LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
LabSampleId : VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_U\Method\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.385	6	14	28	rBV	167448	180863	5.65%	0.229%
2	1.520	49	56	71	rVB	173953	194943	6.09%	0.246%
3	1.607	75	83	90	rBV	208327	226224	7.07%	0.286%
4	1.684	99	107	118	rBV	123934	144817	4.52%	0.183%
5	1.829	145	152	169	rVB	138588	150165	4.69%	0.190%
6	1.912	169	178	194	rVB	127889	178873	5.59%	0.226%
7	2.128	234	245	266	rVB	276168	421775	13.18%	0.533%
8	2.379	312	323	342	rVB	233221	340828	10.65%	0.431%
9	2.488	347	357	370	rVB	43968	70668	2.21%	0.089%
10	2.578	370	385	393	rBV	531239	922146	28.81%	1.165%
11	2.629	393	401	418	rVV	316579	538883	16.84%	0.681%
12	2.719	418	429	441	rVV	102848	184368	5.76%	0.233%
13	2.790	441	451	472	rVB	206569	359072	11.22%	0.454%
14	2.925	472	493	517	rBV2	271622	864932	27.02%	1.093%
15	3.047	517	531	555	rVB	255675	502090	15.69%	0.635%
16	3.202	559	579	600	rBV2	125311	332287	10.38%	0.420%
17	3.318	600	615	621	rVV	474493	976847	30.52%	1.235%
18	3.359	622	628	658	rVB2	541477	1236376	38.63%	1.563%
19	3.871	769	787	800	rBV	184720	436917	13.65%	0.552%
20	3.957	800	814	842	rBV2	769455	2550629	79.69%	3.224%
21	4.671	1016	1036	1041	rBV	461384	1055791	32.99%	1.334%
22	4.777	1058	1069	1084	rBV2	264327	770895	24.08%	0.974%
23	4.977	1115	1131	1143	rBV2	402704	870305	27.19%	1.100%
24	5.054	1143	1155	1164	rBV	501431	1175604	36.73%	1.486%
25	5.314	1214	1236	1246	rBV2	291482	903541	28.23%	1.142%
26	5.385	1246	1258	1271	rVV2	555947	1358038	42.43%	1.716%
27	5.462	1271	1282	1291	rVV	276738	567118	17.72%	0.717%
28	5.530	1291	1303	1327	rVB	522064	1090450	34.07%	1.378%
29	5.707	1343	1358	1368	rBV	197783	417774	13.05%	0.528%
30	5.780	1368	1381	1406	rVV2	586413	1474410	46.06%	1.863%
31	5.916	1409	1423	1456	rVB	301368	595408	18.60%	0.753%
32	6.253	1511	1528	1552	rBV	405124	763242	23.85%	0.965%
33	6.546	1604	1619	1647	rBV	351385	654808	20.46%	0.828%
34	6.768	1671	1688	1714	rBV3	482487	1542396	48.19%	1.949%
35	6.922	1722	1736	1741	rBV	216401	380417	11.89%	0.481%
36	6.964	1742	1749	1763	rVV2	436500	768570	24.01%	0.971%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
LabSampleId : VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_U\Method\82U092821W.M
Title : SW846 8260

