LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
Sample : P1002-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1209

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\82X121323W.M
Title : SW846 8260

Signal : TIC: VX039597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB2	16830	18900	3.04%	0.358%
2	1.246	21	26	28	rBV	4187	6395	1.03%	0.121%
3	1.453	56	60	66	rBV	29582	34305	5.51%	0.649%
4	1.563	68	78	79	rBV6	7179	17643	2.83%	0.334%
5	2.105	159	167	178	rVV	5091	12073	1.94%	0.228%
6	2.288	191	197	206	rBV	7746	13689	2.20%	0.259%
7	2.386	206	213	223	rBV	24555	45653	7.33%	0.864%
8	2.581	236	245	253	rBV	5086	13880	2.23%	0.263%
9	2.703	261	265	274	rBV	7187	12981	2.08%	0.246%
10	3.014	303	316	319	rBV3	2702	7554	1.21%	0.143%
11	4.227	505	515	523	rBV2	39478	108048	17.35%	2.045%
12	4.306	524	528	544	rVB4	9889	33585	5.39%	0.636%
13	4.574	563	572	586	rBV	4556	15882	2.55%	0.301%
14	5.385	693	705	720	rBV	66933	197085	31.65%	3.730%
15	5.544	720	731	744	rBV	96700	280604	45.06%	5.311%
16	5.952	789	798	817	rBV2	77512	209307	33.61%	3.961%
17	6.153	822	831	844	rBV3	5080	16589	2.66%	0.314%
18	6.757	921	930	946	rBV	185667	448191	71.98%	8.483%
19	7.232	1000	1008	1023	rBV	27735	74582	11.98%	1.412%
20	7.964	1121	1128	1135	rBV4	3056	7055	1.13%	0.134%
21	8.647	1233	1240	1250	rBV	396216	622689	100.00%	11.785%
22	8.787	1257	1263	1273	rVB5	3061	7454	1.20%	0.141%
23	9.256	1333	1340	1349	rBV3	3667	9505	1.53%	0.180%
24	10.049	1465	1470	1484	rBV	417433	616565	99.02%	11.669%
25	10.159	1484	1488	1498	rVB3	4503	9113	1.46%	0.172%
26	10.506	1542	1545	1555	rVB2	6179	9605	1.54%	0.182%
27	10.683	1570	1574	1581	rVB	8665	11736	1.88%	0.222%
28	10.756	1581	1586	1595	rBV3	23326	42419	6.81%	0.803%
29	11.079	1634	1639	1645	rBV	367798	473003	75.96%	8.952%
30	11.134	1645	1648	1653	rVB2	9065	11828	1.90%	0.224%
31	11.390	1683	1690	1694	rBV	16976	23667	3.80%	0.448%
32	11.567	1714	1719	1733	rBV	277533	370117	59.44%	7.005%
33	11.683	1733	1738	1748	rVV	193865	231985	37.26%	4.391%
34	11.829	1757	1762	1767	rBV	39501	55770	8.96%	1.056%
35	11.884	1767	1771	1776	rVB4	8528	13567	2.18%	0.257%
36	11.988	1779	1788	1789	rBV2	31517	39156	6.29%	0.741%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
Sample : P1002-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1209

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\82X121323W.M
Title : SW846 8260

37	12.018	1789	1793	1802	rVV	441704	585911	94.09%	11.089%
38	12.097	1802	1806	1810	rVB3	5133	7433	1.19%	0.141%
39	12.219	1820	1826	1837	rBV	209092	330496	53.08%	6.255%
40	12.305	1837	1840	1850	rVB6	11339	23697	3.81%	0.448%
41	13.676	2059	2065	2069	rBV	50518	61120	9.82%	1.157%
42	13.750	2071	2077	2079	rBV6	7543	11322	1.82%	0.214%
43	14.030	2119	2123	2129	rBB	17521	20800	3.34%	0.394%
44	14.140	2136	2141	2146	rBV	20437	25445	4.09%	0.482%
45	14.268	2158	2162	2166	rBV	12825	15696	2.52%	0.297%
46	14.378	2174	2180	2186	rBV4	7664	9972	1.60%	0.189%
47	14.993	2276	2281	2288	rBV4	8124	13395	2.15%	0.254%
48	15.133	2300	2304	2309	rBV2	4857	7623	1.22%	0.144%
49	15.304	2327	2332	2336	rBV2	4098	6788	1.09%	0.128%
50	15.676	2385	2393	2399	rVB8	3783	7849	1.26%	0.149%
51	15.969	2434	2441	2451	rBV3	17807	33939	5.45%	0.642%

