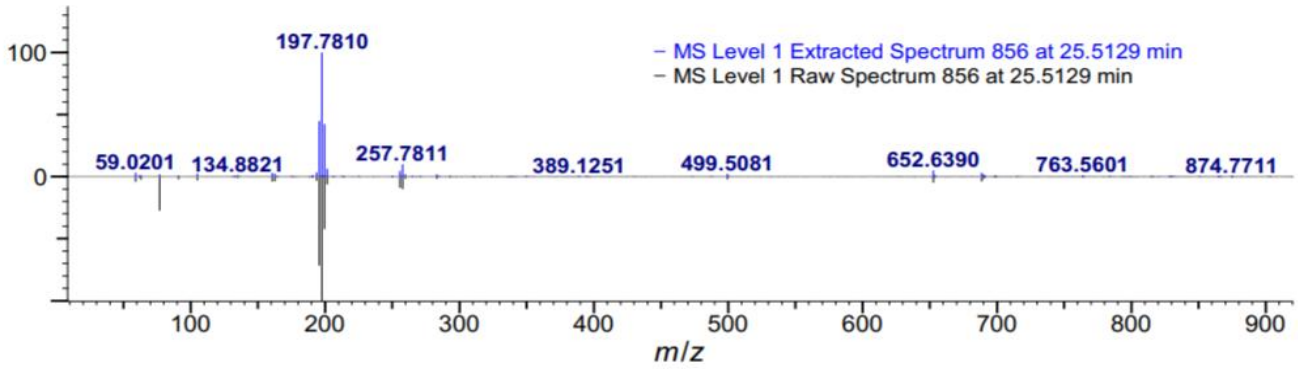


Figure 6.1 Mass spectra of Dehydrovariabilin.

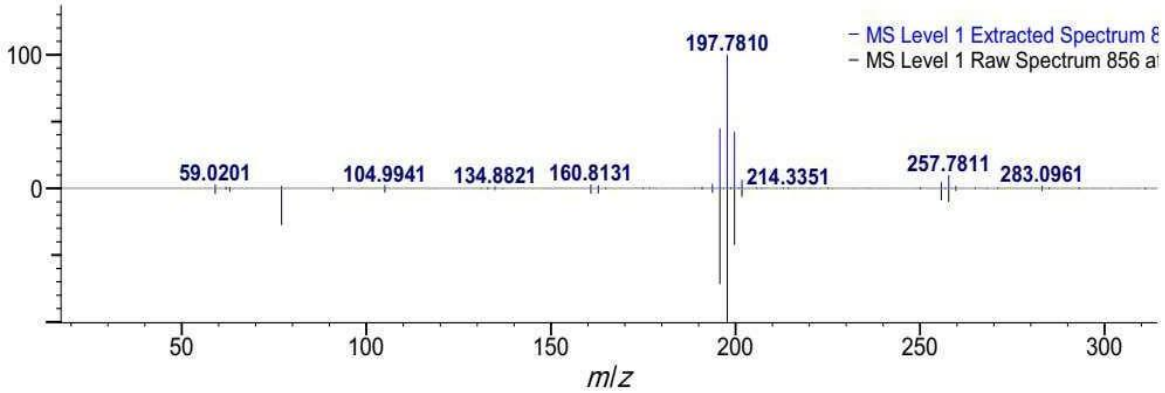


Figure 6.2 Mass spectra of Dehydrovariabilin.

Table 2. uknowing compounds extract by Mnova softwera

Compound	Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error ppm	Error (mDa)	Error (ppm)	Fitness	RT
X1	$C_{16}H_{24}NOS$	279.16514	279.16507	5.5	0.24	-0.07	-0.24	0.925	0.36
X2	$C_7H_{12}N$	111.10425	111.10406	2.5	1.76	-0.19	-1.76	0.987	0.48
X3	$C_{16}H_{30}O_4$	287.22169	287.22305	2.0	4.78	1.37	4.78	0.938	0.54
X4	$C_{14}H_{30}N_4S$	287.22639	287.22604	2.0	1.22	-0.35	-1.22	0.938	0.60
X5	$C_{16}H_{32}N_2OS$	301.23081	301.23206	2.0	4.15	1.24	4.15	0.990	0.78
X6	$C_6H_{19}N_{10}O_6$	328.15618	328.15607	2.5	0.35	-0.11	-0.35	0.977	1.67
X7	$C_{22}H_{21}N_3$	328.18082	328.18106	14.0	0.72	0.24	0.72	0.883	1.85
X8	$C_{10}H_{23}N_4O_6S$	328.14111	328.14105	1.5	0.17	-0.05	-0.17	0.956	1.91
X9	$C_{54}H_{91}N_3O_8S_2$	974.63203	974.63208	11.0	0.05	0.05	0.05	0.517	18.32
X10	$C_{63}H_{91}NOS_3$	974.63356	974.63208	19.0	1.51	-1.47	-1.51	0.426	18.32
X11	$C_{56}H_{87}OS_3$	872.59918	872.60303	13.5	4.41	3.85	4.41	0.420	18.38
X12	$C_{53}H_{83}N_4O_2S_2$	872.60302	872.60303	14.5	0.01	0.01	0.01	0.466	18.35
X13	$C_{40}H_{54}OS_5$	711.28510	711.28601	14.01	1.29	0.91	1.29	0.538	18.44
X14	$C_{26}H_{48}N_9O_8S_3$	711.28607	711.28601	7.5	0.09	-0.06	-0.09	0.732	18.44
X15	$C_{40}H_{75}N_8O_7$	780.58315	780.58307	7.5	0.10	-0.08	-0.10	0.664	18.50
X16	$C_{23}H_{30}N_8O_8S$	579.19801	579.19806	13.0	0.09	0.05	0.09	0.831	18.56
X17	$C_{19}H_{37}NO$	296.29479	296.29605	2.0	4.27	1.26	4.27	0.913	18.56
X18	$C_{14}H_{31}NOS_2$	294.19198	294.19205	0.0	0.22	0.06	0.22	0.920	19.69
X19	$C_{14}H_{23}N_5O_6$	358.17211	358.17206	6.0	0.15	-0.05	-0.15	0.977	19.69
X20	$C_{20}H_{20}N$	275.16685	275.16705	11.5	0.74	0.20	0.74	0.994	18.98
X21	$C_{38}H_{81}N_7O_7S$	780.59910	780.59906	2.0	0.04	-0.04	-0.04	0.621	19.10
X22	$C_{41}H_{83}N_7O_3S_2$	786.60716	786.60706	4.0	0.13	-0.10	-0.13	0.957	19.57
X23	$C_{86}H_{165}N_6O_{10}S_3$	1539.18221	1539.18201	7.5	0.13	-0.20	-0.13	0.155	19.63
X24	$C_{40}H_{87}N_4O_4S_3$	784.59622	784.59705	-0.5	1.05	0.83	1.05	0.826	19.69
X25	C_8H_{10}	107.08553	107.08601	4.0	4.59	0.49	4.59	0.985	19.75
X26	$C_{47}H_{81}N_3O_6$	784.61981	784.62006	9.0	0.31	0.24	0.31	0.362	19.75
X27	$C_{44}H_{81}N_7O_5$	788.63720	788.63702	8.0	0.22	-0.17	-0.22	0.995	19.93
X28	$C_{51}H_{83}N_2O_2S$	788.62480	788.62506	11.5	0.33	0.26	0.33	0.973	19.99
X29	$C_{51}H_{83}N_2O_2S$	788.62480	788.62506	11.5	0.33	0.26	0.33	0.973	19.99
X30	$C_{46}H_{78}N_9O_2$	789.63512	789.63507	12.5	0.07	-0.05	-0.07	0.900	20.05
X31	$C_{64}H_{90}O_4S$	955.66326	955.66101	20.0	2.35	-2.25	-2.35	0.811	20.11
X32	$C_{41}H_{88}N_3O_4S_3$	783.60097	783.59802	-0.5	3.77	-2.95	-3.77	0.846	20.17
X33	$C_{45}H_{85}N_7S_2$	788.63806	788.63800	7.0	0.08	-0.06	-0.08	0.588	20.41
X34	$C_{52}H_{95}N_3OS_4$	906.64307	906.64307	7.0	0.01	-0.01	-0.01	0.779	21.01
X35	$C_{47}H_{86}N_9O_{10}$	937.65704	937.65704	9.5	0.00	0.00	0.00	0.916	12.31
X36	$C_{53}H_{97}N_3O_2S_4$	936.65364	936.65380	7.0	0.17	0.16	0.17	0.551	21.36
X37	$C_{50}H_{79}N_7O_4S_2$	906.57077	906.57073	15.0	0.05	-0.05	-0.05	0.88	21.54
X38	$C_{58}H_{89}N_7O_3$	932.70997	932.70976	18.0	0.22	-0.20	-0.22	0.89	21.66
X39	$C_{55}H_{99}N_3O_7$	914.75558	914.75579	8.0	0.23	0.21	0.23	0.490	21.72
X40	$C_{61}H_{105}NOS_2$	932.77103	932.77106	10.0	0.02	0.02	0.02	0.390	21.72
X41	$C_{74}H_{143}N_4O_8S_4$	1344.98615	1344.98608	5.5	0.05	-0.07	-0.05	0.552	21.90
X42	$C_{74}H_{136}N_9O_4S_4$	1343.96709	1343.96704	11.5	0.04	-0.05	-0.04	0.207	22.14
X43	$C_{61}H_{105}NOS_2$	932.77103	932.77106	10.0	0.02	0.02	0.02	0.852	23.04
X44	$C_{58}H_{107}O_7$	916.80896	916.80908	5.5	5.5	0.14	0.12	0.14	23.33

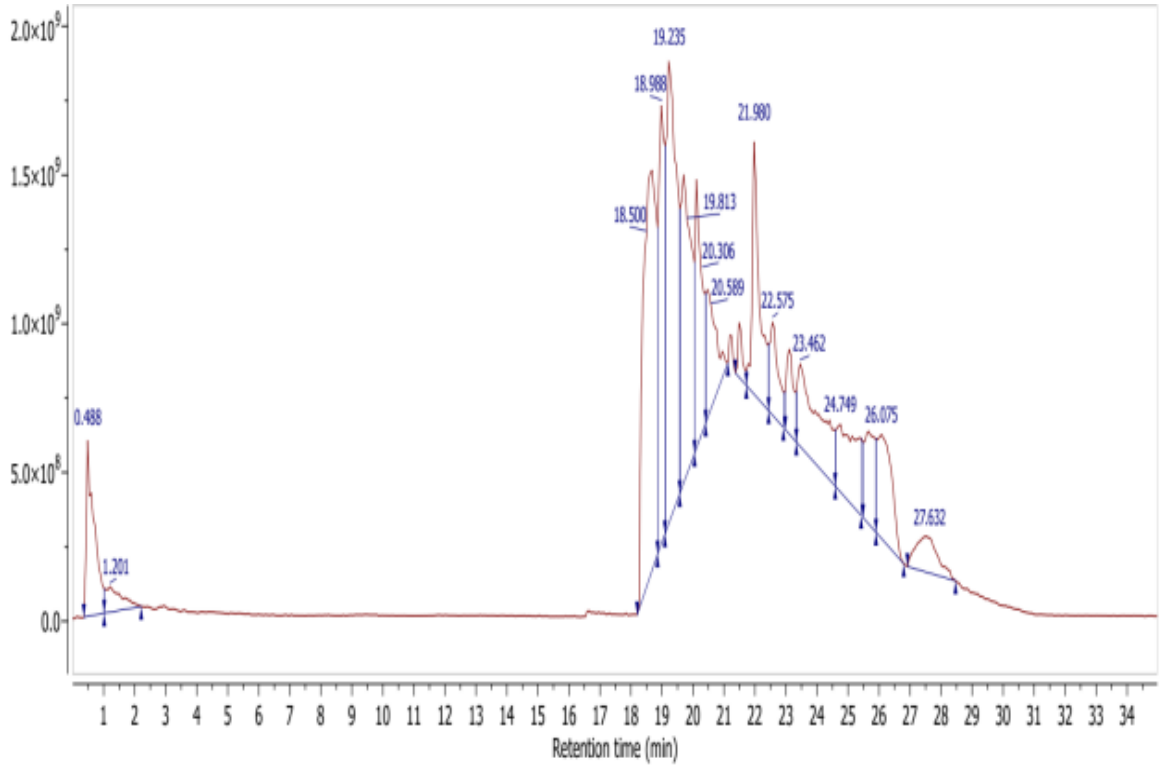
X45	$C_{55}H_{107}N_6S_2$	916.80714	916.80701	5.5	0.15	-0.13	-0.15	0.436	23.45
X46	$C_{54}H_{109}NO_7S$	916.79975	916.80005	1.0	0.32	0.30	0.32	0.484	23.57
X47	$C_{53}H_{113}N_5OS_3$	932.81800	932.81805	0.0	0.06	0.05	0.06	0.431	23.63
X48	$C_{58}H_{109}NO_4S$	916.81501	916.81506	5.0	0.06	0.06	0.06	0.901	24.59
X49	$C_{58}H_{111}N_2O_3S$	916.83882	916.83905	4.5	0.25	0.23	0.25	0.440	24.65
X50	$C_{50}H_{109}N_9OS_2$	916.82693	916.82703	1.0	0.11	0.10	0.11	0.435	24.83
X51	$C_{49}H_{105}N_9O_6$	916.82606	916.82605	2.0	0.01	-0.01	-0.01	0.536	25.42
X52	$C_{51}H_{97}N_6O_8$	922.74407	922.74402	6.5	0.05	-0.05	-0.05	0.351	25.48
X53	$C_{48}H_{94}N_{10}O_7$	923.73797	923.73804	7.0	0.07	0.07	0.07	0.484	25.54
X54	$C_{60}H_{94}N_2OS_2$	923.68803	923.68805	15.0	0.02	0.02	0.02	0.825	25.66
X55	$C_{59}H_{94}N_4O_2S$	923.71703	923.71704	15.0	0.02	0.02	0.02	0.318	52.72
X56	$C_{47}H_{88}N_9O_7S$	923.66002	923.66003	8.5	0.02	0.02	0.02	0.535	25.90
X57	$C_{49}H_{100}N_3O_4S_4$	923.66694	923.66705	1.5	0.12	0.11	0.12	0.466	25.96
X58	$C_{55}H_{96}N_5S_3$	923.69006	923.69000	10.5	0.06	-0.06	-0.06	0.41	26.14
X59	$C_{48}H_{97}N_6S_5$	918.64510	918.64502	3.5	0.09	-0.08	-0.09	0.520	26.50
X60	$C_{10}H_{31}N_8O_2$	296.26427	296.26306	-0.5	4.11	-1.21	-4.11	0.960	26.98
X61	$C_{17}H_{35}N_4$	296.29401	296.29401	5.2	1.89	0.56	1.89	0.922	27.93

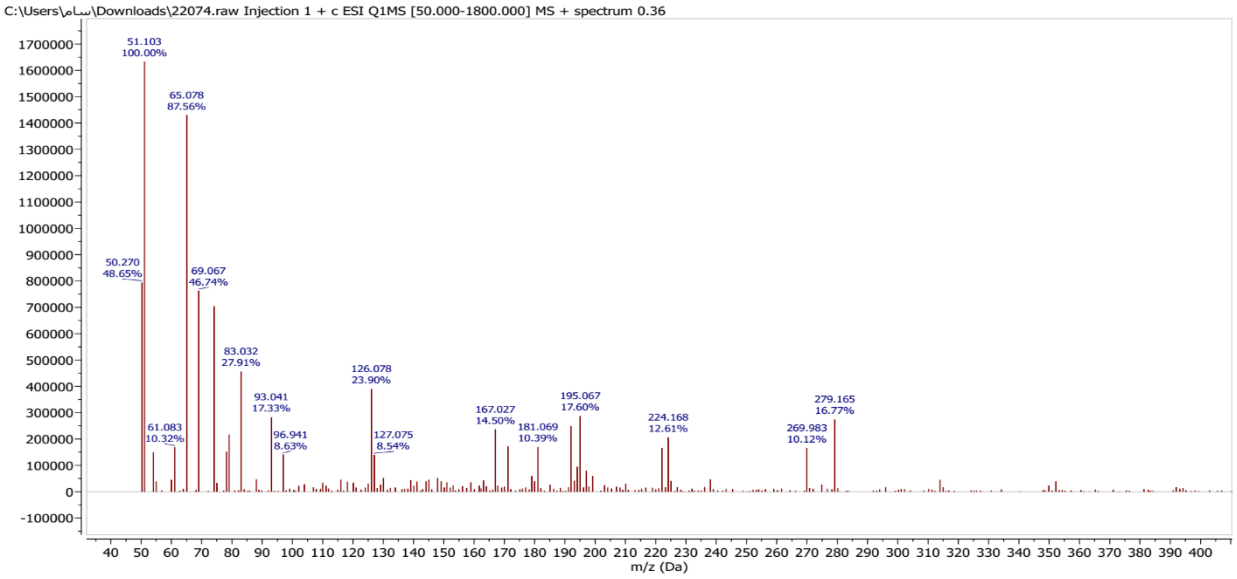
Table 3. slected uknowing compounds extract by Mnova softwera

Compound	Formula	Calculated Mass	Double Bond Equivalence	Absolute Error ppm	Error (mDa)	Error (ppm)	Fitness	RT
X1	C_{16} H_{24} N O S	279.16514	5.5	0.24	-0.07	-0.24	0.925	0.36
X2	C_7 H_{12} N	111.10425	2.5	1.76	-0.19	-1.76	0.987	0.48
X3	C_{16} H_{30} O_4	287.22169	2.0	4.78	1.37	4.78	0.938	0.54
X4	C_{14} H_{30} N_4 S	287.22639	2.0	1.22	-0.35	-1.22	0.938	0.60
X5	C_{16} H_{32} N_2 O S	301.23081	2.0	4.15	1.24	4.15	0.990	0.78
X6	C_6 H_{19} N_{10} O_6	328.15618	2.5	0.35	-0.11	-0.35	0.977	1.67
X7	C_{22} H_{21} N_3	328.18082	14.0	0.72	0.24	0.72	0.883	1.85
X8	C_{10} H_{23} N_4 O_6 S	328.14111	1.5	0.17	-0.05	-0.17	0.956	1.91
X14	C_{26} H_{48} N_9 O_8 S_3	711.28607	7.5	0.09	-0.06	-0.09	0.732	18.44
X16	C_{23} H_{30} N_8 O_8 S	579.19801	13.0	0.09	0.05	0.09	0.831	18.56
X17	C_{19} H_{37} N O	296.29479	2.0	4.27	1.26	4.27	0.913	18.56
X18	C_{14} H_{31} N O S_2	294.19198	0.0	0.22	0.06	0.22	0.920	19.69
X19	C_{14} H_{23} N_5 O_6	358.17211	6.0	0.15	-0.05	-0.15	0.977	19.69
X20	C_{20} H_{20} N	275.16685	11.5	0.74	0.20	0.74	0.994	18.98
X22	C_{41} H_{83} N_7 O_3 S_2	786.60716	4.0	0.13	-0.10	-0.13	0.957	19.57
X24	C_{40} H_{87} N_4 O_4 S_3	784.59622	-0.5	1.05	0.83	1.05	0.826	19.69
X25	C_8 H_{10}	107.08553	4.0	4.59	0.49	4.59	0.985	19.75
X27	C_{44} H_{81} N_7 O_5	788.63720	8.0	0.22	-0.17	-0.22	0.995	19.93
X28	C_{51} H_{83} N_2 O_2 S	788.62480	11.5	0.33	0.26	0.33	0.973	19.99
X29	C_{51} H_{83} N_2 O_2 S	788.62480	11.5	0.33	0.26	0.33	0.973	19.99
X30	C_{46} H_{78} N_9 O_2	789.63512	12.5	0.07	-0.05	-0.07	0.900	20.05
X31	C_{64} H_{90} O_4 S	955.66326	20.0	2.35	-2.25	-2.35	0.811	20.11
X32	C_{41} H_{88} N_3 O_4 S_3	783.60097	-0.5	3.77	-2.95	-3.77	0.846	20.17
X34	C_{52} H_{95} N_3 O S_4	906.64307	7.0	0.01	-0.01	-0.01	0.779	21.01
X35	C_{47} H_{86} N_9 O_{10}	937.65704	9.5	0.00	0.00	0.00	0.916	12.31
X37	C_{50} H_{79} N_7 O_4 S_2	906.57077	15.0	0.05	-0.05	-0.05	0.886	21.54
X38	C_{58} H_{89} N_7 O_3	932.70997	18.0	0.22	-0.20	-0.22	0.898	21.66
X43	C_{61} H_{105} N O S_2	932.77103	10.0	0.02	0.02	0.02	0.852	23.04
X48	C_{58} H_{109} N O_4 S	916.81501	5.0	0.06	0.06	0.06	0.901	24.59
X54	C_{60} H_{94} N_2 O S_2	923.68803	15.0	0.02	0.02	0.02	0.825	25.66
X60	C_{10} H_{31} N_8 O_2	296.26427	-0.5	4.11	-1.21	-4.11	0.960	26.98
X61	$C_{17}H_{35}N_4$	296.29401	5.2	1.89	0.56	1.89	0.922	27.93

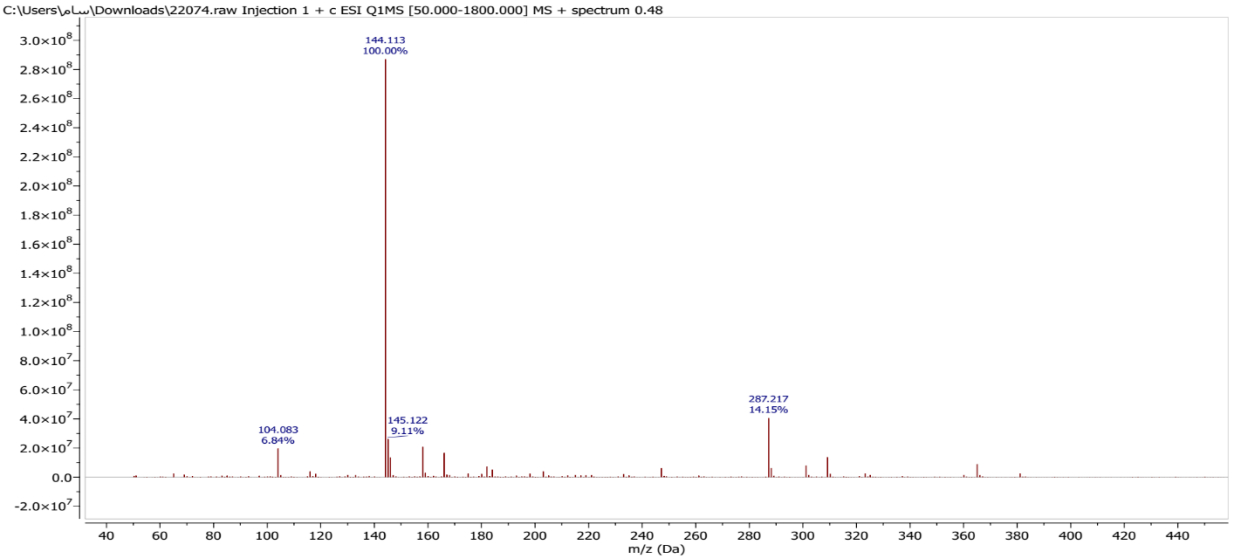
Table 4. slected uknowing compounds extract by Mnova softwera represented by CP symbio

