LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

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\SOMUTR101719WMA.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	1.507	45	52	72	rVB	160823	195042	6.16%	1.145%
2	1.620	76	87	97	rBV3	694941	787003	24.86%	4.620%
3	1.935	177	185	197	rVB	81838	107061	3.38%	0.629%
4	2.015	199	210	231	rBV	2310261	3166357	100.00%	18.588%
5	2.231	268	277	294	rVB3	47377	100829	3.18%	0.592%
6	2.494	350	359	370	rBV2	26799	42549	1.34%	0.250%
7	2.597	380	391	421	rVB2	130673	295374	9.33%	1.734%
8	3.073	519	539	549	rBV2	109282	262928	8.30%	1.544%
9	3.170	557	569	586	rVB	477100	965647	30.50%	5.669%
10	3.427	626	649	673	rBV	1182661	2848705	89.97%	16.724%
11	4.134	857	869	884	rVB5	14758	34893	1.10%	0.205%
12	4.382	931	946	962	rBV3	22197	54932	1.73%	0.322%
13	4.578	989	1007	1019	rBV2	63653	152477	4.82%	0.895%
14	4.658	1019	1032	1037	rVV2	77830	163384	5.16%	0.959%
15	4.703	1038	1046	1074	rVB	156554	402318	12.71%	2.362%
16	5.115	1158	1174	1199	rBV	138186	330989	10.45%	1.943%
17	5.433	1256	1273	1286	rBV3	34544	78464	2.48%	0.461%
18	5.771	1360	1378	1387	rBV3	268878	689882	21.79%	4.050%
19	5.819	1389	1393	1406	rVB	113104	188774	5.96%	1.108%
20	6.292	1525	1540	1560	rBV	264784	557898	17.62%	3.275%
21	6.597	1619	1635	1656	rVB7	25522	72258	2.28%	0.424%
22	6.735	1664	1678	1707	rBV	187270	383208	12.10%	2.250%
23	7.604	1933	1948	1966	rBV	81899	172561	5.45%	1.013%
24	7.790	1996	2006	2021	rVB4	19643	37545	1.19%	0.220%
25	7.935	2030	2051	2068	rBV	283859	527127	16.65%	3.095%
26	8.218	2126	2139	2152	rBV2	45987	87043	2.75%	0.511%
27	8.690	2271	2286	2318	rBV	267428	902610	28.51%	5.299%
28	8.832	2319	2330	2364	rVB	278654	565074	17.85%	3.317%
29	9.449	2509	2522	2532	rBV	346941	619926	19.58%	3.639%
30	9.861	2625	2650	2677	rBV	407419	799082	25.24%	4.691%
31	10.070	2697	2715	2730	rBV9	22648	62305	1.97%	0.366%
32	10.314	2779	2791	2804	rBV2	35915	66586	2.10%	0.391%
33	10.398	2805	2817	2827	rVV6	37335	72382	2.29%	0.425%
34	10.456	2827	2835	2847	rVB3	19030	32888	1.04%	0.193%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

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\SOMUTR101719WMA.M
Title : TRACE VOA SOM01.0

35	10.787	2922	2938	2947	rBV2	158824	289471	9.14%	1.699%
36	11.446	3132	3143	3166	rVB8	23484	48248	1.52%	0.283%
37	11.845	3254	3267	3285	rBV	229597	450595	14.23%	2.645%
38	12.224	3373	3385	3404	rVB	227700	419716	13.26%	2.464%

Sum of corrected areas: 17034131

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Acq On : 23 Oct 2019 23:47
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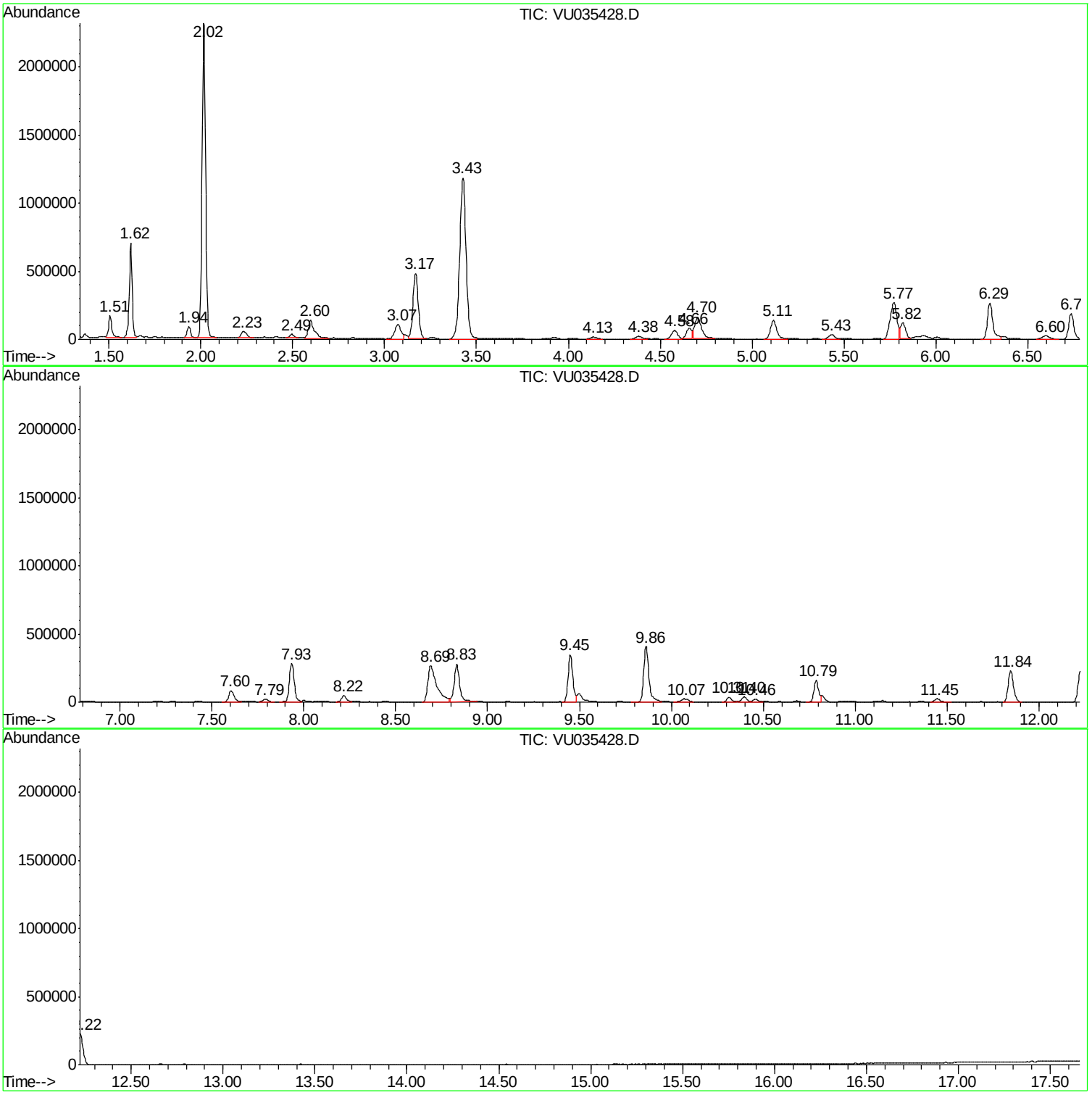
Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.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\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
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Quant Title : TRACE VOA SOM01.0

