LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066189.D
Acq On : 12 Mar 2021 18:13
Operator : JC/MD
Sample : M1647-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41145

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_N\methods\82N031221W.M
Title : SW846 8260

Signal : TIC: VN066189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.783	25	35	51	rVB	117730	151513	2.02%	0.421%
2	3.205	550	565	592	rBV2	137799	334688	4.46%	0.930%
3	3.738	742	764	804	rBV	2918426	7505988	100.00%	20.863%
4	3.991	847	858	876	rVB2	43929	120868	1.61%	0.336%
5	4.237	933	950	972	rVB2	49714	139142	1.85%	0.387%
6	5.852	1522	1552	1582	rBV3	75258	280690	3.74%	0.780%
7	6.453	1753	1776	1799	rBV3	139414	423407	5.64%	1.177%
8	6.748	1866	1886	1913	rBV	89970	264485	3.52%	0.735%
9	7.509	2150	2170	2184	rBV2	310447	762976	10.16%	2.121%
10	7.587	2184	2199	2226	rVB	581291	1376476	18.34%	3.826%
11	7.952	2308	2335	2358	rBV	428523	1036676	13.81%	2.881%
12	8.515	2525	2545	2569	rBV	886045	1834942	24.45%	5.100%
13	10.028	3092	3109	3120	rBV	1383192	2472565	32.94%	6.873%
14	10.092	3120	3133	3166	rVB	4033852	7163510	95.44%	19.911%
15	10.795	3385	3395	3414	rVB3	40925	78701	1.05%	0.219%
16	11.350	3585	3602	3621	rBV	1203304	2150733	28.65%	5.978%
17	11.452	3628	3640	3661	rVB	387468	647339	8.62%	1.799%
18	11.562	3664	3681	3708	rBV	1797699	3321706	44.25%	9.233%
19	11.892	3788	3804	3820	rBV	934500	1684293	22.44%	4.682%
20	12.345	3958	3973	3998	rBV	809015	1421355	18.94%	3.951%
21	13.050	4222	4236	4248	rBV3	99172	232669	3.10%	0.647%
22	13.286	4310	4324	4348	rBV	849444	1478847	19.70%	4.111%
23	13.396	4353	4365	4389	rBV	552290	1093594	14.57%	3.040%

