LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

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_D\Method\82D021324S.M
Title : SW846 8260

Signal : TIC: VD078439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.734	19	25	35	rBV	71853	121823	30.88%	4.070%
2	1.893	49	52	57	rVB3	3489	4310	1.09%	0.144%
3	2.164	91	98	100	rBV2	3700	7252	1.84%	0.242%
4	2.252	108	113	119	rBV4	6838	11481	2.91%	0.384%
5	2.422	136	142	149	rVB	16199	28430	7.21%	0.950%
6	2.564	161	166	169	rBV2	4168	8778	2.23%	0.293%
7	4.034	403	416	418	rBV3	4619	9836	2.49%	0.329%
8	4.799	539	546	548	rBV4	2842	4460	1.13%	0.149%
9	6.805	880	887	897	rBV4	5659	14496	3.68%	0.484%
10	7.075	923	933	944	rBV3	8267	24384	6.18%	0.815%
11	7.805	1048	1057	1063	rBV	44572	107557	27.27%	3.593%
12	7.875	1063	1069	1077	rVB2	60242	138523	35.12%	4.628%
13	8.234	1121	1130	1140	rBV	38997	91784	23.27%	3.066%
14	8.775	1215	1222	1233	rVB	103024	210273	53.31%	7.025%
15	9.352	1310	1320	1331	rVB2	15585	33977	8.61%	1.135%
