LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

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\82U092218W.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	1.402	60	71	79	rBV3	65498	93030	5.93%	0.914%
2	1.472	81	93	101	rBV	56617	77487	4.94%	0.761%
3	1.562	114	121	141	rBV	265665	402061	25.62%	3.949%
4	1.759	172	182	212	rVB	1163916	1569581	100.00%	15.416%
5	1.948	233	241	264	rVB3	84014	148629	9.47%	1.460%
6	2.051	266	273	285	rVB	22845	31714	2.02%	0.311%
7	2.186	307	315	325	rVB3	22463	34770	2.22%	0.341%
8	2.247	326	334	344	rVB	17193	25468	1.62%	0.250%
9	2.321	345	357	367	rBV	126274	200435	12.77%	1.969%
10	2.379	367	375	385	rVB	71638	110075	7.01%	1.081%
11	2.443	385	395	412	rBV	116644	196828	12.54%	1.933%
12	2.636	415	455	467	rBV2	127487	809460	51.57%	7.950%
13	2.997	559	567	583	rVB	21630	45094	2.87%	0.443%
14	3.186	616	626	643	rVB2	16485	35502	2.26%	0.349%
15	3.305	653	663	680	rVB4	7305	17206	1.10%	0.169%
16	3.993	860	877	894	rBV3	20823	55381	3.53%	0.544%
17	4.099	894	910	926	rVV3	24865	70090	4.47%	0.688%
18	4.263	929	961	988	rVV2	59679	232324	14.80%	2.282%
19	4.566	1043	1055	1078	rBV3	27607	69534	4.43%	0.683%
20	4.884	1139	1154	1170	rBV	122338	276307	17.60%	2.714%
21	4.987	1171	1186	1204	rVV2	201313	463698	29.54%	4.554%
22	5.083	1206	1216	1232	rVB2	10751	26970	1.72%	0.265%
23	5.312	1273	1287	1302	rBV	149391	310698	19.79%	3.052%
24	5.392	1304	1312	1324	rVB2	12458	26054	1.66%	0.256%
25	5.540	1345	1358	1372	rVB2	46455	106136	6.76%	1.042%
26	5.887	1451	1466	1483	rBV	267393	524372	33.41%	5.150%
27	6.421	1613	1632	1644	rBV4	34012	73526	4.68%	0.722%
28	6.537	1658	1668	1678	rBV2	11695	21407	1.36%	0.210%
29	6.929	1773	1790	1808	rBV2	18489	37776	2.41%	0.371%
30	7.051	1814	1828	1839	rBV3	23219	46978	2.99%	0.461%
31	7.340	1896	1918	1950	rBV	78523	237925	15.16%	2.337%
32	7.527	1964	1976	1977	rBV2	11663	16073	1.02%	0.158%
33	7.565	1977	1988	2003	rVV	512296	906203	57.74%	8.900%
34	7.639	2005	2011	2024	rVB2	25931	45746	2.91%	0.449%

LSC Area Percent Report

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Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

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\82U092218W.M
Title : SW846 8260

35	8.369	2229	2238	2256	rBV2	9964	20200	1.29%	0.198%
36	9.089	2450	2462	2485	rBV	381559	646650	41.20%	6.351%
37	9.253	2503	2513	2525	rVB	22415	34629	2.21%	0.340%
38	9.376	2540	2551	2564	rBV2	60320	102662	6.54%	1.008%
39	9.781	2666	2677	2689	rBV	13312	24380	1.55%	0.239%
40	9.855	2690	2700	2713	rVV8	7480	18966	1.21%	0.186%
41	10.051	2747	2761	2778	rVB5	7346	19471	1.24%	0.191%
42	10.308	2829	2841	2857	rBV	351704	566826	36.11%	5.567%
43	10.684	2949	2958	2963	rBV2	11764	18648	1.19%	0.183%
44	10.774	2980	2986	2993	rVB	11859	16426	1.05%	0.161%
45	10.970	3032	3047	3055	rBV4	10778	19056	1.21%	0.187%
46	11.028	3055	3065	3079	rVB3	16060	29605	1.89%	0.291%
47	11.151	3087	3103	3114	rVB2	29608	49528	3.16%	0.486%
48	11.257	3125	3136	3150	rBV	100725	160872	10.25%	1.580%
49	11.337	3150	3161	3185	rVV	121876	202232	12.88%	1.986%
50	11.485	3195	3207	3225	rVV	438317	677684	43.18%	6.656%
51	11.572	3226	3234	3243	rVB	14185	21177	1.35%	0.208%
52	11.742	3276	3287	3306	rBV	95493	168844	10.76%	1.658%
53	12.456	3499	3509	3516	rBV2	10966	18323	1.17%	0.180%
54	12.501	3516	3523	3534	rVB2	13343	20958	1.34%	0.206%

