LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

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\SOMUTR021119WMA.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	1.183	23	29	36	rBV3	13940	15283	1.49%	0.173%
2	1.302	59	66	78	rBV	52157	55154	5.39%	0.624%
3	1.386	84	92	108	rBV2	899822	1022696	100.00%	11.568%
4	1.540	135	140	148	rBV5	9559	13788	1.35%	0.156%
5	1.682	176	184	193	rBV	99182	121731	11.90%	1.377%
6	2.273	358	368	377	rBV	234804	357912	35.00%	4.049%
7	2.322	377	383	399	rVB	47370	79086	7.73%	0.895%
8	2.444	413	421	439	rVB	36989	64996	6.36%	0.735%
9	2.836	531	543	559	rVB	89891	184035	18.00%	2.082%
10	3.987	881	901	927	rBV2	70117	200849	19.64%	2.272%
11	4.190	950	964	1002	rBV2	94976	395720	38.69%	4.476%
12	4.646	1087	1106	1127	rBV2	126343	306987	30.02%	3.473%
13	4.987	1195	1212	1229	rBV2	111876	265574	25.97%	3.004%
14	5.334	1297	1320	1349	rBV2	264921	723905	70.78%	8.189%
15	5.884	1471	1491	1522	rBV	251247	508707	49.74%	5.754%
16	6.328	1614	1629	1648	rBV2	160563	324148	31.70%	3.667%
17	6.781	1757	1770	1780	rBV	62818	128961	12.61%	1.459%
18	7.225	1894	1908	1935	rBV	98526	182655	17.86%	2.066%
19	7.563	1997	2013	2031	rBV	375132	661479	64.68%	7.482%
20	7.849	2090	2102	2119	rBV	58956	107642	10.53%	1.218%
21	8.177	2194	2204	2214	rBV2	13851	23757	2.32%	0.269%
22	8.312	2234	2246	2283	rBV	395600	736980	72.06%	8.337%
23	8.472	2288	2296	2309	rVB8	6659	12222	1.20%	0.138%
24	9.087	2472	2487	2506	rBV	358034	606456	59.30%	6.860%
25	10.032	2771	2781	2790	rBV4	8273	14956	1.46%	0.169%
26	10.431	2892	2905	2921	rBV2	127916	211118	20.64%	2.388%
27	10.607	2941	2960	2970	rBV2	24732	45308	4.43%	0.513%
28	11.482	3220	3232	3258	rBV	403697	662031	64.73%	7.489%
29	11.752	3305	3316	3325	rBV7	5666	11213	1.10%	0.127%
30	11.858	3336	3349	3371	rBV	377587	631915	61.79%	7.148%
31	12.469	3527	3539	3552	rBV5	11144	27841	2.72%	0.315%
32	13.987	3998	4011	4029	rBV2	64116	107175	10.48%	1.212%
33	14.588	4187	4198	4204	rBV8	5297	10640	1.04%	0.120%
34	16.340	4734	4743	4755	rBV8	9587	17465	1.71%	0.198%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

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\SOMUTR021119WMA.M
Title : TRACE VOA SOM01.0

