LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072718\
Data File : VU025709.D
Acq On : 28 Jul 2018 07:42
Operator : MD/SY
Sample : J4208-06
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U072718W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.088	138	155	180	rBV	308201	352762	31.65%	3.981%
2	1.760	357	364	372	rVB3	9157	13136	1.18%	0.148%
3	1.950	416	423	431	rBV	10614	13744	1.23%	0.155%
4	2.310	525	535	550	rVB5	11251	26056	2.34%	0.294%
5	2.442	564	576	597	rVB	11223	20922	1.88%	0.236%
6	2.747	648	671	698	rBV2	41620	108369	9.72%	1.223%
7	3.001	736	750	764	rBV2	47694	99387	8.92%	1.121%
8	3.310	830	846	863	rBV3	21694	45918	4.12%	0.518%
9	4.101	1073	1092	1112	rVB3	53269	142451	12.78%	1.607%
10	4.889	1320	1337	1353	rBV	174842	393959	35.35%	4.445%
11	4.989	1353	1368	1387	rVV2	279629	653257	58.61%	7.371%
12	5.088	1388	1399	1415	rVB4	11125	27292	2.45%	0.308%
13	5.223	1424	1441	1451	rBV5	18332	44349	3.98%	0.500%
14	5.313	1456	1469	1497	rVB2	173019	375467	33.69%	4.237%
15	5.487	1507	1523	1535	rBV6	12938	30246	2.71%	0.341%
16	5.558	1535	1545	1556	rVV4	10165	22847	2.05%	0.258%
17	5.628	1556	1567	1582	rVB5	15512	34042	3.05%	0.384%
18	5.892	1634	1649	1678	rBV	335100	664476	59.62%	7.498%
19	6.419	1793	1813	1830	rBV2	93852	201949	18.12%	2.279%
20	6.644	1873	1883	1897	rVB4	8295	15062	1.35%	0.170%
21	7.570	2148	2171	2193	rBV	628938	1114592	100.00%	12.577%
22	7.921	2269	2280	2294	rVB5	10477	19453	1.75%	0.220%
23	8.548	2467	2475	2486	rVB3	9188	14997	1.35%	0.169%
24	9.094	2631	2645	2667	rBV	504147	839561	75.32%	9.474%
25	9.255	2684	2695	2705	rVB	12613	19558	1.75%	0.221%
26	9.381	2723	2734	2752	rVB2	23205	42141	3.78%	0.476%
27	10.168	2968	2979	2996	rVB	35169	52006	4.67%	0.587%
28	10.310	3003	3023	3047	rBV	512696	825221	74.04%	9.312%
29	10.590	3099	3110	3124	rBV	47056	74518	6.69%	0.841%
30	10.709	3129	3147	3158	rBV	69500	109810	9.85%	1.239%
31	10.776	3158	3168	3188	rVB	79578	121202	10.87%	1.368%
32	10.975	3219	3230	3245	rBV	93027	144800	12.99%	1.634%
33	11.152	3273	3285	3301	rVB	242211	375934	33.73%	4.242%
34	11.326	3333	3339	3349	rVB2	8887	13926	1.25%	0.157%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Title : SW846 8260

