LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112420\
Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

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_X\METHOD\82X112120W.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	1.465	59	62	69	rBV	13652702	18091958	100.00%	36.918%
2	1.520	69	71	97	rVB	1509264	3500122	19.35%	7.142%
3	2.130	162	171	193	rBV	2399041	4236125	23.41%	8.644%
4	2.422	214	219	236	rVB	202618	377642	2.09%	0.771%
5	5.464	704	718	733	rBV	178492	524153	2.90%	1.070%
6	5.623	733	744	760	rVV	310647	876275	4.84%	1.788%
7	6.025	801	810	816	rBV	194444	503158	2.78%	1.027%
8	6.111	816	824	838	rVB	533574	1410698	7.80%	2.879%
9	6.824	930	941	955	rBV	474946	1137772	6.29%	2.322%
10	8.696	1241	1248	1253	rBV	963920	1548004	8.56%	3.159%
11	8.763	1253	1259	1276	rVB	2334533	3601691	19.91%	7.350%
12	9.055	1299	1307	1315	rBV	163661	245807	1.36%	0.502%
13	9.482	1369	1377	1381	rBV2	293945	519919	2.87%	1.061%
14	9.531	1381	1385	1395	rVB	1047101	1505479	8.32%	3.072%
15	10.098	1466	1478	1481	rBV	915633	1308370	7.23%	2.670%
16	10.134	1481	1484	1490	rVB	321197	431843	2.39%	0.881%
17	10.342	1509	1518	1528	rVB2	581602	899458	4.97%	1.835%
18	10.445	1528	1535	1540	rBV2	154604	251539	1.39%	0.513%
19	10.683	1569	1574	1583	rVB	564321	784174	4.33%	1.600%
20	10.915	1602	1612	1616	rBV4	141195	332686	1.84%	0.679%
21	11.122	1640	1646	1651	rBV	780963	996073	5.51%	2.033%
22	11.793	1751	1756	1761	rVB	233977	303379	1.68%	0.619%
23	12.061	1794	1800	1806	rBV	1004619	1207737	6.68%	2.464%
24	12.451	1859	1864	1869	rBV	761776	904045	5.00%	1.845%
25	12.835	1923	1927	1933	rVB	462324	581888	3.22%	1.187%
26	13.817	2082	2088	2093	rVB	2149310	2692352	14.88%	5.494%
27	13.908	2099	2103	2110	rVB2	154195	233442	1.29%	0.476%

Sum of corrected areas: 49005789

LSC Report - Integrated Chromatogram

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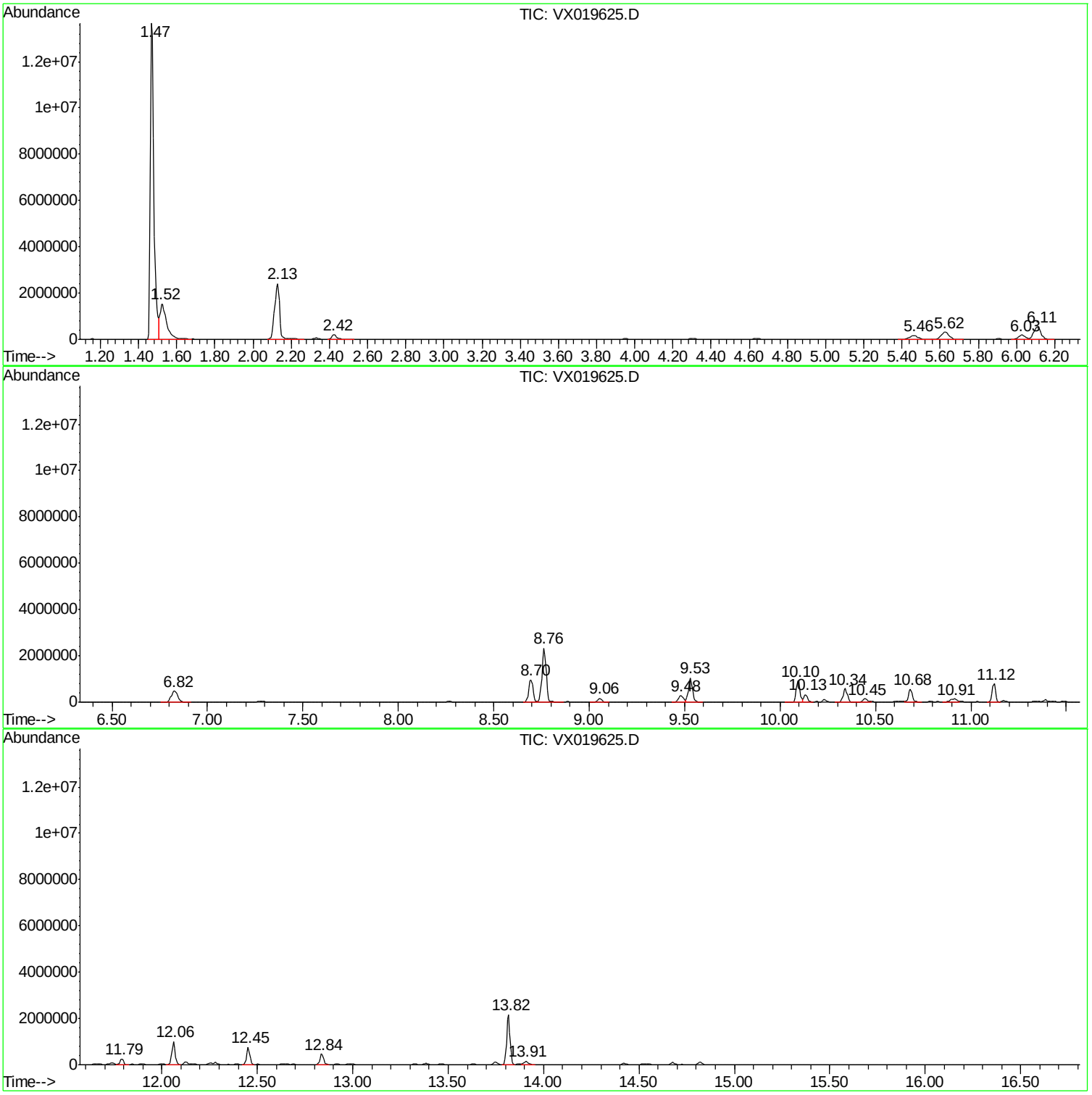
Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112420\
Data File : VX019625.D
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

