LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039608.D
Acq On : 21 Jul 2020 19:38
Operator : SY/MD
Sample : L3347-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

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\SOMUTR072120WMA.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	1.366	3	8	13	rBV	246066	229537	45.84%	4.223%
2	1.398	13	18	28	rVB	172972	179606	35.86%	3.305%
3	1.449	29	34	42	rVB2	7060	7761	1.55%	0.143%
4	1.498	42	49	55	rBV	22839	23272	4.65%	0.428%
5	1.597	70	80	91	rBV3	158627	272103	54.34%	5.006%
6	1.668	97	102	107	rVB	4864	5416	1.08%	0.100%
7	1.742	118	125	136	rVB3	21222	27446	5.48%	0.505%
8	1.922	166	181	193	rBV2	58763	84141	16.80%	1.548%
9	2.006	197	207	220	rVB	41620	57066	11.40%	1.050%
10	2.166	246	257	265	rBV	45950	64071	12.79%	1.179%
11	2.224	265	275	292	rVB4	40210	90727	18.12%	1.669%
12	2.330	301	308	316	rBV5	5311	8008	1.60%	0.147%
13	2.427	324	338	347	rBV4	13961	26435	5.28%	0.486%
14	2.481	347	355	368	rVB2	11903	18635	3.72%	0.343%
15	2.581	374	386	398	rBV	92172	150826	30.12%	2.775%
16	2.655	400	409	418	rBV3	8901	19875	3.97%	0.366%
17	2.816	448	459	466	rBV6	3189	5985	1.20%	0.110%
18	2.874	468	477	490	rVB	9365	17633	3.52%	0.324%
19	2.986	502	512	514	rBV4	3701	5260	1.05%	0.097%
20	3.153	554	564	575	rVB4	7871	13657	2.73%	0.251%
21	3.379	618	634	649	rVB3	9126	20133	4.02%	0.370%
22	3.607	691	705	717	rVB6	13224	32331	6.46%	0.595%
23	3.719	728	740	752	rBV4	4957	10672	2.13%	0.196%
24	3.845	764	779	792	rBV6	2620	6014	1.20%	0.111%
25	4.218	888	895	906	rVB8	3374	6838	1.37%	0.126%
26	4.465	957	972	984	rVB6	2707	6950	1.39%	0.128%
27	4.559	988	1001	1012	rVV5	5400	12529	2.50%	0.231%
28	4.655	1015	1031	1075	rVV2	67640	231296	46.19%	4.256%
29	4.835	1075	1087	1107	rVB3	5588	13993	2.79%	0.257%
30	5.083	1149	1164	1189	rBV3	79258	196222	39.18%	3.610%
31	5.401	1248	1263	1274	rBV8	4230	11488	2.29%	0.211%
32	5.481	1274	1288	1303	rVB5	7728	20028	4.00%	0.368%
33	5.610	1315	1328	1341	rBV6	2877	5830	1.16%	0.107%
34	5.742	1346	1369	1395	rBV2	163652	443450	88.55%	8.159%

LSC Area Percent Report

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Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

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\SOMUTR072120WMA.M
Title : TRACE VOA SOM01.0