Compound	Formula	Calculated Mass	Double Bond Equivalence	Absolute Error ppm	Error (mDa)	Error (ppm)	Fitness	RT
CP1	C_{16} H_{24} N O S	279.16514	5.5	0.24	-0.07	-0.24	0.925	0.36
CP2	C_7 H_{12} N	111.10425	2.5	1.76	-0.19	-1.76	0.987	0.48
CP3	C_{16} H_{30} O_4	287.22169	2.0	4.78	1.37	4.78	0.938	0.54
CP4	C_{14} H_{30} N_4 S	287.22639	2.0	1.22	-0.35	-1.22	0.938	0.60
CP5	C_{16} H_{32} N_2 O S	301.23081	2.0	4.15	1.24	4.15	0.990	0.78
CP6	C_6 H_{19} N_{10} O_6	328.15618	2.5	0.35	-0.11	-0.35	0.977	1.67
CP7	C_{22} H_{21} N_3	328.18082	14.0	0.72	0.24	0.72	0.883	1.85
CP8	C_{10} H_{23} N_4 O_6 S	328.14111	1.5	0.17	-0.05	-0.17	0.956	1.91
CP9	C_{26} H_{48} N_9 O_8 S_3	711.28607	7.5	0.09	-0.06	-0.09	0.732	18.44
CP10	C_{23} H_{30} N_8 O_8 S	579.19801	13.0	0.09	0.05	0.09	0.831	18.56
CP11	C_{19} H_{37} N O	296.29479	2.0	4.27	1.26	4.27	0.913	18.56
CP12	C_{14} H_{31} N O S_2	294.19198	0.0	0.22	0.06	0.22	0.920	19.69
CP13	C_{14} H_{23} N_5 O_6	358.17211	6.0	0.15	-0.05	-0.15	0.977	19.69
CP14	C_{20} H_{20} N	275.16685	11.5	0.74	0.20	0.74	0.994	18.98
CP15	C_{41} H_{83} N_7 O_3 S_2	786.60716	4.0	0.13	-0.10	-0.13	0.957	19.57
CP16	C_{40} H_{87} N_4 O_4 S_3	784.59622	-0.5	1.05	0.83	1.05	0.826	19.69
CP17	C_8 H_{10}	107.08553	4.0	4.59	0.49	4.59	0.985	19.75
CP18	C_{44} H_{81} N_7 O_5	788.63720	8.0	0.22	-0.17	-0.22	0.995	19.93
CP19	C_{51} H_{83} N_2 O_2 S	788.62480	11.5	0.33	0.26	0.33	0.973	19.99
CP20	C_{51} H_{83} N_2 O_2 S	788.62480	11.5	0.33	0.26	0.33	0.973	19.99
CP21	C_{46} H_{78} N_9 O_2	789.63512	12.5	0.07	-0.05	-0.07	0.900	20.05
CP22	C_{64} H_{90} O_4 S	955.66326	20.0	2.35	-2.25	-2.35	0.811	20.11
CP23	C_{41} H_{88} N_3 O_4 S_3	783.60097	-0.5	3.77	-2.95	-3.77	0.846	20.17
CP24	C_{52} H_{95} N_3 O S_4	906.64307	7.0	0.01	-0.01	-0.01	0.779	21.01
CP25	C_{47} H_{86} N_9 O_{10}	937.65704	9.5	0.00	0.00	0.00	0.916	12.31
CP26	C_{50} H_{79} N_7 O_4 S_2	906.57077	15.0	0.05	-0.05	-0.05	0.886	21.54
CP27	C_{58} H_{89} N_7 O_3	932.70997	18.0	0.22	-0.20	-0.22	0.898	21.66
CP28	C_{61} H_{105} N O S_2	932.77103	10.0	0.02	0.02	0.02	0.852	23.04
CP29	C_{58} H_{109} N O_4 S	916.81501	5.0	0.06	0.06	0.06	0.901	24.59
CP30	C_{60} H_{94} N_2 O S_2	923.68803	15.0	0.02	0.02	0.02	0.825	25.66
CP32	C_{10} H_{31} N_8 O_2	296.26427	-0.5	4.11	-1.21	-4.11	0.960	26.98
CP33	$C_{17}H_{35}N_4$	296.29401	5.2	1.89	0.56	1.89	0.922	27.93

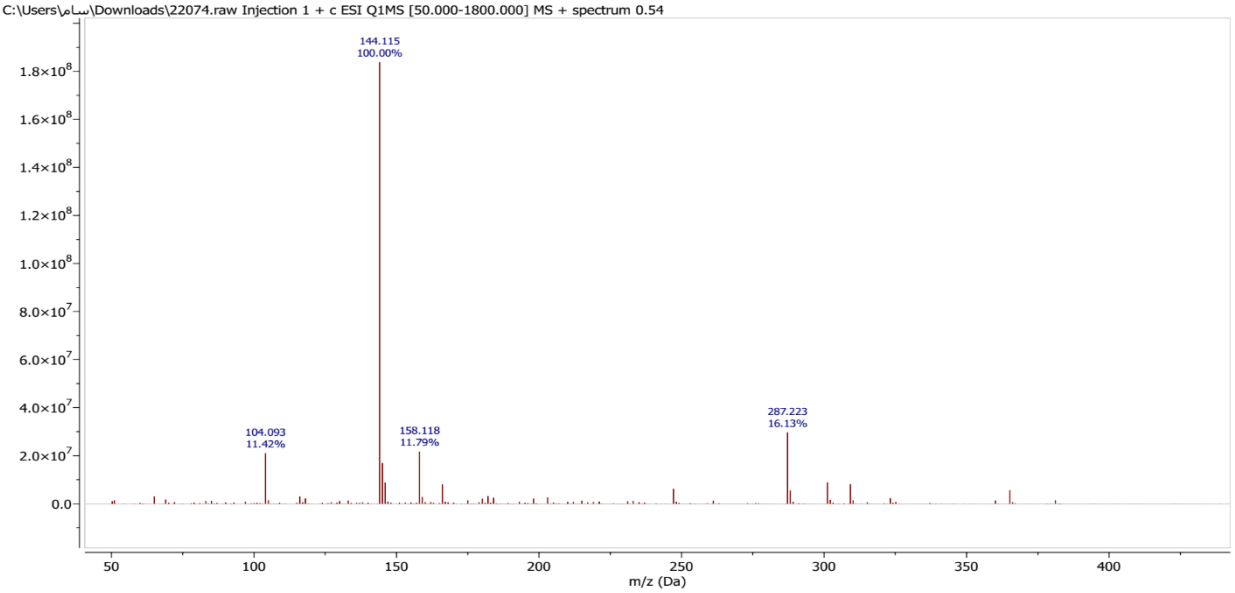




Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C16 H24 N O S	279.16514	279.16507	5.5	0.24	-0.07	-0.24	0.925



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C10 H24 N9 O	287.21766	287.21704	3.5	2.16	-0.62	-2.16	0.999



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C17 H26 N4	287.22302	287.22305	7.0	0.10	0.03	0.10	0.923

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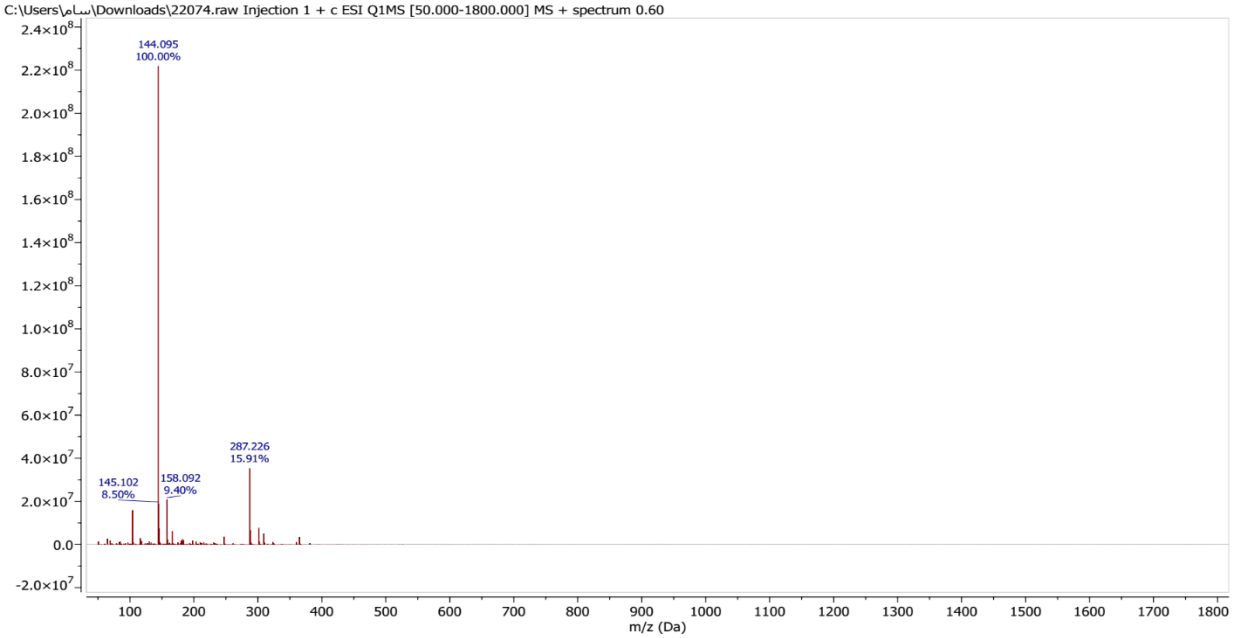

Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C14 H30 N4 S	287.22639	287.22604	2.0	1.22	-0.35	-1.22	0.938

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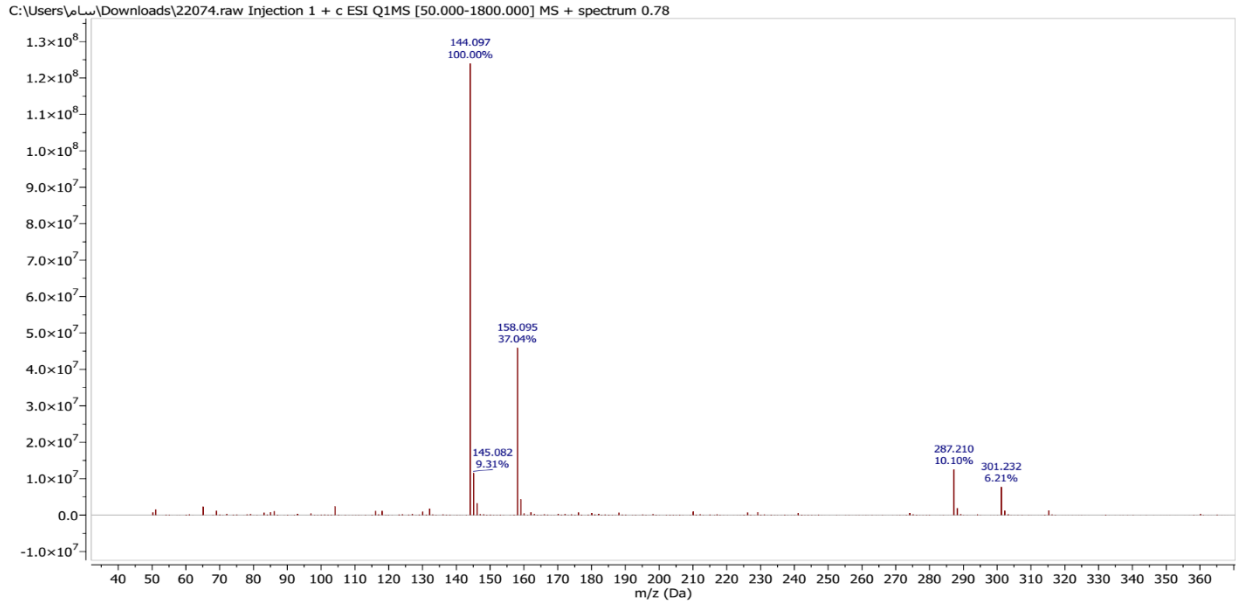

Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C16 H24 N5	287.21045	287.21005	7.5	1.38	-0.39	-1.38	0.928

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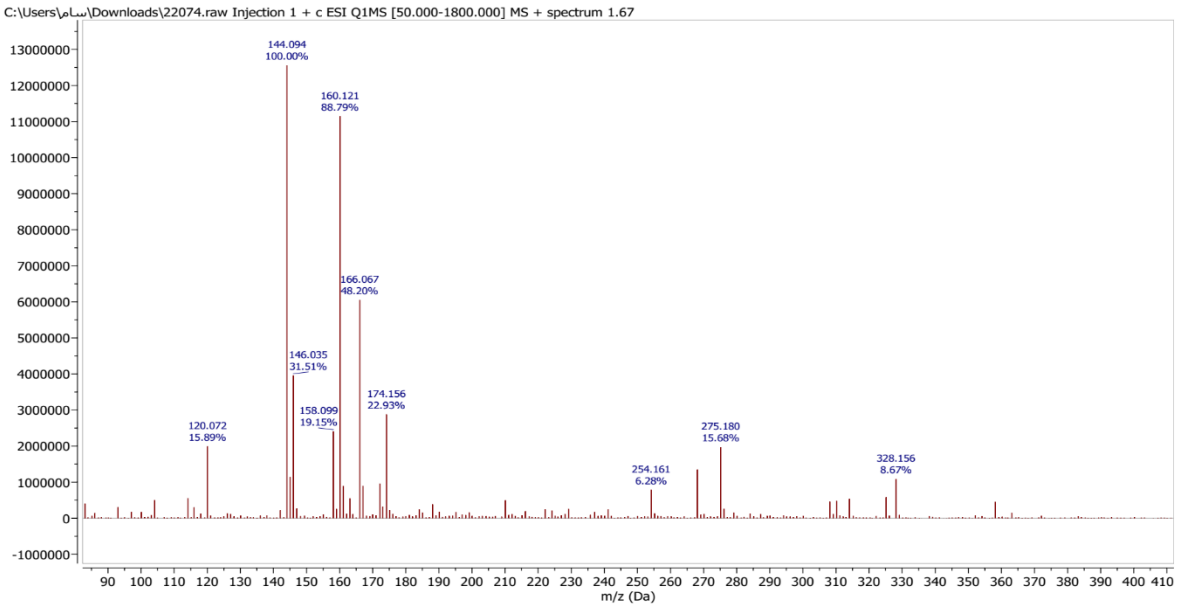
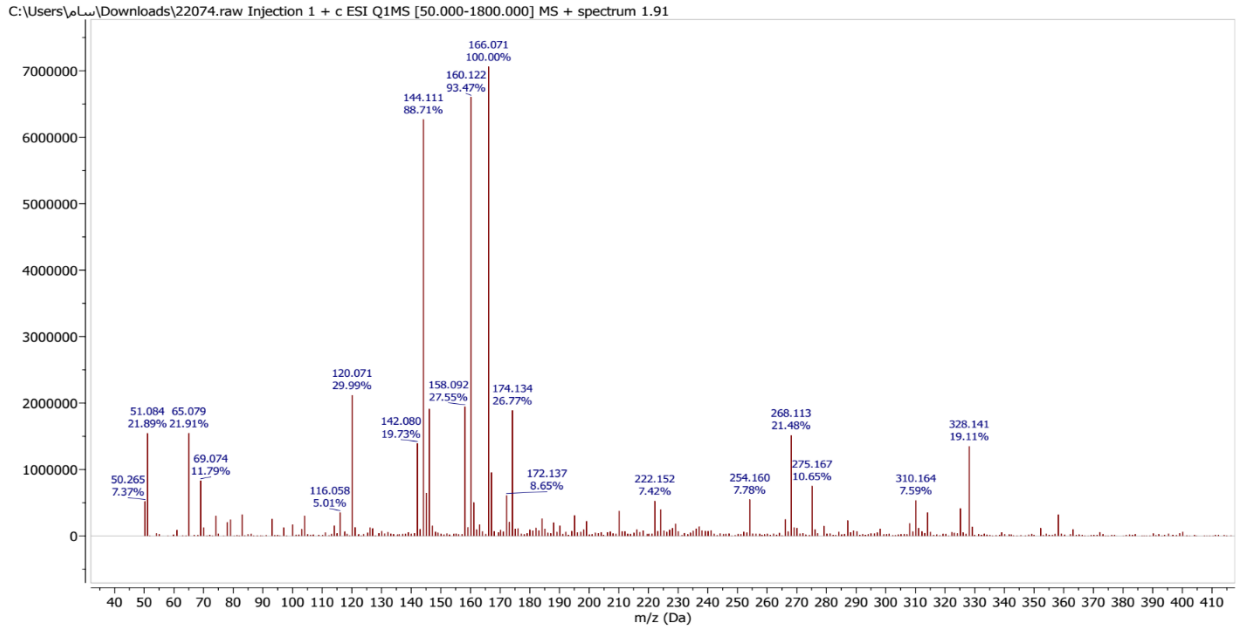
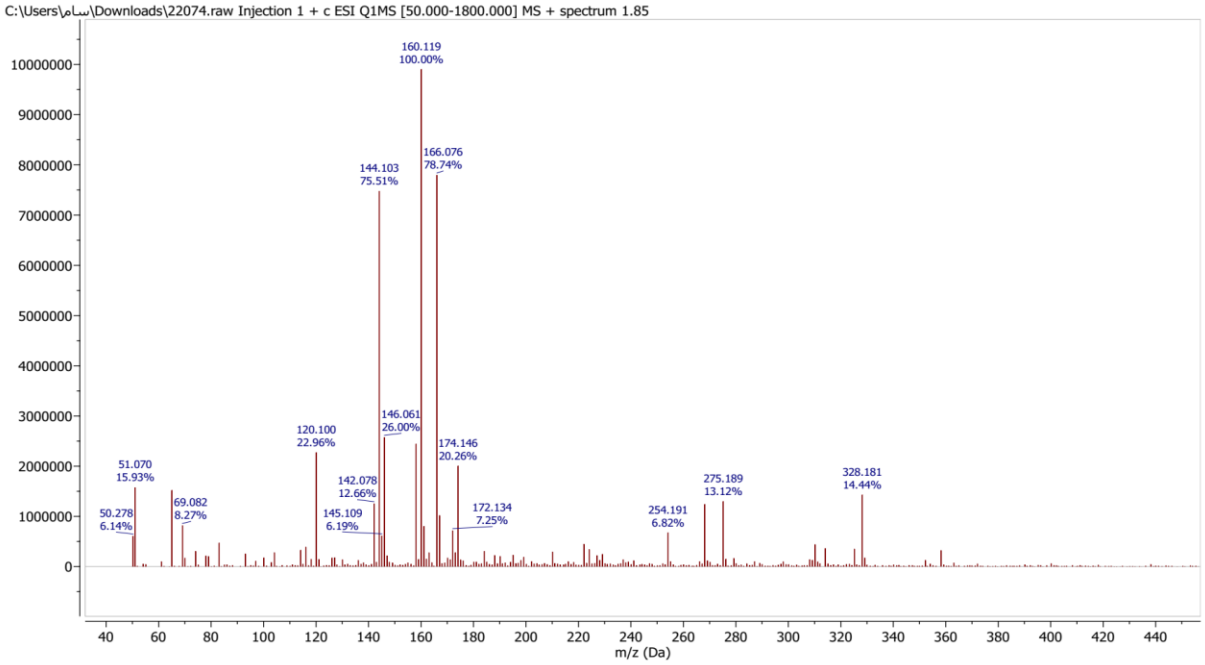


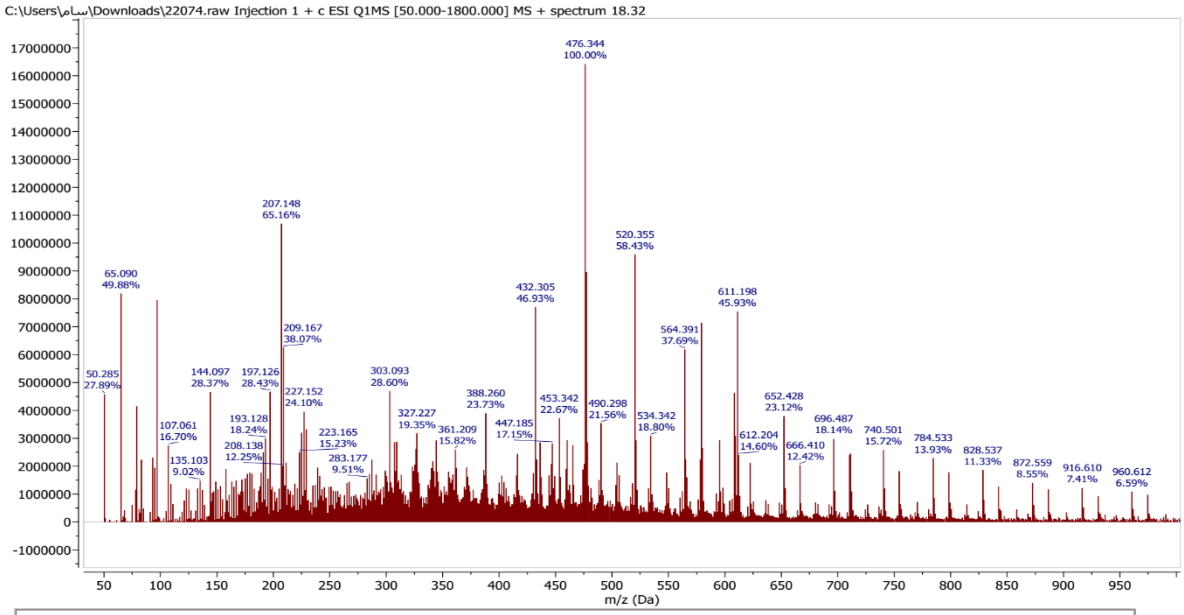
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C6 H19 N10 O6	328.15618	328.15607	2.5	0.35	-0.11	-0.35	0.977



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C10 H23 N4 O6 S	328.14111	328.14105	1.5	0.17	-0.05	-0.17	0.956



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C22 H21 N3	328.18082	328.18106	14.0	0.72	0.24	0.72	0.883



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C54 H91 N3 O8 S2	974.63203	974.63208	11.0	0.05	0.05	0.05	0.517

