

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD053119\
 Data File : VD062564.D
 Acq On : 31 May 2019 15:26
 Operator : VA/AP
 Sample : K3125-21
 Misc : 5.04g/5ml/MSVOA D/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 13903

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_D\METHOD\82D053019S.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.499	3	7	28	rVB	706814	2545521	100.00%	18.151%
2	1.775	28	35	36	rBV	18371	54982	2.16%	0.392%
3	3.832	238	244	250	rBV	12390	35040	1.38%	0.250%
4	3.950	250	256	262	rVV3	11702	38842	1.53%	0.277%
5	4.718	328	334	342	rBV3	9692	33303	1.31%	0.237%
6	6.195	475	484	491	rVB2	16826	62839	2.47%	0.448%
7	6.943	551	560	566	rBV	314419	924683	36.33%	6.593%
8	7.061	566	572	582	rVB2	465270	1289924	50.67%	9.198%
9	7.475	603	614	626	rBV	251478	714876	28.08%	5.097%
10	8.233	685	691	702	rBV	630777	1578949	62.03%	11.259%
11	10.418	908	913	919	rVV	440493	1002198	39.37%	7.146%
12	10.526	919	924	939	rVB	805960	1938608	76.16%	13.823%
13	11.245	992	997	1002	rBV2	32785	87435	3.43%	0.623%
14	11.885	1059	1062	1071	rVB	16786	33177	1.30%	0.237%
15	12.377	1108	1112	1123	rVB	700447	1111821	43.68%	7.928%
16	12.672	1139	1142	1146	rBV	29815	55490	2.18%	0.396%
17	13.558	1227	1232	1236	rBV	379395	580057	22.79%	4.136%
18	13.716	1245	1248	1257	rVB4	24892	56093	2.20%	0.400%
19	13.903	1264	1267	1269	rVV2	33250	56617	2.22%	0.404%
20	13.942	1269	1271	1279	rVB4	42376	77323	3.04%	0.551%
21	14.238	1299	1301	1305	rVB	30866	39416	1.55%	0.281%
22	14.523	1327	1330	1333	rVV	418922	512825	20.15%	3.657%
23	14.592	1335	1337	1340	rVB2	49841	63987	2.51%	0.456%
24	14.691	1344	1347	1354	rVB	237080	339794	13.35%	2.423%
25	14.887	1364	1367	1370	rBV	30256	39450	1.55%	0.281%
26	15.291	1404	1408	1410	rBV3	26968	44922	1.76%	0.320%
27	15.429	1420	1422	1425	rBV	30384	45952	1.81%	0.328%
28	15.655	1442	1445	1446	rBV2	28540	44318	1.74%	0.316%
29	15.813	1458	1461	1466	rVB6	38936	69141	2.72%	0.493%
30	15.892	1466	1469	1471	rBV3	21580	33857	1.33%	0.241%
31	16.148	1492	1495	1497	rBV4	31832	57228	2.25%	0.408%
32	16.216	1500	1502	1508	rVB7	35192	78369	3.08%	0.559%
33	16.315	1508	1512	1516	rBV7	21315	52162	2.05%	0.372%
34	16.384	1516	1519	1525	rVB8	22205	67897	2.67%	0.484%

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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

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Title : SW846 8260

35	16.492	1528	1530	1531	rBV2	18115	30170	1.19%	0.215%
36	16.650	1542	1546	1549	rVB6	15956	45552	1.79%	0.325%
37	16.728	1549	1554	1557	rVB6	28671	68794	2.70%	0.491%
38	16.886	1567	1570	1572	rBV3	24177	38957	1.53%	0.278%
39	17.053	1584	1587	1591	rVB5	16130	37907	1.49%	0.270%
40	17.250	1605	1607	1612	rVV5	17725	35772	1.41%	0.255%