35	5.915	1413	1423	1435	rVB	10904	23383	4.67%	0.430%
36	6.041	1454	1462	1476	rVB7	4039	9342	1.87%	0.172%
37	6.263	1516	1531	1555	rBV	152921	297832	59.47%	5.480%
38	6.706	1654	1669	1684	rBV2	102989	205413	41.02%	3.779%
39	6.771	1684	1689	1701	rVB6	3015	5886	1.18%	0.108%
40	7.263	1827	1842	1857	rVB7	7176	16133	3.22%	0.297%
41	7.391	1872	1882	1892	rBV4	5085	11104	2.22%	0.204%
42	7.575	1928	1939	1954	rBV2	53910	94935	18.96%	1.747%
43	7.906	2029	2042	2056	rBV	199491	340221	67.94%	6.260%
44	7.976	2056	2064	2074	rVB	23711	38393	7.67%	0.706%
45	8.189	2118	2130	2143	rBV2	33133	54910	10.96%	1.010%
46	8.642	2252	2271	2301	rBV	265836	500785	100.00%	9.214%
47	9.420	2501	2513	2528	rBV	223360	370787	74.04%	6.822%
48	9.574	2551	2561	2571	rBV	9939	14954	2.99%	0.275%
49	9.697	2588	2599	2610	rBV2	32439	52806	10.54%	0.972%
50	10.105	2712	2726	2744	rBV2	13035	22233	4.44%	0.409%
51	10.758	2917	2929	2942	rBV	81265	132129	26.38%	2.431%
52	10.906	2966	2975	2986	rVB2	5237	7820	1.56%	0.144%
53	11.002	2993	3005	3008	rBV2	5086	8101	1.62%	0.149%
54	11.086	3024	3031	3041	rVB2	7933	10635	2.12%	0.196%
55	11.291	3083	3095	3105	rBV3	7947	11683	2.33%	0.215%
56	11.465	3137	3149	3161	rBV2	36933	56092	11.20%	1.032%
57	11.809	3244	3256	3270	rBV	220140	353430	70.58%	6.503%
58	11.889	3272	3281	3291	rVB	9210	13341	2.66%	0.245%
59	12.057	3324	3333	3336	rBV3	6515	8947	1.79%	0.165%
60	12.089	3336	3343	3358	rVV3	18712	34359	6.86%	0.632%
61	12.188	3362	3374	3388	rVB	205267	336434	67.18%	6.190%
62	12.565	3482	3491	3499	rBV	7174	10801	2.16%	0.199%
63	12.674	3517	3525	3534	rBV3	8061	11852	2.37%	0.218%
64	12.963	3606	3615	3623	rBV2	5046	7188	1.44%	0.132%
65	13.018	3623	3632	3640	rVB2	5860	8120	1.62%	0.149%
66	13.285	3708	3715	3724	rVB5	5947	8396	1.68%	0.154%
67	13.449	3756	3766	3779	rVB4	12236	20122	4.02%	0.370%
68	13.931	3909	3916	3927	rVB8	3288	5608	1.12%	0.103%
69	14.079	3951	3962	3971	rBV2	3471	5748	1.15%	0.106%