35	11.487	3377	3389	3406	rBV	669516	1060748	95.17%	11.969%
36	11.573	3406	3416	3434	rVB	89251	138761	12.45%	1.566%
37	11.776	3468	3479	3498	rBV5	19533	41039	3.68%	0.463%
38	11.876	3498	3510	3526	rVV5	25588	52261	4.69%	0.590%
39	12.059	3558	3567	3576	rVB2	15675	22977	2.06%	0.259%
40	12.149	3585	3595	3600	rBV2	18232	28281	2.54%	0.319%
41	12.178	3600	3604	3616	rVB2	19407	26638	2.39%	0.301%
42	12.255	3616	3628	3635	rBV	25721	39712	3.56%	0.448%
43	12.358	3647	3660	3681	rBV2	23457	56263	5.05%	0.635%
44	12.554	3710	3721	3732	rVB4	15797	28055	2.52%	0.317%
45	12.654	3736	3752	3760	rBV	22958	36464	3.27%	0.411%
46	12.705	3760	3768	3781	rVB	31641	45965	4.12%	0.519%
47	12.969	3843	3850	3864	rVB3	10218	16437	1.47%	0.185%
48	13.123	3888	3898	3909	rBV3	64511	101694	9.12%	1.148%
49	13.290	3940	3950	3962	rVB	23160	35725	3.21%	0.403%
50	13.747	4082	4092	4102	rBV	11297	20131	1.81%	0.227%
51	14.885	4436	4446	4461	rBV2	13732	28514	2.56%	0.322%
52	15.069	4493	4503	4520	rBV3	14669	29053	2.61%	0.328%

Sum of corrected areas: 8862128

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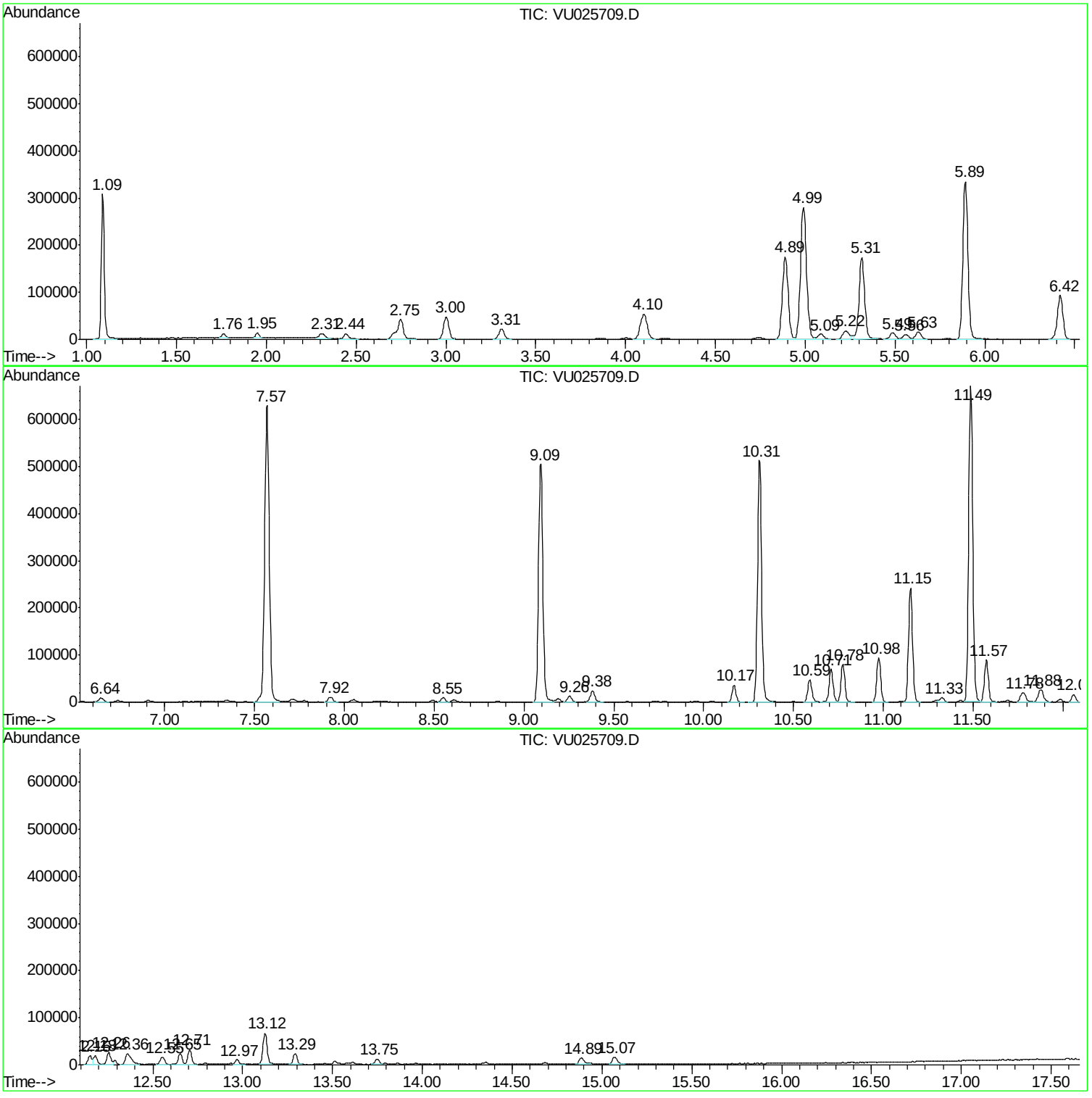
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072718\
Data File : VU025709.D
Acq On : 28 Jul 2018 07:42
Operator : MD/SY
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ALS Vial : 55 Sample Multiplier: 1

