LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

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_U\Method\82U110521W.M
Title : SW846 8260

Signal : TIC: VU045607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.588	70	77	92	rBV	26193	29082	1.69%	0.220%
2	2.623	387	399	422	rBV	94731	161679	9.40%	1.225%
3	2.752	427	439	464	rVB	18534	37181	2.16%	0.282%
4	3.173	552	570	594	rBV	742734	1597321	92.86%	12.099%
5	4.449	951	967	985	rBV3	7912	20831	1.21%	0.158%
6	4.703	1033	1046	1067	rVB	62744	137766	8.01%	1.044%
7	4.973	1116	1130	1151	rBV2	20067	46301	2.69%	0.351%
8	5.292	1213	1229	1243	rBV	136987	286046	16.63%	2.167%
9	5.375	1243	1255	1273	rVB	205856	420121	24.42%	3.182%
10	5.706	1342	1358	1372	rBV	152165	306932	17.84%	2.325%
11	6.153	1484	1497	1510	rBV2	13921	30293	1.76%	0.229%
12	6.253	1513	1528	1558	rVV	327438	620920	36.10%	4.703%
13	6.767	1677	1688	1707	rVB2	15997	30525	1.77%	0.231%
14	7.166	1786	1812	1851	rBV	866421	1720199	100.00%	13.030%
15	7.793	1995	2007	2022	rBV	44521	79563	4.63%	0.603%
16	7.899	2027	2040	2053	rVV	508966	890927	51.79%	6.748%
17	7.970	2053	2062	2075	rVB	84579	143304	8.33%	1.085%
18	8.221	2122	2140	2178	rBV	299771	563407	32.75%	4.268%
19	8.488	2211	2223	2232	rBV2	45719	83979	4.88%	0.636%
20	8.539	2232	2239	2254	rVB	21445	38763	2.25%	0.294%
21	8.719	2290	2295	2305	rVV2	11704	18441	1.07%	0.140%
22	9.420	2500	2513	2539	rBV	476657	792238	46.06%	6.001%
23	9.574	2550	2561	2569	rBV	30016	47179	2.74%	0.357%
24	9.693	2588	2598	2609	rBV	85656	137525	7.99%	1.042%
25	9.745	2609	2614	2632	rVB3	12538	24517	1.43%	0.186%
26	10.102	2713	2725	2747	rVB	52320	87363	5.08%	0.662%
27	10.237	2755	2767	2786	rBV2	14094	26752	1.56%	0.203%
28	10.635	2879	2891	2915	rVB	392517	623454	36.24%	4.722%
29	10.906	2962	2975	2984	rBV4	13561	25987	1.51%	0.197%
30	10.999	2994	3004	3010	rBV	33886	55131	3.20%	0.418%
31	11.089	3026	3032	3035	rBV2	19171	22774	1.32%	0.173%
32	11.295	3087	3096	3108	rVB	20131	33123	1.93%	0.251%
33	11.359	3108	3116	3126	rBV3	12928	21413	1.24%	0.162%
34	11.468	3140	3150	3164	rVB	73397	120164	6.99%	0.910%
35	11.635	3190	3202	3222	rVV2	85807	202182	11.75%	1.531%
36	11.812	3245	3257	3272	rVB	532315	839221	48.79%	6.357%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

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_U\Method\82U110521W.M
Title : SW846 8260

37	11.896	3273	3283	3295	rBV	26024	47596	2.77%	0.361%
38	12.057	3323	3333	3348	rBV	198646	386621	22.48%	2.928%
39	12.140	3349	3359	3365	rBV5	73419	152867	8.89%	1.158%
40	12.327	3409	3417	3425	rVB	62948	85887	4.99%	0.651%
41	12.677	3513	3526	3535	rBV5	9172	22638	1.32%	0.171%
42	13.031	3627	3636	3651	rVB3	16811	47067	2.74%	0.357%
43	13.291	3710	3717	3728	rVB3	22849	40261	2.34%	0.305%
44	13.436	3753	3762	3766	rBV	50881	80396	4.67%	0.609%
45	13.590	3804	3810	3814	rBV2	14373	19939	1.16%	0.151%
46	13.790	3865	3872	3880	rBV8	10585	21920	1.27%	0.166%
47	13.844	3881	3889	3900	rVV9	24084	47452	2.76%	0.359%
48	14.076	3952	3961	3972	rBV2	57141	131639	7.65%	0.997%
49	14.455	4073	4079	4087	rBV3	35576	63130	3.67%	0.478%
50	15.214	4307	4315	4327	rBV2	144216	282348	16.41%	2.139%
51	16.198	4615	4621	4632	rVB	383102	573487	33.34%	4.344%
52	16.545	4724	4729	4739	rVB	583739	876302	50.94%	6.638%