Sum of corrected areas: 5283666

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Instrument :
MSVOA_X
ClientSampleId :
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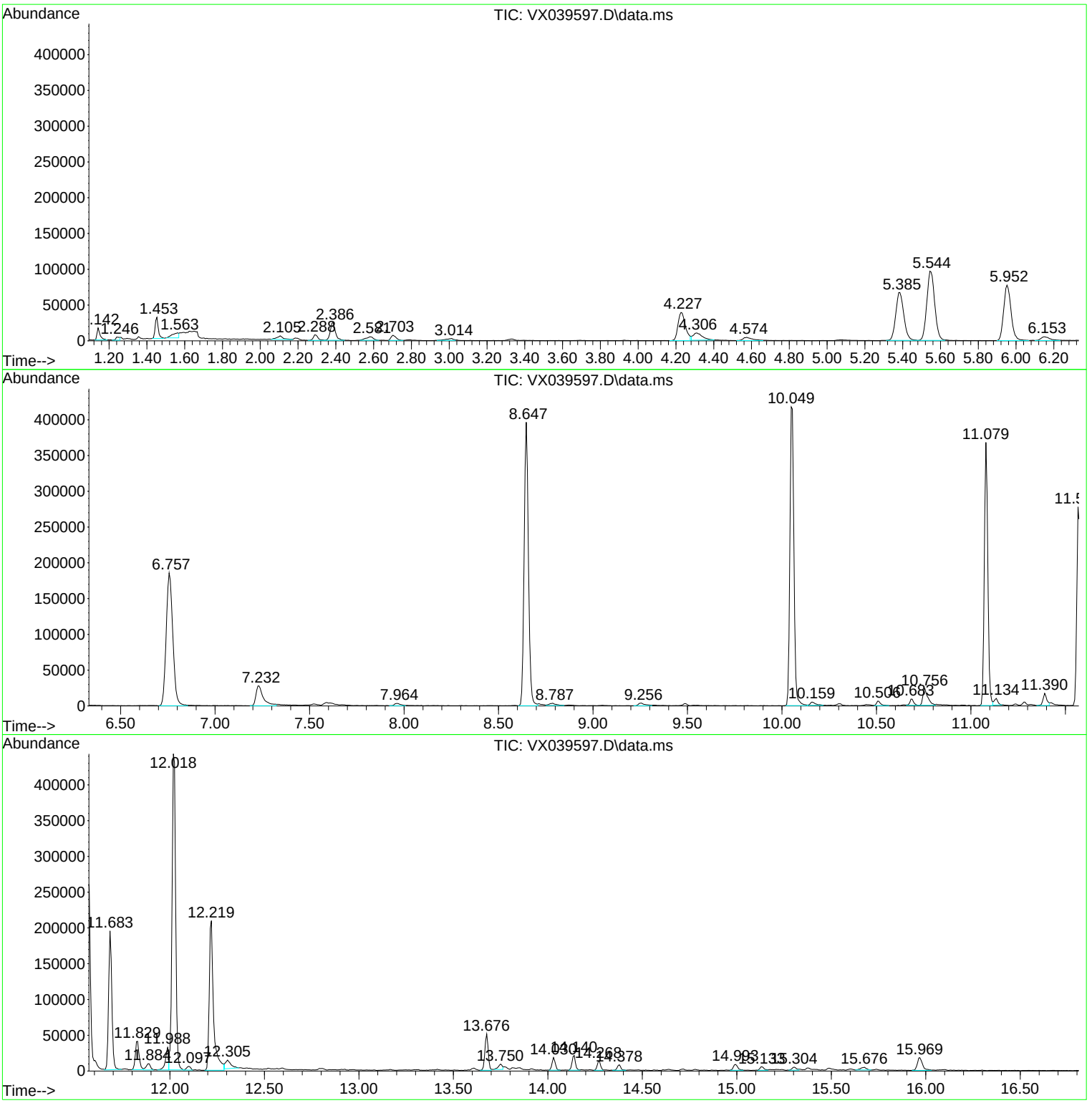
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
Sample : P1002-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

