LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045363.D
Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-PIT-SOIL

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\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045363.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.761	102	131	173	rBV	50093	277242	5.78%	1.294%
2	3.041	517	529	551	rVB	33320	67727	1.41%	0.316%
3	5.292	1195	1229	1242	rBV	188091	427076	8.91%	1.994%
4	5.375	1242	1255	1279	rVB	333823	702355	14.65%	3.279%
5	5.706	1342	1358	1384	rBV	226184	481119	10.03%	2.246%
6	5.922	1410	1425	1455	rBV2	22173	62397	1.30%	0.291%
7	6.250	1513	1527	1582	rVB	517006	1101461	22.97%	5.143%
8	6.951	1724	1745	1761	rBV3	22682	73486	1.53%	0.343%
9	7.050	1761	1776	1811	rVV	1263099	3408076	71.07%	15.913%
10	7.751	1979	1994	2015	rBV	190633	495486	10.33%	2.314%
11	7.902	2027	2041	2058	rBV	787053	1410712	29.42%	6.587%
12	8.484	2205	2222	2229	rBV2	69834	175952	3.67%	0.822%
13	8.587	2246	2254	2268	rVB4	186385	432470	9.02%	2.019%
14	8.745	2287	2303	2322	rBV	2284780	4795134	100.00%	22.389%
15	8.854	2323	2337	2362	rVB	238481	491443	10.25%	2.295%
16	9.227	2437	2453	2483	rBV	1528377	2780716	57.99%	12.984%
17	9.423	2488	2514	2540	rVB	669705	1261963	26.32%	5.892%
18	10.086	2706	2720	2737	rBV	56912	97854	2.04%	0.457%
19	10.642	2880	2893	2915	rVB	549131	903566	18.84%	4.219%
20	10.909	2963	2976	2988	rBV2	40876	75359	1.57%	0.352%
21	11.819	3245	3259	3275	rBV	717130	1128723	23.54%	5.270%
22	15.404	4365	4374	4385	rBV2	51893	80319	1.68%	0.375%
23	16.294	4645	4651	4662	rVB	141620	201039	4.19%	0.939%
24	16.886	4827	4835	4841	rBV	60815	98975	2.06%	0.462%
25	17.137	4904	4913	4925	rVB	265244	386360	8.06%	1.804%

Sum of corrected areas: 21417010

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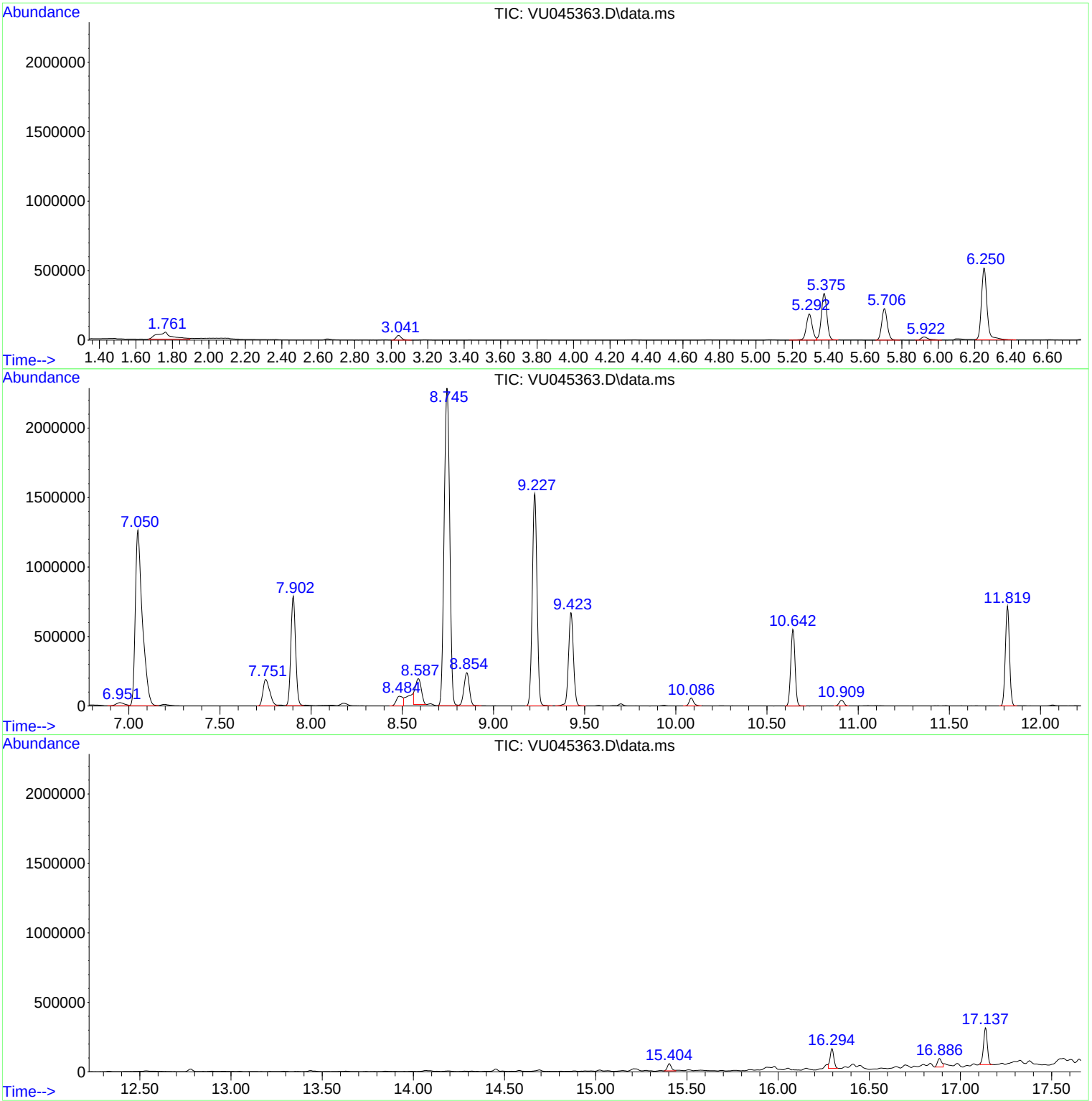
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-PIT-SOIL