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

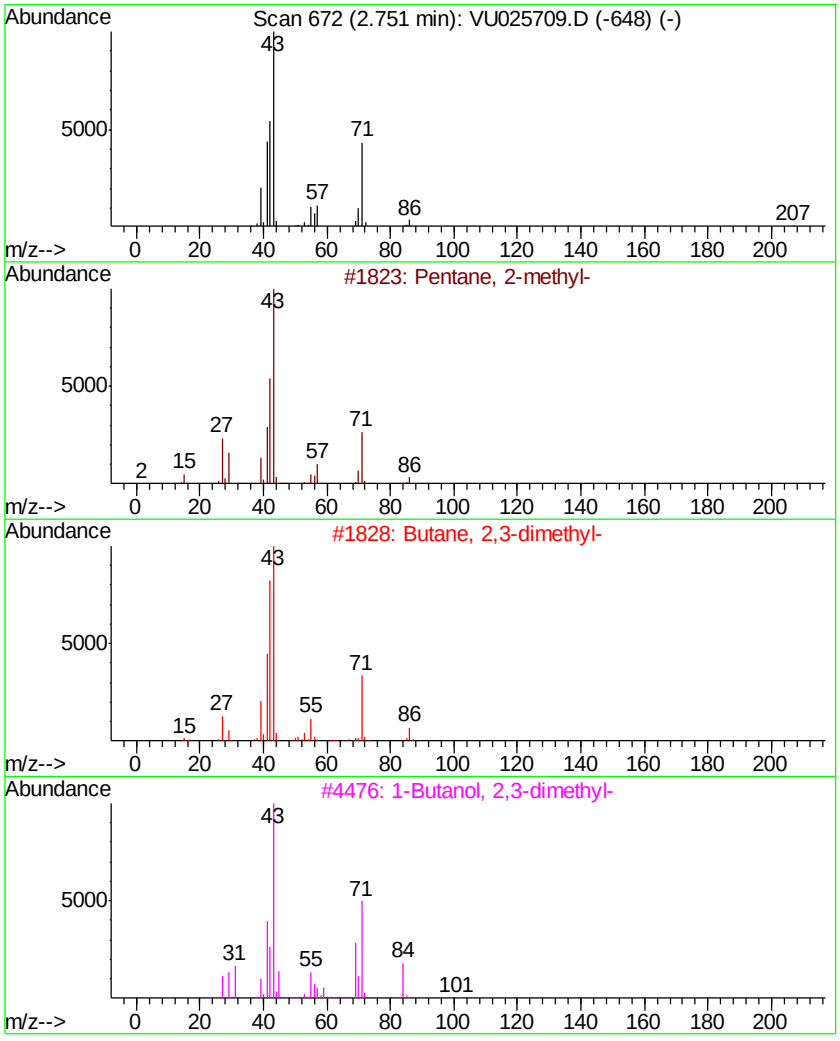
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