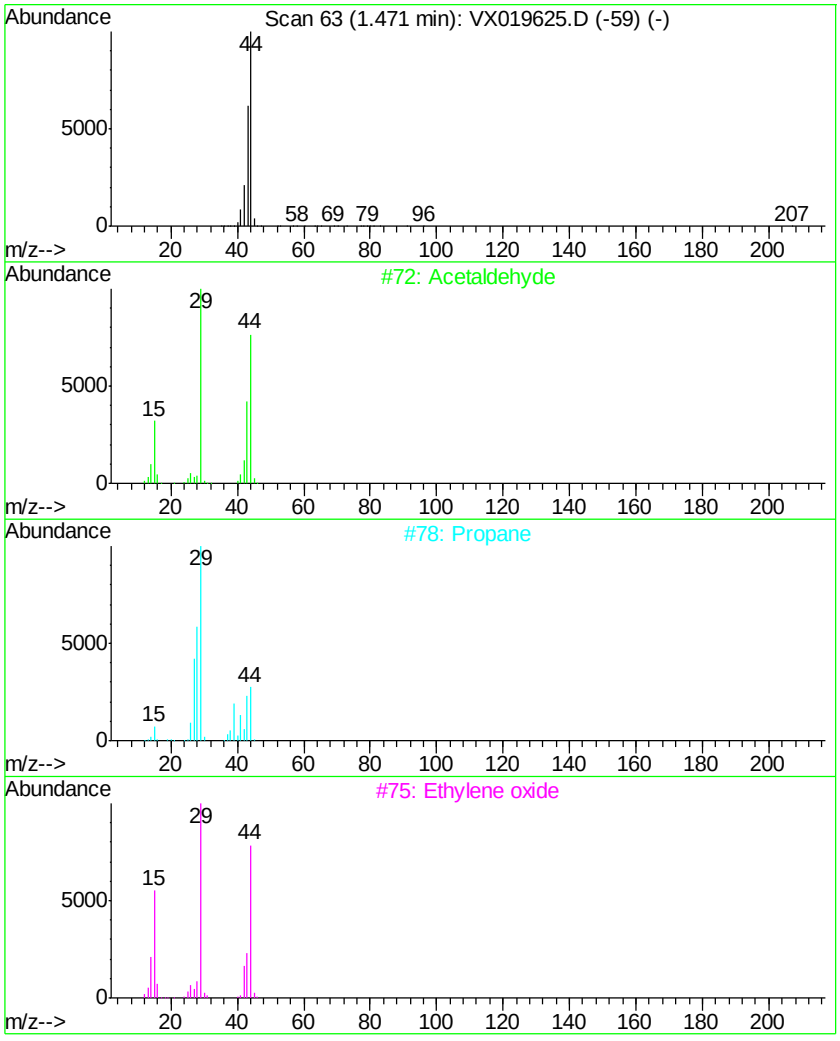
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

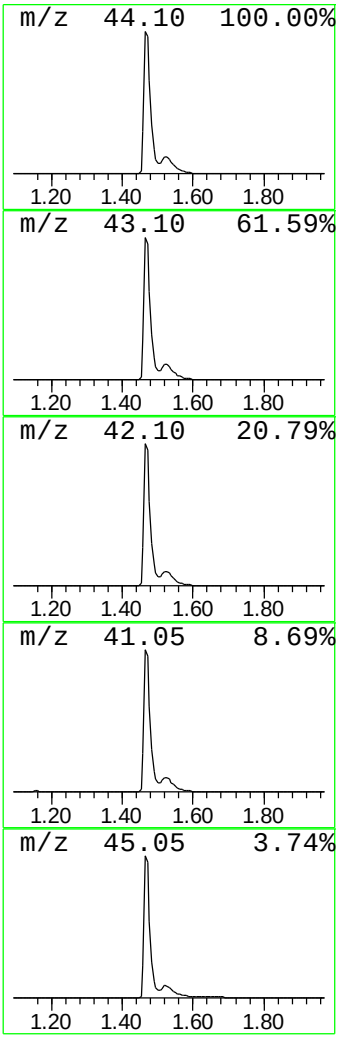
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	1032.32 ug/l	18092000	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Carbon dioxide	44	CO2	000124-38-9	3