16	10.157	1452	1457	1464	rBV3	24720	43437	11.01%	1.451%
17	10.269	1468	1476	1483	rBV	175364	323743	82.08%	10.816%
18	10.328	1483	1486	1491	rVB	5064	7868	1.99%	0.263%
19	10.669	1539	1544	1548	rBV3	5418	7585	1.92%	0.253%
20	11.022	1598	1604	1611	rBV2	83539	141847	35.96%	4.739%
21	11.581	1693	1699	1705	rBV	201420	345114	87.49%	11.530%
22	11.628	1705	1707	1713	rVB5	11105	16878	4.28%	0.564%
23	11.787	1729	1734	1745	rBV4	11953	23835	6.04%	0.796%
24	12.122	1785	1791	1798	rBV3	26273	46066	11.68%	1.539%
25	12.193	1798	1803	1811	rBV2	18163	31227	7.92%	1.043%
26	12.298	1815	1821	1825	rBV3	24792	42055	10.66%	1.405%
27	12.434	1837	1844	1845	rBV3	3114	5604	1.42%	0.187%
28	12.475	1846	1851	1852	rBV5	4089	4887	1.24%	0.163%
29	12.575	1862	1868	1876	rVB	169819	292305	74.11%	9.765%
30	12.828	1907	1911	1914	rVB3	5032	7003	1.78%	0.234%
31	12.904	1919	1924	1930	rVB3	15906	26763	6.79%	0.894%
32	13.063	1946	1951	1955	rVB4	7102	12595	3.19%	0.421%
33	13.169	1963	1969	1970	rBV4	6934	10327	2.62%	0.345%