Sum of corrected areas: 35977163

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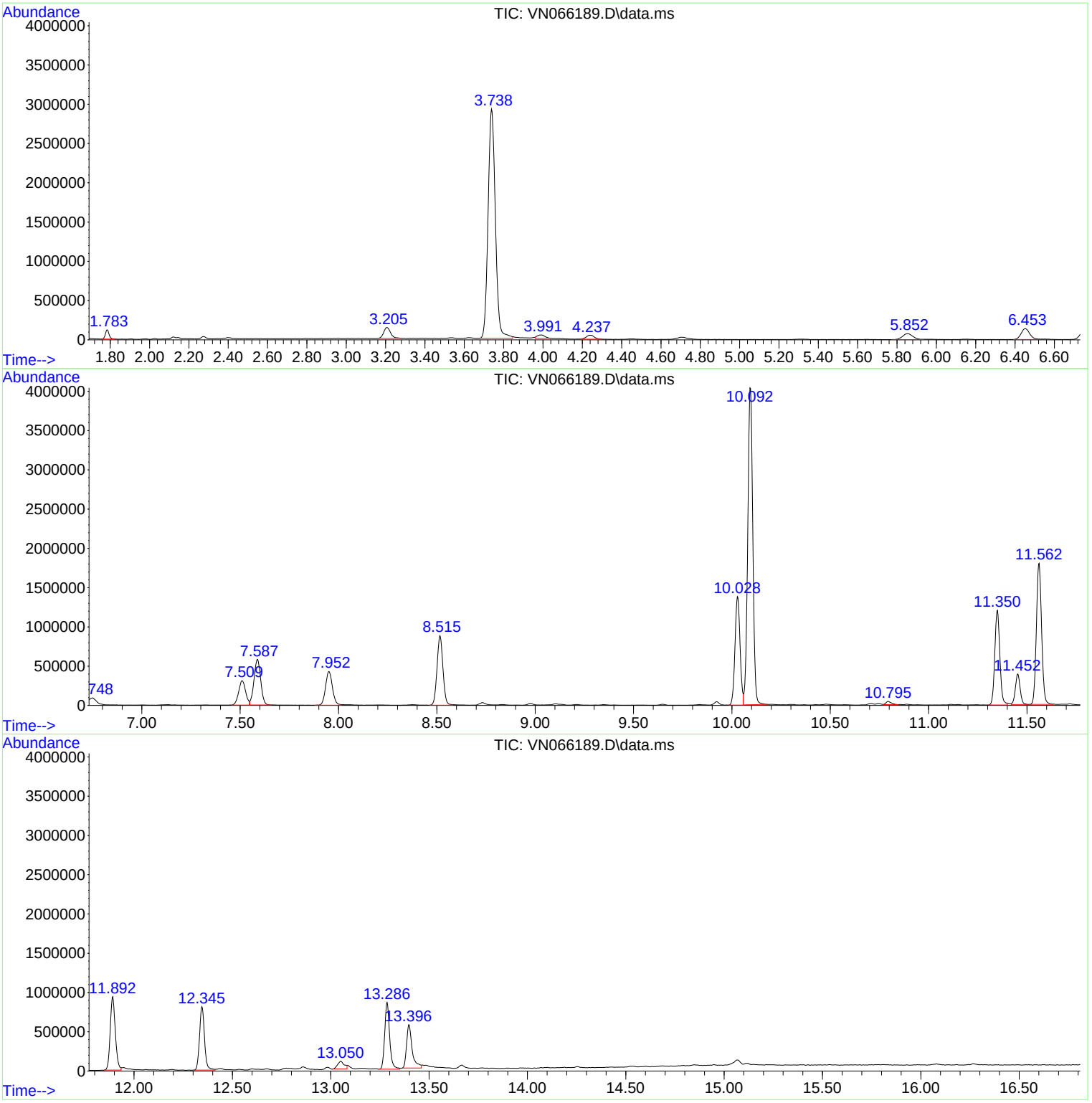
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

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



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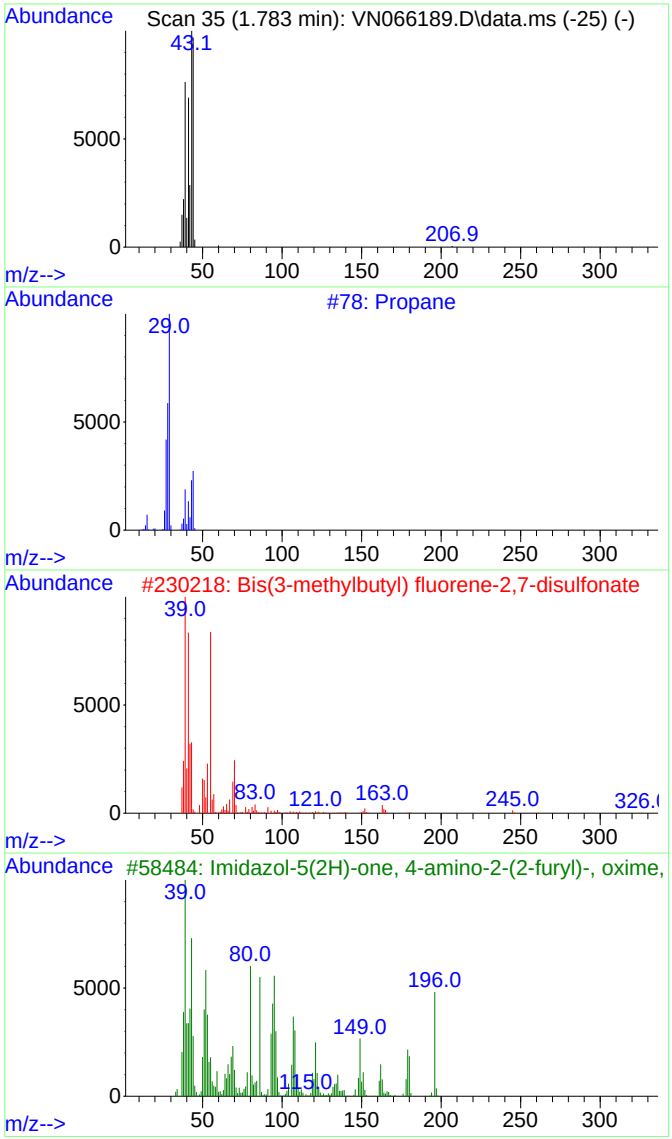
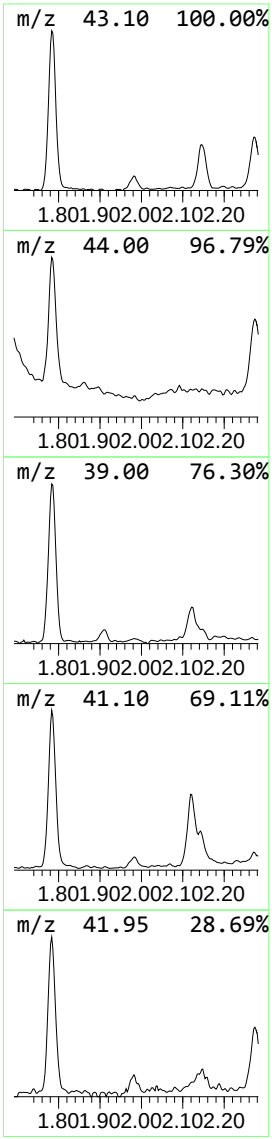
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.783	5.50 ug/l	151513	Pentafluorobenzene	7.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	50
3	Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	50
4	2-Hexynoic acid	112	C6H8O2	000764-33-0	43
5	Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	39