Sum of corrected areas: 10181675

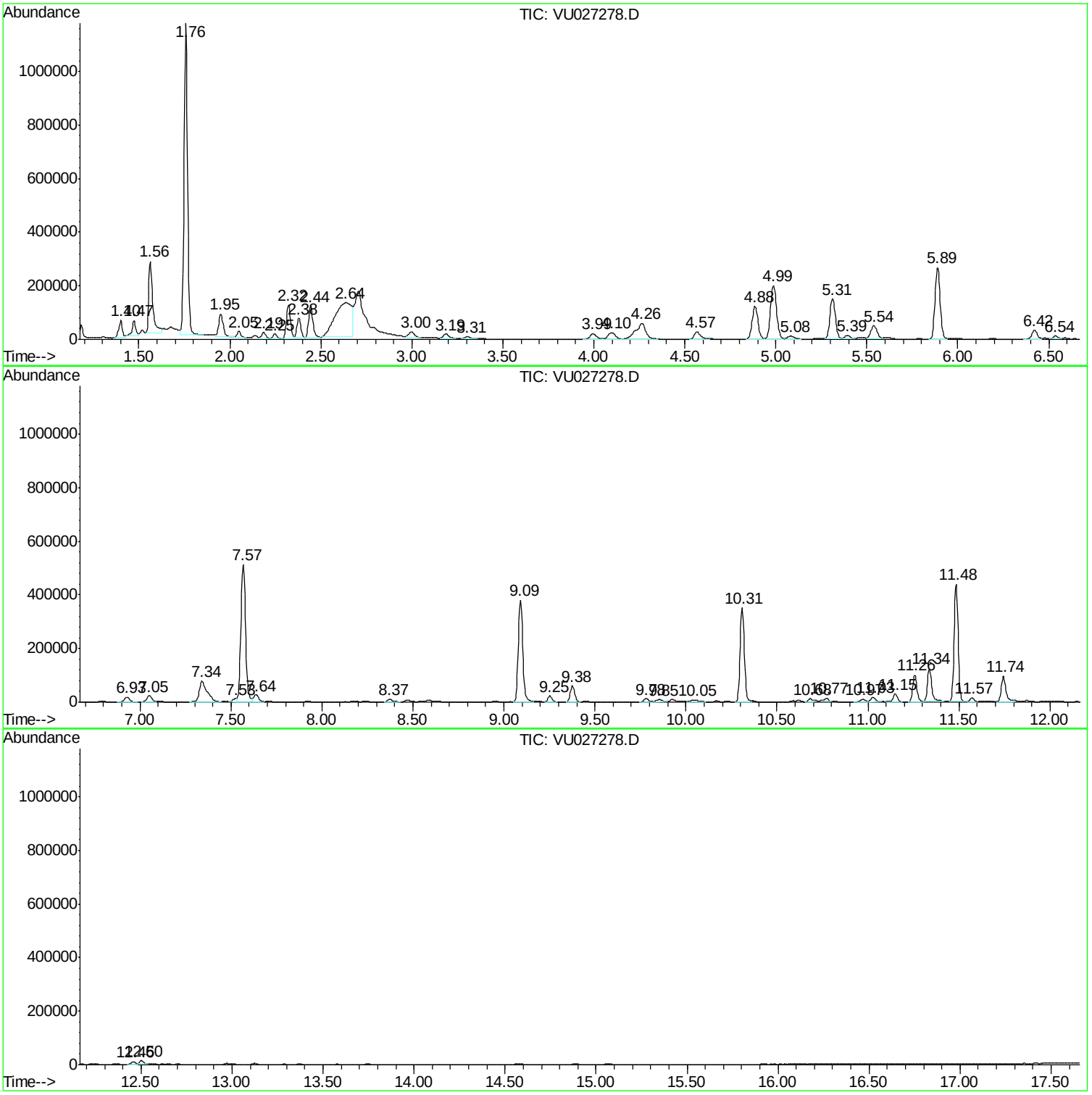
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

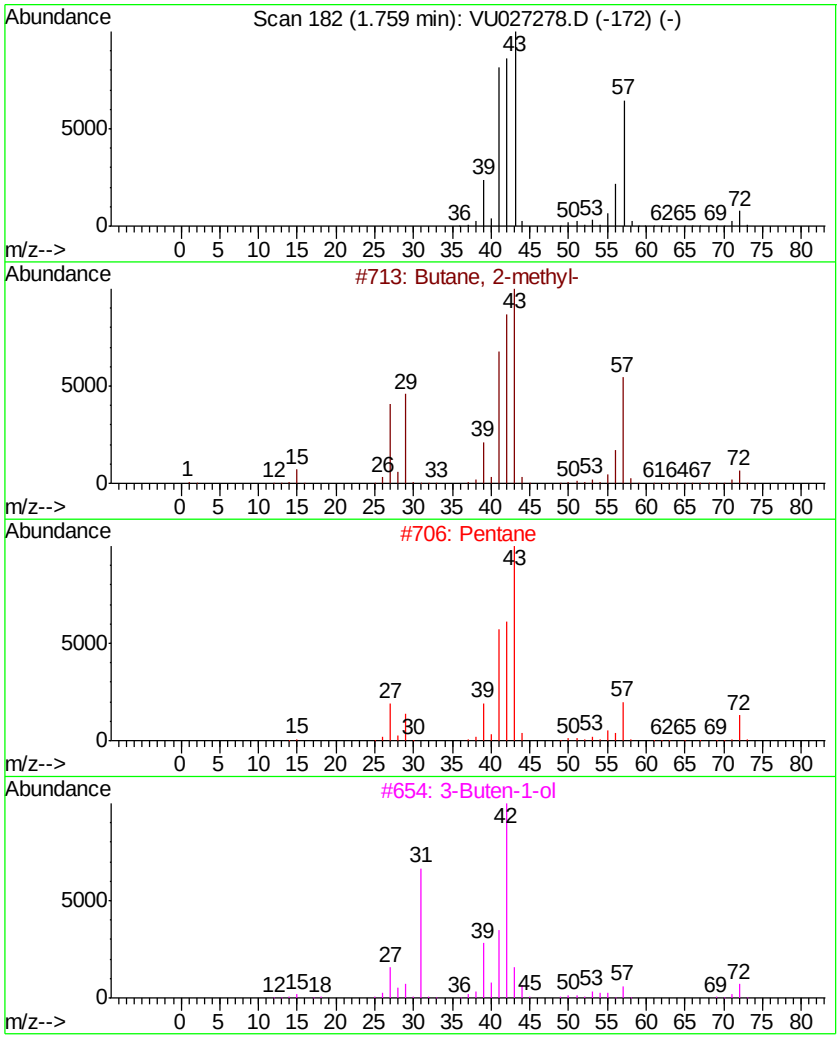
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

