LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

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\82X101922W.M
Title : SW846 8260

Signal : TIC: VX032270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	31	rBV	10666	9533	1.26%	0.161%
2	1.367	42	46	50	rVB	34679	34590	4.57%	0.585%
3	1.416	50	54	59	rBV	33423	36608	4.84%	0.619%
4	1.752	104	109	117	rVB	49413	67243	8.89%	1.137%
5	2.343	197	206	224	rVB	93236	184705	24.41%	3.122%
6	2.782	267	278	287	rBV	174040	374755	49.52%	6.335%
7	2.867	287	292	300	rVB2	10570	21651	2.86%	0.366%
8	3.111	323	332	345	rVB3	20062	49593	6.55%	0.838%
9	4.215	502	513	522	rBV	27952	81728	10.80%	1.382%
10	4.306	522	528	537	rVB2	6780	17941	2.37%	0.303%
11	4.446	537	551	563	rBV6	5065	20662	2.73%	0.349%
12	5.123	648	662	663	rBV	4890	9998	1.32%	0.169%
13	5.385	692	705	716	rBV3	86715	255598	33.78%	4.321%
14	5.550	722	732	740	rBV	166605	474983	62.77%	8.029%
15	5.623	740	744	758	rVB2	44052	119189	15.75%	2.015%
16	5.848	772	781	789	rBV3	3743	10518	1.39%	0.178%
17	5.958	789	799	808	rVV	95699	258434	34.15%	4.369%
18	6.043	808	813	826	rVB	8180	22384	2.96%	0.378%
19	6.190	826	837	838	rBV3	3995	8715	1.15%	0.147%
20	6.251	838	847	859	rVB2	40642	120391	15.91%	2.035%
21	6.763	916	931	946	rBV	237235	560319	74.05%	9.472%
22	7.372	1023	1031	1038	rVB4	5465	13740	1.82%	0.232%
23	7.988	1122	1132	1139	rBV	20474	40942	5.41%	0.692%
24	8.110	1144	1152	1162	rBV2	40748	88036	11.63%	1.488%
25	8.513	1211	1218	1225	rVB4	5445	11414	1.51%	0.193%
26	8.647	1229	1240	1249	rBV	472662	756710	100.00%	12.792%
27	9.159	1320	1324	1332	rVB	6851	10569	1.40%	0.179%
28	10.055	1460	1471	1478	rBV	487373	646903	85.49%	10.935%
29	10.195	1490	1494	1500	rVV	46178	58972	7.79%	0.997%
30	10.963	1613	1620	1625	rVB2	5999	7586	1.00%	0.128%
31	11.079	1634	1639	1646	rBV	387932	510929	67.52%	8.637%
32	11.305	1673	1676	1685	rVB	5945	8568	1.13%	0.145%
33	11.866	1764	1768	1776	rVB2	5853	7733	1.02%	0.131%
34	12.024	1788	1794	1802	rBV	500128	610882	80.73%	10.327%
35	12.250	1825	1831	1837	rVV	122625	157717	20.84%	2.666%
36	12.317	1837	1842	1850	rVV	29364	36619	4.84%	0.619%

LSC Area Percent Report

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Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

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\82X101922W.M
Title : SW846 8260

37	12.408	1852	1857	1862	rVV	25804	32291	4.27%	0.546%
38	12.463	1862	1866	1874	rVB	17017	21694	2.87%	0.367%
39	12.713	1901	1907	1912	rBV3	11755	21275	2.81%	0.360%
40	12.920	1934	1941	1947	rVV	60635	72458	9.58%	1.225%
41	13.030	1953	1959	1965	rVB3	5314	7838	1.04%	0.132%
42	13.292	1995	2002	2007	rBV4	6285	9004	1.19%	0.152%
43	13.579	2046	2049	2053	rVB	7241	7780	1.03%	0.132%
44	13.640	2053	2059	2060	rVV2	9309	10843	1.43%	0.183%
45	13.664	2060	2063	2068	rVB	13861	17163	2.27%	0.290%
46	14.213	2149	2153	2158	rBV2	6192	8440	1.12%	0.143%