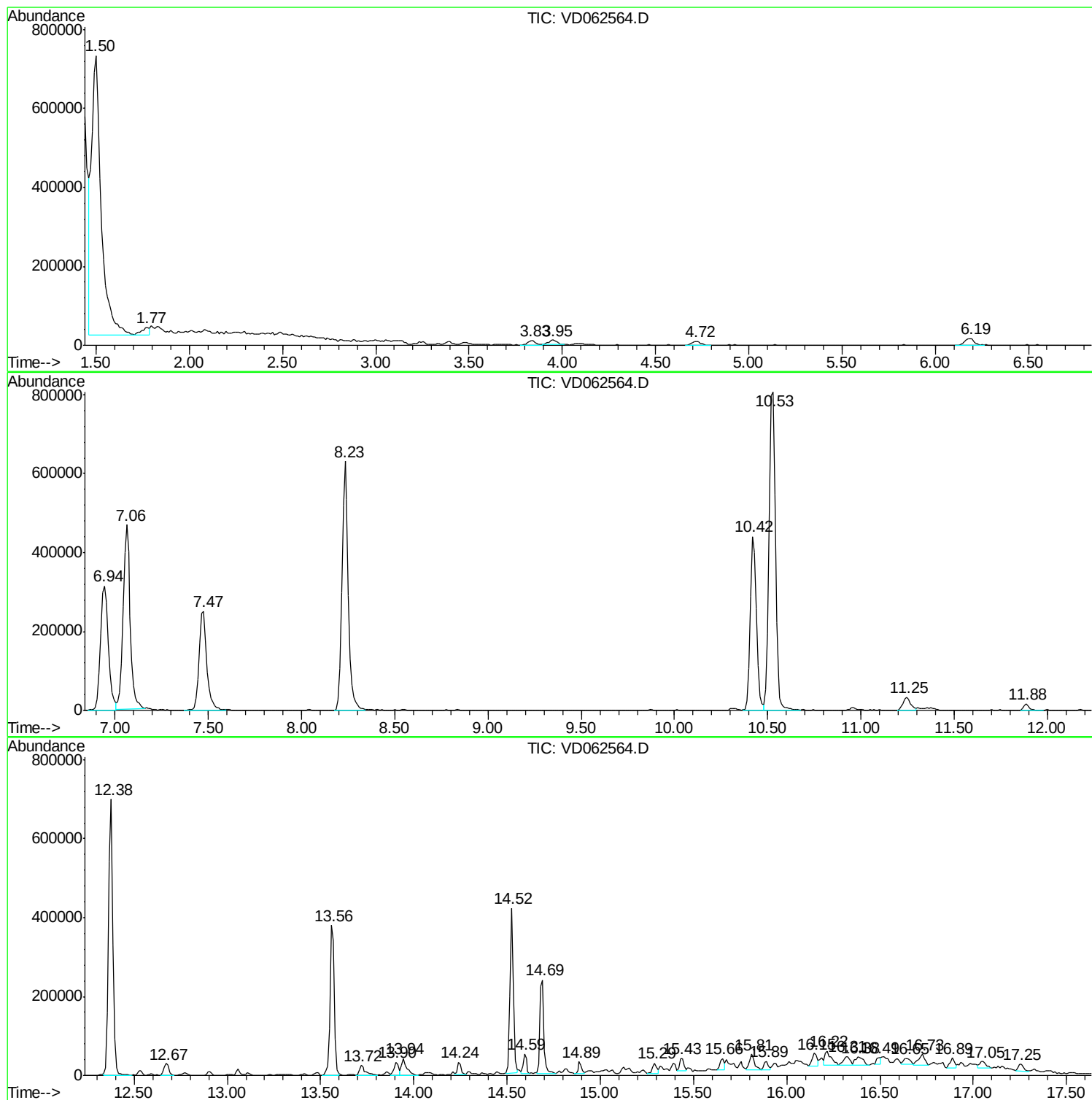
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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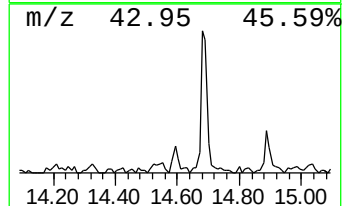
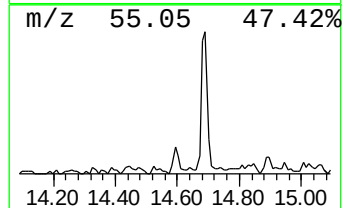
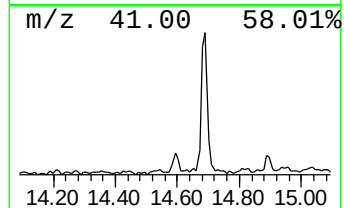
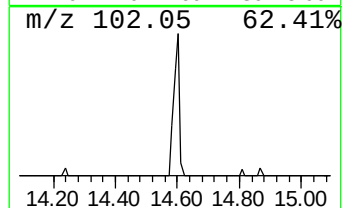
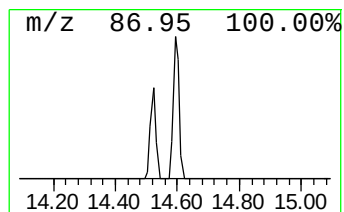
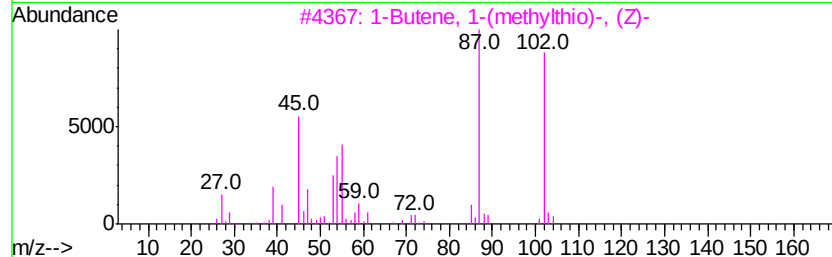
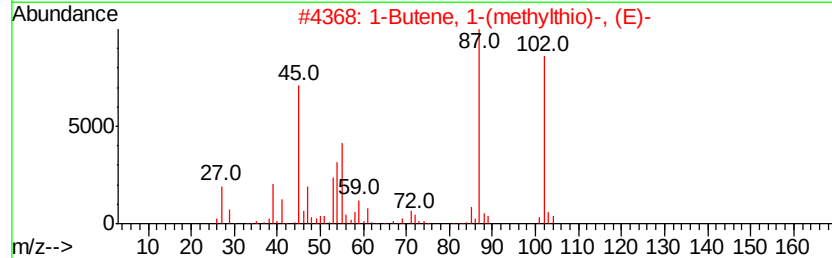
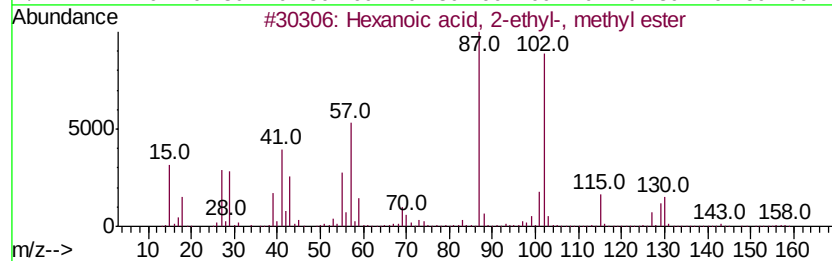
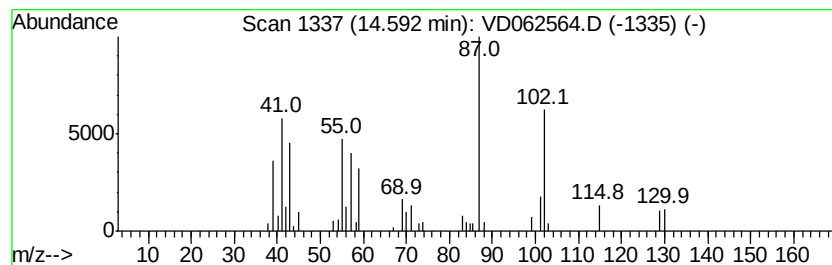
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanoic acid, 2-ethyl-, me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	6.24 ug/l	63987	1,4-Dichlorobenzene-d4	14.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	83
2	1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	53
3	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	42
4	Neodecanoic acid	172	C10H20O2	026896-20-8	40
5	2-O-Methyl-d-xylose	164	C6H12O5	1000130-01-3	37