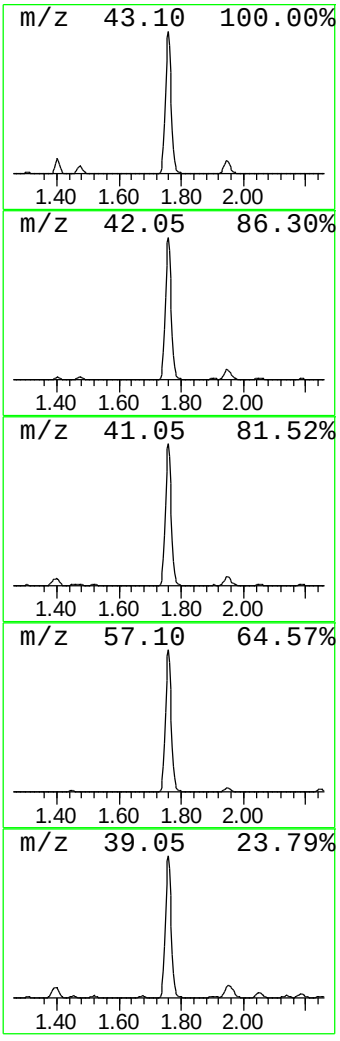
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	169.25 ug/l	1569580	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	39
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5	1-Butene	56	C4H8	000106-98-9	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

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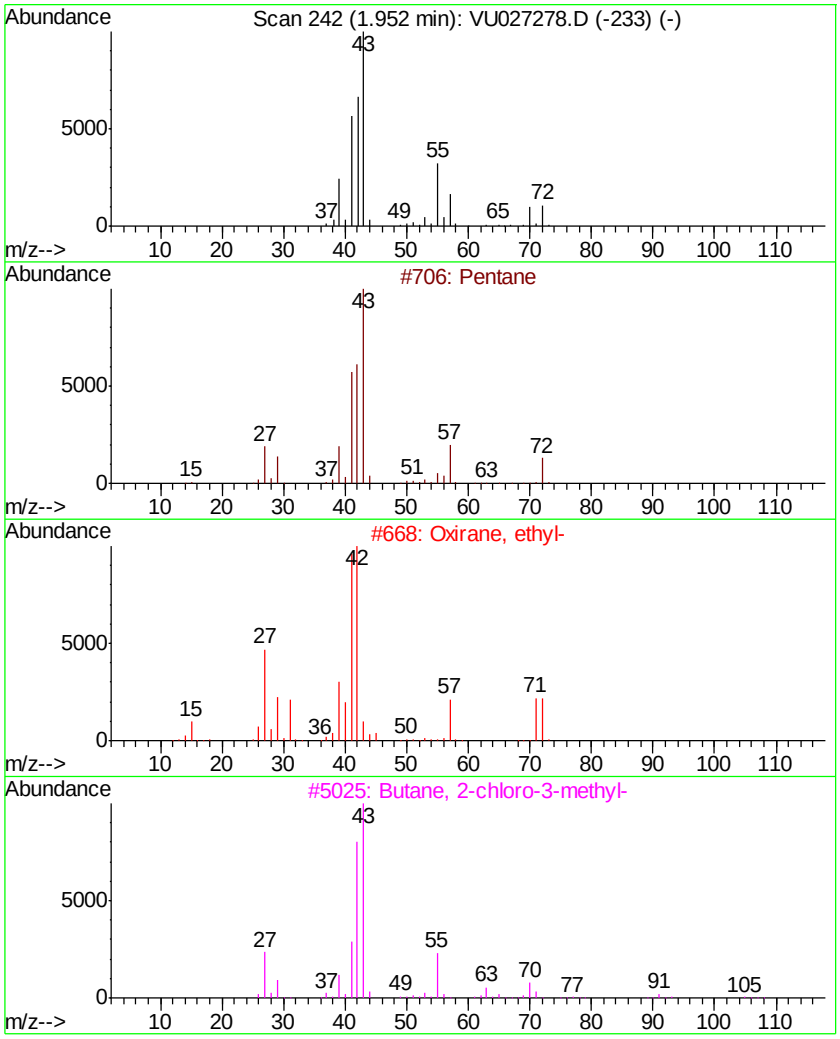
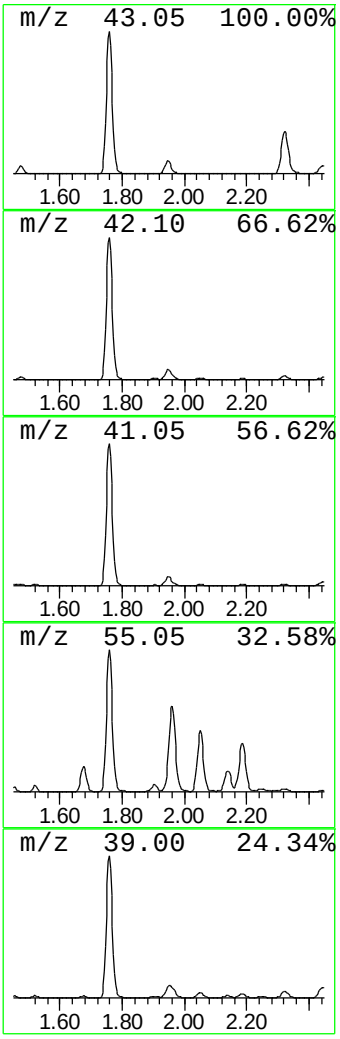
Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.95	16.03 ug/l	148629	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	47
3	Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	33
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