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



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Data File : VU045363.D
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Operator : SY/MD
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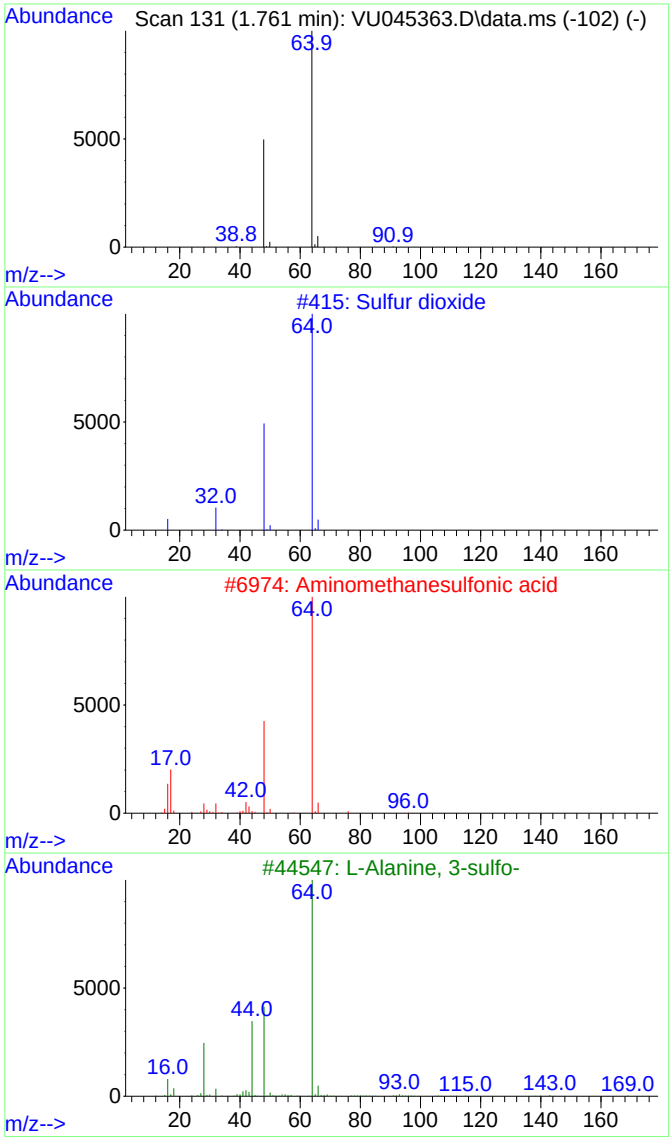
Quant Title : SW846 8260

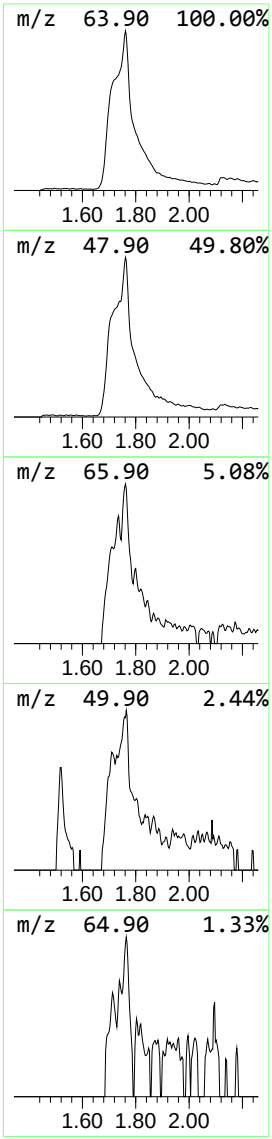
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.761	19.74 ug/l	277242	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	4





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Data File : VU045363.D
Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-PIT-SOIL