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

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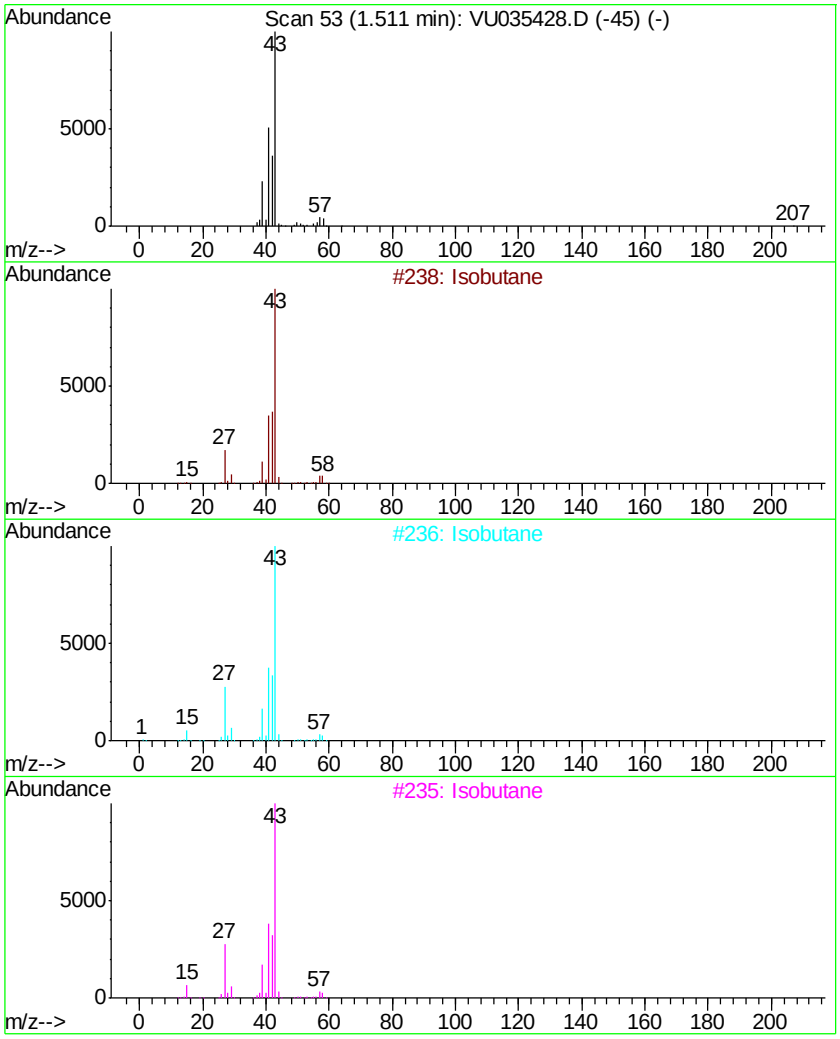
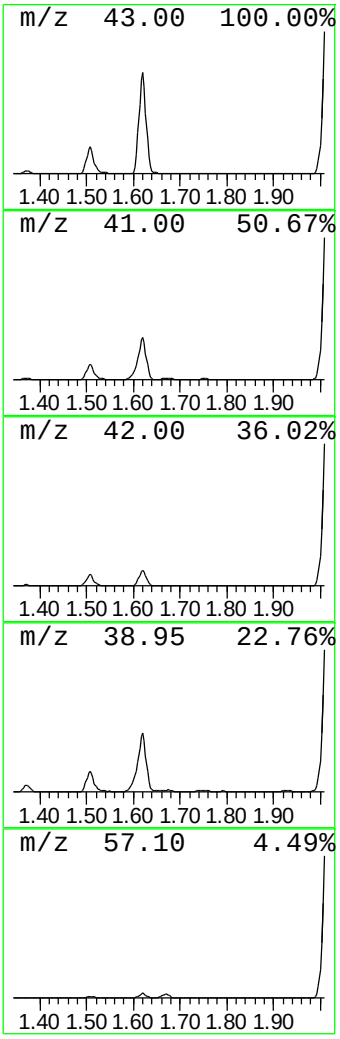
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	1.75 ug/L	195042	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Isobutane	58	C4H10	000075-28-5	64
3	Isobutane	58	C4H10	000075-28-5	64
4	Isobutane	58	C4H10	000075-28-5	50
5	3-Butenoic acid, ethyl ester	114	C6H10O2	001617-18-1	4