37	7.044	1763	1774	1783	rVV	306214	554794	17.33%	0.701%
38	7.108	1784	1794	1826	rVB	298383	614934	19.21%	0.777%
39	7.369	1859	1875	1892	rBV	99211	190924	5.96%	0.241%
40	7.465	1892	1905	1924	rVB	810155	1360693	42.51%	1.720%
41	7.610	1937	1950	1976	rVB	367359	631523	19.73%	0.798%
42	7.796	1991	2008	2028	rBV	1847876	3200755	100.00%	4.045%
43	7.903	2028	2041	2052	rVV	649669	1130038	35.31%	1.428%
44	7.973	2052	2063	2085	rVB	737760	1246686	38.95%	1.576%
45	8.214	2122	2138	2156	rBV	372968	611825	19.12%	0.773%
46	8.337	2164	2176	2186	rBV	460120	716971	22.40%	0.906%
47	8.404	2186	2197	2225	rVB	423340	730666	22.83%	0.923%
48	8.558	2232	2245	2263	rBV2	551934	1482857	46.33%	1.874%
49	8.690	2273	2286	2312	rBV	1493995	2429529	75.90%	3.071%
50	8.835	2312	2331	2348	rVV2	506639	1165728	36.42%	1.473%
51	8.928	2348	2360	2379	rVB	209407	349770	10.93%	0.442%
52	9.420	2499	2513	2518	rBV	618108	1058119	33.06%	1.337%
53	9.539	2537	2550	2554	rBV	438701	705937	22.06%	0.892%
54	9.575	2554	2561	2580	rVB	870377	1381294	43.16%	1.746%
55	9.697	2584	2599	2628	rVB	1658115	2715703	84.85%	3.432%
56	10.111	2709	2728	2743	rBV4	1352074	2661989	83.17%	3.364%
57	10.295	2772	2785	2788	rBV	234575	340350	10.63%	0.430%
58	10.324	2788	2794	2822	rVB	558541	905826	28.30%	1.145%
59	10.488	2832	2845	2855	rBV	946687	1457619	45.54%	1.842%
60	10.549	2855	2864	2880	rVV	331844	537499	16.79%	0.679%
61	10.636	2880	2891	2911	rVB	511874	800587	25.01%	1.012%
62	10.787	2924	2938	2945	rBV	1033971	1688639	52.76%	2.134%
63	10.828	2945	2951	2966	rVV2	541808	1209858	37.80%	1.529%
64	10.909	2966	2976	2989	rVV	958474	1459275	45.59%	1.844%
65	10.989	2989	3001	3016	rVB	792585	1243852	38.86%	1.572%
66	11.095	3021	3034	3052	rVB3	1584299	2694510	84.18%	3.405%
67	11.423	3116	3136	3144	rBV2	1226671	2142898	66.95%	2.708%
68	11.472	3144	3151	3165	rVB	960652	1479685	46.23%	1.870%
69	11.645	3187	3205	3220	rBV	968600	1494439	46.69%	1.889%
70	11.748	3224	3237	3244	rBV	696739	1076394	33.63%	1.360%
71	11.800	3244	3253	3261	rBV3	1023513	2085322	65.15%	2.636%
72	12.214	3367	3382	3402	rBV2	1555690	2416046	75.48%	3.054%
73	12.478	3449	3464	3478	rBV	451039	733160	22.91%	0.927%
74	12.999	3610	3626	3646	rVB2	227315	401383	12.54%	0.507%
75	13.208	3679	3691	3711	rVB	23130	39161	1.22%	0.049%
76	13.449	3753	3766	3786	rVB	917639	1391061	43.46%	1.758%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
LabSampleId : VSTDCCC050

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_U\Method\82U092821W.M
Title : SW846 8260

77	13.841	3876	3888	3904	rBV	523616	829169	25.91%	1.048%
78	14.025	3933	3945	3954	rBV2	359915	555791	17.36%	0.702%
79	14.089	3954	3965	3986	rVB	726721	1166029	36.43%	1.474%
80	14.333	4028	4041	4060	rVB	528655	831199	25.97%	1.051%