Sum of corrected areas: 5915644

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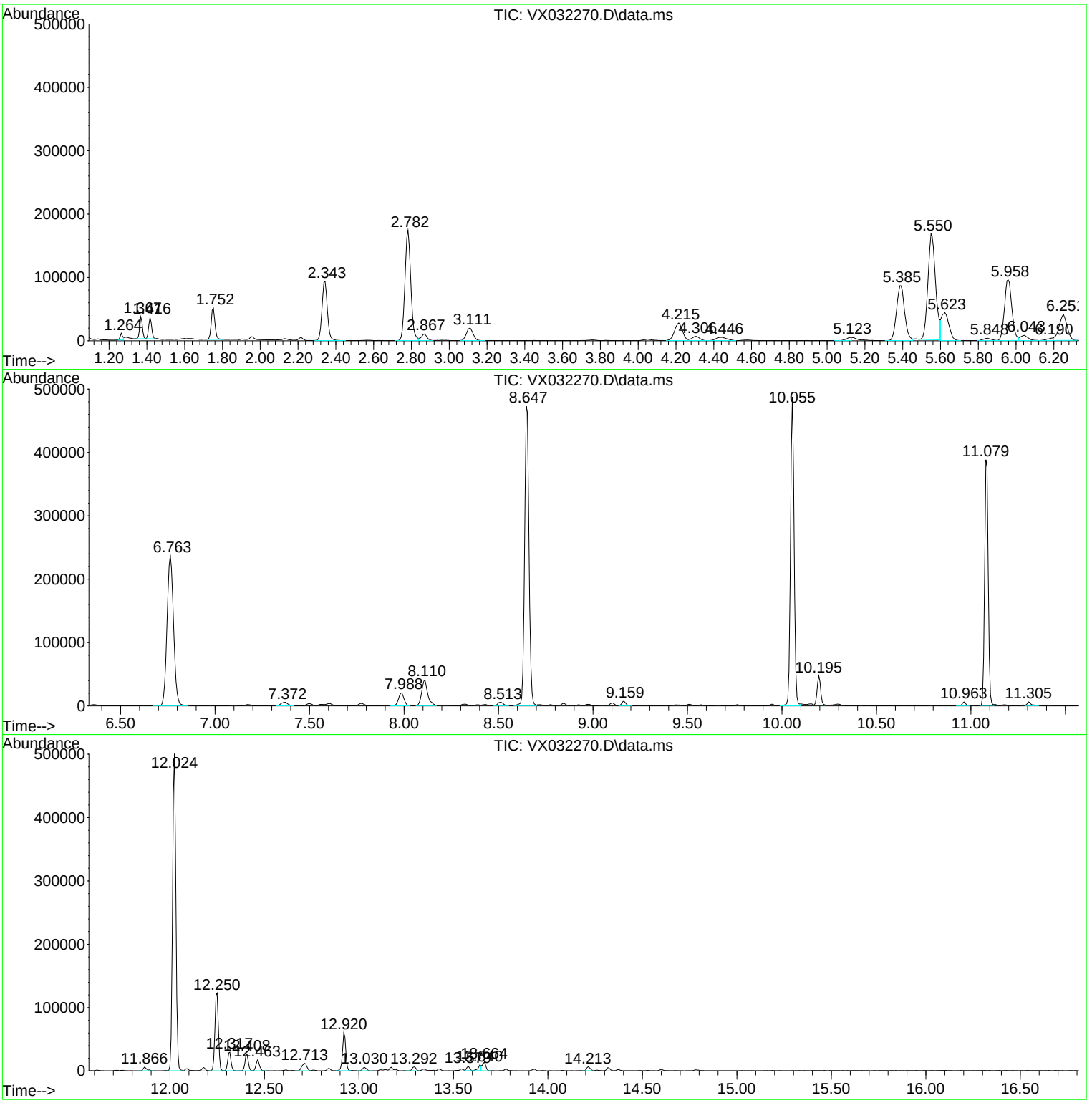
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

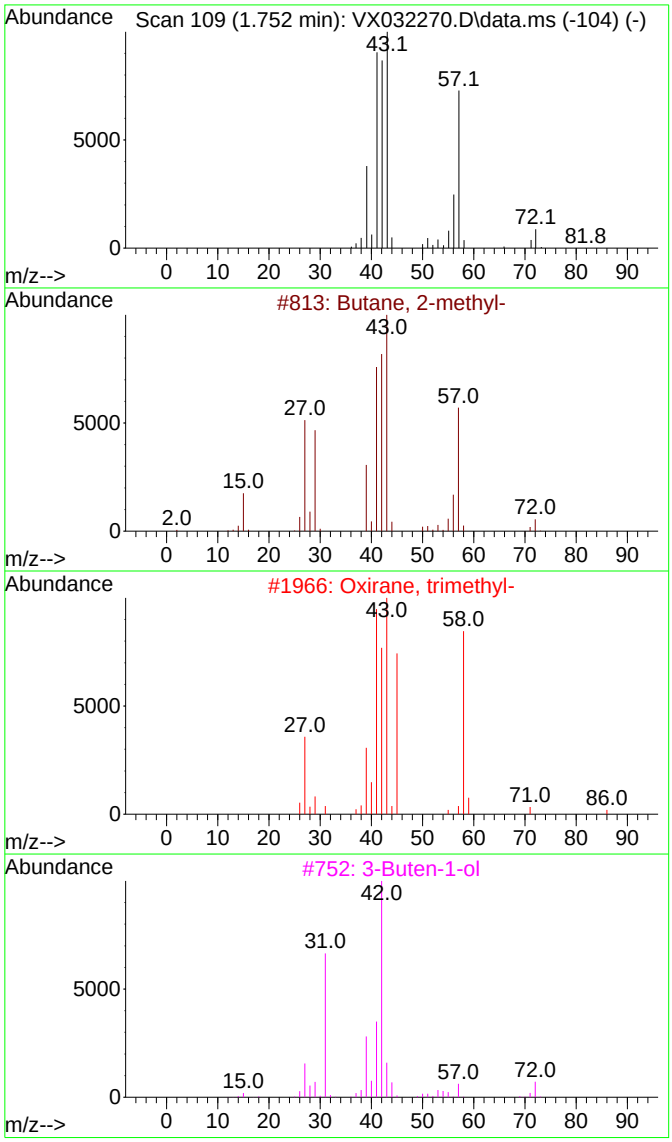
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