Library Search Compound Report

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Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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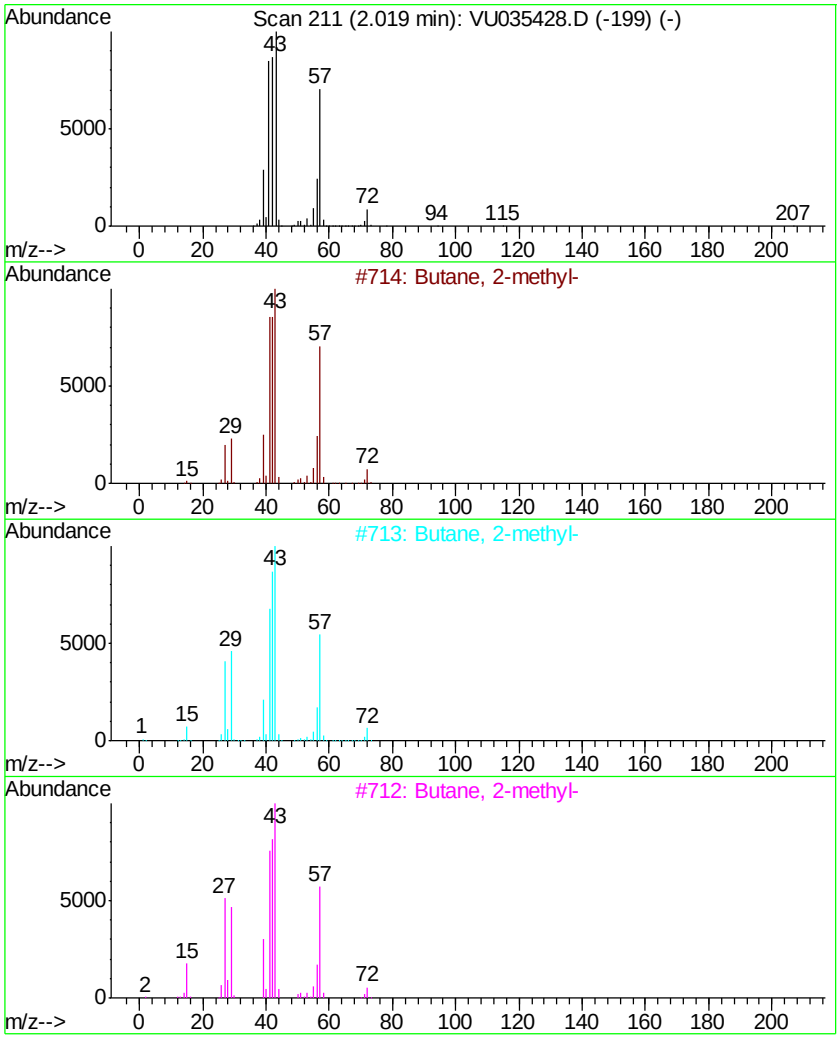
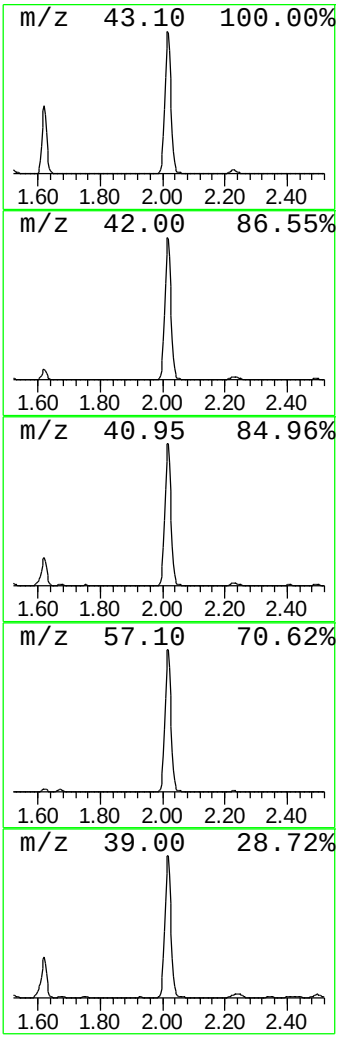
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	28.38 ug/L	3166360	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Butane, 2-methyl-	72	C5H12	000078-78-4	91
3	Butane, 2-methyl-	72	C5H12	000078-78-4	86
4	Pentane	72	C5H12	000109-66-0	50
5	3-Buten-1-ol	72	C4H8O	000627-27-0	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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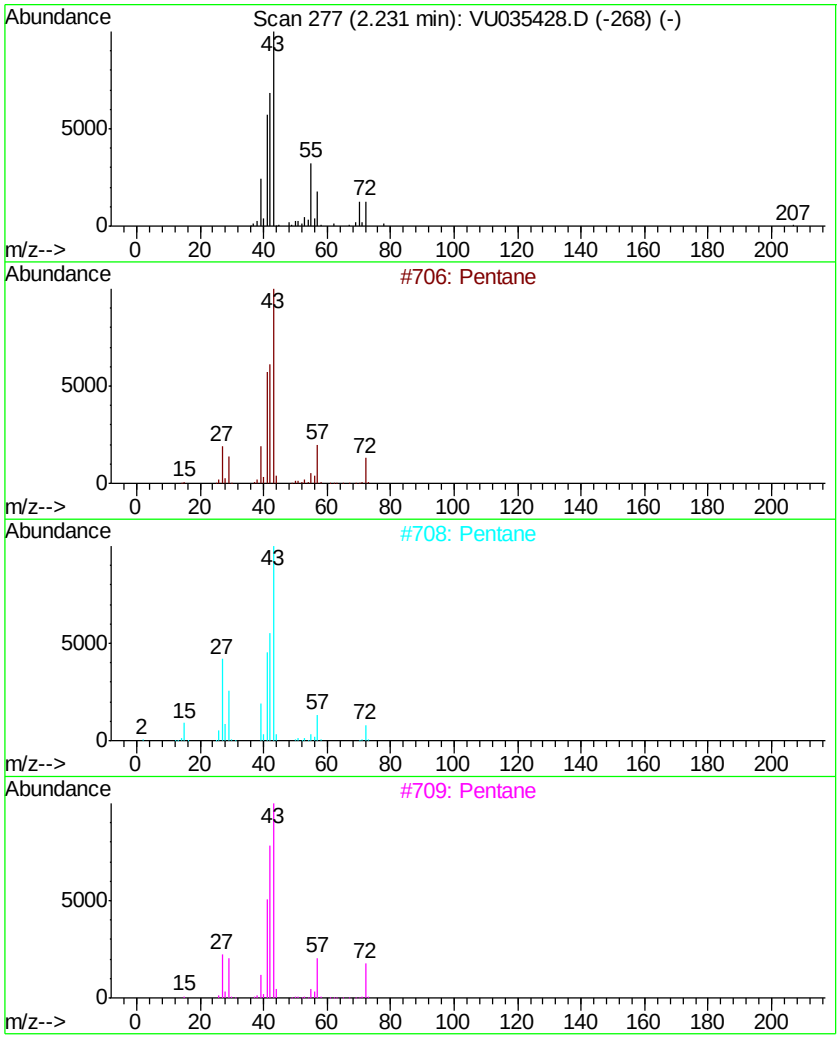
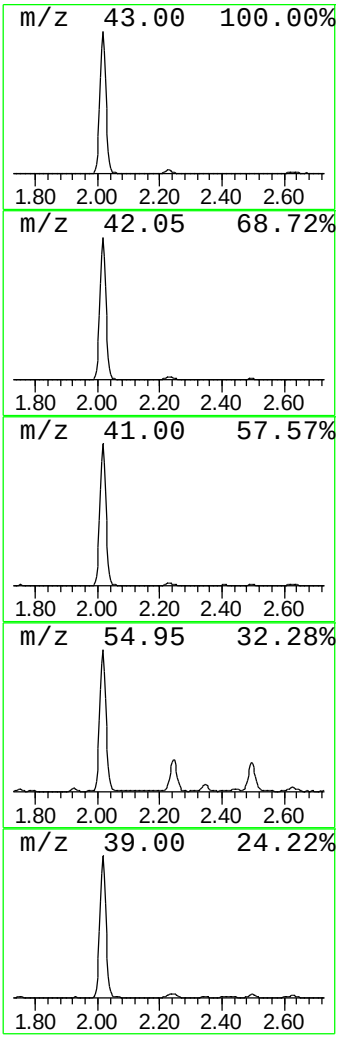
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	0.90 ug/L	100829	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	80
2	Pentane	72	C5H12	000109-66-0	64
3	Pentane	72	C5H12	000109-66-0	64
4	Pentane	72	C5H12	000109-66-0	64
5	Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

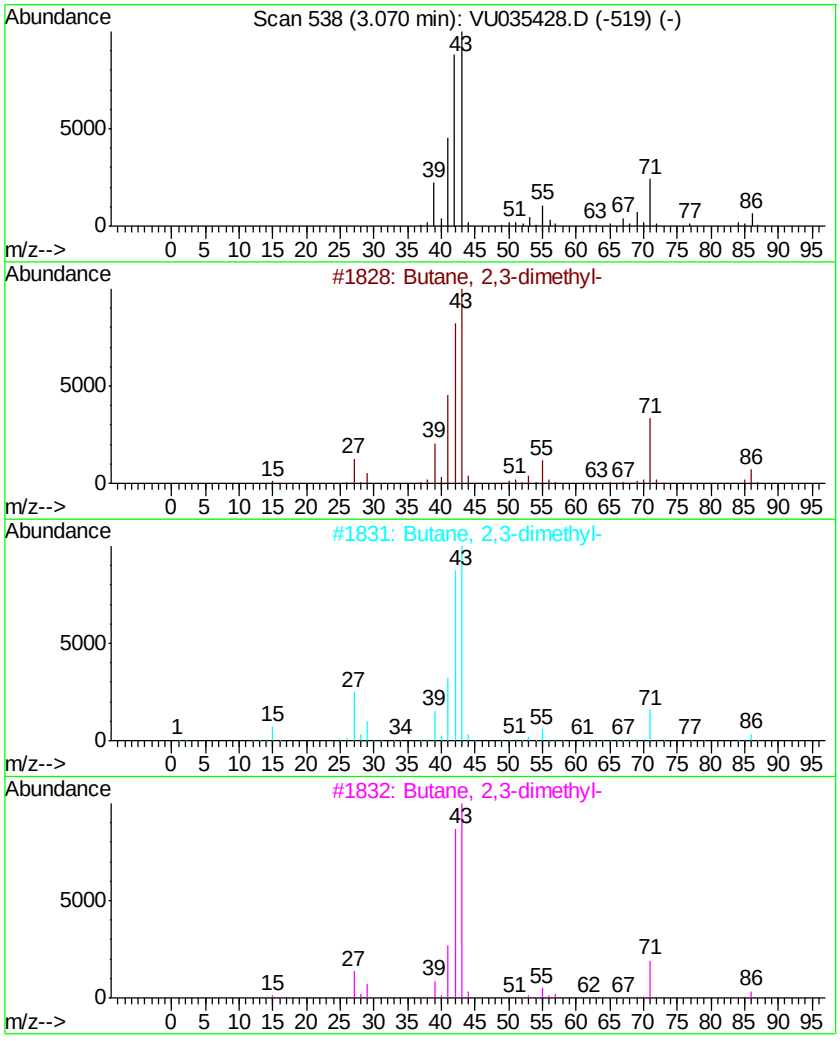
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