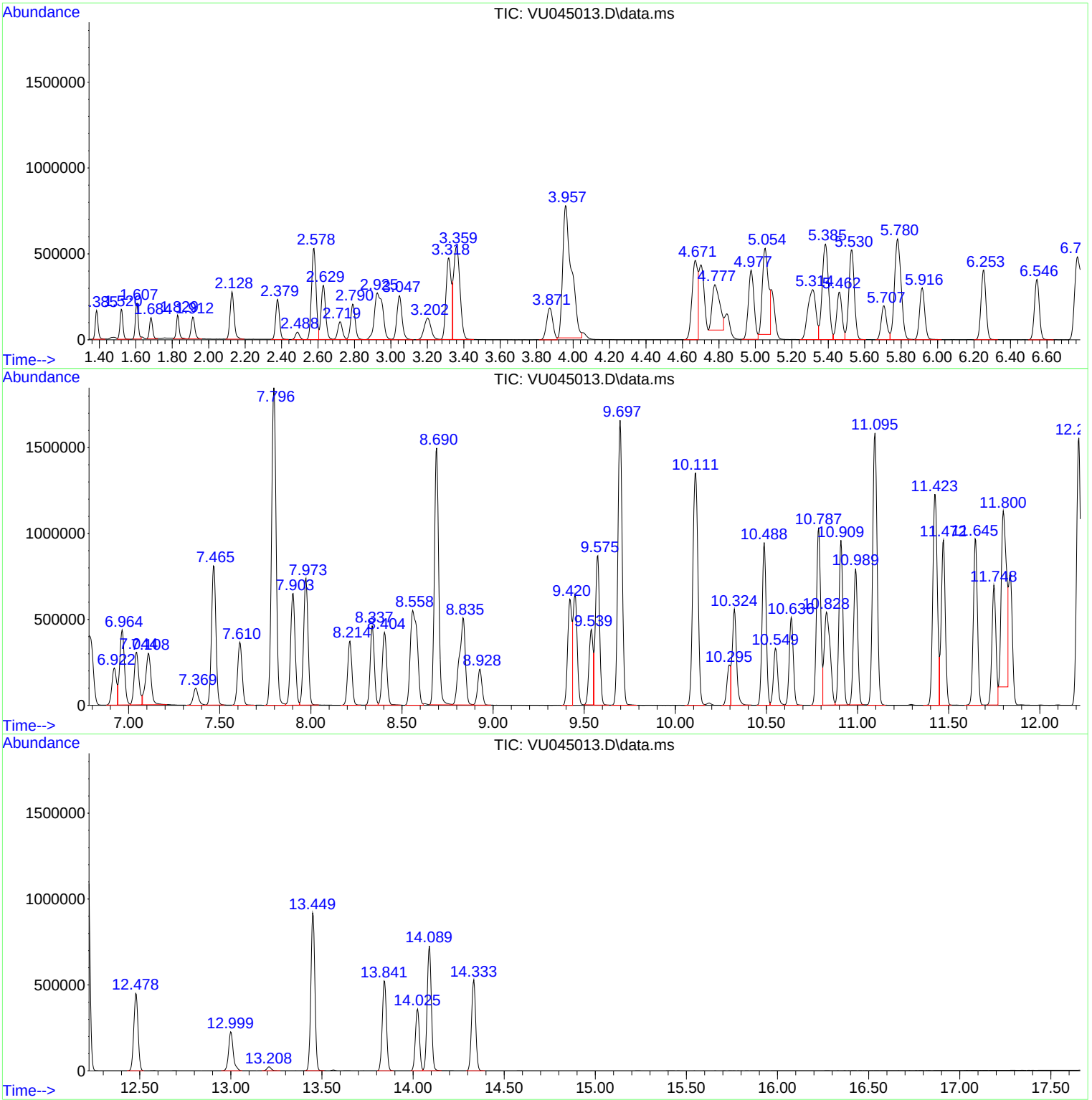
Sum of corrected areas: 79122957

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

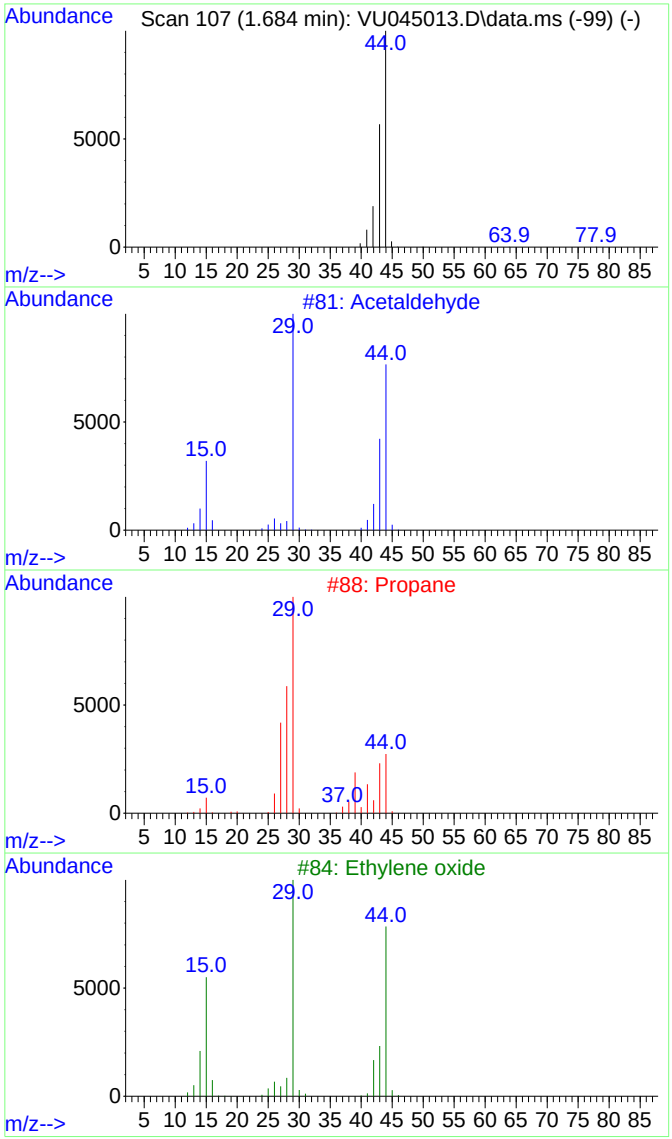
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