Sum of corrected areas: 5435157

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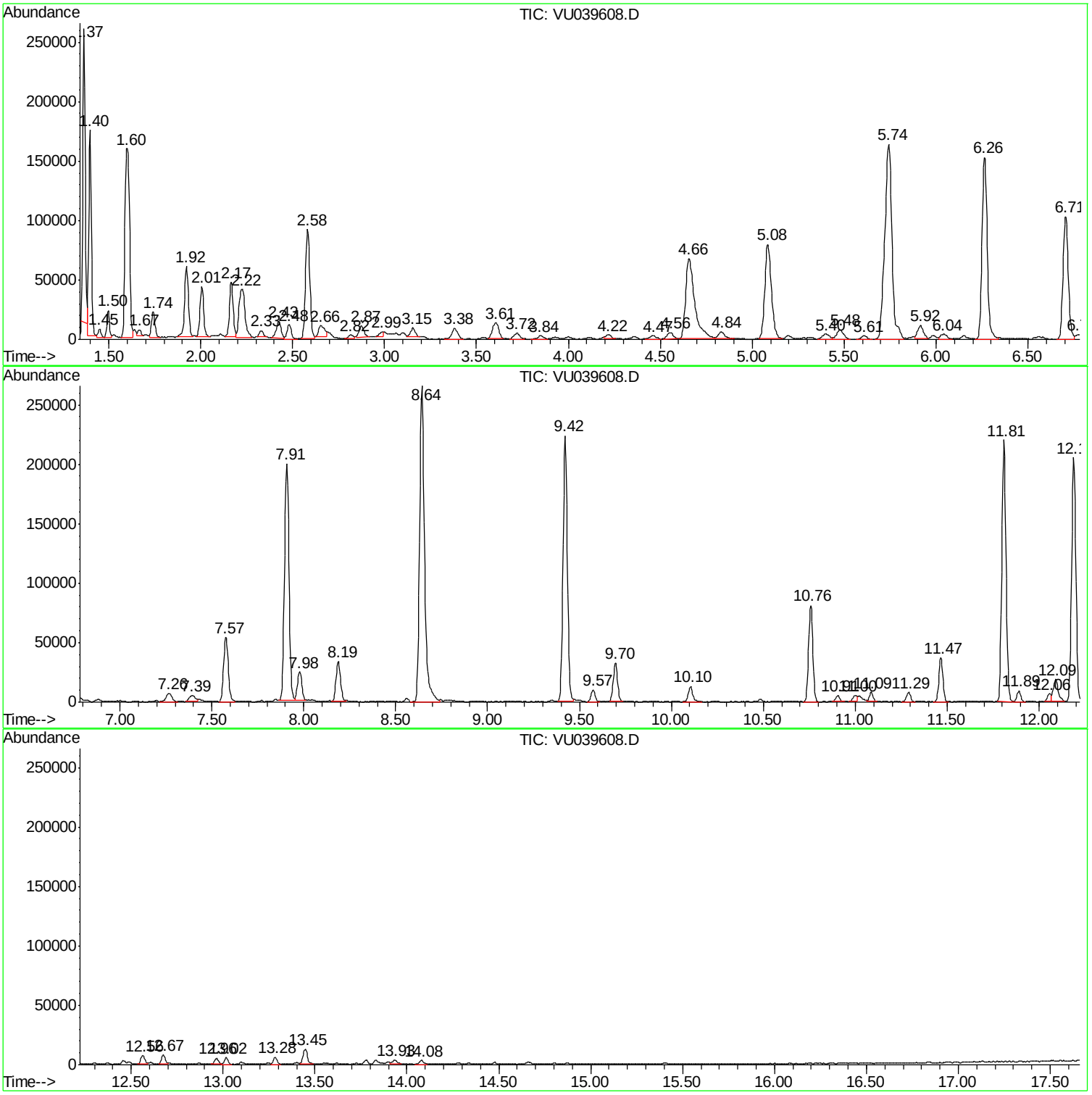
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039608.D
Acq On : 21 Jul 2020 19:38
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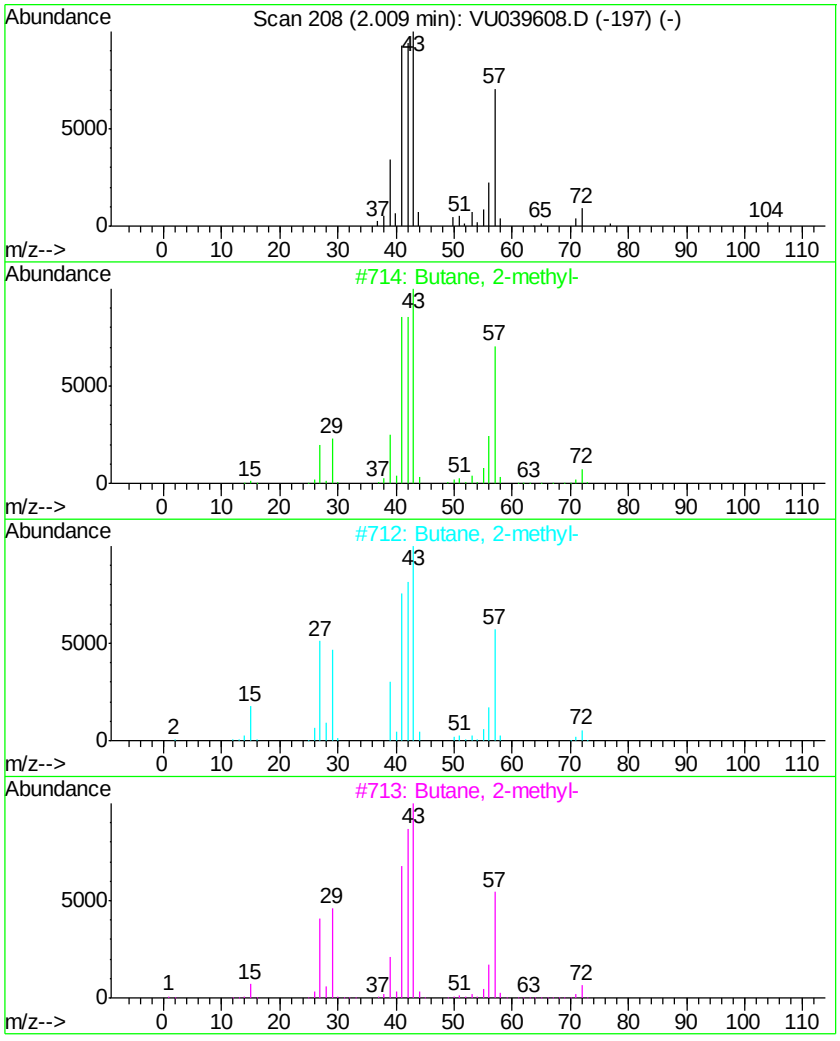
Quant Title : TRACE VOA SOM01.0