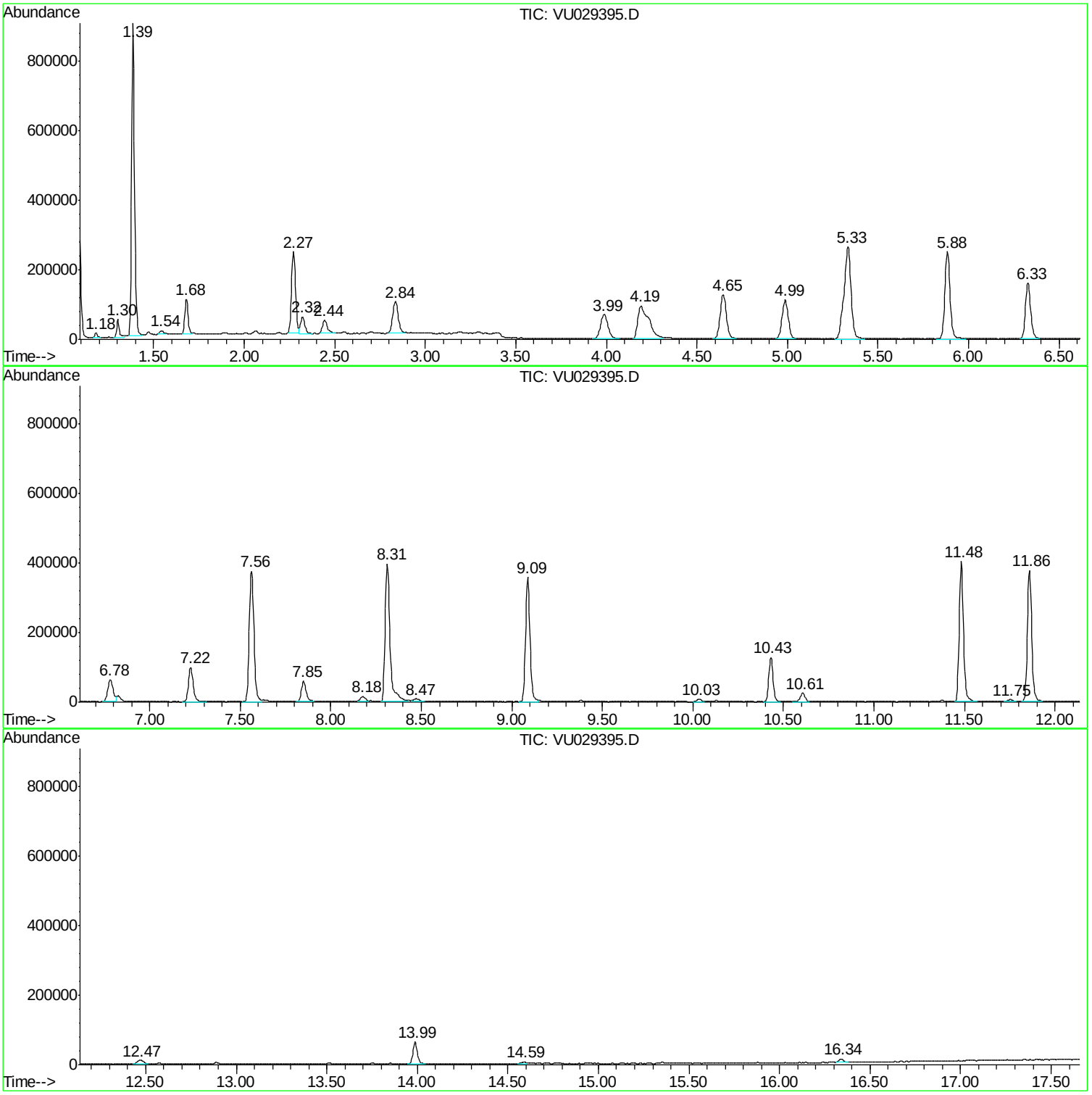
Sum of corrected areas: 8840385

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

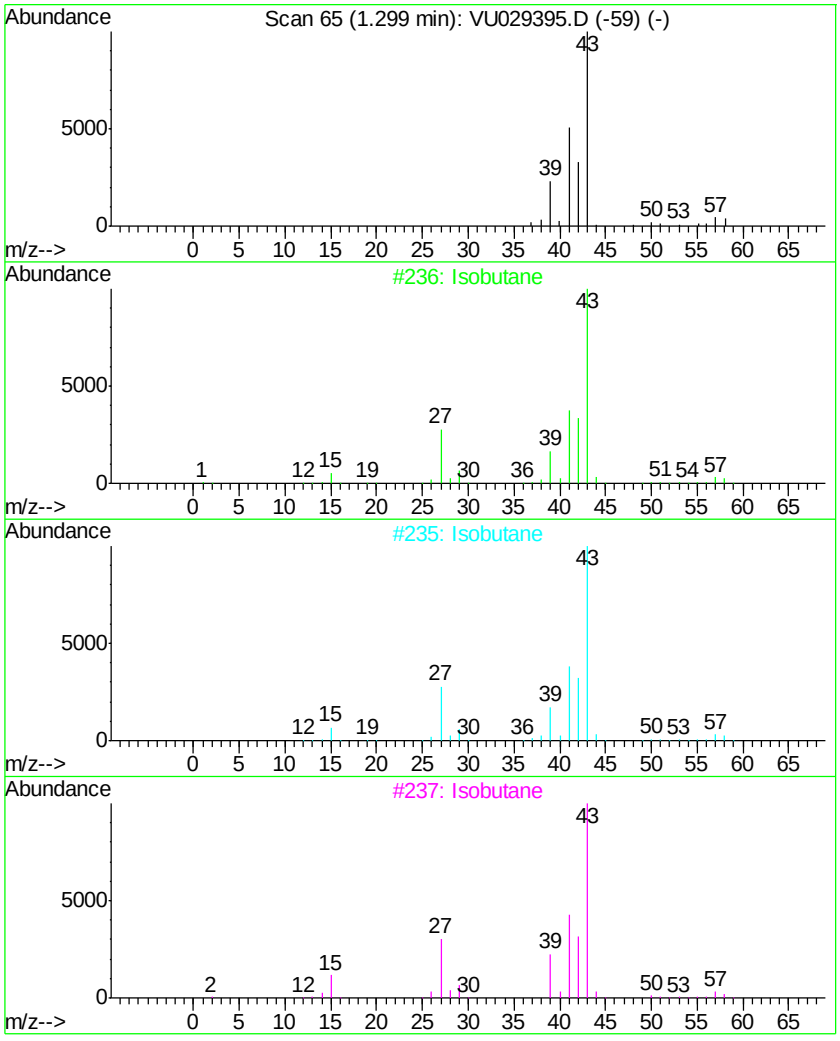
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

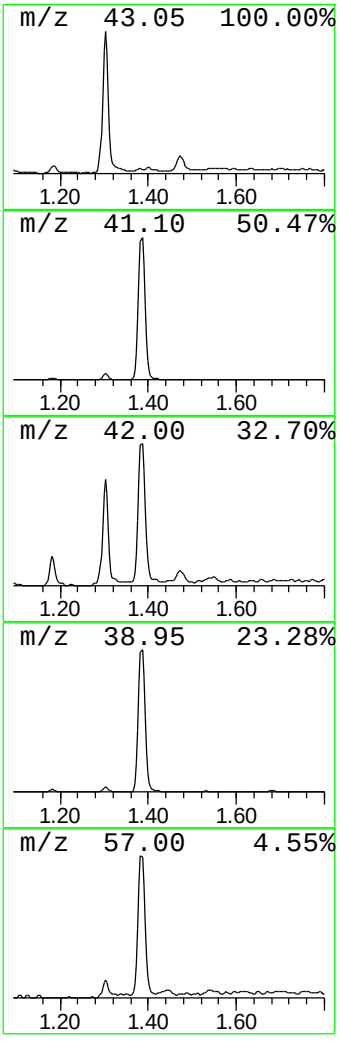
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	0.54 ug/L	55154	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	50
2	Isobutane	58	C4H10	000075-28-5	50
3	Isobutane	58	C4H10	000075-28-5	45
4	Isobutane	58	C4H10	000075-28-5	42
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