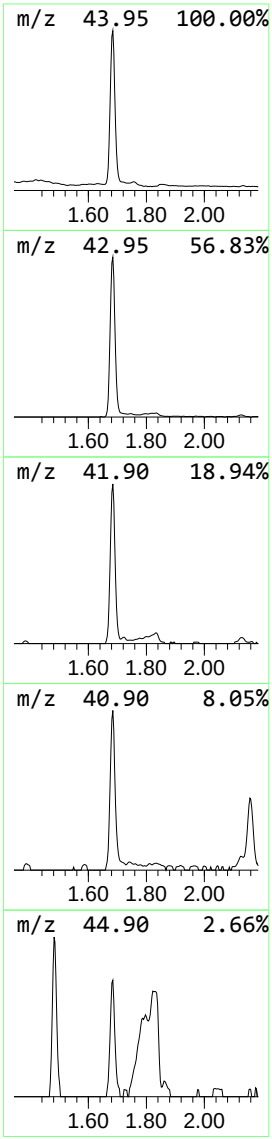
****

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.684	5.33 ug/l	144817	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
LabSampleId : VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

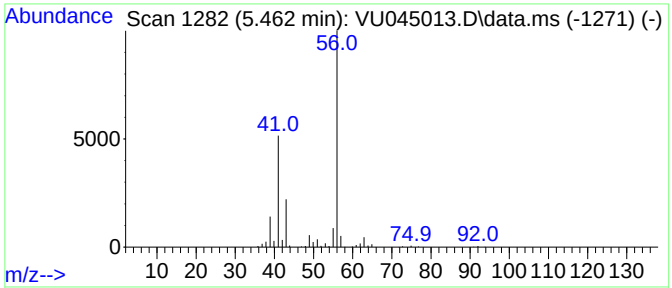
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

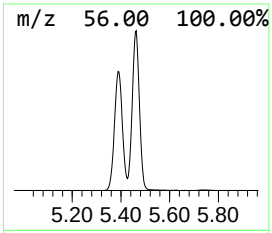
****

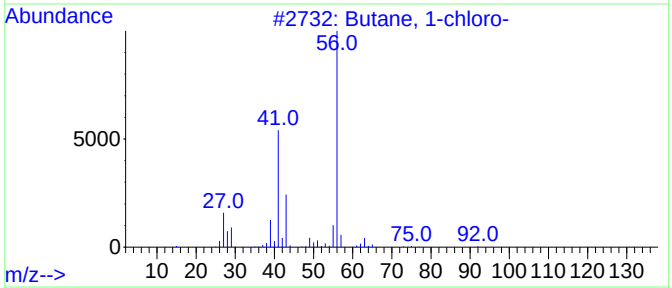
Peak Number 2 Butane, 1-chloro- Concentration Rank 3

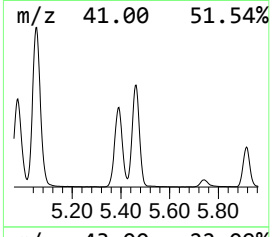
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.462	20.88 ug/l	567118	Pentafluorobenzene	5.375

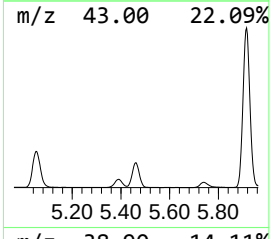
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	91
2	Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	72
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	39
4	Ethane, diazo-	56	C2H4N2	001117-96-0	9
5	Butane, 2-chloro-	92	C4H9Cl	000078-86-4	9