Sum of corrected areas: 13202154

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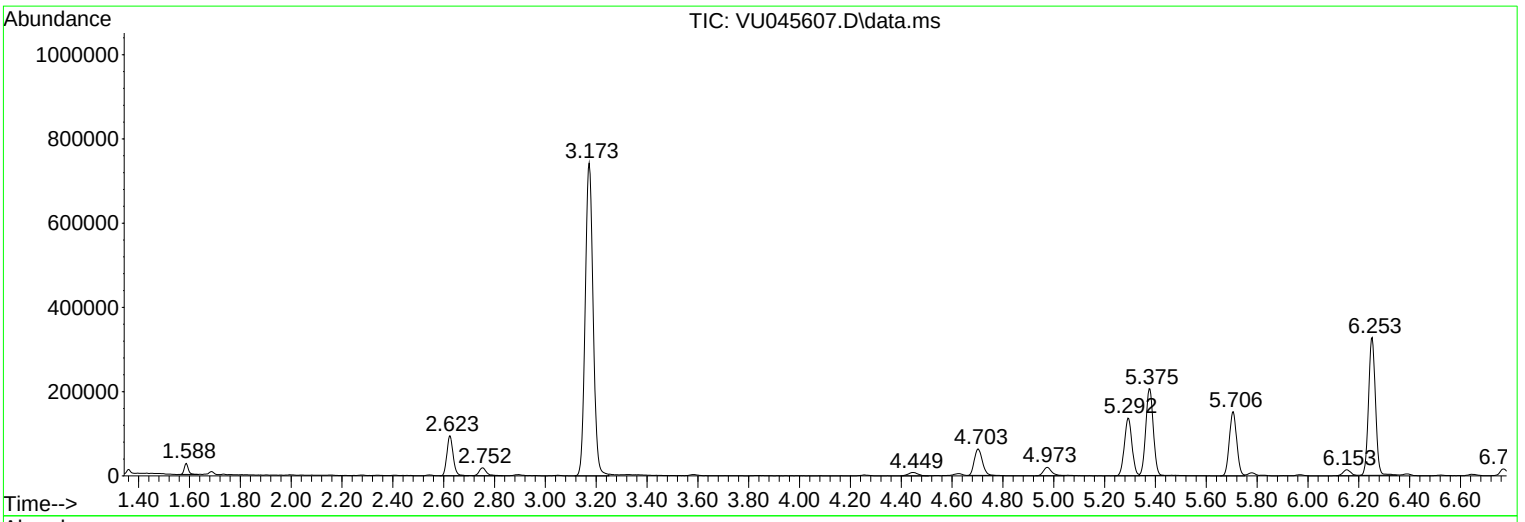
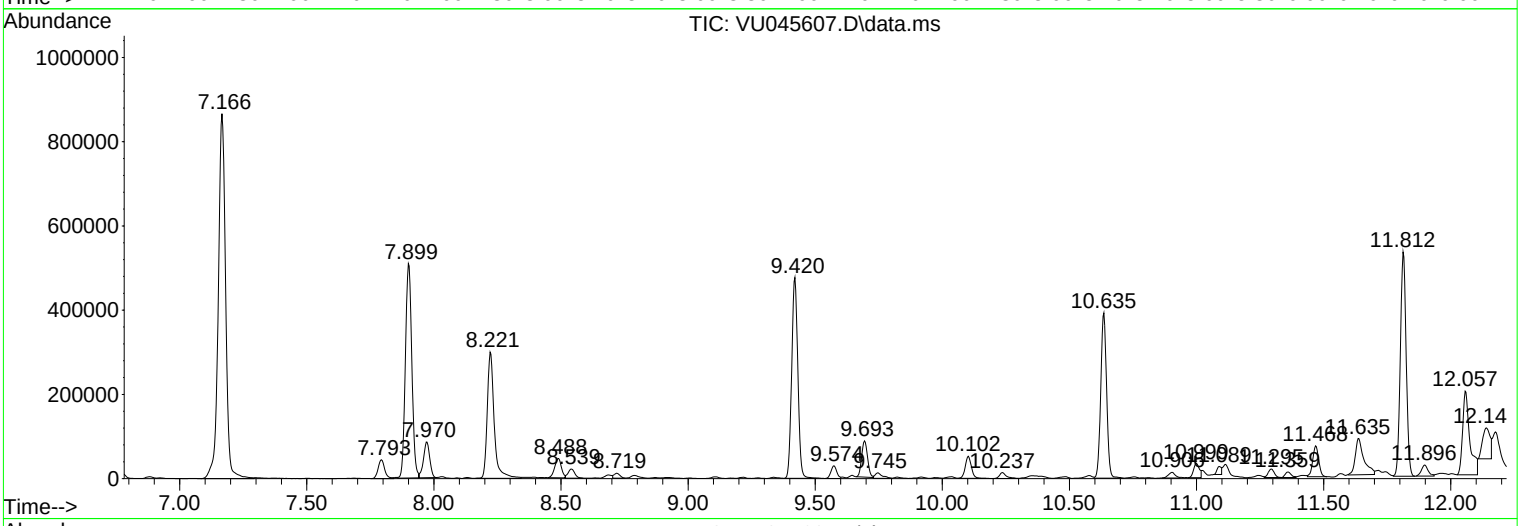
ALS Vial : 8 Sample Multiplier: 1

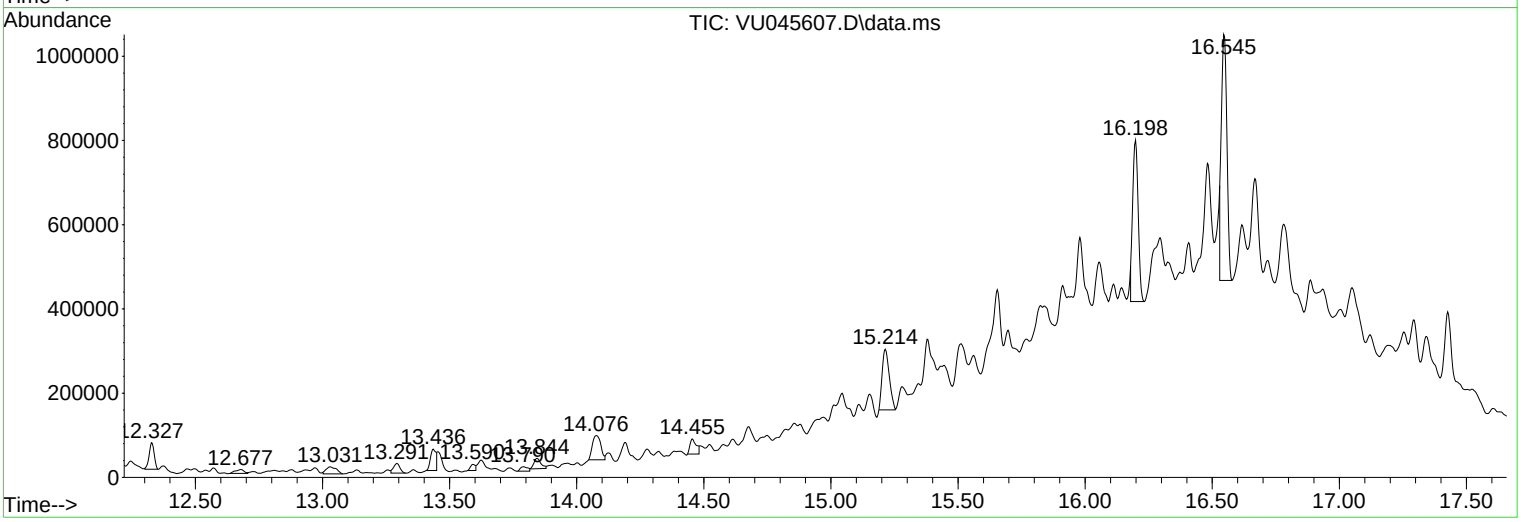
Instrument :
MSVOA_U
ClientSampleId :
2229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