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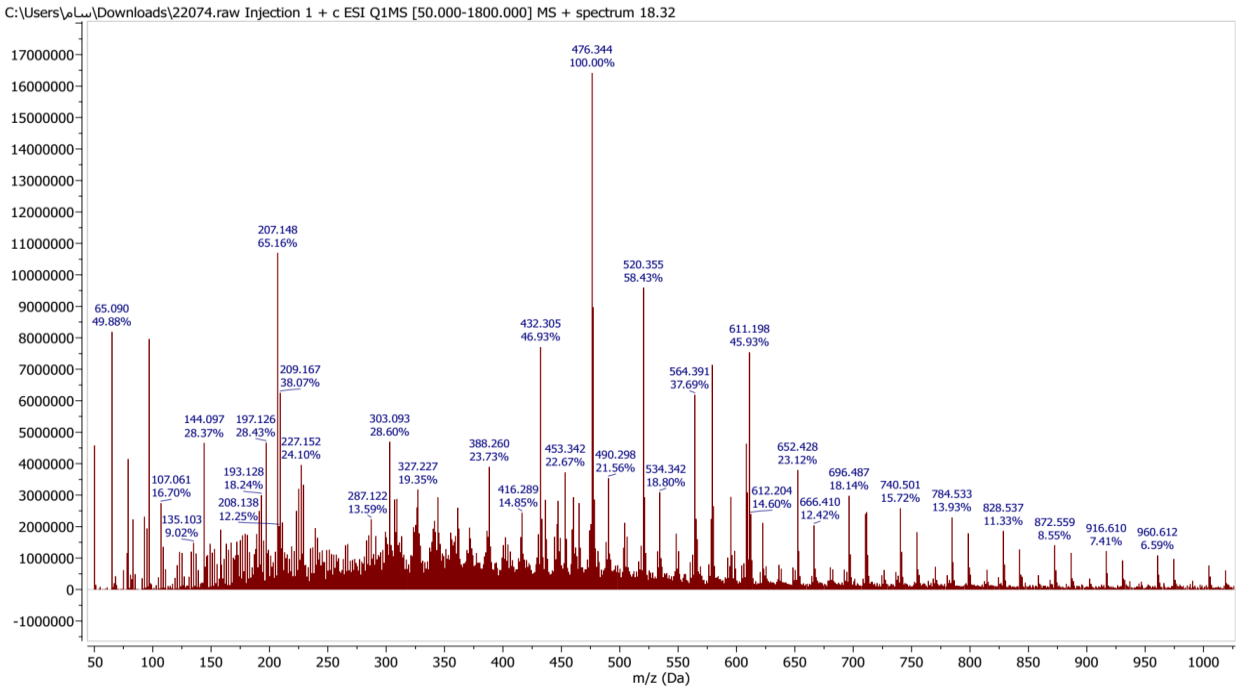
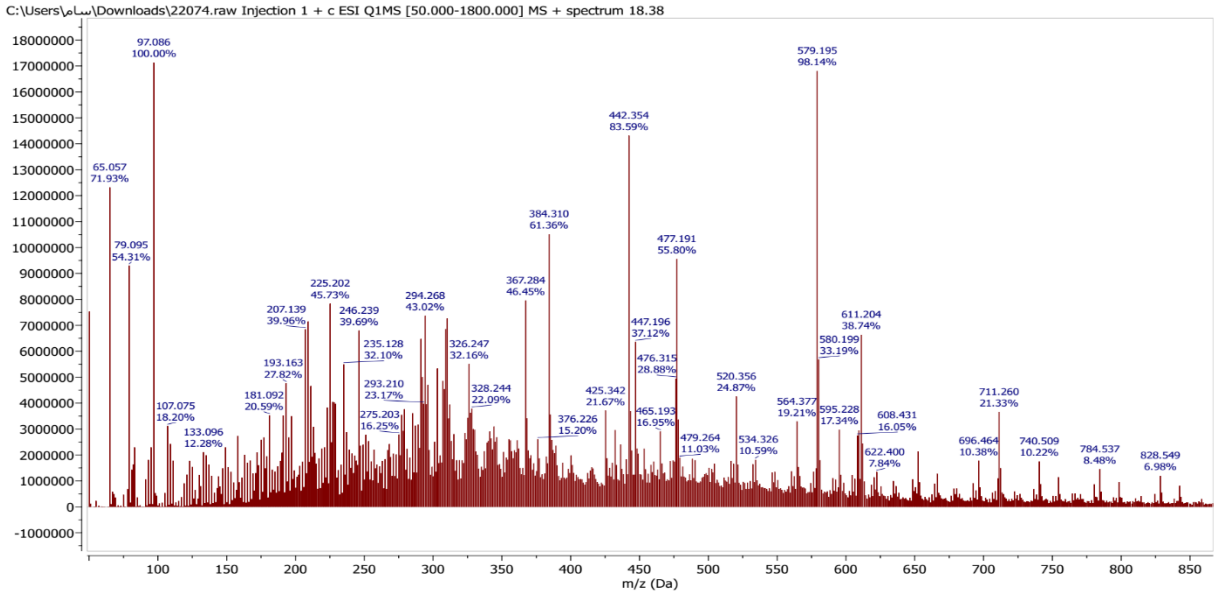
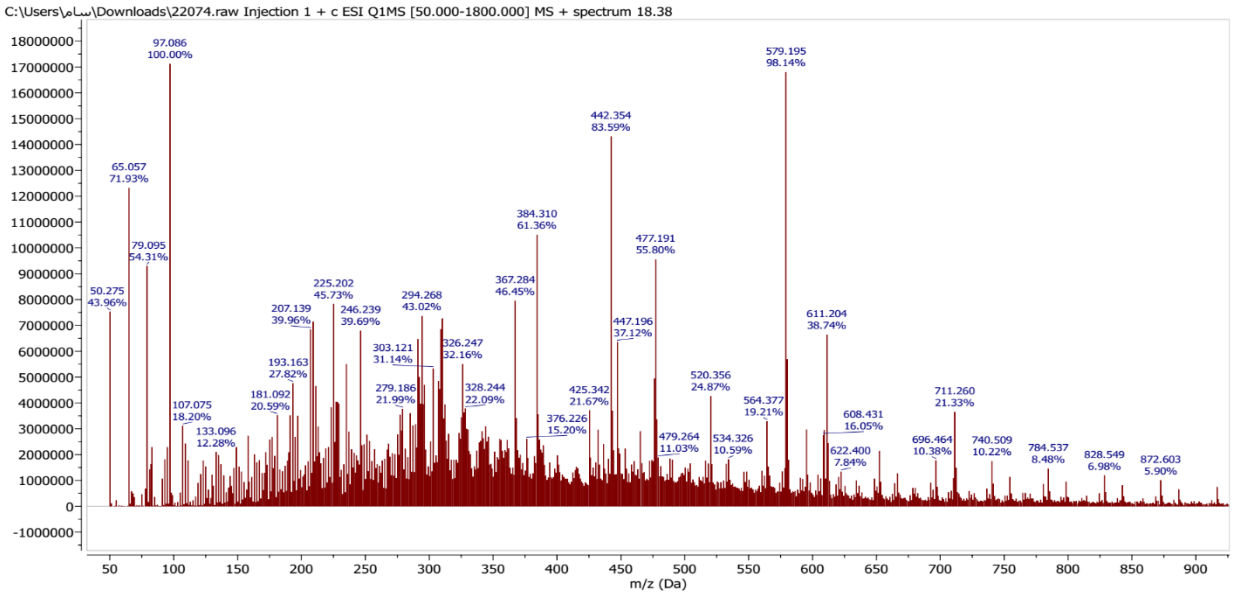


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C63 H91 N O S3	974.63356	974.63208	19.0	1.51	-1.47	-1.51	0.426

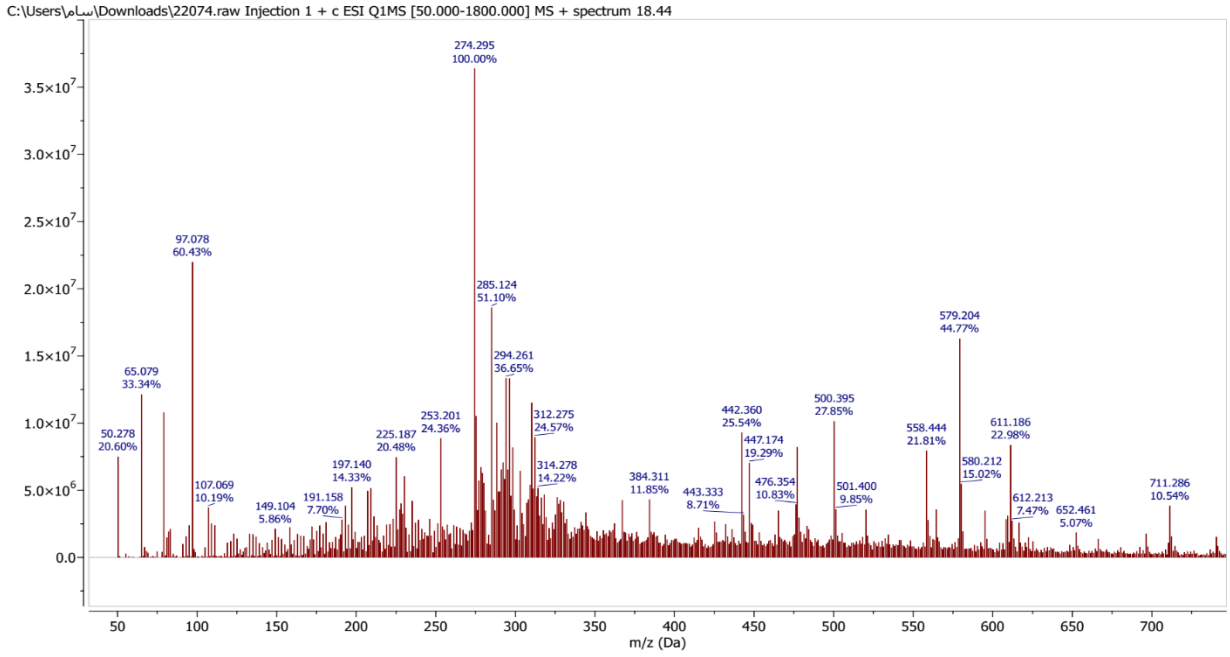


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C56 H87 O S3	872.59918	872.60303	13.5	4.41	3.85	4.41	0.420

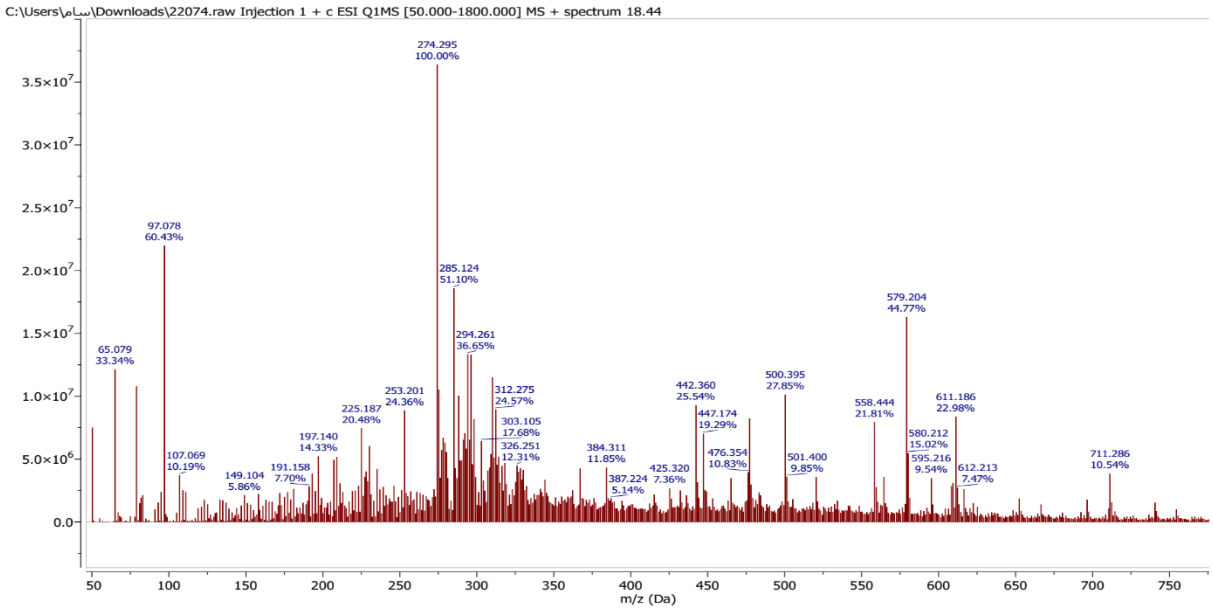
und.



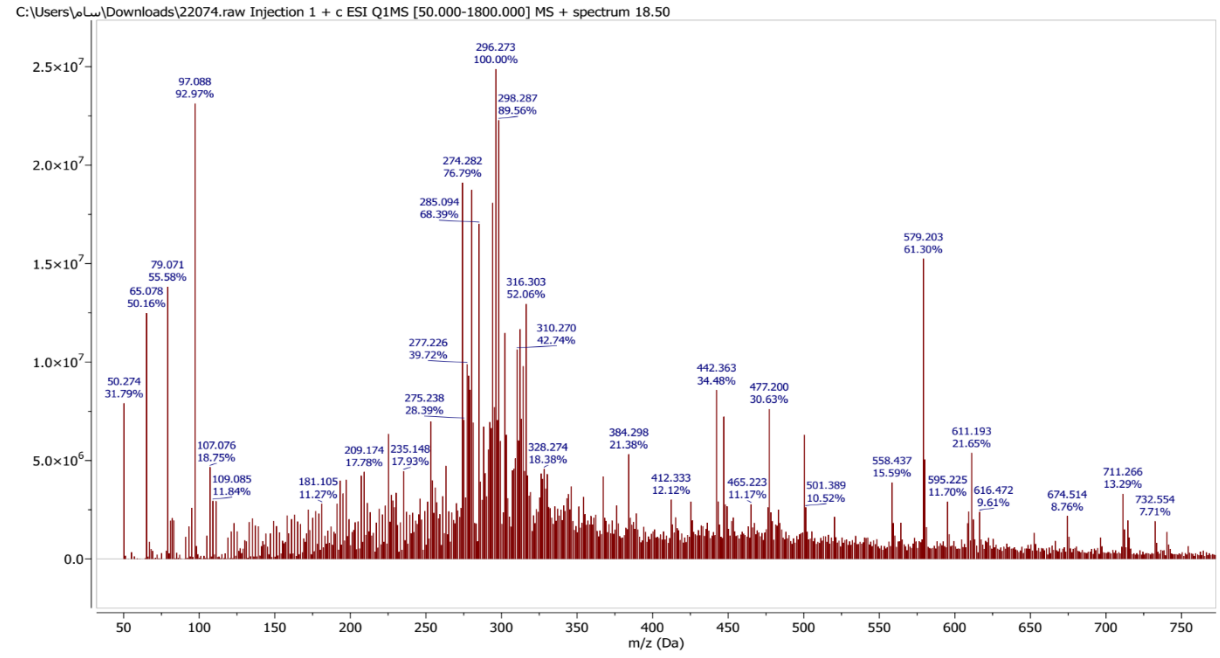
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C53 H83 N4 O2 S2	872.60302	872.60303	14.5	0.01	0.01	0.01	0.466



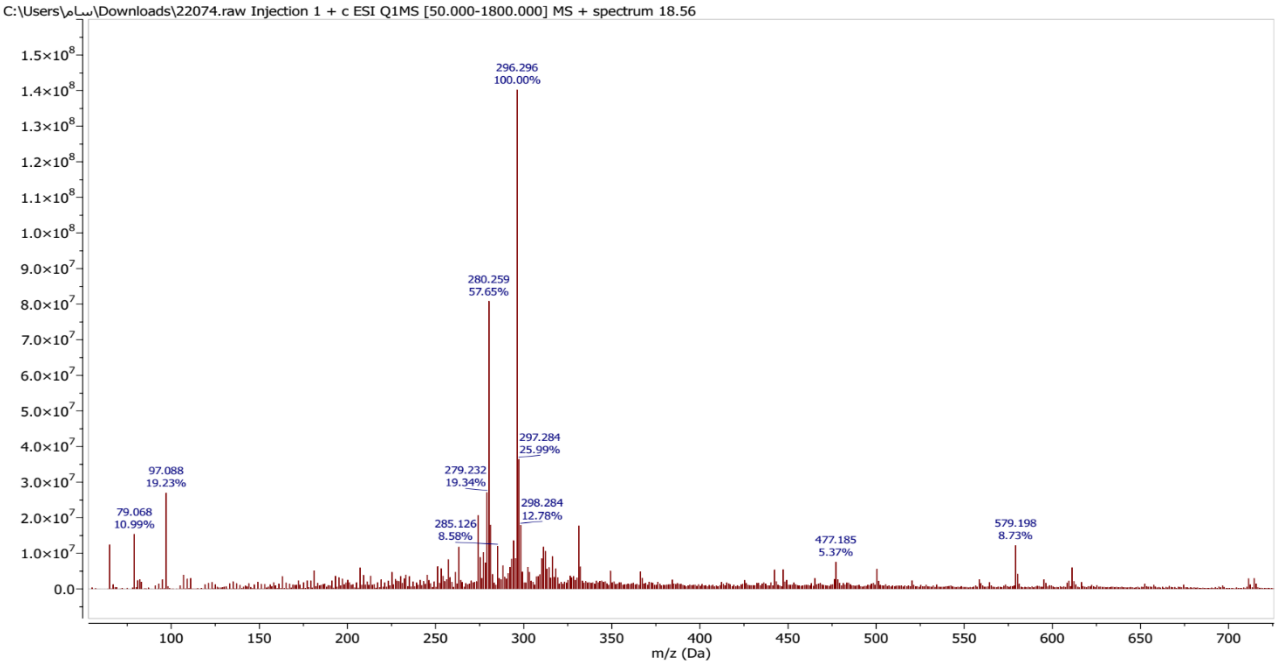
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C40 H54 O S5	711.28510	711.28601	14.0	1.29	0.91	1.29	0.538



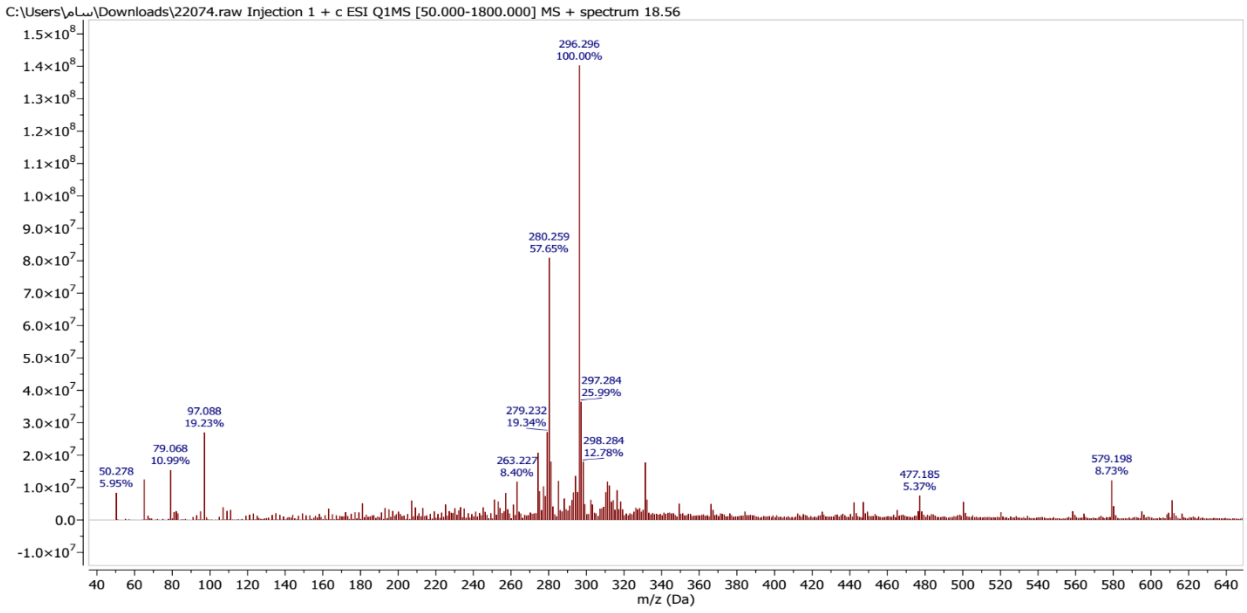
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C26 H48 N9 O8 S3	711.28607	711.28601	7.5	0.09	-0.06	-0.09	0.732



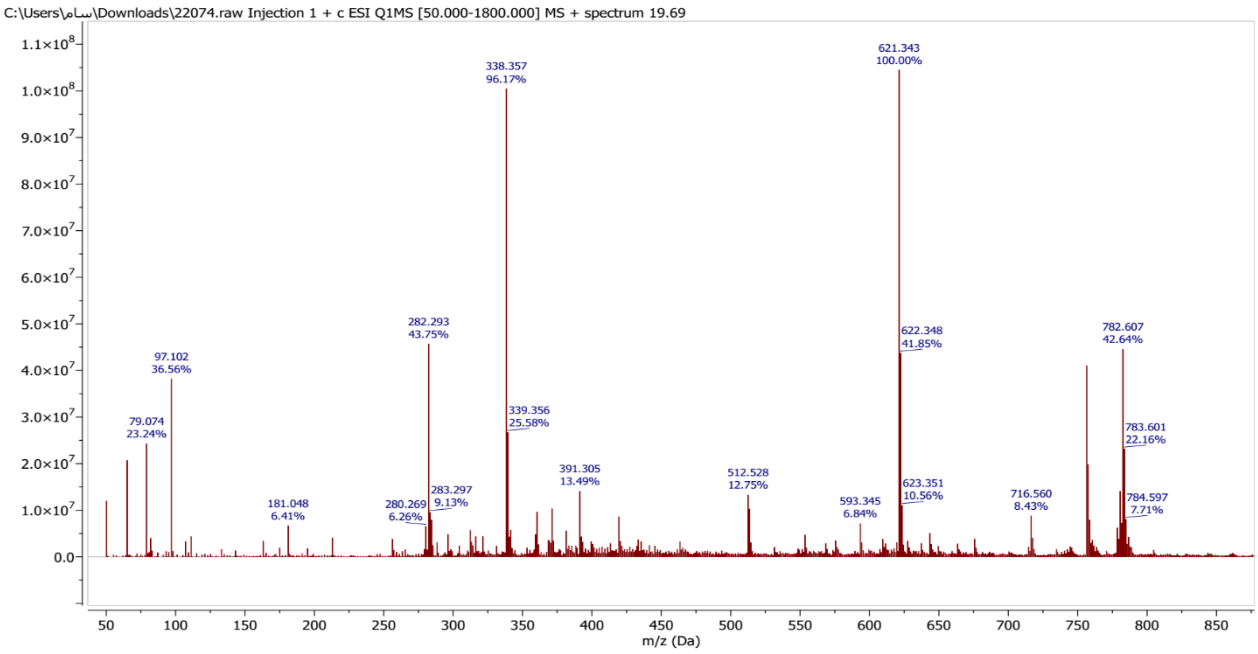
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C40 H75 N8 O7	780.58315	780.58307	7.5	0.10	-0.08	-0.10	0.664



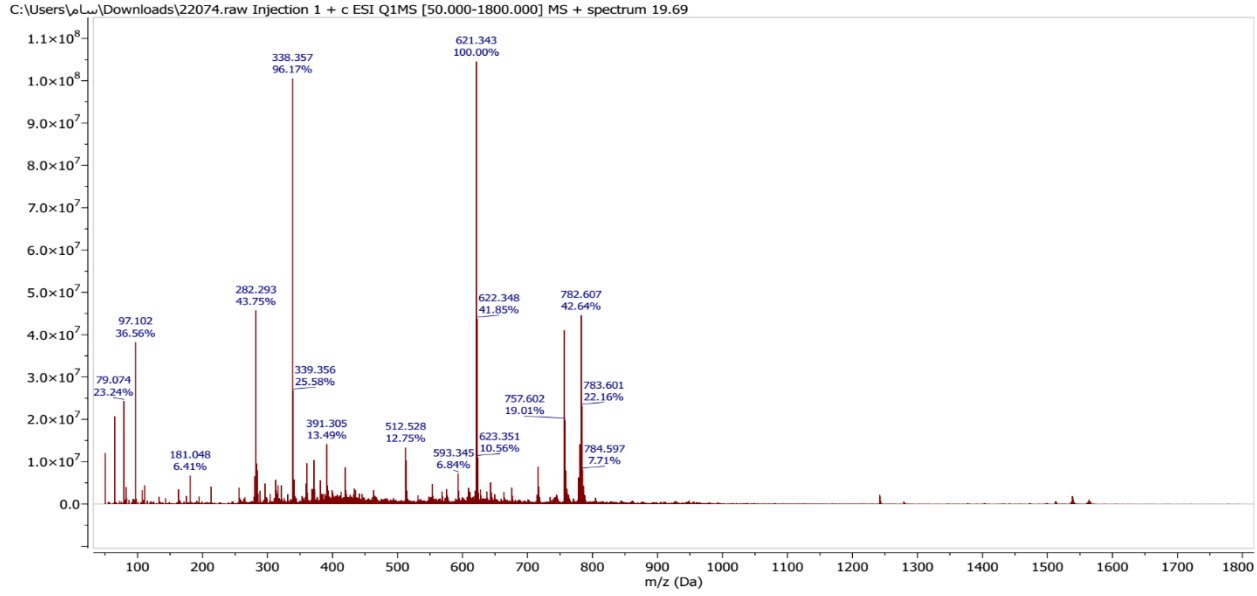
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C23 H30 N8 O8 S	579.19801	579.19806	13.0	0.09	0.05	0.09	0.831



