

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU051420\
 Data File : VU038180.D
 Acq On : 14 May 2020 19:23
 Operator : JC/MD
 Sample : L2653-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AD9

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.388	8	15	31	rBV2	80104	83573	4.64%	0.713%
2	1.517	50	55	60	rBV	28279	25712	1.43%	0.219%
3	1.610	76	84	102	rBV2	233655	417662	23.18%	3.563%
4	1.758	123	130	139	rBV	74346	103758	5.76%	0.885%
5	1.941	180	187	196	rVB	148301	183995	10.21%	1.569%
6	2.600	381	392	407	rVB	239720	383872	21.30%	3.274%
7	4.767	1042	1066	1113	rBV	161823	668550	37.10%	5.703%
8	5.134	1164	1180	1201	rVB	219920	470817	26.13%	4.016%
9	5.780	1358	1381	1408	rBV2	487307	1187356	65.89%	10.128%
10	6.298	1527	1542	1563	rBV	413316	773472	42.92%	6.597%
11	6.738	1662	1679	1698	rBV	292583	571087	31.69%	4.871%
12	7.600	1934	1947	1962	rBV	141736	246087	13.66%	2.099%
13	7.928	2034	2049	2065	rBV	534954	938770	52.09%	8.007%
14	8.211	2116	2137	2149	rBV2	85433	148261	8.23%	1.265%