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

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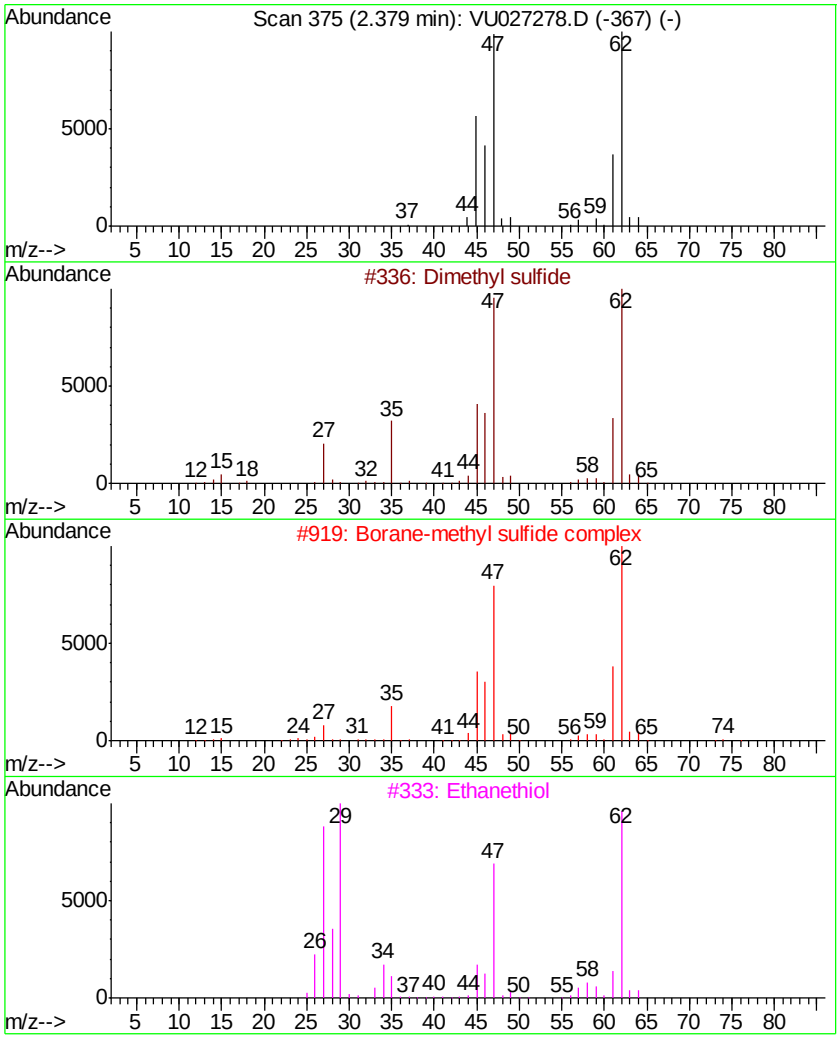
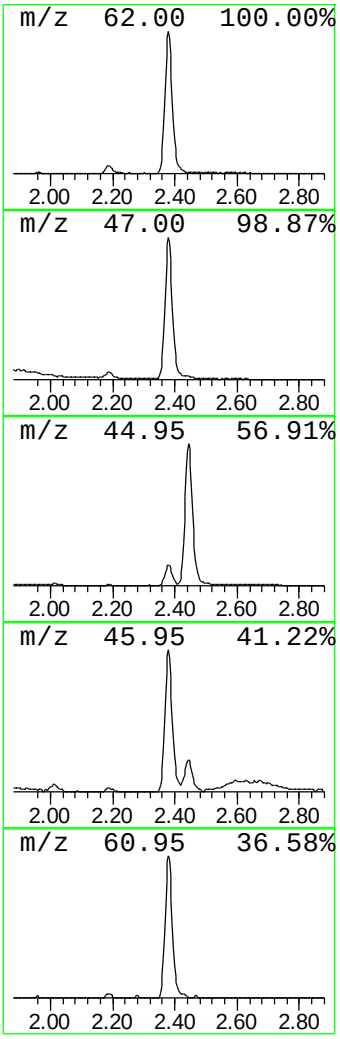
Peak Number 4 Dimethyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	11.87 ug/l	110075	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3	Ethanethiol	62	C2H6S	000075-08-1	72
4	Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5	Propane, 2-fluoro-	62	C3H7F	000420-26-8	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

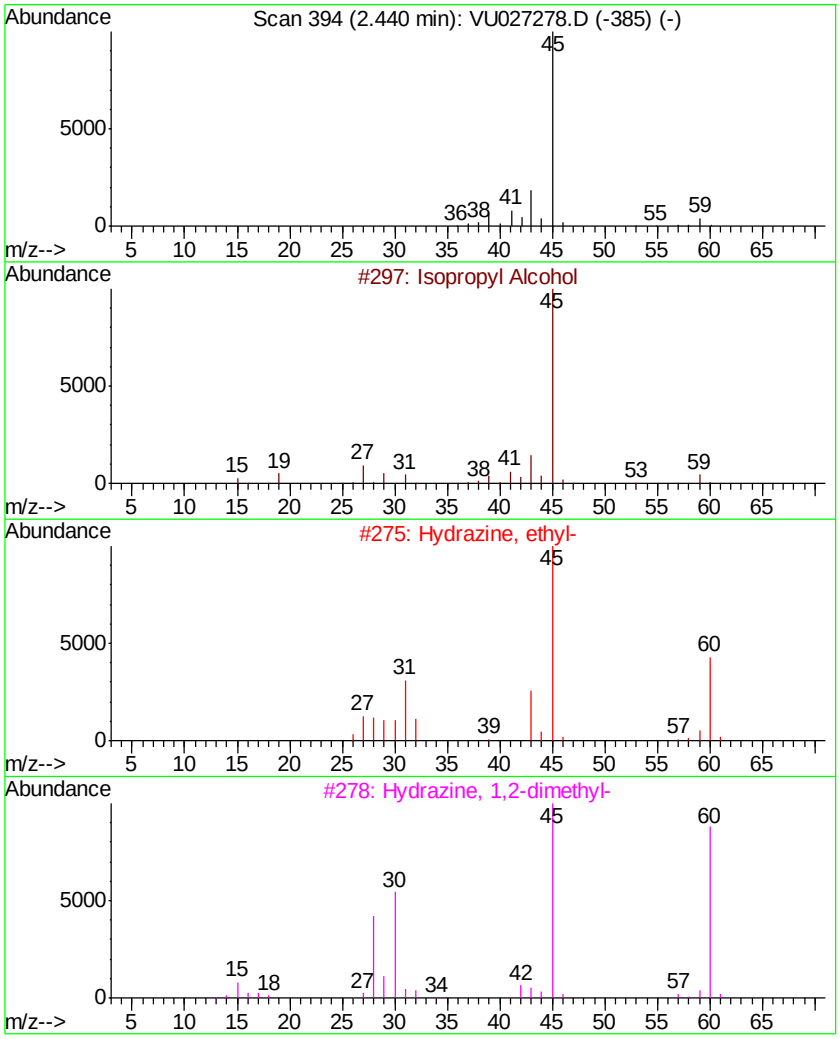
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

