LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101823\
Data File : VX038366.D
Acq On : 18 Oct 2023 16:35
Operator : JC/MD
Sample : 04936-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1027

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\82X100523W.M
Title : SW846 8260

Signal : TIC: VX038366.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	16	rBV	19101	19005	1.27%	0.248%
2	2.380	206	212	222	rVB	27106	44094	2.94%	0.576%
3	3.331	360	368	378	rBV2	8296	19668	1.31%	0.257%
4	4.227	504	515	536	rBV	574967	1501090	100.00%	19.602%
5	4.550	559	568	586	rBV	204470	573995	38.24%	7.495%
6	4.995	631	641	655	rBV2	19386	68474	4.56%	0.894%
7	5.385	694	705	721	rBV	78241	234167	15.60%	3.058%
8	5.550	721	732	754	rVB2	124383	356763	23.77%	4.659%
9	5.952	789	798	809	rBV	88423	236536	15.76%	3.089%
10	6.117	818	825	839	rVB2	6277	18453	1.23%	0.241%
11	6.763	922	931	944	rBV	204118	490357	32.67%	6.403%
12	7.208	997	1004	1023	rBV	69380	175162	11.67%	2.287%
13	7.580	1059	1065	1073	rBV	24703	49346	3.29%	0.644%
14	8.647	1234	1240	1248	rBV	451761	707616	47.14%	9.240%
15	8.720	1248	1252	1257	rVV2	12231	21849	1.46%	0.285%
16	10.055	1465	1471	1485	rBV	489090	683376	45.53%	8.924%
17	10.299	1506	1511	1521	rVB	12988	20010	1.33%	0.261%
18	10.506	1541	1545	1554	rVB	12115	16195	1.08%	0.211%
19	10.750	1581	1585	1595	rBV	61144	104259	6.95%	1.361%
20	11.079	1634	1639	1645	rBV	423241	544447	36.27%	7.110%
21	11.134	1645	1648	1660	rVB	15091	22571	1.50%	0.295%
22	11.573	1712	1720	1723	rBV	27936	41974	2.80%	0.548%
23	11.604	1723	1725	1736	rVB2	26792	41776	2.78%	0.546%
24	11.872	1765	1769	1781	rVB	17304	31779	2.12%	0.415%
25	12.018	1788	1793	1802	rVB	565637	749402	49.92%	9.786%
26	12.219	1821	1826	1840	rBV	518882	810133	53.97%	10.579%
27	13.756	2073	2078	2086	rBV5	16376	39535	2.63%	0.516%
28	13.841	2090	2092	2100	rVV4	9421	18645	1.24%	0.243%
29	13.914	2100	2104	2117	rVB5	7933	17327	1.15%	0.226%

