

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD012424\
 Data File : VD078229.D
 Acq On : 24 Jan 2024 17:59
 Operator : RP/MD
 Sample : P1235-04
 Misc : 5.05G/5.0ml/MSVOA_D/SOIL/A
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 143

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\82D012224S.M
 Title : SW846 8260

Signal : TIC: VD078229.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	19	27	40	rVB	946706	1477858	100.00%	21.954%
2	4.799	538	546	557	rBV5	8587	27213	1.84%	0.404%
3	7.069	923	932	941	rBV3	5100	16544	1.12%	0.246%
4	7.810	1047	1058	1064	rBV	116861	288821	19.54%	4.291%
5	7.881	1064	1070	1081	rVB	172456	394360	26.68%	5.858%
6	8.040	1090	1097	1105	rBV3	6763	15460	1.05%	0.230%
7	8.234	1122	1130	1143	rVB	97603	221361	14.98%	3.288%
8	8.781	1213	1223	1232	rBV	319373	648433	43.88%	9.633%
9	10.269	1467	1476	1486	rBV	540711	954333	64.58%	14.177%
10	11.581	1691	1699	1712	rBV	501079	857553	58.03%	12.739%
11	12.575	1859	1868	1875	rBV	348886	576625	39.02%	8.566%
12	13.516	2021	2028	2036	rBV	463130	743428	50.30%	11.044%
13	14.945	2260	2271	2273	rBV5	15241	34105	2.31%	0.507%
14	14.981	2273	2277	2284	rVV3	39249	102551	6.94%	1.523%
15	15.051	2284	2289	2297	rVV4	49727	134606	9.11%	2.000%
16	15.128	2297	2302	2307	rVV6	26430	56050	3.79%	0.833%
17	15.186	2307	2312	2317	rVV5	11765	24434	1.65%	0.363%
18	15.275	2318	2327	2333	rVV6	26371	80337	5.44%	1.193%
19	15.369	2335	2343	2354	rVB5	29467	77550	5.25%	1.152%