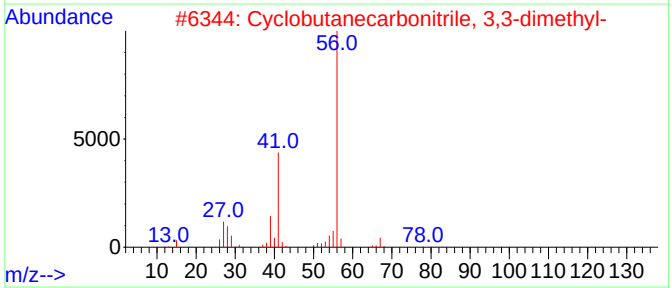


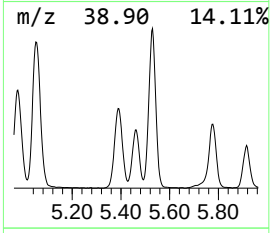


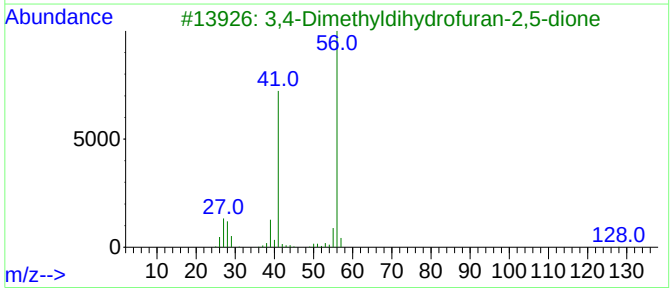


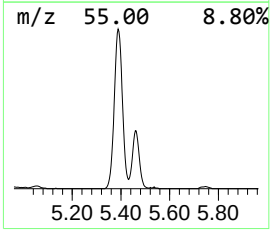












Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

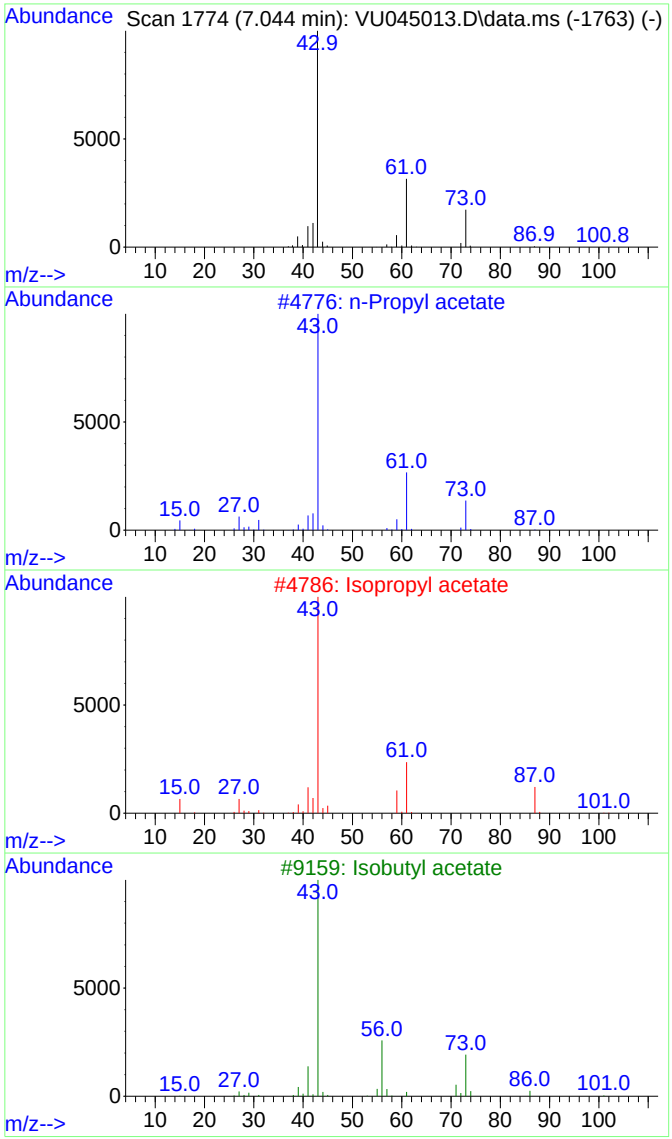
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