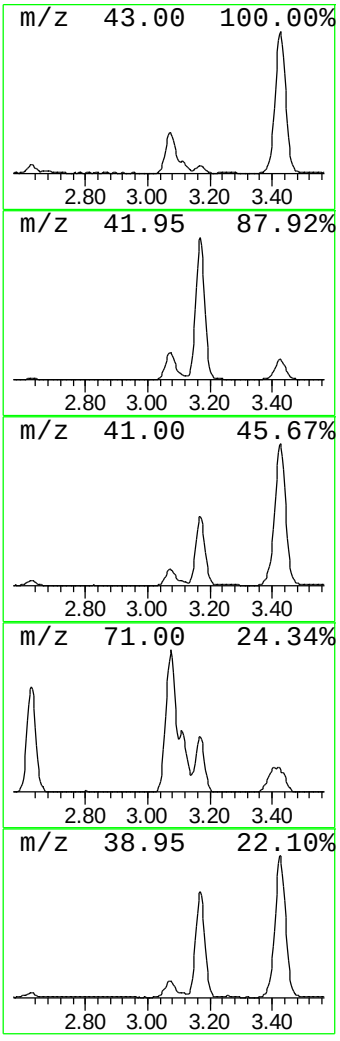
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.07	2.36 ug/L	262928	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
5	Pentane	72	C5H12	000109-66-0	36





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

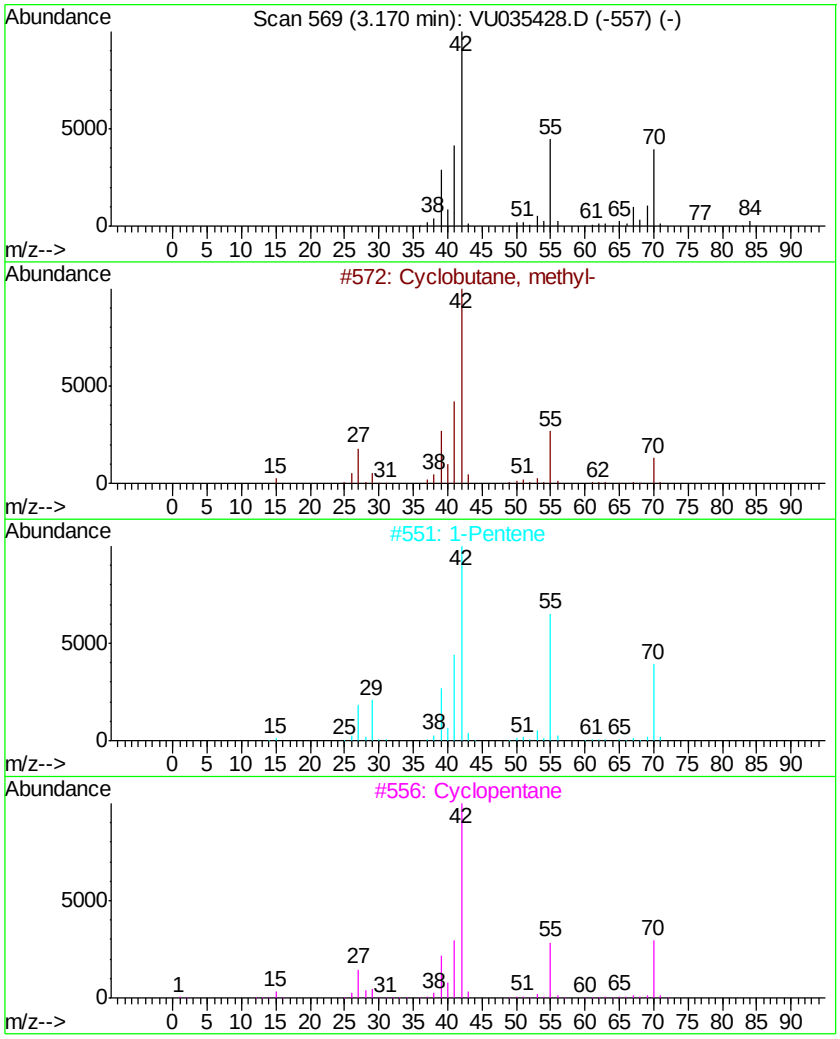
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

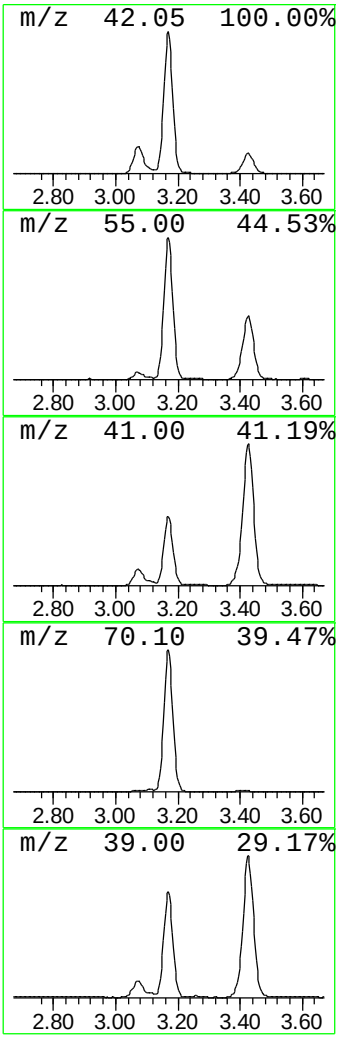
****

Peak Number 5 (DEL) Alkane: Cyclic3.17 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	8.65 ug/L	965647	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2	1-Pentene	70	C5H10	000109-67-1	64
3	Cyclopentane	70	C5H10	000287-92-3	64
4	Cyclopentane	70	C5H10	000287-92-3	50
5	1-Pentene	70	C5H10	000109-67-1	45





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ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