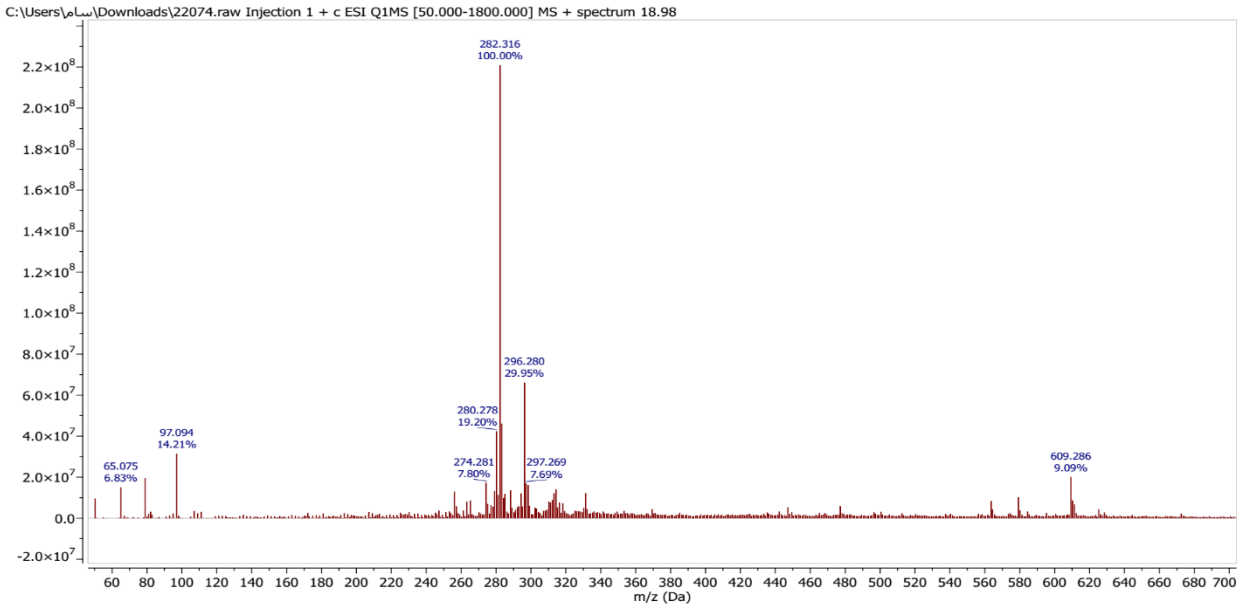
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C23 H30 N8 O8 S	579.19801	579.19806	13.0	0.09	0.05	0.09	0.831



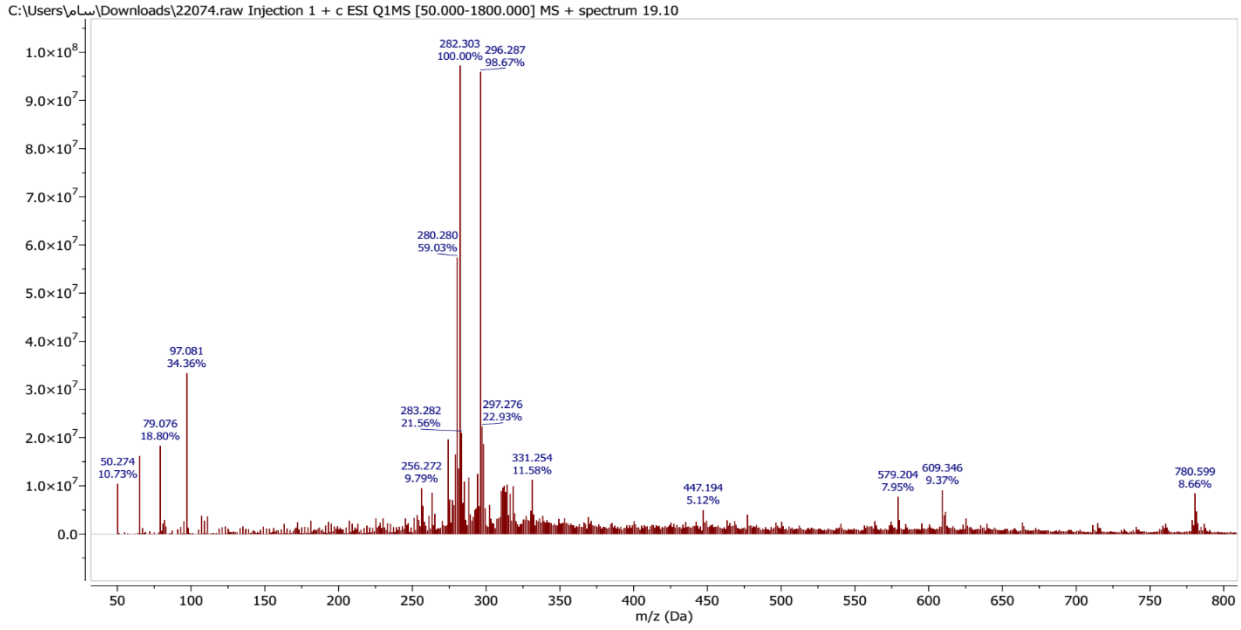
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C51 H73 N7	784.60002	784.59705	19.0	3.80	-2.98	-3.80	0.804



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C48 H83 N2 O2 S2	784.59687	784.59705	8.5	0.22	0.17	0.22	0.808



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C32 H36 N10 O S	609.28670	609.28607	20.0	1.04	-0.63	-1.04	0.727



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C38 H81 N7 O7 S	780.59910	780.59906	2.0	0.04	-0.04	-0.04	0.621

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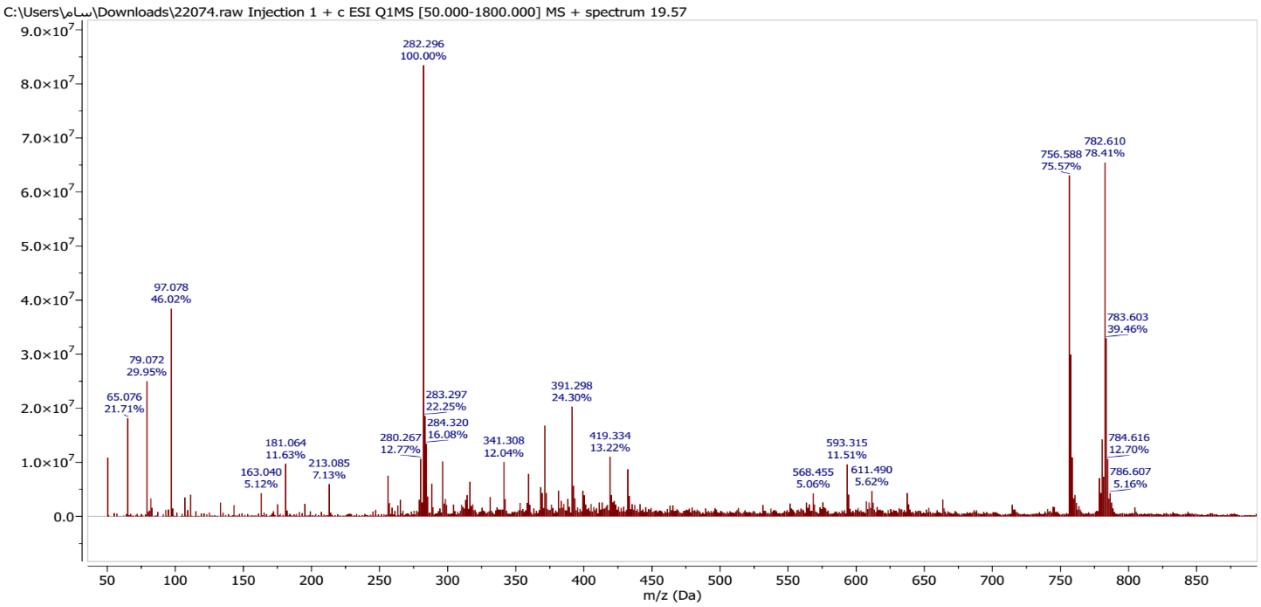
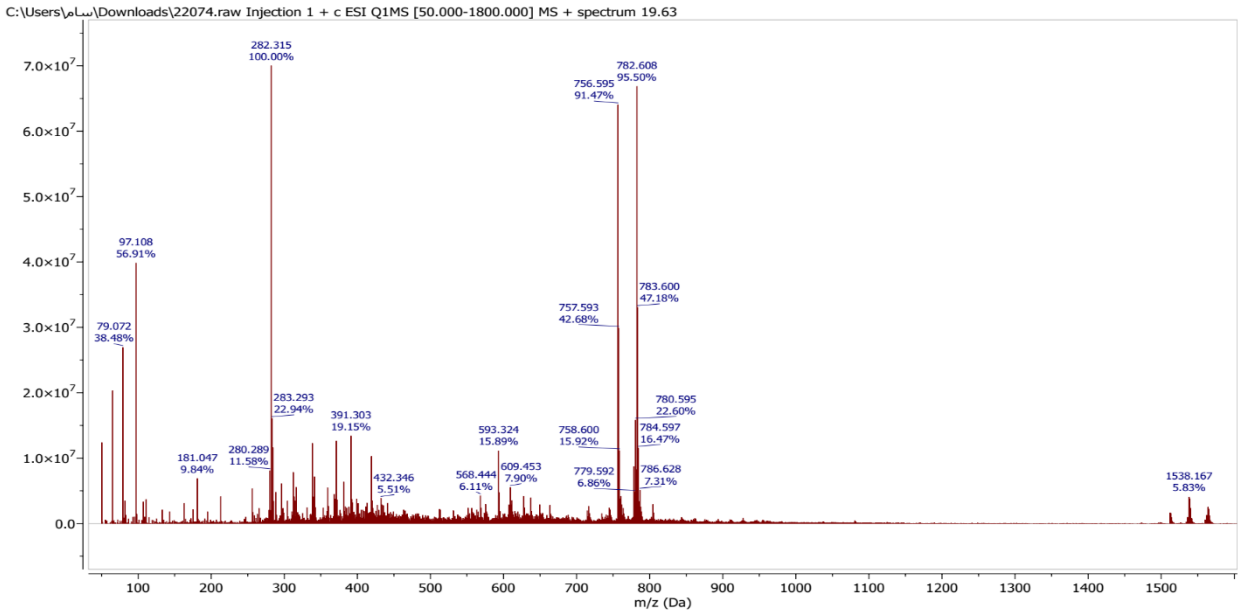
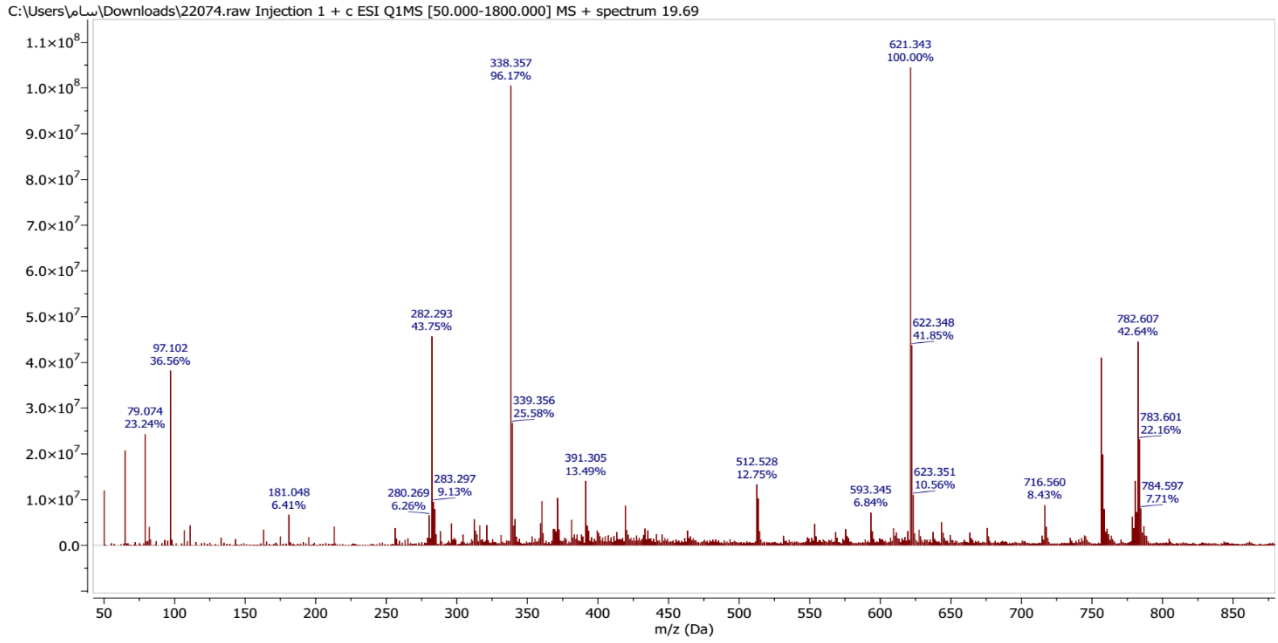


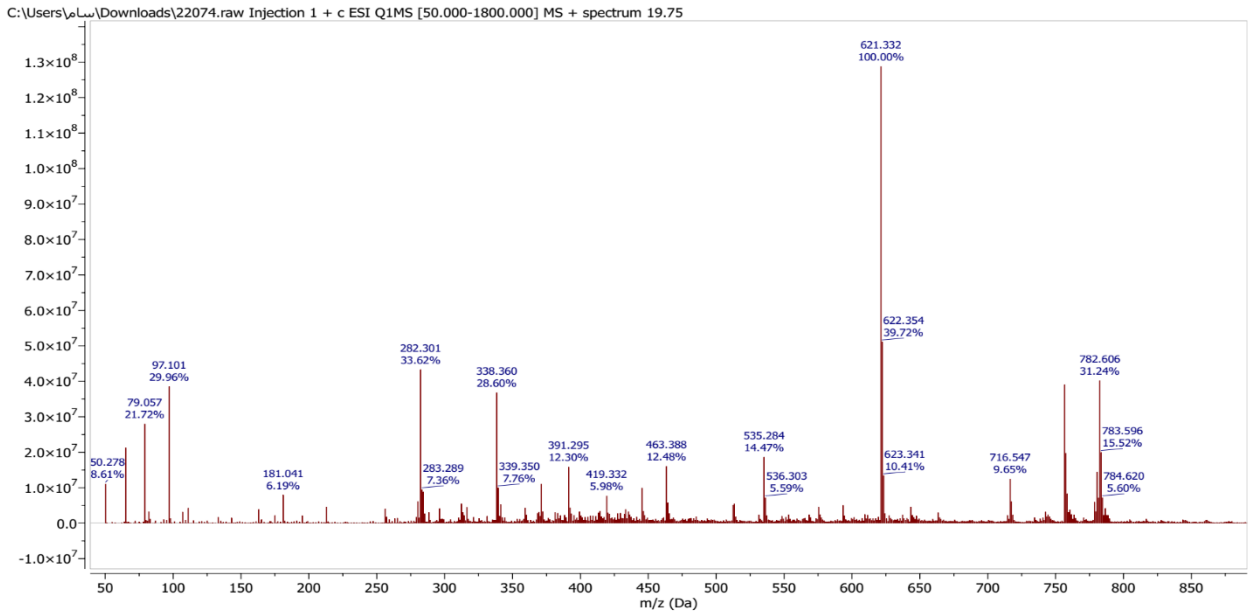
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C41 H83 N7 O3 S2	786.60716	786.60706	4.0	0.13	-0.10	-0.13	0.957



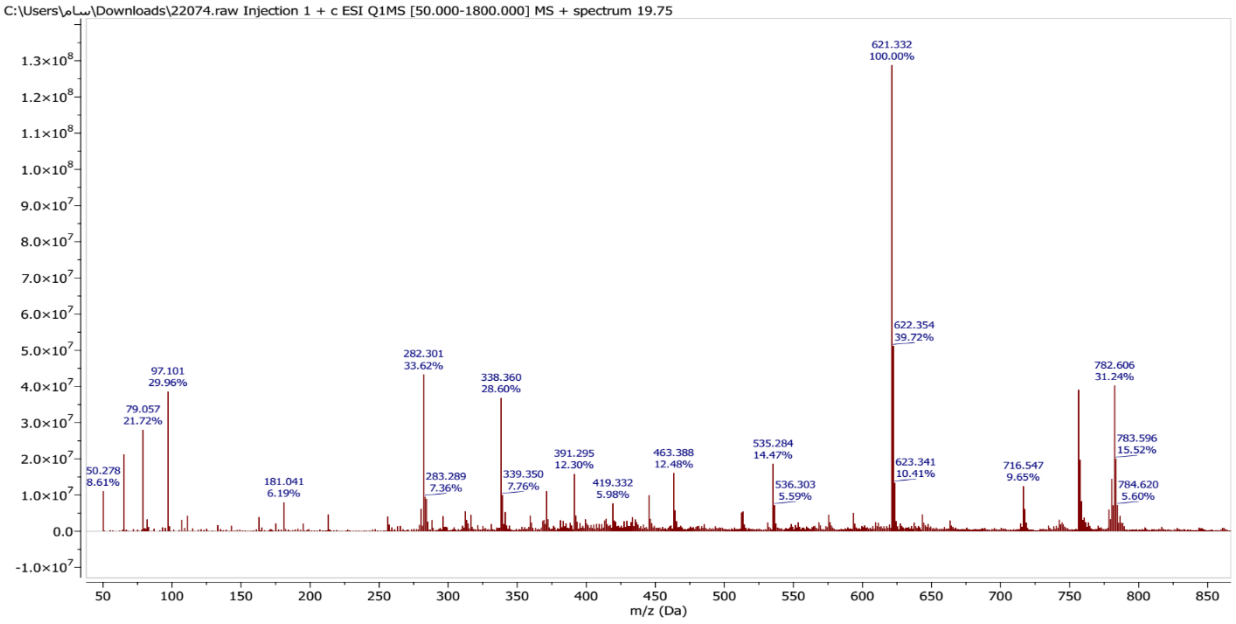
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C86 H165 N6 O10 S3	1539.18221	1539.18201	7.5	0.13	-0.20	-0.13	0.155



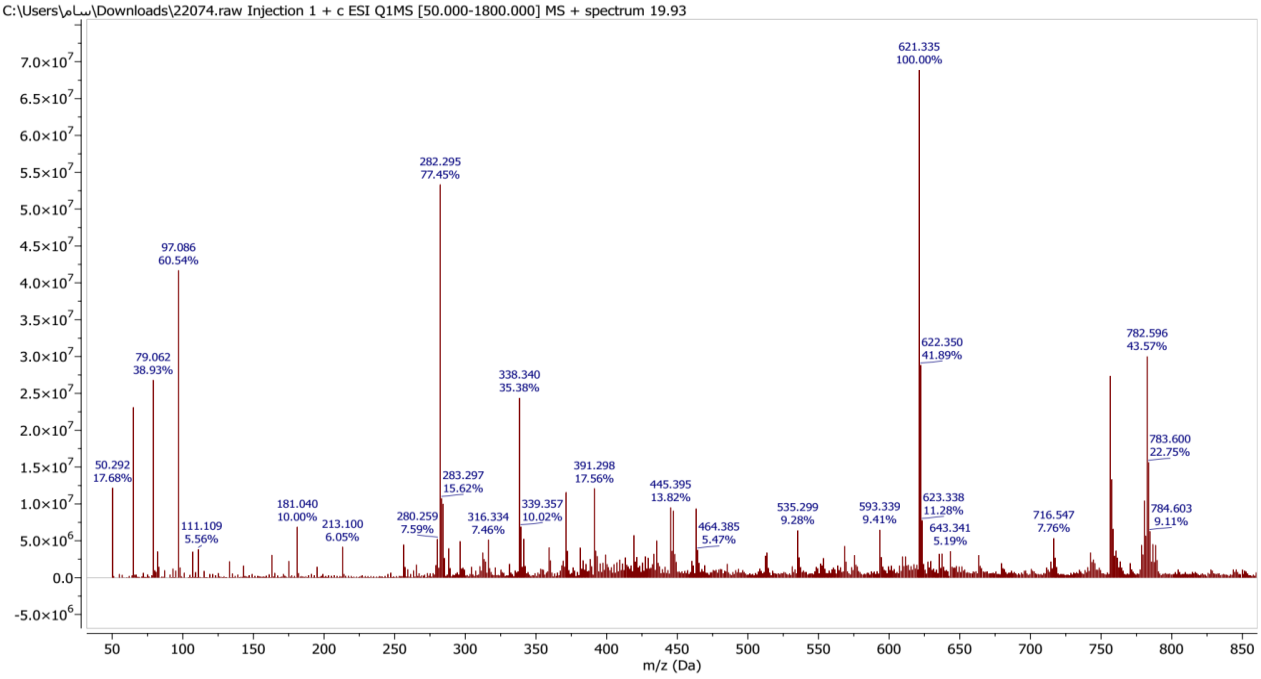
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C40 H87 N4 O4 S3	784.59622	784.59705	-0.5	1.05	0.83	1.05	0.826



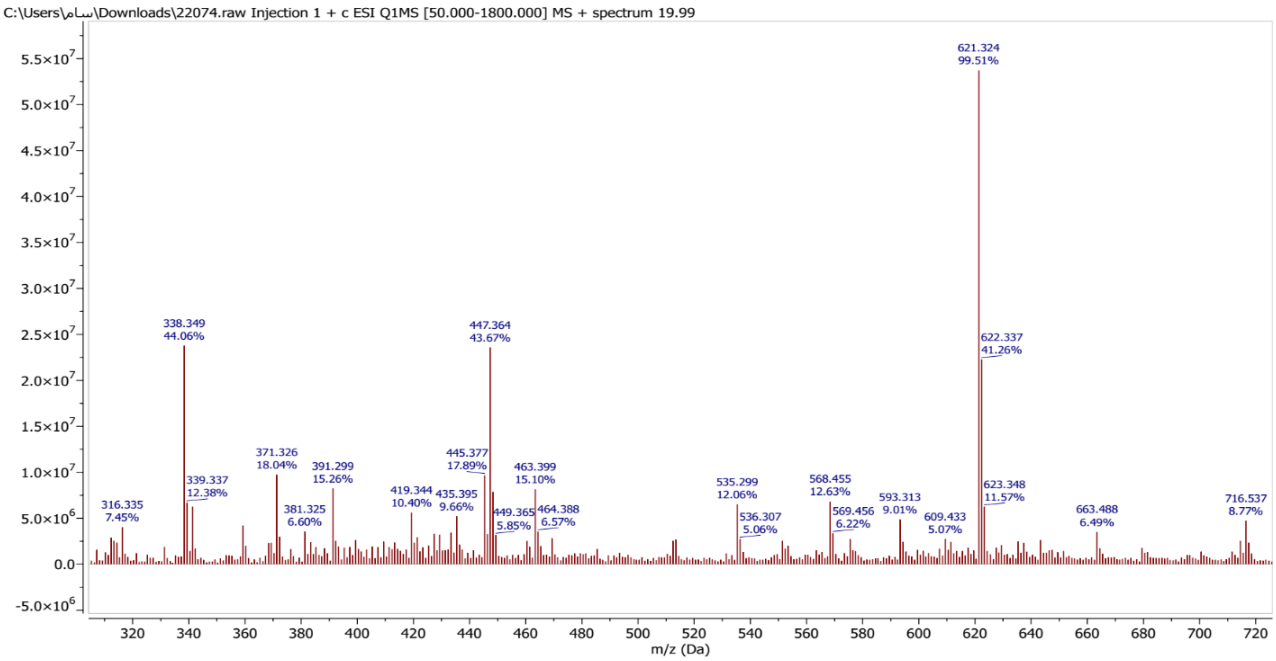
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C48 H77 N7 O2	784.62115	784.62006	14.0	1.40	-1.10	-1.40	0.351