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

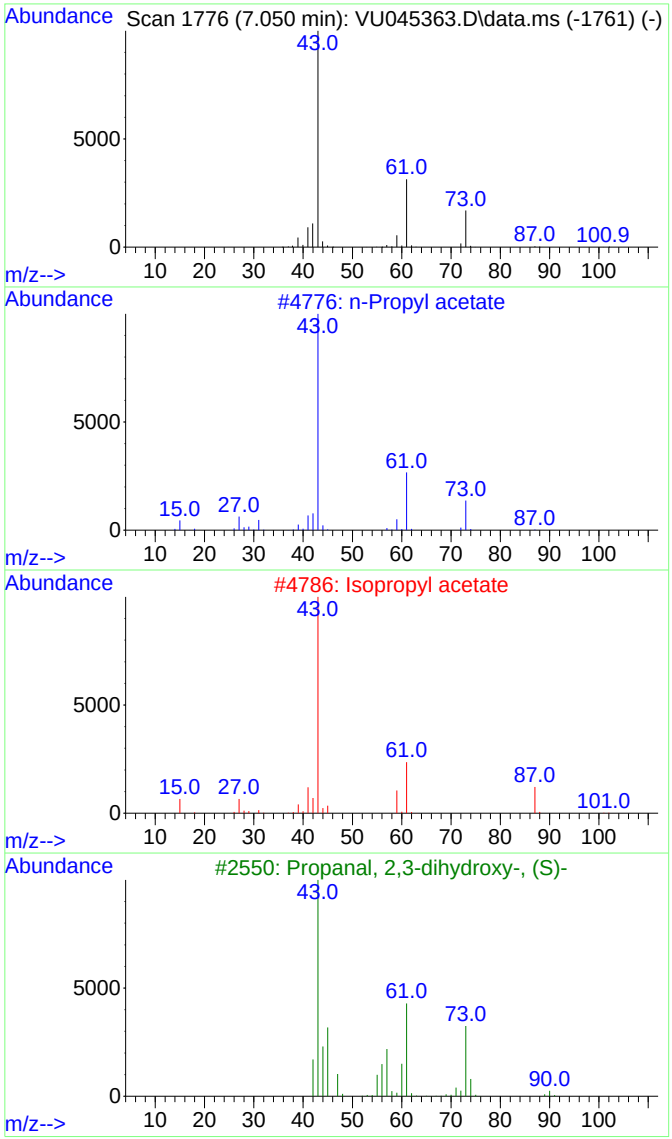
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

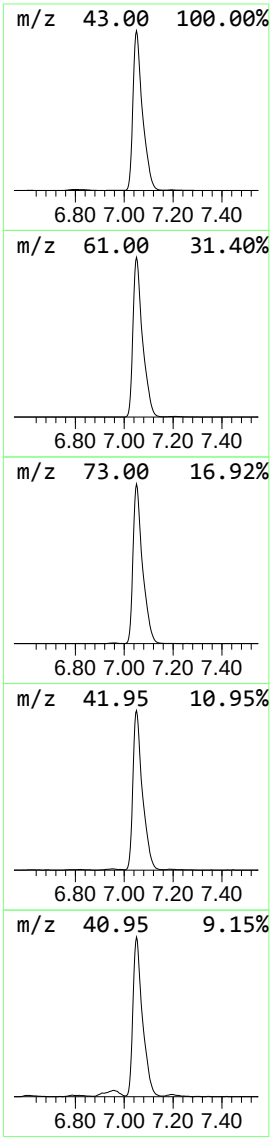
****

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.050	154.71 ug/l	3408080	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	38
3	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Data File : VU045363.D
Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-PIT-SOIL

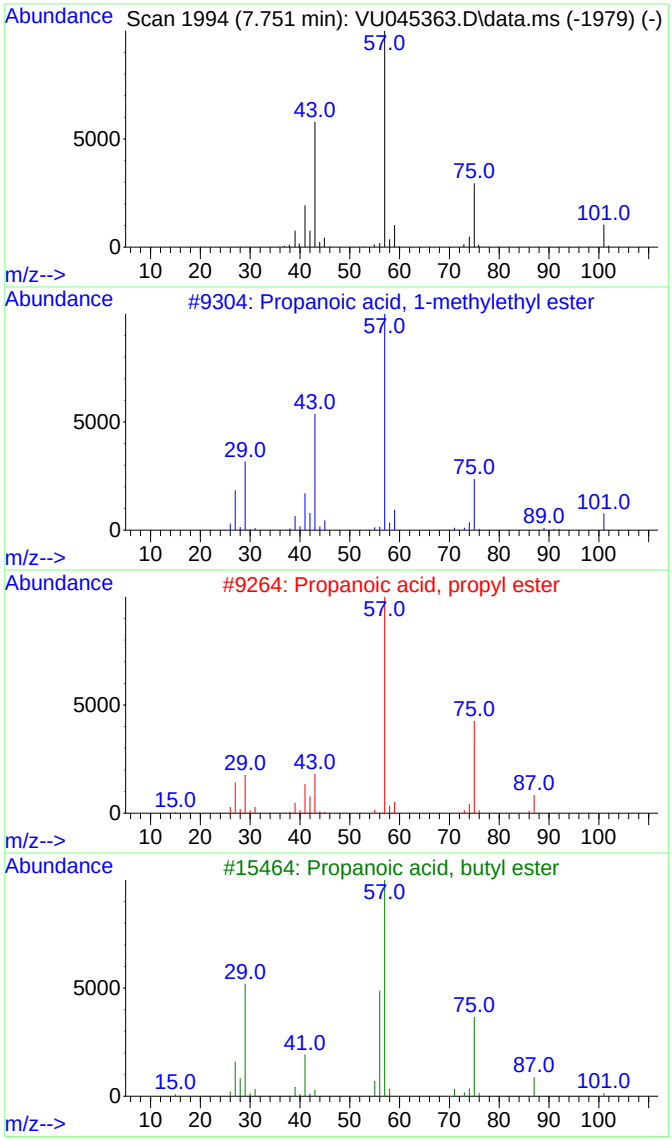
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