15	8.671	2262	2280	2314	rBV	949823	1802080	100.00%	15.371%
16	8.812	2314	2324	2335	rVB4	32033	58450	3.24%	0.499%
17	9.439	2503	2519	2543	rBV	576004	966023	53.61%	8.240%
18	10.774	2922	2934	2946	rBV	236536	385138	21.37%	3.285%
19	11.825	3248	3261	3275	rBV	598785	944021	52.39%	8.052%
20	12.079	3329	3340	3355	rBV9	13223	36321	2.02%	0.310%
21	12.204	3366	3379	3401	rVB	553944	903222	50.12%	7.704%
22	12.629	3504	3511	3526	rVB9	12728	22871	1.27%	0.195%
23	12.905	3589	3597	3608	rVB7	10553	20114	1.12%	0.172%
24	13.047	3633	3641	3655	rVB7	8342	20816	1.16%	0.178%
25	13.864	3887	3895	3906	rBV7	11062	22468	1.25%	0.192%
26	14.108	3959	3971	3978	rBV3	15398	34106	1.89%	0.291%
27	14.156	3979	3986	3995	rVB8	11095	20208	1.12%	0.172%
28	14.217	3995	4005	4023	rVB4	40441	72557	4.03%	0.619%
29	14.314	4023	4035	4051	rBV2	78091	143323	7.95%	1.222%
30	14.851	4193	4202	4213	rBV8	10568	19078	1.06%	0.163%
31	14.909	4213	4220	4233	rVB8	16063	31073	1.72%	0.265%