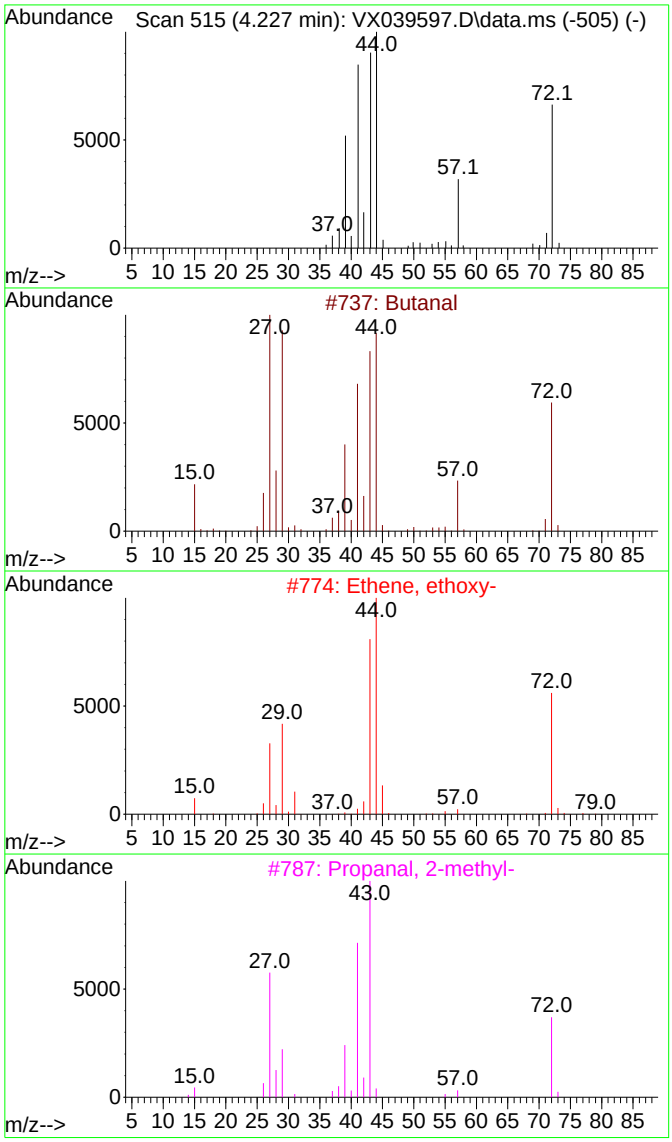
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

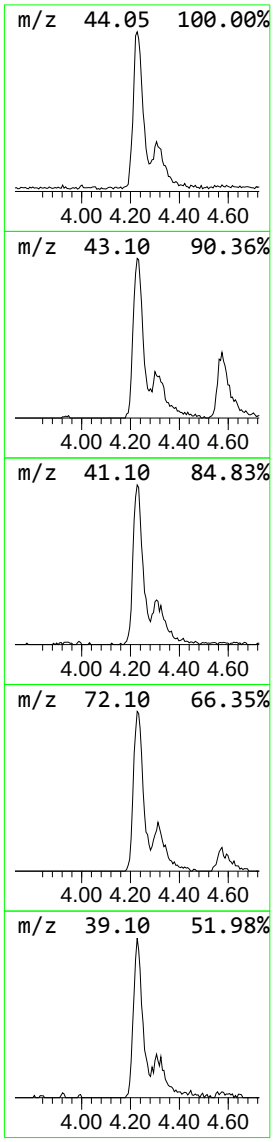
****

Peak Number 2 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	19.25 ug/l	108048	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5	Methacrolein	70	C4H6O	000078-85-3	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