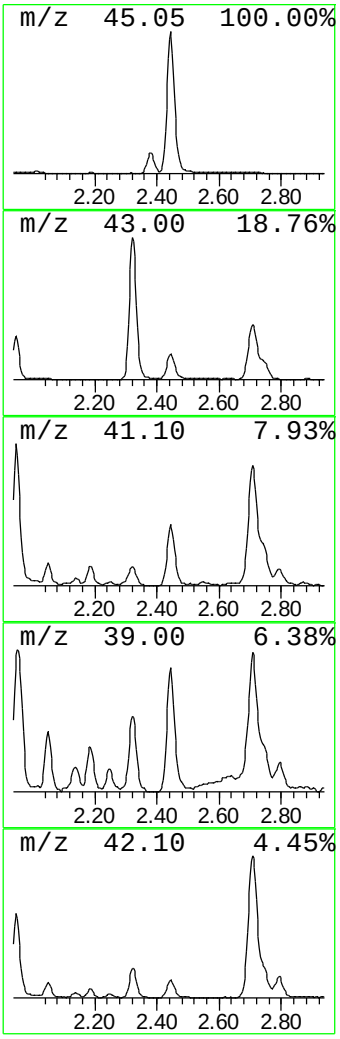
****

Peak Number 5 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	21.22 ug/l	196828	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Formamide	45	CH3NO	000075-12-7	4
5	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
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Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

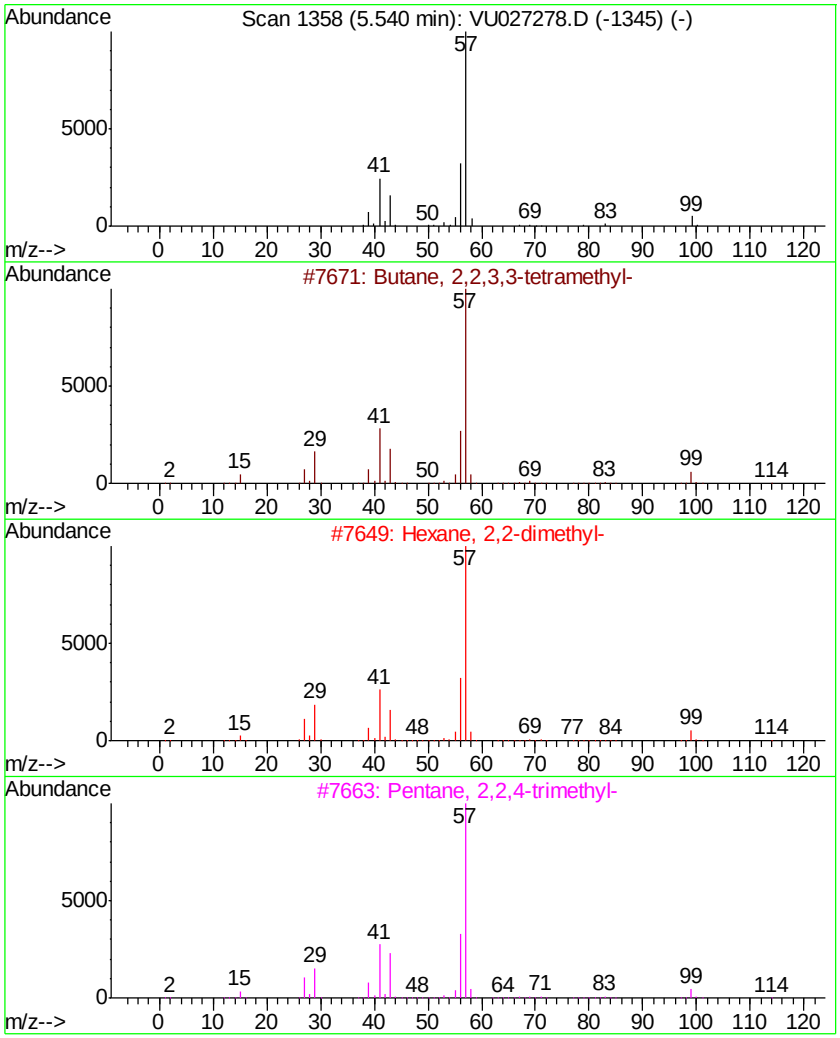
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

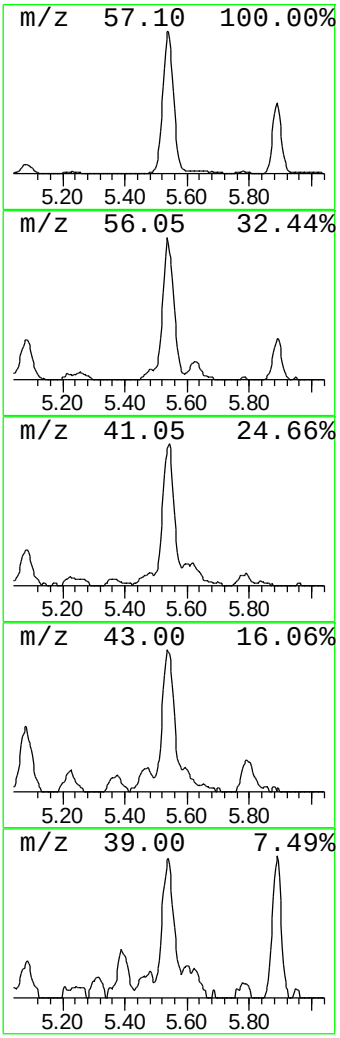
****

Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	10.12 ug/l	106136	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	72





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Operator : MD/SY
Sample : J5104-03
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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