Sum of corrected areas: 7658004

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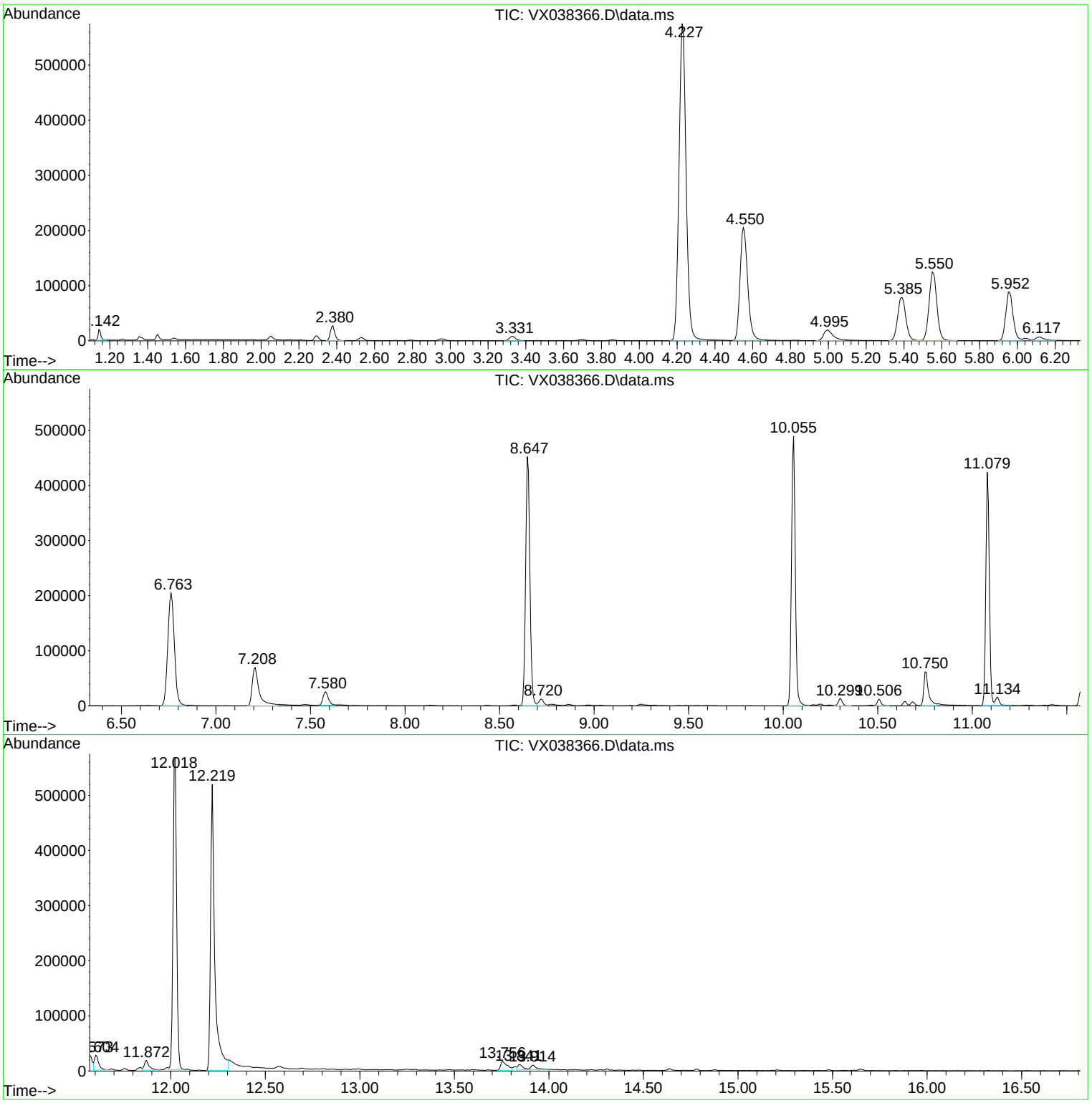
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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



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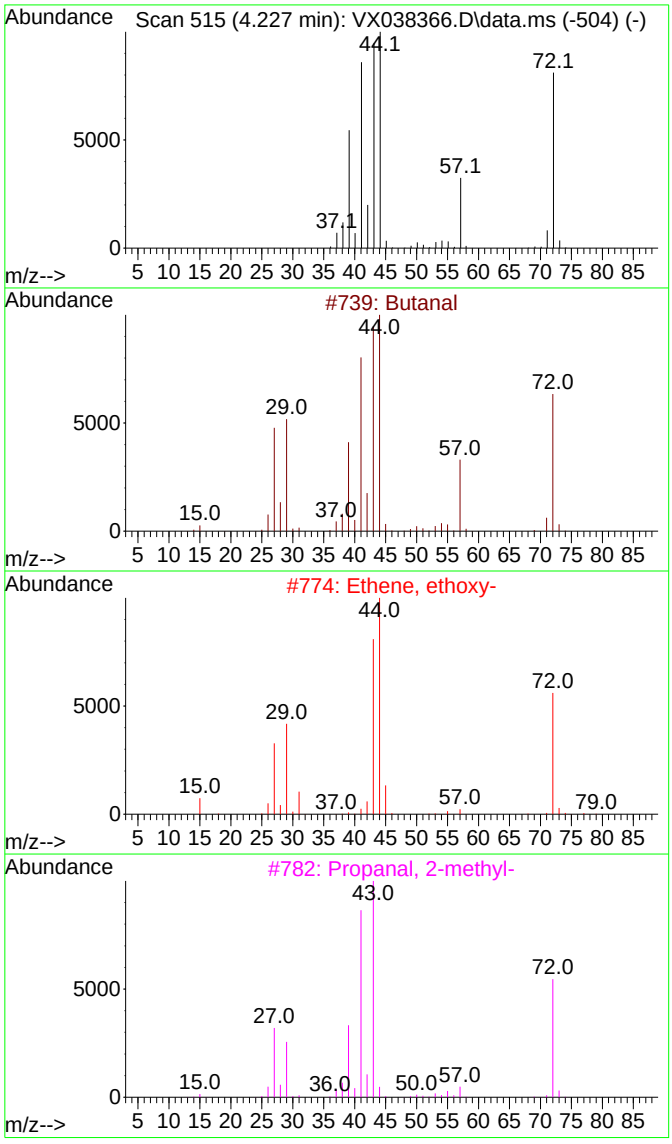
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

