

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112219\
 Data File : VN059360.D
 Acq On : 22 Nov 2019 13:35
 Operator : JC/SP
 Sample : K5957-03
 Misc : 5.21g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2-(12-14)

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_N\METHODS\82N112019W.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	2.442	188	208	210	rBV	13456	33784	2.16%	0.352%
2	7.567	1782	1802	1813	rBV	190210	470191	30.02%	4.904%
3	7.641	1813	1825	1852	rVB	386381	917761	58.59%	9.573%
4	8.005	1922	1938	1962	rBV	218901	510768	32.61%	5.327%
5	8.567	2094	2113	2133	rBV	550616	1146426	73.19%	11.958%
6	10.082	2568	2584	2601	rBV	853879	1566329	100.00%	16.337%
7	10.297	2639	2651	2668	rBV2	6258	19026	1.21%	0.198%
8	11.406	2981	2996	3016	rBV	733698	1282810	81.90%	13.380%
9	11.931	3144	3159	3170	rVV10	16135	41174	2.63%	0.429%
10	12.046	3186	3195	3206	rVB	52019	82981	5.30%	0.866%
11	12.123	3206	3219	3221	rBV6	23721	39906	2.55%	0.416%
12	12.156	3222	3229	3239	rVB2	50590	87319	5.57%	0.911%
13	12.297	3262	3273	3280	rBV9	20470	45554	2.91%	0.475%
14	12.336	3281	3285	3294	rVB	26770	35052	2.24%	0.366%
15	12.403	3294	3306	3319	rBV	540250	927566	59.22%	9.675%
16	12.561	3347	3355	3368	rVB2	49916	104583	6.68%	1.091%
17	12.651	3370	3383	3393	rBV10	30842	84542	5.40%	0.882%
18	12.734	3395	3409	3412	rBV6	59844	118682	7.58%	1.238%
19	12.876	3446	3453	3460	rBV4	44955	64182	4.10%	0.669%
20	12.931	3463	3470	3473	rBV4	50590	66614	4.25%	0.695%
21	12.966	3473	3481	3494	rVB	314537	532150	33.97%	5.551%
22	13.095	3514	3521	3529	rBV	79402	121662	7.77%	1.269%
23	13.146	3531	3537	3550	rBV4	81645	132511	8.46%	1.382%
24	13.213	3553	3558	3562	rBV6	33686	43559	2.78%	0.454%
25	13.345	3589	3599	3610	rVB	610721	1021273	65.20%	10.652%
26	14.339	3903	3908	3917	rVB4	66393	91018	5.81%	0.949%