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







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Operator : SY/MD
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MSVOA_U
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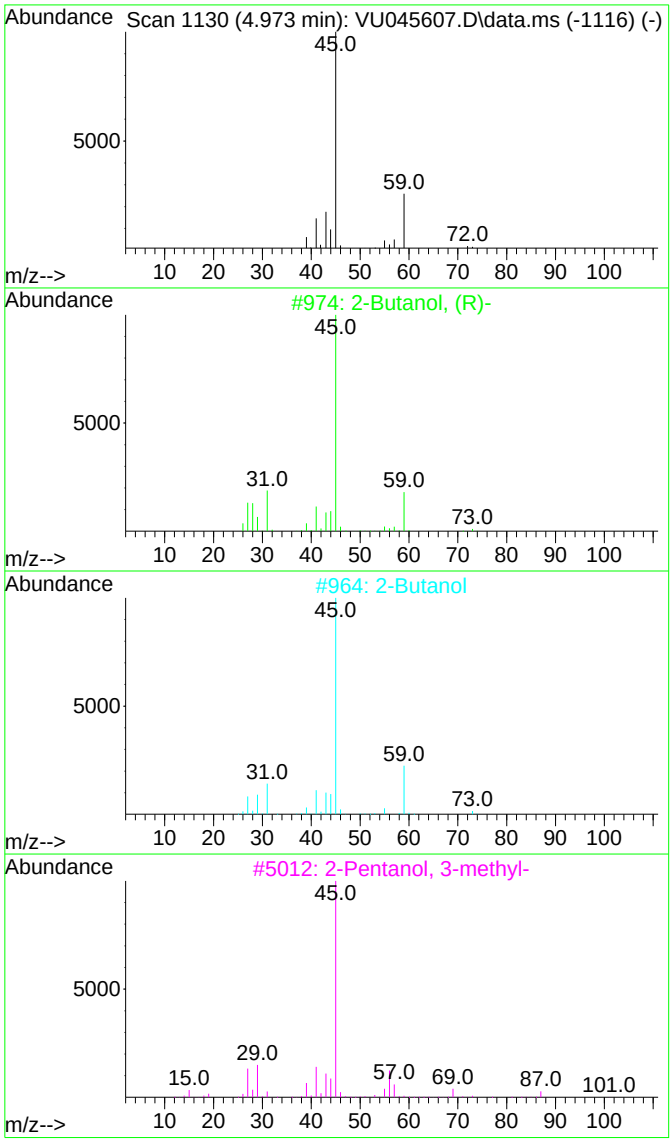
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

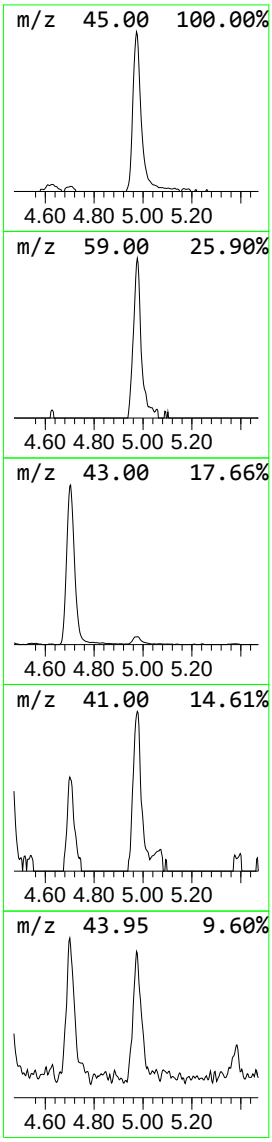
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Butanol, (R)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.973	5.51 ug/l	46301	Pentafluorobenzene	5.378

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	78
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	64
4	2-Hexanol	102	C6H14O	000626-93-7	38
5	2-Pentanol	88	C5H12O	006032-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

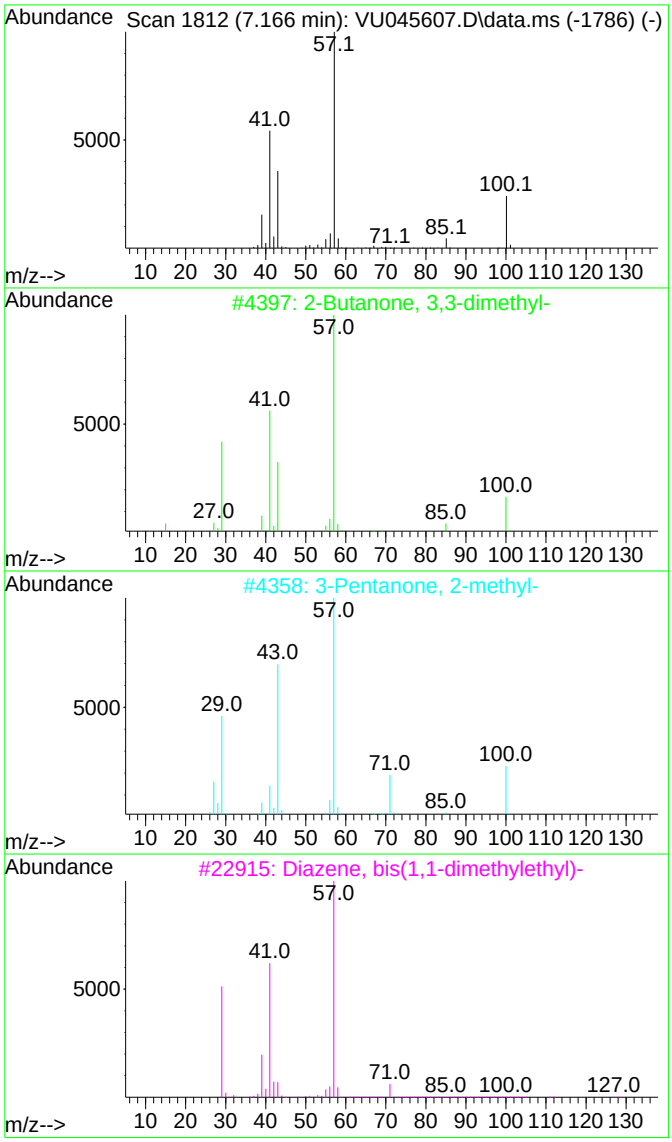
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