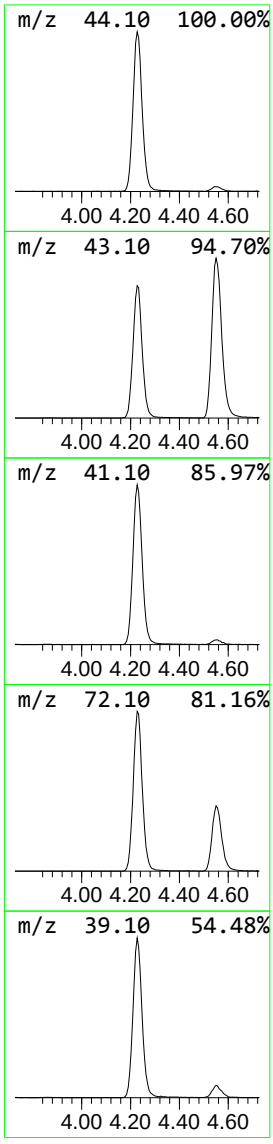
****

Peak Number 1 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	210.38 ug/l	1501090	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5	Propane	44	C3H8	000074-98-6	38





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Instrument :
MSVOA_X
ClientSampleId :
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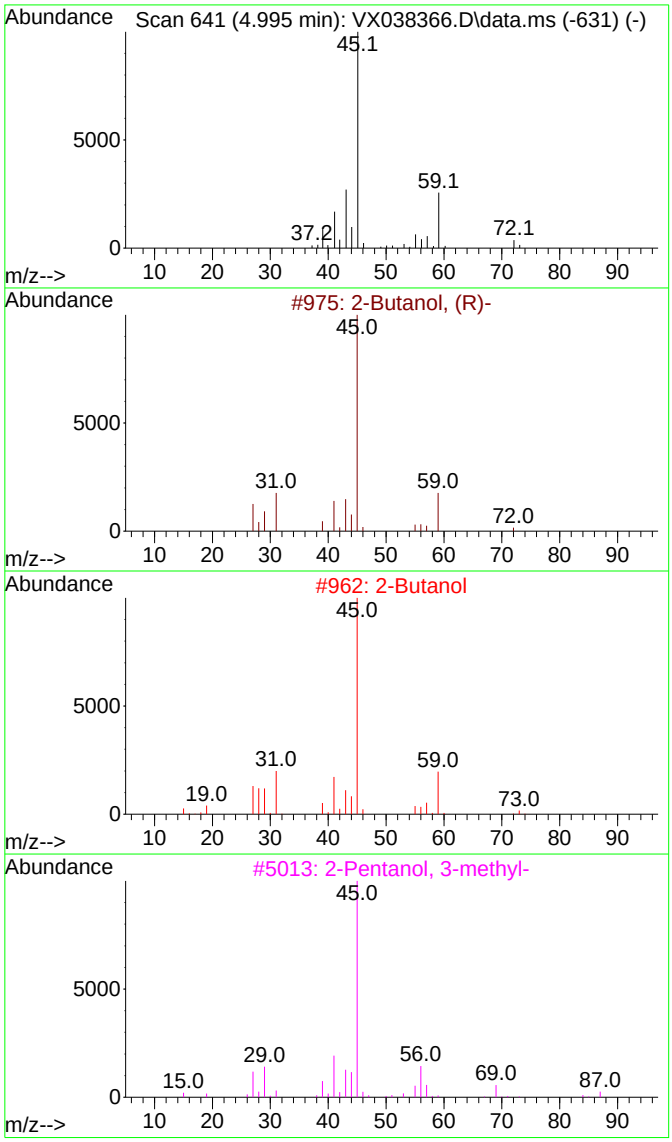
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