32	15.976	4543	4552	4560	rBV8	10475	18949	1.05%	0.162%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

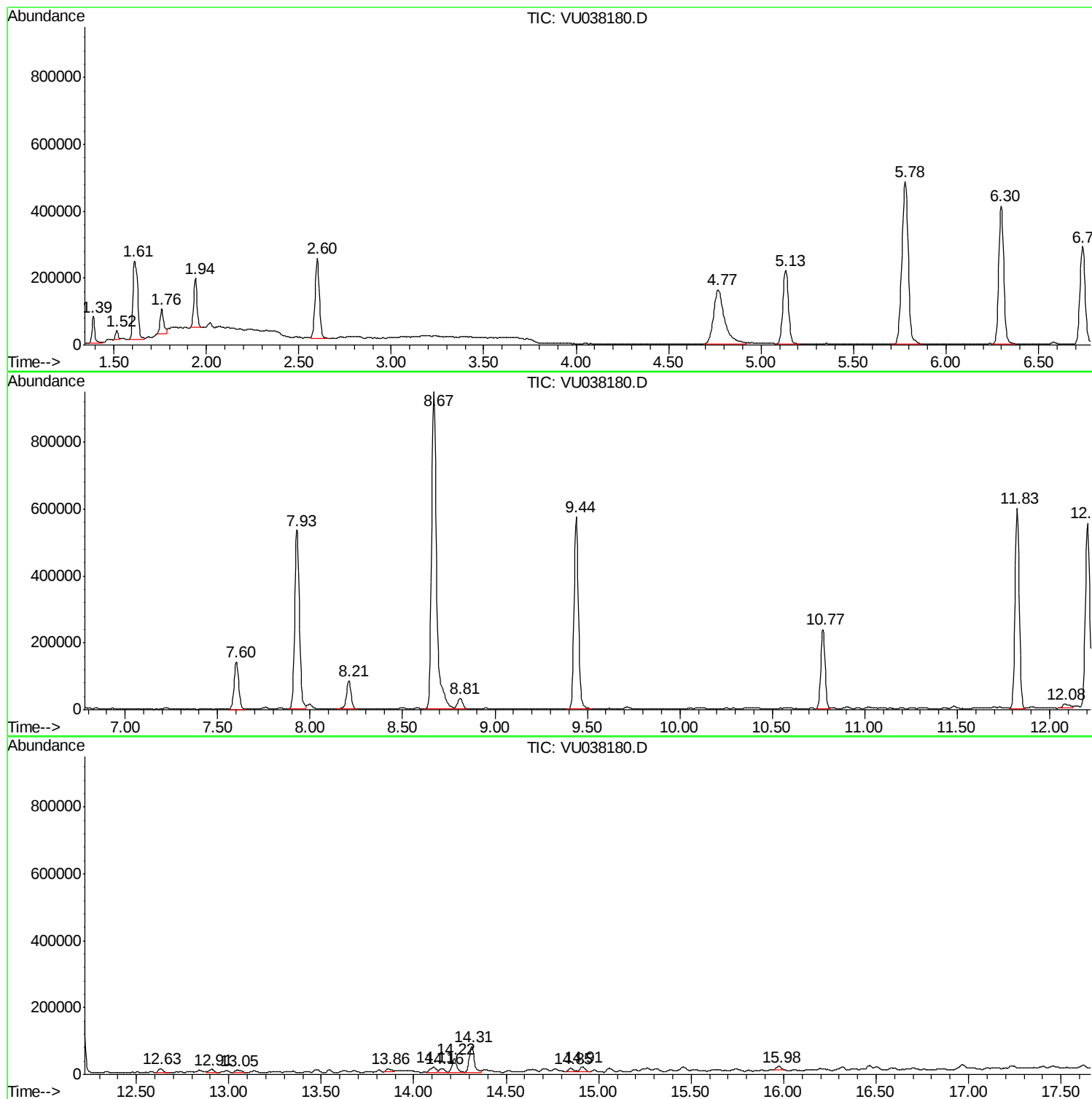
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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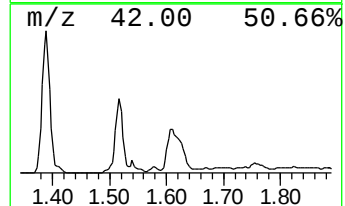
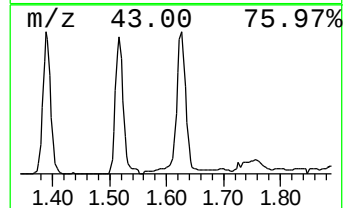
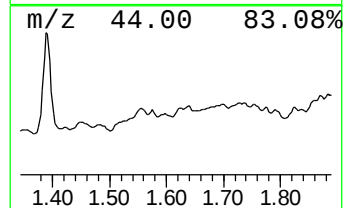
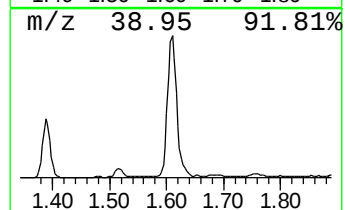
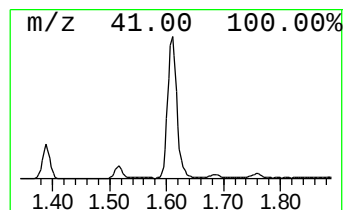
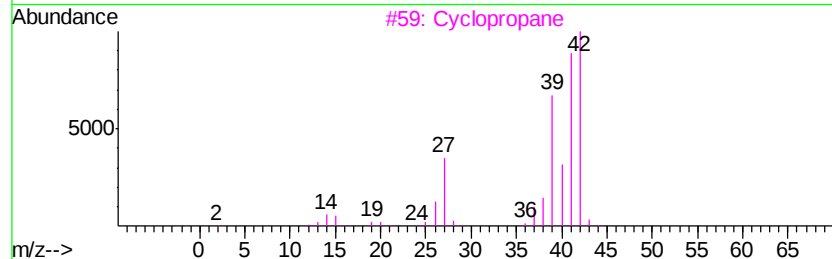
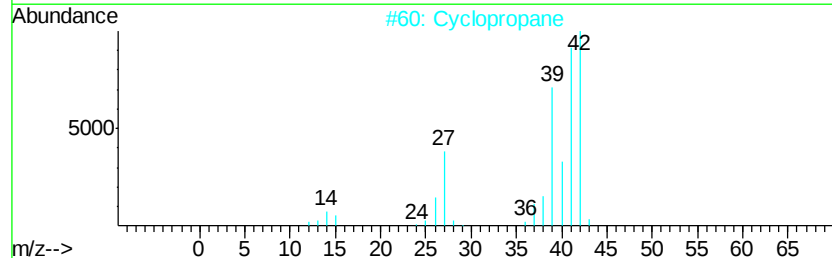
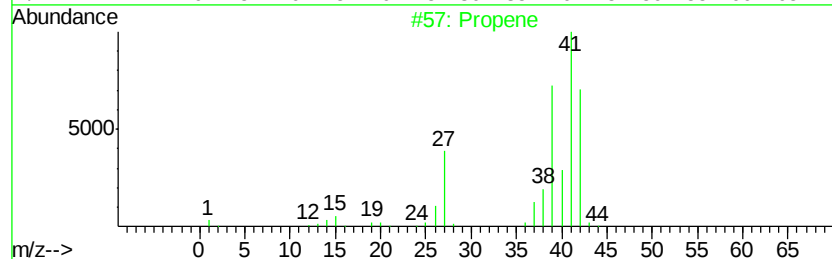
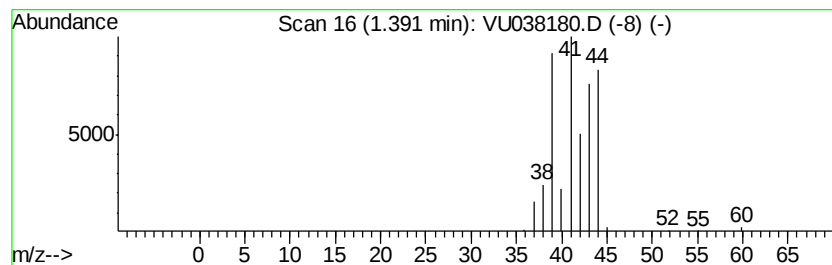
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.39	0.54 ug/L	83573	1,4-Difluorobenzene	6.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	9
2			Cyclopropane	42	C3H6	000075-19-4	9
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Propane	44	C3H8	000074-98-6	5
5			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4



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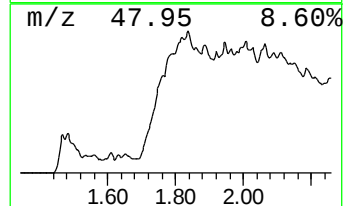