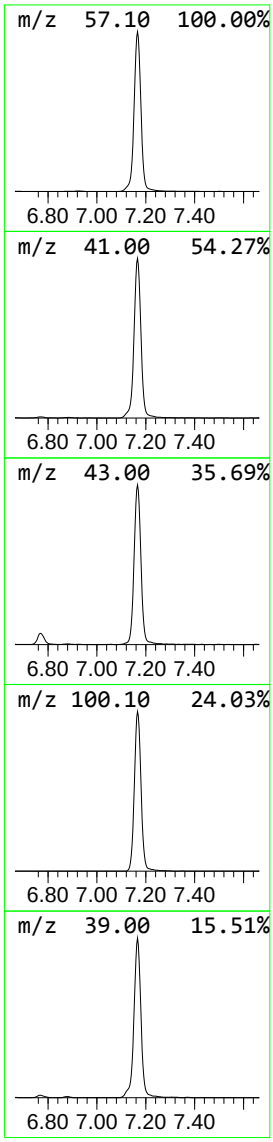
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.166	138.52 ug/l	1720200	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
3	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	47
4	Methyl methacrylate	100	C5H8O2	000080-62-6	47
5	Neopentane	72	C5H12	000463-82-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

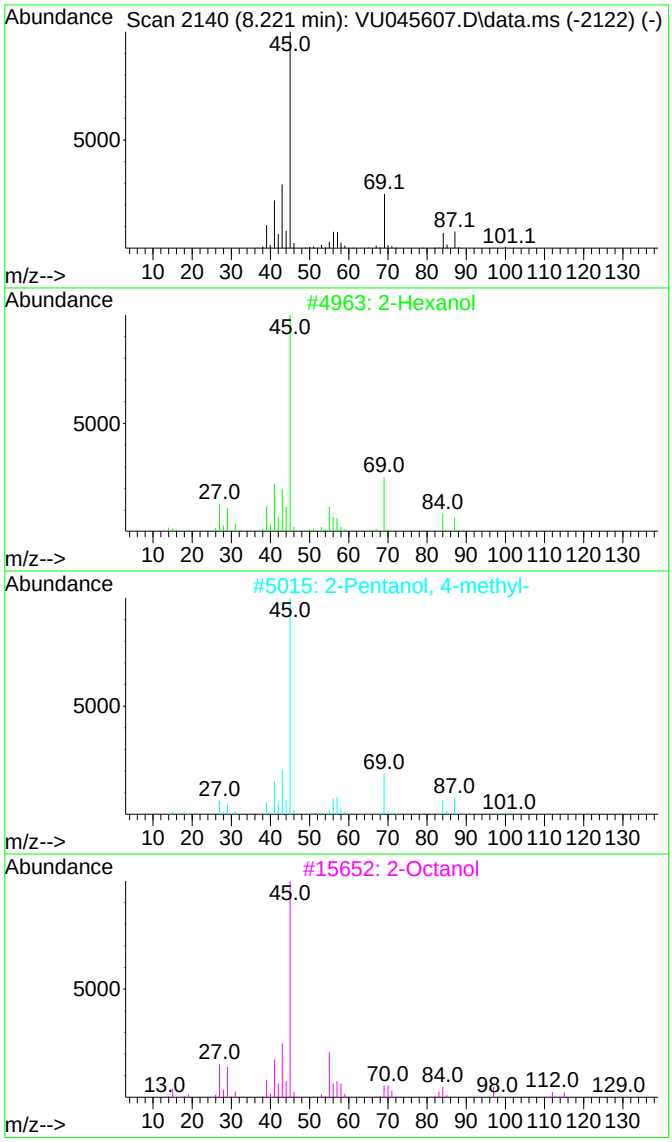
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

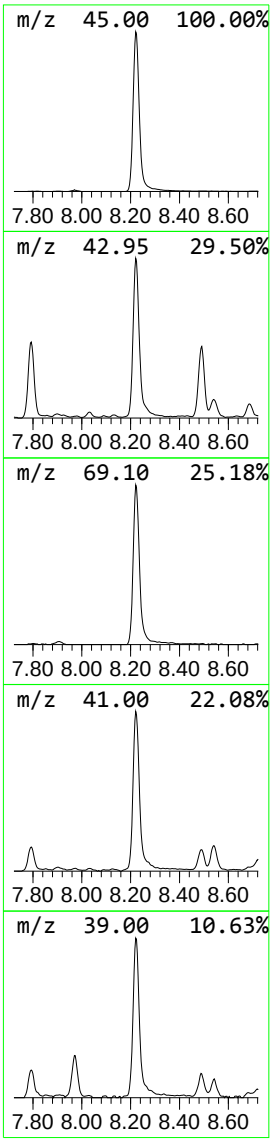
****

Peak Number 3 2-Hexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.221	35.56 ug/l	563407	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol	102	C6H14O	000626-93-7	83
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3	2-Octanol	130	C8H18O	000123-96-6	78
4	2-Octanol, (S)-	130	C8H18O	006169-06-8	64
5	2-Octanol, (R)-	130	C8H18O	005978-70-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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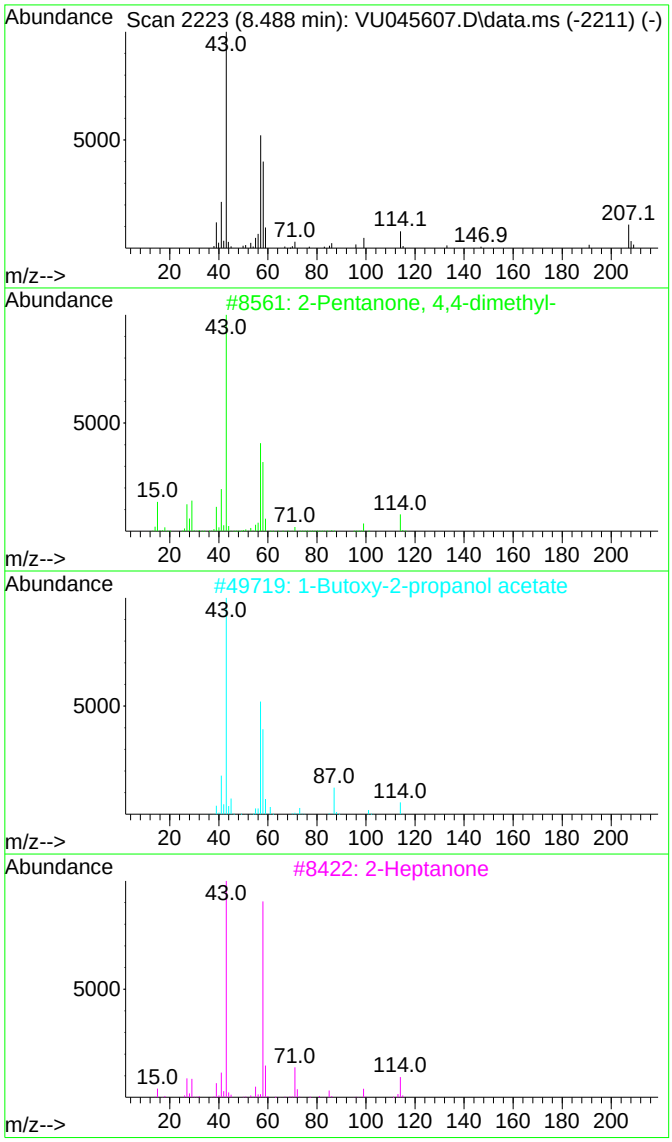
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