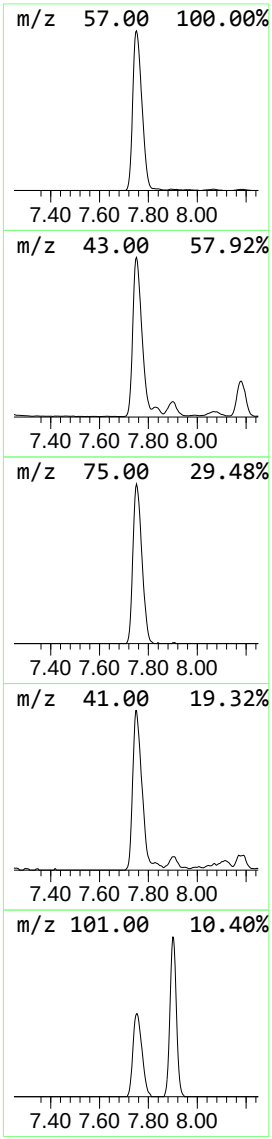
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.751	22.49 ug/l	495486	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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Data File : VU045363.D
Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-PIT-SOIL

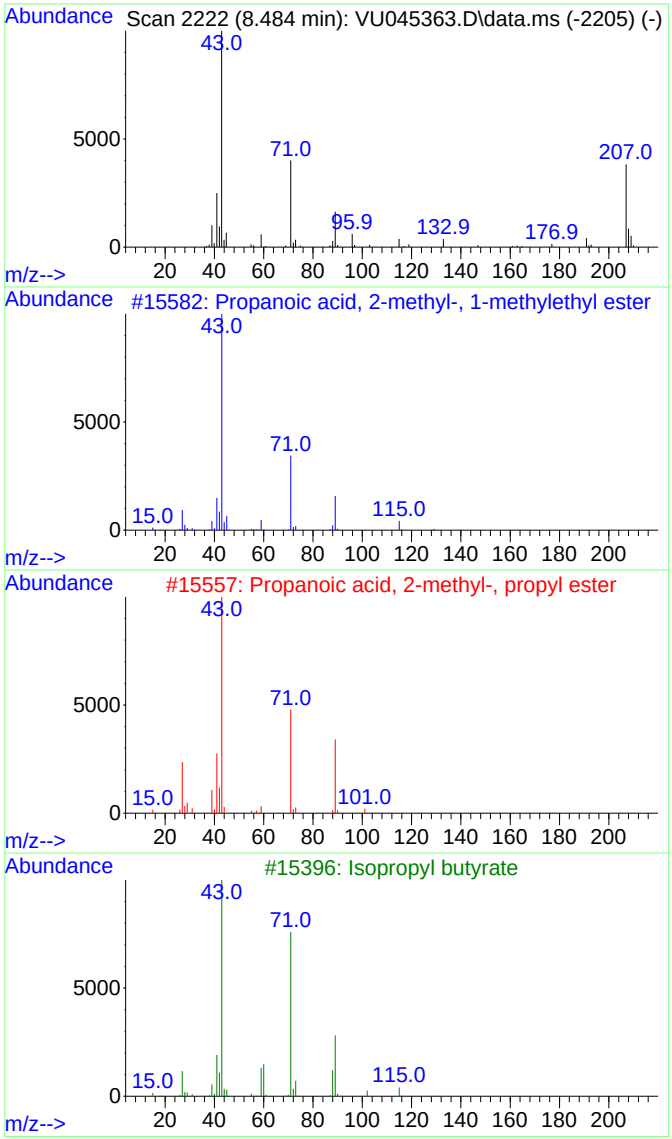
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

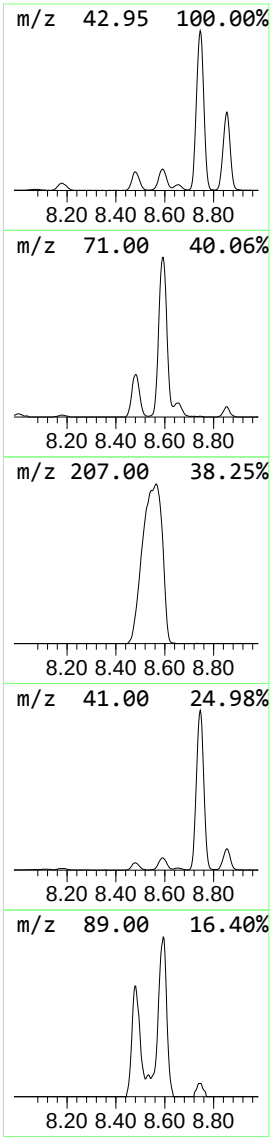
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown8.484 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.484	6.97 ug/l	175952	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	35
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	35
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	25
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	25
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
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Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MH-PIT-SOIL