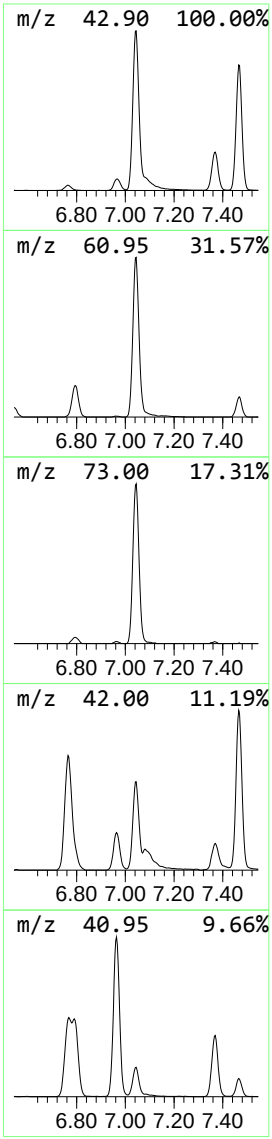
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	36.34 ug/l	554794	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	36
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

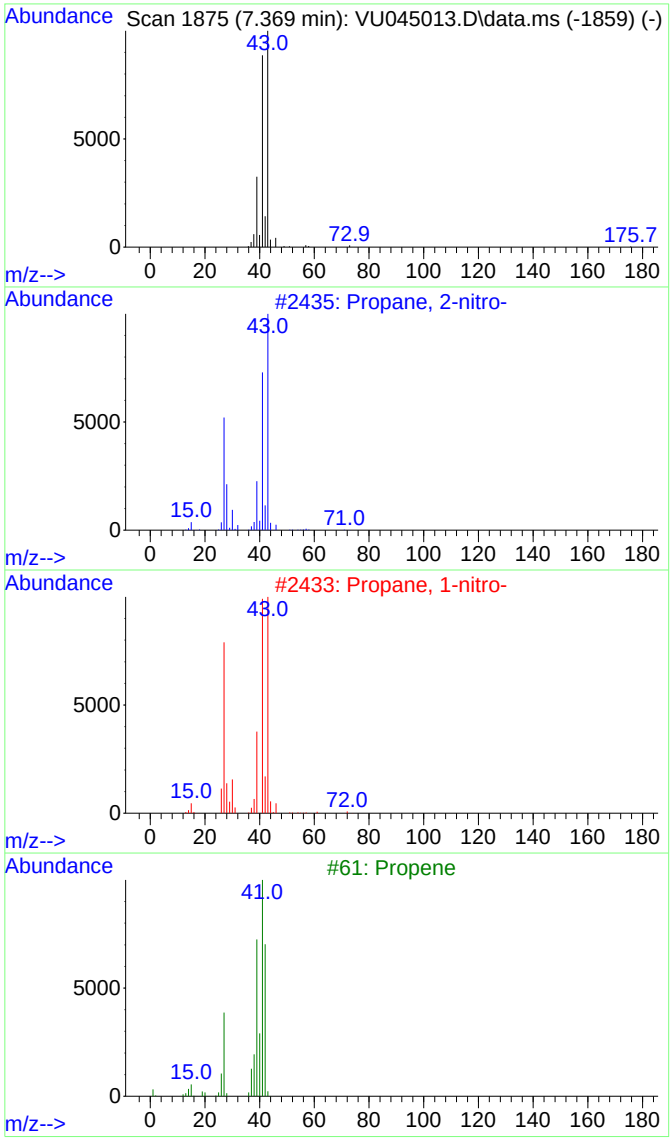
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

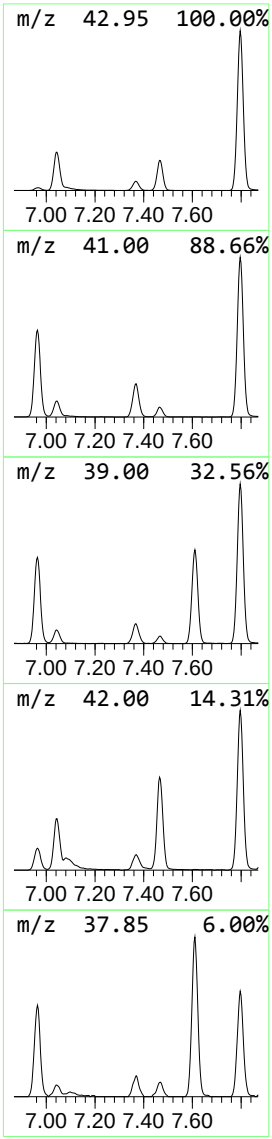
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propane, 2-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.369	12.51 ug/l	190924	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	64
2	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	45
3	Propene	42	C3H6	000115-07-1	9
4	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
5	1H-Pyrazol-1-amine, 5-methyl-3-n...	142	C4H6N4O2	151588-03-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
LabSampleId :
VSTDCCC050