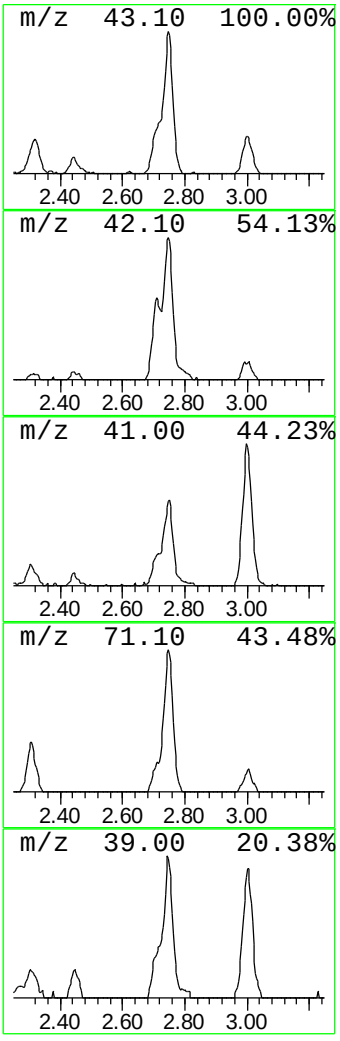
****

Peak Number 2 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.75	8.29 ug/l	108369	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	50
4	Pentane	72	C5H12	000109-66-0	43
5	Hexane, 3-ethyl-	114	C8H18	000619-99-8	38





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Data File : VU025709.D
Acq On : 28 Jul 2018 07:42
Operator : MD/SY