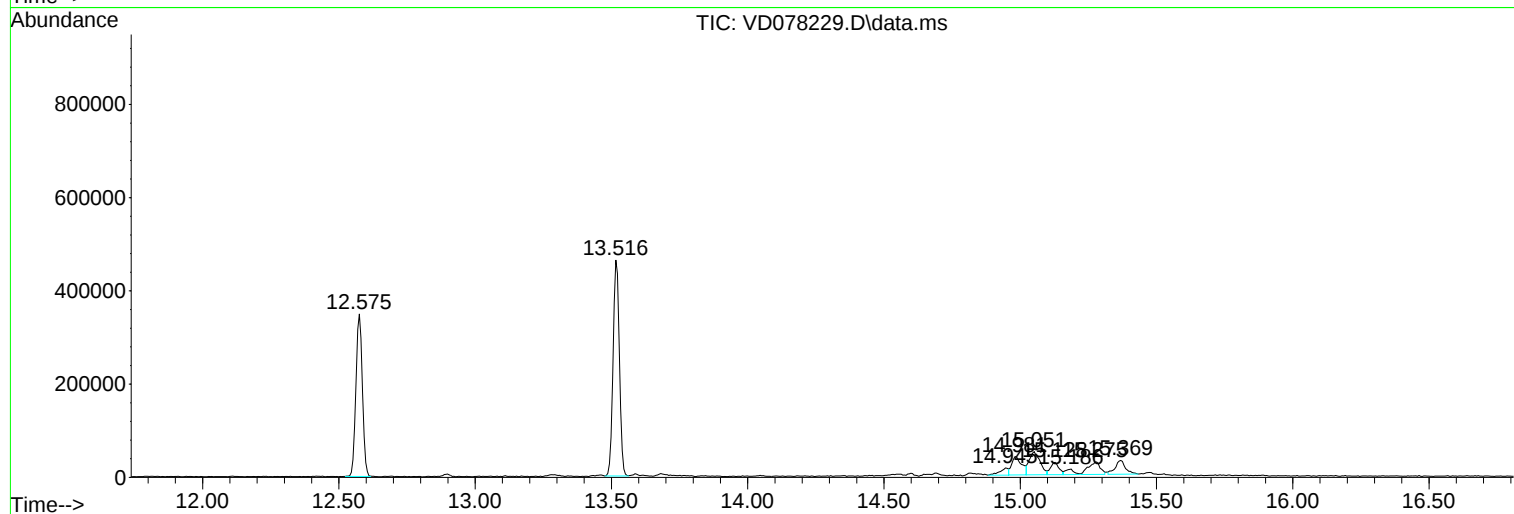
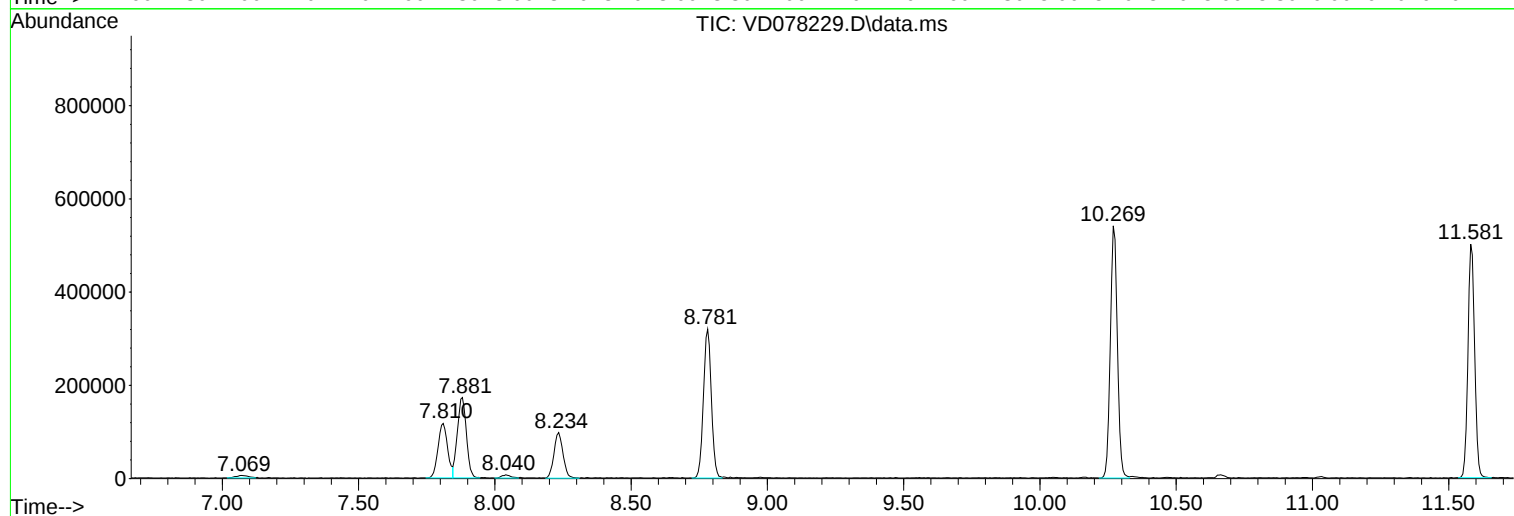
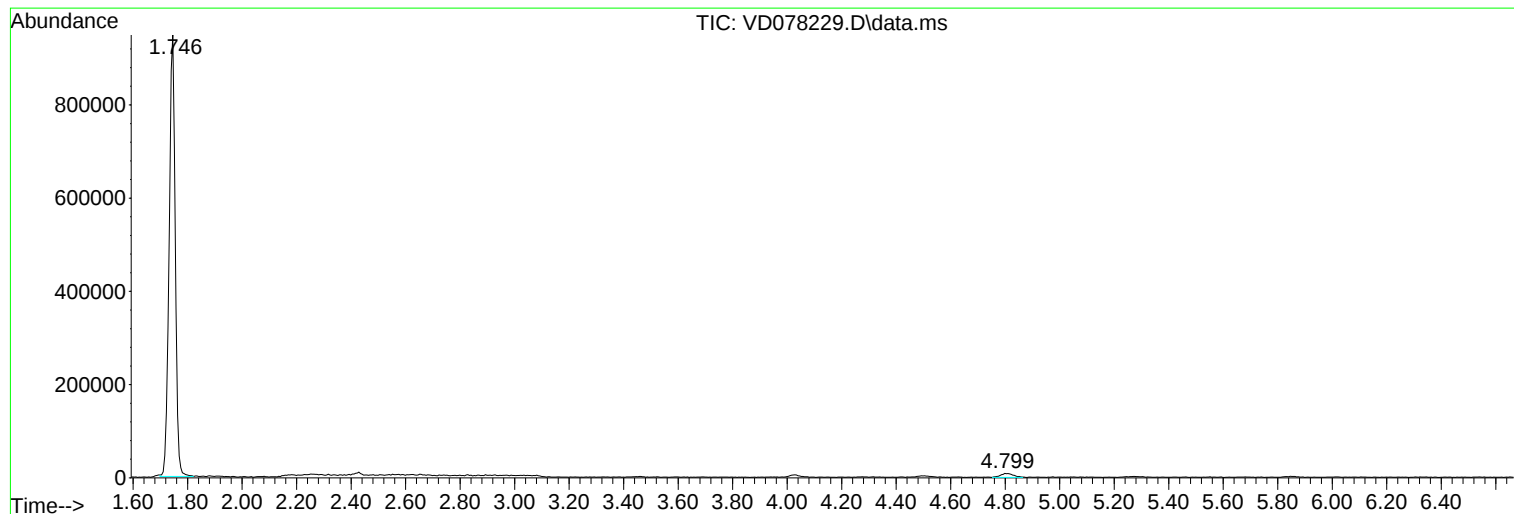
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D012224S.M
Quant Title : SW846 8260