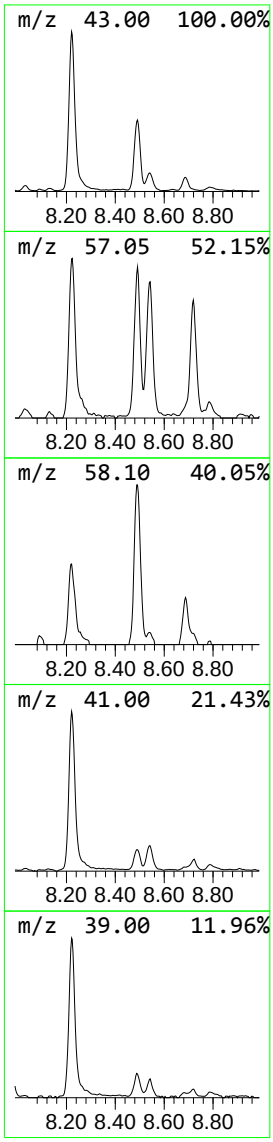
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.488	5.30 ug/l	83979	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	81
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	64
3	2-Heptanone	114	C7H14O	000110-43-0	58
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	50





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Operator : SY/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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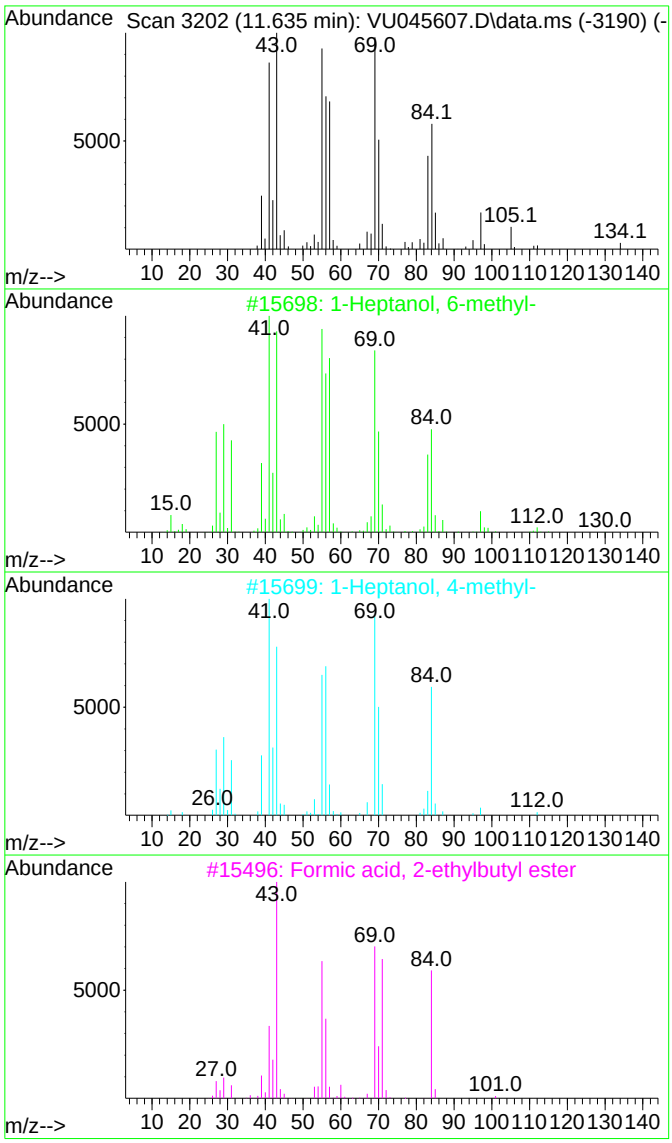
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

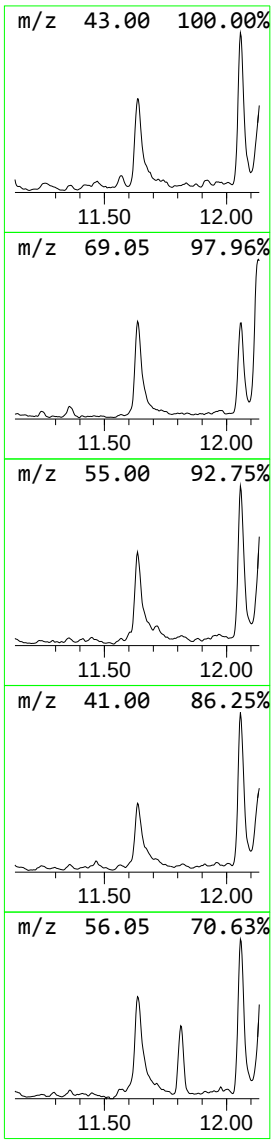
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Heptanol, 6-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.635	12.05 ug/l	202182	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
3	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	53
4	Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	50
5	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	50