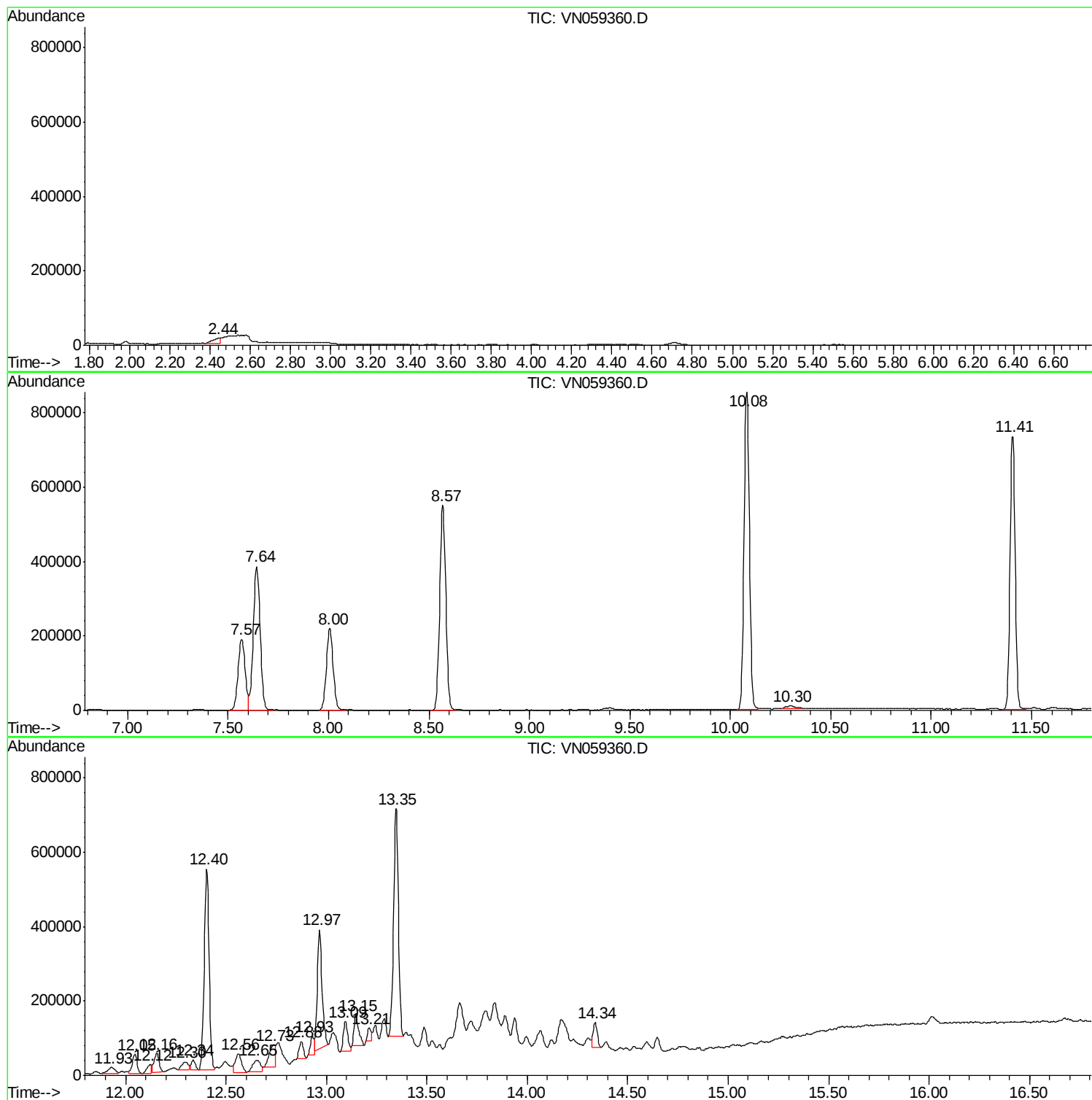
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-2-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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