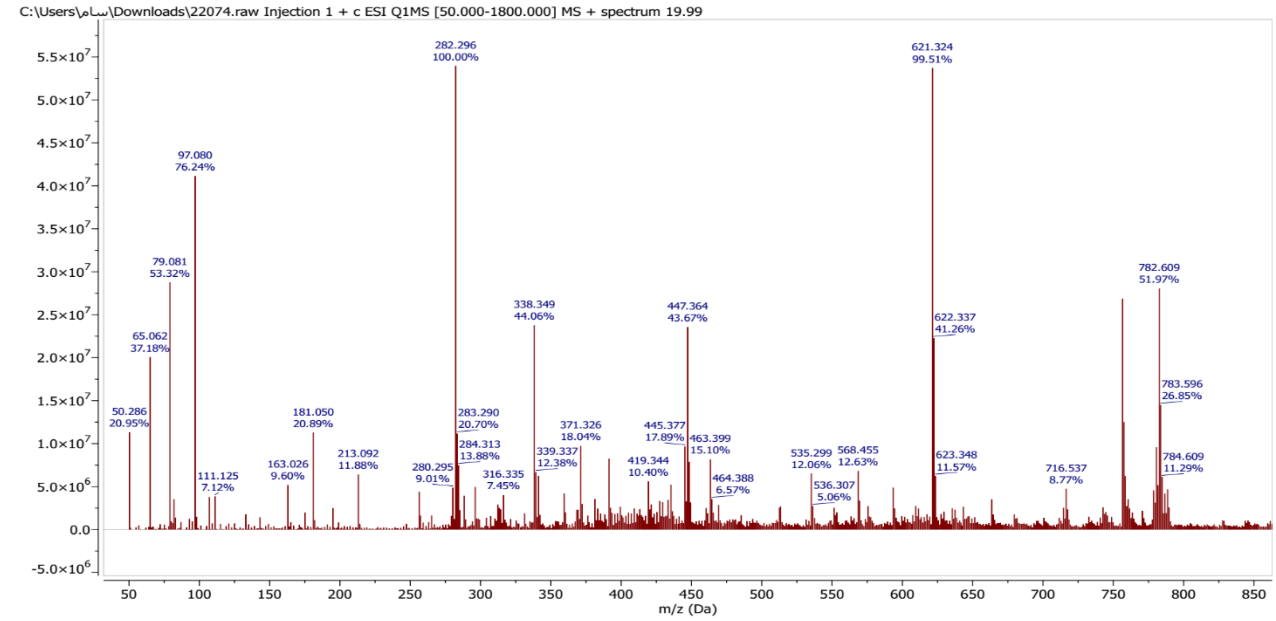
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C47 H81 N3 O6	784.61981	784.62006	9.0	0.31	0.24	0.31	0.362



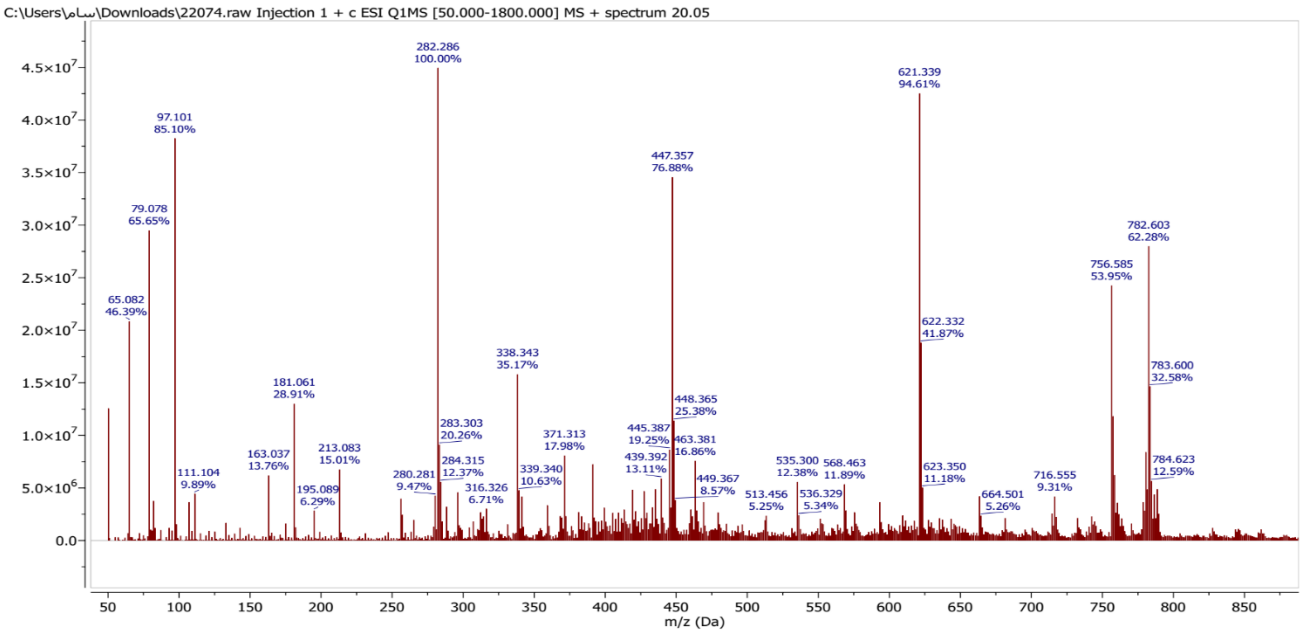
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C44 H81 N7 O5	788.63720	788.63702	8.0	0.22	-0.17	-0.22	0.995



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C51 H83 N2 O2 S	788.62480	788.62506	11.5	0.33	0.26	0.33	0.973



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C51 H83 N2 O2 S	788.62480	788.62506	11.5	0.33	0.26	0.33	0.973



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C46 H94 N S4	789.63419	789.63507	0.5	1.12	0.88	1.12	0.739

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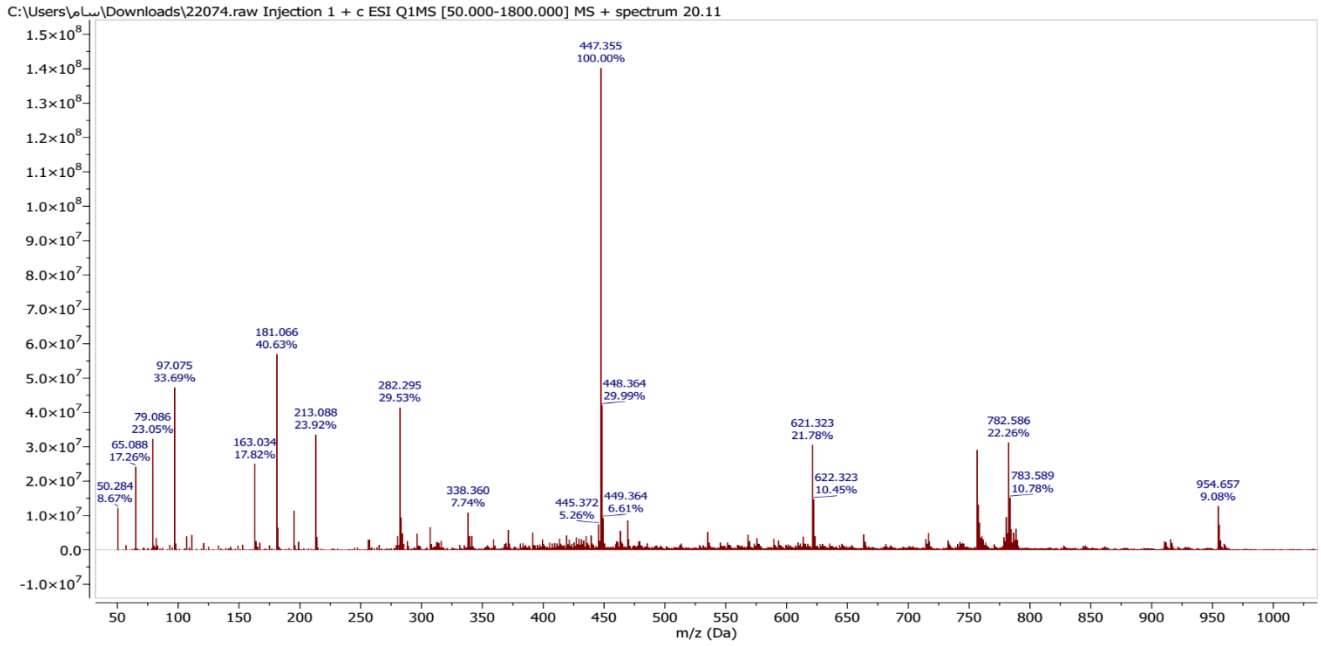
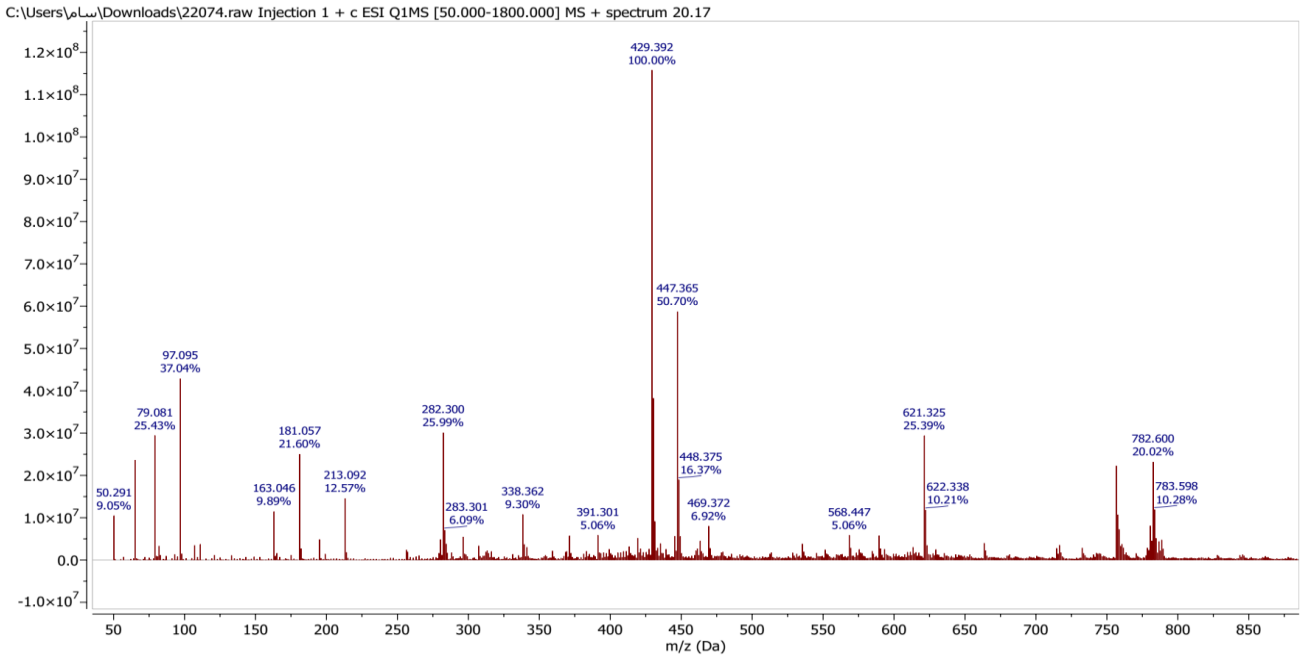


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C64 H90 O4 S	955.66326	955.66101	20.0	2.35	-2.25	-2.35	0.811



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C41 H88 N3 O4 S3	783.60097	783.59802	-0.5	3.77	-2.95	-3.77	0.846

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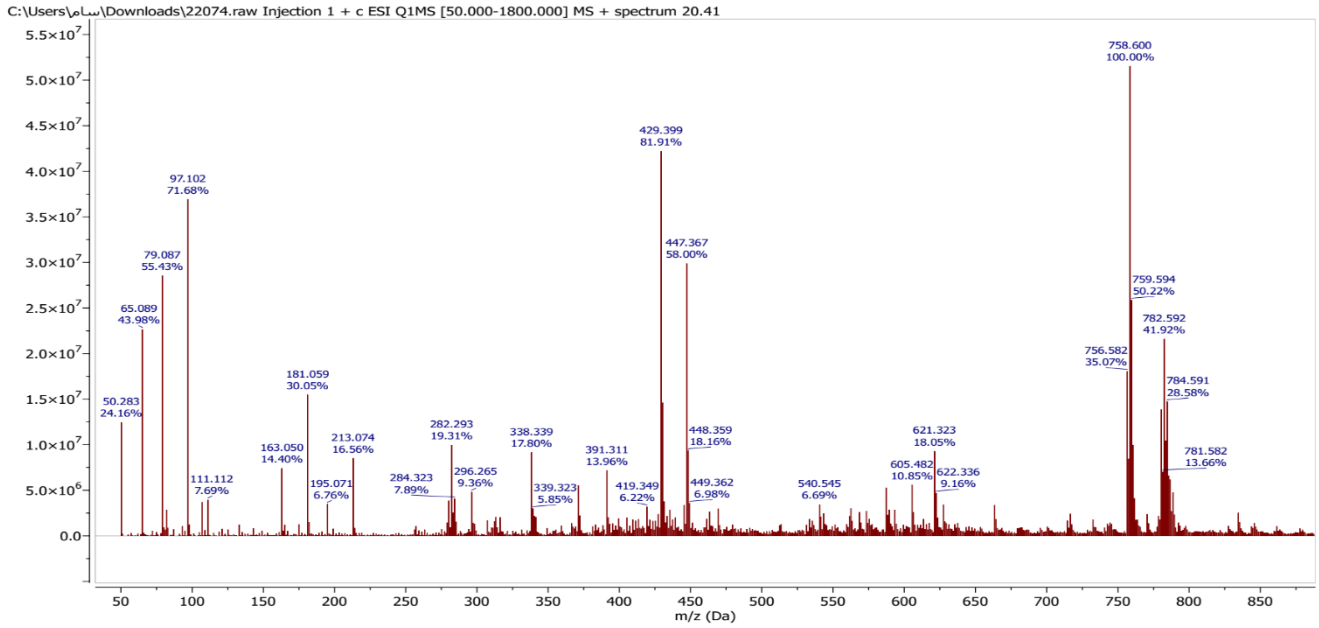
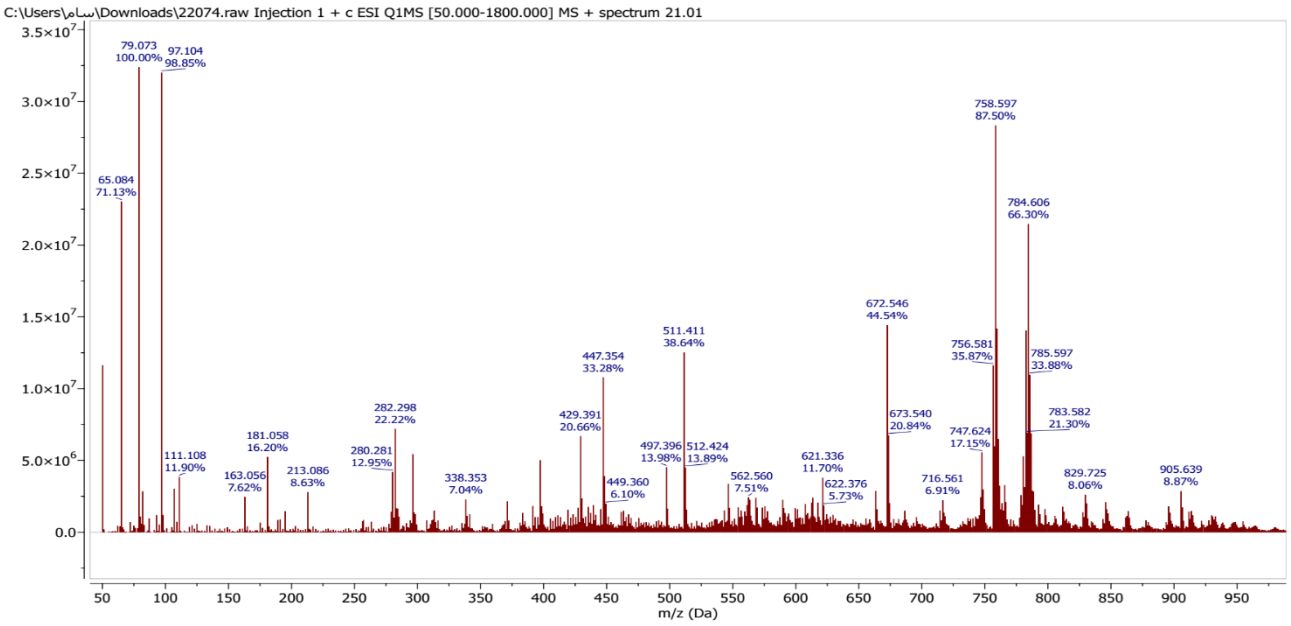
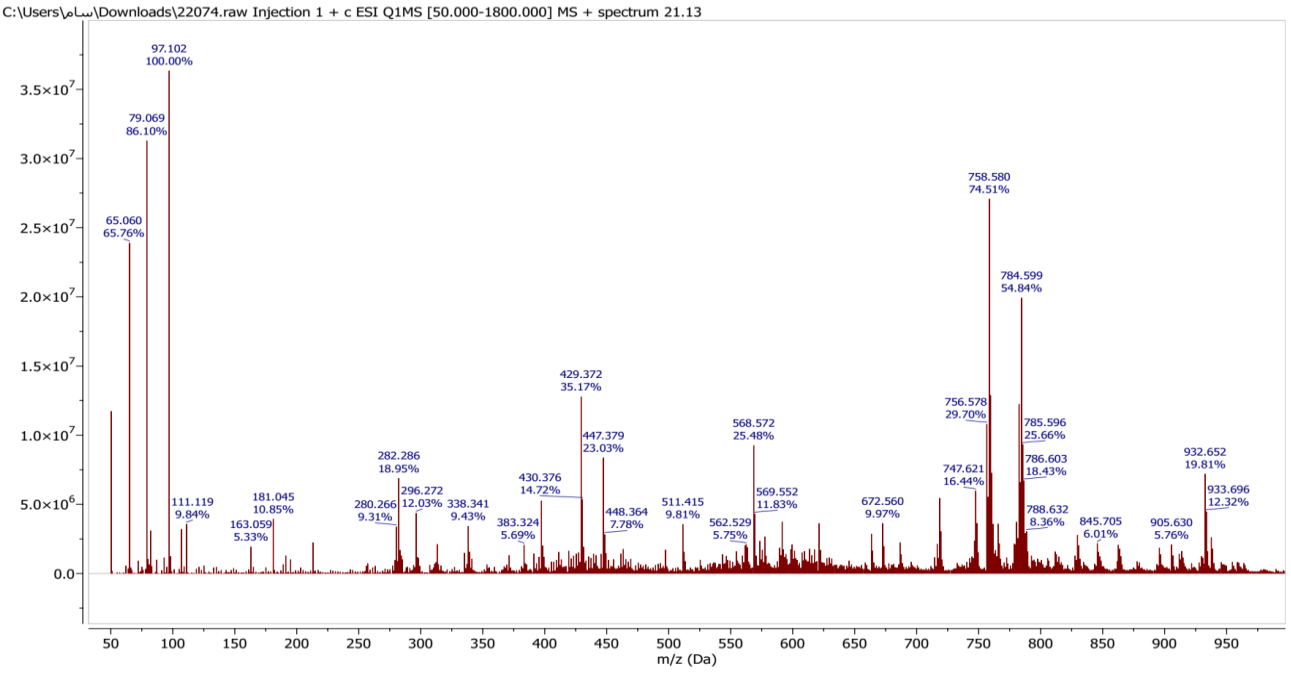


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C45 H85 N7 S2	788.63806	788.63800	7.0	0.08	-0.06	-0.08	0.588



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C52 H95 N3 O S4	906.64307	906.64307	7.0	0.01	-0.01	-0.01	0.779



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C47 H86 N9 O10	937.65704	937.65704	9.5	0.00	0.00	0.00	0.916