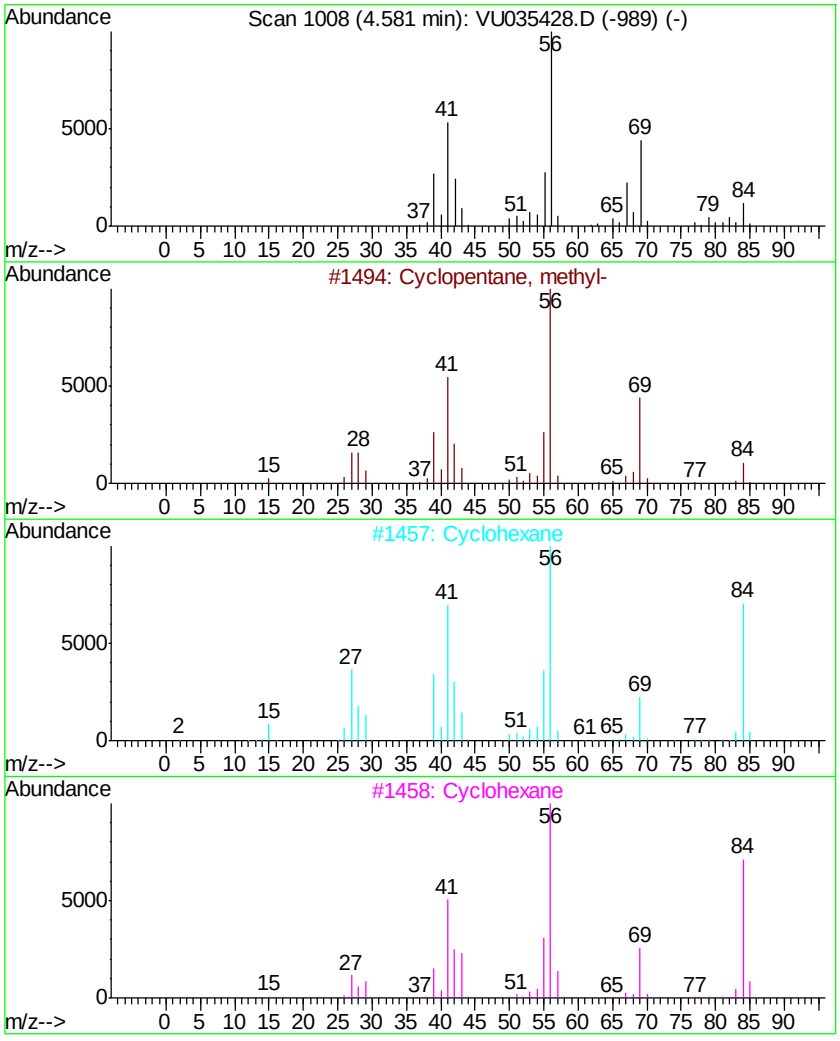
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

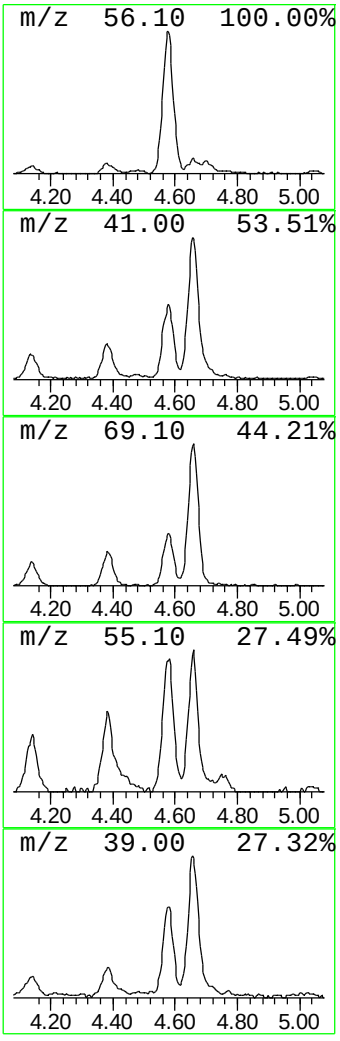
****

Peak Number 6 (DEL) Alkane: Cyclic4.58 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	1.37 ug/L	152477	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2	Cyclohexane	84	C6H12	000110-82-7	64
3	Cyclohexane	84	C6H12	000110-82-7	64
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
5	Cyclohexane	84	C6H12	000110-82-7	59





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Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

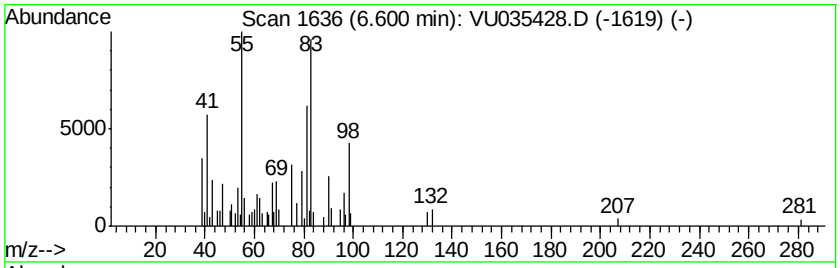
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

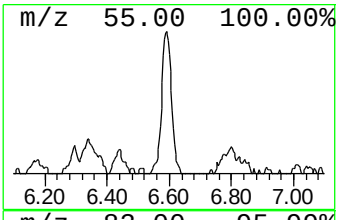
****

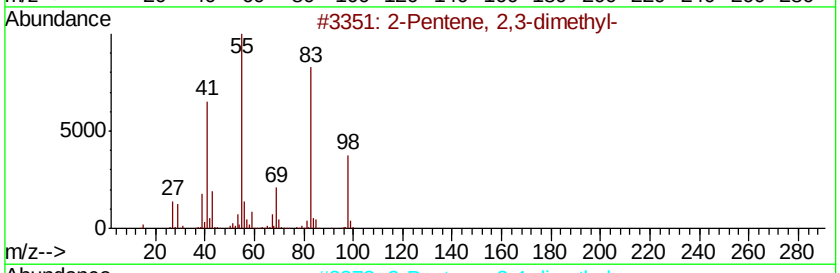
Peak Number 7 (DEL) Alkane: Cyclic6.60 Concentration Rank 10

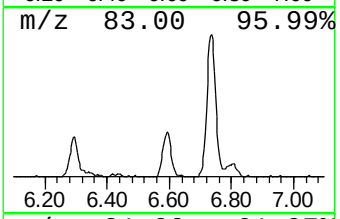
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	0.65 ug/L	72258	1,4-Difluorobenzene	6.29

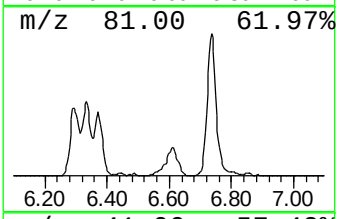
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	41
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	38
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	38
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	38
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	38