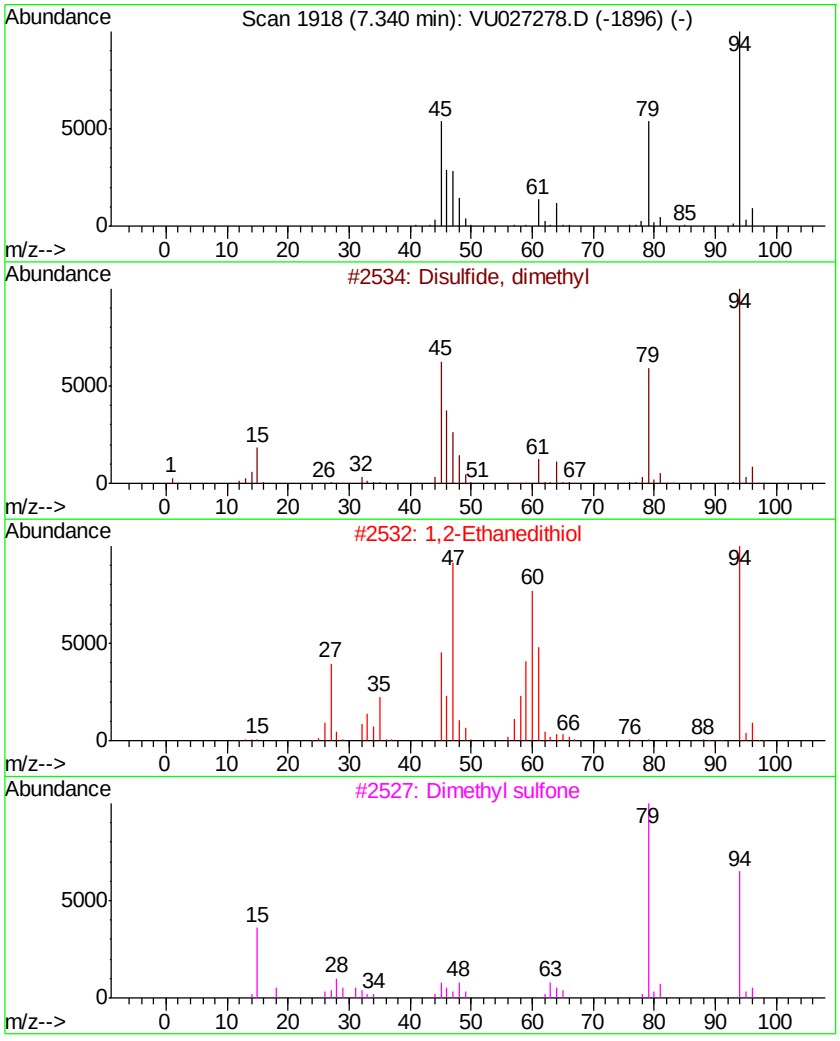
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

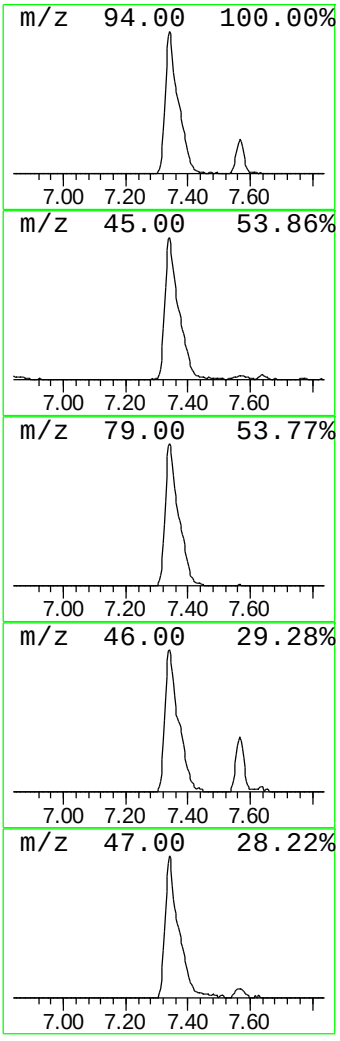
****

Peak Number 7 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	22.69 ug/l	237925	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	50
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	43
4	Methanesulfonylacetic acid	138	C3H6O4S	002516-97-4	9
5	Dimethyl ether	46	C2H6O	000115-10-6	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

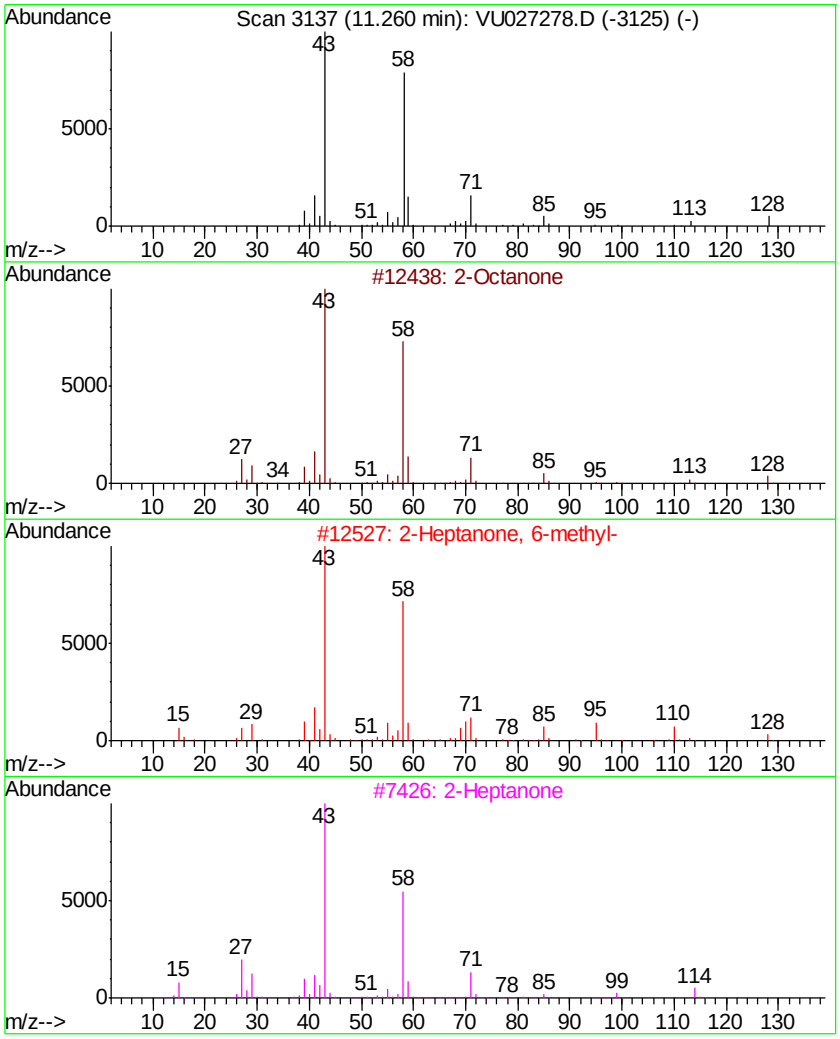
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