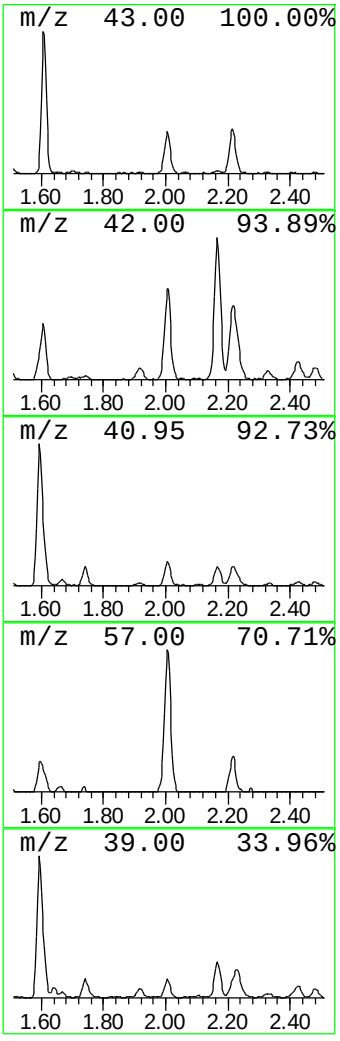
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	0.96 ug/L	57066	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	90
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	45
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	38





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Data File : VU039608.D
Acq On : 21 Jul 2020 19:38
Operator : SY/MD
Sample : L3347-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

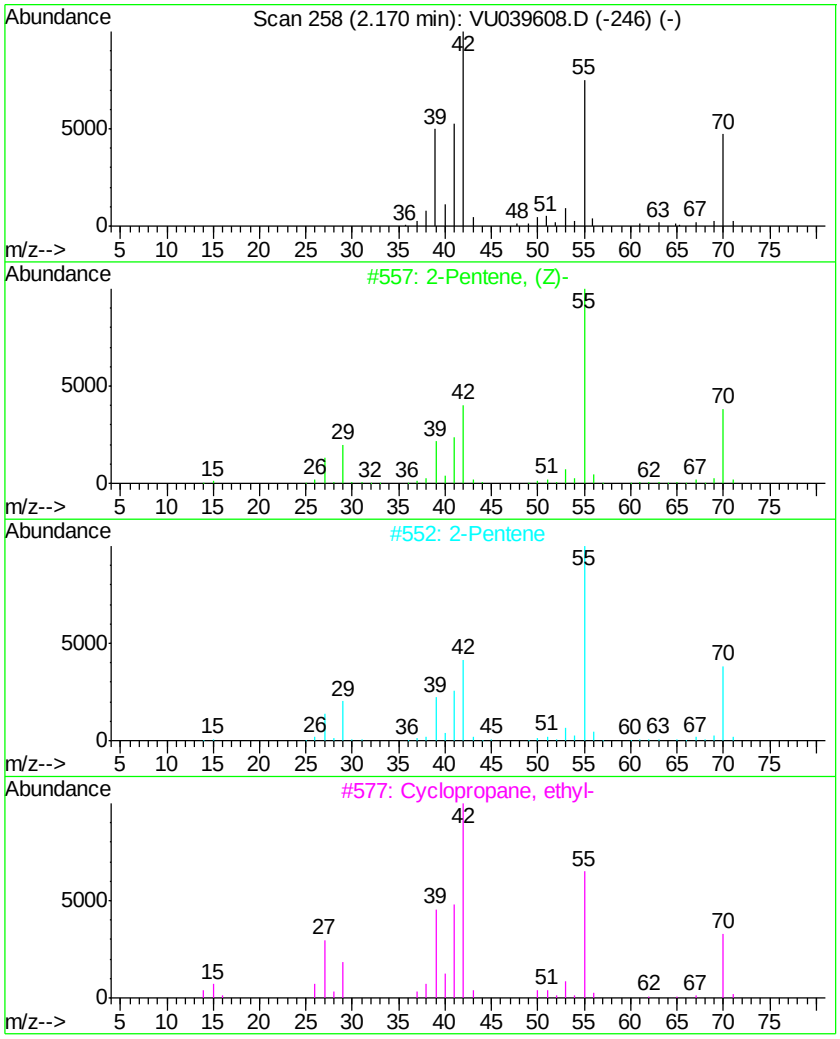
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