34	13.210	1970	1976	1981	rVV2	32316	69714	17.67%	2.329%
35	13.251	1981	1983	1988	rVV4	12532	18521	4.70%	0.619%
36	13.328	1992	1996	1997	rVV4	6117	7867	1.99%	0.263%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

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_D\Method\82D021324S.M
Title : SW846 8260

37	13.357	1997	2001	2006	rVV3	30904	51355	13.02%	1.716%
38	13.434	2010	2014	2022	rVB6	14826	26031	6.60%	0.870%
39	13.516	2022	2028	2038	rBV	232746	394441	100.00%	13.177%
40	13.616	2041	2045	2049	rBV4	8929	13762	3.49%	0.460%
41	13.745	2065	2067	2073	rVB5	5303	10420	2.64%	0.348%
42	13.845	2077	2084	2093	rBV5	7504	22882	5.80%	0.764%
43	13.981	2103	2107	2115	rVV7	9688	19142	4.85%	0.639%
44	14.057	2116	2120	2124	rVB4	4250	6299	1.60%	0.210%
45	14.192	2135	2143	2146	rBV4	11577	21360	5.42%	0.714%
46	14.298	2155	2161	2167	rBV3	28616	46745	11.85%	1.562%
47	14.698	2225	2229	2232	rBV4	3980	4712	1.19%	0.157%
48	14.769	2236	2241	2248	rVB8	2968	6810	1.73%	0.228%
49	15.051	2283	2289	2293	rVB7	8798	16607	4.21%	0.555%