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Instrument :
MSVOA_U
ClientSampleId :
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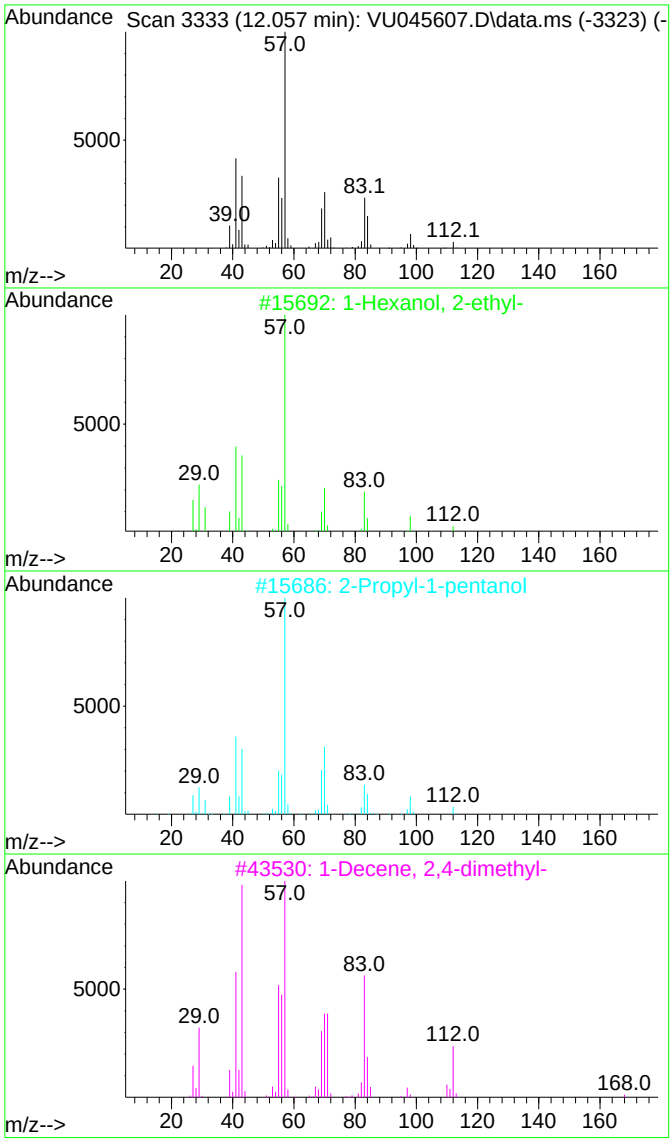
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

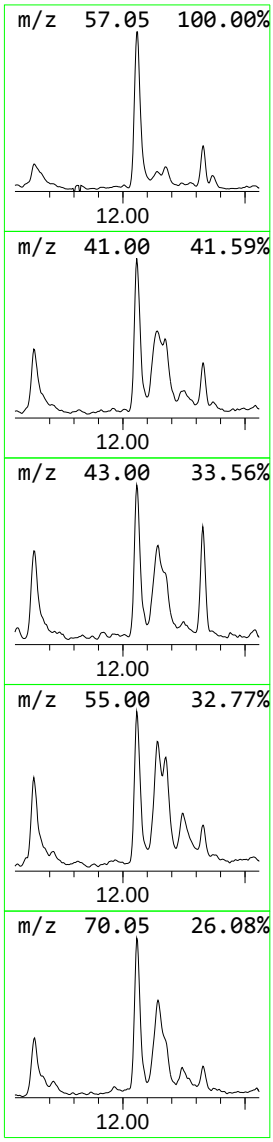
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	23.03 ug/l	386621	1,4-Dichlorobenzene-d4	11.812

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	59
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

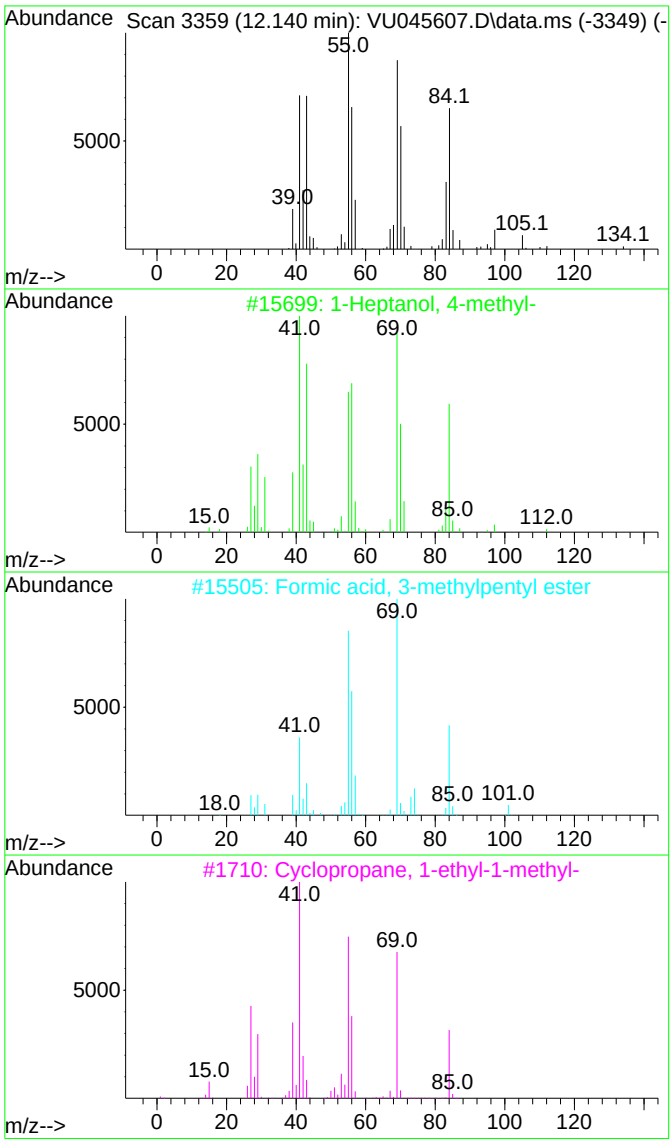
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