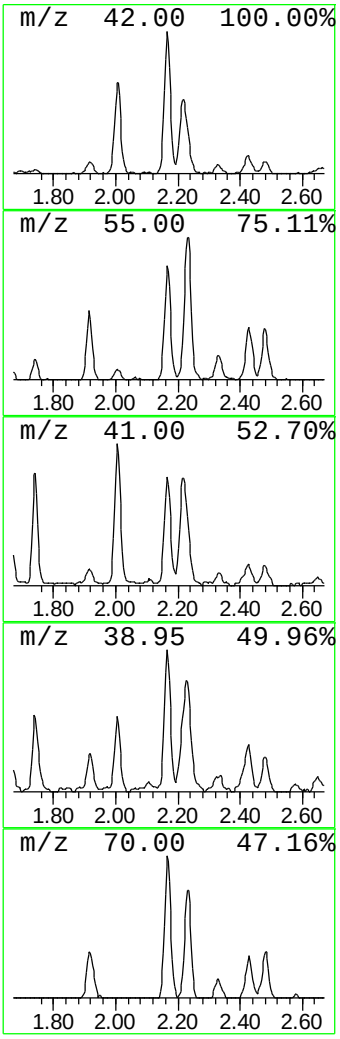
****

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	1.08 ug/L	64071	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
2	2-Pentene	70	C5H10	000109-68-2	90
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	90
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	70
5	1-Pentene	70	C5H10	000109-67-1	68





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072120\
Data File : VU039608.D
Acq On : 21 Jul 2020 19:38
Operator : SY/MD
Sample : L3347-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