50	15.328	2327	2336	2343	rBV6	6770	19328	4.90%	0.646%
51	15.686	2395	2397	2401	rBV5	3323	4378	1.11%	0.146%
52	16.257	2489	2494	2499	rVB5	3795	6773	1.72%	0.226%
53	16.404	2512	2519	2523	rBV6	5002	8854	2.24%	0.296%
54	16.592	2546	2551	2559	rBV5	5113	10789	2.74%	0.360%

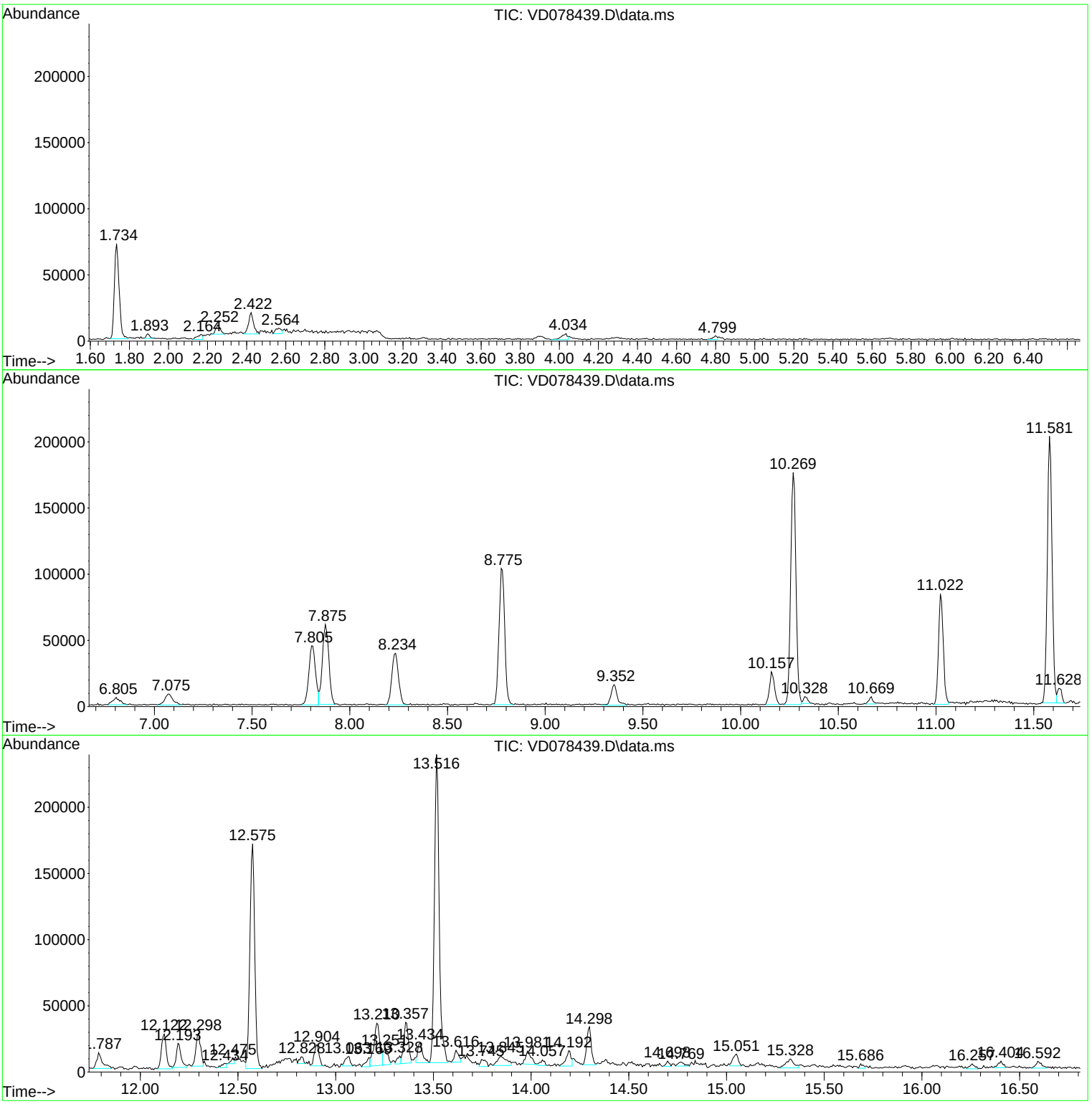
Sum of corrected areas: 2993293

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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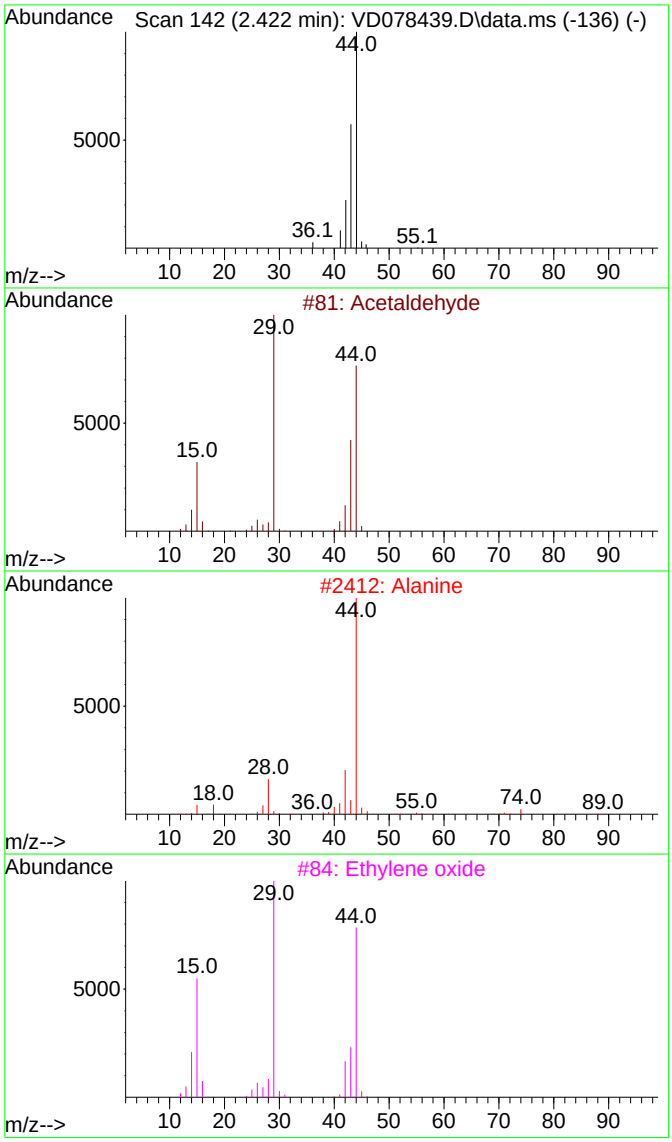
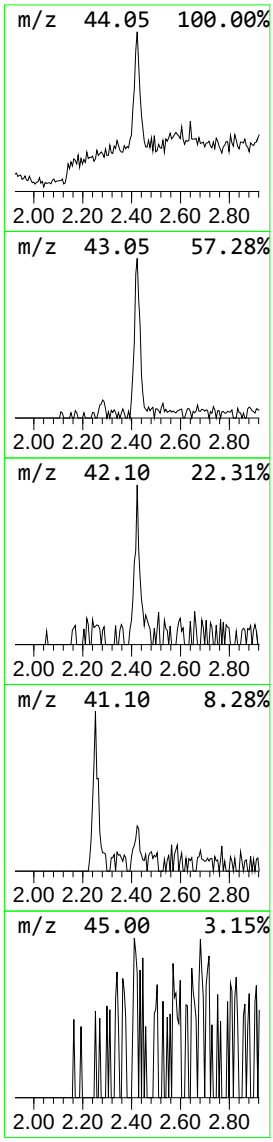
Peak Number 2 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.422	10.26 ug/l	28430	Pentafluorobenzene	7.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Alanine	89	C3H7NO2	000056-41-7	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Acetonitrile-d3	44	C2D3N	002206-26-0	5
5	Propane	44	C3H8	000074-98-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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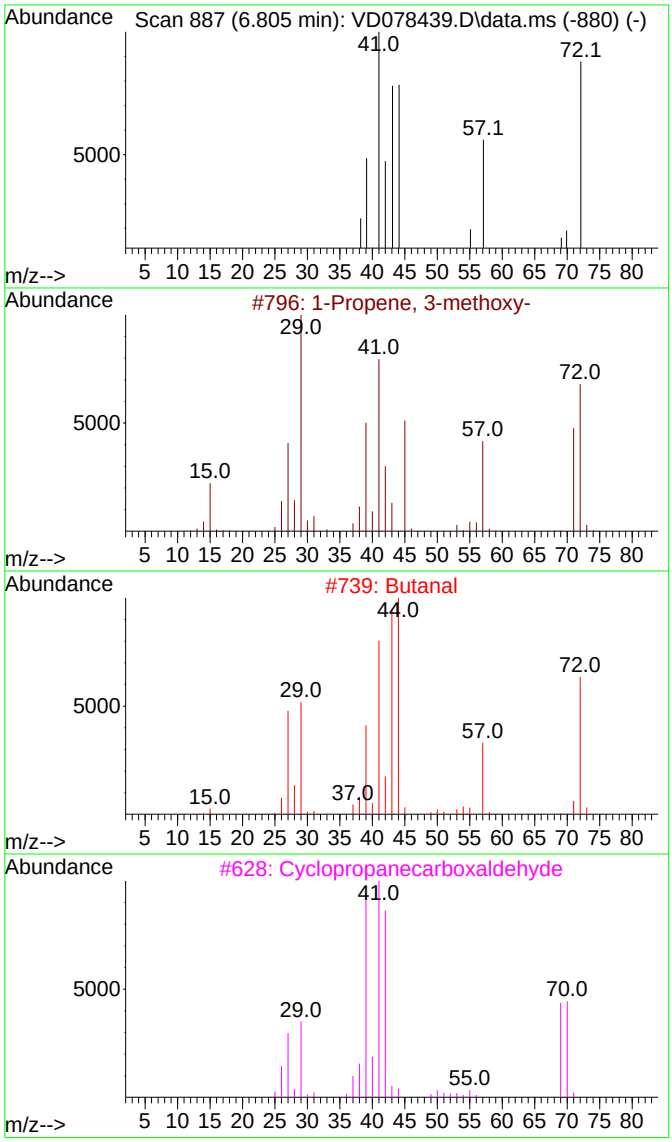