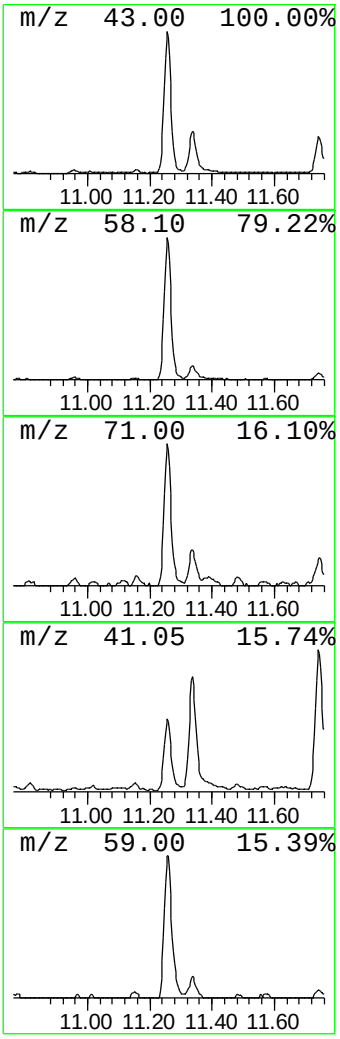
****

Peak Number 8 2-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	11.87 ug/l	160872	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90
3	2-Heptanone	114	C7H14O	000110-43-0	72
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
5	Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

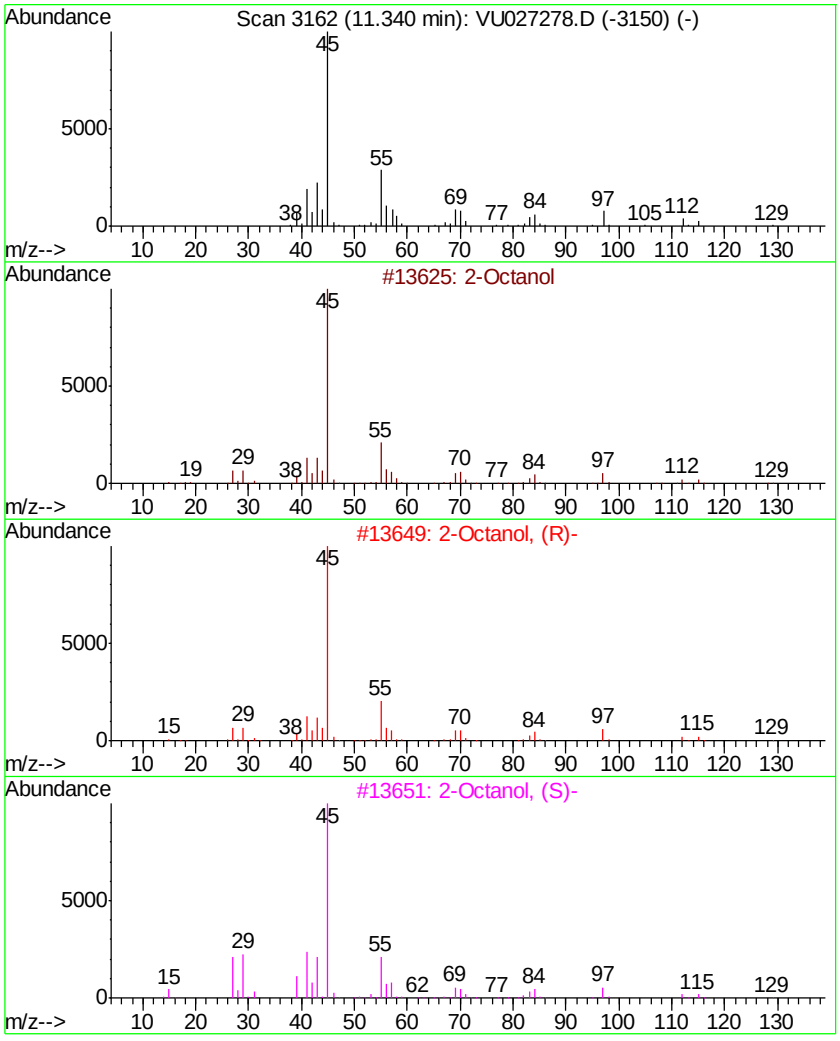
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

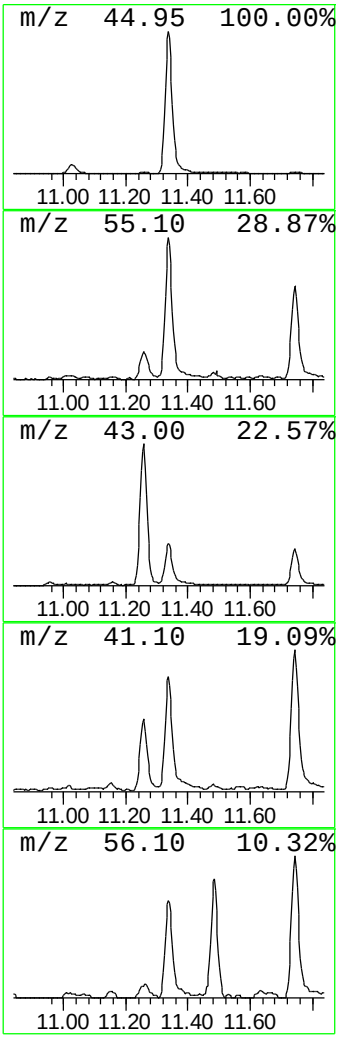
****

Peak Number 9 2-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	14.92 ug/l	202232	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol	130	C8H18O	000123-96-6	90
2	2-Octanol, (R)-	130	C8H18O	005978-70-1	90
3	2-Octanol, (S)-	130	C8H18O	006169-06-8	83
4	2-Decanol	158	C10H22O	001120-06-5	78
5	2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	78