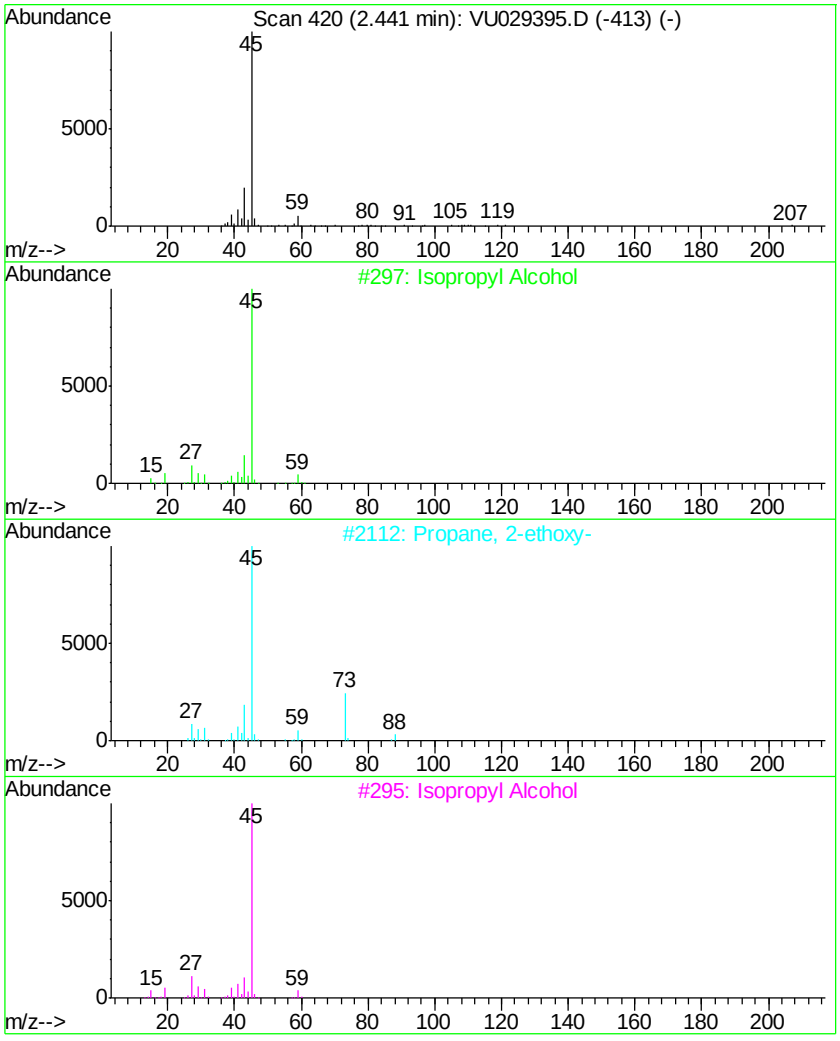
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

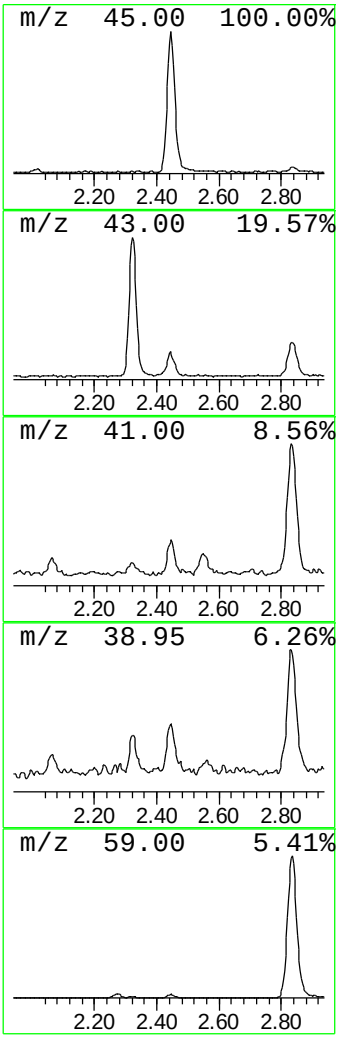
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	0.64 ug/L	64996	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

