LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

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\82X090122W.M
Title : SW846 8260

Signal : TIC: VX031132.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	72	rBV	502945	576177	13.47%	2.966%
2	2.111	156	168	194	rBV	1322728	4278829	100.00%	22.025%
3	2.385	206	213	228	rVB	787001	1301732	30.42%	6.701%
4	2.562	234	242	255	rBV	79339	211675	4.95%	1.090%
5	2.977	298	310	321	rBV2	33199	87062	2.03%	0.448%
6	4.007	472	479	490	rVB2	18761	47279	1.10%	0.243%
7	4.233	503	516	530	rBV2	84164	248116	5.80%	1.277%
8	4.562	561	570	584	rBV	193166	551911	12.90%	2.841%
9	4.720	585	596	608	rVB3	55689	172055	4.02%	0.886%
10	5.031	634	647	663	rBV2	15507	62650	1.46%	0.322%
11	5.391	695	706	721	rBV2	139992	409746	9.58%	2.109%
12	5.556	721	733	745	rBV2	214445	616863	14.42%	3.175%
13	5.958	789	799	810	rBV	132662	352816	8.25%	1.816%
14	6.641	897	911	921	rBV	28852	82693	1.93%	0.426%
15	6.769	921	932	944	rBV	311981	771405	18.03%	3.971%
16	7.458	1038	1045	1058	rVB	243726	474076	11.08%	2.440%
17	7.641	1070	1075	1082	rVB	30107	48963	1.14%	0.252%
18	8.579	1221	1229	1234	rBV	46698	75718	1.77%	0.390%
19	8.653	1234	1241	1247	rBV	718808	1096703	25.63%	5.645%
20	8.720	1247	1252	1258	rVV3	21574	45987	1.07%	0.237%
21	8.805	1258	1266	1275	rVB6	17917	50274	1.17%	0.259%
22	9.311	1342	1349	1353	rBV	40426	54977	1.28%	0.283%
23	9.433	1364	1369	1375	rBV	149950	200247	4.68%	1.031%
24	10.055	1458	1471	1485	rBV	634938	881031	20.59%	4.535%
25	10.390	1519	1526	1529	rBV	42228	61935	1.45%	0.319%
26	10.506	1541	1545	1555	rVB	35774	46513	1.09%	0.239%
27	10.683	1569	1574	1581	rVB	242047	295581	6.91%	1.521%
28	10.768	1581	1588	1594	rBV	259941	324800	7.59%	1.672%
29	10.884	1600	1607	1614	rVB5	17804	43950	1.03%	0.226%
30	11.085	1634	1640	1645	rVV	571370	757501	17.70%	3.899%
31	11.359	1681	1685	1690	rVV	88580	111267	2.60%	0.573%
32	11.475	1700	1704	1713	rVB	275500	336023	7.85%	1.730%
33	11.561	1714	1718	1722	rBV2	40044	64121	1.50%	0.330%
34	11.603	1722	1725	1732	rVV3	41438	73896	1.73%	0.380%
35	11.841	1760	1764	1768	rVV	85563	111828	2.61%	0.576%
36	11.902	1770	1774	1782	rVV7	22233	56794	1.33%	0.292%

LSC Area Percent Report

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

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\82X090122W.M
Title : SW846 8260

37	11.987	1782	1788	1790	rVV2	37480	61668	1.44%	0.317%
38	12.024	1790	1794	1801	rVB	682451	825901	19.30%	4.251%
39	12.219	1822	1826	1850	rBV	1626072	2459340	57.48%	12.659%
40	12.420	1854	1859	1862	rVV2	66972	121808	2.85%	0.627%
41	12.457	1862	1865	1870	rVV4	32739	65797	1.54%	0.339%
42	12.518	1871	1875	1878	rVV	59768	78447	1.83%	0.404%
43	12.768	1912	1916	1919	rBV2	38791	50910	1.19%	0.262%
44	13.164	1970	1981	1990	rBV8	36060	92288	2.16%	0.475%
45	13.280	1995	2000	2009	rVB6	23187	45395	1.06%	0.234%
46	13.658	2058	2062	2067	rBV	31769	43688	1.02%	0.225%
47	13.895	2094	2101	2111	rVB2	44587	127108	2.97%	0.654%
48	14.328	2167	2172	2175	rBV	63311	97787	2.29%	0.503%
49	14.530	2200	2205	2208	rBV	78808	117266	2.74%	0.604%
50	14.566	2208	2211	2218	rVB	94759	146772	3.43%	0.756%
51	14.956	2272	2275	2279	rVV2	31416	49882	1.17%	0.257%
52	15.145	2301	2306	2311	rBV4	28303	59767	1.40%	0.308%