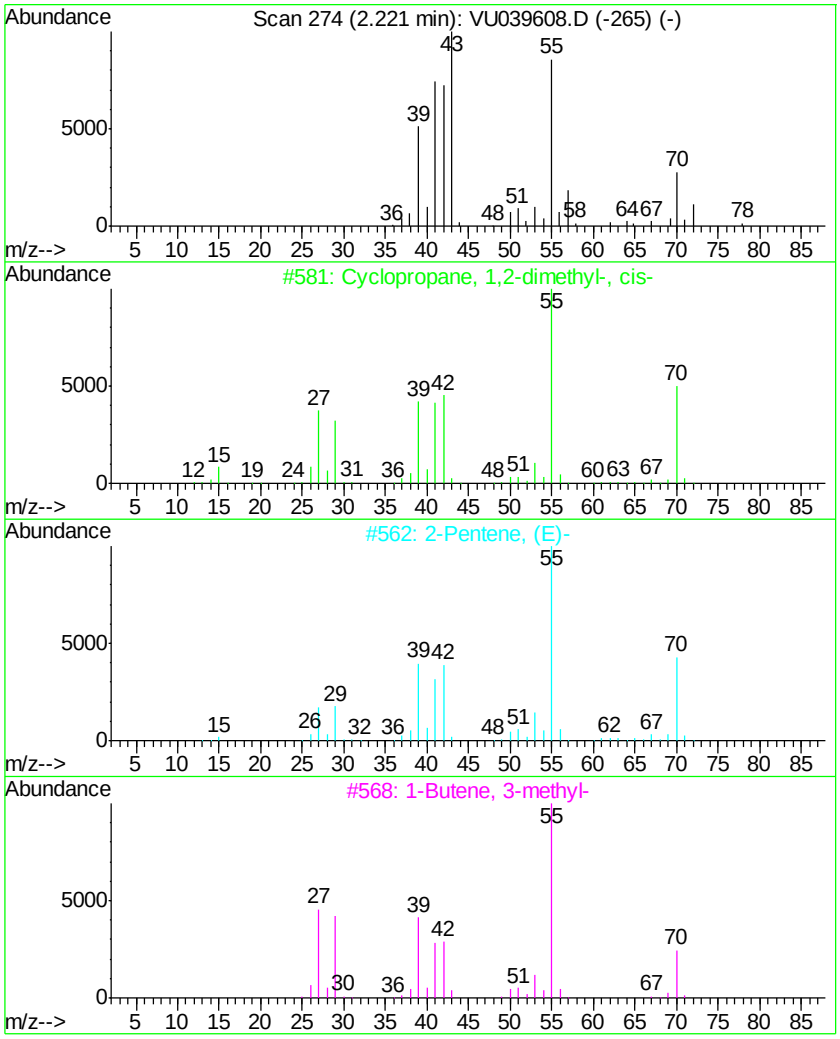
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

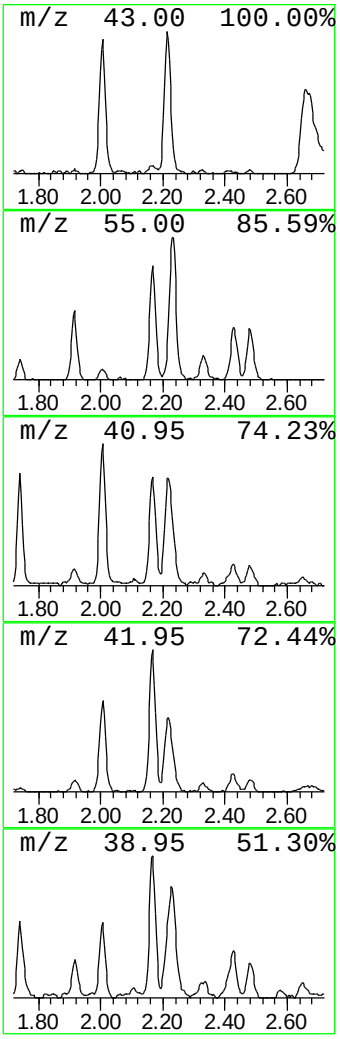
****

Peak Number 3 (DEL) Alkane: Cyclic2.22 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	1.52 ug/L	90727	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	72
2	2-Pentene, (E)-	70	C5H10	000646-04-8	72
3	1-Butene, 3-methyl-	70	C5H10	000563-45-1	64
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	58
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	58