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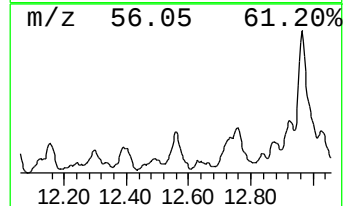
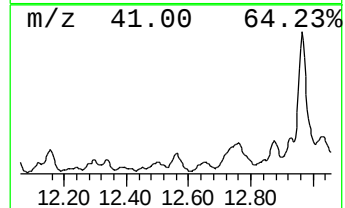
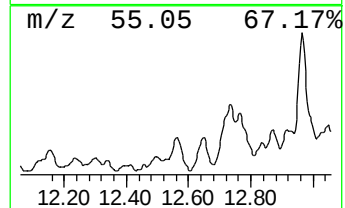
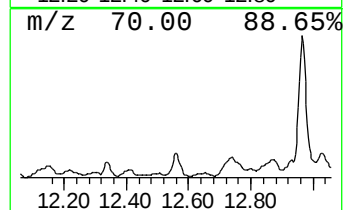
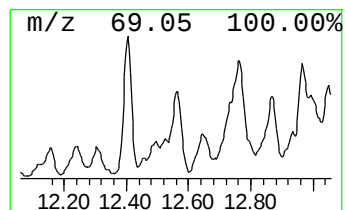
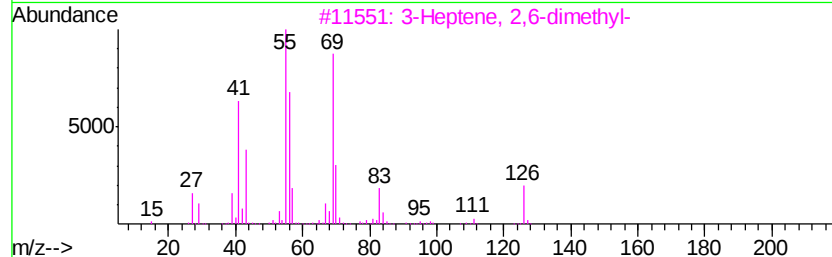
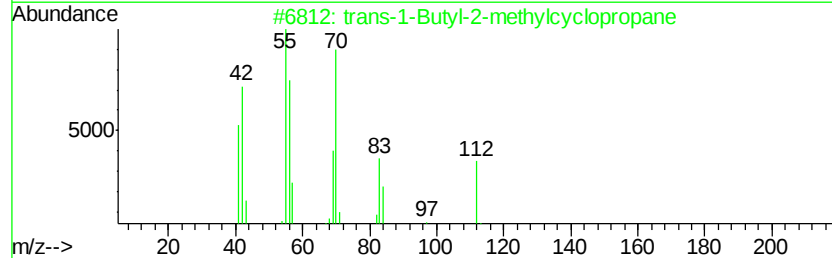
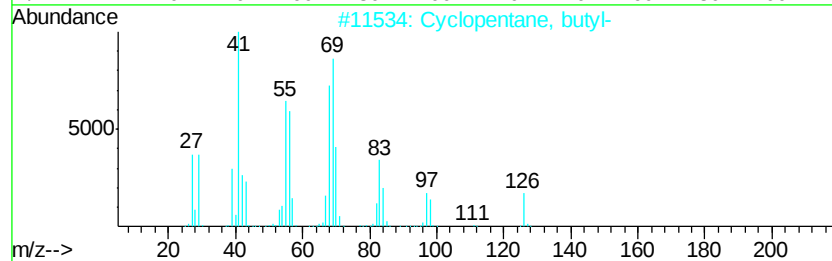
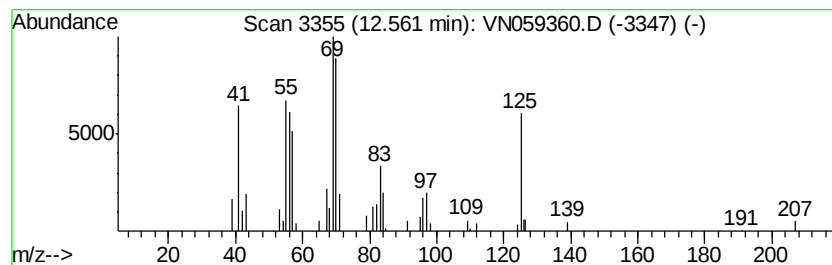
Instrument :
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ClientSampleId :
MW-2-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	5.12 ug/l	104583	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, butyl-	126	C9H18	002040-95-1	70
2	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	50
3	3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	46
4	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	45
5	Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	38