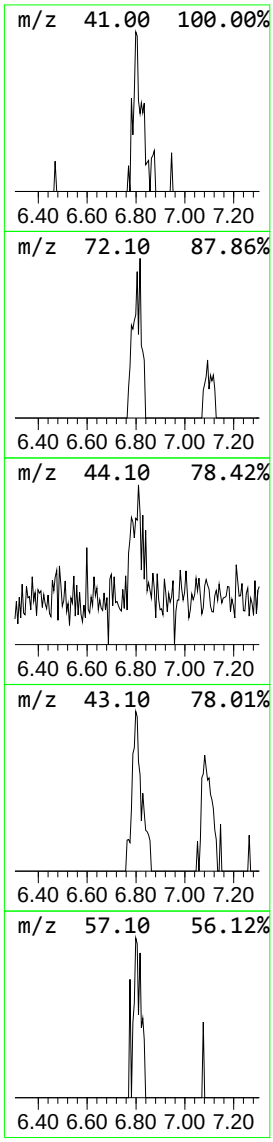
Peak Number 3 unknown6.805 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.805	5.23 ug/l	14496	Pentafluorobenzene	7.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
2	Butanal	72	C4H8O	000123-72-8	17
3	Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	10
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	9
5	2-Methylene-1,3-propanediol	88	C4H8O2	003513-81-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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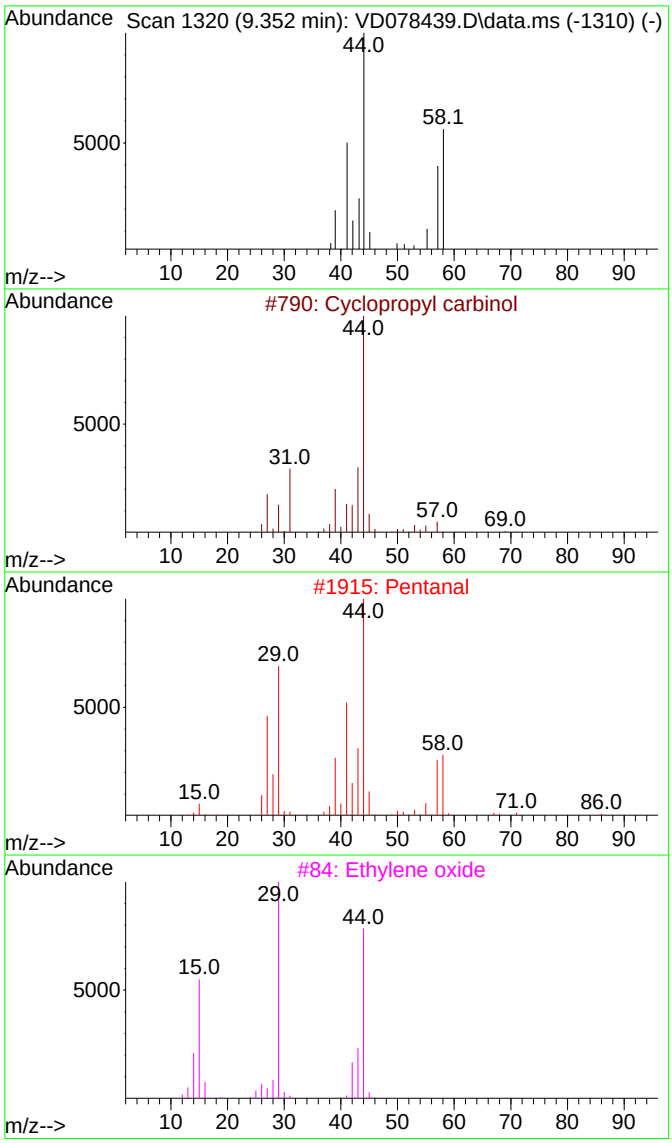
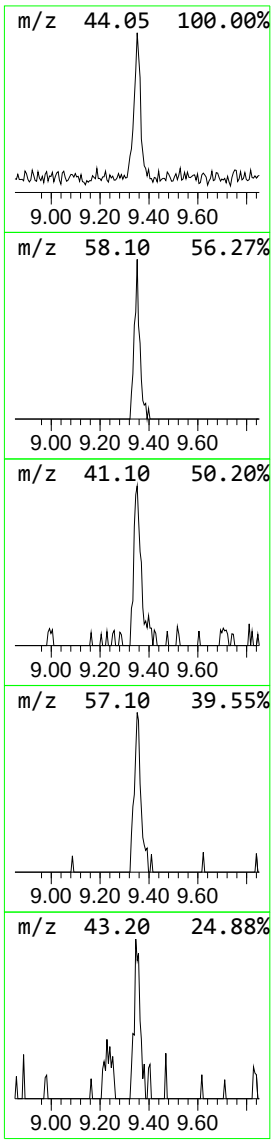
Peak Number 5 unknown9.352 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.352	8.08 ug/l	33977	1,4-Difluorobenzene	8.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
2	Pentanal	86	C5H10O	000110-62-3	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Acetaldehyde	44	C2H4O	000075-07-0	5
5	Ethene, methoxy-	58	C3H6O	000107-25-5	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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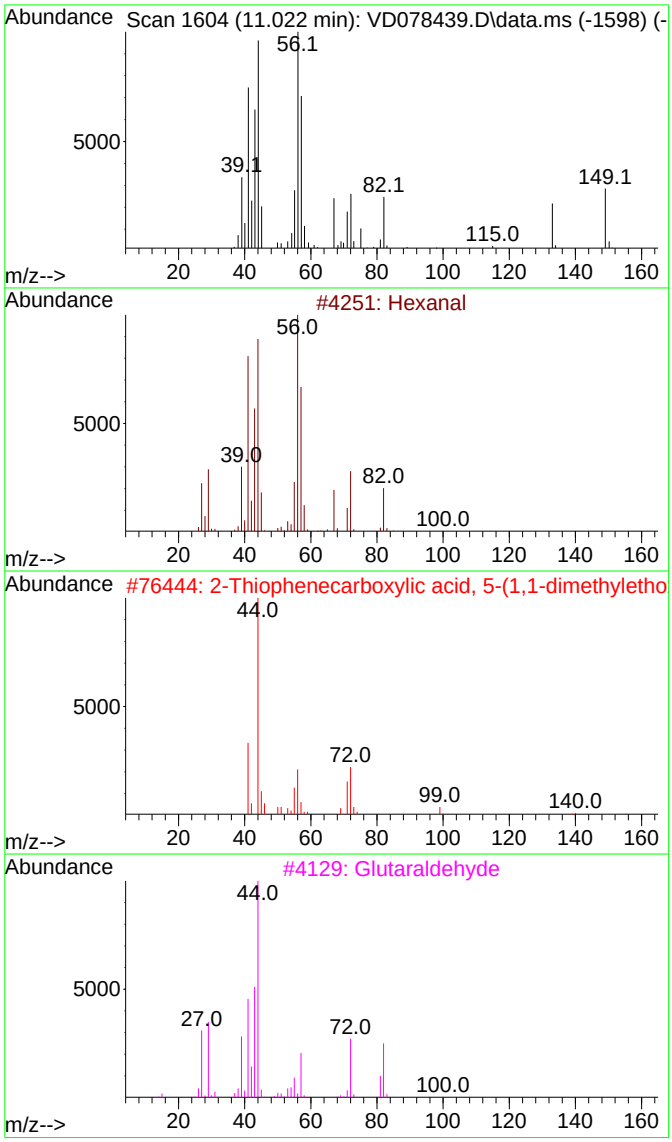