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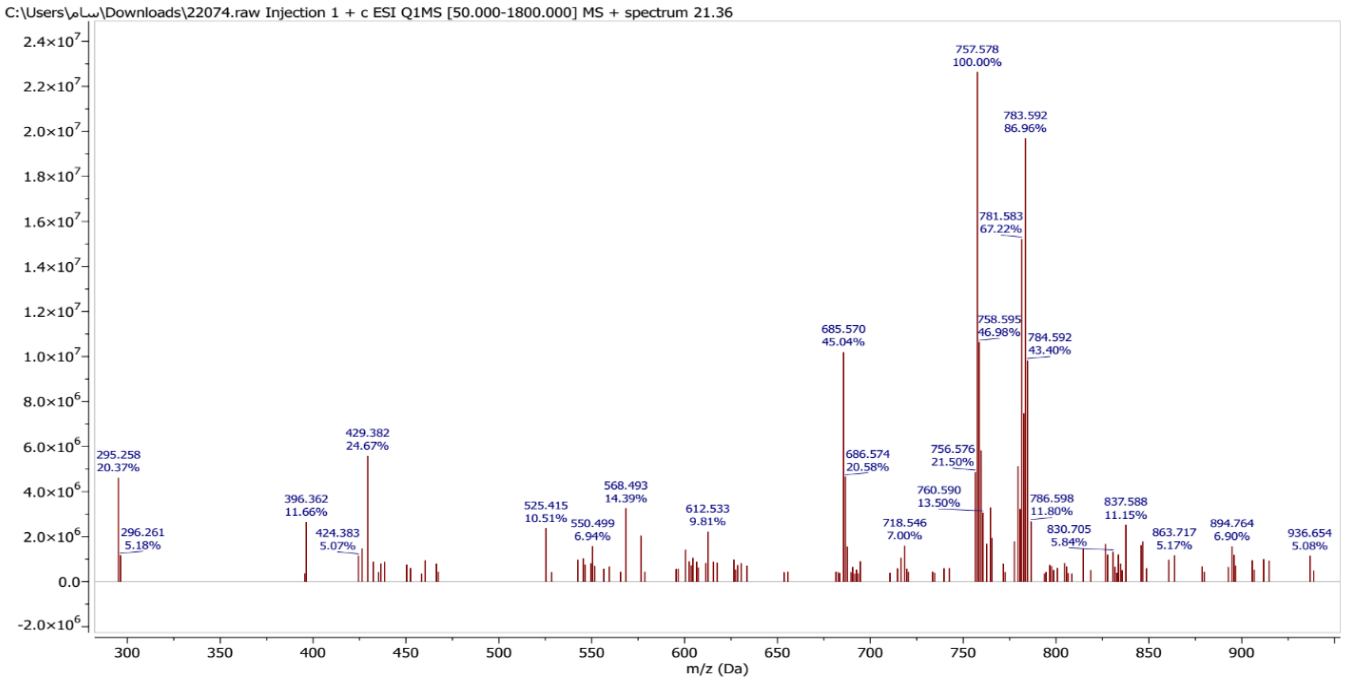
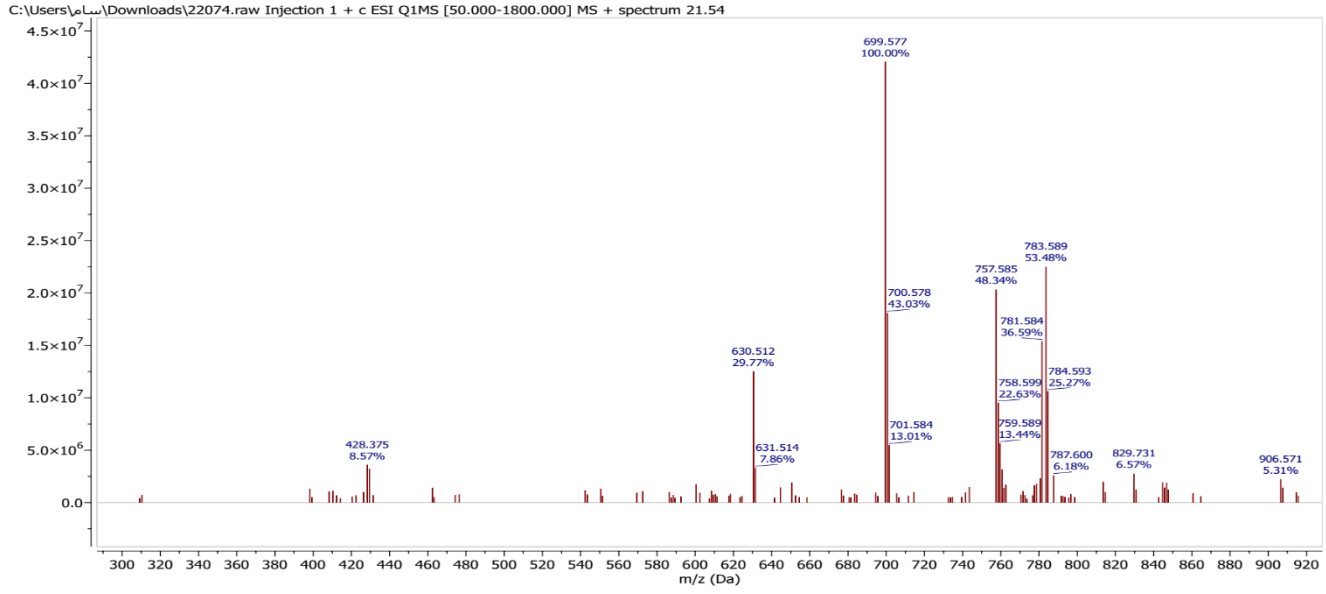
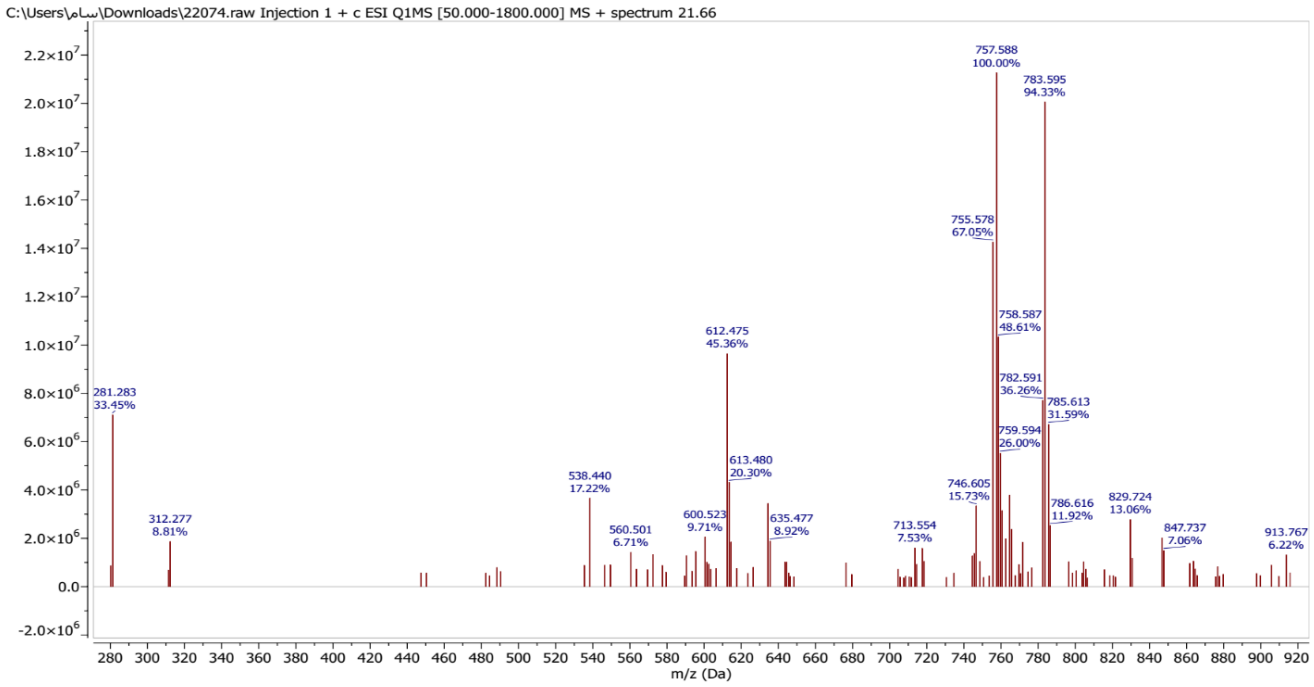


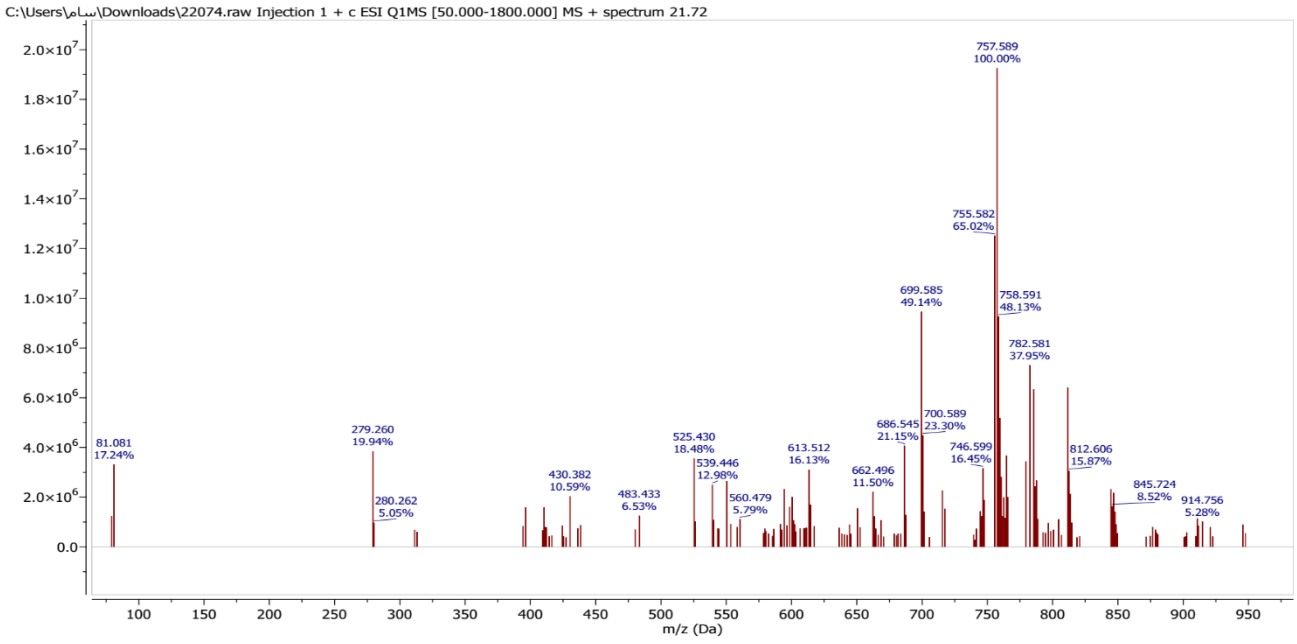
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C53 H97 N3 O2 S4	936.65364	936.65380	7.0	0.17	0.16	0.17	0.551



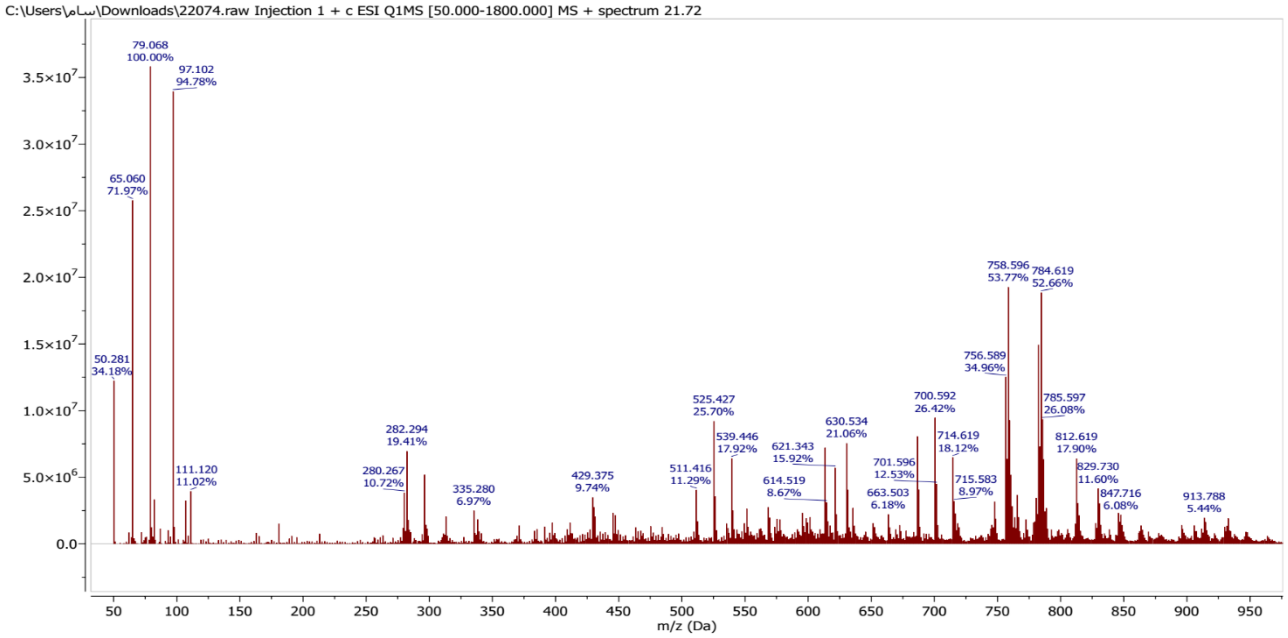
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C50 H79 N7 O4 S2	906.57077	906.57073	15.0	0.05	-0.05	-0.05	0.887



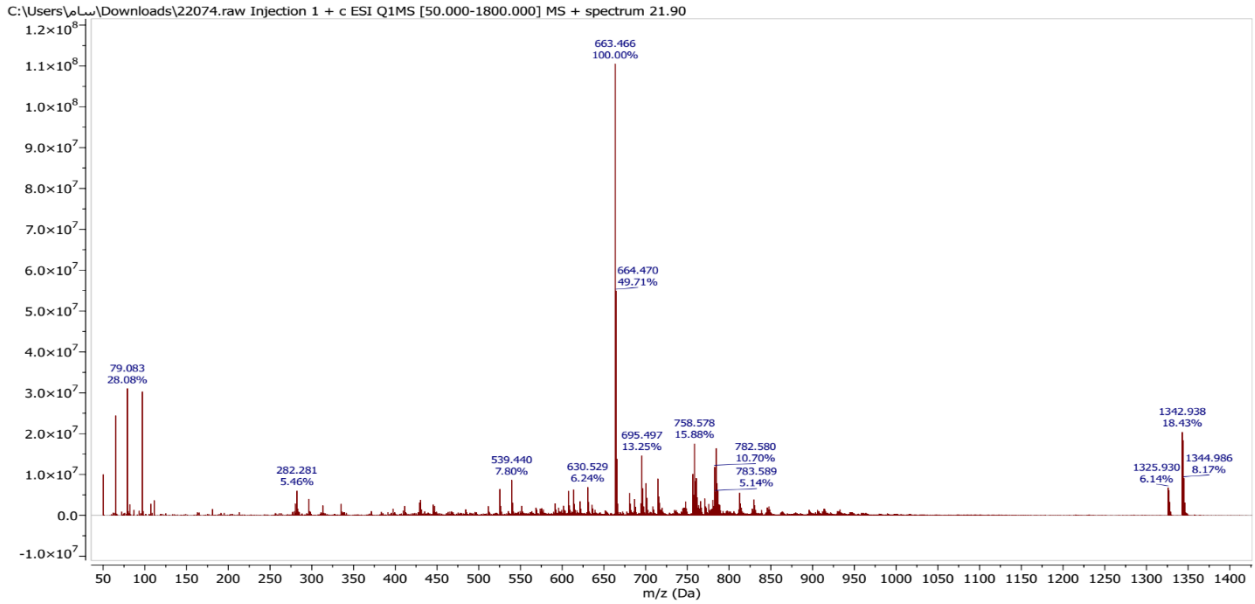
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C58 H89 N7 O3	932.70997	932.70976	18.0	0.22	-0.20	-0.22	0.899



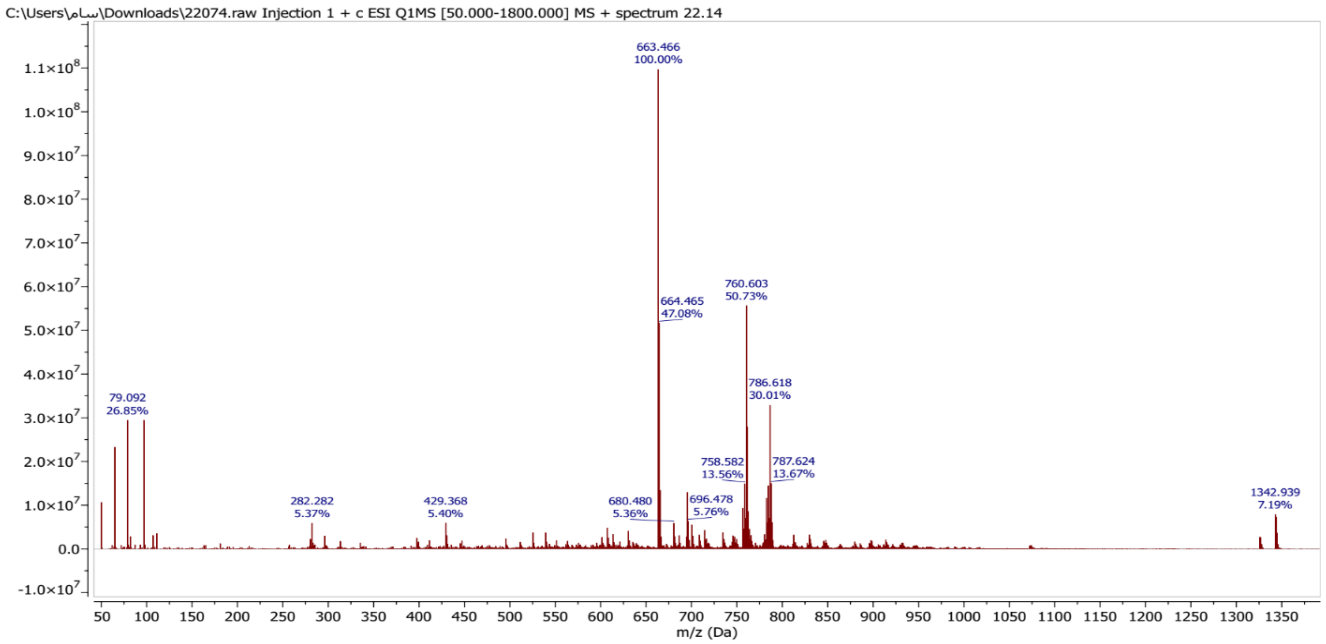
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C55 H99 N3 O7	914.75558	914.75579	8.0	0.23	0.21	0.23	0.490



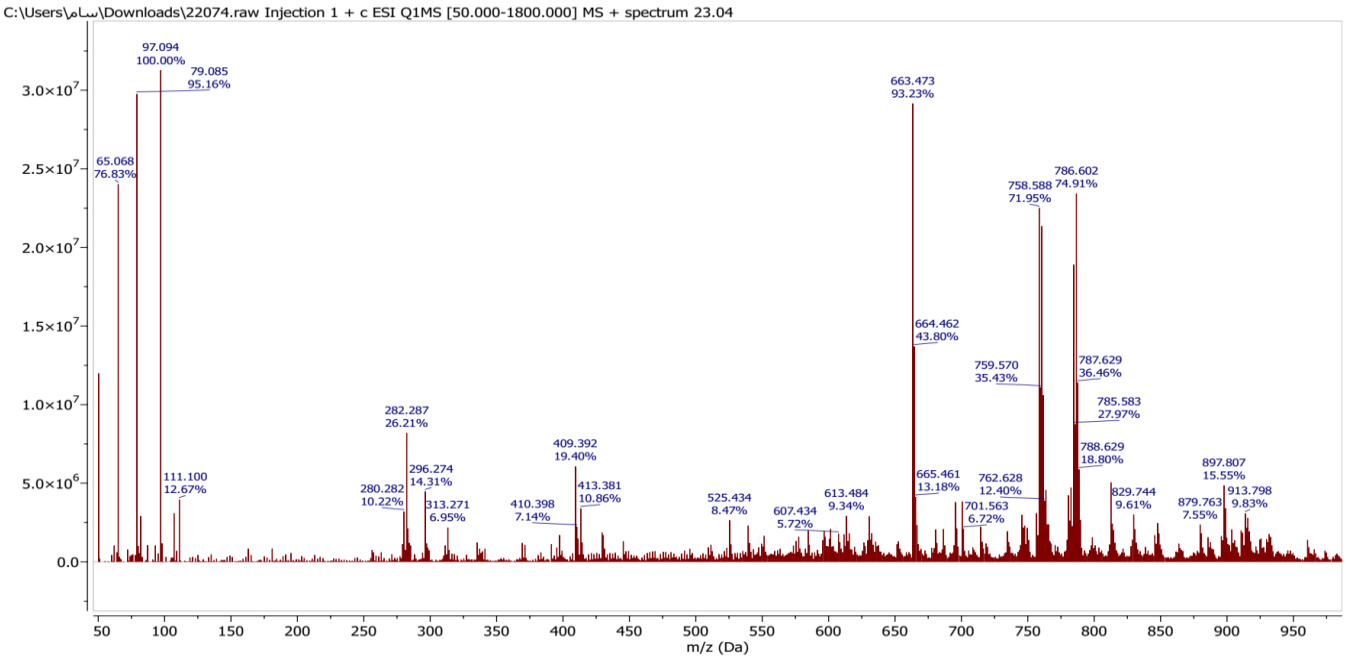
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C61 H105 N O S2	932.77103	932.77106	10.0	0.02	0.02	0.02	0.390



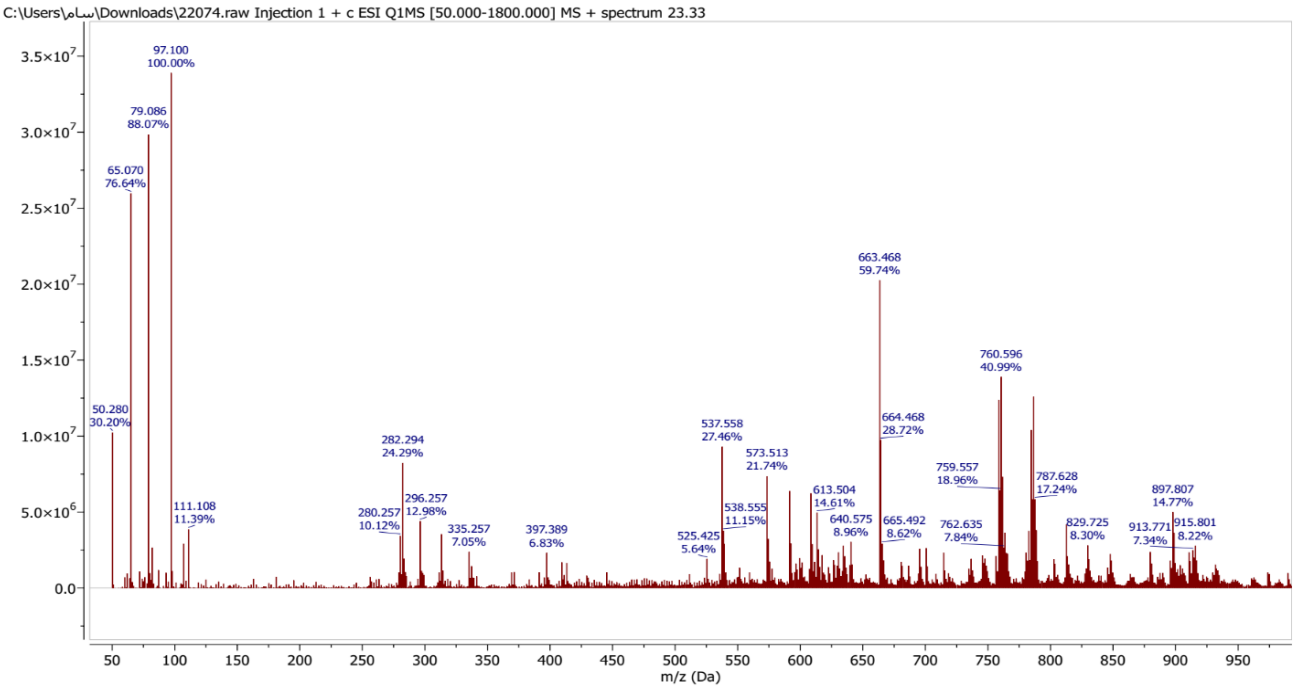
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C74 H143 N4 O8 S4	1344.98615	1344.98608	5.5	0.05	-0.07	-0.05	0.552