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



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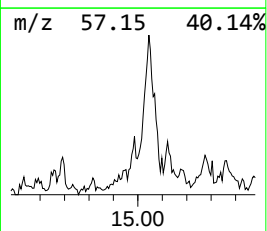
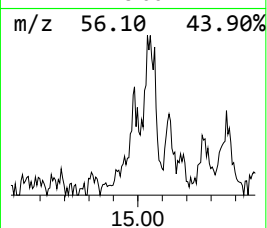
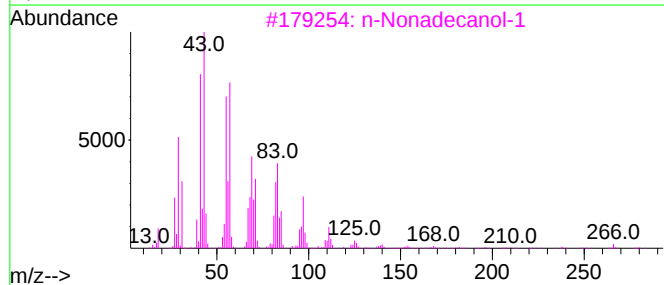
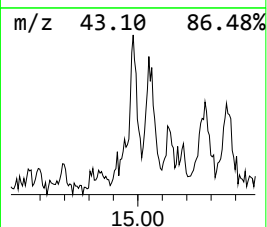
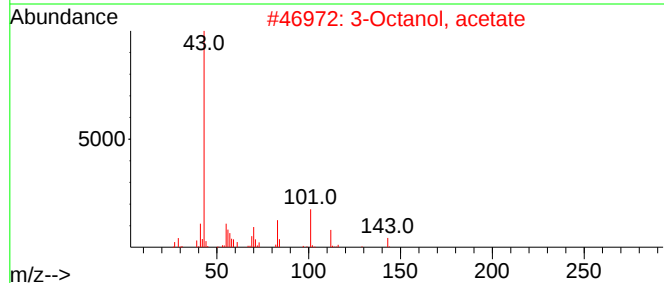
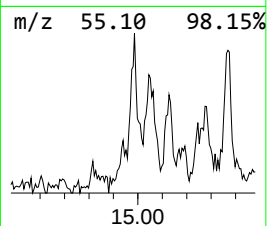
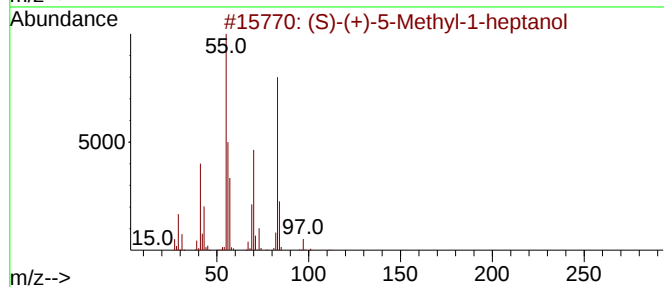
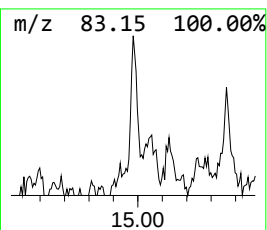
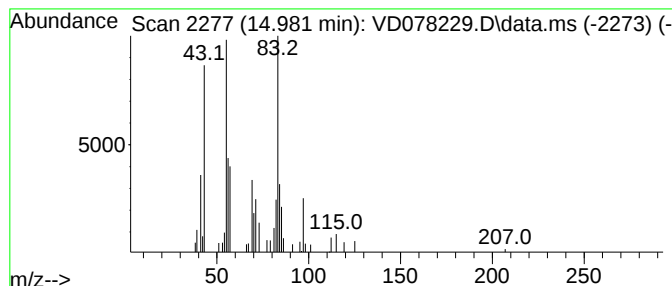
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D012224S.M
Quant Title : SW846 8260

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

Peak Number 2 (S)-(+)-5-Methyl-1-heptanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.981	6.90 ug/l	102551	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	53		
2	3-Octanol, acetate	172	C10H20O2	004864-61-3	40		
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	35		
4	1-Hexanol, 5-methyl-2-(1-methyle...	200	C12H24O2	040853-55-2	35		
5	Hexane, 3-methyl-4-methylene-	112	C8H16	003404-67-9	35		