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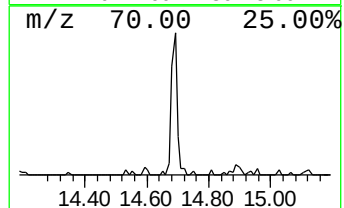
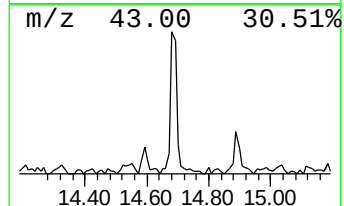
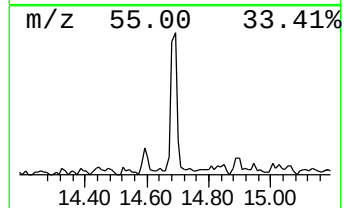
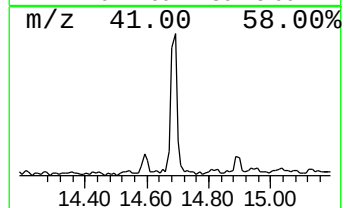
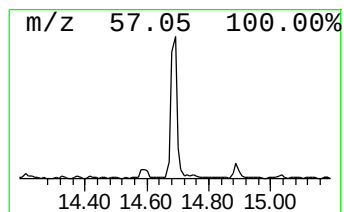
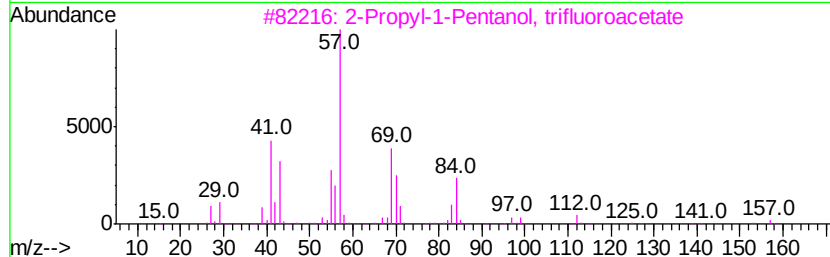
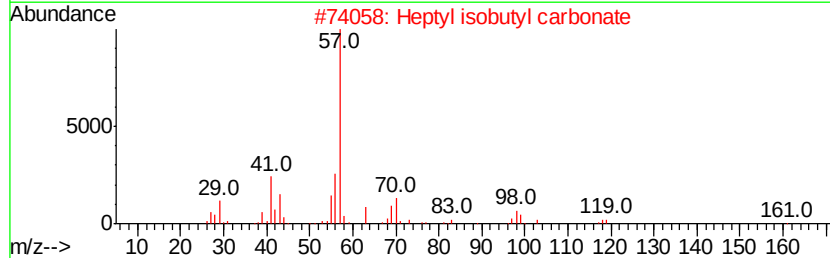
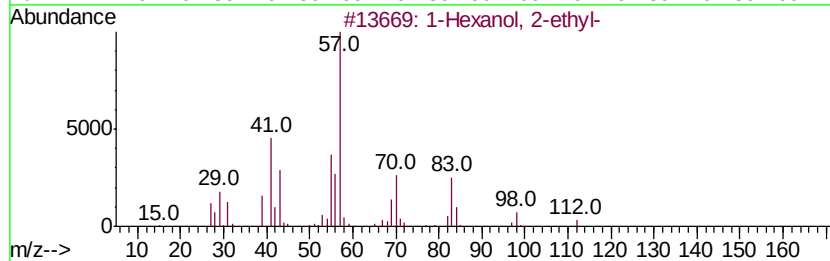
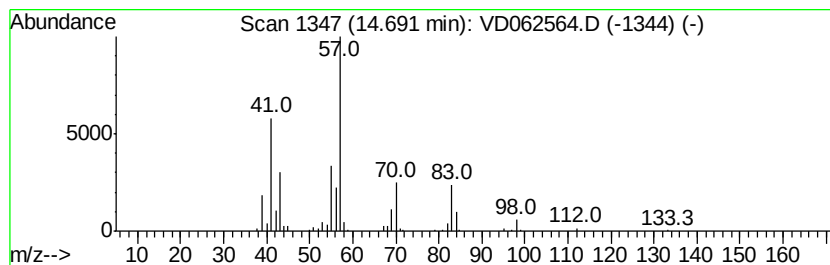
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D053019S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	33.13 ug/l	339794	1,4-Dichlorobenzene-d4	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7 83
2		Heptyl isobutyl carbonate	216 C12H24O3	959068-08-7 50
3		2-Propyl-1-Pentanol, trifluoroac...	226 C10H17F3O2	1000365-19-7 47
4		2-Decenal, (Z)-	154 C10H18O	002497-25-8 43
5		Octane, 2,3-dimethyl-	142 C10H22	007146-60-3 42



