LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032797.D
Acq On : 14 Nov 2022 16:13
Operator : JC/MD
Sample : N5572-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31911

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032797.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	206	214	228	rBV	75596	146707	6.60%	2.161%
2	2.959	297	307	330	rBV6	6159	23947	1.08%	0.353%
3	3.696	416	428	439	rBV	10130	27555	1.24%	0.406%
4	4.227	505	515	534	rBV	301800	820697	36.93%	12.089%
5	4.562	561	570	591	rVB	94451	278055	12.51%	4.096%
6	5.385	695	705	719	rBV	65217	192587	8.67%	2.837%
7	5.556	722	733	749	rVB	107015	301475	13.57%	4.441%
8	5.958	788	799	815	rBV	71466	186345	8.39%	2.745%
9	6.763	920	931	943	rBV	161483	382409	17.21%	5.633%
10	7.245	1002	1010	1029	rBV3	15738	60196	2.71%	0.887%
11	7.574	1056	1064	1074	rBV	48977	97752	4.40%	1.440%
12	8.647	1234	1240	1248	rBV	334717	535014	24.08%	7.881%
13	10.055	1465	1471	1482	rBV	332509	457999	20.61%	6.746%
14	10.756	1581	1586	1593	rBV	29186	42037	1.89%	0.619%
15	11.079	1634	1639	1645	rBV	307817	388821	17.50%	5.727%
16	11.421	1690	1695	1701	rBV	22972	30689	1.38%	0.452%
17	11.988	1784	1788	1790	rVV3	16568	24368	1.10%	0.359%
18	12.024	1790	1794	1802	rVB	346035	439229	19.77%	6.470%
19	12.219	1821	1826	1837	rBV	1832435	2222169	100.00%	32.732%
20	12.305	1837	1840	1851	rVB3	39985	77480	3.49%	1.141%
21	13.609	2046	2054	2060	rBV4	16129	22712	1.02%	0.335%