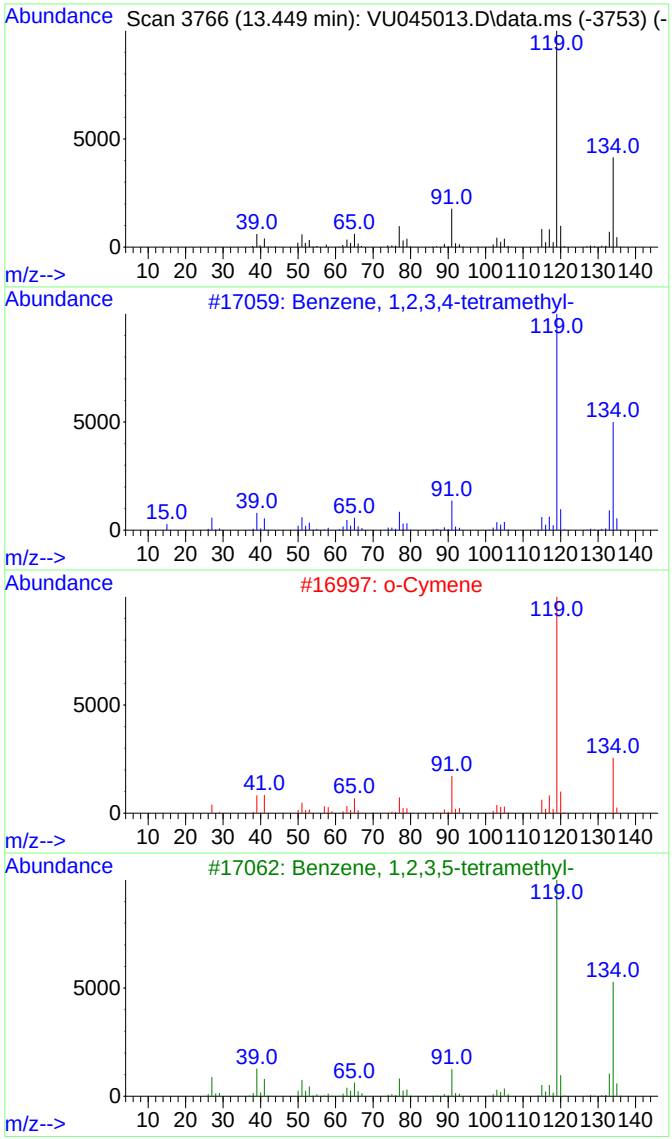
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

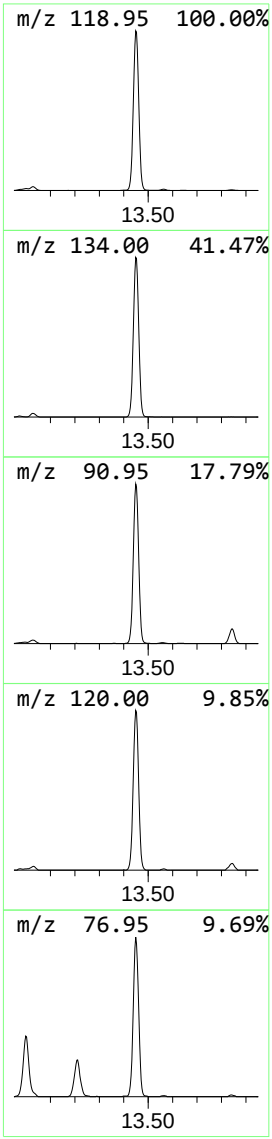
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.449	33.35 ug/l	1391060	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045013.D
Acq On : 29 Sep 2021 23:31
Operator : SY/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument : MSVOA_U
LabSampleId : VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.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	1.684	5.3	ug/l	144817	1	5.375	1358040	50.0
Butane, 1-chloro-	5.462	20.9	ug/l	567118	1	5.375	1358040	50.0
n-Propyl acetate	7.044	36.3	ug/l	554794	2	6.253	763242	50.0
Propane, 2-nitro-	7.369	12.5	ug/l	190924	2	6.253	763242	50.0
Benzene, 1,2,3,...	13.449	33.4	ug/l	1391060	4	11.816	2085320	50.0