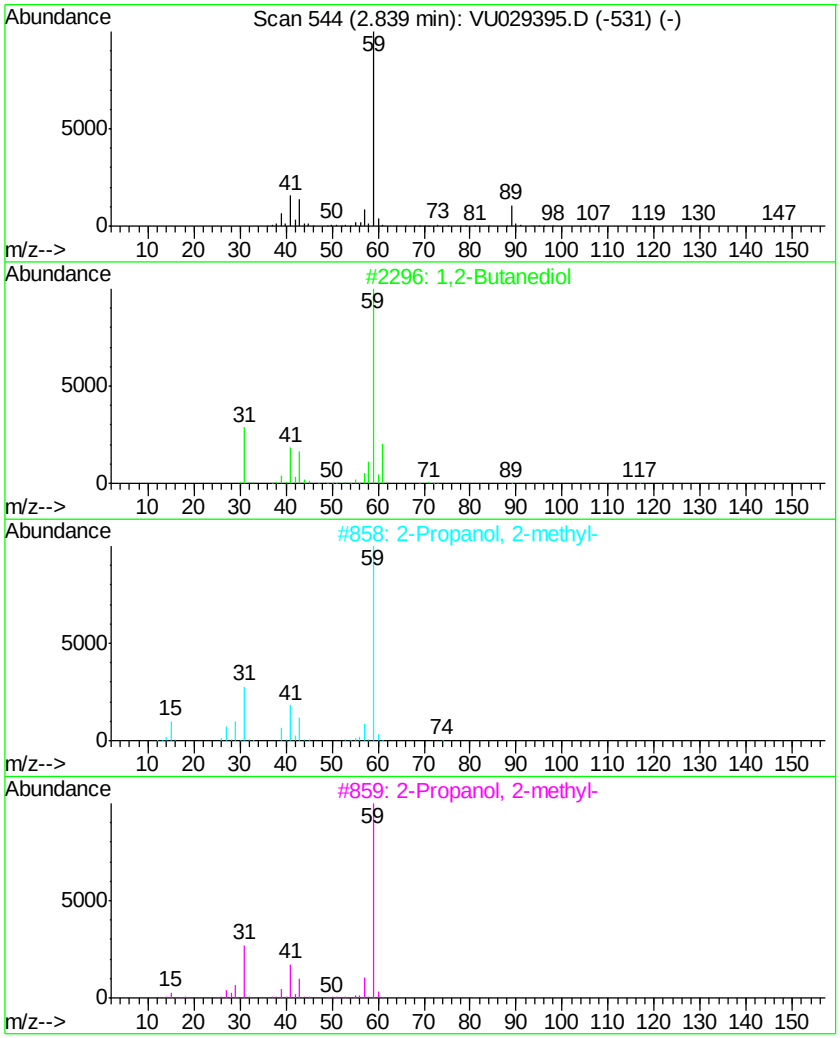
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

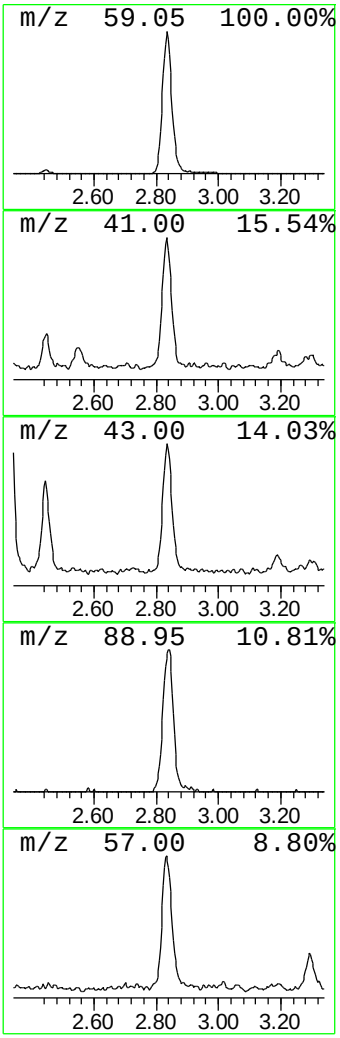
****

Peak Number 3 1,2-Butanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	1.81 ug/L	184035	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Butanediol	90	C4H10O2	000584-03-2	59
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	38
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021119\
Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