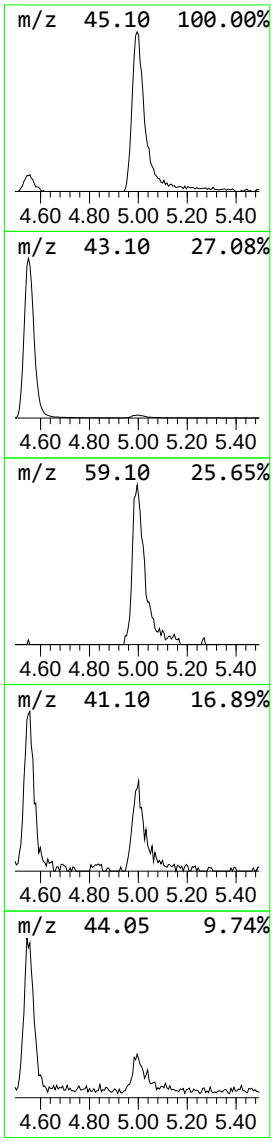
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanol, (R)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.995	9.60 ug/l	68474	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
2	2-Butanol	74	C4H10O	000078-92-2	83
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	45
4	1-Pentanol, 5-methoxy-	118	C6H14O2	004799-62-6	38
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	36





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Instrument :
MSVOA_X
ClientSampleId :
1027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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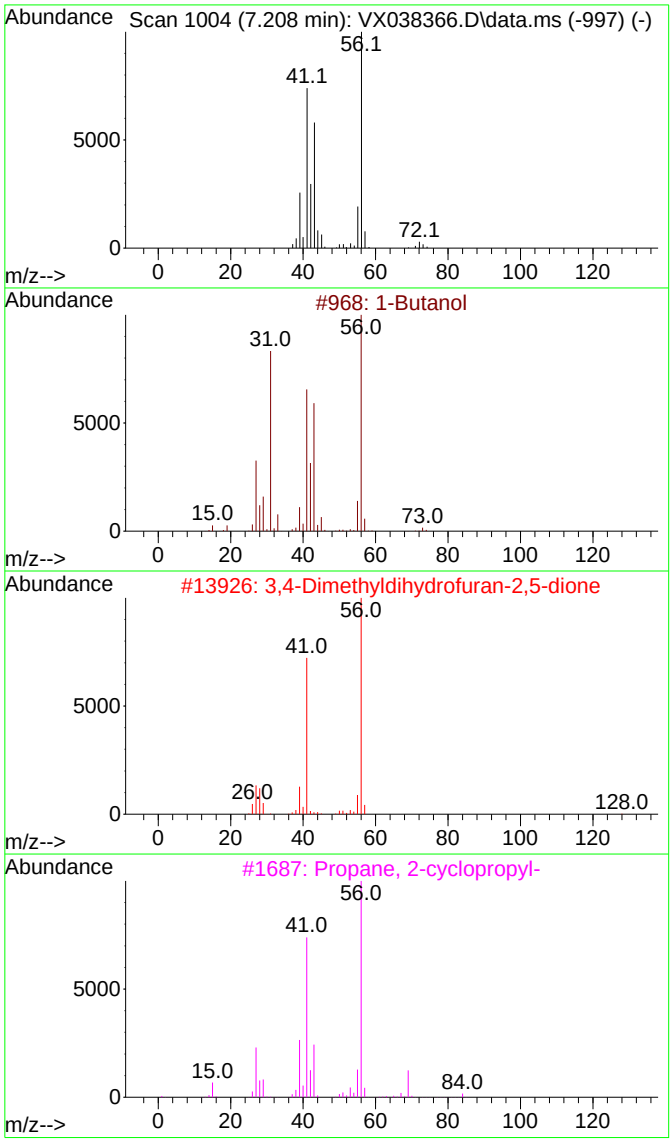
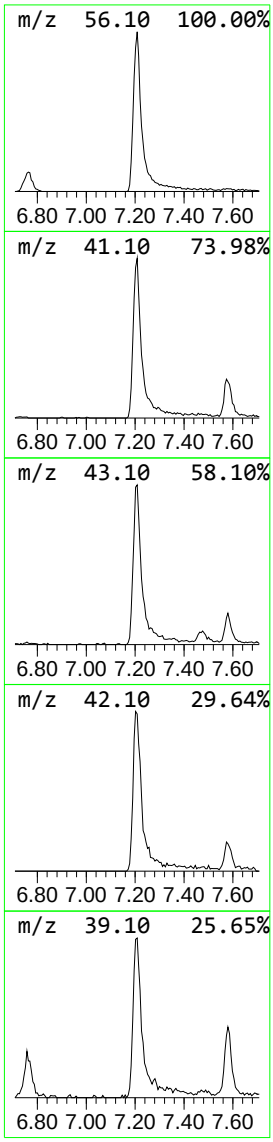