Sample : J4208-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

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

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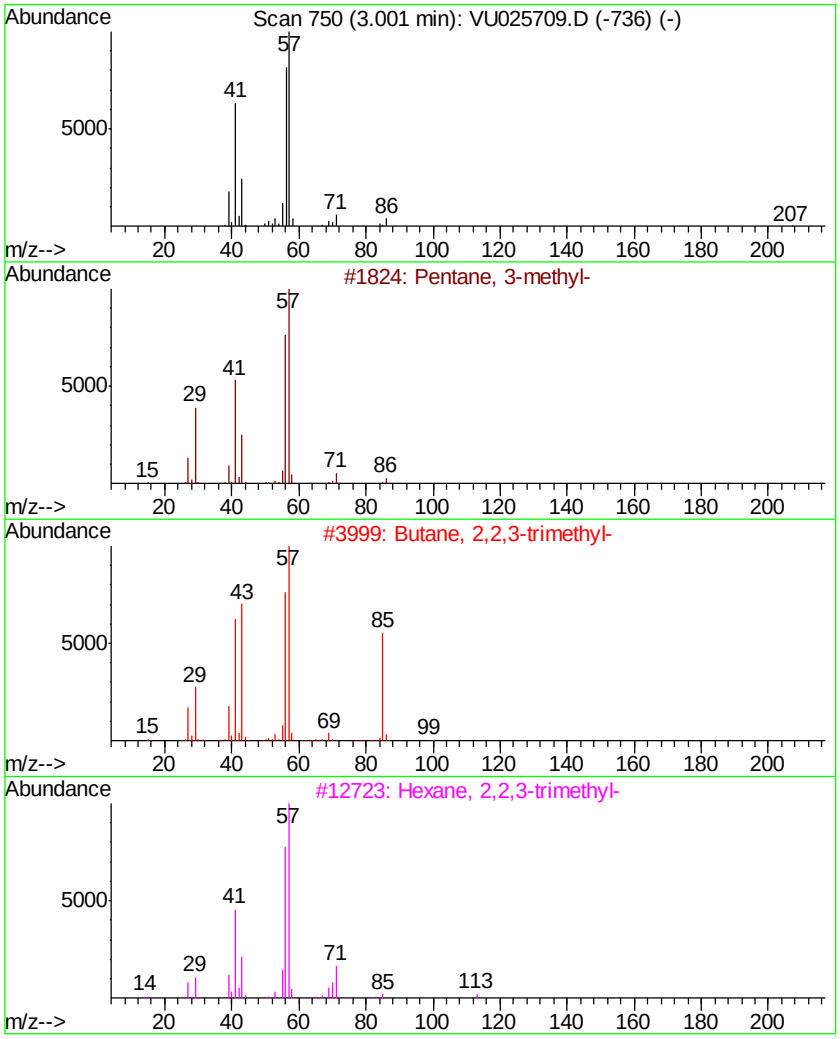
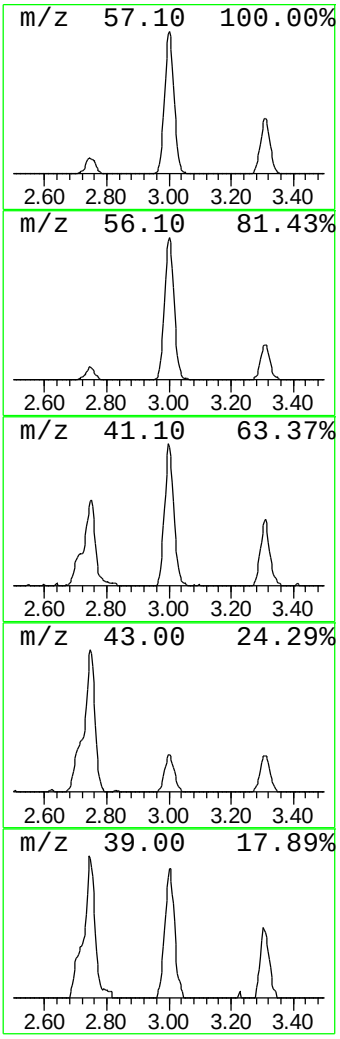
Peak Number 3 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	7.61 ug/l	99387	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	83
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45