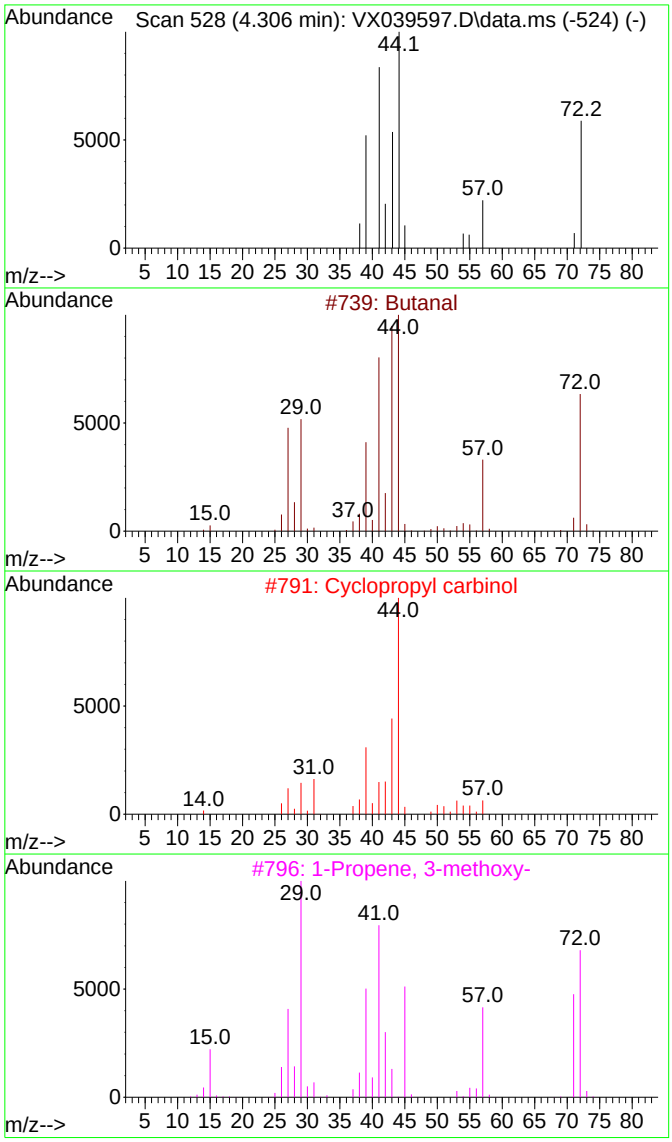
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

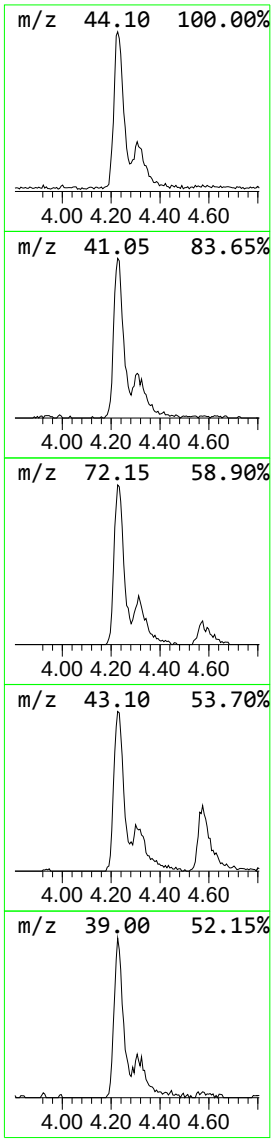
****

Peak Number 3 unknown4.306 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.98 ug/l	33585	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	90
2	Cyclopropyl carbinol	72	C4H8O	002516-33-8	23
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	17
4	Propane	44	C3H8	000074-98-6	9
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9





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Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
Sample : P1002-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

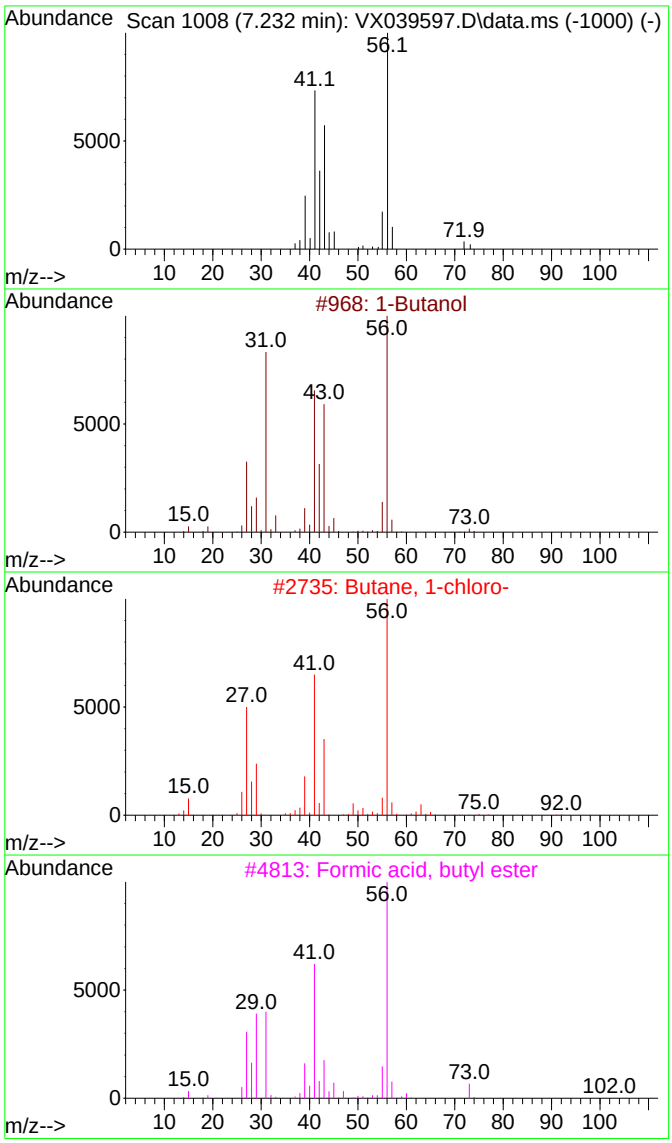
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