****
Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	17.86 ug/l	175162	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	45
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
4	.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	9
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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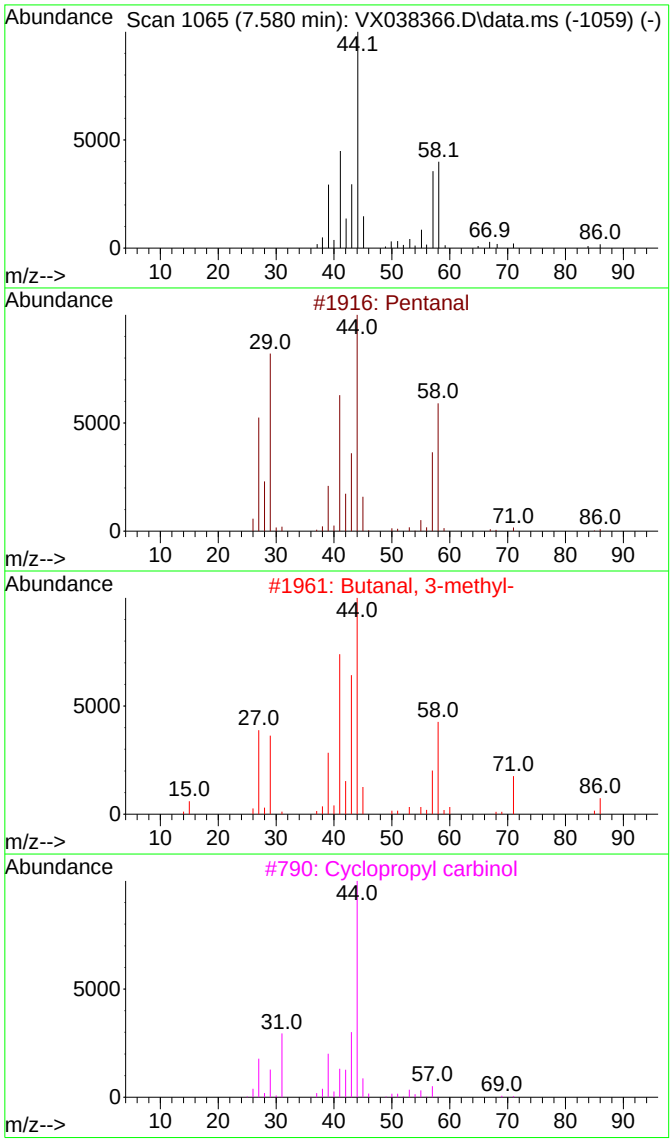
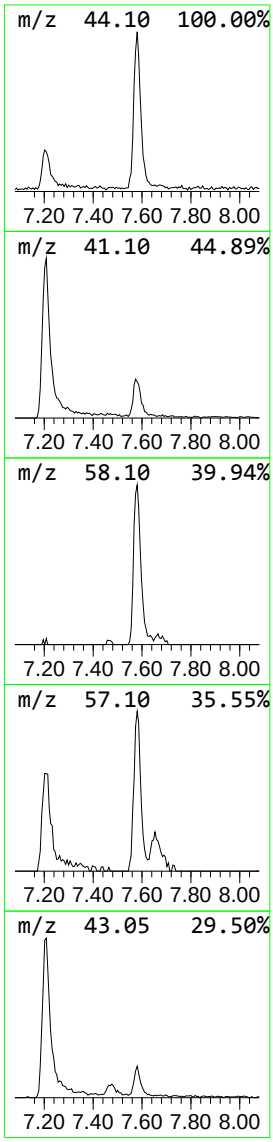
Peak Number 4 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.580	5.03 ug/l	49346	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	78
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	42
4	2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5	(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	9