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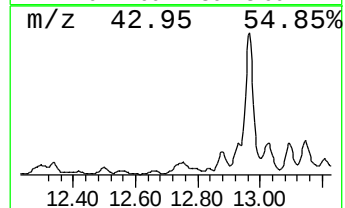
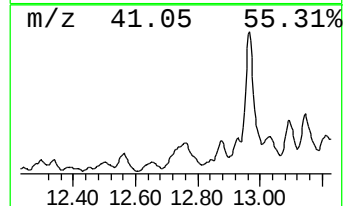
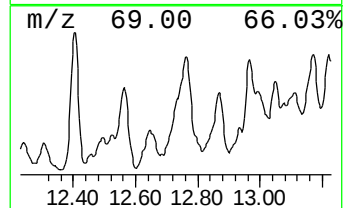
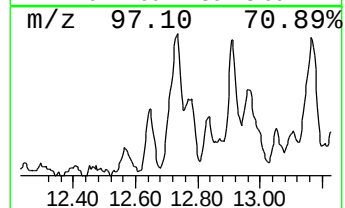
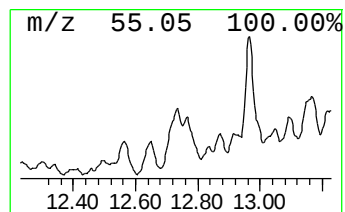
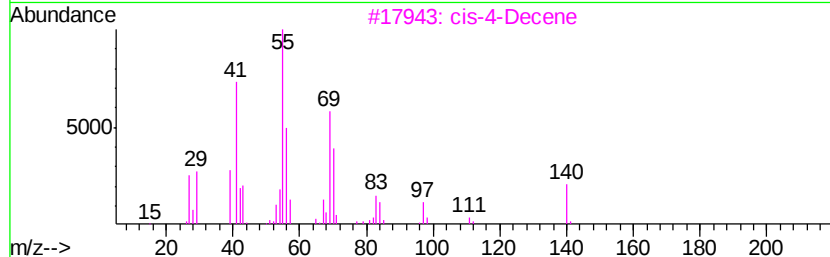
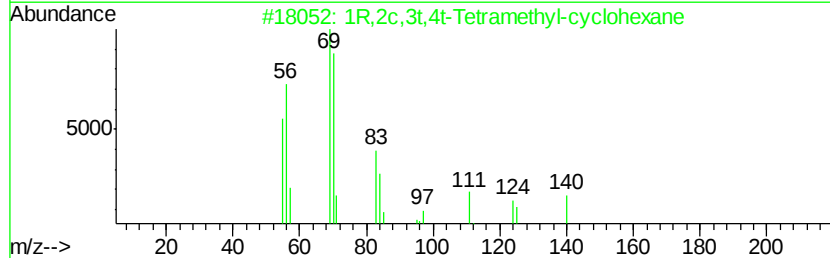
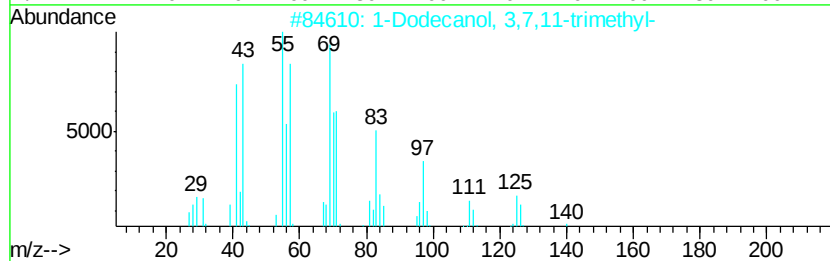
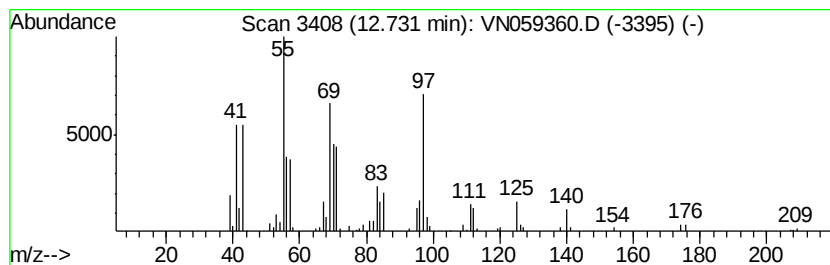
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Quant Title : SW846 8260

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

Peak Number 2 1-Dodecanol, 3,7,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	5.81 ug/l	118682	1,4-Dichlorobenzene-d4	13.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	74
2			1R,2c,3t,4t-Tetramethyl-cyclohexane	140	C10H20	1000144-07-3	49
3			cis-4-Decene	140	C10H20	019398-88-0	46
4			4-Decene	140	C10H20	019689-18-0	45
5			3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	41