Sum of corrected areas: 19427018

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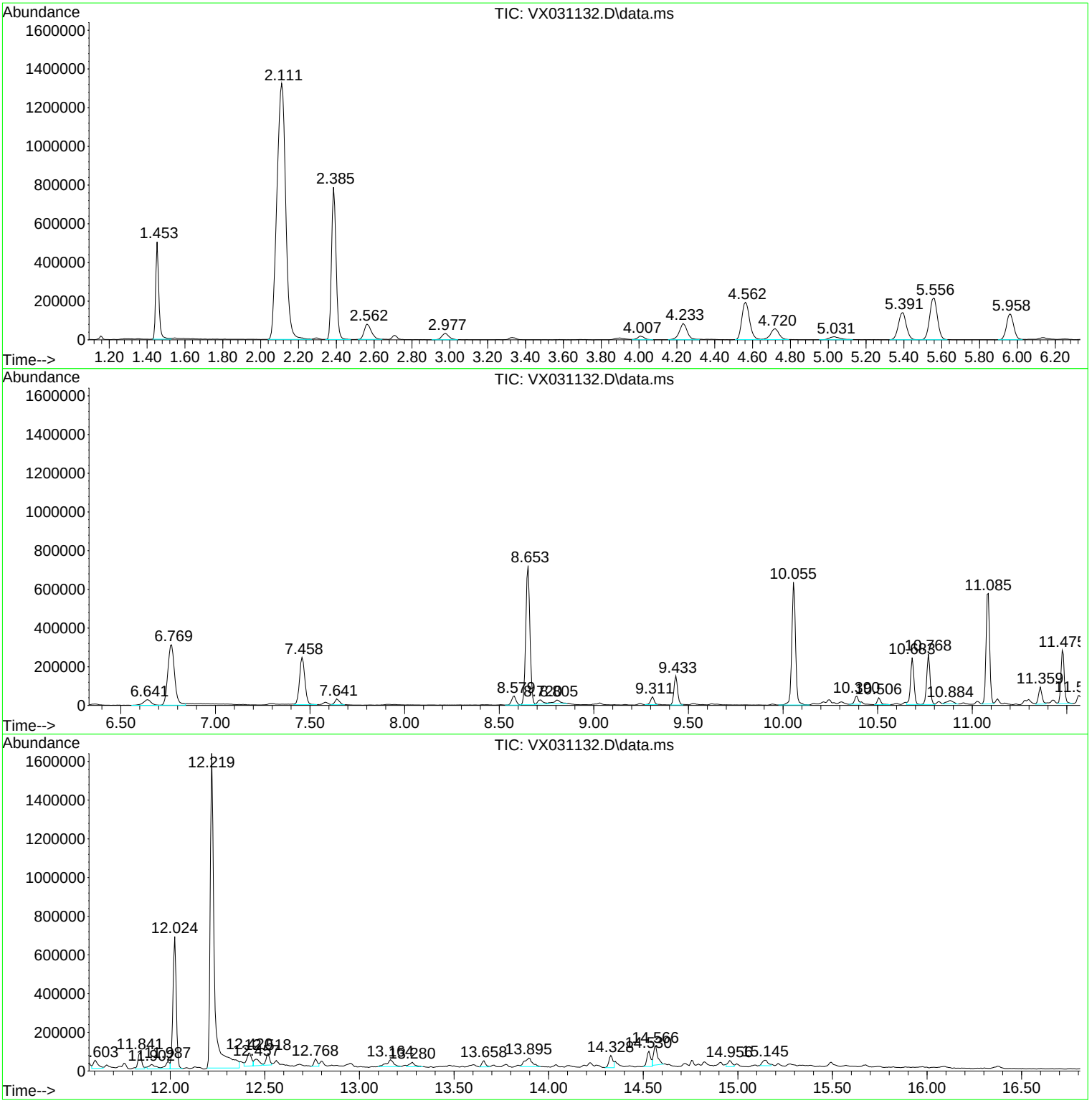
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

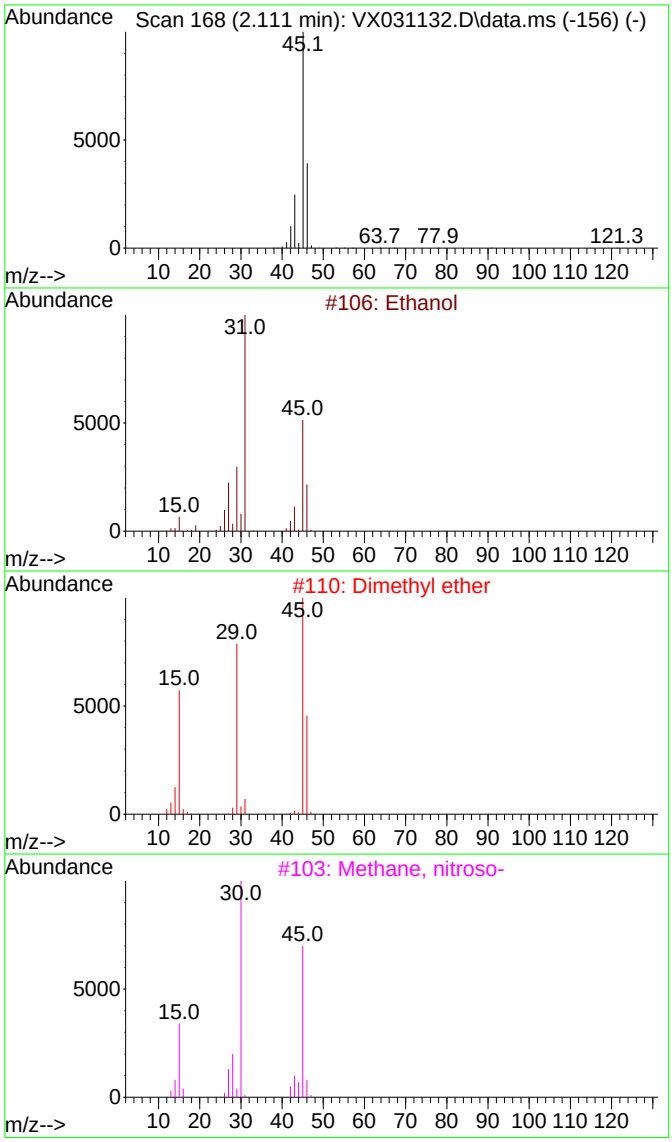
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