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Data File : VU025709.D
Acq On : 28 Jul 2018 07:42
Operator : MD/SY
Sample : J4208-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

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

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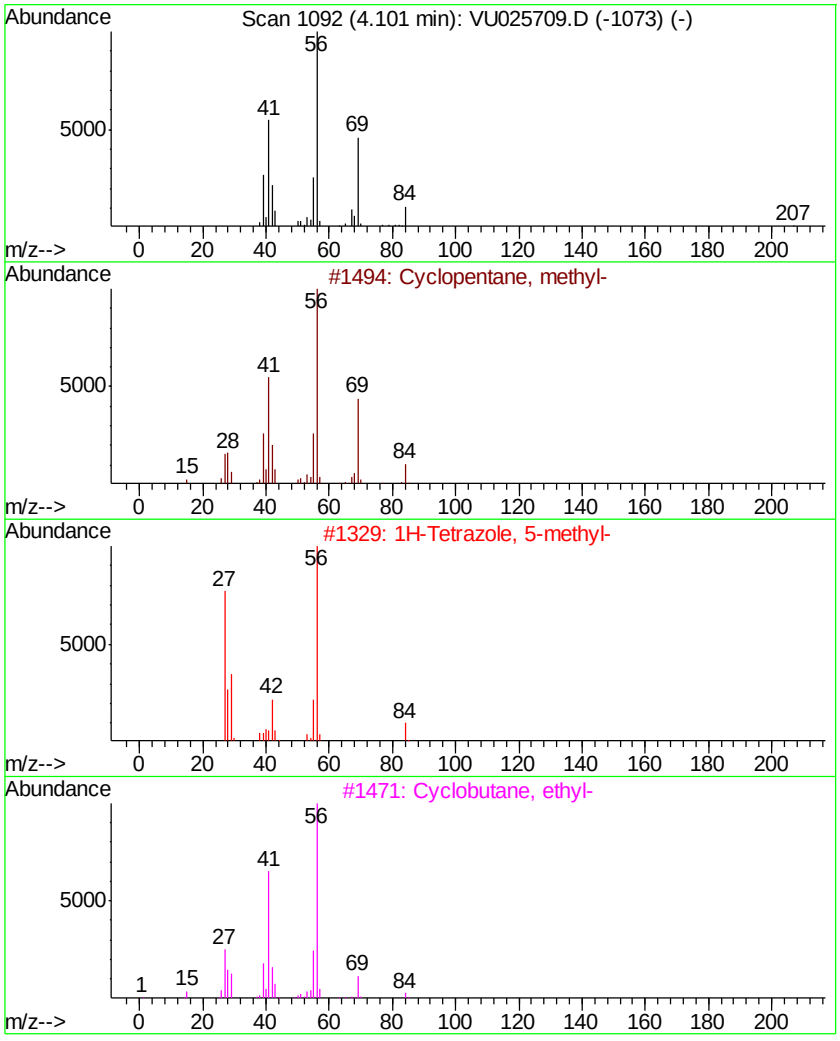
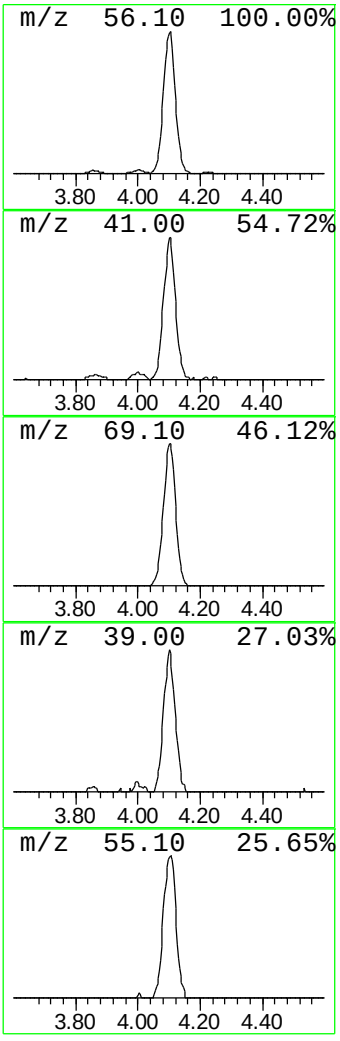
Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	10.90 ug/l	142451	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclobutane	56	C4H8	000287-23-0	50





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Data File : VU025709.D
Acq On : 28 Jul 2018 07:42
Operator : MD/SY
Sample : J4208-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