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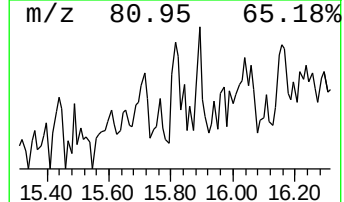
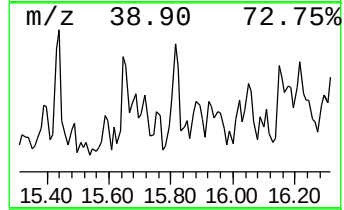
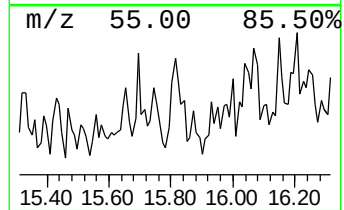
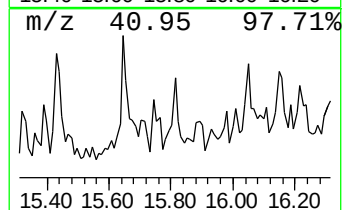
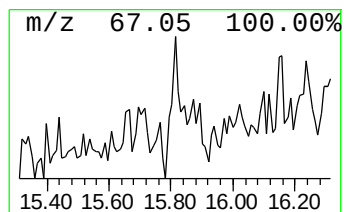
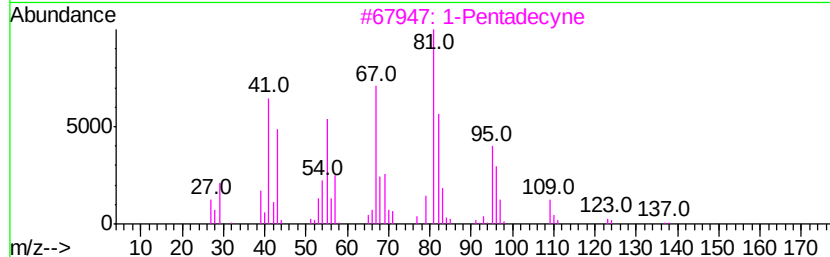
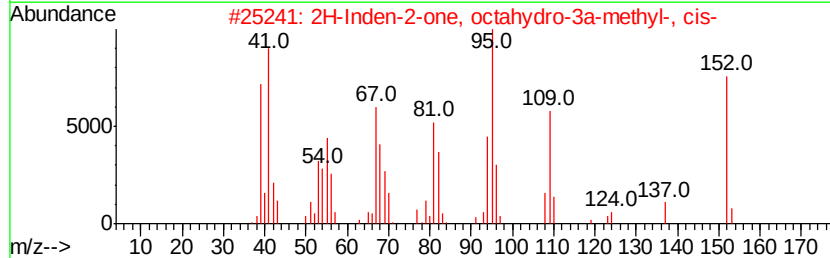
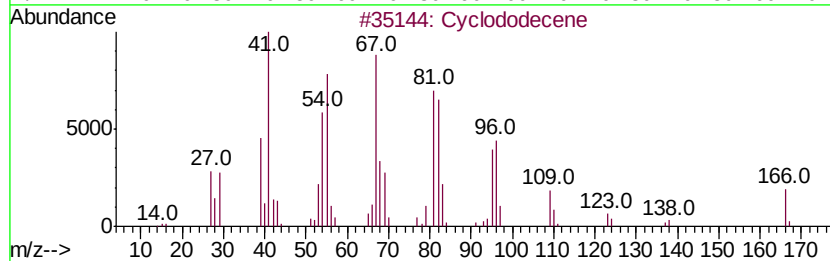
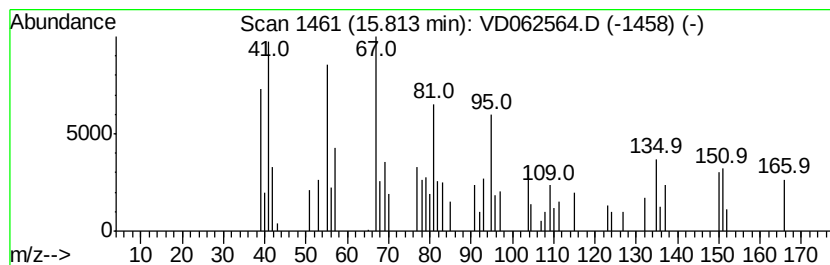
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.81 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	6.74 ug/l	69141	1,4-Dichlorobenzene-d4	14.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclododecene	166	C12H22	001501-82-2	46
2		2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	013351-29-6	38
3		1-Pentadecyne	208	C15H28	000765-13-9	38
4		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	38
5		3-Octyne, 6-methyl-	124	C9H16	062108-34-3	38