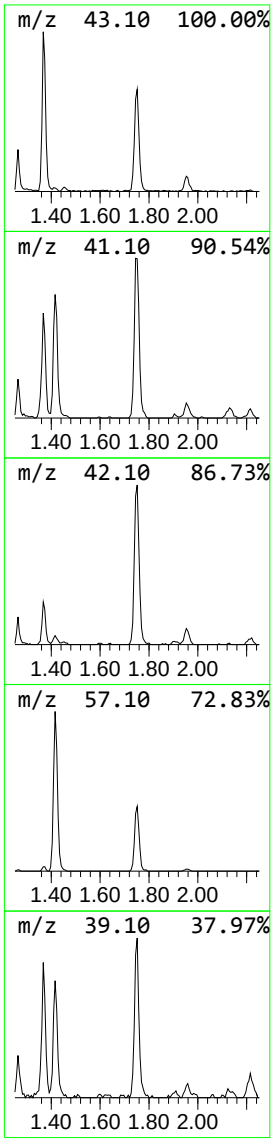
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	7.08 ug/l	67243	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	Pentane	72	C5H12	000109-66-0	36
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33





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Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

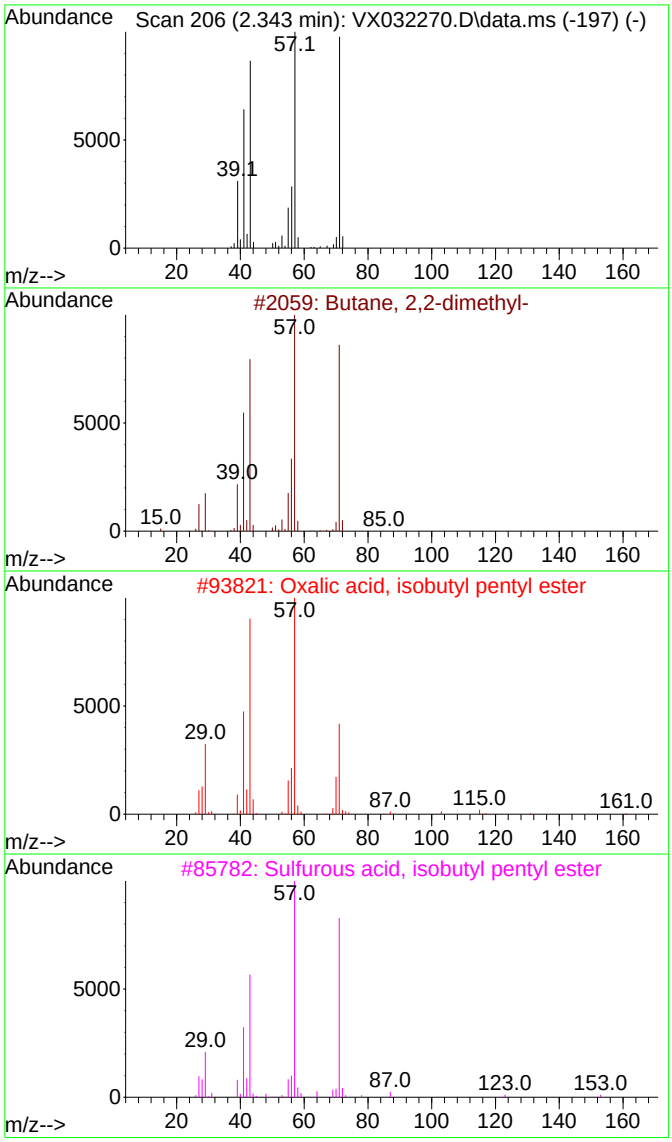
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

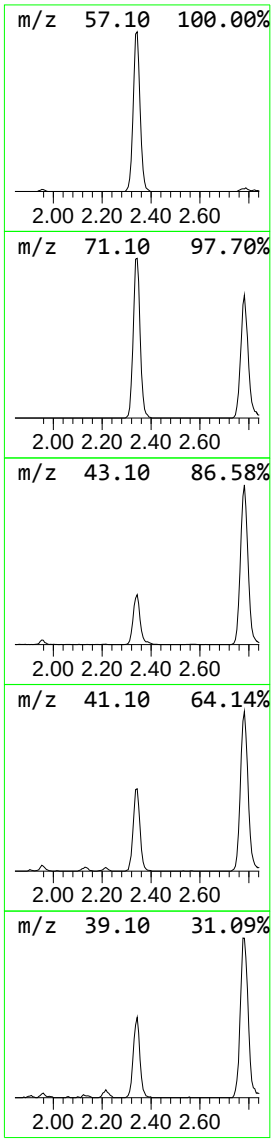
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.343	19.44 ug/l	184705	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	90
2	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	78
3	Sulfurous acid, isobutyl pentyl ...	208	C9H20O3S	1000309-13-8	50
4	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	50
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