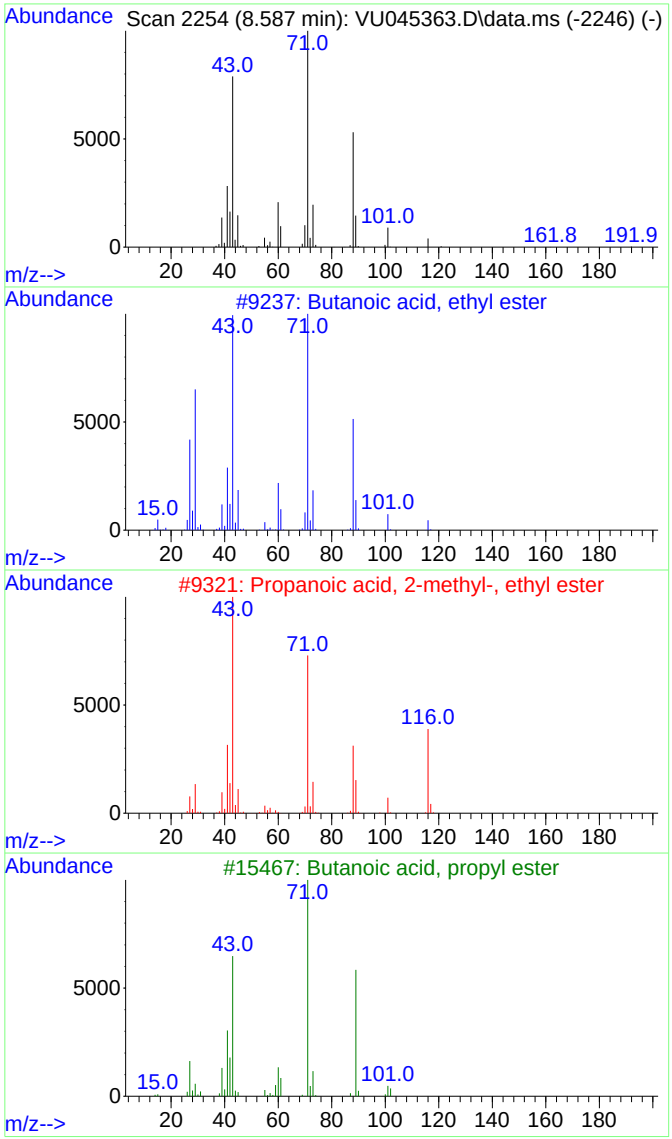
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

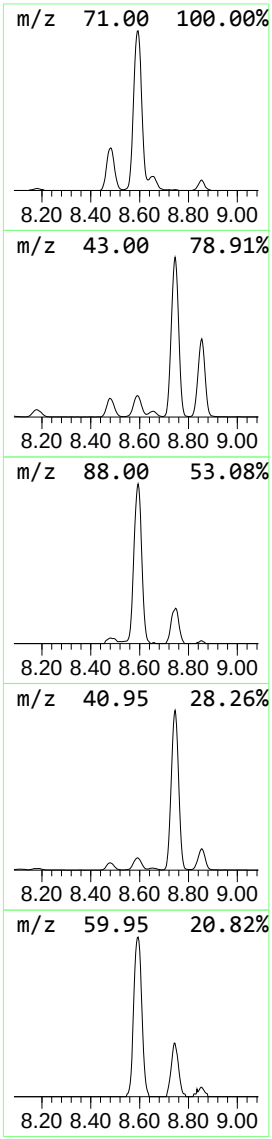
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.587	17.13 ug/l	432470	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
4	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37
5	Ethyl 6-bromohexanoate	222	C8H15BrO2	025542-62-5	35





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Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-PIT-SOIL

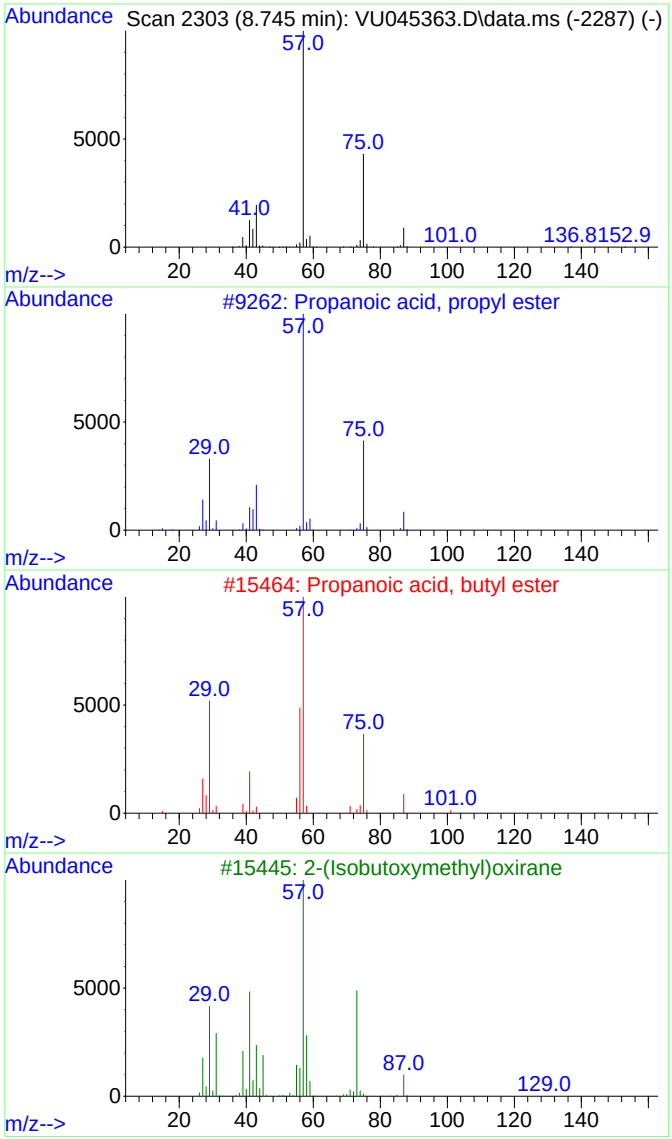
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