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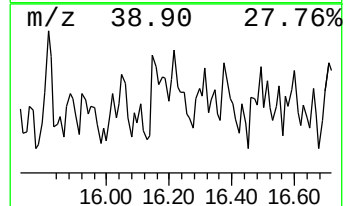
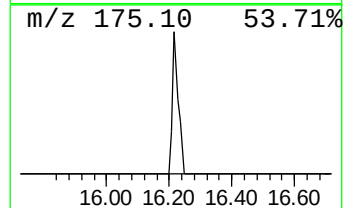
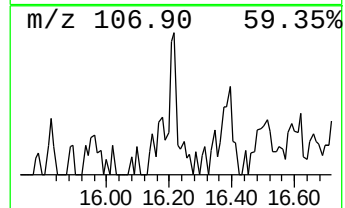
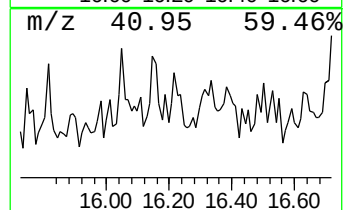
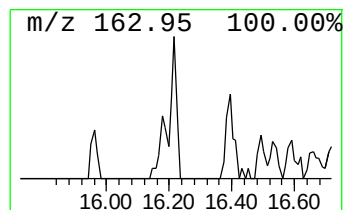
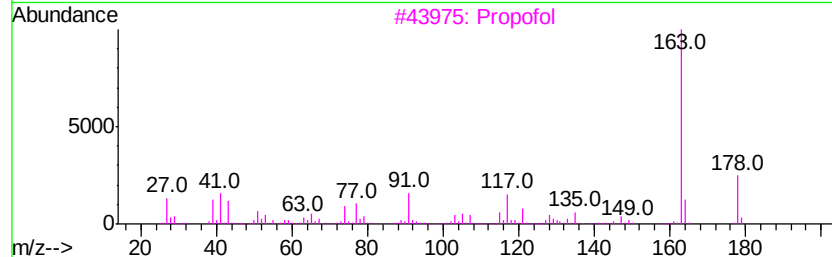
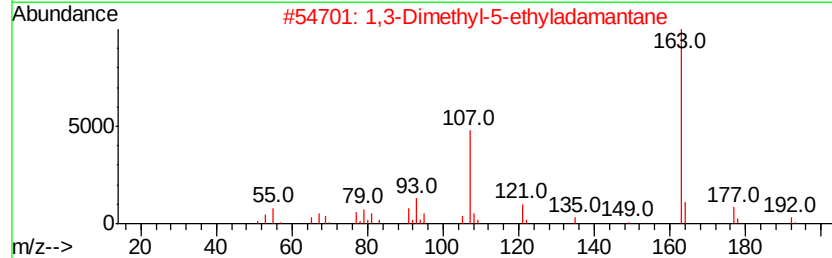
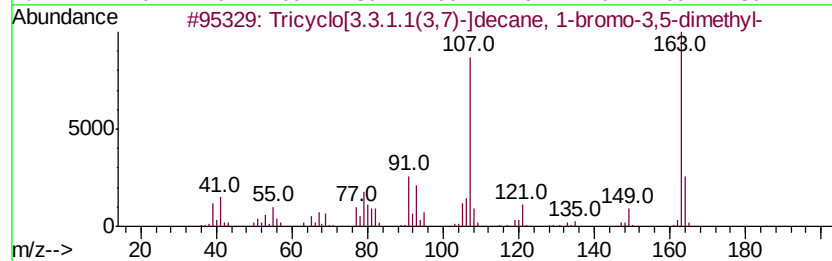
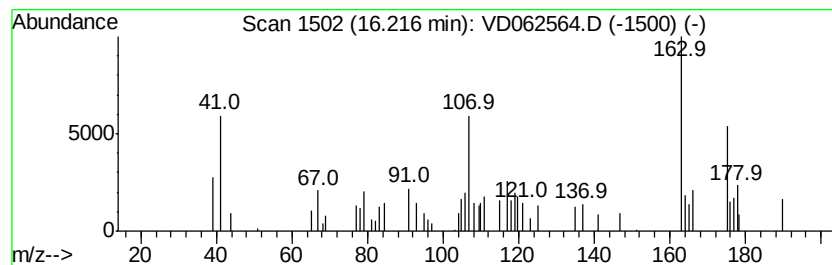
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown16.22 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	7.64 ug/l	78369	1,4-Dichlorobenzene-d4	14.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tricyclo[3.3.1.1(3,7)]decane, 1...	242 C12H19Br	000941-37-7 35
2		1,3-Dimethyl-5-ethyladamantane	192 C14H24	001687-35-0 35
3		Propofol	178 C12H18O	002078-54-8 30
4		1,3-Disilaindan, 1,3-dimethyl-	178 C9H14Si2	017864-73-2 27
5		Formamide, N-(4-methyl-3-nitroph...	180 C8H8N2O3	1000319-41-8 27