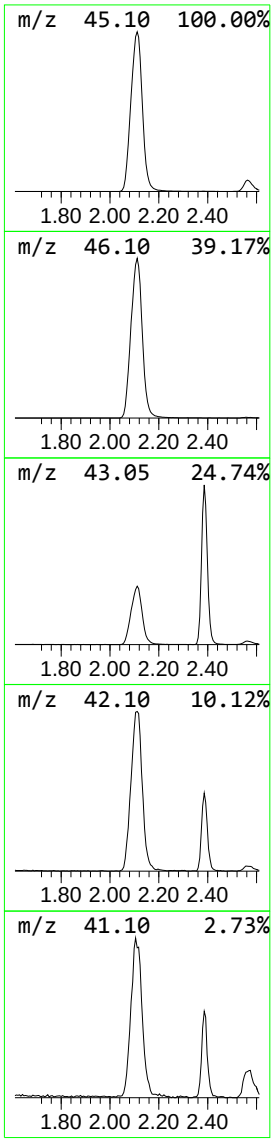
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.111	346.82 ug/l	4278830	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
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\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

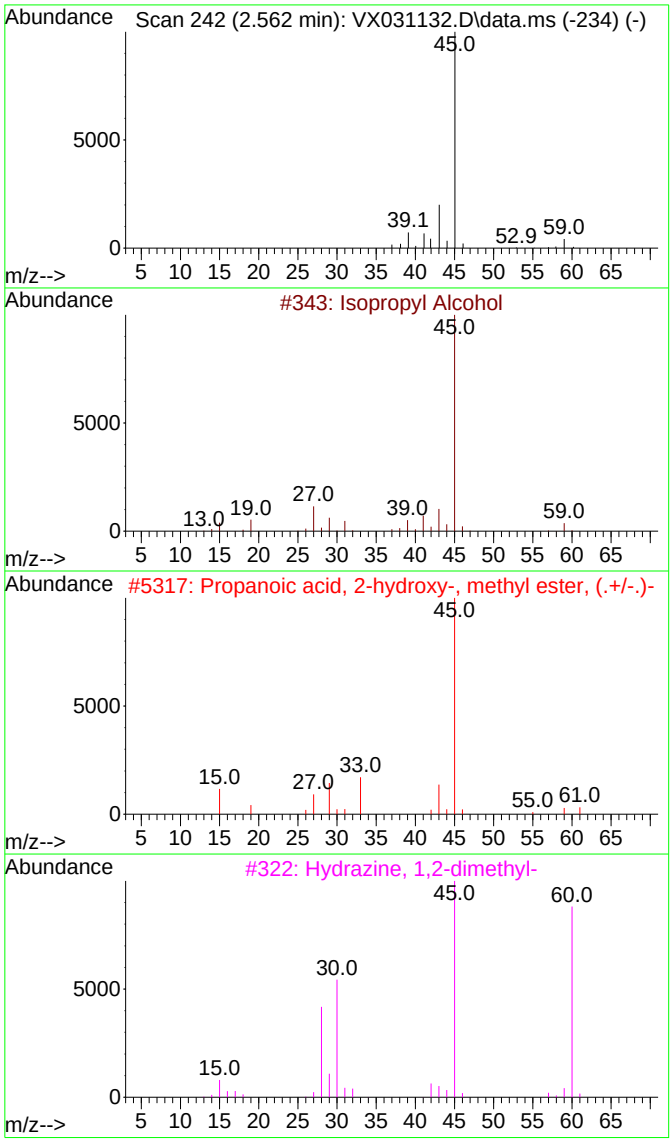
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

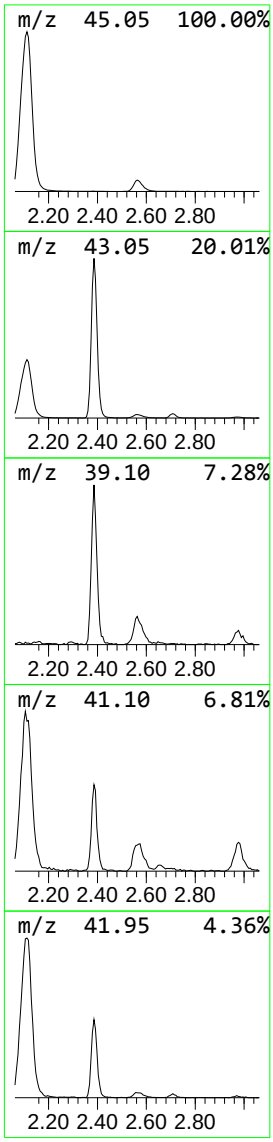
****

Peak Number 3 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.562	17.16 ug/l	211675	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Formamide	45	CH3NO	000075-12-7	5
5	2-Butanol	74	C4H10O	000078-92-2	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