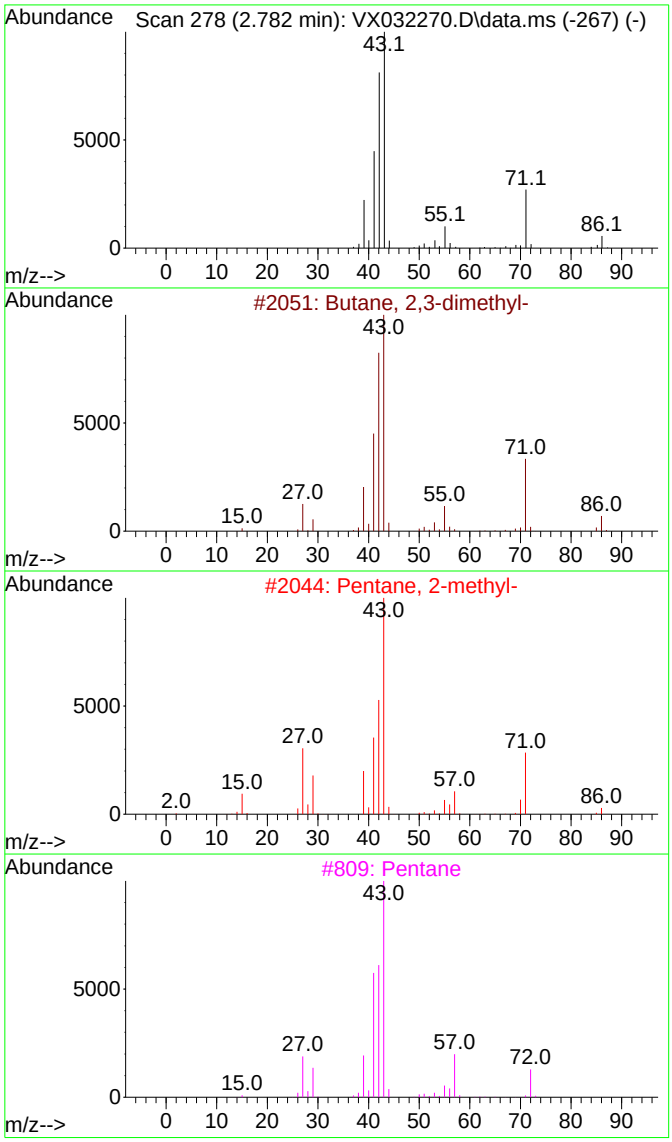
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

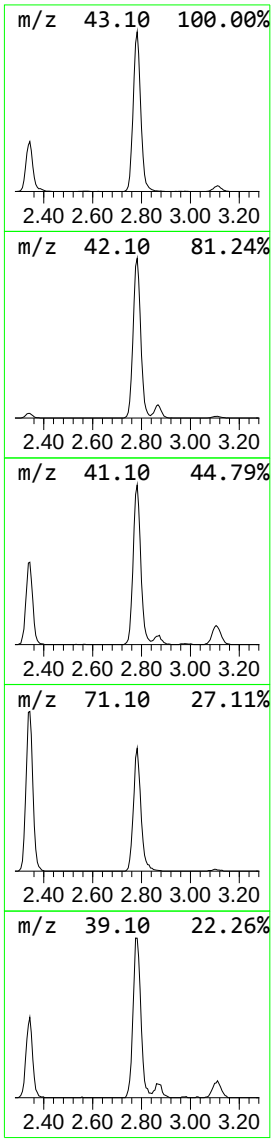
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	39.45 ug/l	374755	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pentane	72	C5H12	000109-66-0	36
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	33
5	1-Pentene	70	C5H10	000109-67-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
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Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

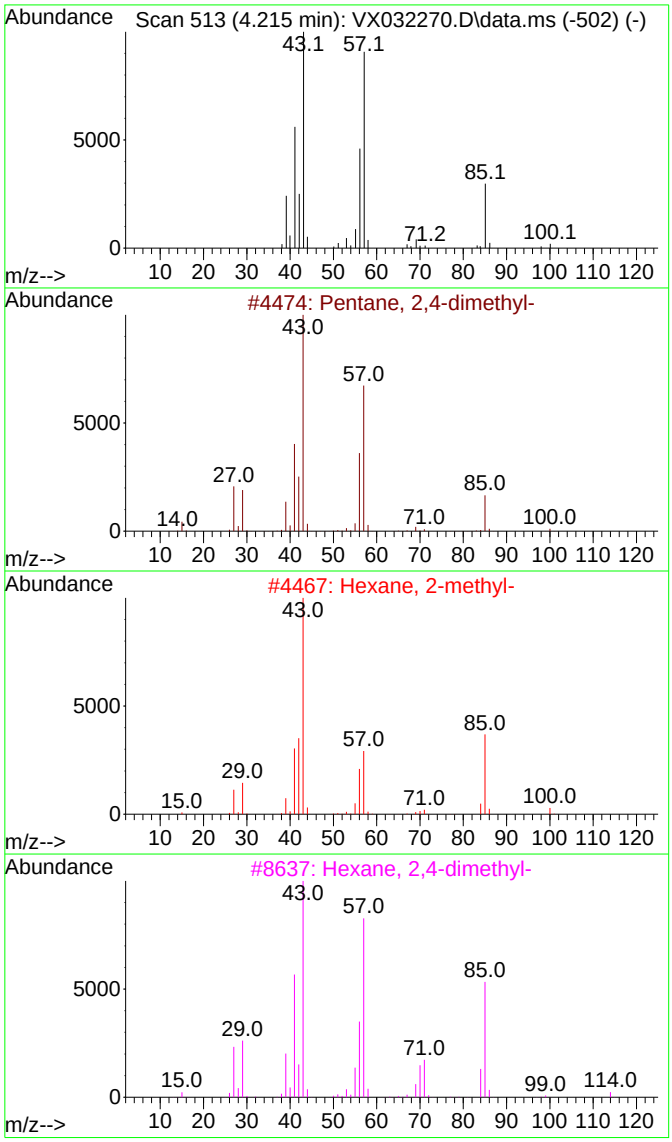
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