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Instrument :
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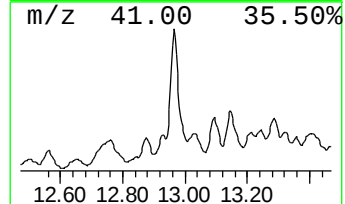
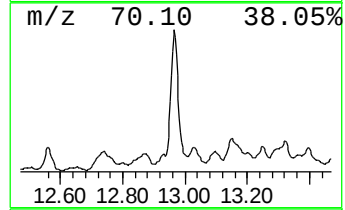
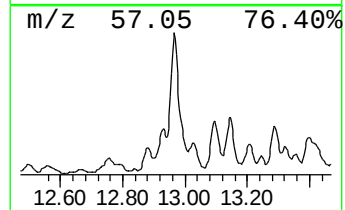
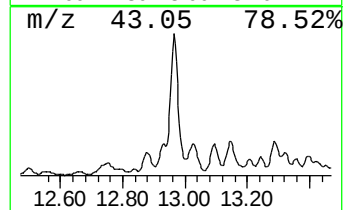
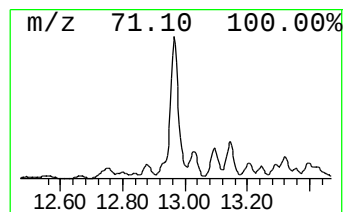
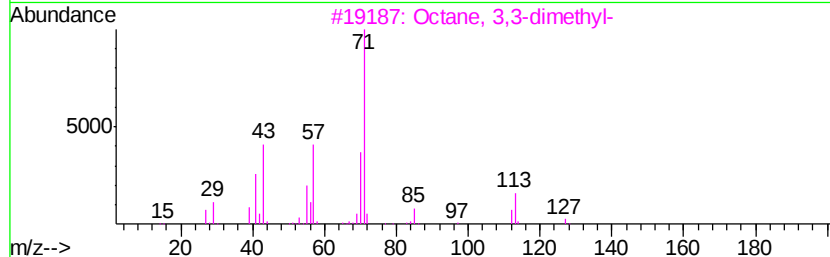
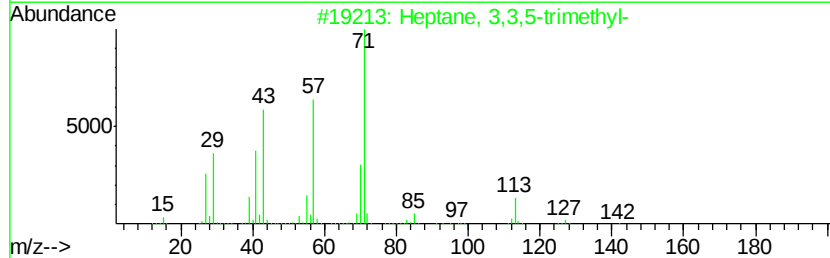
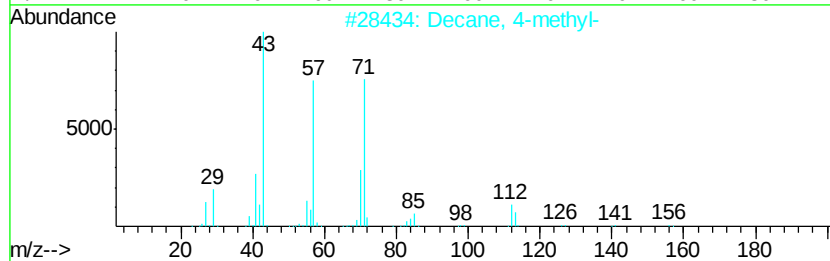
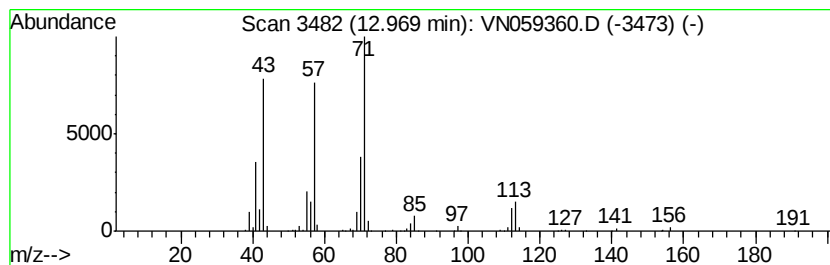
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Quant Title : SW846 8260

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

Peak Number 3 Decane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	26.05 ug/l	532150	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 4-methyl-	156	C11H24	002847-72-5	91
2		Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	78
3		Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
4		4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	72
5		Octane, 3-ethyl-	142	C10H22	005881-17-4	64