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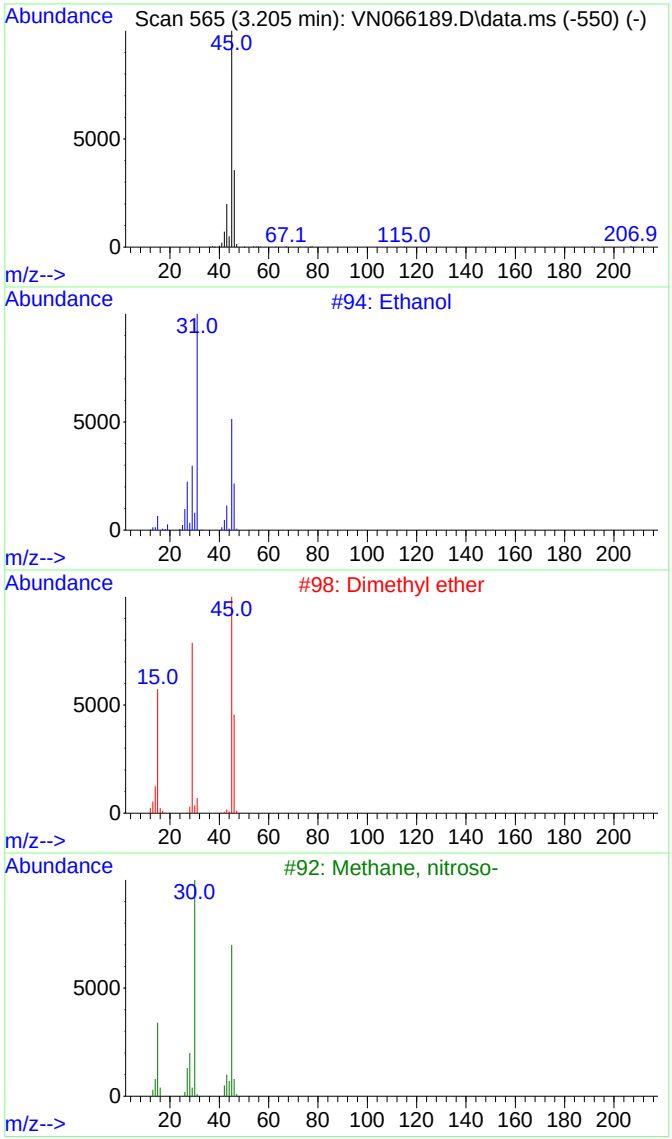
Quant Title : SW846 8260