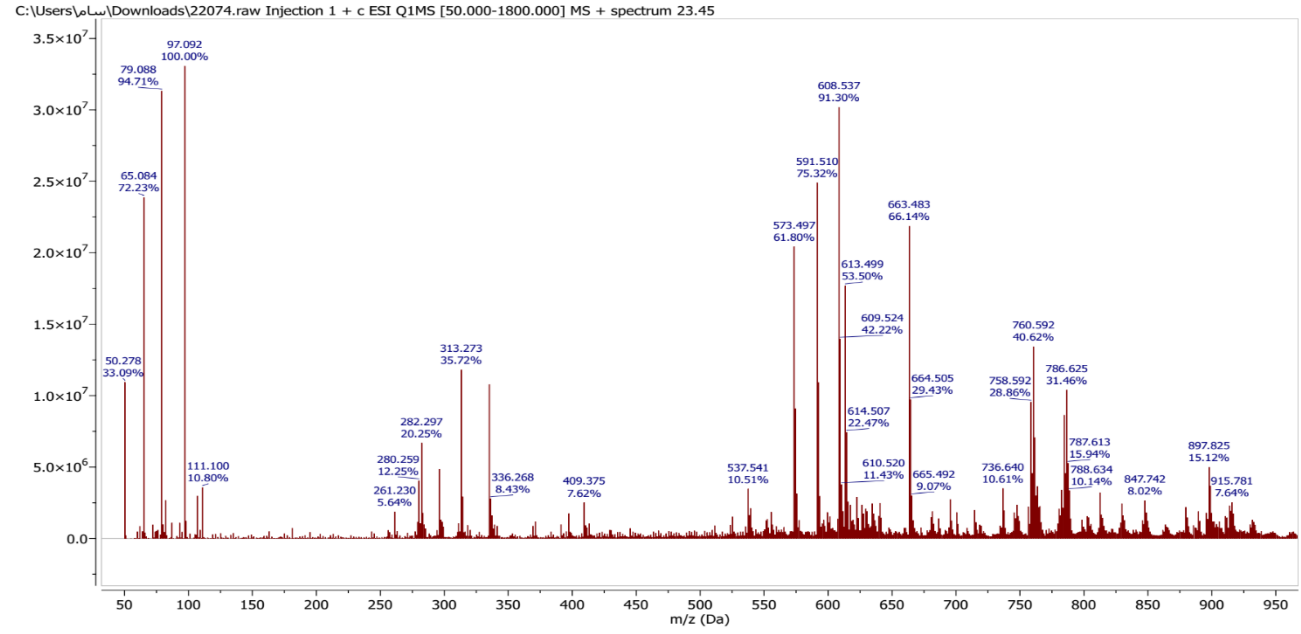
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C74 H136 N9 O4 S4	1343.96709	1343.96704	11.5	0.04	-0.05	-0.04	0.207



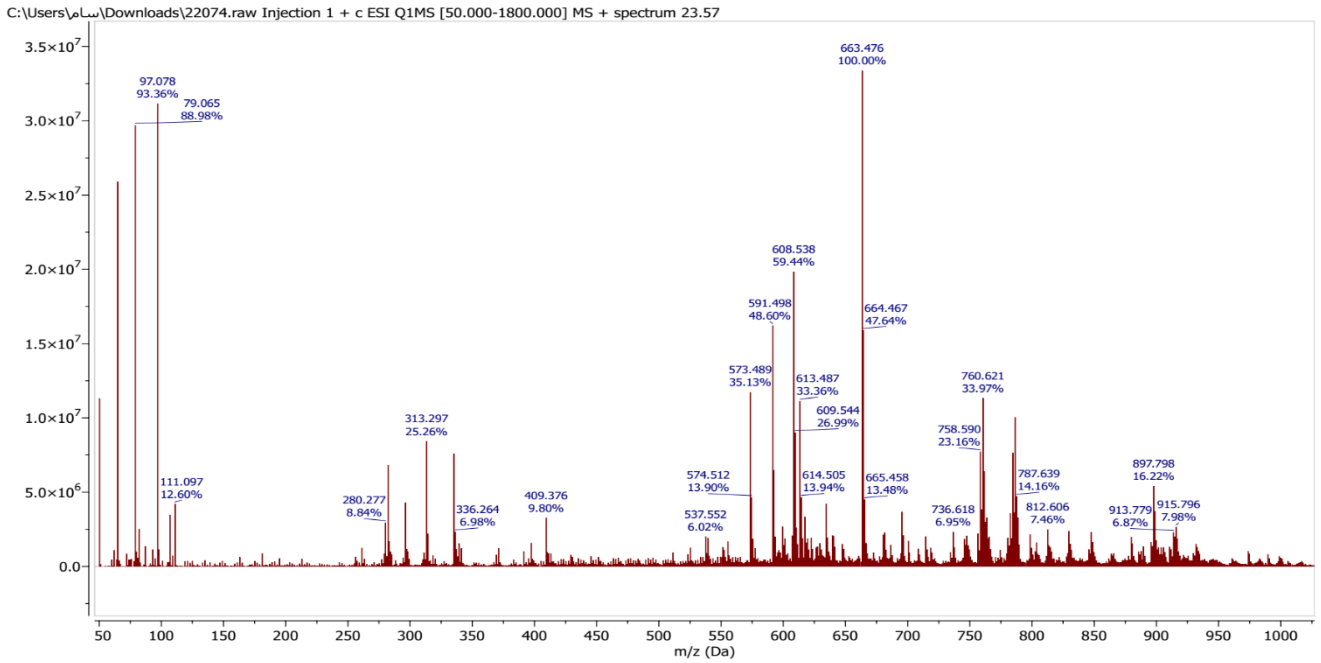
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C61 H105 N O S2	932.77103	932.77106	10.0	0.02	0.02	0.02	0.852



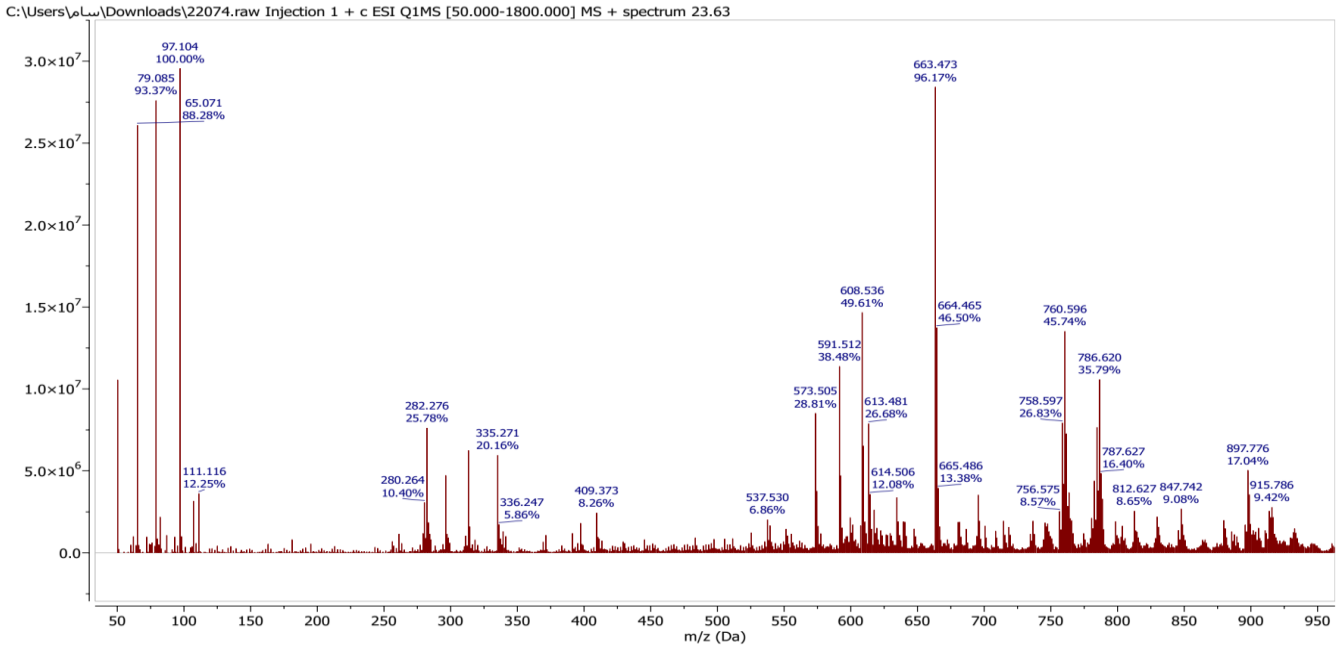
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C58 H107 O7	916.80896	916.80908	5.5	0.14	0.12	0.14	0.509



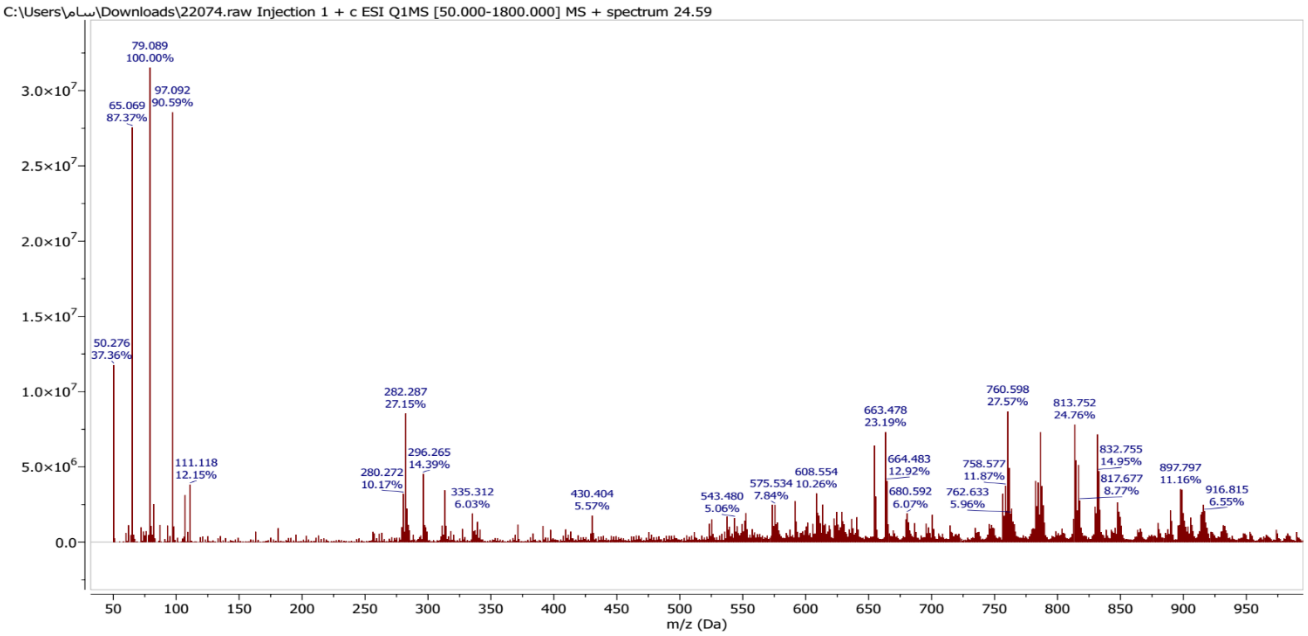
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C55 H107 N6 S2	916.80714	916.80701	5.5	0.15	-0.13	-0.15	0.436



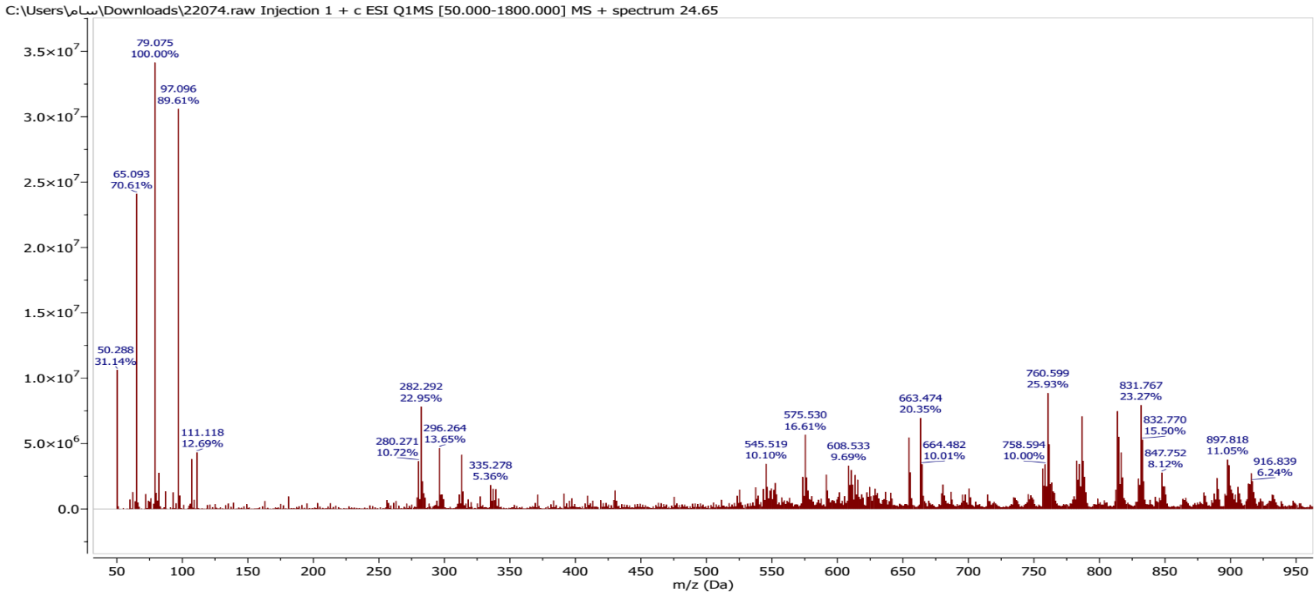
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C54 H109 N O7 S	916.79975	916.80005	1.0	0.32	0.30	0.32	0.484



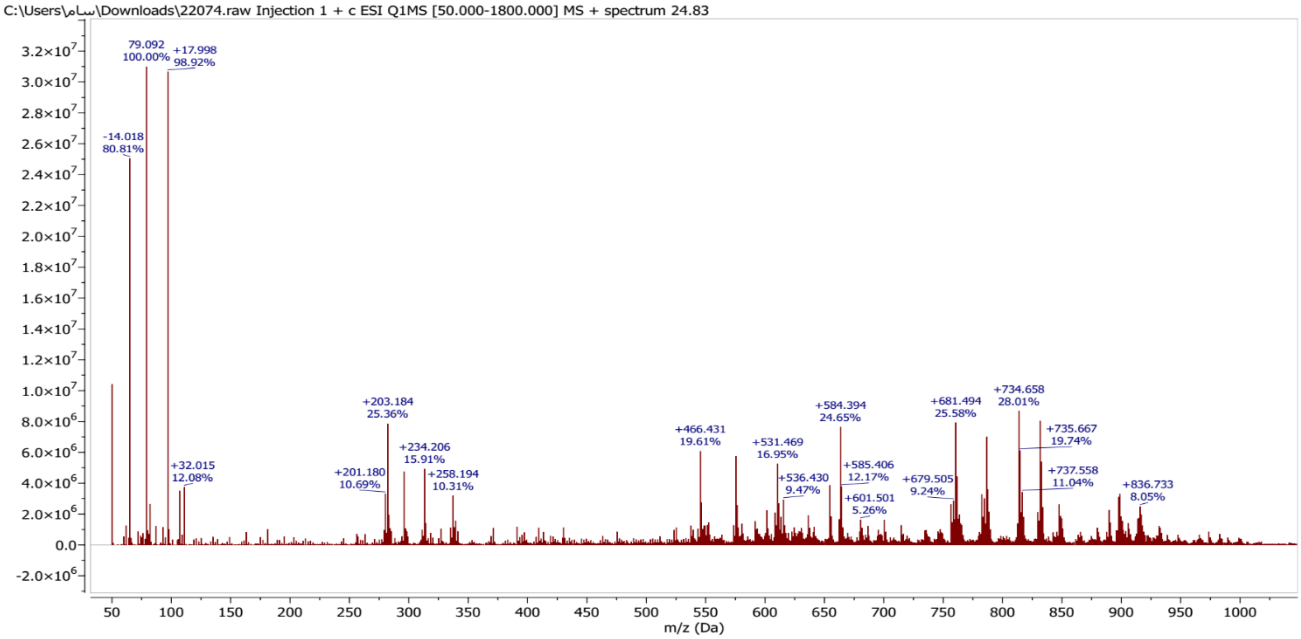
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C53 H113 N5 O S3	932.81800	932.81805	0.0	0.06	0.05	0.06	0.431



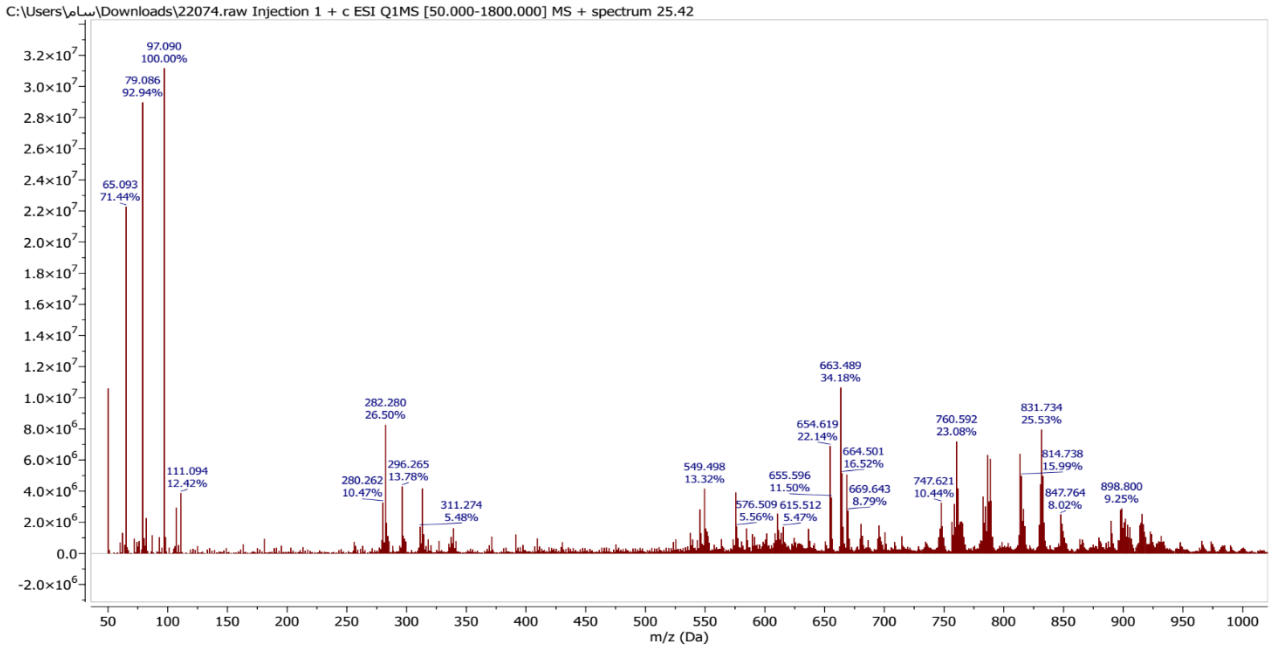
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C58 H109 N O4 S	916.81501	916.81506	5.0	0.06	0.06	0.06	0.901



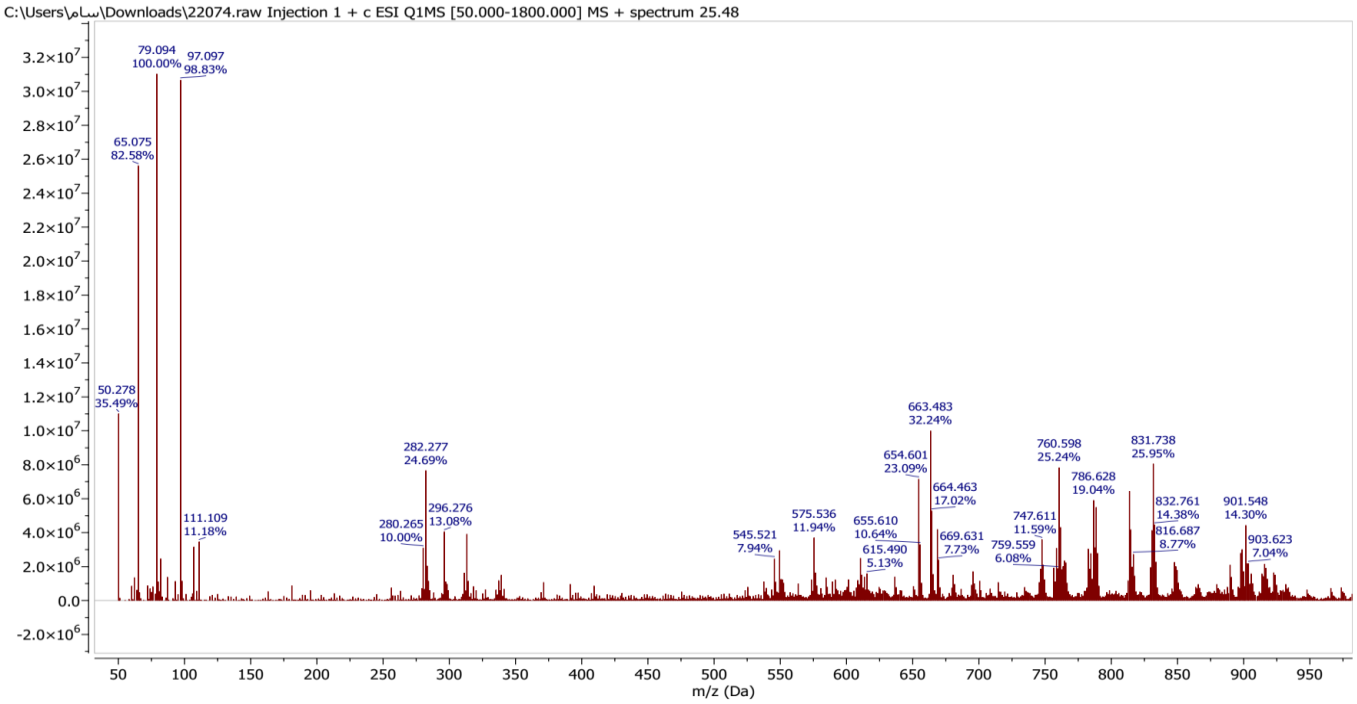
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C58 H111 N2 O3 S	916.83882	916.83905	4.5	0.25	0.23	0.25	0.440



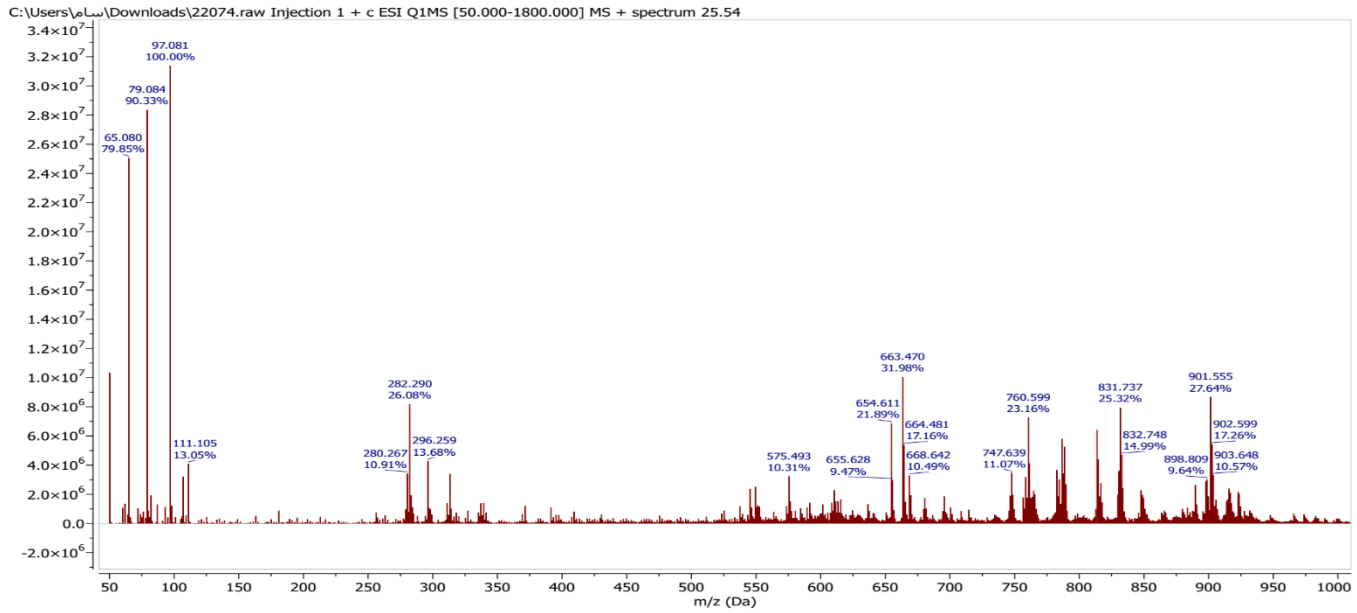
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C50 H109 N9 O S2	916.82693	916.82703	1.0	0.11	0.10	0.11	0.435