22	14.755	2234	2242	2245	rBV	25655	30775	1.38%	0.453%

Sum of corrected areas: 6789018

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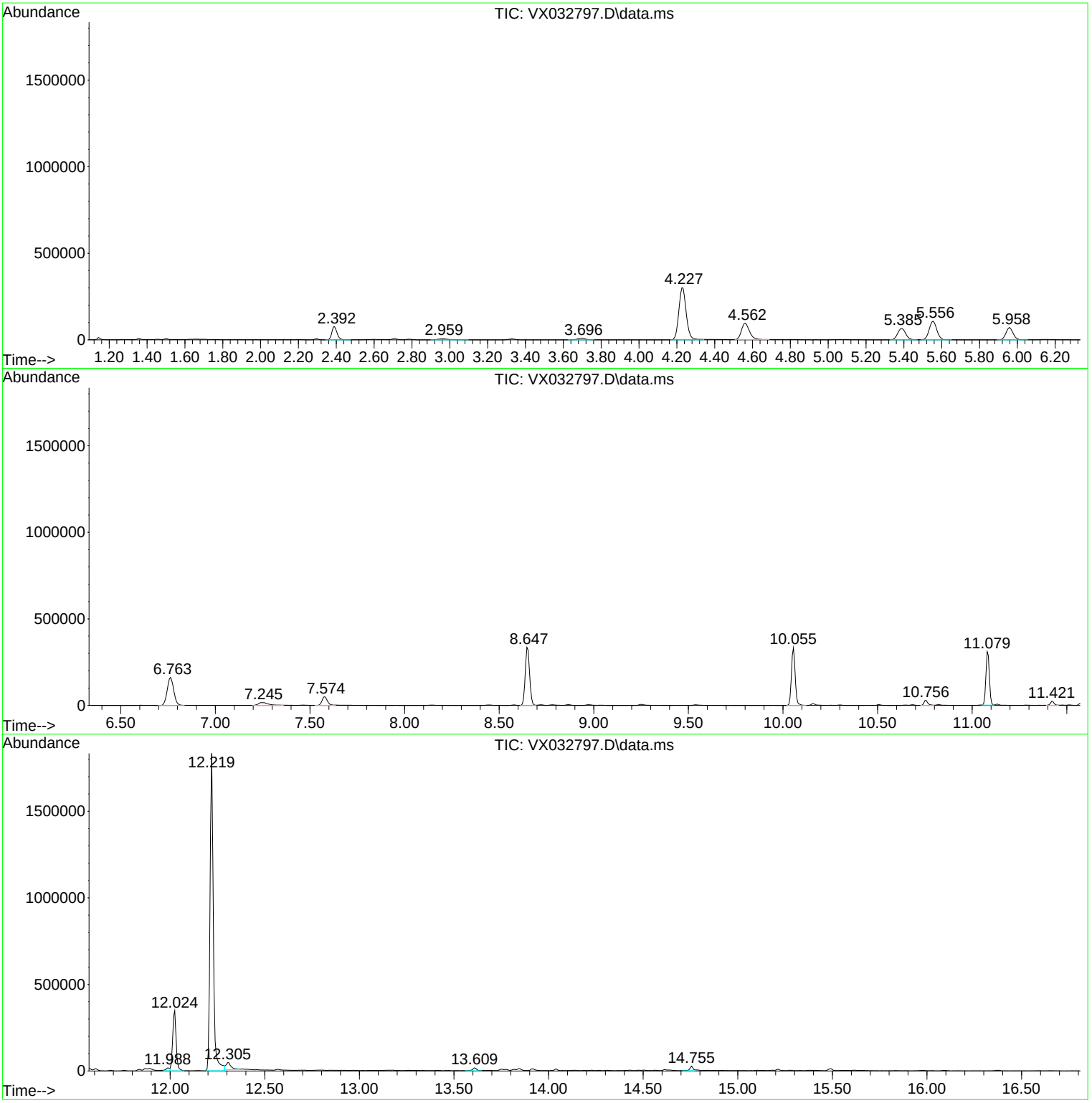
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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



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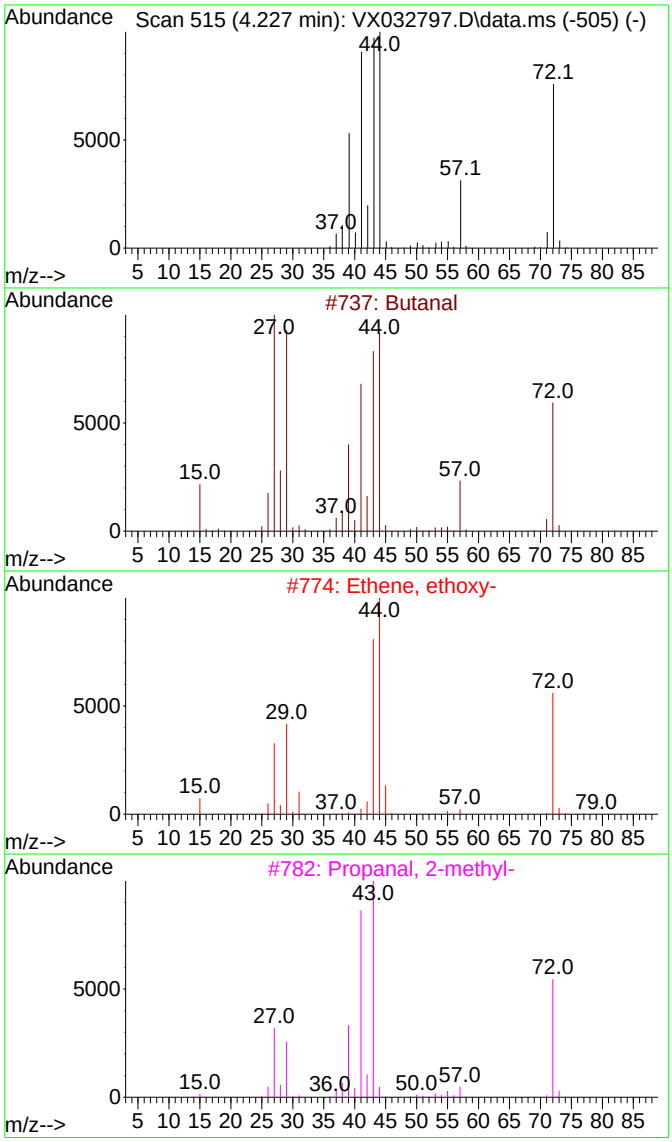
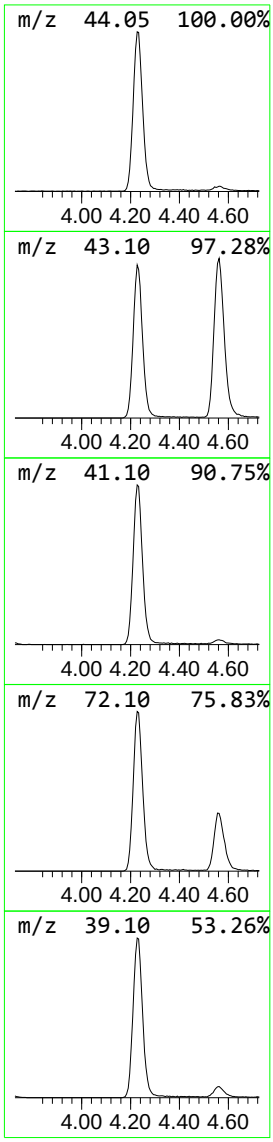
Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	136.11 ug/l	820697	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	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	Isobutylene epoxide	72	C4H8O	000558-30-5	27
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25