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

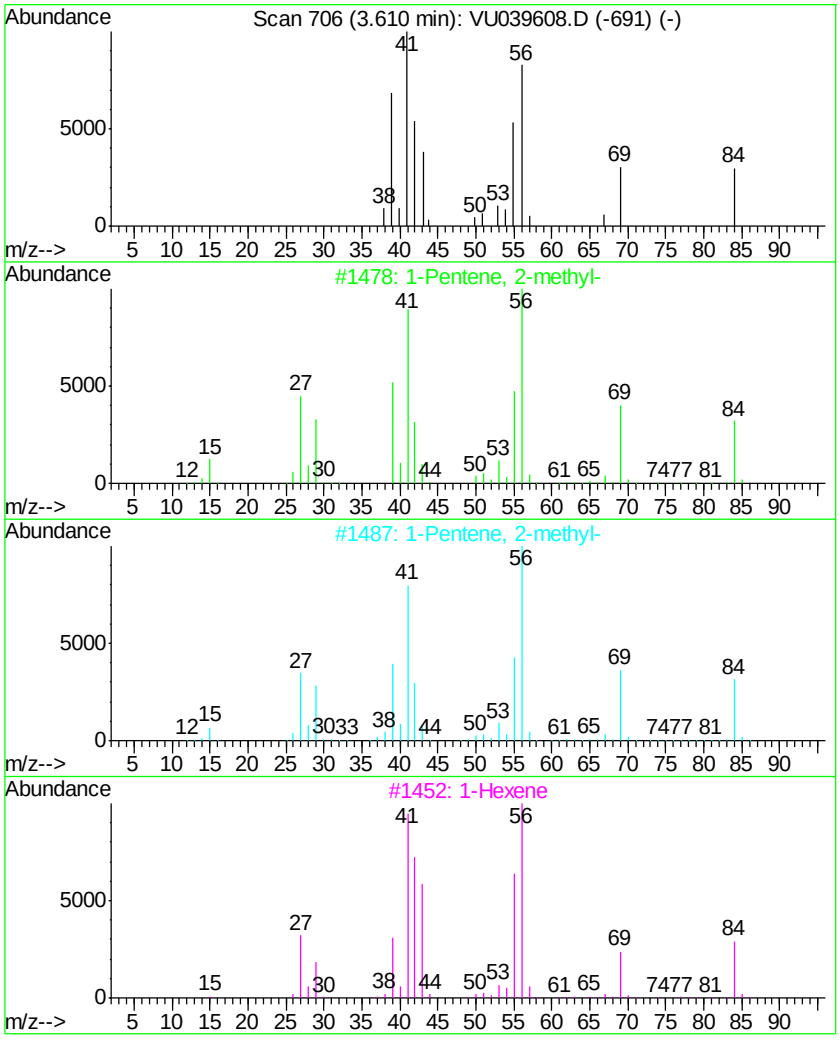
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

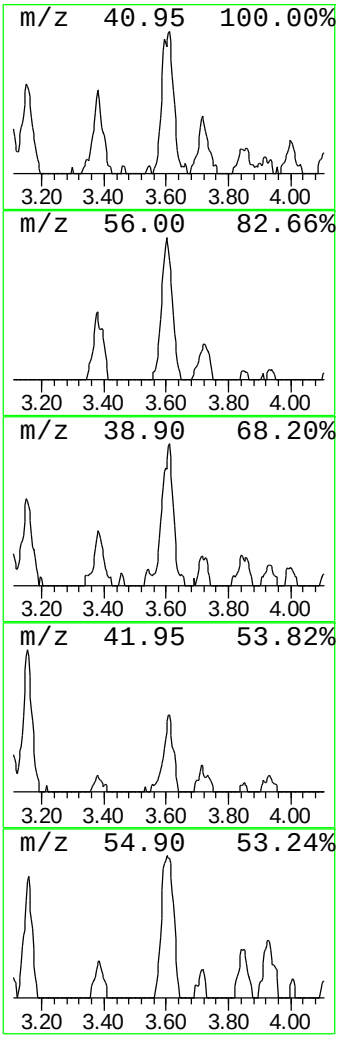
****

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	0.54 ug/L	32331	1,4-Difluorobenzene	6.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	58
3	1-Hexene	84	C6H12	000592-41-6	58
4	1-Hexene	84	C6H12	000592-41-6	53
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	50





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAY04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