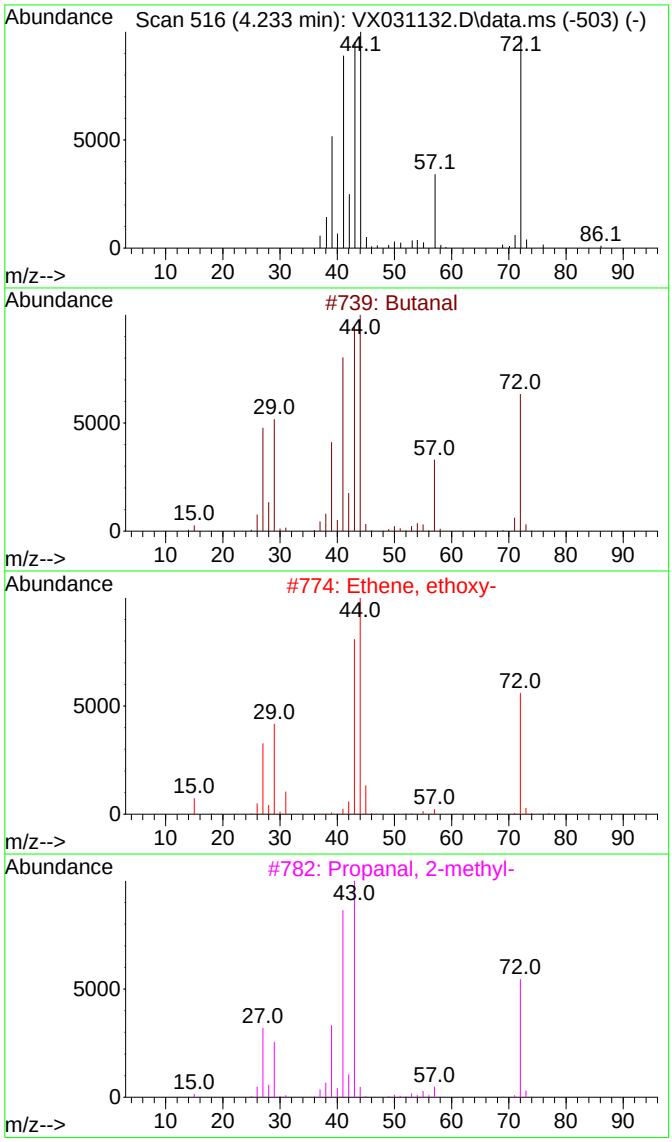
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

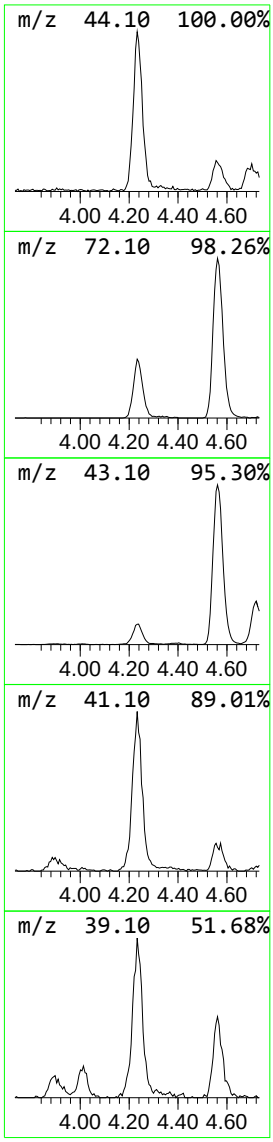
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	20.11 ug/l	248116	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	64
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

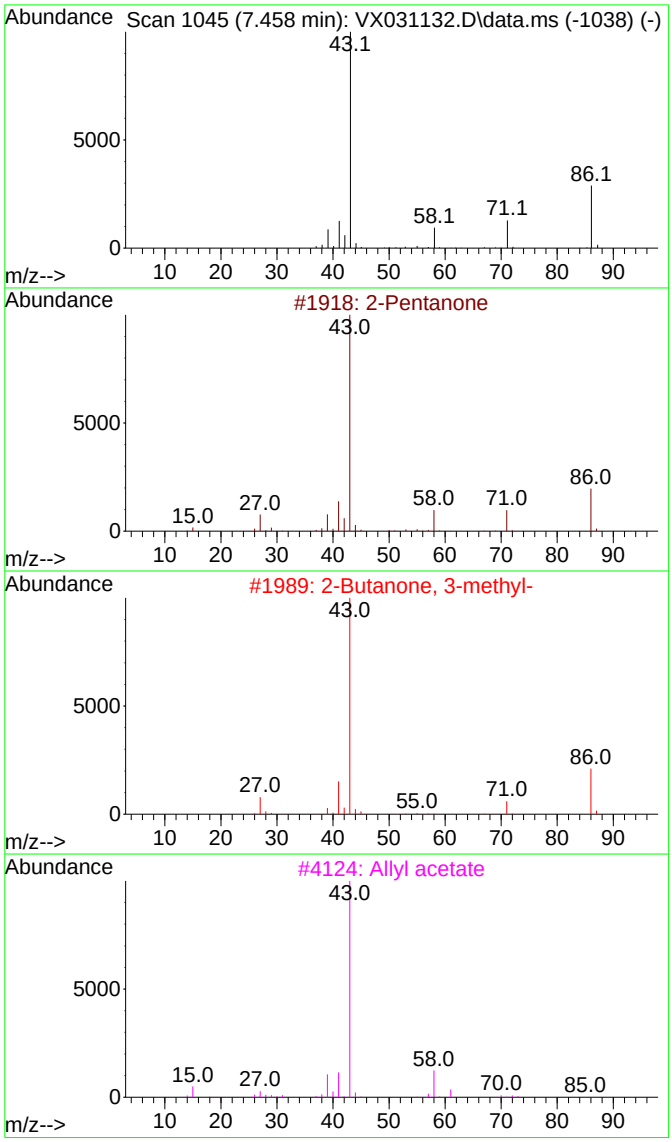
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