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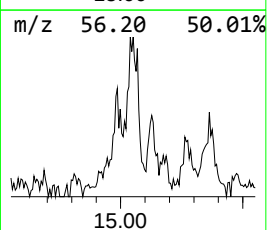
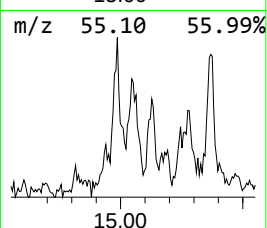
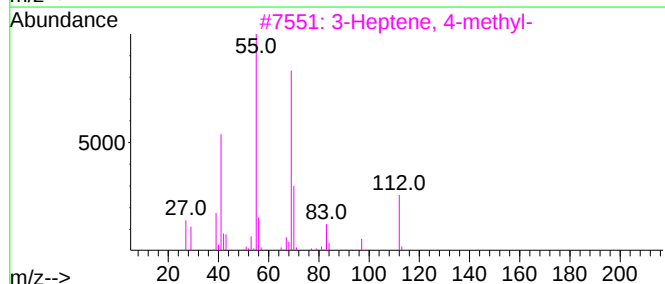
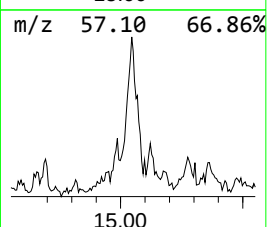
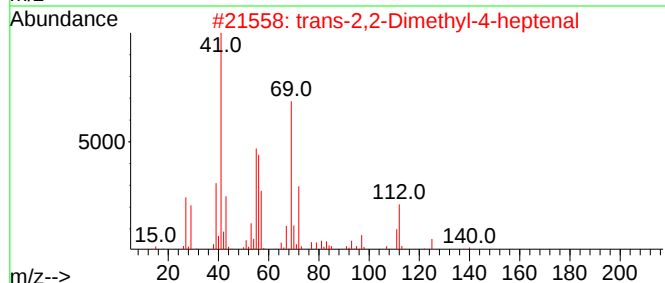
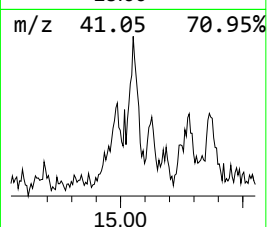
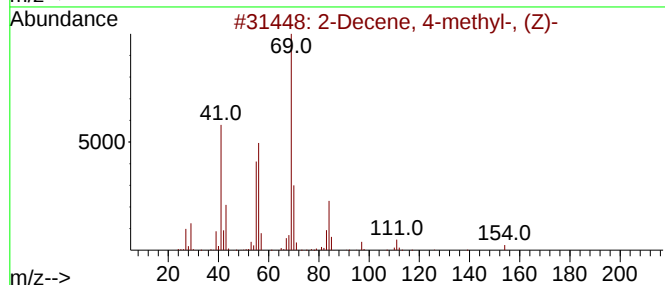
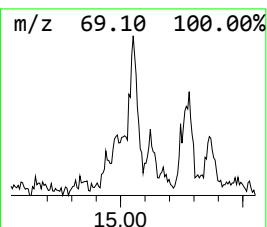
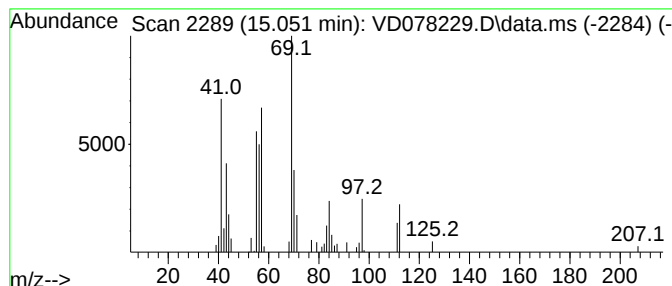
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D012224S.M
Quant Title : SW846 8260

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

Peak Number 3 2-Decene, 4-methyl-, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	9.05 ug/l	134606	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	59
2			trans-2,2-Dimethyl-4-heptenal	140	C9H16O	091296-58-1	53
3			3-Heptene, 4-methyl-	112	C8H16	004485-16-9	50
4			2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	49
5			4-Methyl-2-heptene	112	C8H16	003404-56-6	47