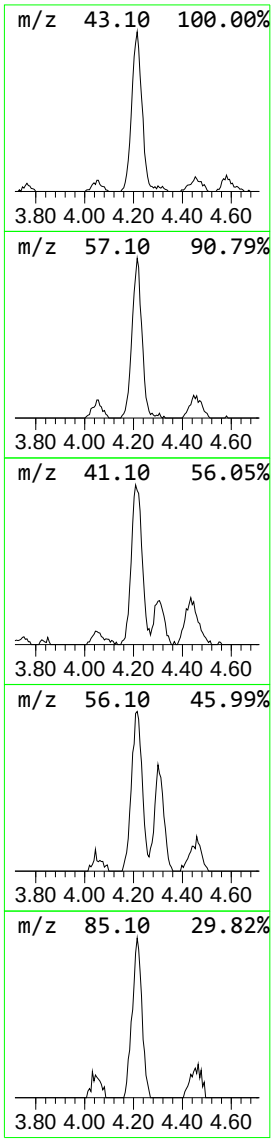
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.215	8.60 ug/l	81728	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
2	Hexane, 2-methyl-	100	C7H16	000591-76-4	72
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
5	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
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Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

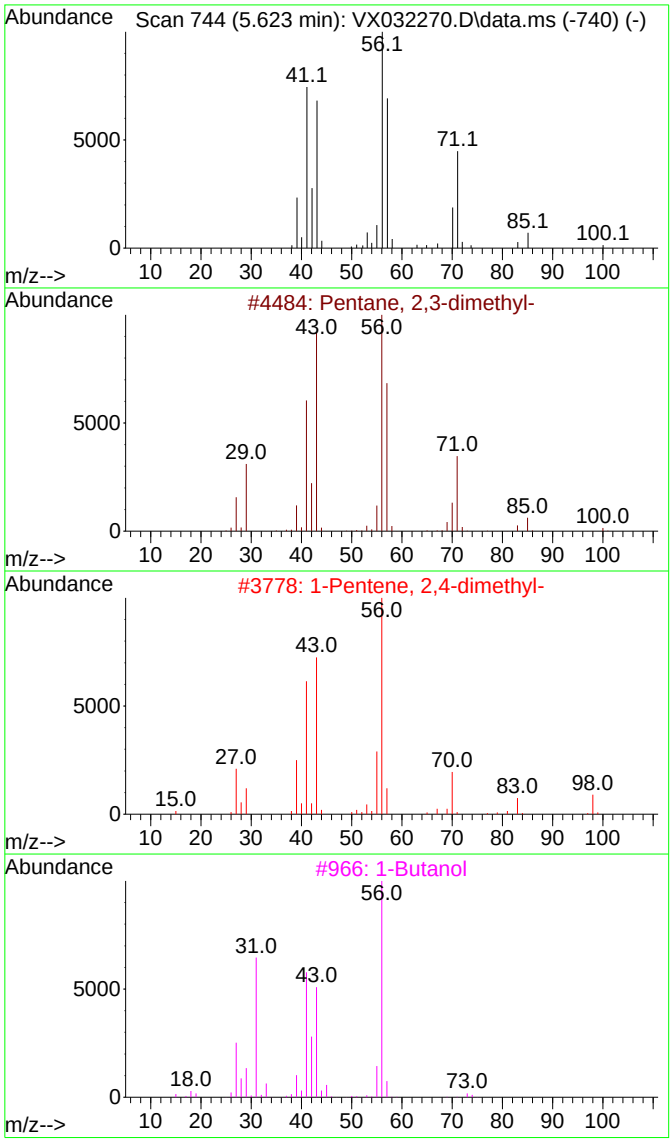
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

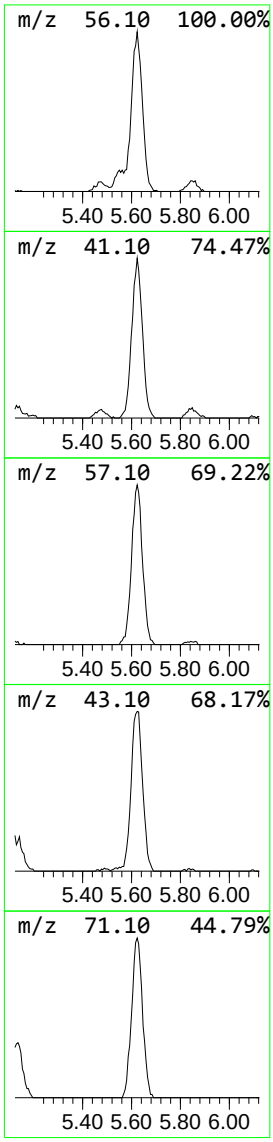
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.623	12.55 ug/l	119189	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	50
3	1-Butanol	74	C4H10O	000071-36-3	50
4	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	43