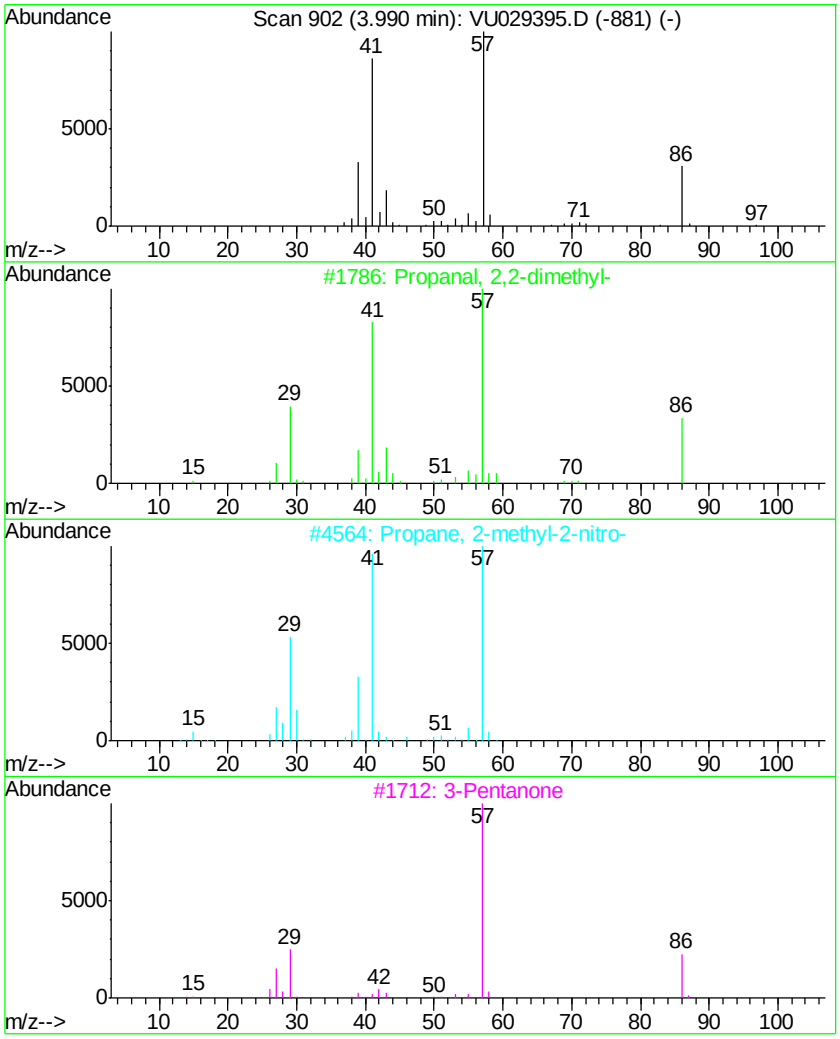
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

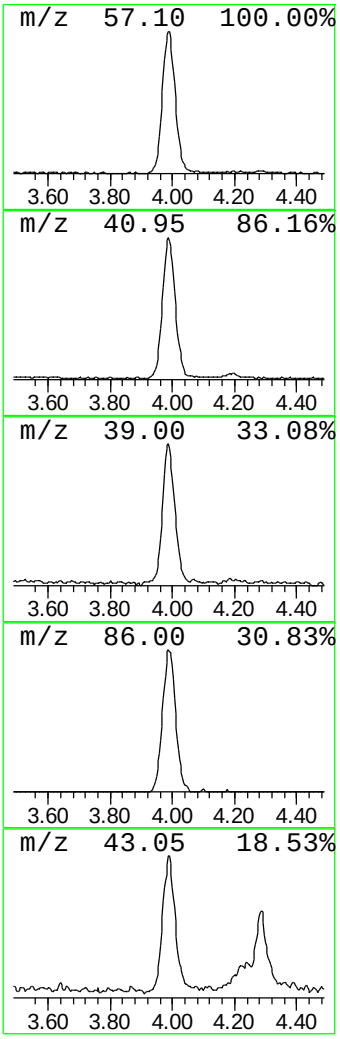
****

Peak Number 4 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	1.97 ug/L	200849	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	80
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3	3-Pentanone	86	C5H10O	000096-22-0	40
4	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	40
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021119\
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Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