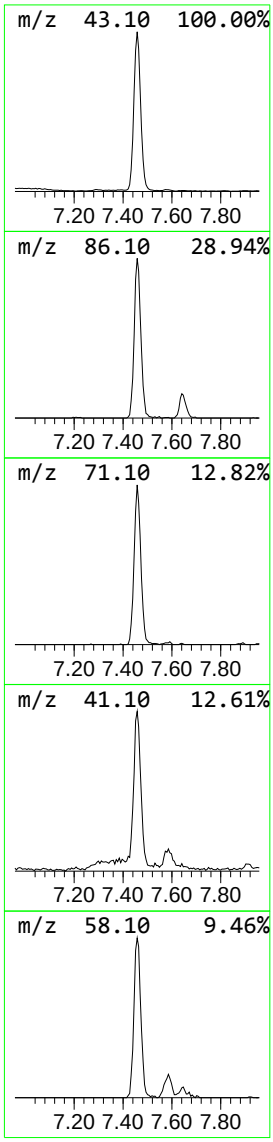
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	30.73 ug/l	474076	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	Allyl acetate	100	C5H8O2	000591-87-7	9
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

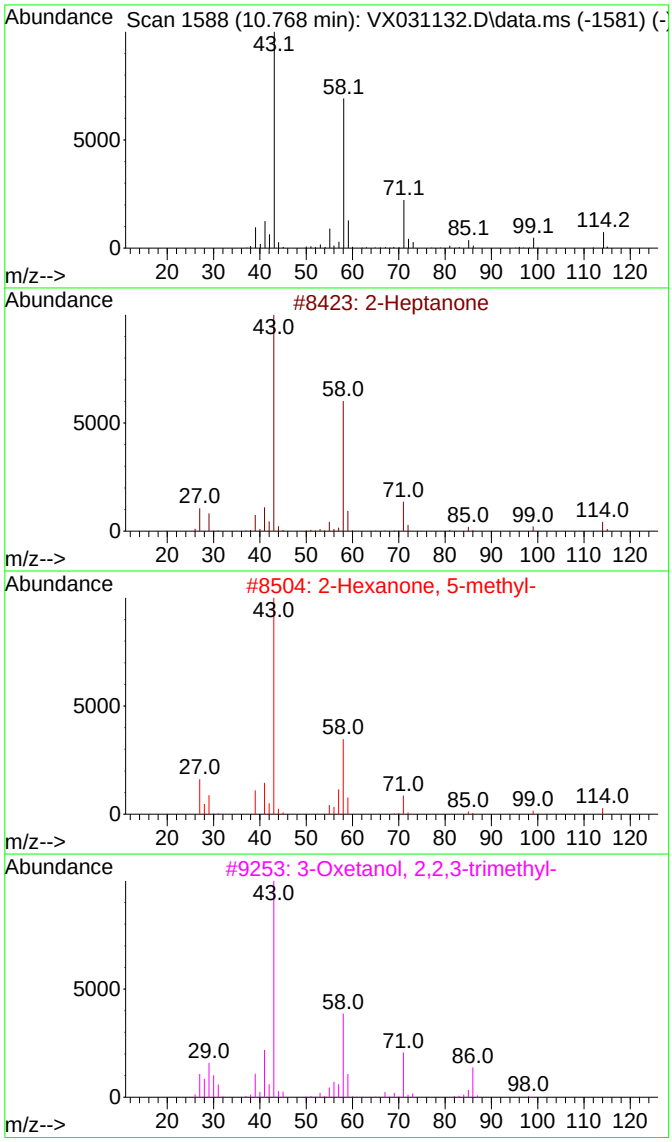
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

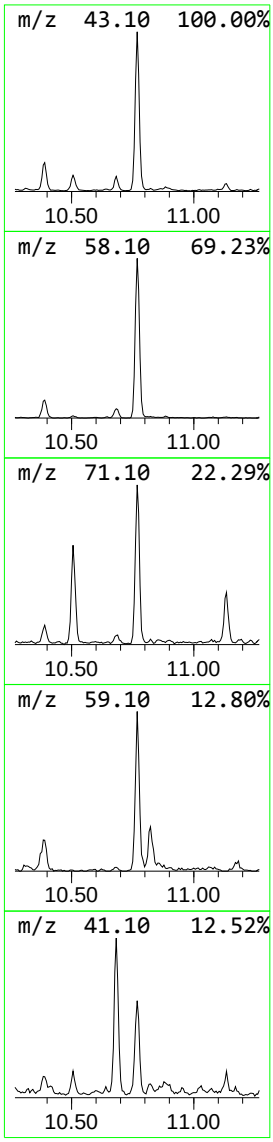
****

Peak Number 6 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	18.43 ug/l	324800	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86
3	3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	025910-96-7	56
4	Butane, 2-(ethenyloxy)-2-methyl-	114	C7H14O	029281-39-8	38
5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
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Operator : JC/MD
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