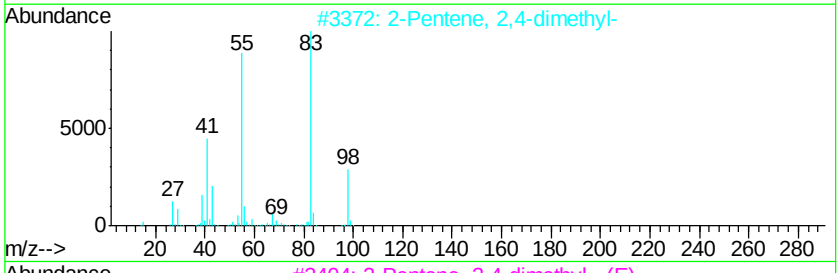


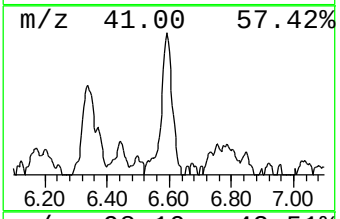


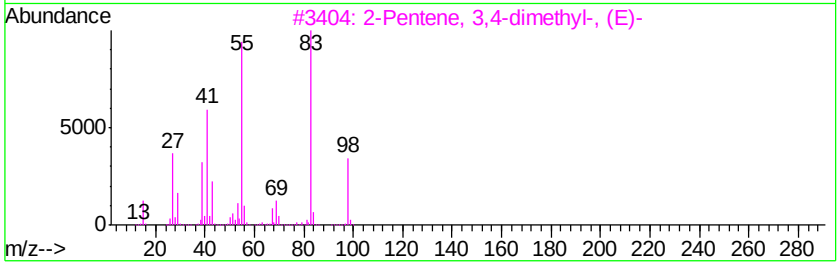


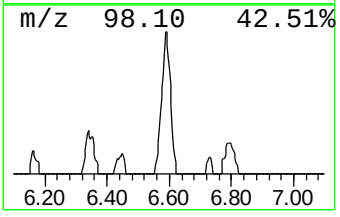












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Sample : K5488-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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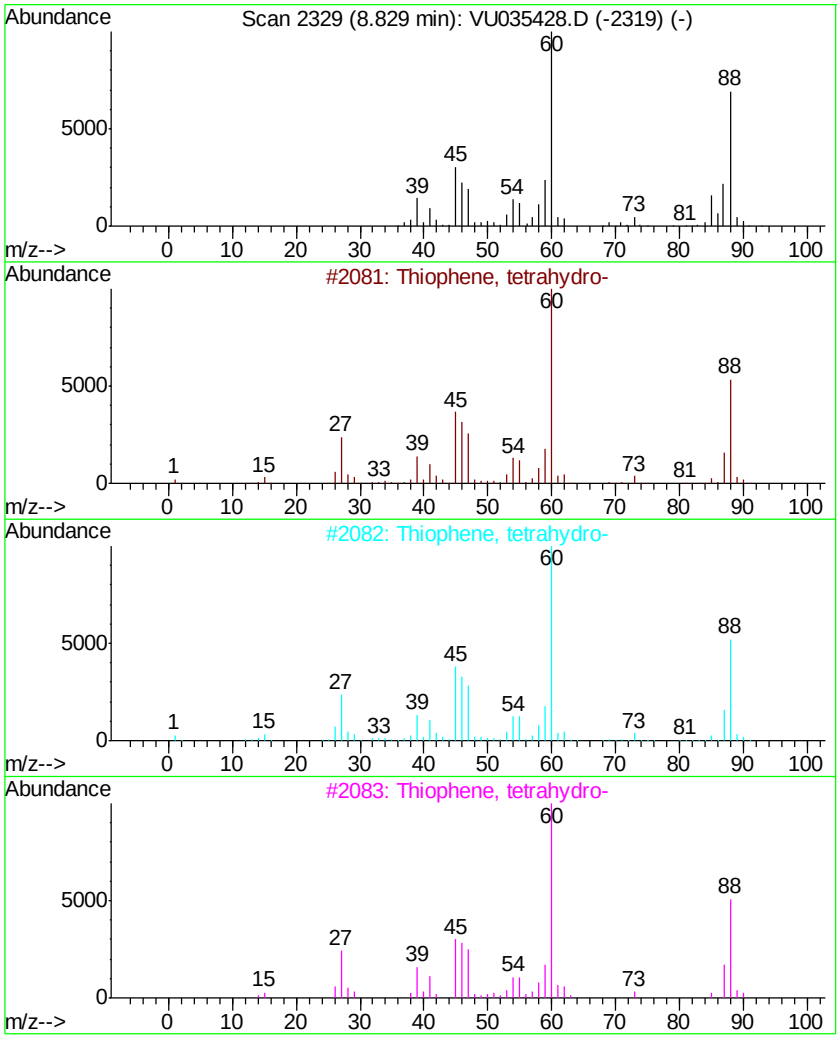
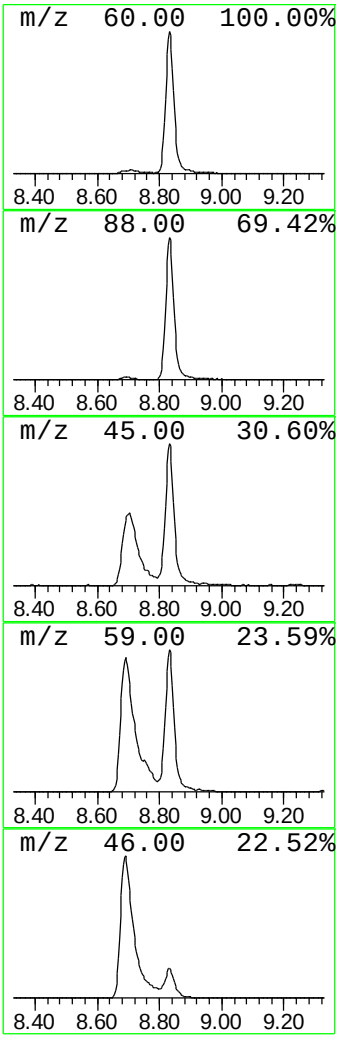
Peak Number 9 Thiophene, tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	4.56 ug/L	565074	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	95
2	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
3	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	64
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	50
5	Thietane, 2-methyl-	88	C4H8S	017837-41-1	49





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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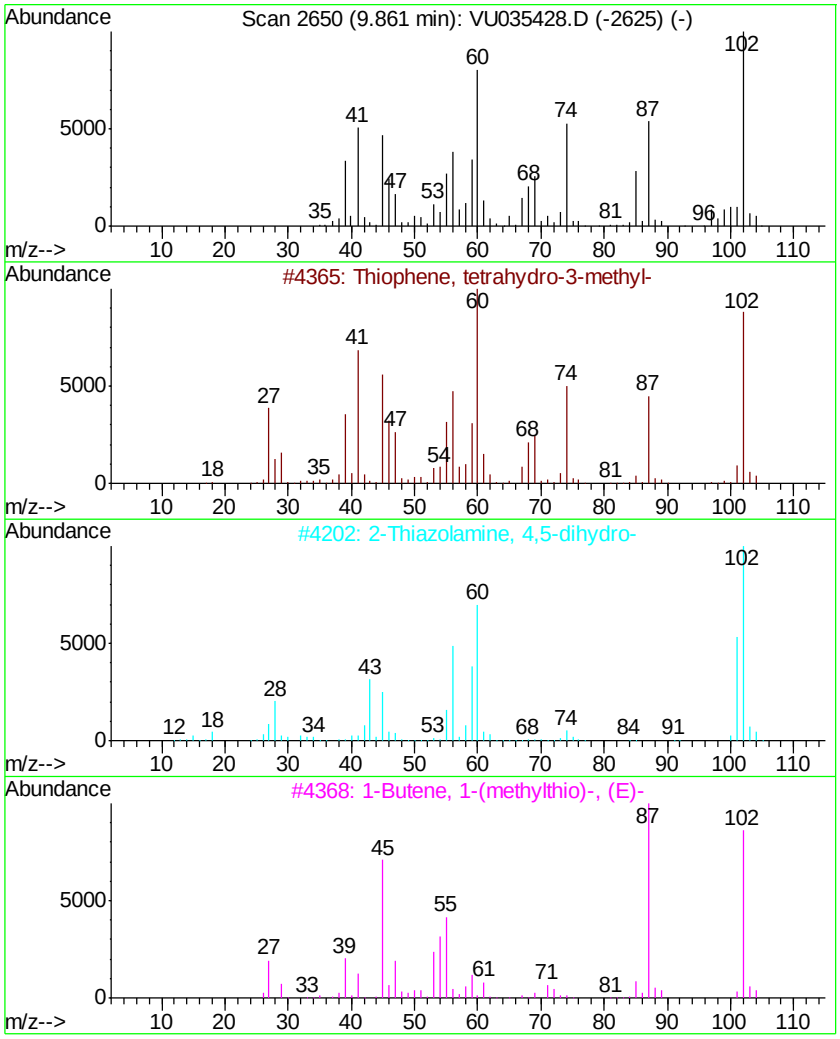
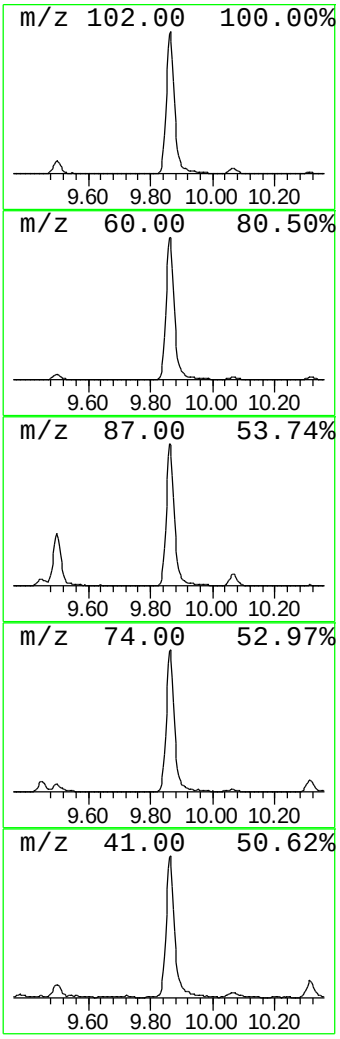
Peak Number 10 Thiophene, tetrahydro-3-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	6.44 ug/L	799082	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	96
2	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	49
3	1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	46
4	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	43
5	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43