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Instrument :
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ClientSampleId :
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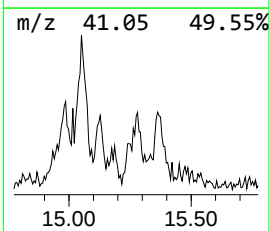
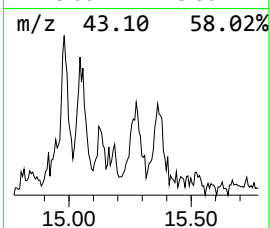
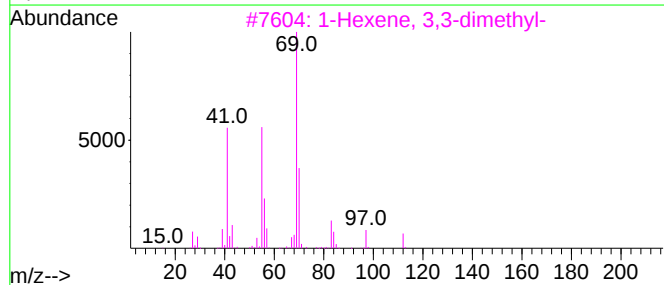
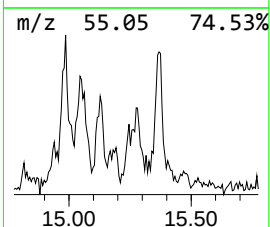
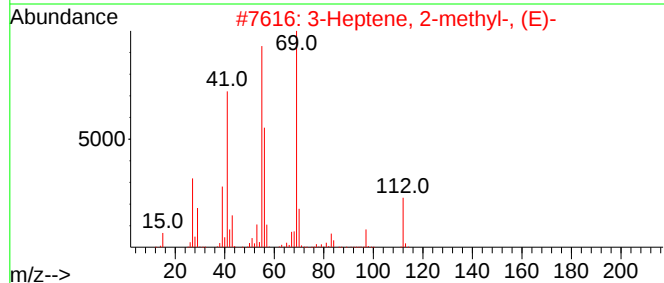
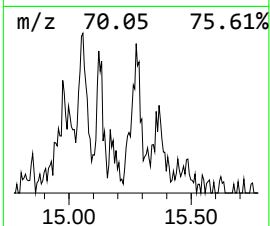
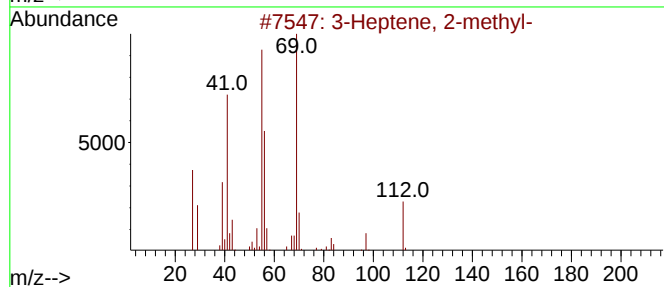
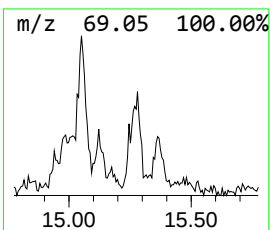
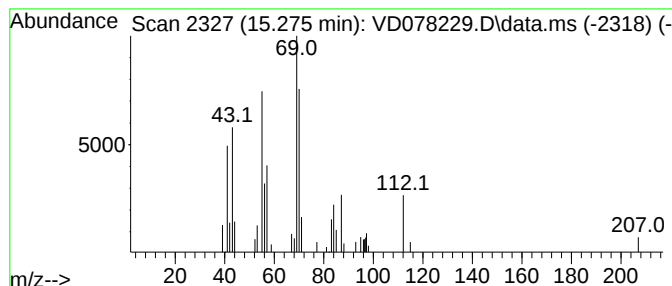
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D012224S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown15.275 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.275	5.40 ug/l	80337	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptene, 2-methyl-	112	C8H16	017618-76-7	43
2			3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	43
3			1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	43
4			3-Heptene, 4-methyl-	112	C8H16	004485-16-9	38
5			2-Heptene, 3-methyl-	112	C8H16	003404-75-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD012424\
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Operator : RP/MD
Sample : P1235-04