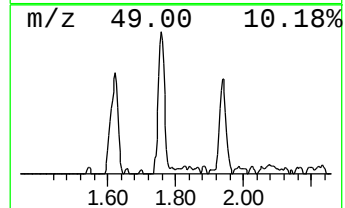
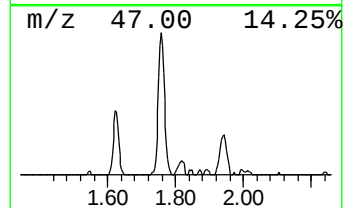
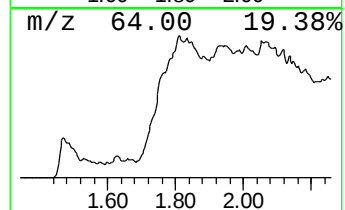
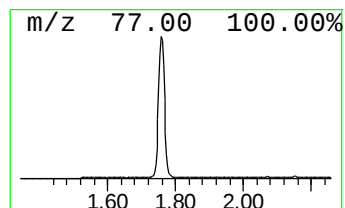
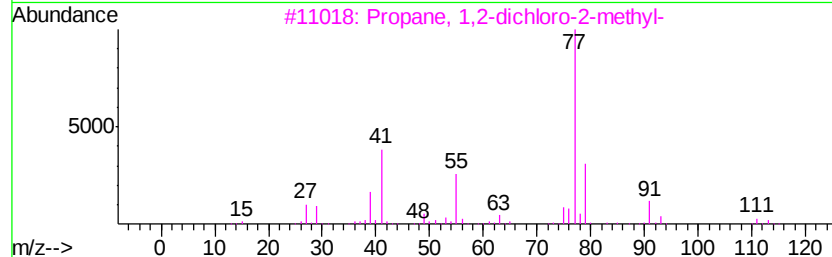
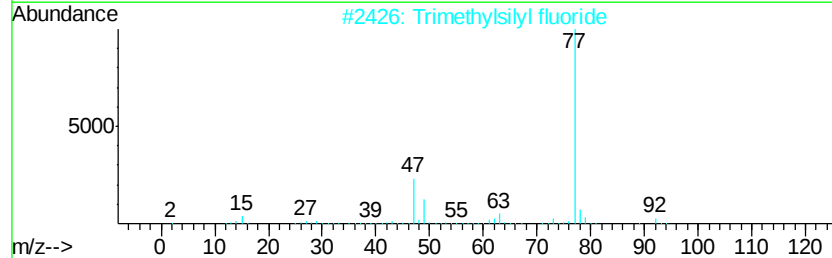
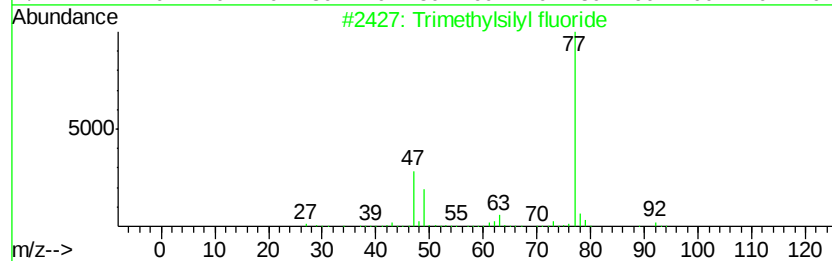
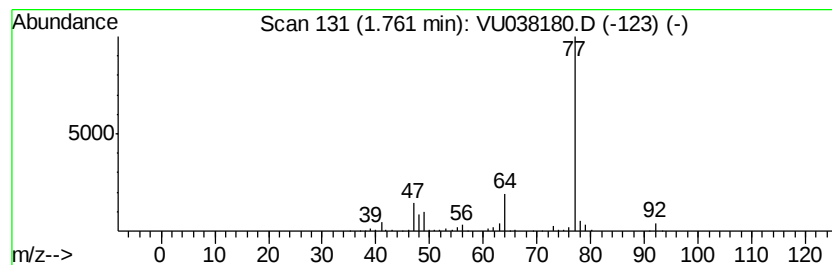
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Trimethylsilyl fluoride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	0.67 ug/L	103758	1,4-Difluorobenzene	6.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trimethylsilyl fluoride	92	C3H9FSi	000420-56-4	83
2			Trimethylsilyl fluoride	92	C3H9FSi	000420-56-4	46
3			Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	9
4			Trimethylphosphine oxide	92	C3H9OP	000676-96-0	4
5			Propane, 2-chloro-2-nitro-	123	C3H6ClNO2	000594-71-8	4



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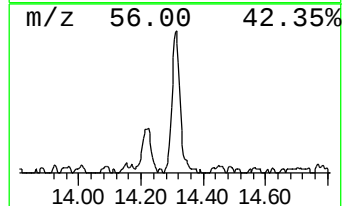
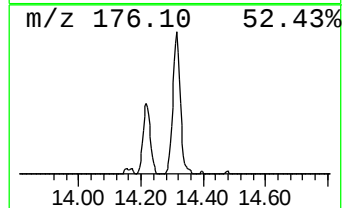