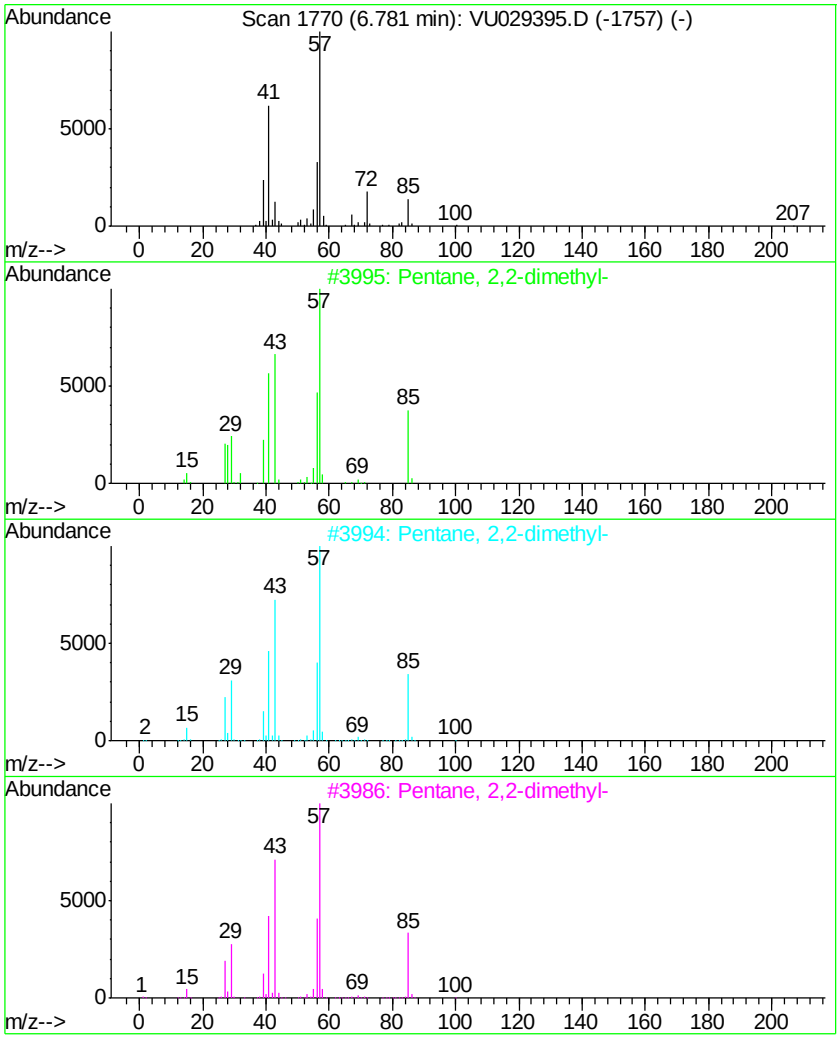
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

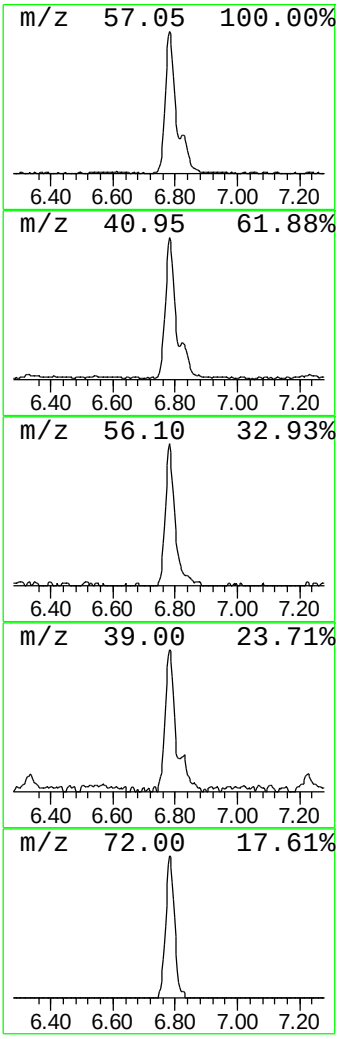
****

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	1.27 ug/L	128961	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
2	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	45
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40





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Data File : VU029395.D
Acq On : 11 Feb 2019 14:21
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.M
Quant Title : TRACE VOA SOM01.0