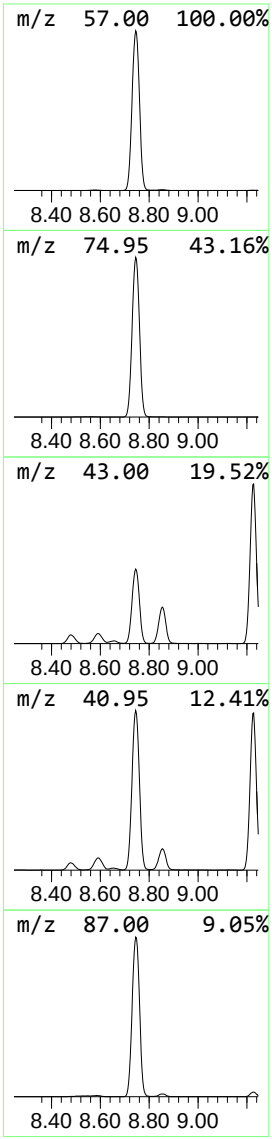
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.745	189.99 ug/l	4795130	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7





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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-PIT-SOIL

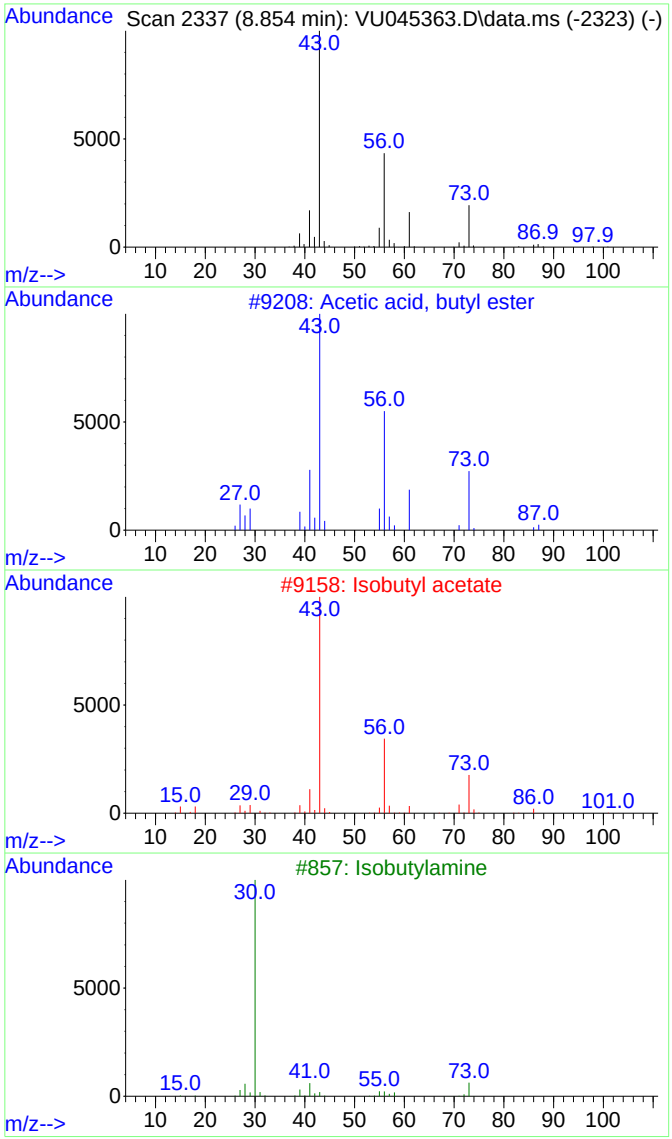
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

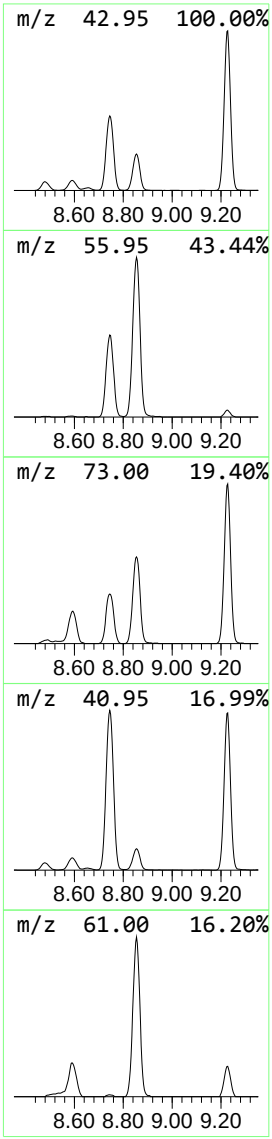
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.854	19.47 ug/l	491443	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





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ClientSampleId : MH-PIT-SOIL