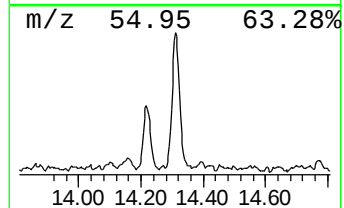
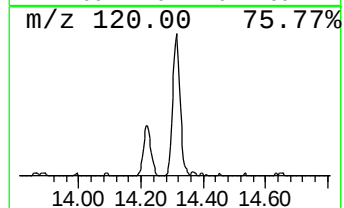
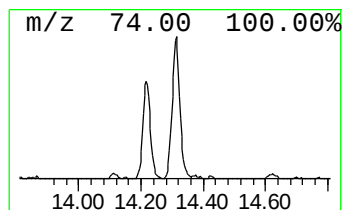
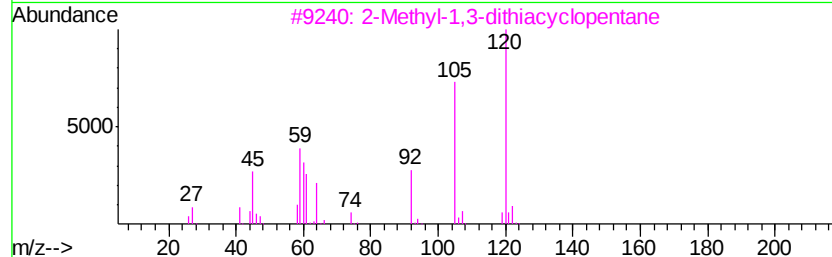
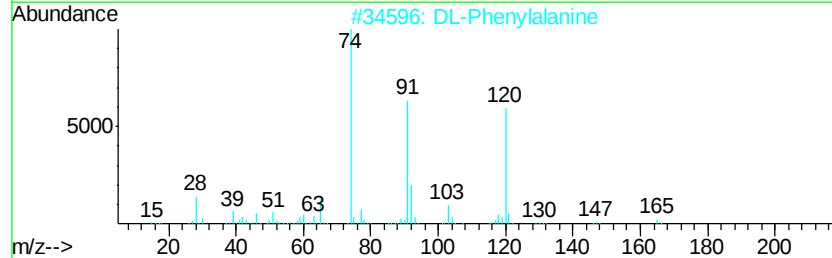
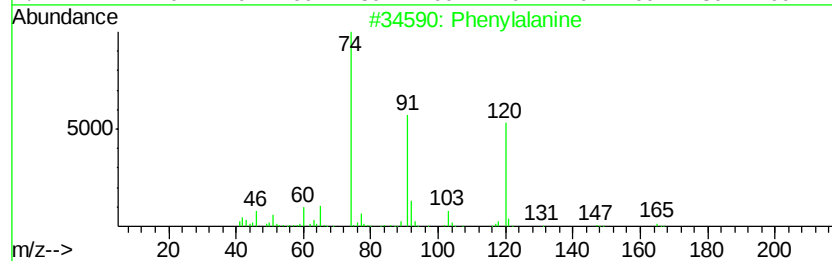
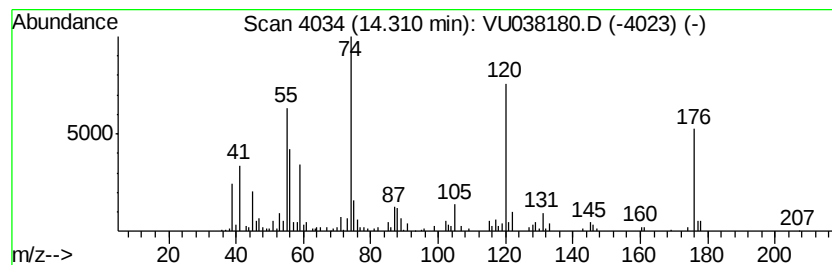
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ClientSampleID :
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Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.31	0.76 ug/L	143323	1,4-Dichlorobenzene-d4	11.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenylalanine	165	C9H11NO2	000063-91-2	32
2		DL-Phenylalanine	165	C9H11NO2	000150-30-1	23
3		2-Methyl-1,3-dithiacyclopentane	120	C4H8S2	005616-51-3	22
4		Methyl isovalerate	116	C6H12O2	000556-24-1	22
5		1,3-Dithiane	120	C4H8S2	000505-23-7	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	1.39	0.5	ug/L	83573	1	6.30	773472	5.0
Trimethylsilyl fl...	1.76	0.7	ug/L	103758	1	6.30	773472	5.0
unknown-01	14.31	0.8	ug/L	143323	3	11.83	944021	5.0