Library Search Compound Report

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Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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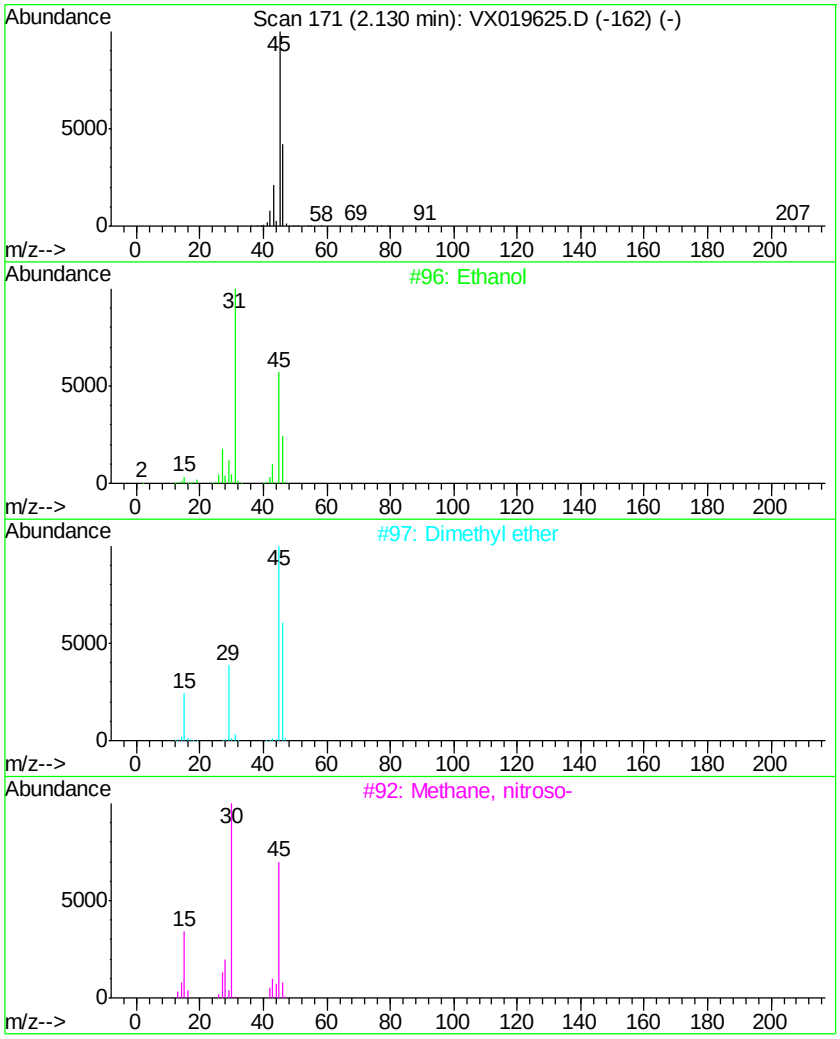
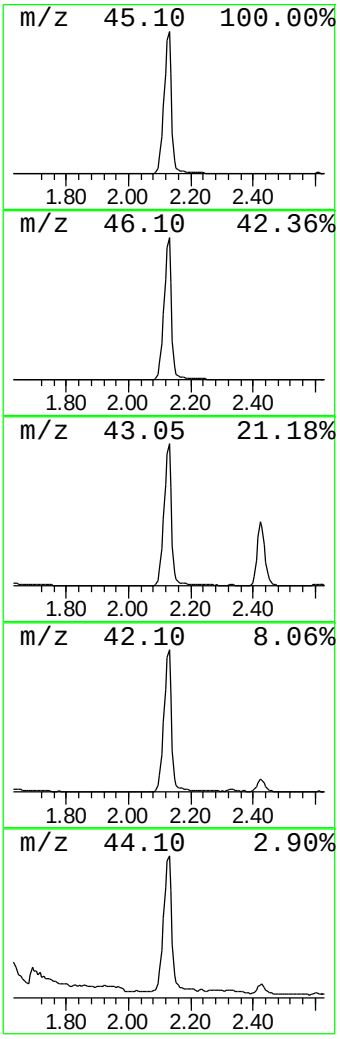
Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	241.71 ug/l	4236130	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112420\
Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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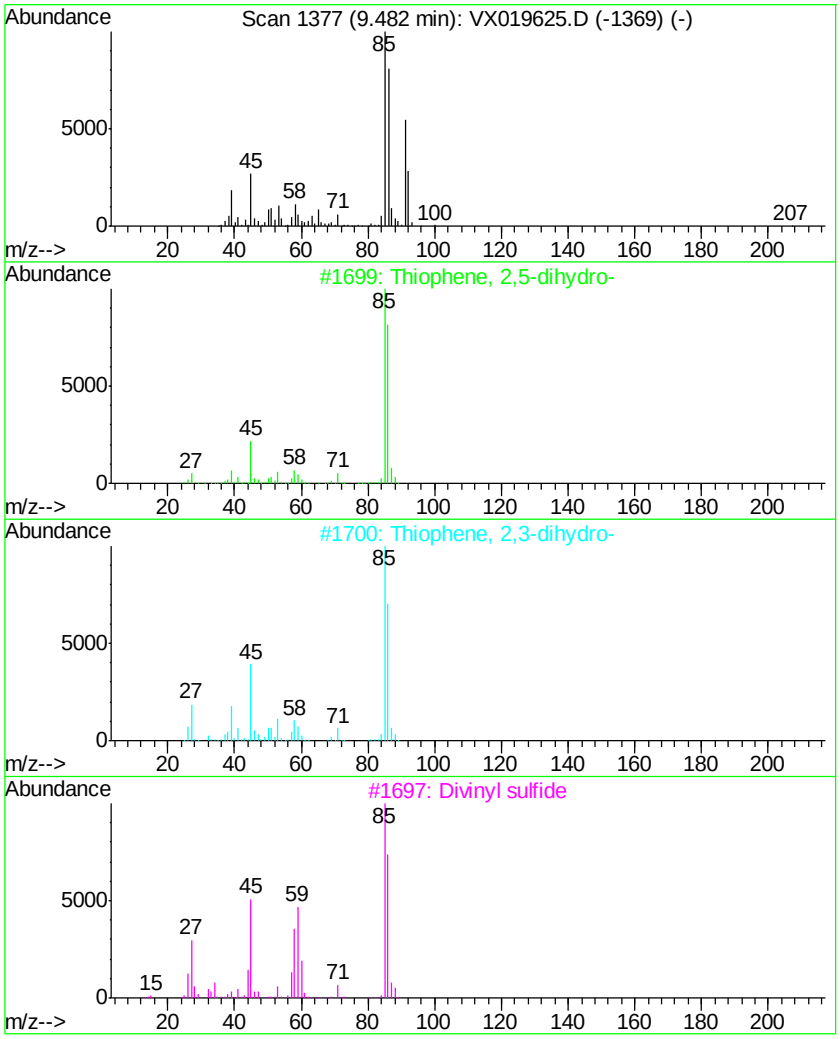
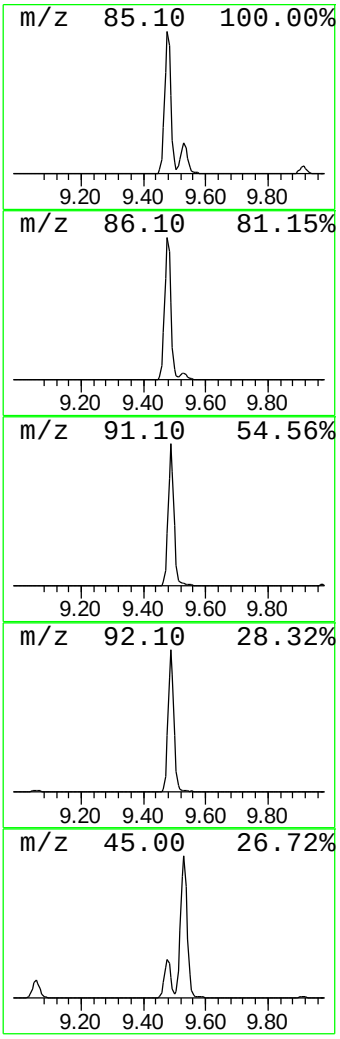
Peak Number 4 Thiophene, 2,5-dihydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	19.87 ug/l	519919	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,5-dihydro-	86	C4H6S	001708-32-3	93