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

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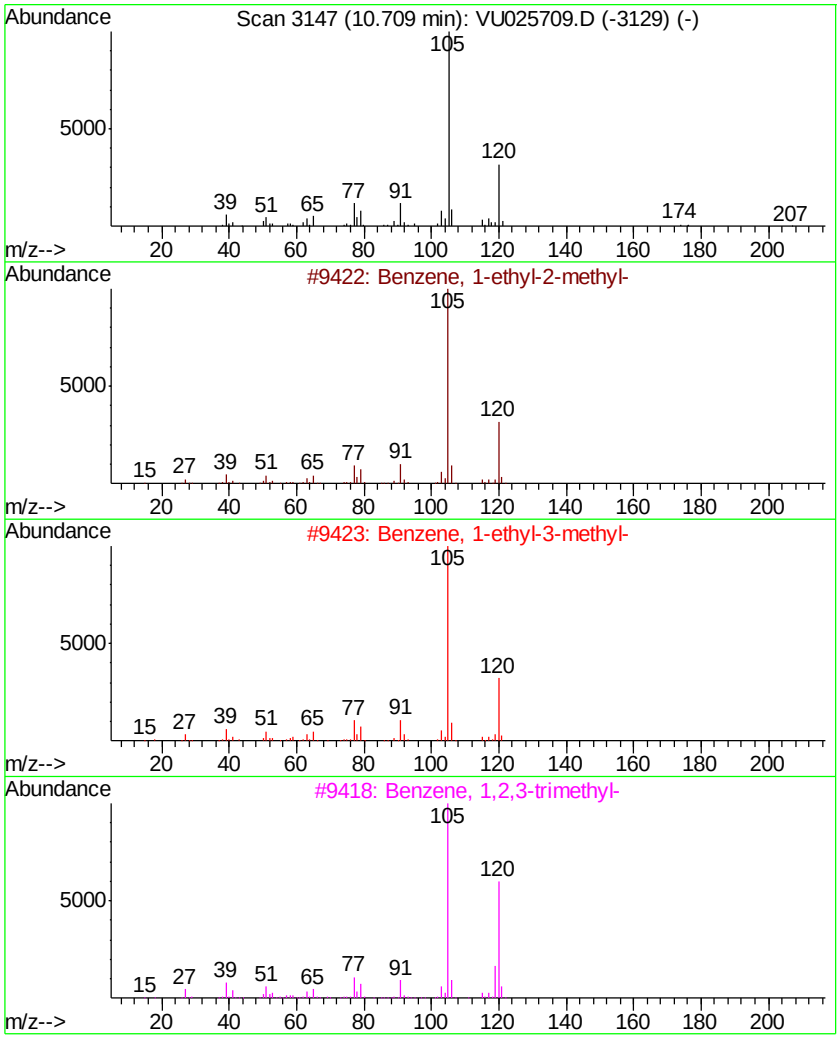
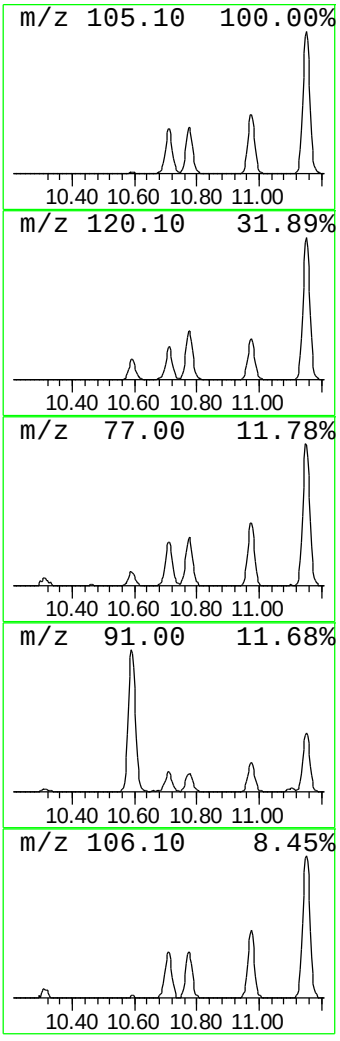
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	5.18 ug/l	109810	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU072718\
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Acq On : 28 Jul 2018 07:42
Operator : MD/SY
Sample : J4208-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 55 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FL-0527