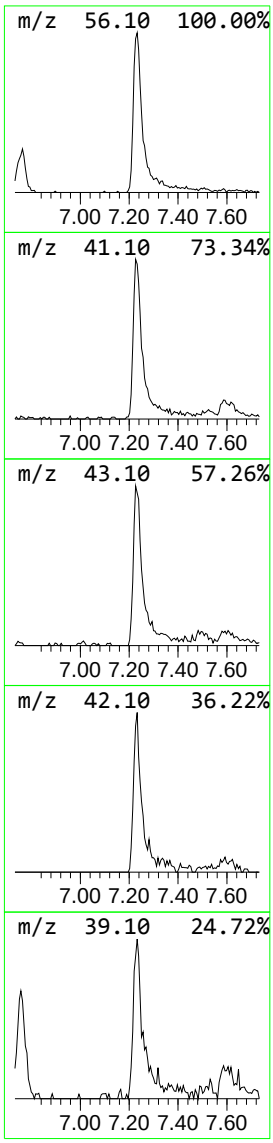
****

Peak Number 4 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.232	8.32 ug/l	74582	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	78
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	36
3	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





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Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
Operator : JC/MD
Sample : P1002-01
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Instrument :
MSVOA_X
ClientSampleId :
1209

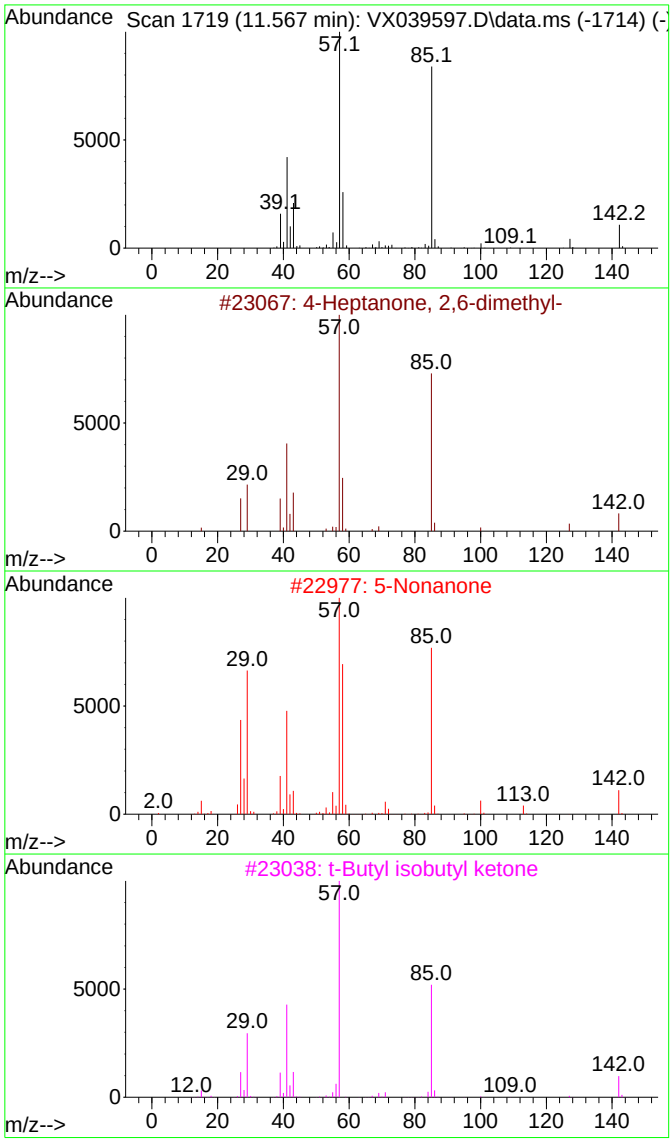
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