2	Thiophene, 2,3-dihydro-	86	C4H6S	001120-59-8	87
3	Divinyl sulfide	86	C4H6S	000627-51-0	59
4	4-Chloro-5-[[2-diethylaminoethyl...	244	C10H17ClN4O	001907-55-7	16
5	2H-Pyran, 2-(4-chlorobutoxy)tetr...	192	C9H17ClO2	041302-05-0	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112420\
Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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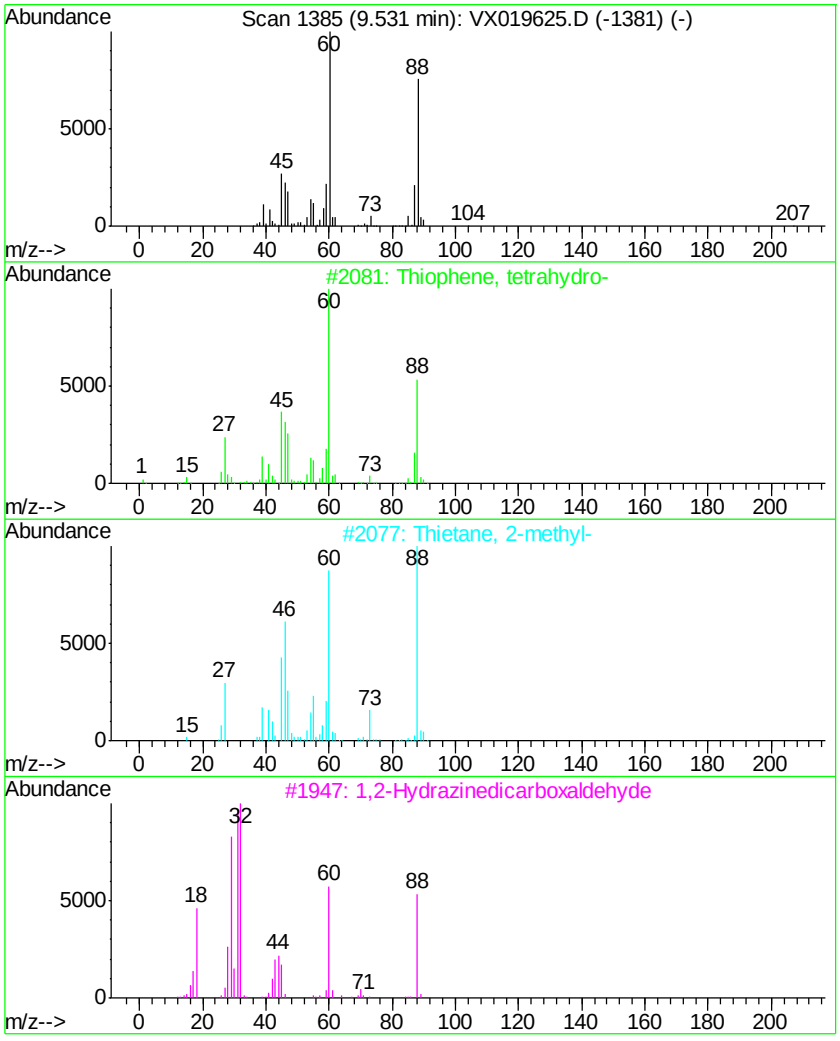
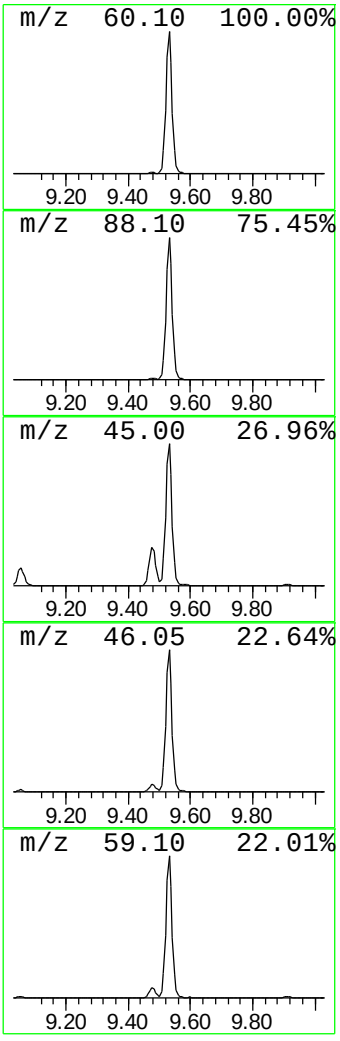
Peak Number 5 Thiophene, tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	57.53 ug/l	1505480	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	53
4	Ethylvinyl sulfide	88	C4H8S	000627-50-9	42