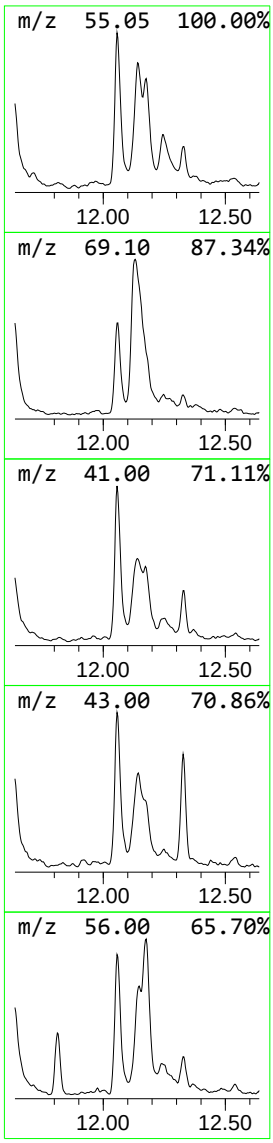
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Heptanol, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.140	9.11 ug/l	152867	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	64
2	Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	53
3	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	53
4	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	53
5	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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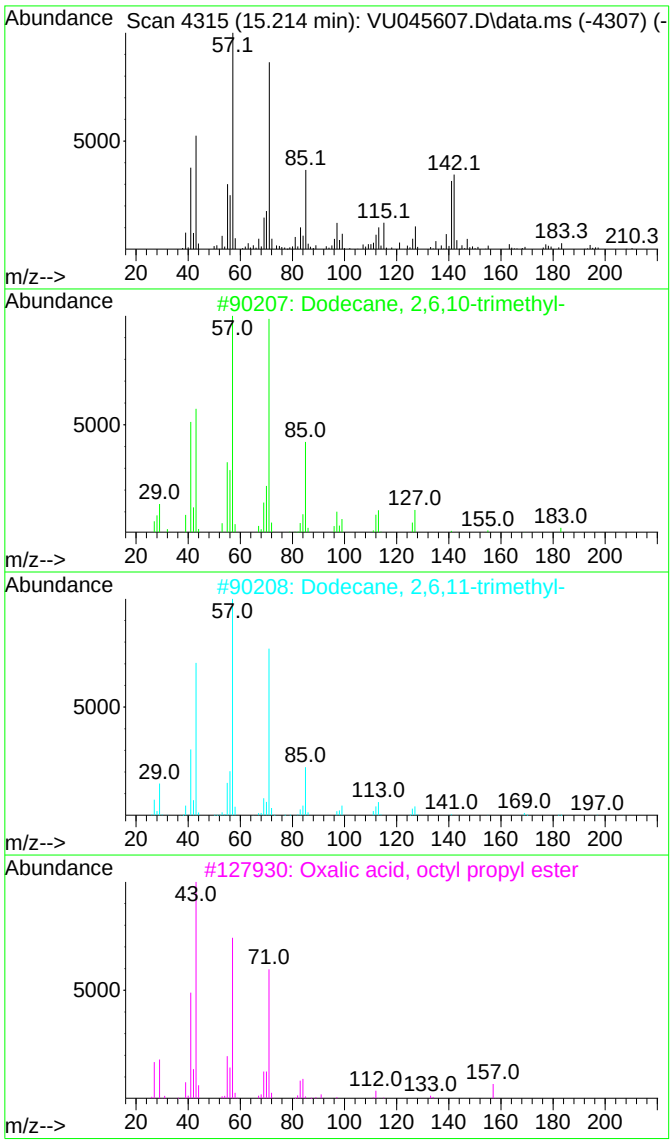
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

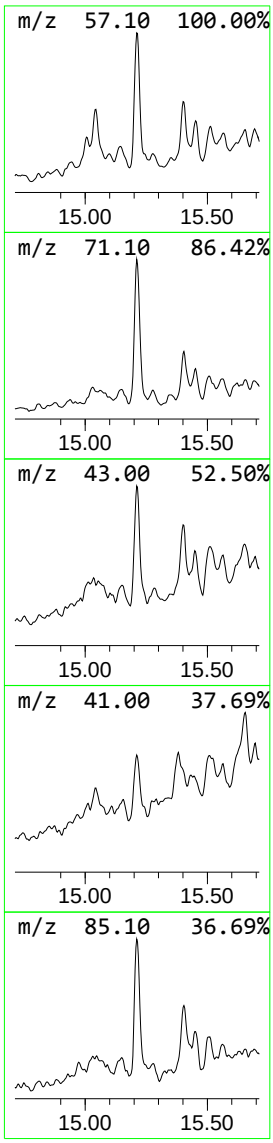
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Dodecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.214	16.82 ug/l	282348	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	68
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
3	Oxalic acid, octyl propyl ester	244	C13H24O4	1010309-26-1	43
4	Hexacosane	366	C26H54	000630-01-3	43
5	Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	43





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Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

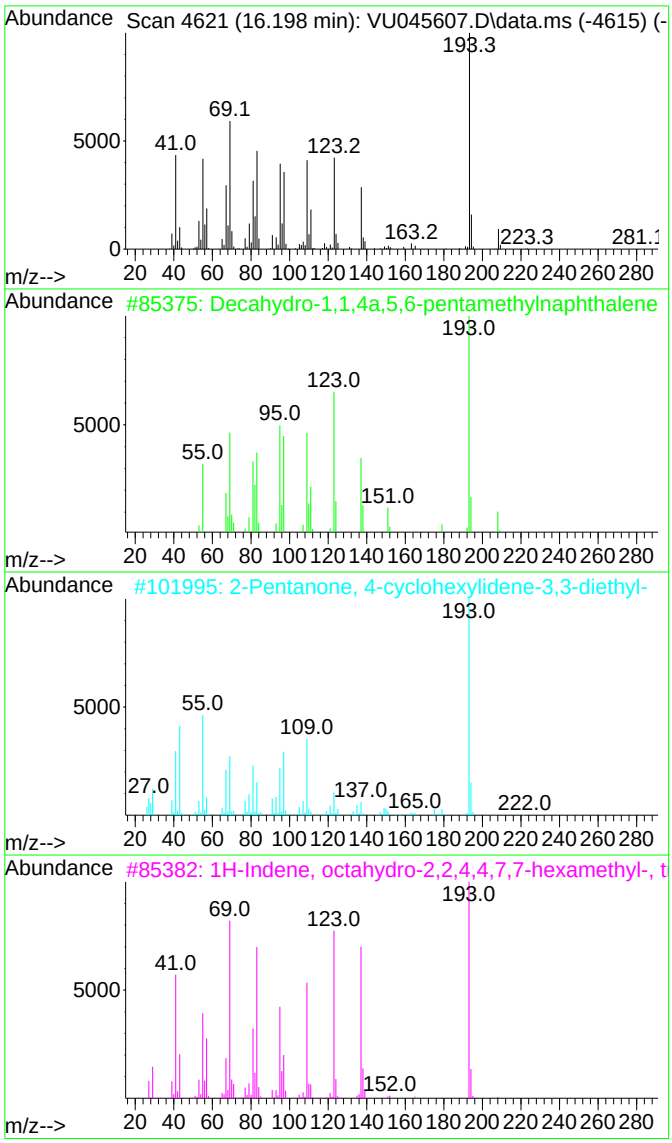
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