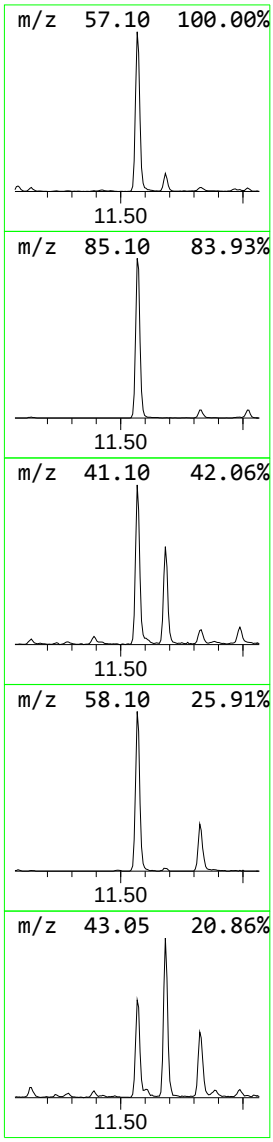
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.567	31.58 ug/l	370117	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	64
4	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	64





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Instrument :
MSVOA_X
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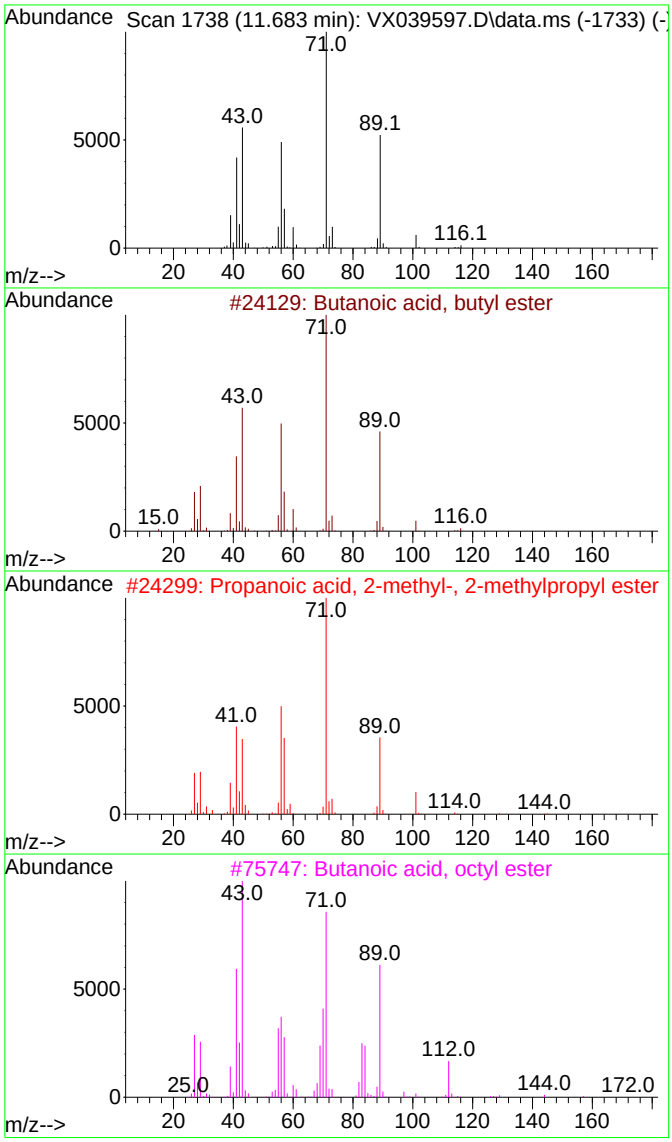
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