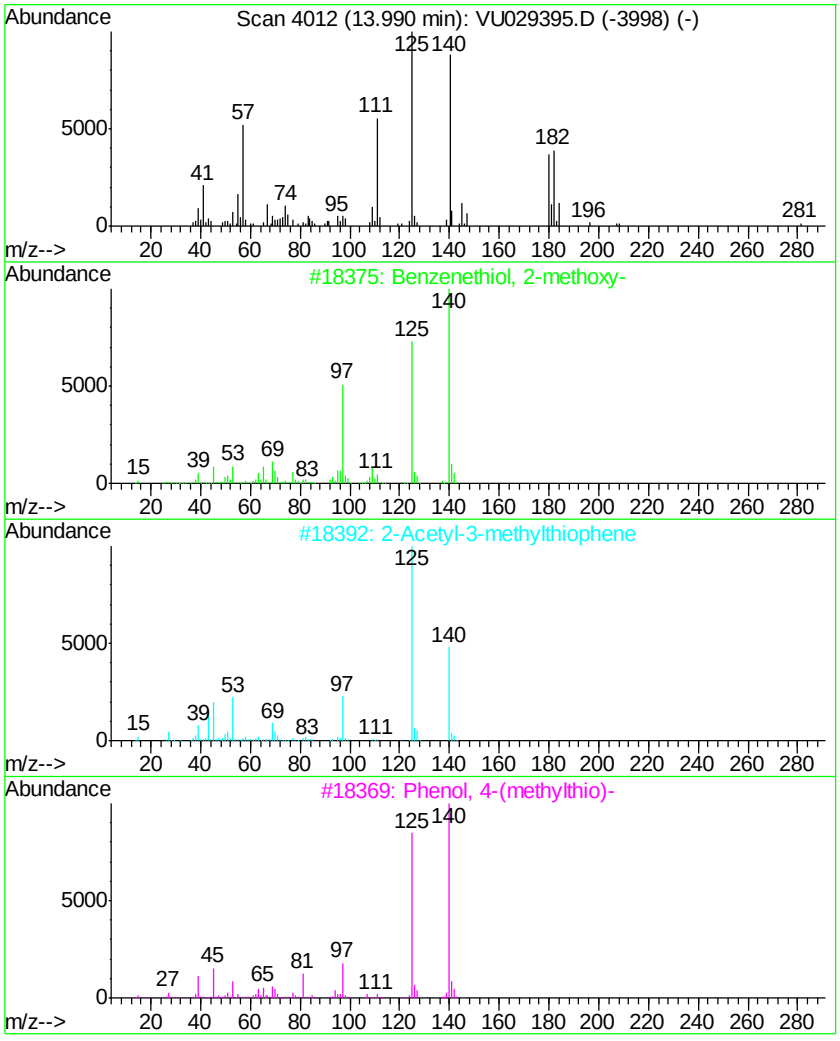
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

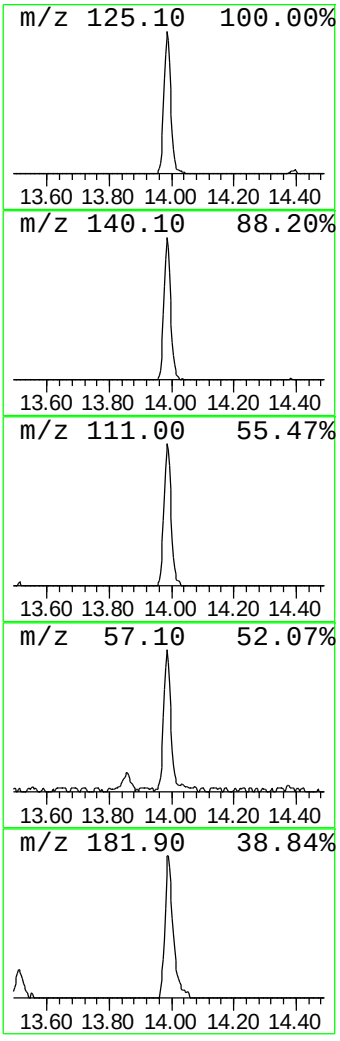
****

Peak Number 7 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	0.81 ug/L	107175	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	47
2	2-Acetyl-3-methylthiophene	140	C7H8OS	013679-72-6	46
3	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	46
4	3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	46
5	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	43





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021119WMA.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...	1.30	0.5	ug/L	55154	1	5.88	508707	5.0
Isopropyl Alcohol	2.44	0.6	ug/L	64996	1	5.88	508707	5.0
1,2-Butanediol	2.84	1.8	ug/L	184035	1	5.88	508707	5.0
Propanal, 2,2-dim...	3.99	2.0	ug/L	200849	1	5.88	508707	5.0
(DEL) Alkane: Str...	6.78	1.3	ug/L	128961	1	5.88	508707	5.0
unknown-01	13.99	0.8	ug/L	107175	3	11.48	662031	5.0