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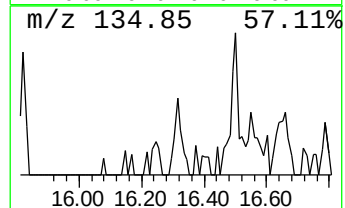
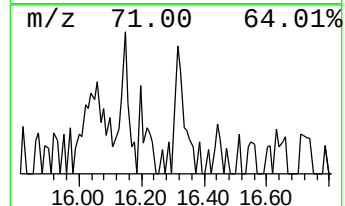
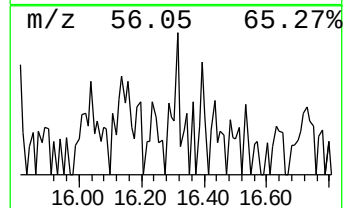
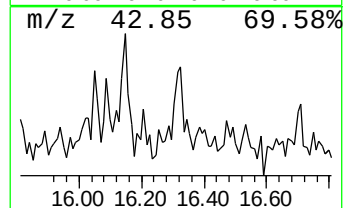
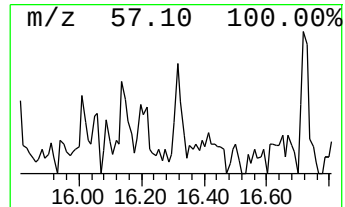
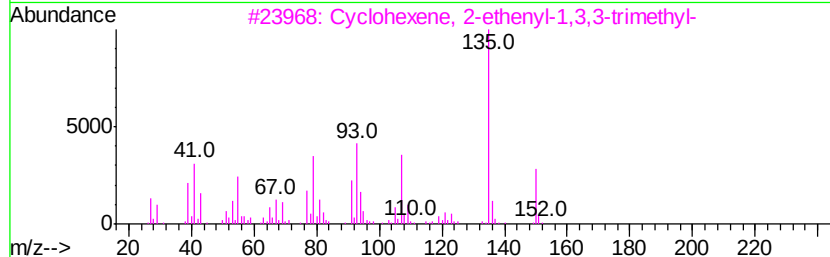
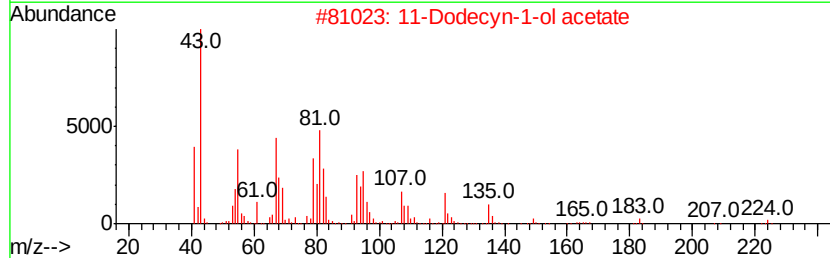
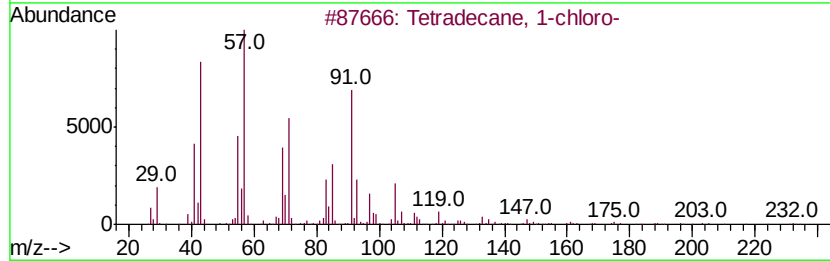
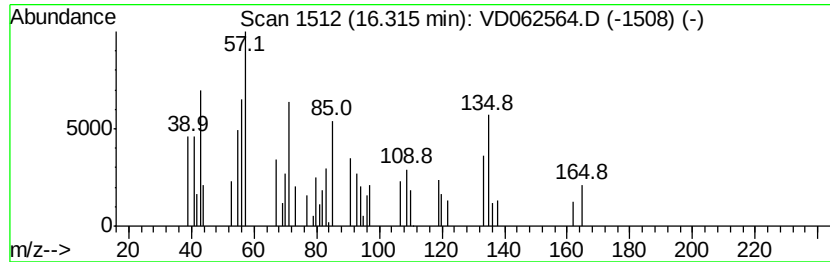
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown16.31 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	5.09 ug/l	52162	1,4-Dichlorobenzene-d4	14.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	10
2		11-Dodecyn-1-ol acetate	224	C14H24O2	053596-78-4	10
3		Cyclohexene, 2-ethenyl-1,3,3-trimethyl-	150	C11H18	005293-90-3	10
4		2-Hydroxymethyl-2-methylbrendane	166	C11H18O	1000139-74-2	10
5		Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	10



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA D\DATA\VD053119\
Data File : VD062564.D
Acq On : 31 May 2019 15:26
Operator : VA/AP
Sample : K3125-21
Misc : 5.04g/5ml/MSVOA D/SOIL
ALS Vial : 8 Sample Multiplier: 1