Misc : 5.05G/5.0ml/MSVOA_D/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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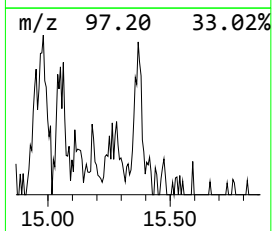
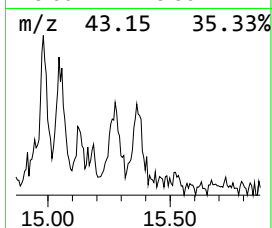
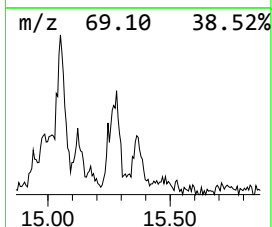
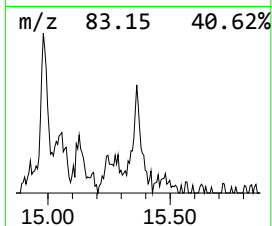
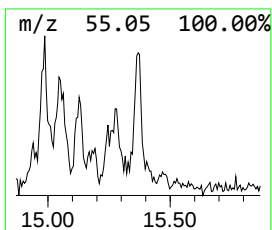
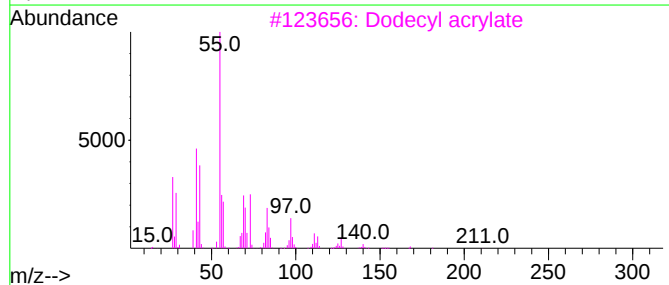
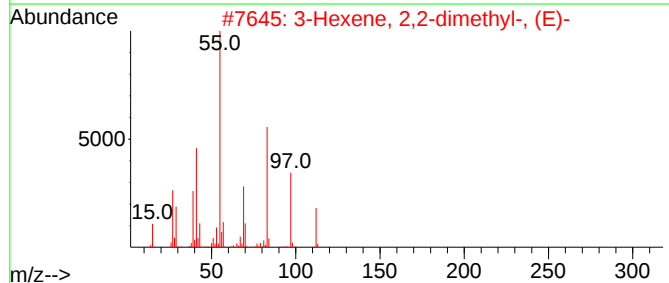
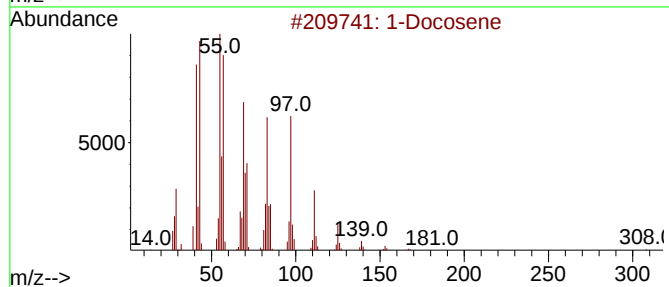
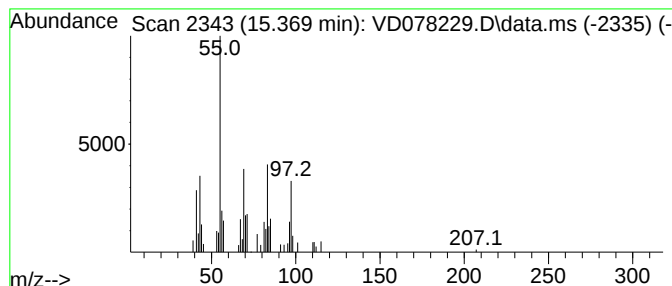
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Quant Title : SW846 8260

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

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.369	5.22 ug/l	77550	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	50
2			3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	000690-93-7	43
3			Dodecyl acrylate	240	C15H28O2	002156-97-0	43
4			3-Ethyl-2-hexene	112	C8H16	000620-00-8	43
5			Carbonic acid, decyl 2,2,2-trich...	332	C13H23Cl3O3	1000314-55-6	38



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(S)-(+)-5-Methy...	14.981	6.9	ug/l	102551	4	13.516	743428	50.0
2-Decene, 4-met...	15.051	9.1	ug/l	134606	4	13.516	743428	50.0
unknown15.275	15.275	5.4	ug/l	80337	4	13.516	743428	50.0
1-Docosene	15.369	5.2	ug/l	77550	4	13.516	743428	50.0