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Instrument :
MSVOA_X
ClientSampleId :
1027

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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

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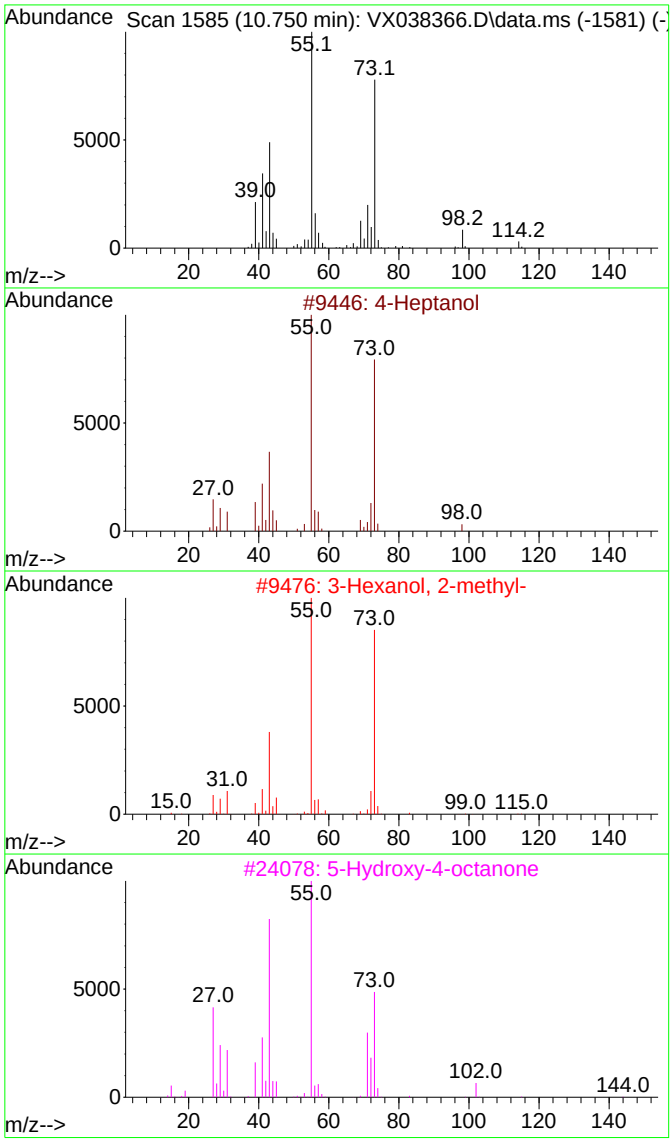
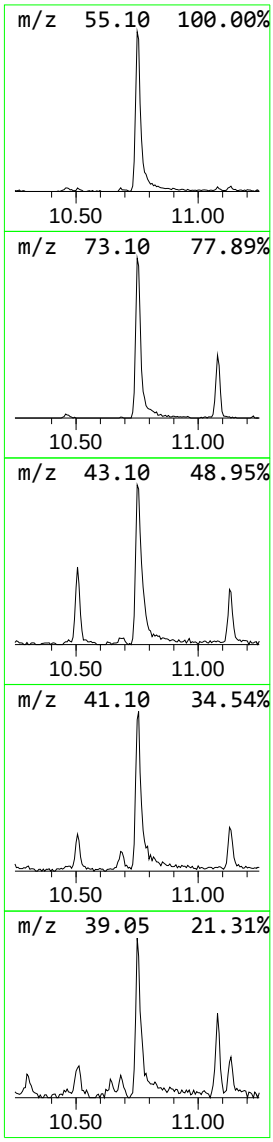
Peak Number 5 4-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	7.63 ug/l	104259	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	53
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	38
3	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	38
4	Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	38
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	35





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MSVOA_X
ClientSampleId :
1027