5	2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112420\
Data File : VX019625.D
Acq On : 24 Nov 2020 23:40
Operator : JC/MD
Sample : L4842-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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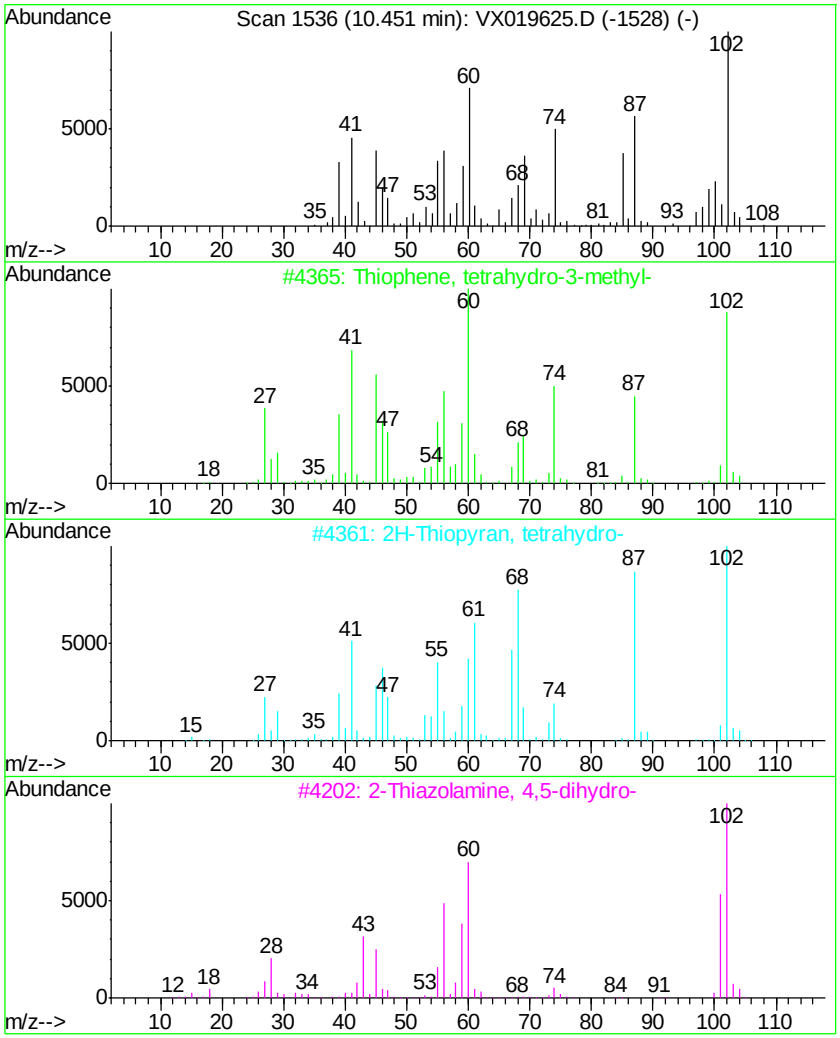
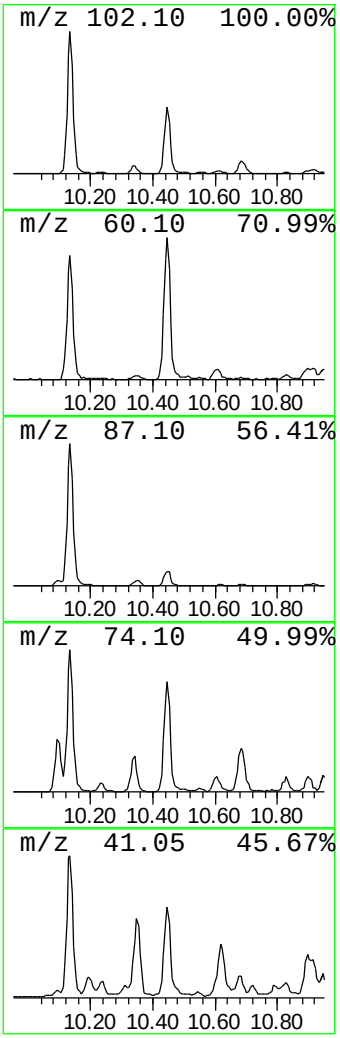
Peak Number 6 Thiophene, tetrahydro-3-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	9.61 ug/l	251539	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	95
2	2H-Thiopyran, tetrahydro-	102	C5H10S	001613-51-0	43
3	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
4	Dihydro-2(3H)-thiophenone	102	C4H6OS	001003-10-7	27
5	Butanamide, N-(aminocarbonyl)-3-...	144	C6H12N2O2	002274-08-0	27