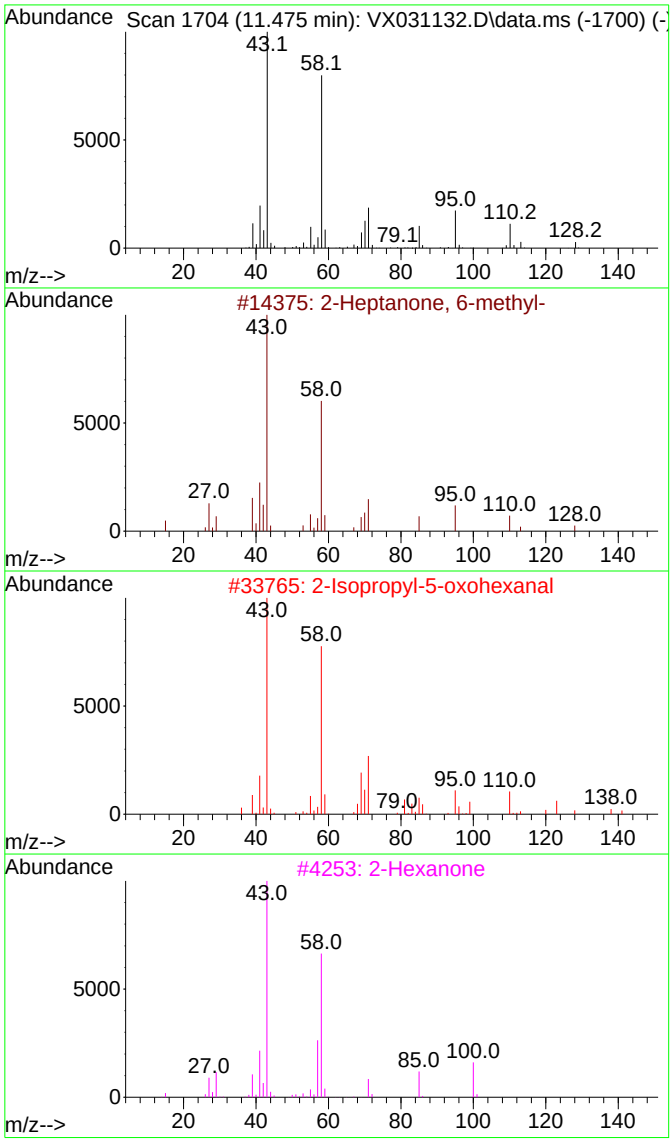
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

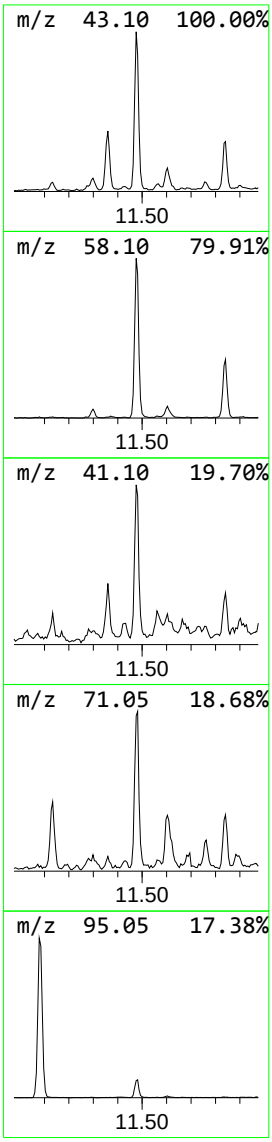
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Heptanone, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	20.34 ug/l	336023	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2	2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	64
3	2-Hexanone	100	C6H12O	000591-78-6	59
4	2-Octanone	128	C8H16O	000111-13-7	59
5	Butanimidamide	86	C4H10N2	000107-90-4	45





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

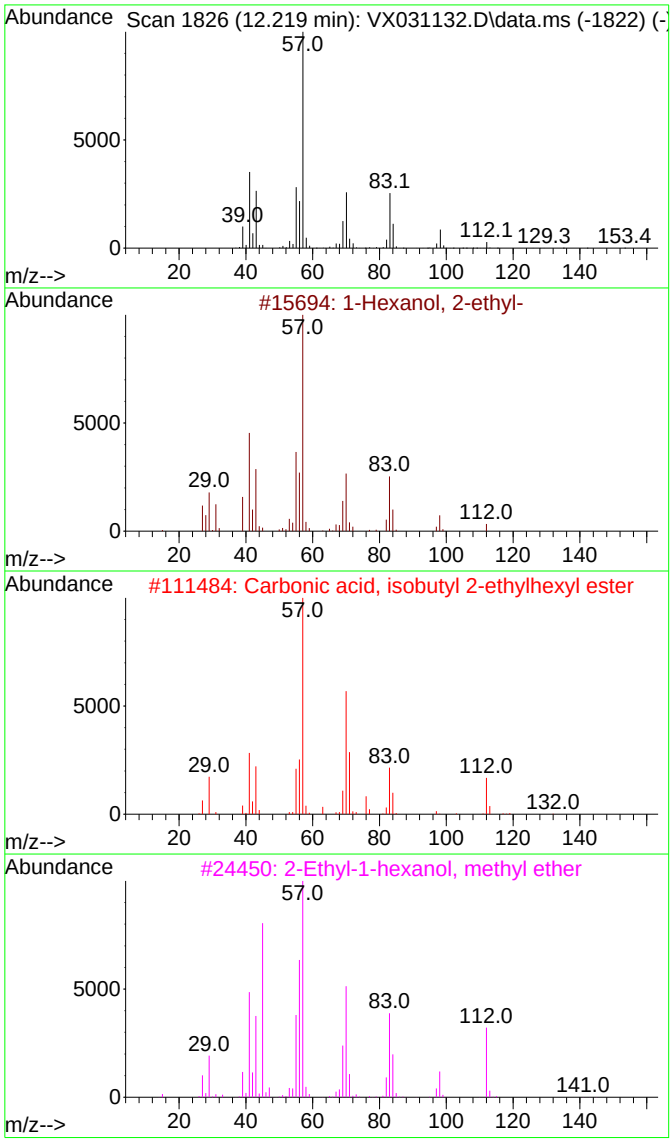
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