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

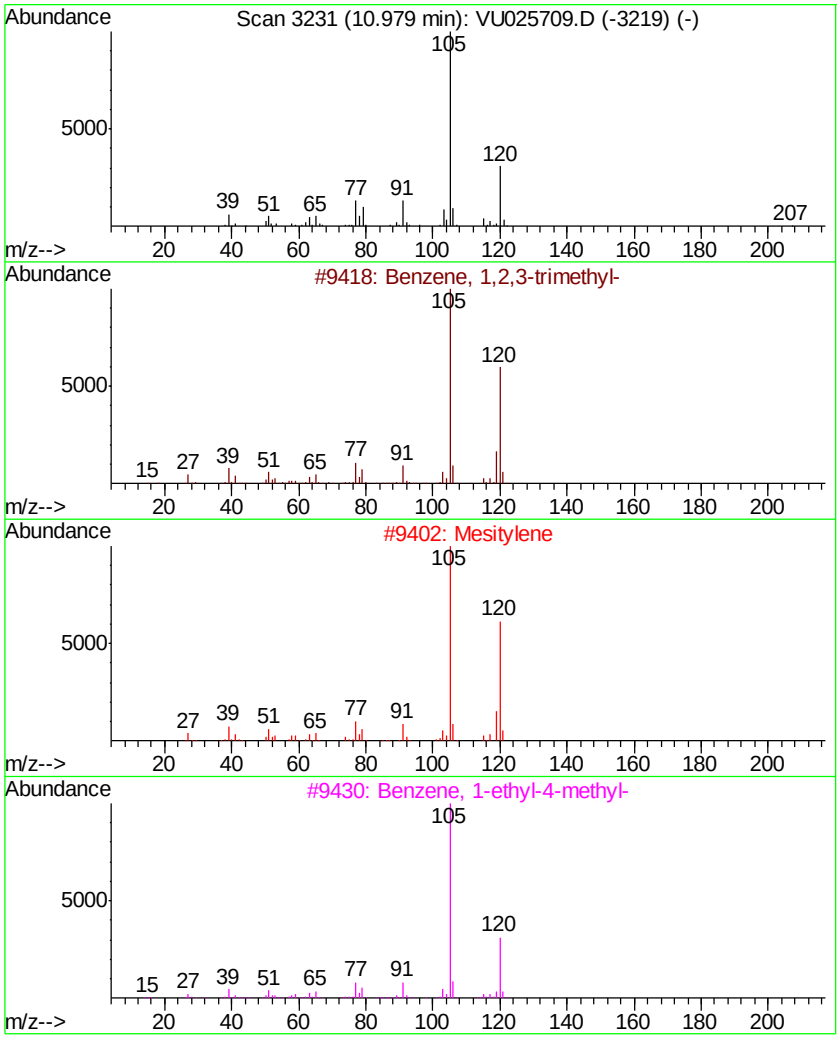
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

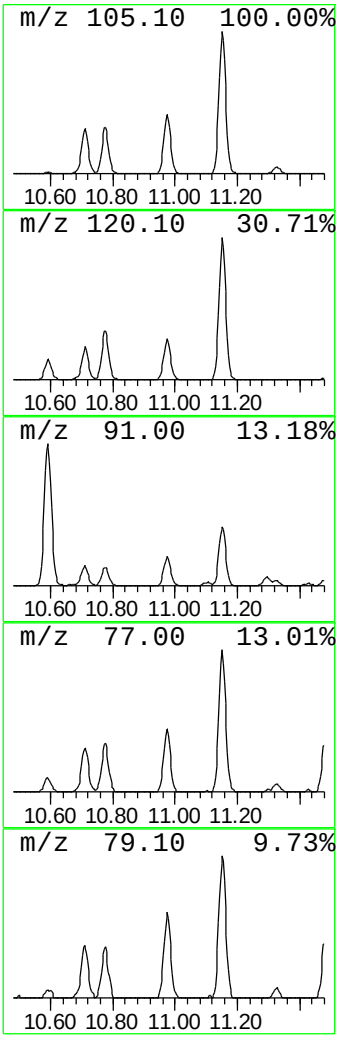
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	6.83 ug/l	144800	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U072718W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2-methyl-	2.75	8.3	ug/l	108369	1	4.99	653257	50.0
Pentane, 3-methyl-	3.00	7.6	ug/l	99387	1	4.99	653257	50.0
Cyclopentane, met...	4.10	10.9	ug/l	142451	1	4.99	653257	50.0
Benzene, 1-ethyl-...	10.71	5.2	ug/l	109810	4	11.49	1060750	50.0
Benzene, 1,2,3-tr...	10.98	6.8	ug/l	144800	4	11.49	1060750	50.0