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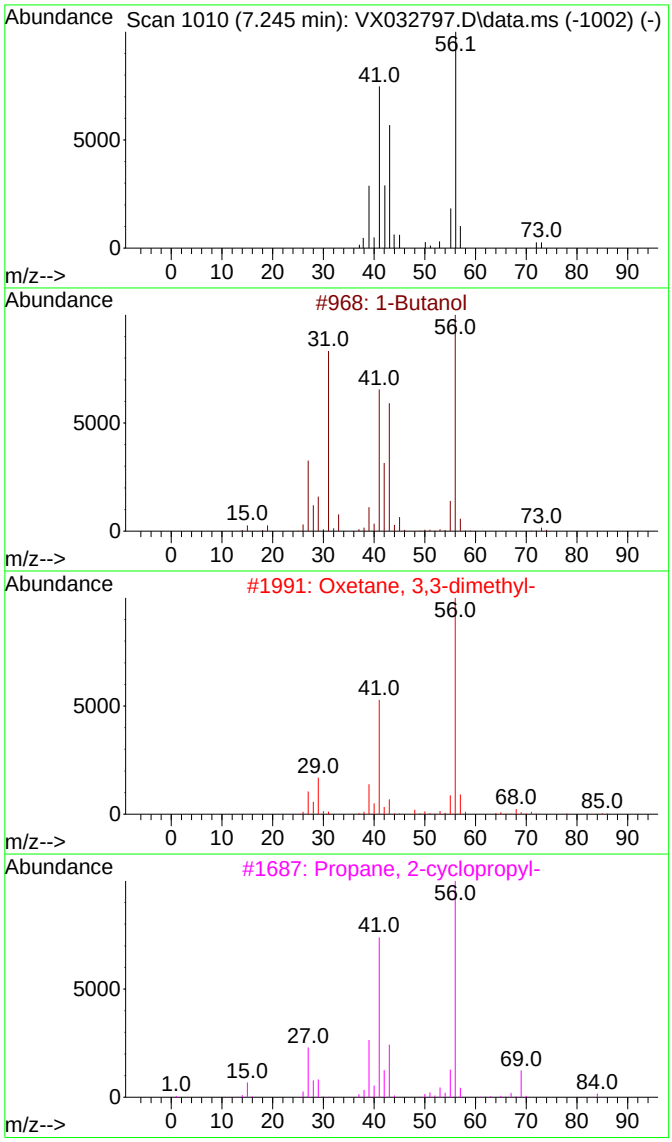
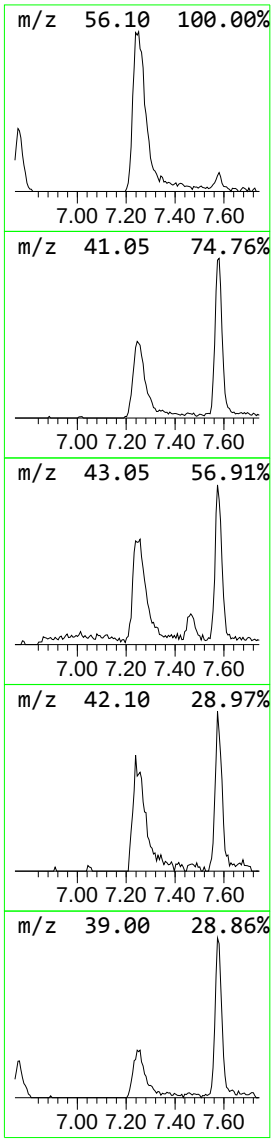
Peak Number 2 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.245	7.87 ug/l	60196	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	9





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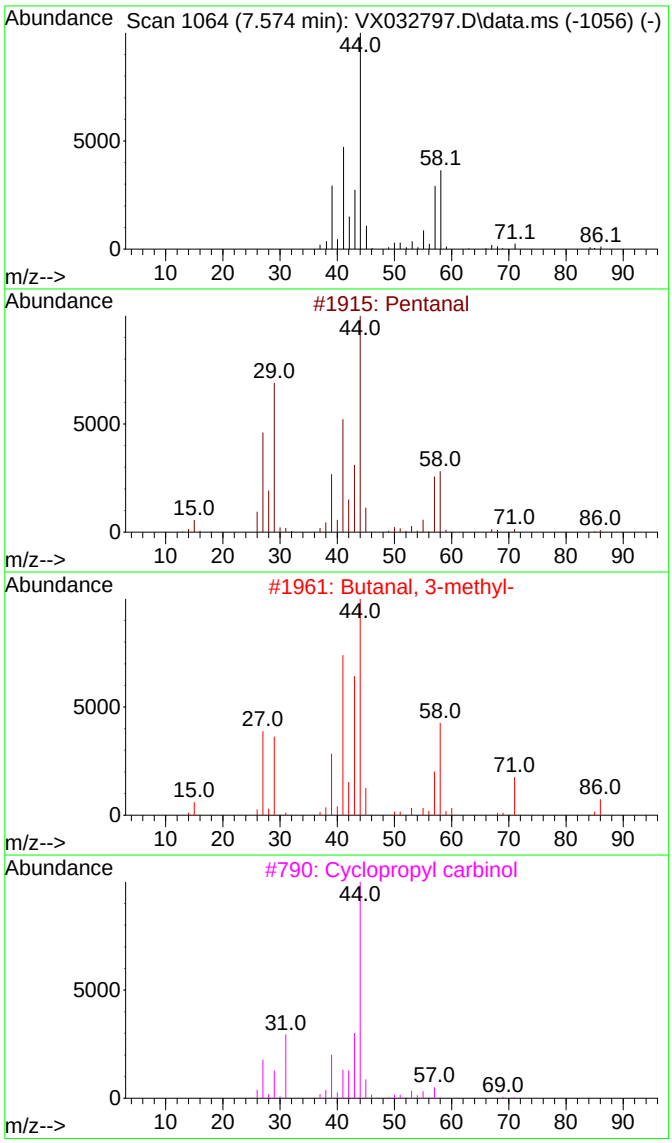
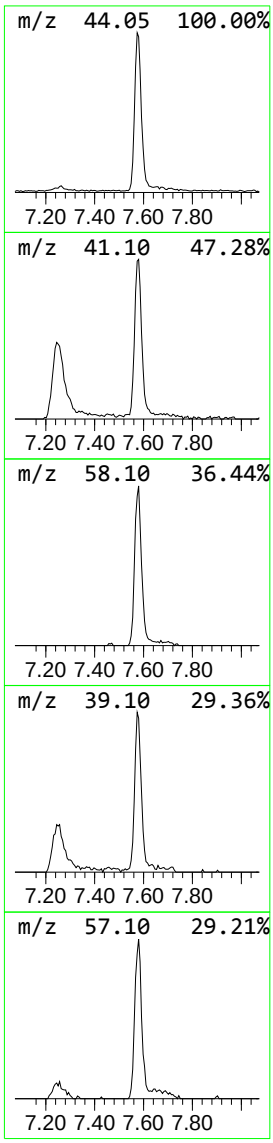
Peak Number 3 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	12.78 ug/l	97752	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	90
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	43
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	38