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Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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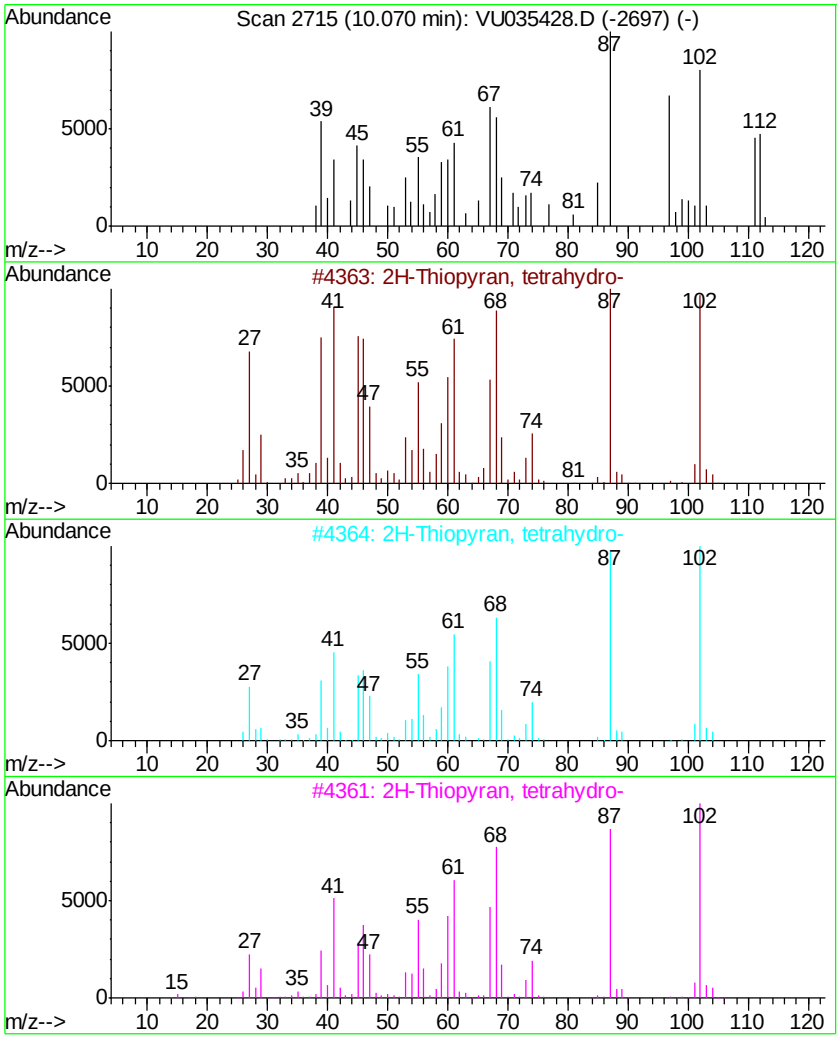
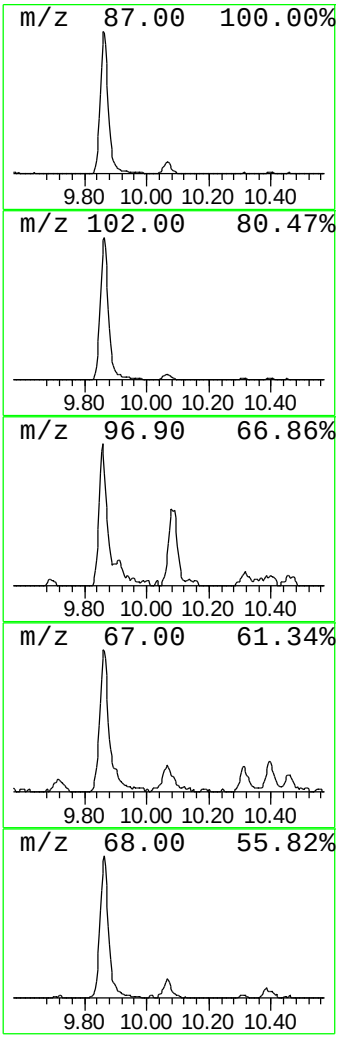
Peak Number 11 2H-Thiopyran, tetrahydro- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	0.50 ug/L	62305	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	64
2	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	64
3	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	55
4	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	38
5	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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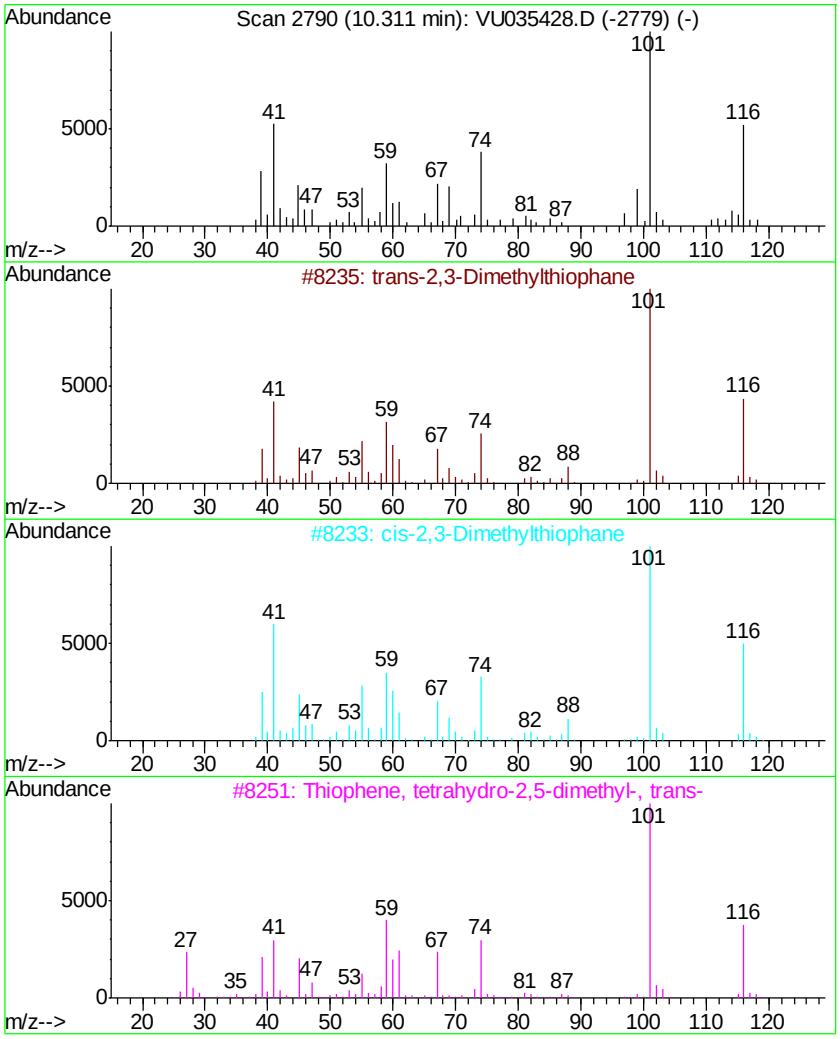
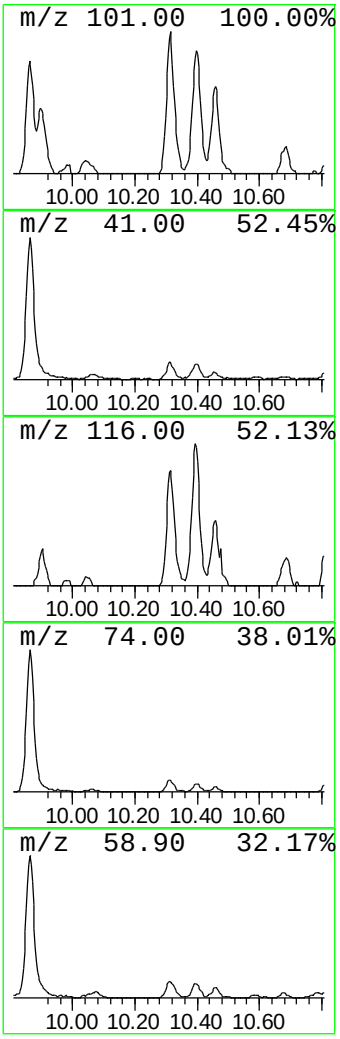
Peak Number 12 trans-2,3-Dimethylthiophane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.31	0.54 ug/L	66586	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	93
2	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	91
3	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	72
4	Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	59
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	59