Library Search Compound Report

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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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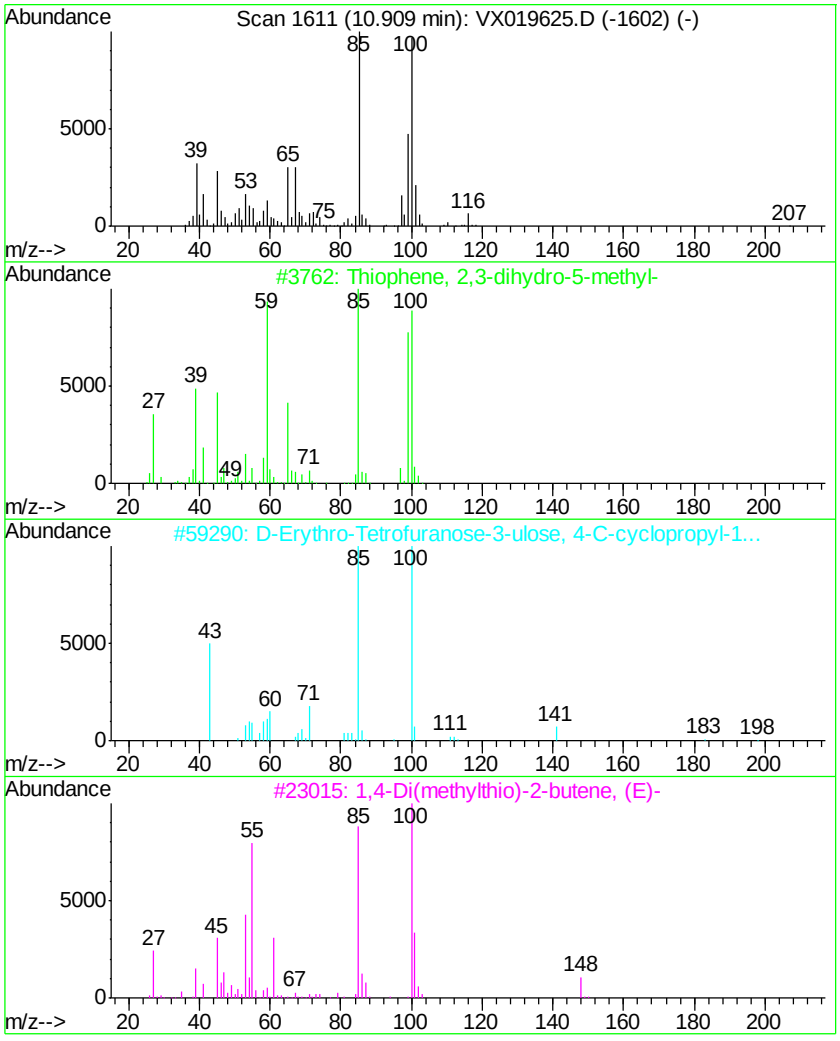
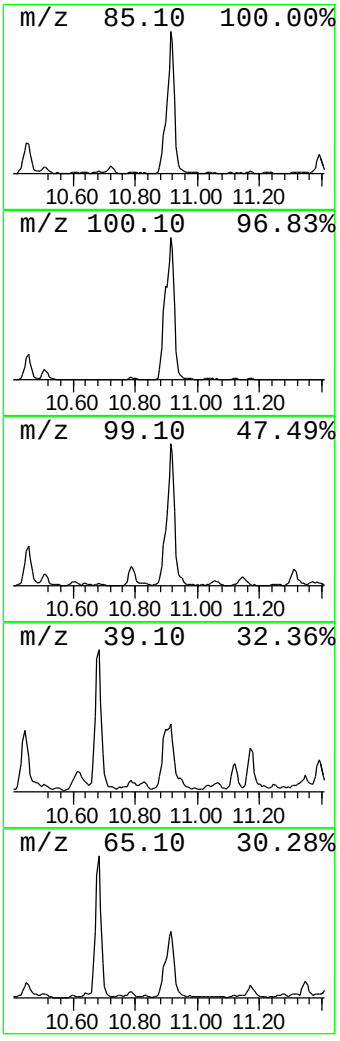
Peak Number 7 Thiophene, 2,3-dihydro-5-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	12.71 ug/l	332686	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2,3-dihydro-5-methyl-	100	C5H8S	004610-02-0	53
2	D-Erythro-Tetrofuranose-3-ulose,...	198	C10H14O4	030645-00-2	50
3	1,4-Di(methylthio)-2-butene, (E)-	148	C6H12S2	052752-62-2	47
4	Imidazole, 5-fluoro-2-methyl-	100	C4H5FN2	071516-19-3	43
5	1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112420\
Data File : VX019625.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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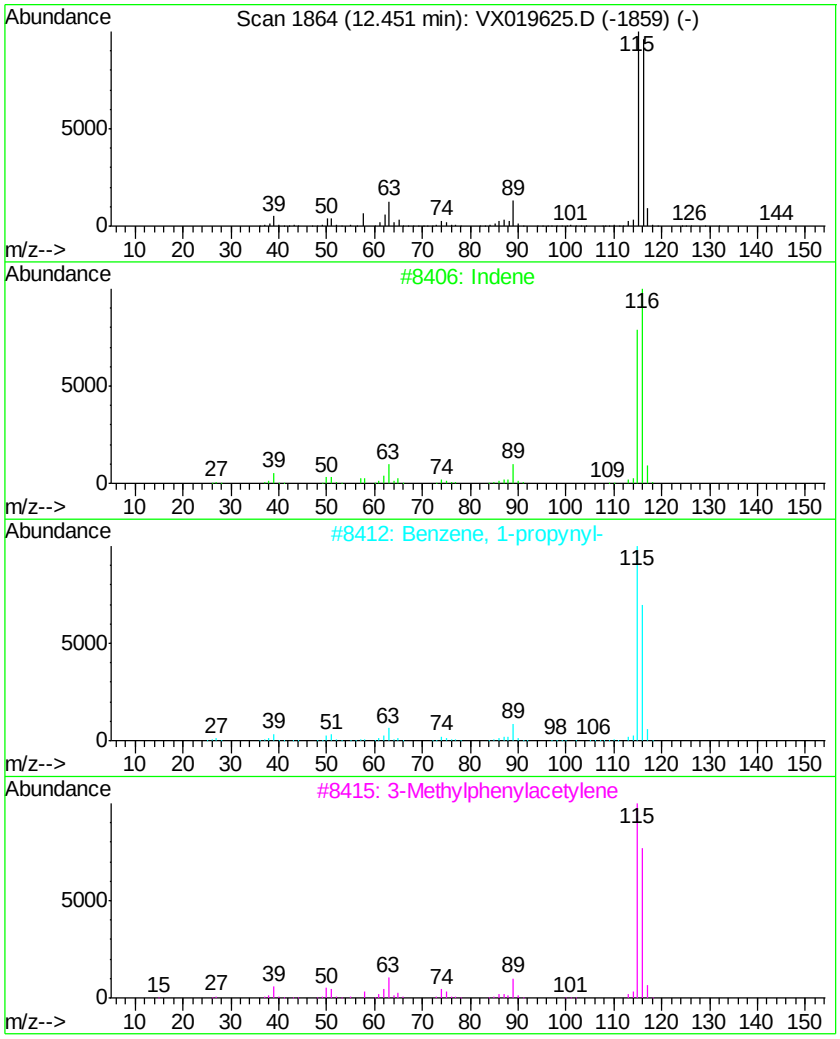
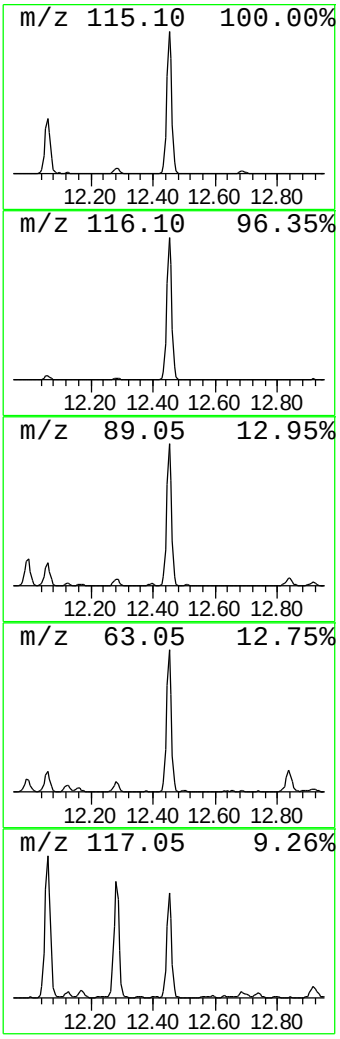
Peak Number 8 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	37.43 ug/l	904045	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	86