4	2-Formylhistamine	139	C6H9N3O	1000132-95-8	33
5	Ethylene oxide	44	C2H4O	000075-21-8	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
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TIC Library : C:\Database\NIST20.L
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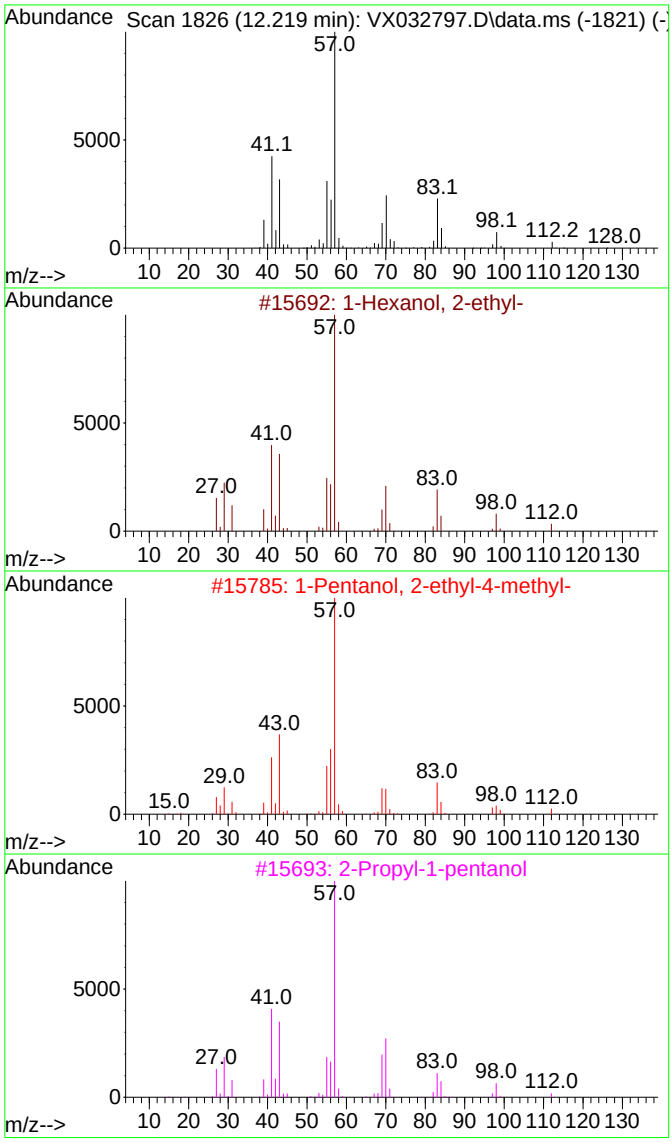
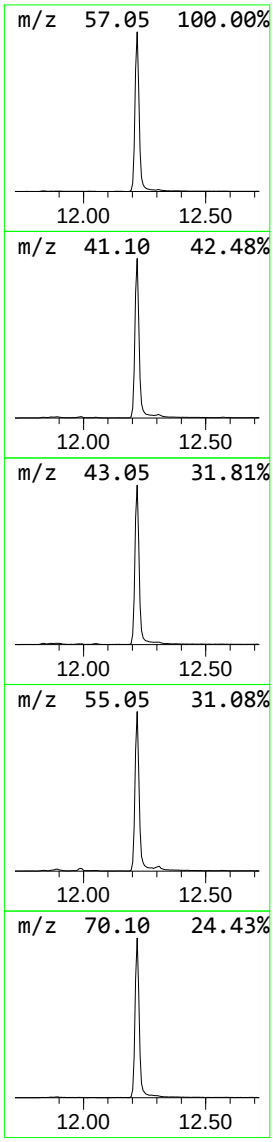
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	252.96 ug/l	2222170	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	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	45





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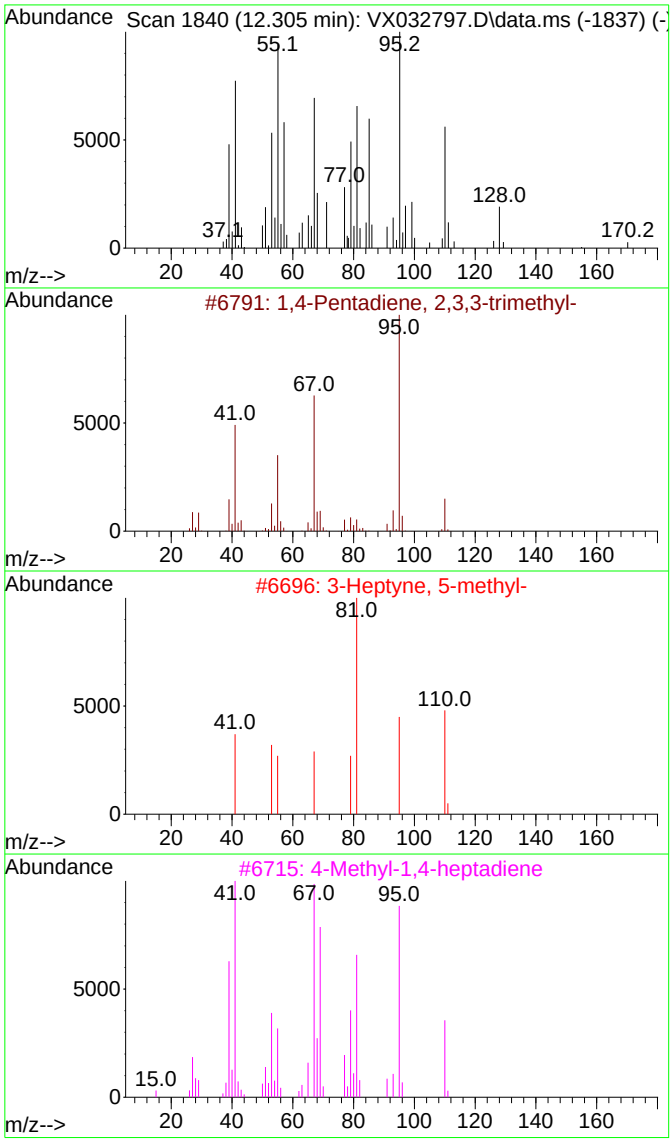
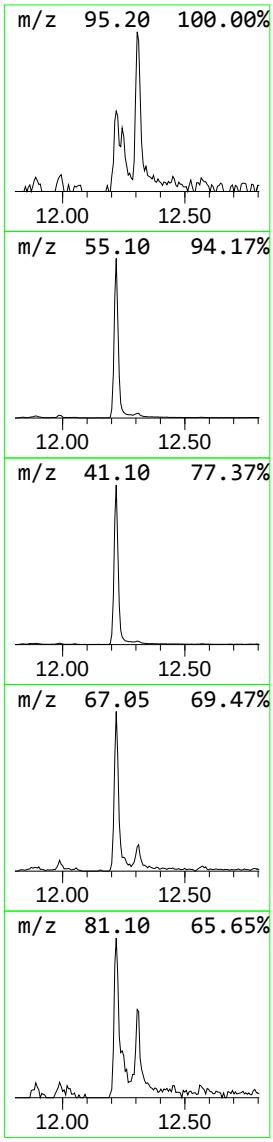
****
Peak Number 5 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.305	8.82 ug/l	77480	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	52
2	3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	46
3	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	42
4	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	38
5	Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	38





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	4.227	136.1	ug/l	820697	1	5.550	301475	50.0
1-Butanol	7.245	7.9	ug/l	60196	2	6.763	382409	50.0
Pentanal	7.574	12.8	ug/l	97752	2	6.763	382409	50.0
1-Hexanol, 2-et...	12.219	253.0	ug/l	2222170	4	12.024	439229	50.0
1,4-Pentadiene,...	12.305	8.8	ug/l	77480	4	12.024	439229	50.0