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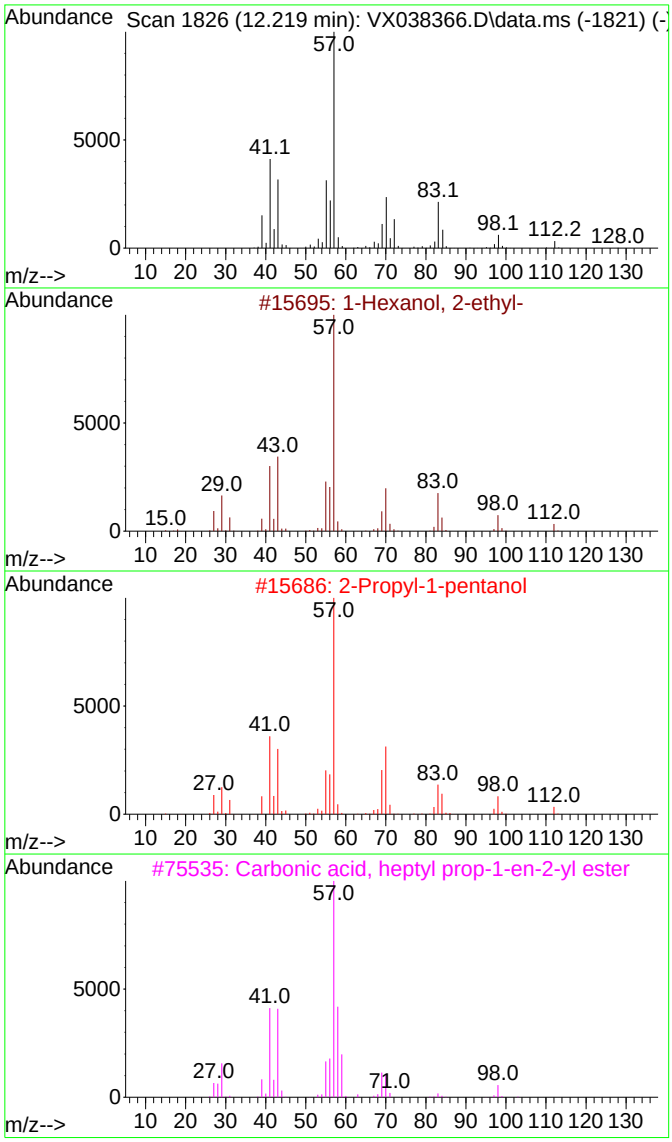
Quant Title : SW846 8260

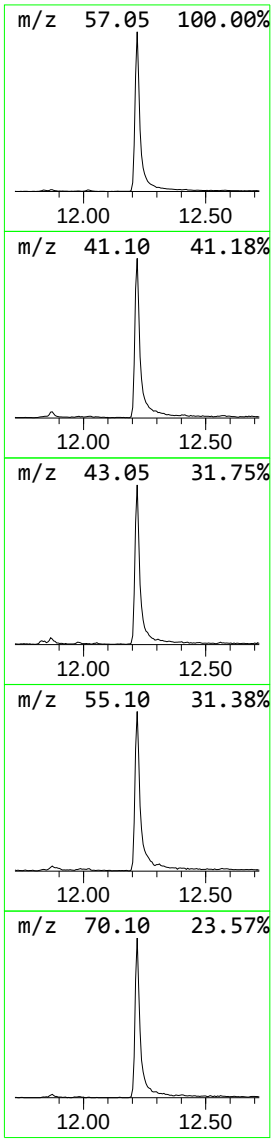
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	54.05 ug/l	810133	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	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
3	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	40





Tentatively Identified Compound (LSC) summary

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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	210.4	ug/l	1501090	1	5.556	356763	50.0
2-Butanol, (R)-	4.995	9.6	ug/l	68474	1	5.556	356763	50.0
1-Butanol	7.208	17.9	ug/l	175162	2	6.763	490357	50.0
Pentanal	7.580	5.0	ug/l	49346	2	6.763	490357	50.0
4-Heptanol	10.750	7.6	ug/l	104259	3	10.055	683376	50.0
1-Hexanol, 2-et...	12.219	54.0	ug/l	810133	4	12.024	749402	50.0