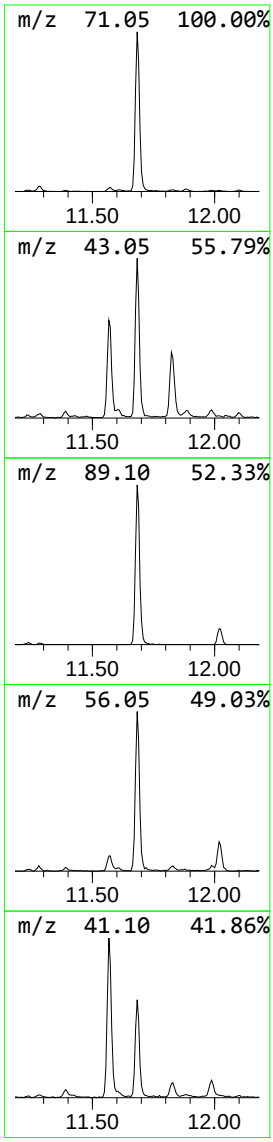
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	19.80 ug/l	231985	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64





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MSVOA_X
ClientSampleId :
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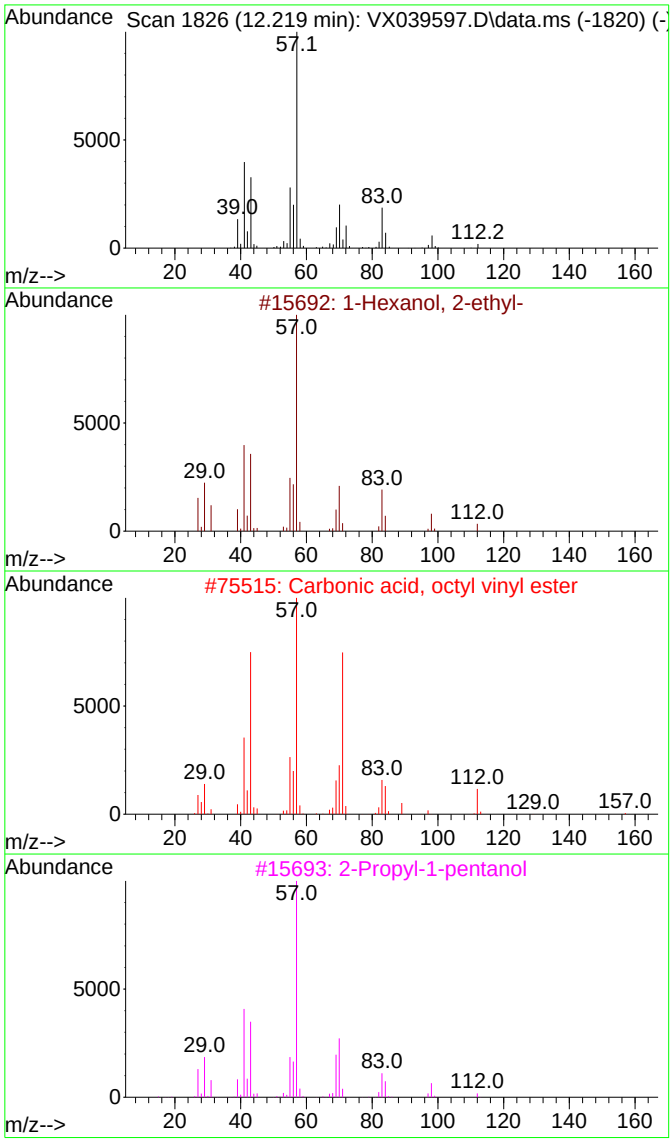
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

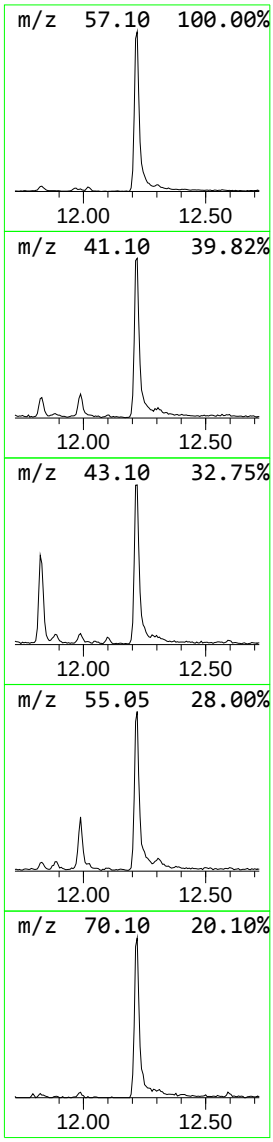
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	28.20 ug/l	330496	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	72
2	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47