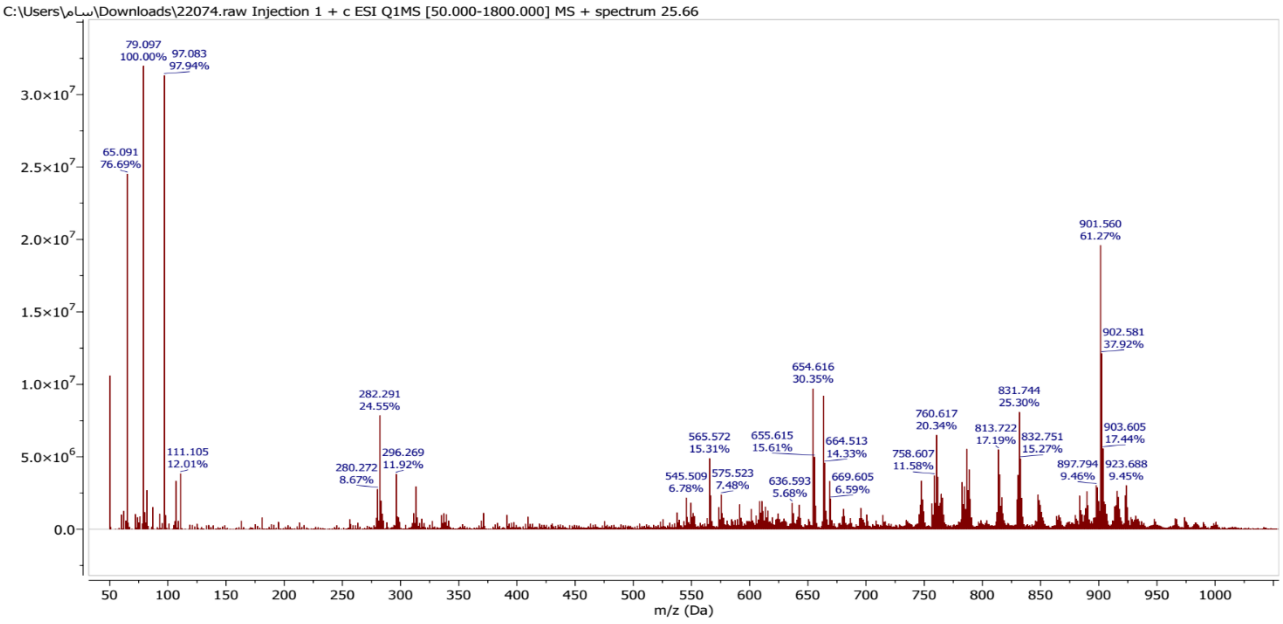
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C49 H105 N9 O6	916.82606	916.82605	2.0	0.01	-0.01	-0.01	0.536



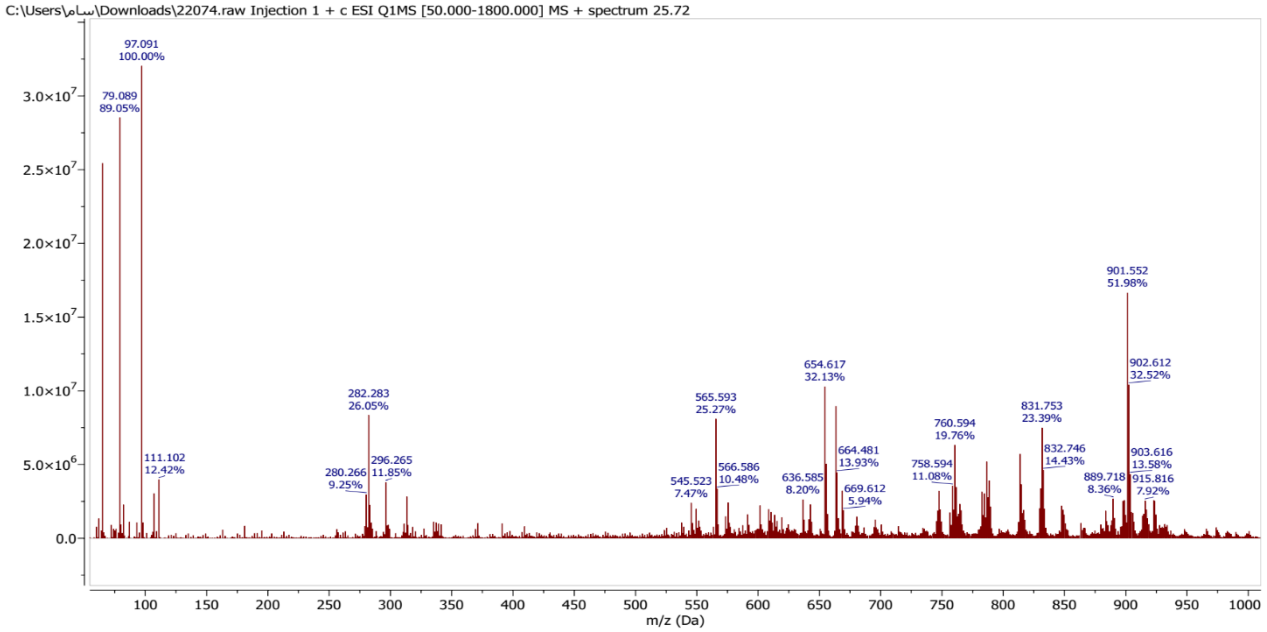
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C51 H97 N6 O8	922.74407	922.74402	6.5	0.05	-0.05	-0.05	0.351



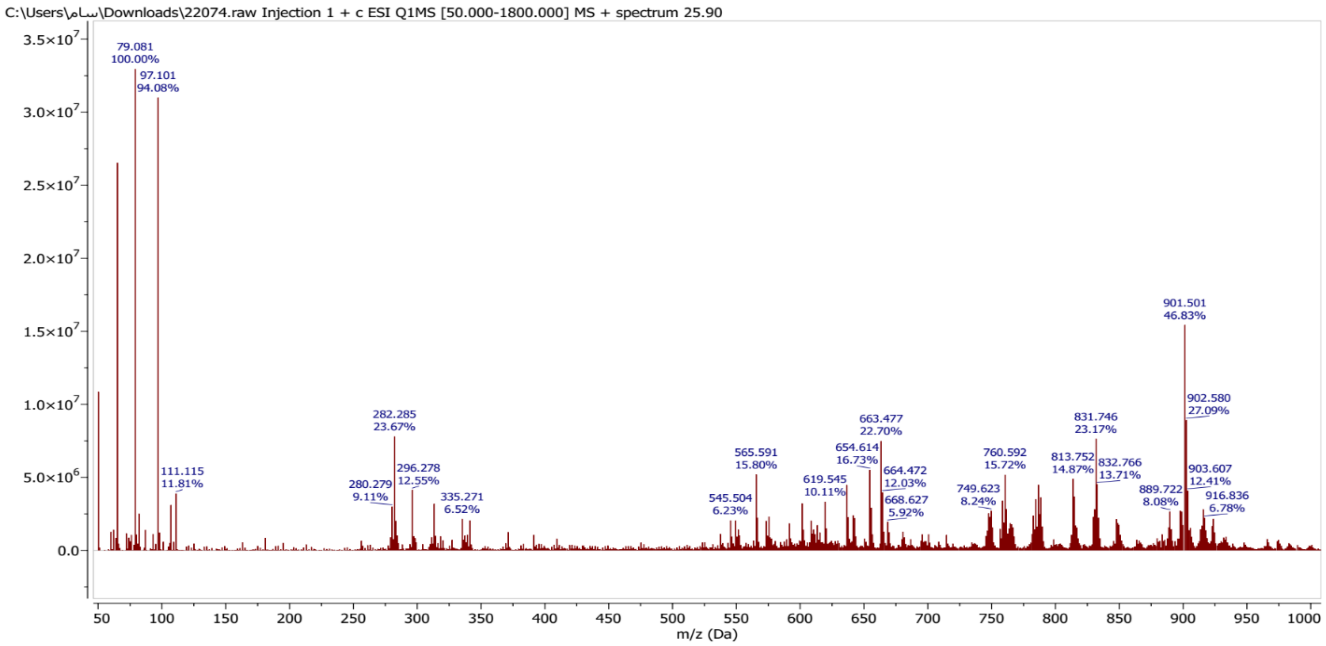
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C48 H94 N10 O7	923.73797	923.73804	7.0	0.07	0.07	0.07	0.484



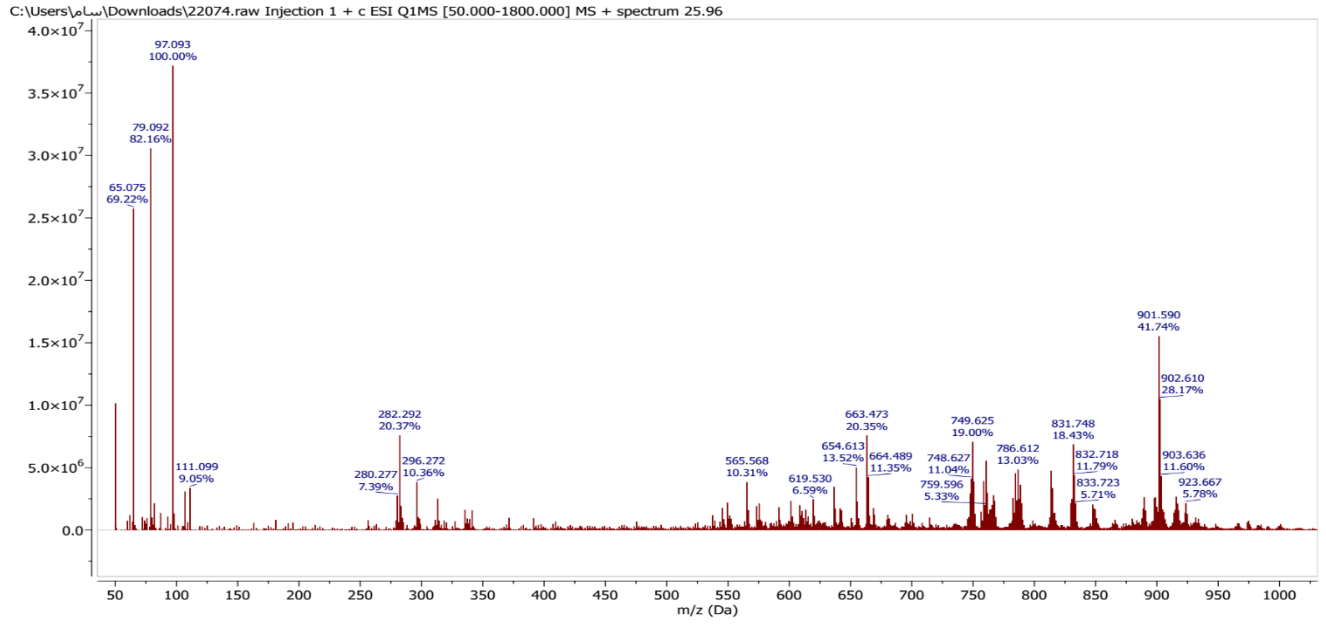
Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C60 H94 N2 O S2	923.68803	923.68805	15.0	0.02	0.02	0.02	0.825



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C59 H94 N4 O2 S	923.71703	923.71704	15.0	0.02	0.02	0.02	0.318



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C47 H88 N9 O7 S	923.66002	923.66003	8.5	0.02	0.02	0.02	0.535



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C49 H100 N3 O4 S4	923.66694	923.66705	1.5	0.12	0.11	0.12	0.466

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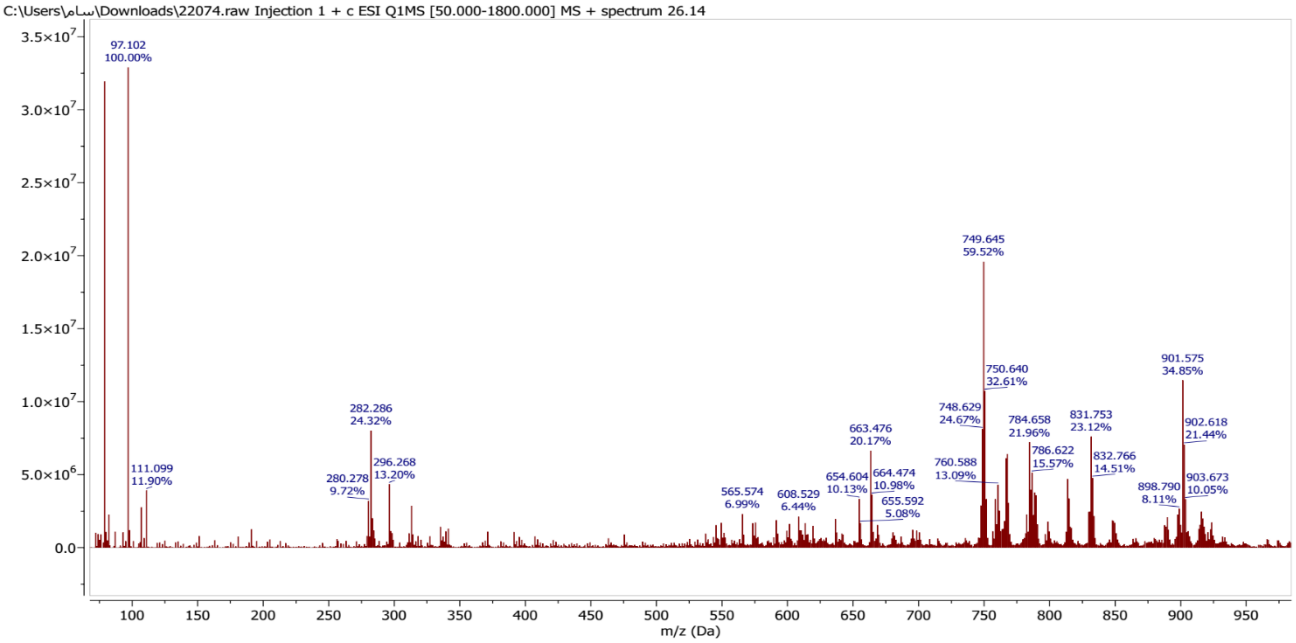
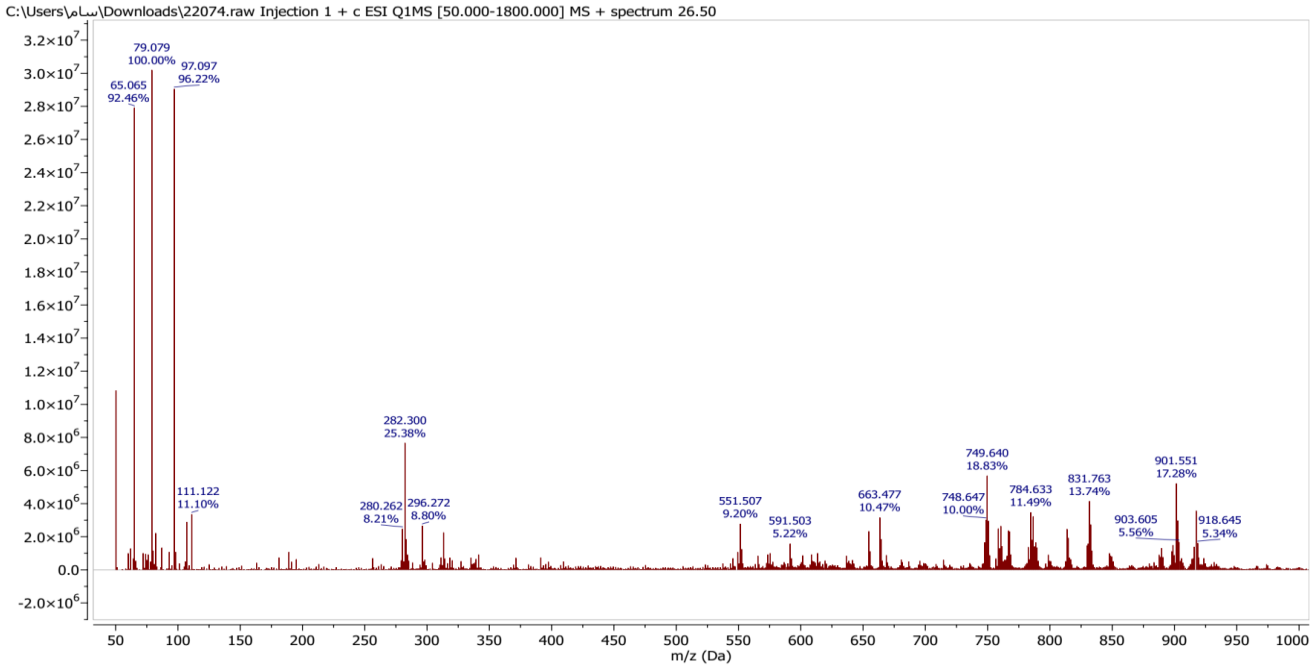
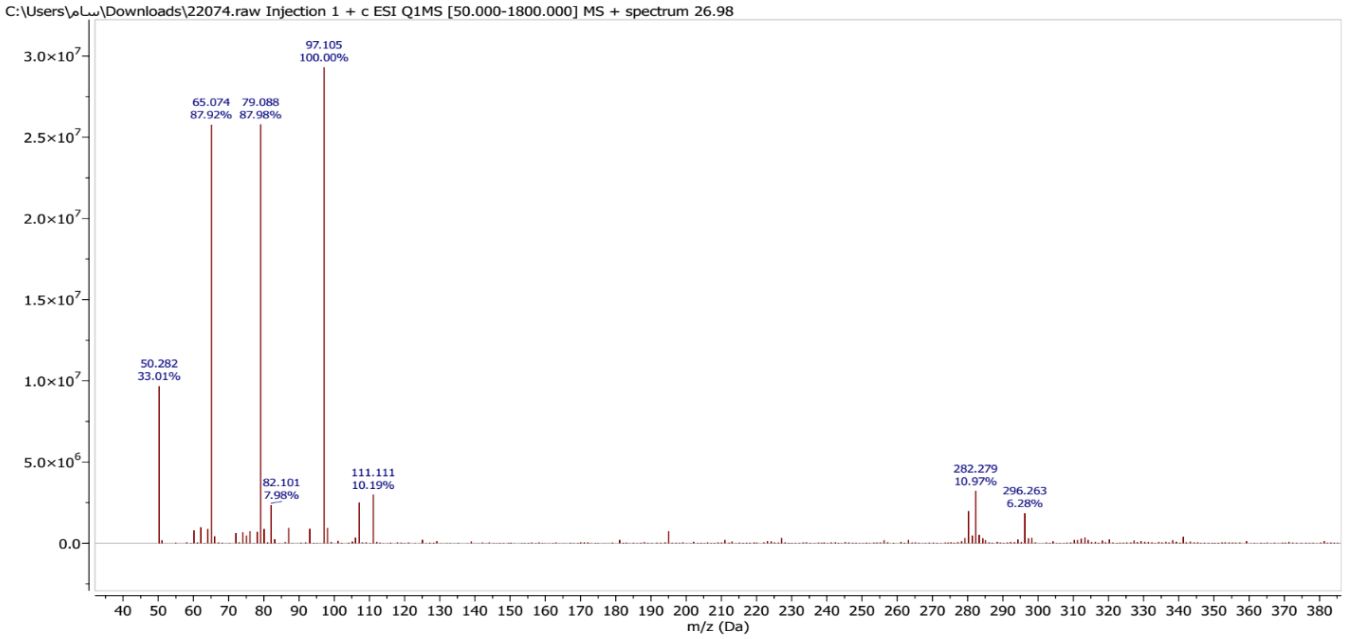


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C55 H96 N5 S3	923.69006	923.69000	10.5	0.06	-0.06	-0.06	0.413

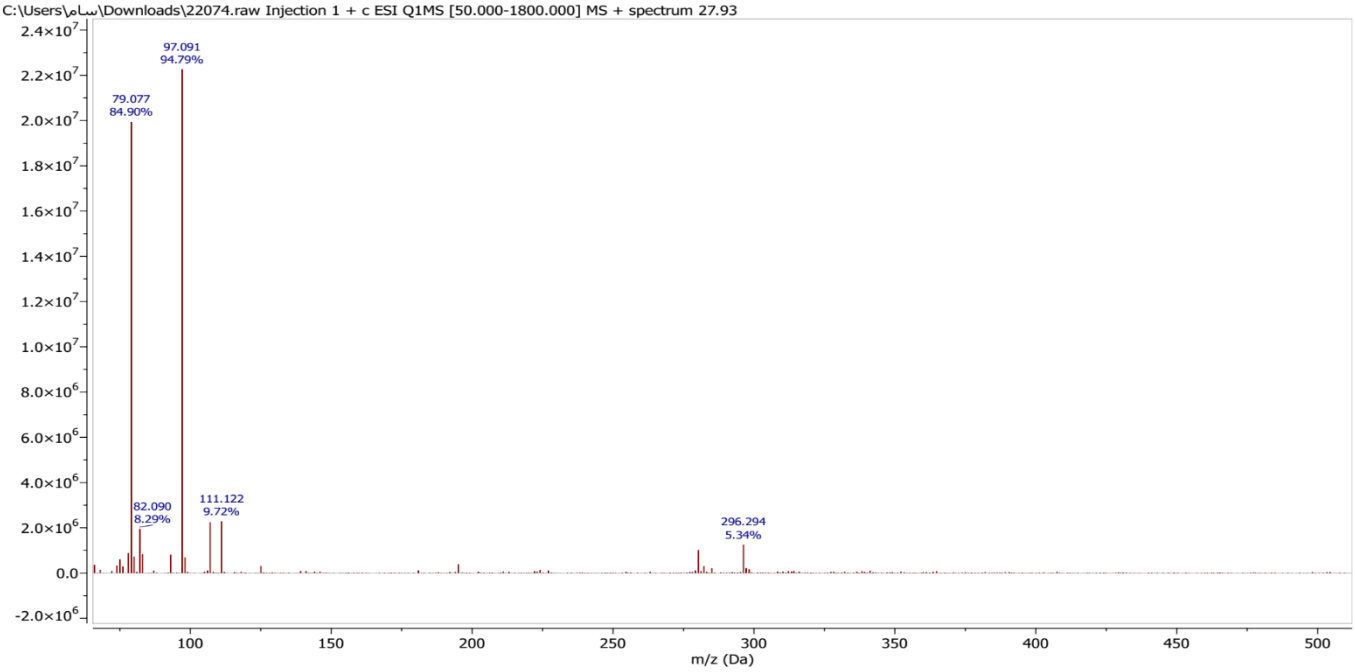


Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C48 H97 N6 S5	918.64510	918.64502	3.5	0.09	-0.08	-0.09	0.520

Figure 3. 95. Mass spectra of **X59** compound.



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C10 H31 N8 O2	296.26427	296.26306	-0.5	4.11	-1.21	-4.11	0.960



Formula	Calculated Mass	Target Mass	Double Bond Equivalence	Absolute Error (ppm)	Error (mDa)	Error (ppm)	Fitness
C17 H35 N4	296.29345	296.29401	2.5	1.89	0.56	1.89	0.922

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