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Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
Sample : K5488-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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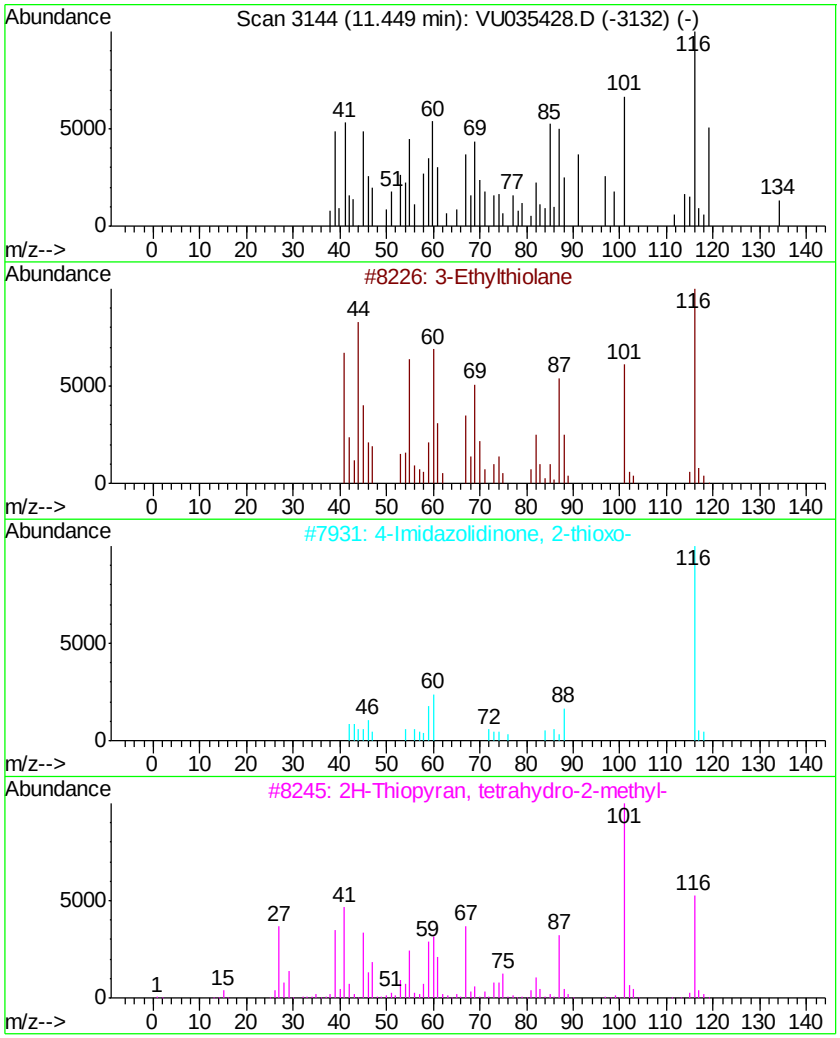
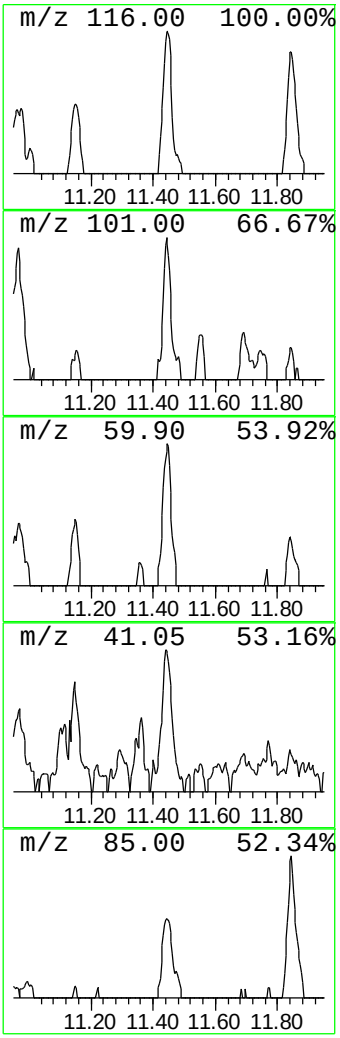
Peak Number 14 3-Ethylthiolane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	0.54 ug/L	48248	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylthiolane	116	C6H12S	062184-67-2	78
2	4-Imidazolidinone, 2-thioxo-	116	C3H4N2OS	000503-87-7	46
3	2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	43
4	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	42
5	Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU102319\
Data File : VU035428.D
Acq On : 23 Oct 2019 23:47
Operator : JC/SP
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

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ClientSampleId : H0G54

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR101719WMA.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...	1.51	1.8	ug/L	195042	1	6.29	557898	5.0
(DEL) Alkane: Str...	2.02	28.4	ug/L	3166360	1	6.29	557898	5.0
(DEL) Alkane: Str...	2.23	0.9	ug/L	100829	1	6.29	557898	5.0
(DEL) Alkane: Str...	3.07	2.4	ug/L	262928	1	6.29	557898	5.0
(DEL) Alkane: Cyc...	3.17	8.7	ug/L	965647	1	6.29	557898	5.0
(DEL) Alkane: Cyc...	4.58	1.4	ug/L	152477	1	6.29	557898	5.0
(DEL) Alkane: Cyc...	6.60	0.7	ug/L	72258	1	6.29	557898	5.0
Thiophene, tetrah...	8.83	4.6	ug/L	565074	2	9.45	619926	5.0
Thiophene, tetrah...	9.86	6.4	ug/L	799082	2	9.45	619926	5.0
2H-Thiopyran, tet...	10.07	0.5	ug/L	62305	2	9.45	619926	5.0
trans-2,3-Dimethy...	10.31	0.5	ug/L	66586	2	9.45	619926	5.0
3-Ethylthiolane	11.45	0.5	ug/L	48248	3	11.84	450595	5.0