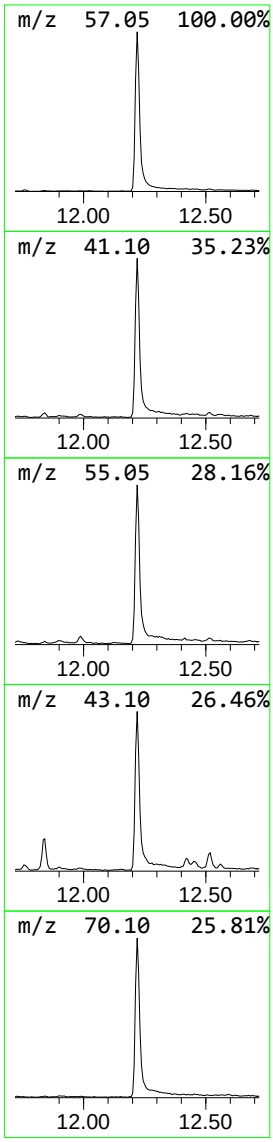
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	148.89 ug/l	2459340	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50





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Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

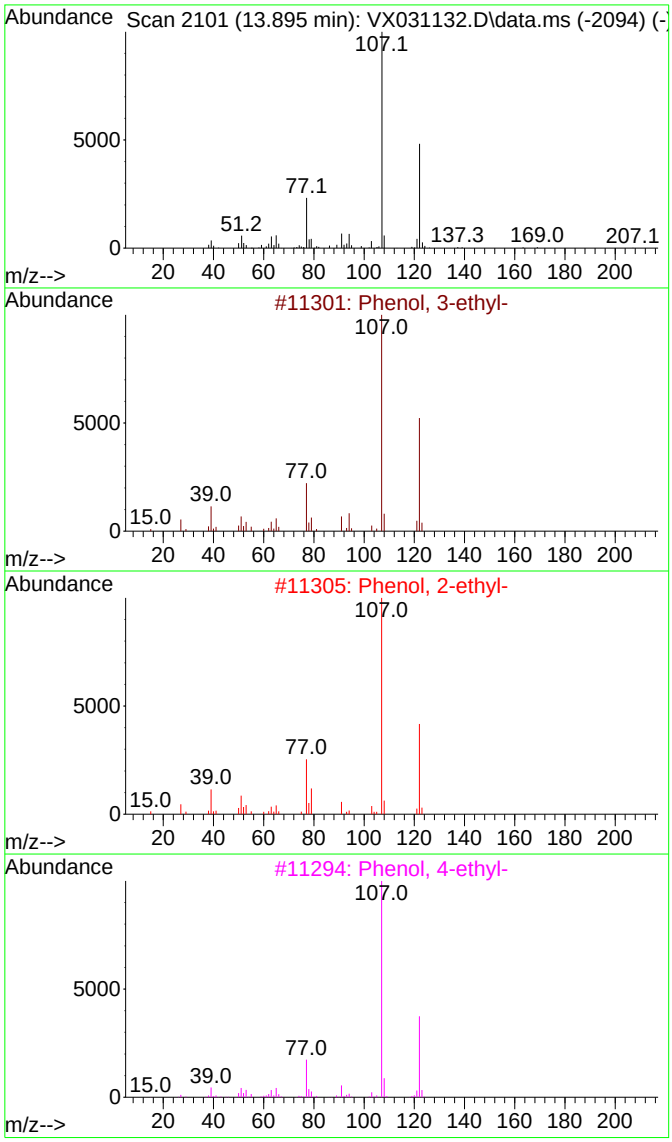
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

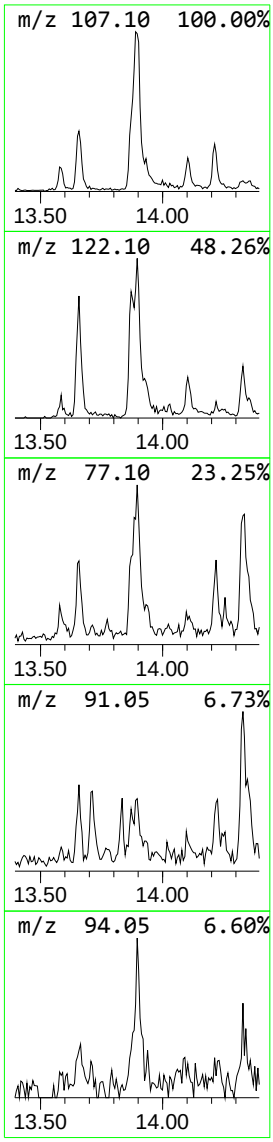
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	7.70 ug/l	127108	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	93
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	90
4	1,3-Cyclopentadiene, 5,5-dimethy...	122	C9H14	1000162-25-6	78
5	Furan, 2-(1-pentenyl)-, (E)-	136	C9H12O	020992-69-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