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Operator : JC/MD
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

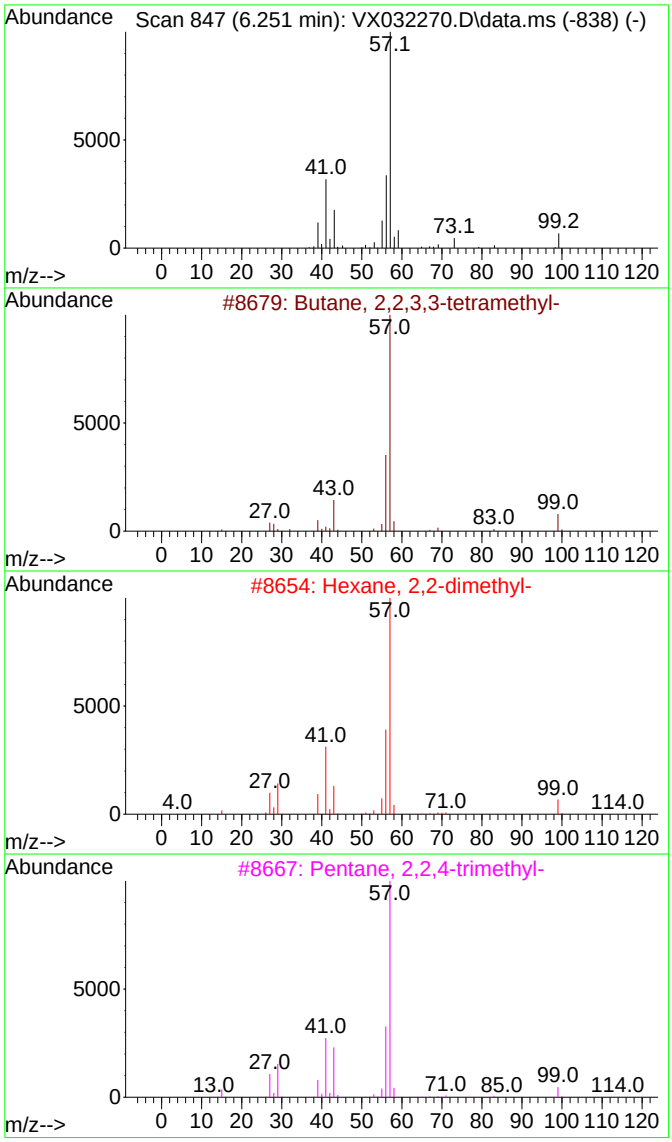
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

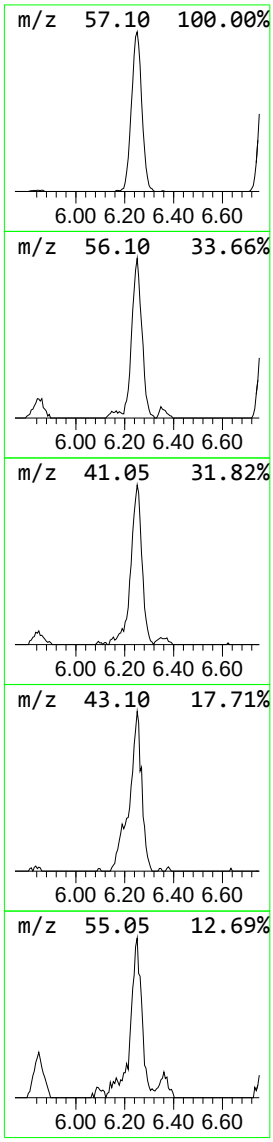
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	10.74 ug/l	120391	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
4	Carbonic acid, bis(2-methylpropy...	174	C9H18O3	000539-92-4	50
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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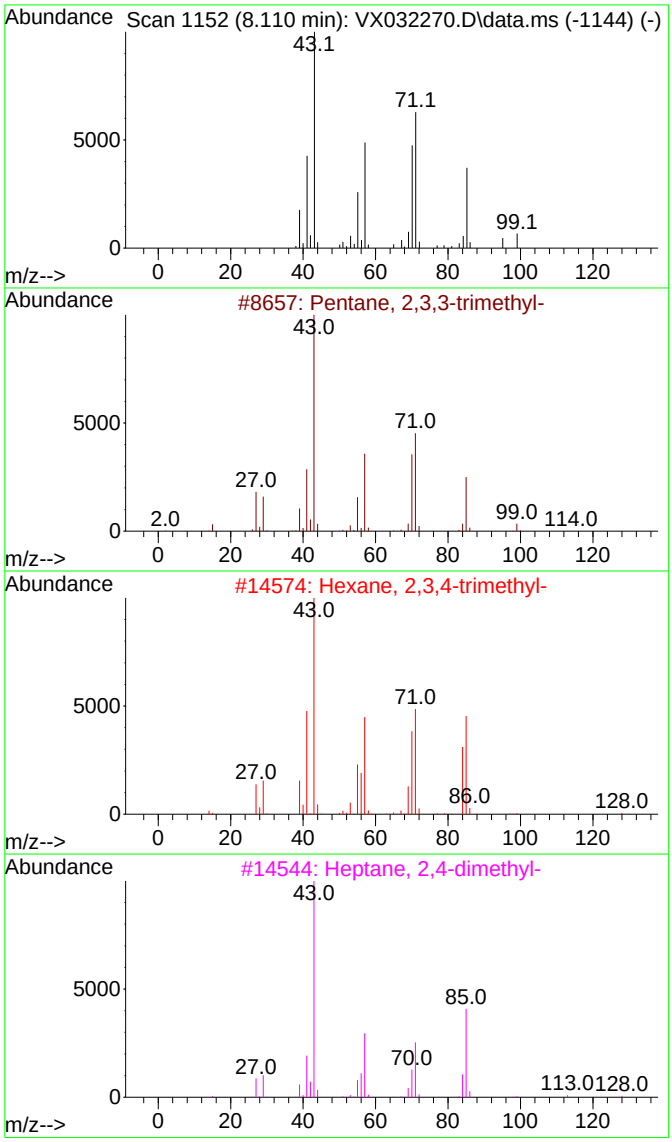
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