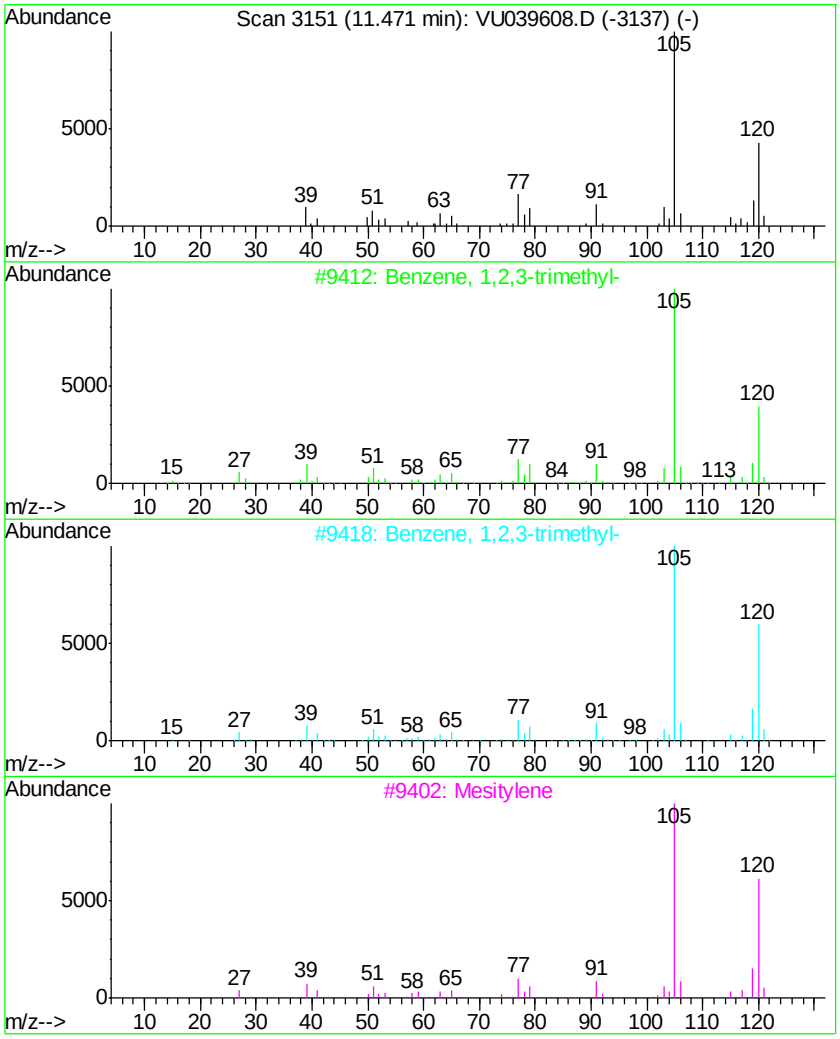
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

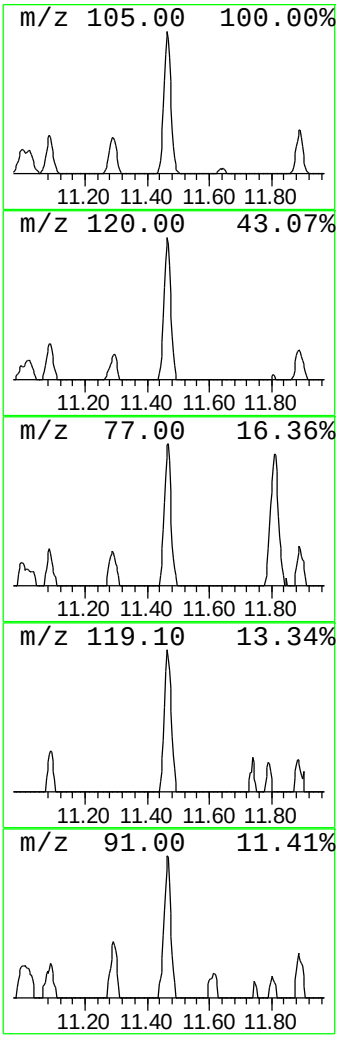
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.79 ug/L	56092	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR072120WMA.M
Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	2.01	1.0	ug/L	57066	1	6.27	297832	5.0
(DEL) Alkane: Str...	2.17	1.1	ug/L	64071	1	6.27	297832	5.0
(DEL) Alkane: Cyc...	2.22	1.5	ug/L	90727	1	6.27	297832	5.0
(DEL) Alkane: Str...	3.61	0.5	ug/L	32331	1	6.27	297832	5.0
Benzene, 1,2,3-tr...	11.47	0.8	ug/L	56092	3	11.81	353430	5.0