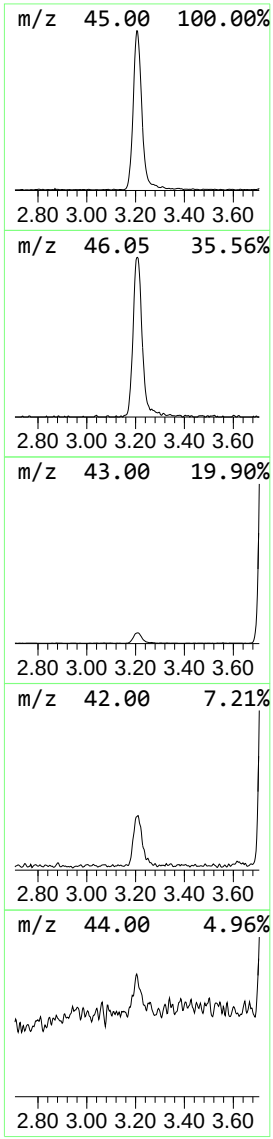
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.205	12.16 ug/l	334688	Pentafluorobenzene	7.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	80
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	7
4	Formic acid	46	CH2O2	000064-18-6	4
5	Fluoroacetic acid	78	C2H3FO2	000144-49-0	2





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MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
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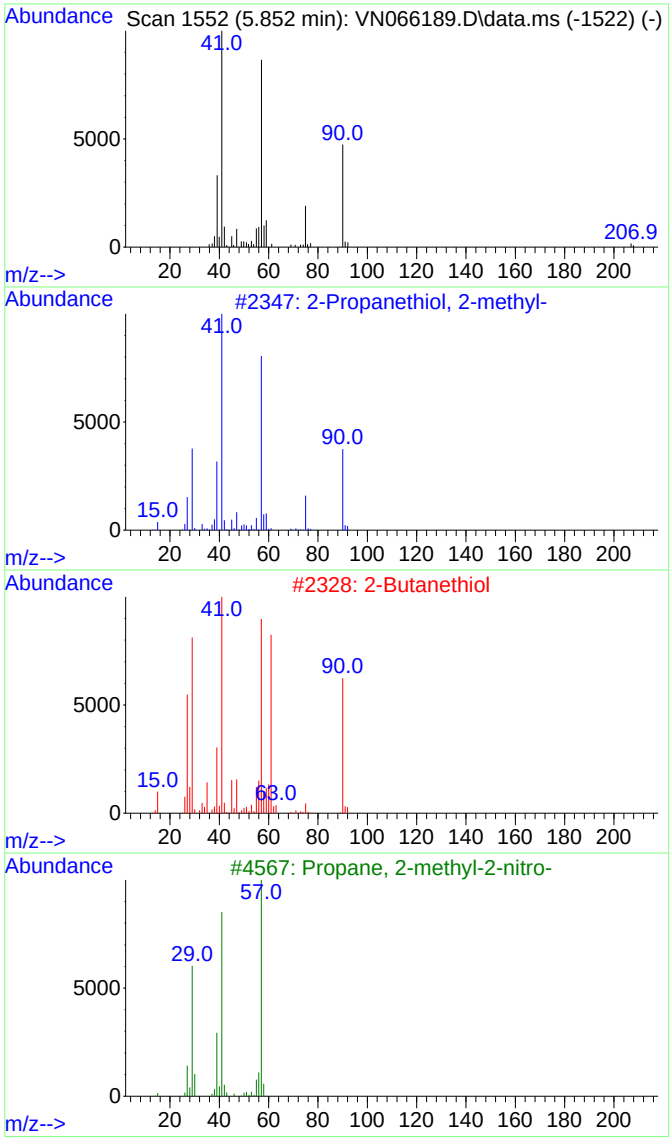
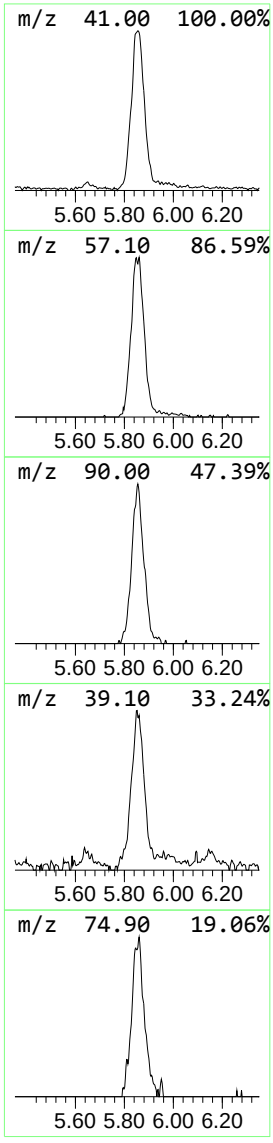
****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.852	10.20 ug/l	280690	Pentafluorobenzene	7.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	87
2	2-Butanethiol	90	C4H10S	000513-53-1	50
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
4	Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	27
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	25