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Quant Title : SW846 8260

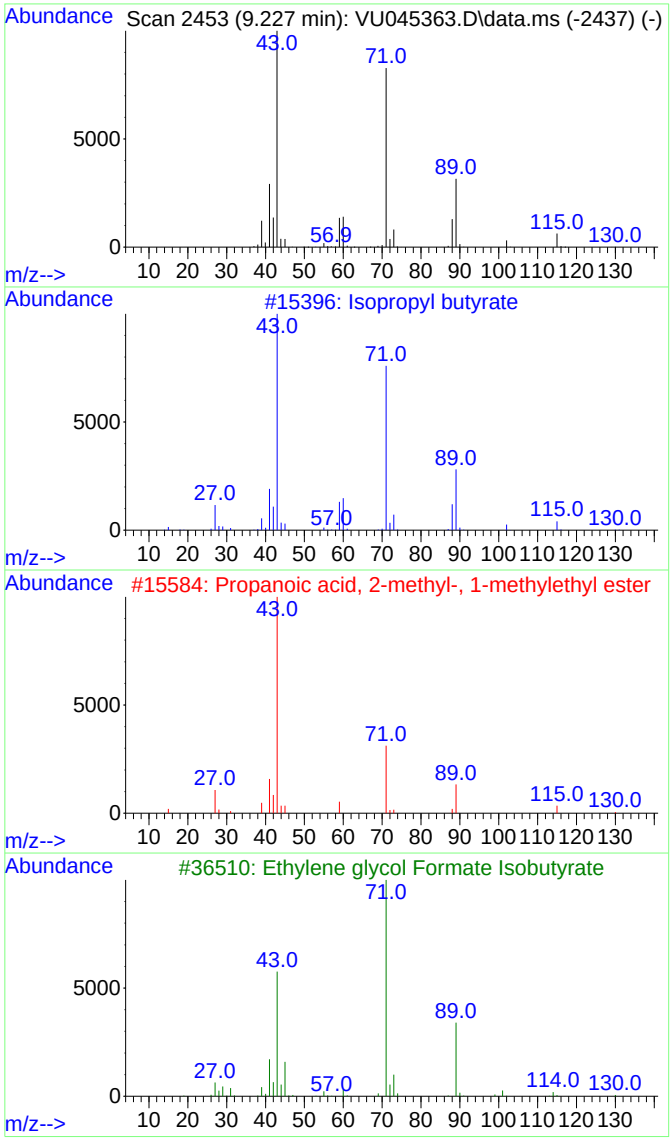
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

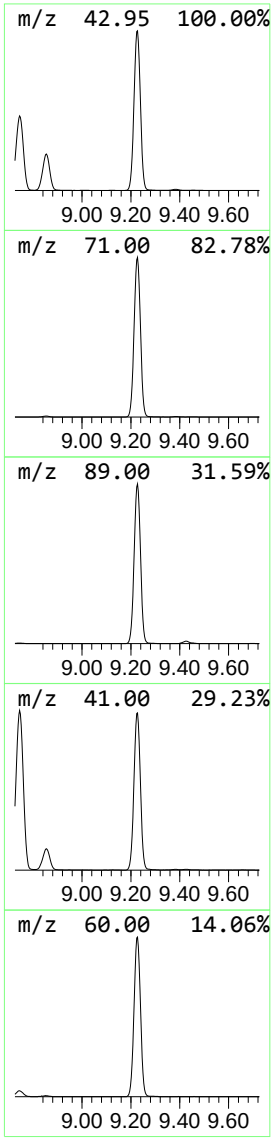
****

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.227	110.17 ug/l	2780720	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





Library Search Compound Report

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ClientSampleId : MH-PIT-SOIL

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

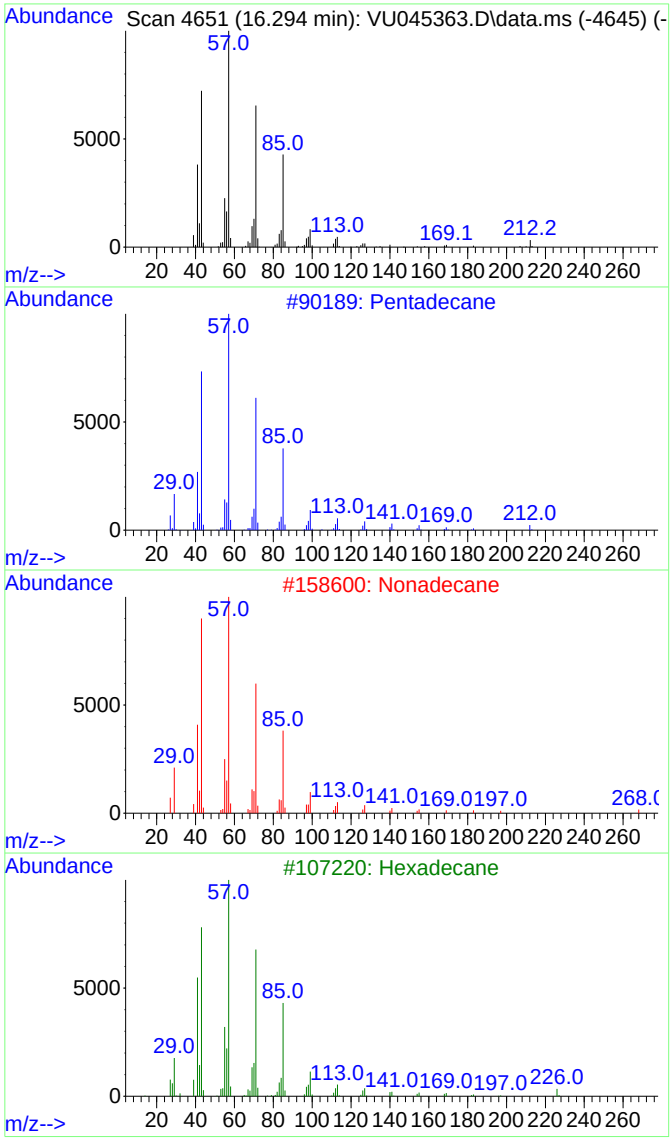
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