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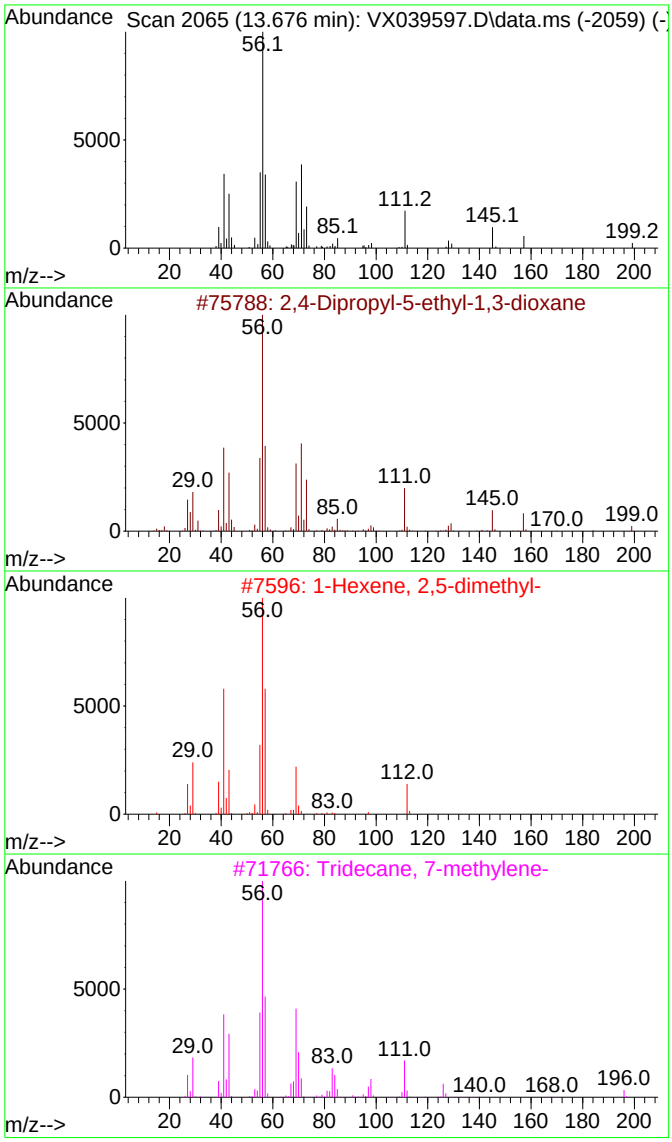
Quant Title : SW846 8260

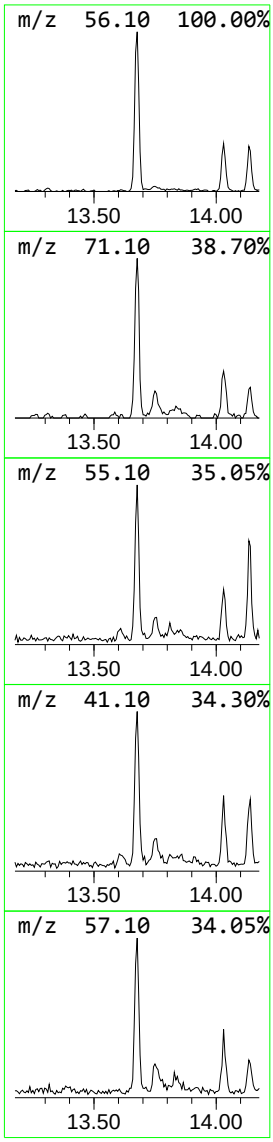
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	5.22 ug/l	61120	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	50
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
3	Tridecane, 7-methylene-	196	C14H28	019780-80-4	32
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
5	2-Methyl-1-nonene	140	C10H20	002980-71-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039597.D
Acq On : 03 Jan 2024 13:20
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Sample : P1002-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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
Butanal	4.227	19.3	ug/l	108048	1	5.550	280604	50.0
unknown4.306	4.306	6.0	ug/l	33585	1	5.550	280604	50.0
1-Butanol	7.232	8.3	ug/l	74582	2	6.757	448191	50.0
4-Heptanone, 2,...	11.567	31.6	ug/l	370117	4	12.024	585911	50.0
Butanoic acid, ...	11.683	19.8	ug/l	231985	4	12.024	585911	50.0
1-Hexanol, 2-et...	12.219	28.2	ug/l	330496	4	12.024	585911	50.0
2,4-Dipropyl-5-...	13.676	5.2	ug/l	61120	4	12.024	585911	50.0