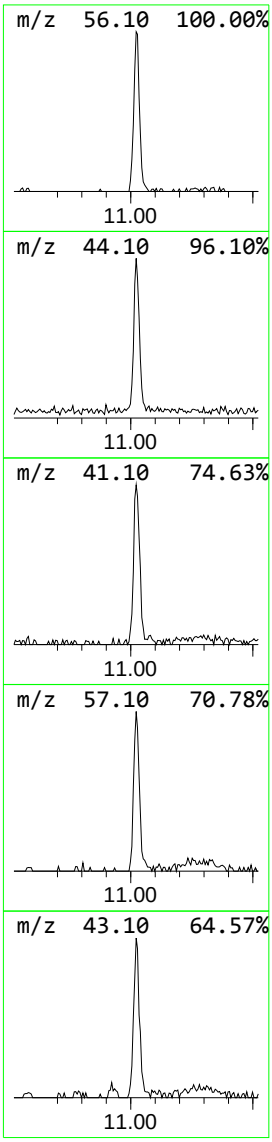
Peak Number 6 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.022	20.55 ug/l	141847	Chlorobenzene-d5	11.581

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	2-Thiophenecarboxylic acid, 5-(1...	200	C9H12O3S	054889-42-8	35
3	Glutaraldehyde	100	C5H8O2	000111-30-8	25
4	Butanal	72	C4H8O	000123-72-8	25
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
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Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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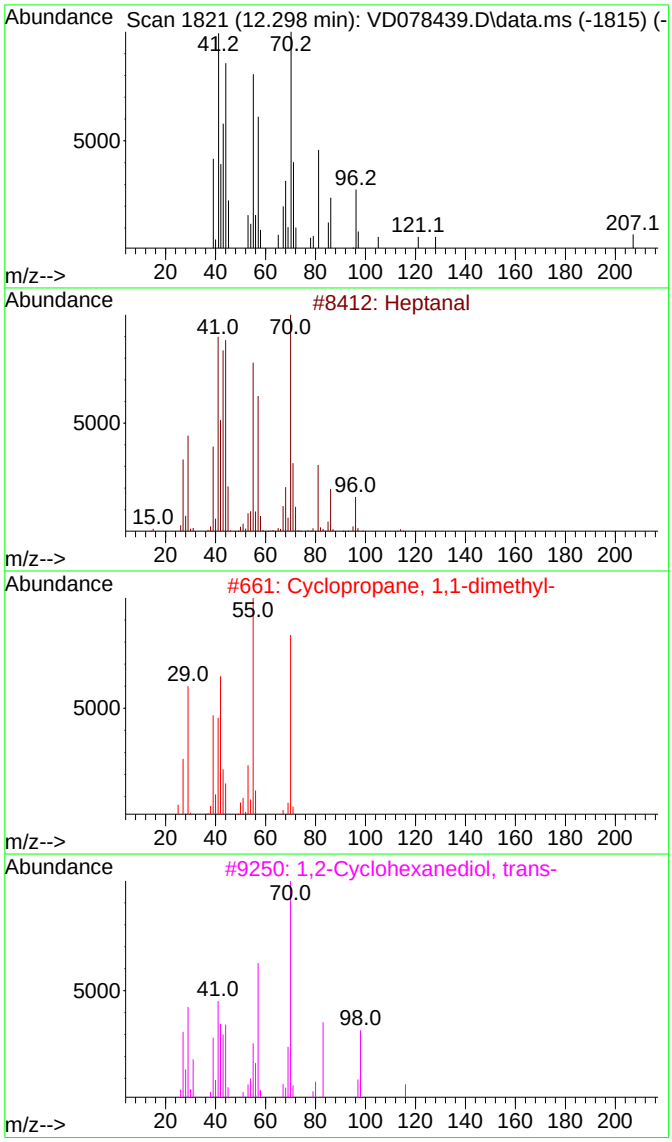
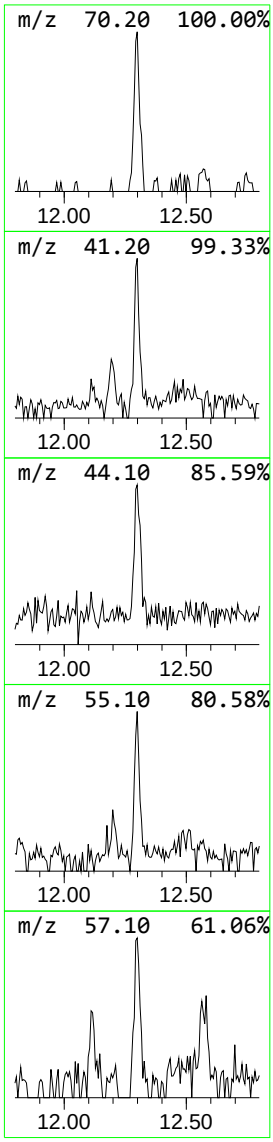
Peak Number 7 Heptanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.298	6.09 ug/l	42055	Chlorobenzene-d5	11.581

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	78
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	30
3	1,2-Cyclohexanediol, trans-	116	C6H12O2	001460-57-7	27