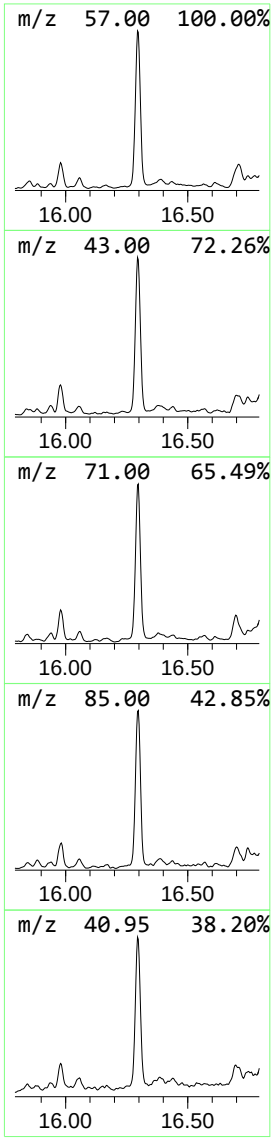
****

Peak Number 9 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.294	8.91 ug/l	201039	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5	Tetradecane	198	C14H30	000629-59-4	90





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ALS Vial : 10 Sample Multiplier: 1

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

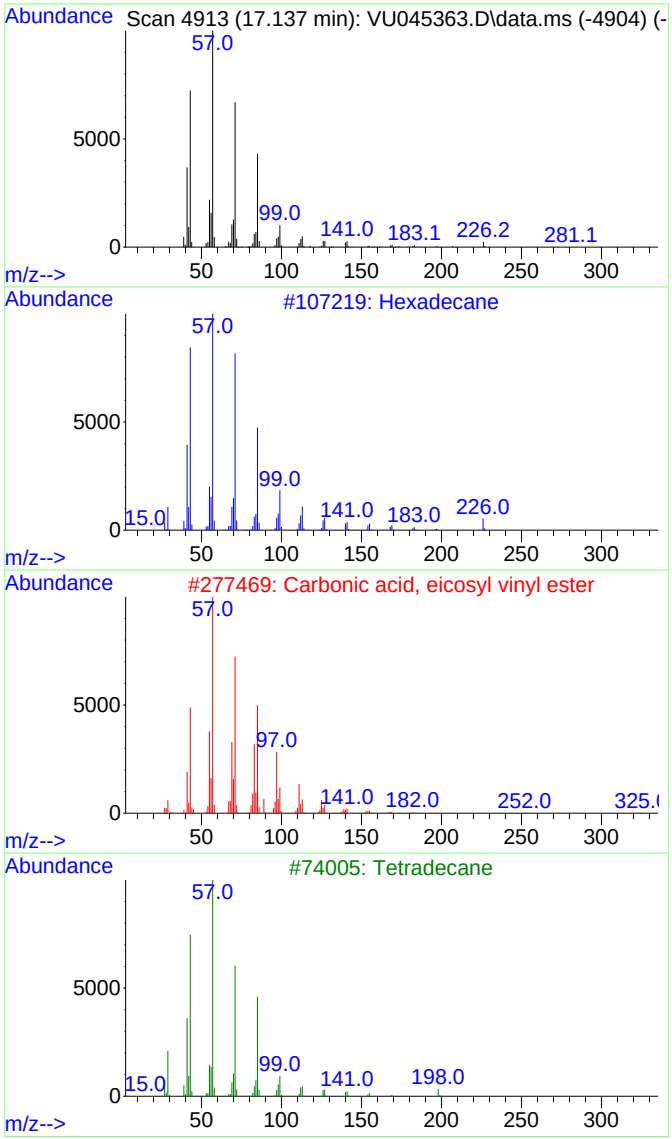
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

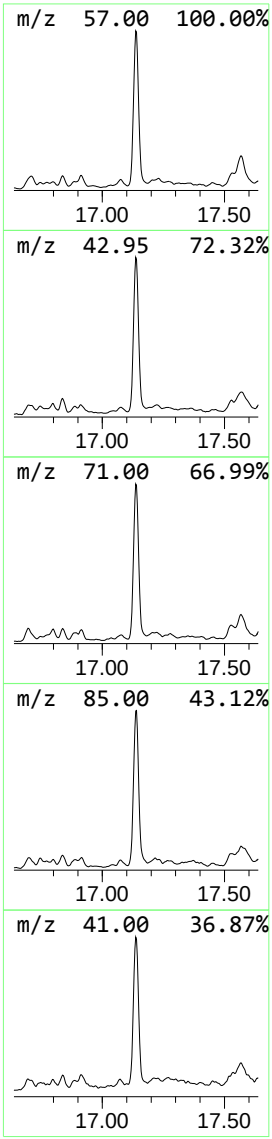
****

Peak Number 10 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.137	17.11 ug/l	386360	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
3	Tetradecane	198	C14H30	000629-59-4	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Nonadecane	268	C19H40	000629-92-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102221\
Data File : VU045363.D
Acq On : 22 Oct 2021 14:37
Operator : SY/MD
Sample : M4306-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MH-PIT-SOIL

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
Sulfur dioxide	1.761	19.7	ug/l	277242	1	5.375	702355	50.0
n-Propyl acetate	7.050	154.7	ug/l	3408080	2	6.253	1101460	50.0
Propanoic acid,...	7.751	22.5	ug/l	495486	2	6.253	1101460	50.0
unknown8.484	8.484	7.0	ug/l	175952	3	9.426	1261960	50.0
Butanoic acid, ...	8.587	17.1	ug/l	432470	3	9.426	1261960	50.0
Propanoic acid,...	8.745	190.0	ug/l	4795130	3	9.426	1261960	50.0
Acetic acid, bu...	8.854	19.5	ug/l	491443	3	9.426	1261960	50.0
Isopropyl butyrate	9.227	110.2	ug/l	2780720	3	9.426	1261960	50.0
Pentadecane	16.294	8.9	ug/l	201039	4	11.819	1128720	50.0
Hexadecane	17.137	17.1	ug/l	386360	4	11.819	1128720	50.0