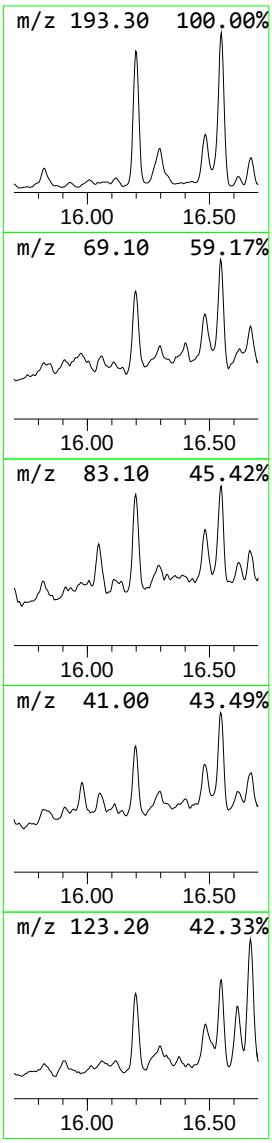
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.198	34.17 ug/l	573487	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	81
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	46
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
5	9-Vinylcarbazole	193	C14H11N	001484-13-5	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

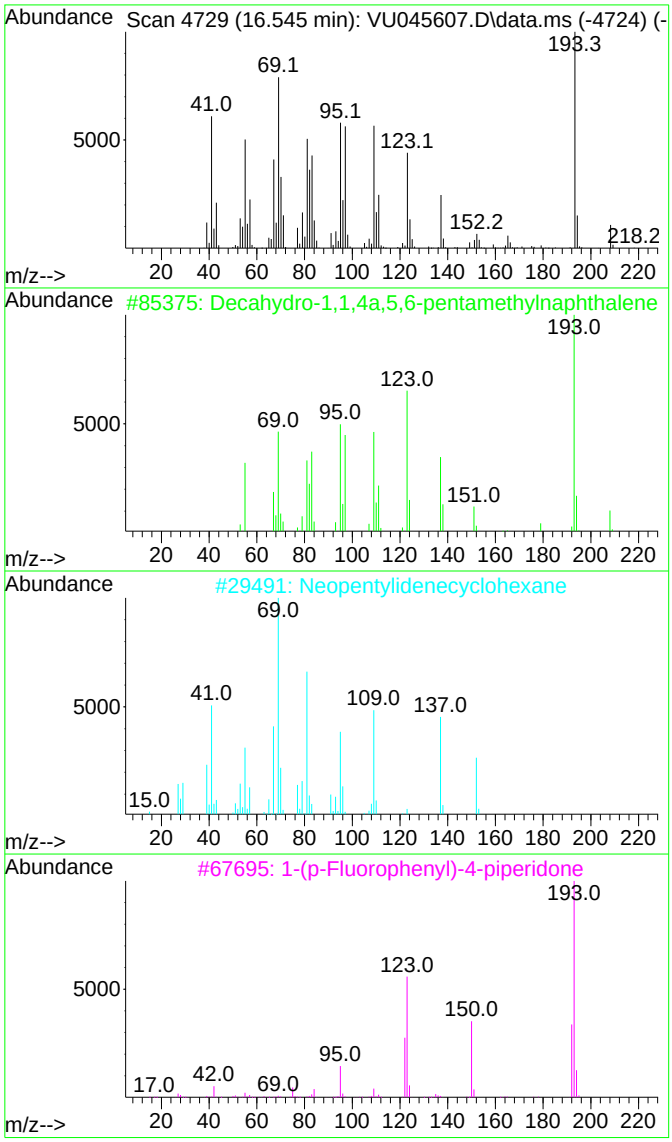
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

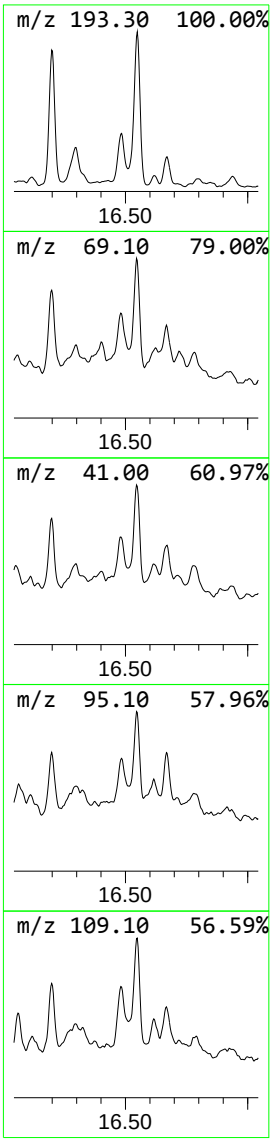
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.545 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.545	52.21 ug/l	876302	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	78
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	27
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
5	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
Data File : VU045607.D
Acq On : 08 Nov 2021 12:05
Operator : SY/MD
Sample : M4434-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
2229

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.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
2-Butanol, (R)-	4.973	5.5	ug/l	46301	1	5.378	420121	50.0
2-Butanone, 3,3...	7.166	138.5	ug/l	1720200	2	6.253	620920	50.0
2-Hexanol	8.221	35.6	ug/l	563407	3	9.420	792238	50.0
2-Pentanone, 4,...	8.488	5.3	ug/l	83979	3	9.420	792238	50.0
1-Heptanol, 6-m...	11.635	12.1	ug/l	202182	4	11.812	839221	50.0
1-Hexanol, 2-et...	12.057	23.0	ug/l	386621	4	11.812	839221	50.0
1-Heptanol, 4-m...	12.140	9.1	ug/l	152867	4	11.812	839221	50.0
Dodecane, 2,6,1...	15.214	16.8	ug/l	282348	4	11.812	839221	50.0
Decahydro-1,1,4...	16.198	34.2	ug/l	573487	4	11.812	839221	50.0
unknown16.545	16.545	52.2	ug/l	876302	4	11.812	839221	50.0