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.M
Quant Title : SW846 8260

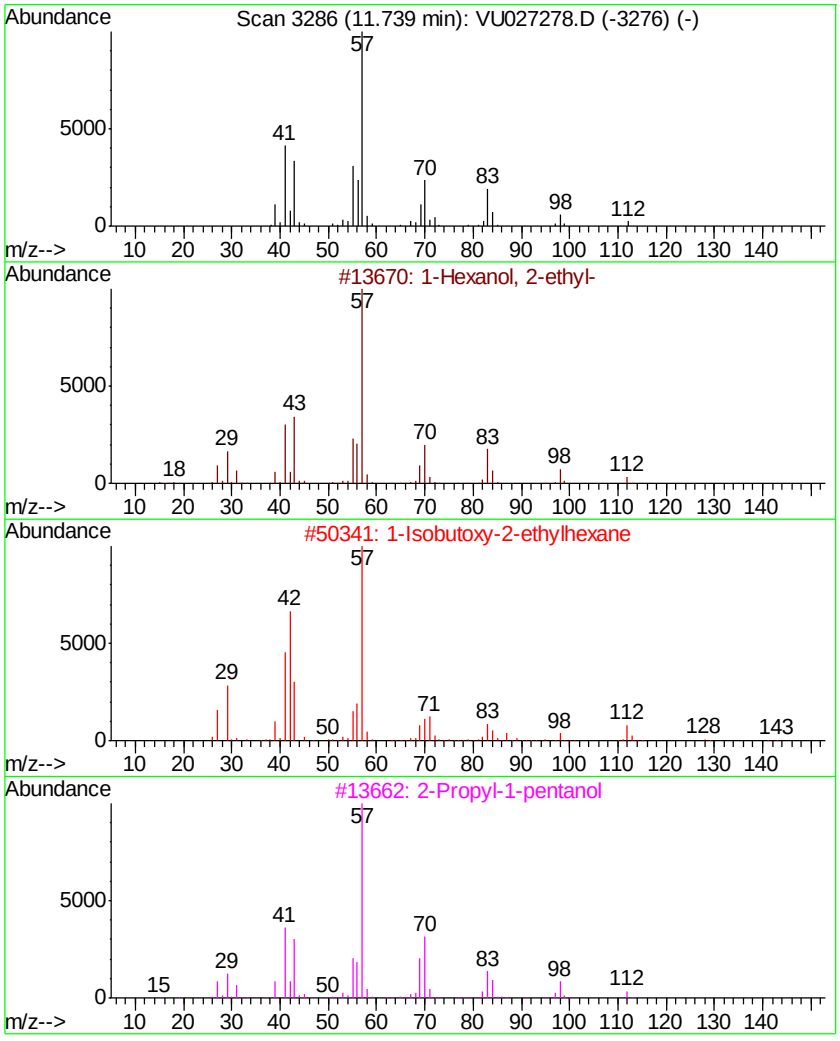
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

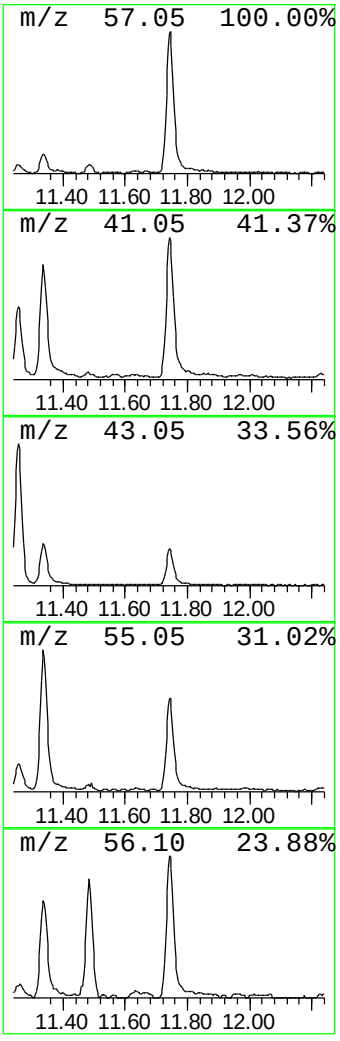
****

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	12.46 ug/l	168844	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU092818\
Data File : VU027278.D
Acq On : 28 Sep 2018 17:48
Operator : MD/SY
Sample : J5104-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : FA18-JEB5-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U092218W.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
Butane, 2-methyl-	1.76	169.3	ug/l	1569580	1	4.99	463698	50.0
Pentane	1.95	16.0	ug/l	148629	1	4.99	463698	50.0
Dimethyl sulfide	2.38	11.9	ug/l	110075	1	4.99	463698	50.0
Isopropyl Alcohol	2.44	21.2	ug/l	196828	1	4.99	463698	50.0
Butane, 2,2,3,3-t...	5.54	10.1	ug/l	106136	2	5.89	524372	50.0
Disulfide, dimethyl	7.34	22.7	ug/l	237925	2	5.89	524372	50.0
2-Octanone	11.26	11.9	ug/l	160872	4	11.48	677684	50.0
2-Octanol	11.34	14.9	ug/l	202232	4	11.48	677684	50.0
1-Hexanol, 2-ethyl-	11.74	12.5	ug/l	168844	4	11.48	677684	50.0