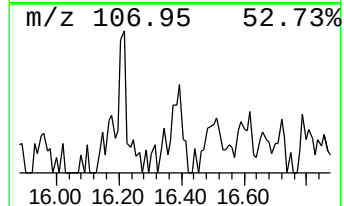
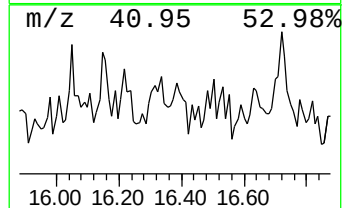
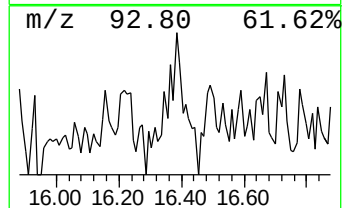
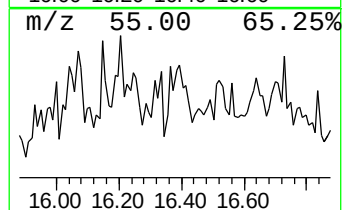
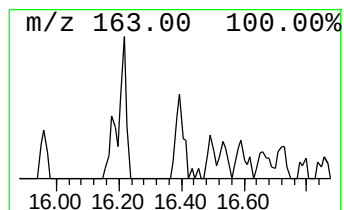
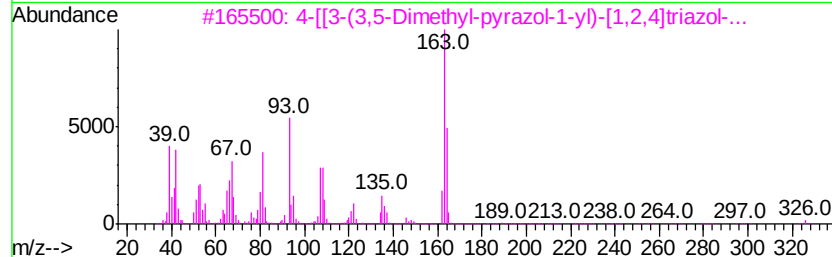
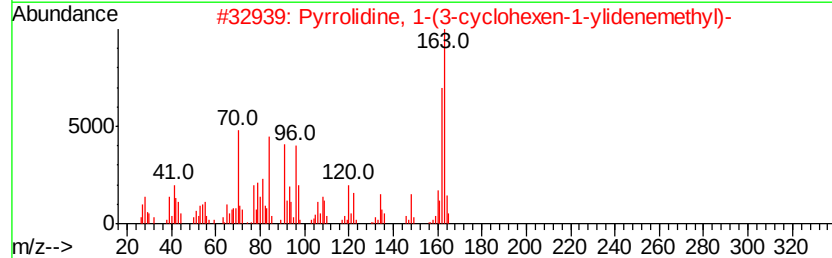
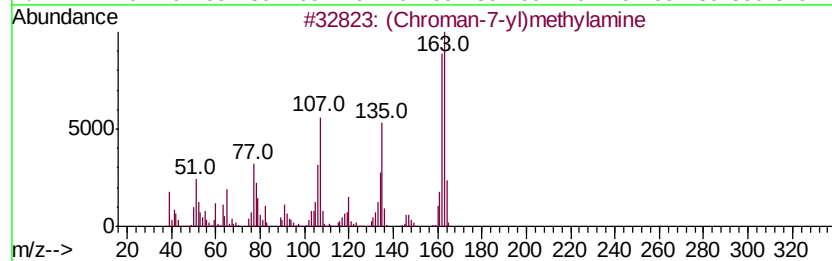
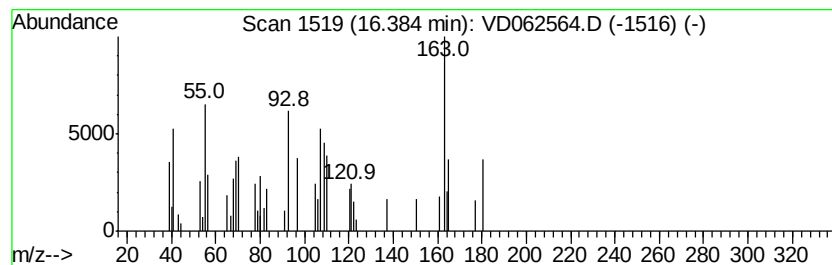
Instrument :
MSVOA_D
ClientSampled :
13903

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D053019S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown16.38 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.38	6.62 ug/l	67897	1,4-Dichlorobenzene-d4	14.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Chroman-7-yl)methylamine	163	C10H13NO	1000306-69-6	35
2	Pyrrolidine, 1-(3-cyclohexen-1-yl)-	163	C11H17N	018205-60-2	22
3	4-[[3-(3,5-Dimethyl-pyrazol-1-yl)-4-methylphenyl]methyl]piperidine	326	C16H18N6O2	1000296-14-6	17
4	1,3,3-Trimethyl-2-(2-methyl-cyclopropyl)propan-1-ol	178	C13H22	285129-06-8	17
5	1,3-Dioxolane, 2-(o-aminophenyl)-	165	C9H11NO2	026908-34-9	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA D\DATA\VD053119\
Data File : VD062564.D
Acq On : 31 May 2019 15:26
Operator : VA/AP
Sample : K3125-21
Misc : 5.04g/5ml/MSVOA D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
13903