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ALS Vial : 35 Sample Multiplier: 1

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Quant Title : SW846 8260

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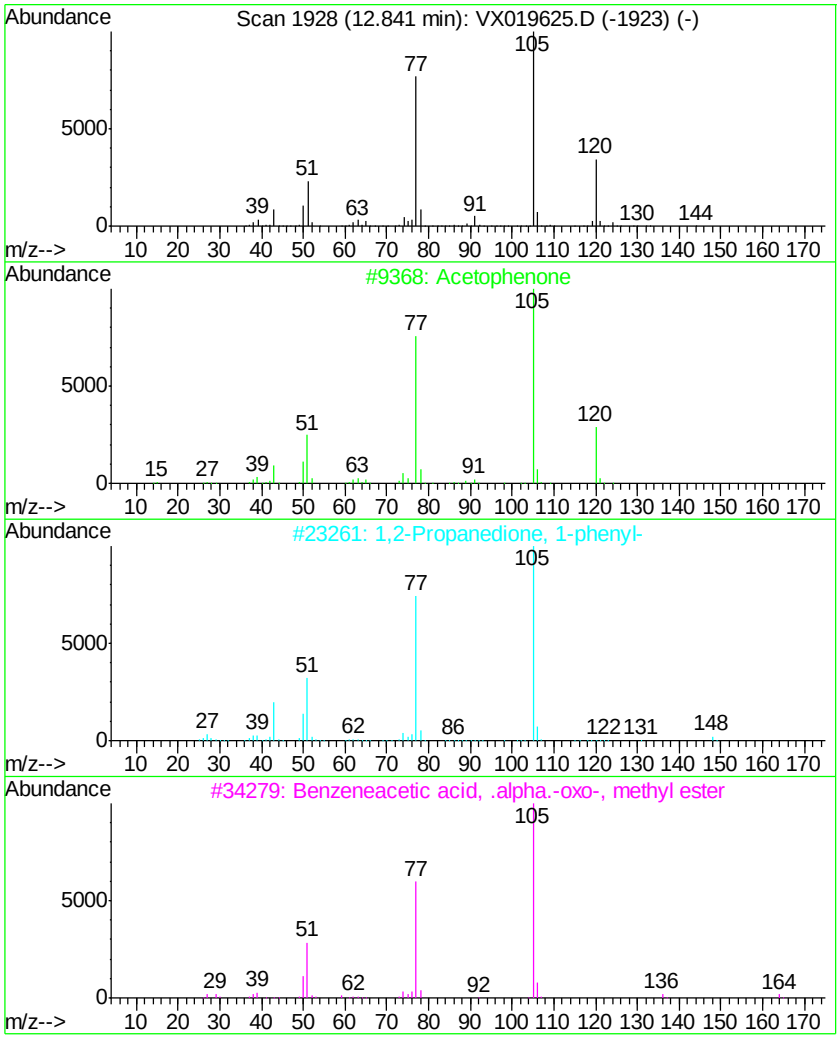
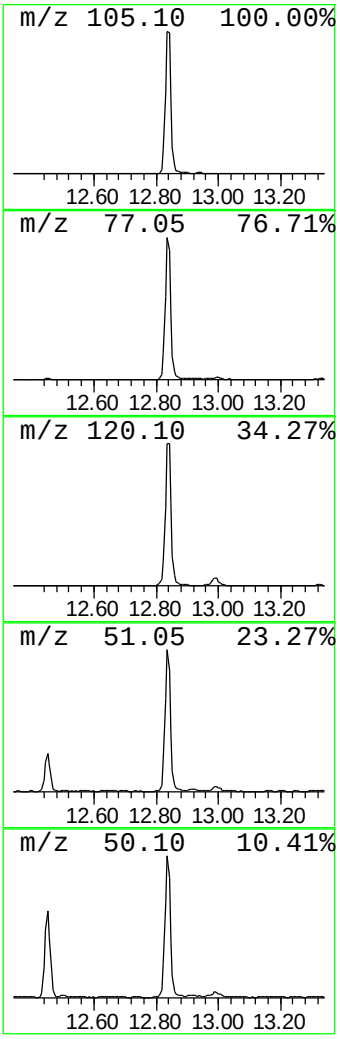
Peak Number 9 Acetophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	24.09 ug/l	581888	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	95
2	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	72
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	72
4	Benzoylformic acid	150	C8H6O3	000611-73-4	72
5	Phenylglyoxal	134	C8H6O2	001074-12-0	72