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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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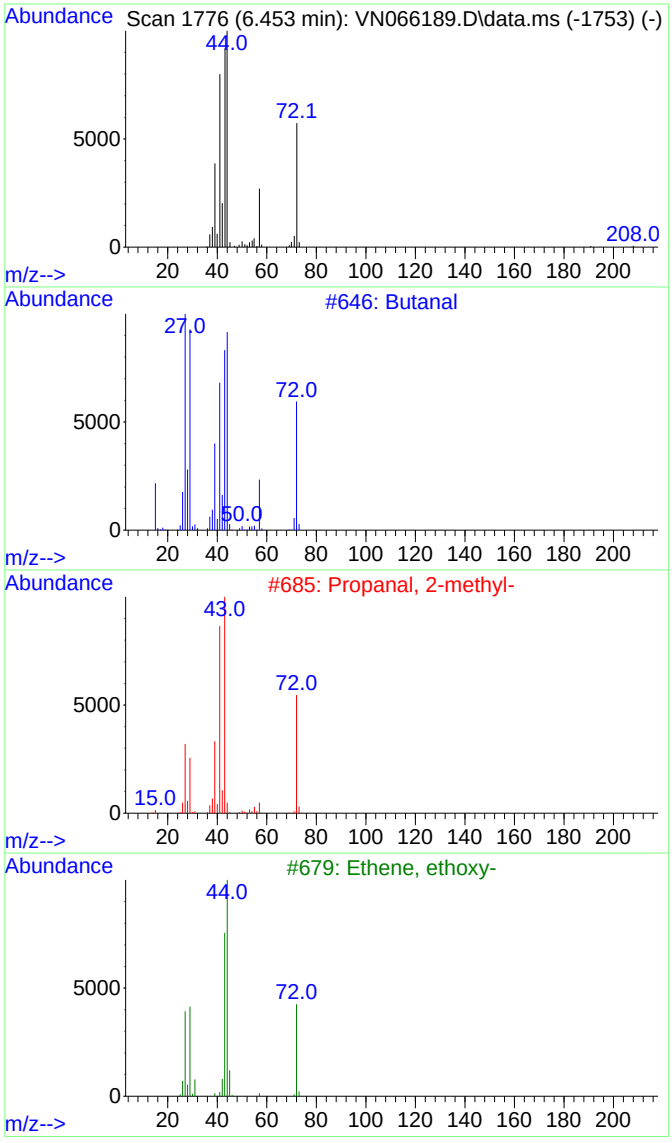
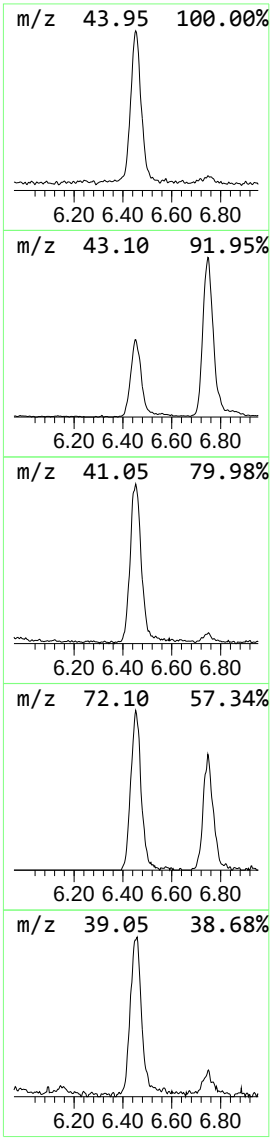
****

Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.453	15.38 ug/l	423407	Pentafluorobenzene	7.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	90
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	2-Formylhistamine	139	C6H9N3O	1000132-95-8	25





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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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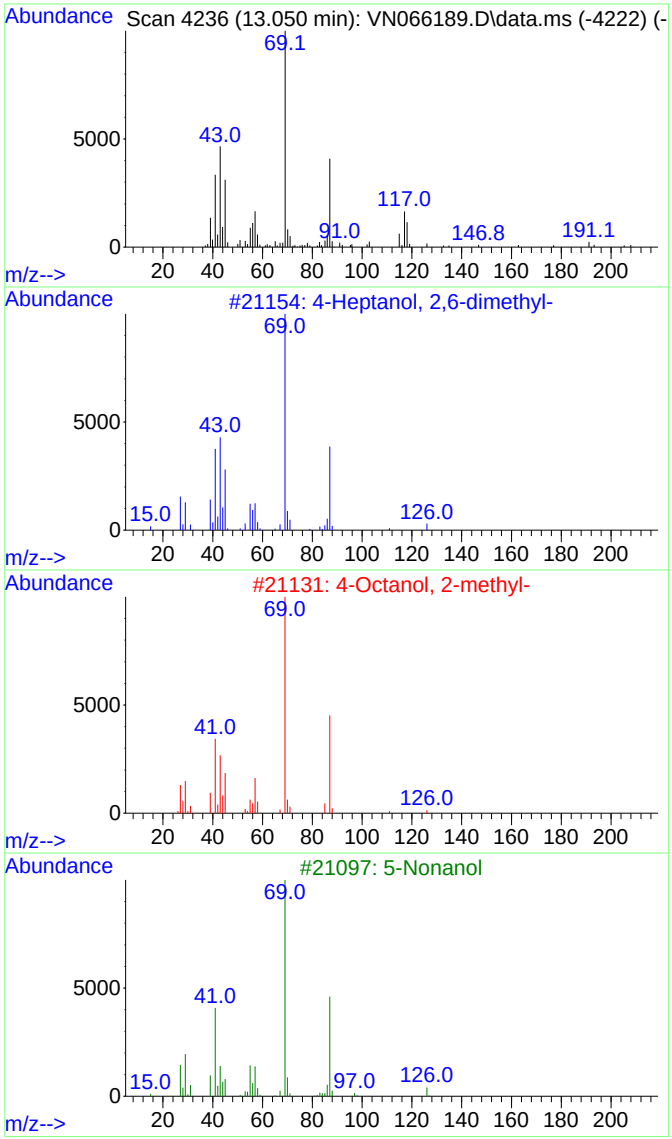
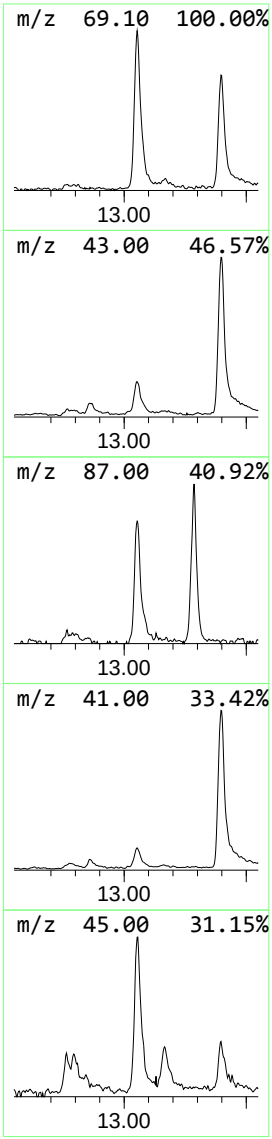
****
Peak Number 5 4-Heptanol, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.050	7.87 ug/l	232669	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	80
2	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	59
3	5-Nonanol	144	C9H20O	000623-93-8	59
4	3-Heptanol, 2,2-dimethyl-	144	C9H20O	019549-70-3	53
5	3-Heptanol, 2-methyl-	130	C8H18O	018720-62-2	53