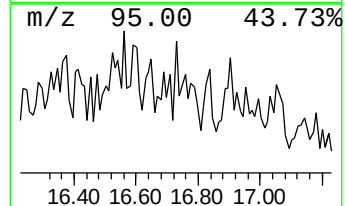
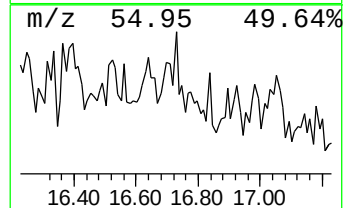
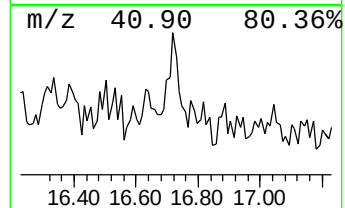
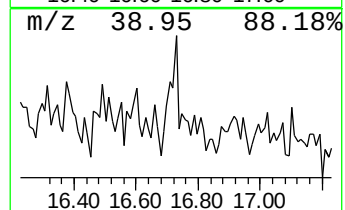
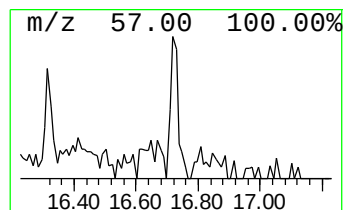
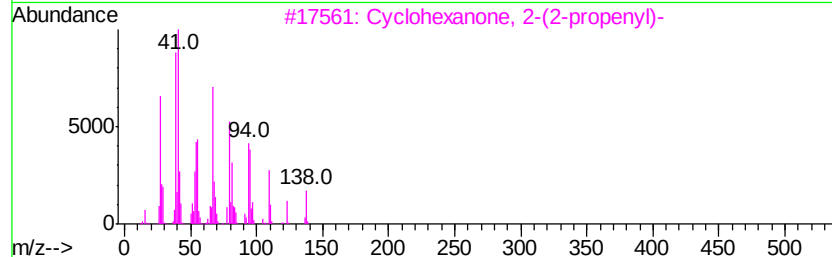
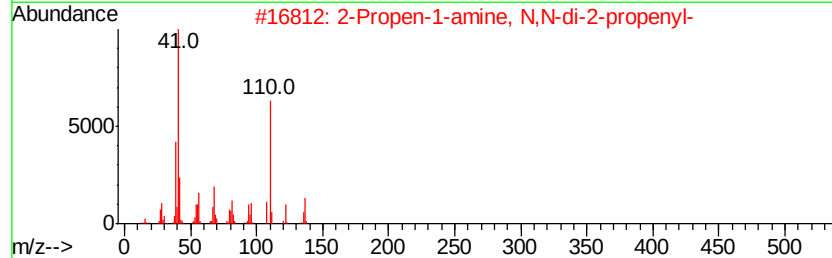
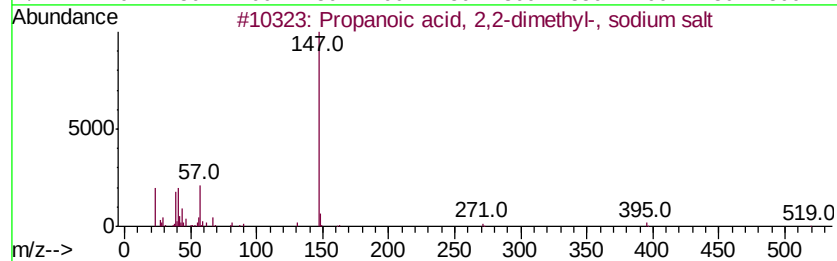
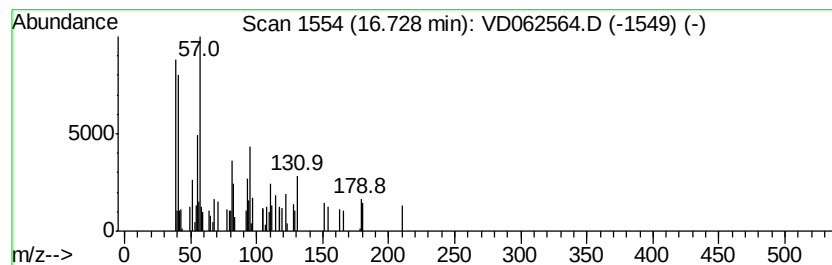
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D053019S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown16.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	6.71 ug/l	68794	1,4-Dichlorobenzene-d4	14.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2,2-dimethyl-, s...	124	C5H9NaO2	001184-88-9	40
2		2-Propen-1-amine, N,N-di-2-prope...	137	C9H15N	000102-70-5	36
3		Cyclohexanone, 2-(2-propenyl)-	138	C9H14O	000094-66-6	34
4		2-Cyclopenten-1-one, 5-hydroxy-2...	126	C7H10O2	058649-31-3	33
5		9-Oxabicyclo[6.1.0]nonan-4-one	140	C8H12O2	028399-88-4	33



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_D\DATA\VD053119\
Data File : VD062564.D
Acq On : 31 May 2019 15:26
Operator : VA/AP
Sample : K3125-21
Misc : 5.04g/5ml/MSVOA_D/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
13903

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D053019S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, 2-...	14.59	6.2	ug/l	63987	4	14.52	512825	50.0
1-Hexanol, 2-ethyl-	14.69	33.1	ug/l	339794	4	14.52	512825	50.0
unknown15.81	15.81	6.7	ug/l	69141	4	14.52	512825	50.0
unknown16.22	16.22	7.6	ug/l	78369	4	14.52	512825	50.0
unknown16.31	16.31	5.1	ug/l	52162	4	14.52	512825	50.0
unknown16.38	16.38	6.6	ug/l	67897	4	14.52	512825	50.0
unknown16.73	16.73	6.7	ug/l	68794	4	14.52	512825	50.0