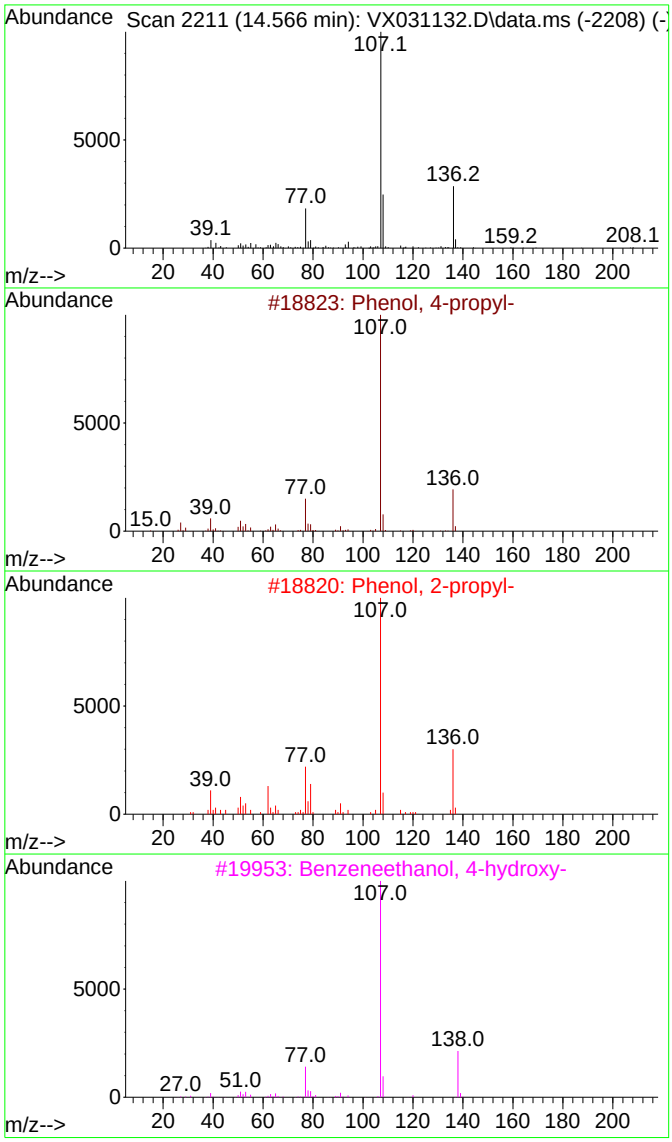
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

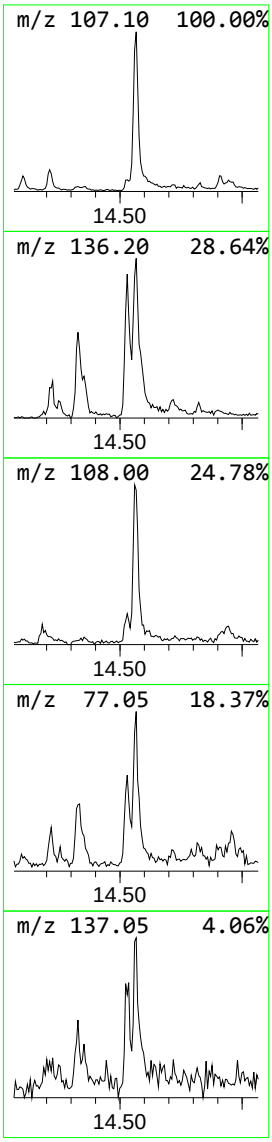
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.566	8.89 ug/l	146772	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-propyl-	136	C9H12O	000645-56-7	72
2	Phenol, 2-propyl-	136	C9H12O	000644-35-9	72
3	Benzeneethanol, 4-hydroxy-	138	C8H10O2	000501-94-0	50
4	1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-1	43
5	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031132.D
Acq On : 06 Sep 2022 16:49
Operator : JC/MD
Sample : N4489-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-0068

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	2.111	346.8	ug/l	4278830	1	5.562	616863	50.0
Isopropyl Alcohol	2.562	17.2	ug/l	211675	1	5.562	616863	50.0
Butanal	4.233	20.1	ug/l	248116	1	5.562	616863	50.0
2-Pentanone	7.458	30.7	ug/l	474076	2	6.769	771405	50.0
2-Heptanone	10.768	18.4	ug/l	324800	3	10.055	881031	50.0
2-Heptanone, 6-...	11.475	20.3	ug/l	336023	4	12.024	825901	50.0
1-Hexanol, 2-et...	12.219	148.9	ug/l	2459340	4	12.024	825901	50.0
Phenol, 3-ethyl-	13.896	7.7	ug/l	127108	4	12.024	825901	50.0
Phenol, 4-propyl-	14.566	8.9	ug/l	146772	4	12.024	825901	50.0