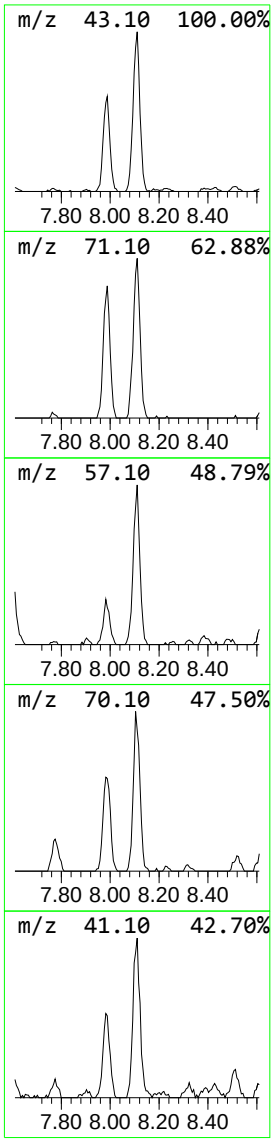
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	7.86 ug/l	88036	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Octane, 4-methyl-	128	C9H20	002216-34-4	56





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Data File : VX032270.D
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Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

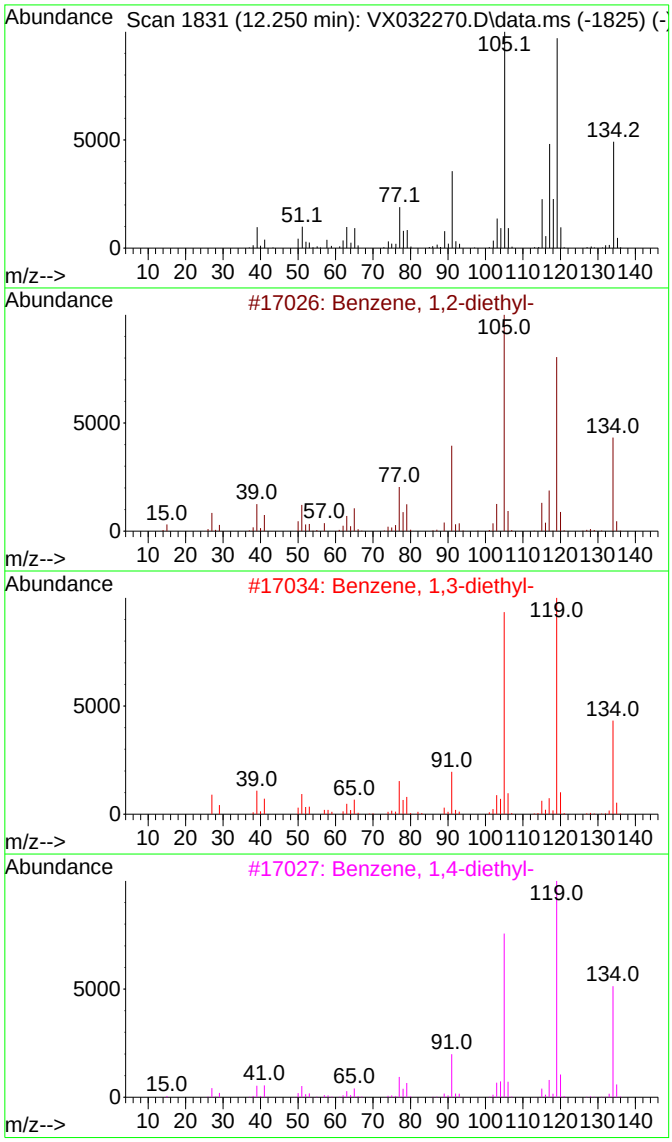
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