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Quant Title : SW846 8260

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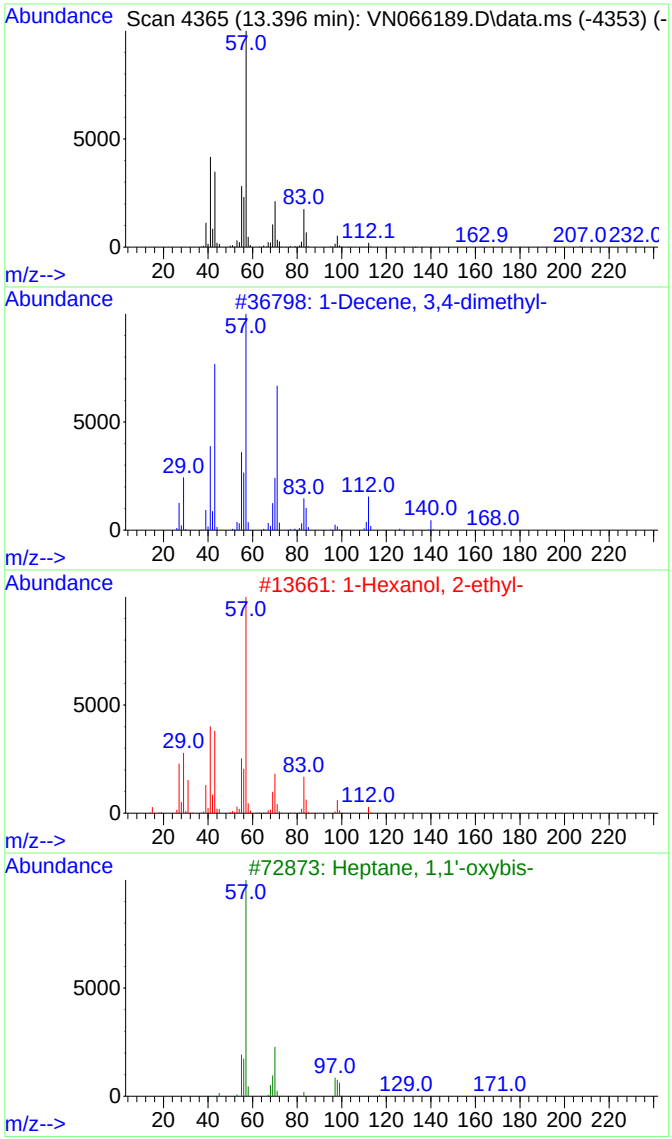
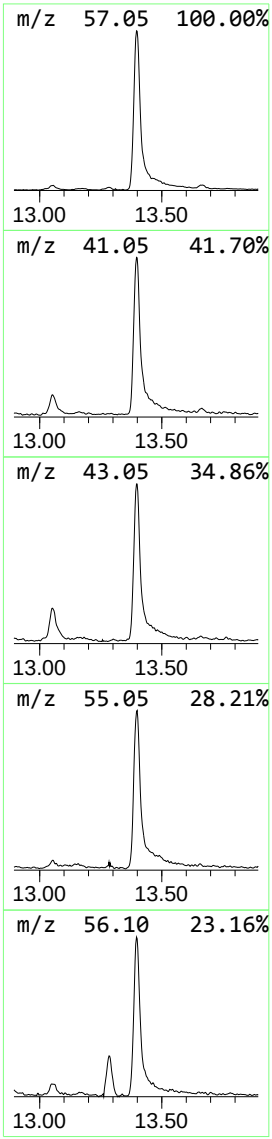
****
Peak Number 6 1-Decene, 3,4-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	36.97 ug/l	1093590	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 3,4-dimethyl-	168	C12H24	050871-03-9	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	47





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.783	5.5	ug/l	151513	1	7.587	1376480	50.0
Ethanol	3.205	12.2	ug/l	334688	1	7.587	1376480	50.0
2-Propanethiol,...	5.852	10.2	ug/l	280690	1	7.587	1376480	50.0
Butanal	6.453	15.4	ug/l	423407	1	7.587	1376480	50.0
4-Heptanol, 2,6...	13.050	7.9	ug/l	232669	4	13.286	1478850	50.0
1-Decene, 3,4-d...	13.396	37.0	ug/l	1093590	4	13.286	1478850	50.0