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ClientSampleId : 16846-41629

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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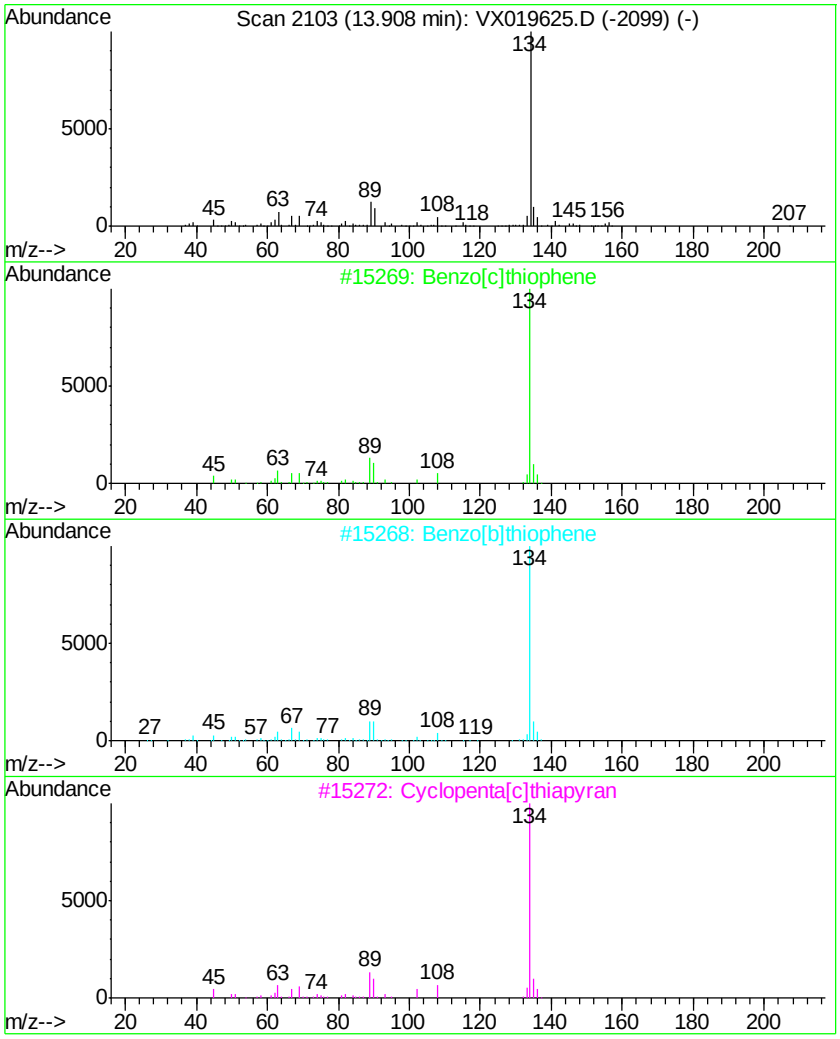
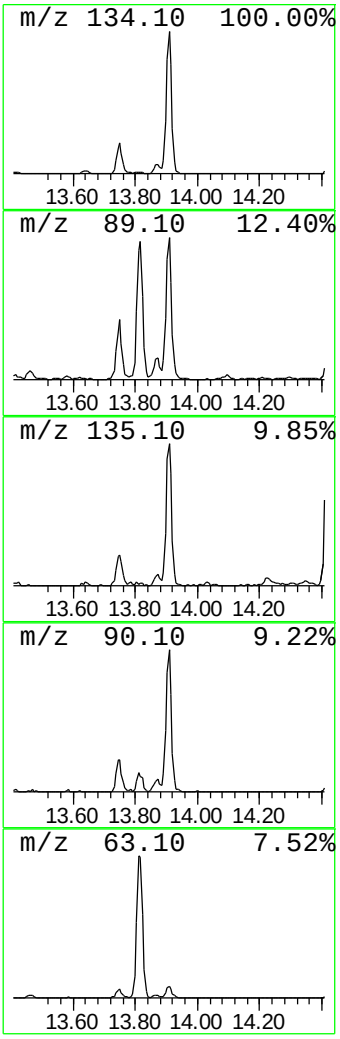
Peak Number 10 Benzo[c]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	9.66 ug/l	233442	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	56
5	Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112420\
Data File : VX019625.D
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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
Acetaldehyde	1.47	1032.3	ug/l	18092000	1	5.62	876275	50.0
Ethanol	2.13	241.7	ug/l	4236130	1	5.62	876275	50.0
Thiophene, 2,5-di...	9.48	19.9	ug/l	519919	3	10.10	1308370	50.0
Thiophene, tetrah...	9.53	57.5	ug/l	1505480	3	10.10	1308370	50.0
Thiophene, tetrah...	10.45	9.6	ug/l	251539	3	10.10	1308370	50.0
Thiophene, 2,3-di...	10.91	12.7	ug/l	332686	3	10.10	1308370	50.0
Indene	12.45	37.4	ug/l	904045	4	12.06	1207740	50.0
Acetophenone	12.84	24.1	ug/l	581888	4	12.06	1207740	50.0
Benzo[c]thiophene	13.91	9.7	ug/l	233442	4	12.06	1207740	50.0