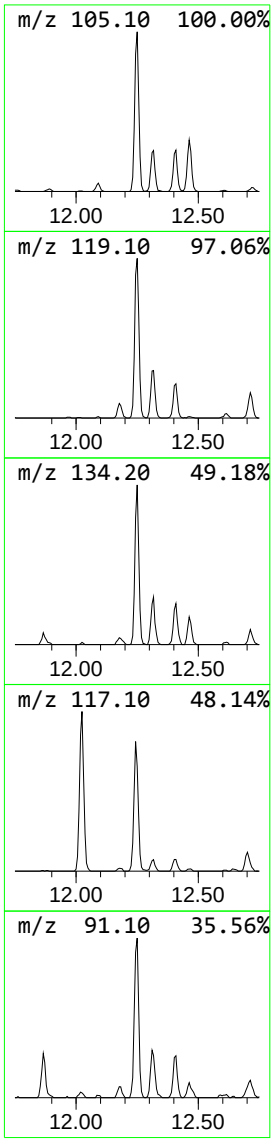
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	12.91 ug/l	157717	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	86
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	76
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	76
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	62
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

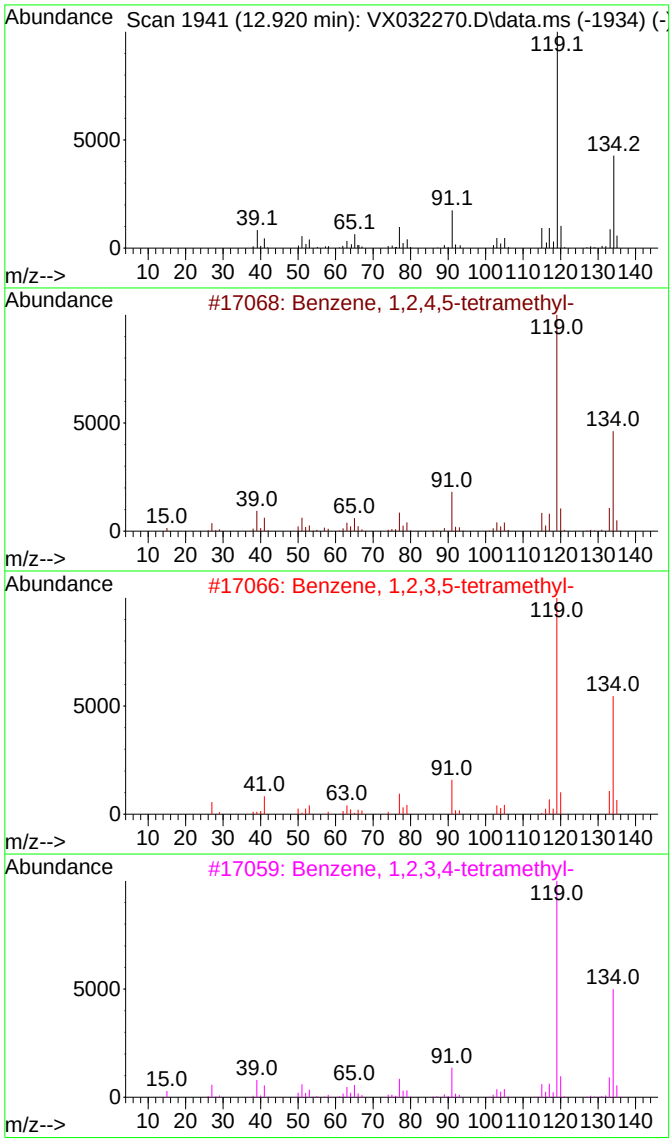
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

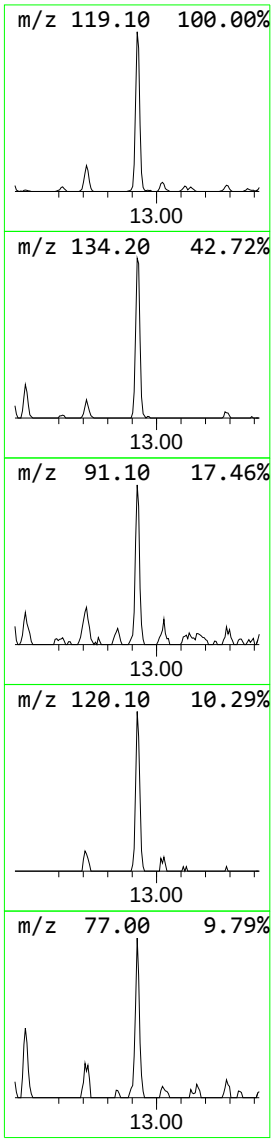
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	5.93 ug/l	72458	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102022\
Data File : VX032270.D
Acq On : 20 Oct 2022 18:00
Operator : JC/MD
Sample : N5185-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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
Butane, 2-methyl-	1.752	7.1	ug/l	67243	1	5.550	474983	50.0
Butane, 2,2-dim...	2.343	19.4	ug/l	184705	1	5.550	474983	50.0
Butane, 2,3-dim...	2.782	39.5	ug/l	374755	1	5.550	474983	50.0
Pentane, 2,4-di...	4.215	8.6	ug/l	81728	1	5.550	474983	50.0
Pentane, 2,3-di...	5.623	12.6	ug/l	119189	1	5.550	474983	50.0
Butane, 2,2,3,3...	6.251	10.7	ug/l	120391	2	6.763	560319	50.0
Pentane, 2,3,3-...	8.110	7.9	ug/l	88036	2	6.763	560319	50.0
Benzene, 1,2-di...	12.250	12.9	ug/l	157717	4	12.024	610882	50.0
Benzene, 1,2,4,...	12.920	5.9	ug/l	72458	4	12.024	610882	50.0