4	cis-1,2-Cyclohexanediol	116	C6H12O2	001792-81-0	27
5	2-Octenal, (E)-	126	C8H14O	002548-87-0	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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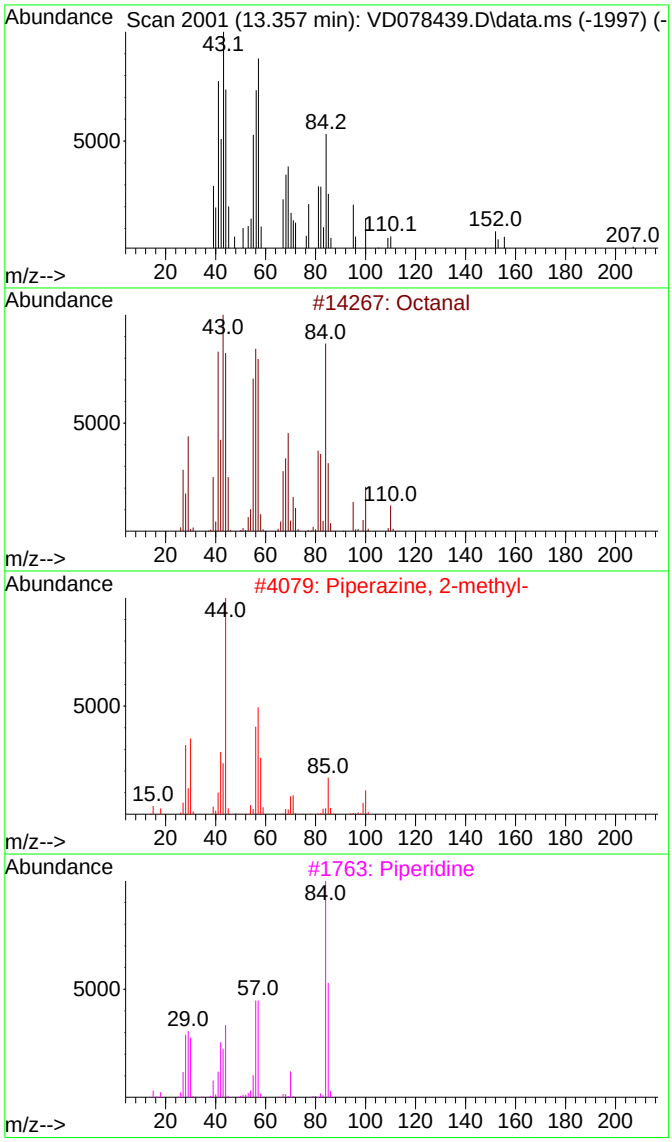
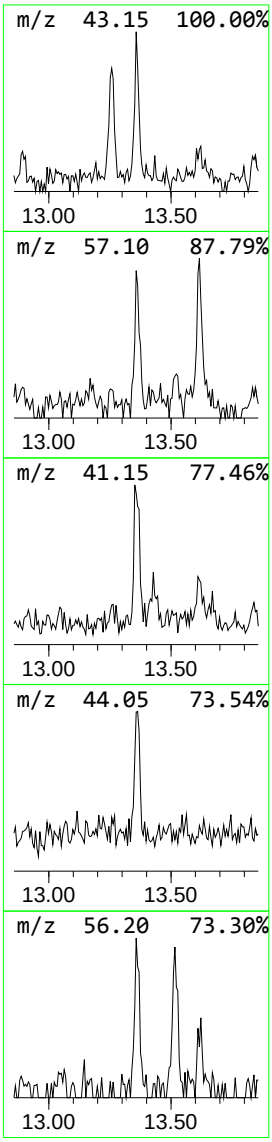
Peak Number 8 Octanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	6.51 ug/l	51355	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	86
2	Piperazine, 2-methyl-	100	C5H12N2	000109-07-9	49
3	Piperidine	85	C5H11N	000110-89-4	47
4	Hexanal	100	C6H12O	000066-25-1	43
5	2-Acetylpiperidine	127	C7H13NO	097073-22-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
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Operator : RP/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.M
Quant Title : SW846 8260

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

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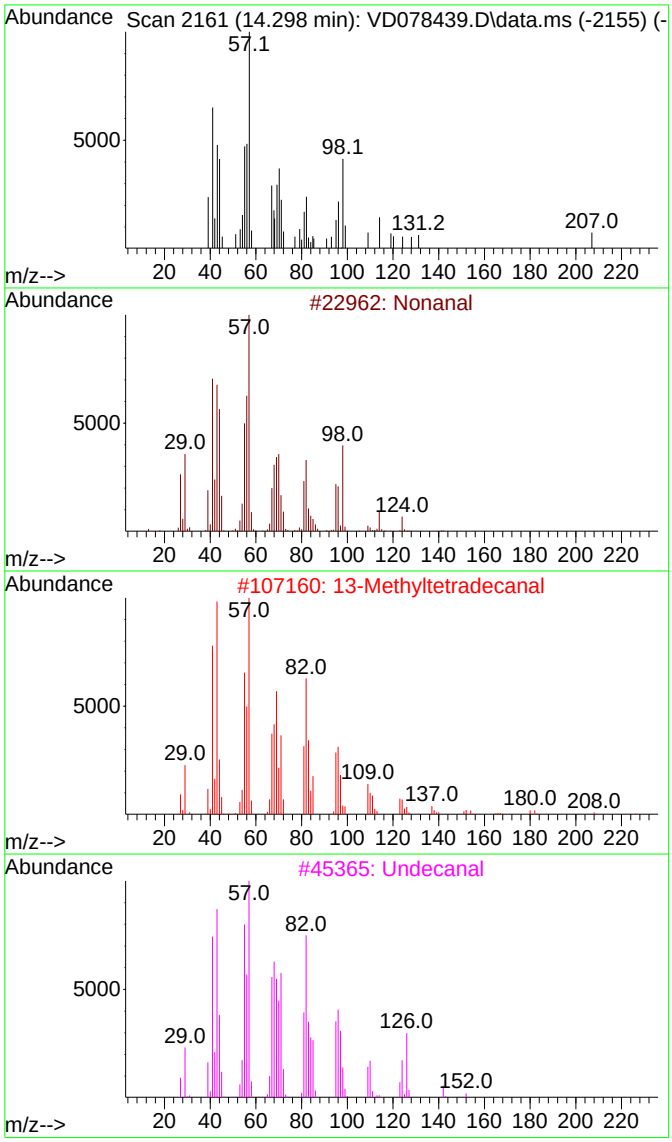
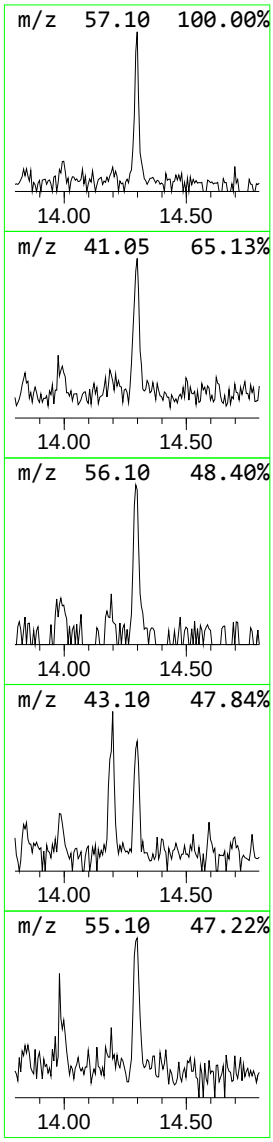
Peak Number 9 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.298	5.93 ug/l	46745	1,4-Dichlorobenzene-d4	13.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	50
2	13-Methyltetradecanal	226	C15H30O	075853-51-9	50
3	Undecanal	170	C11H22O	000112-44-7	47
4	Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	38
5	Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD021524\
Data File : VD078439.D
Acq On : 15 Feb 2024 16:46
Operator : RP/MD
Sample : P1471-01
Misc : 5.03G/5ml/MSVOA_D/SOIL/A
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021324S.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
Acetaldehyde	2.422	10.3	ug/l	28430	1	7.881	138523	50.0
unknown6.805	6.805	5.2	ug/l	14496	1	7.881	138523	50.0
unknown9.352	9.352	8.1	ug/l	33977	2	8.775	210273	50.0
Hexanal	11.022	20.6	ug/l	141847	3	11.581	345114	50.0
Heptanal	12.298	6.1	ug/l	42055	3	11.581	345114	50.0
Octanal	13.357	6.5	ug/l	51355	4	13.516	394441	50.0
Nonanal	14.298	5.9	ug/l	46745	4	13.516	394441	50.0