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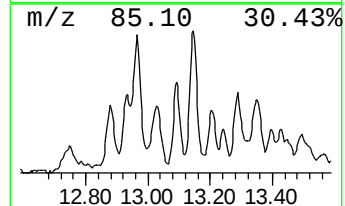
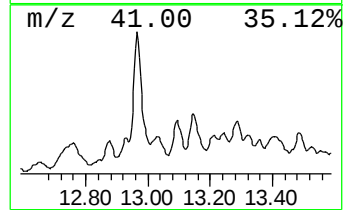
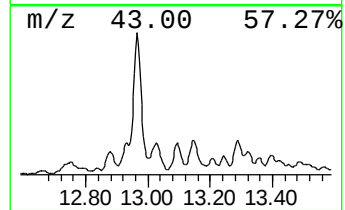
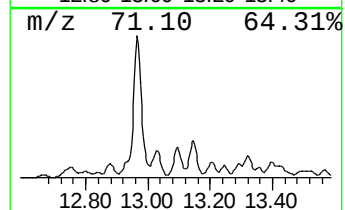
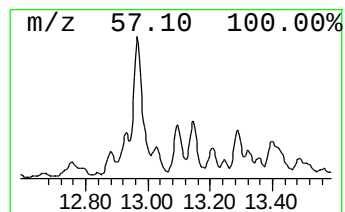
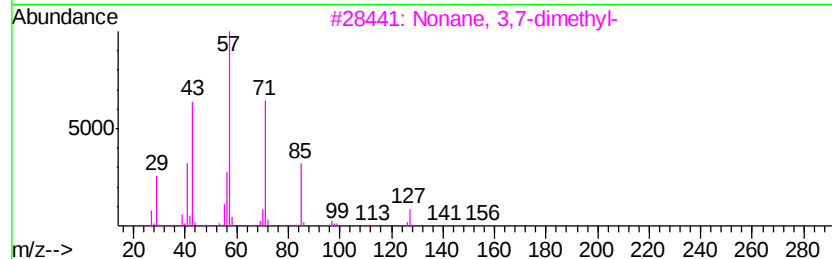
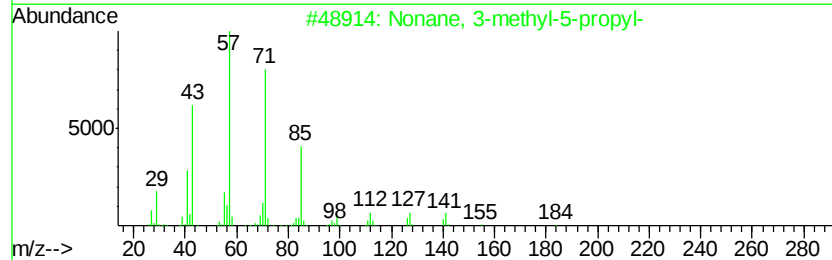
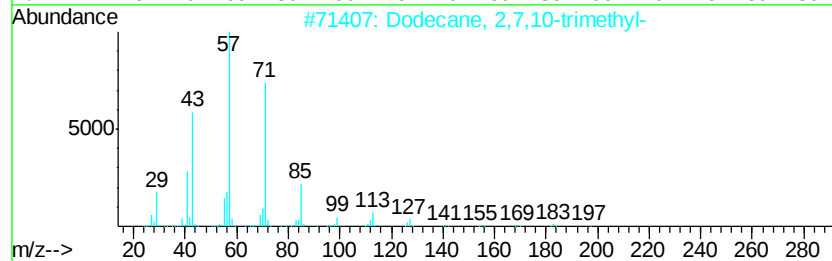
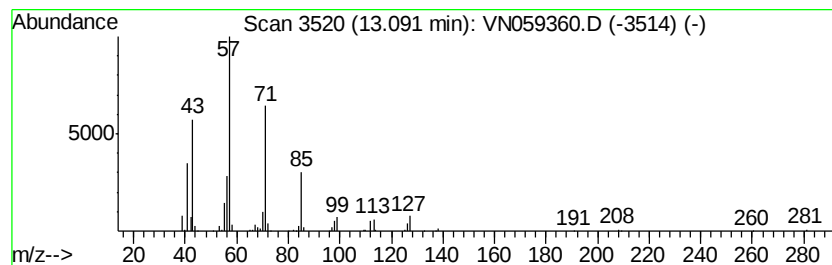
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane, 2,7,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	5.96 ug/l	121662	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
2		Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
3		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5		Decane, 2-methyl-	156	C11H24	006975-98-0	58



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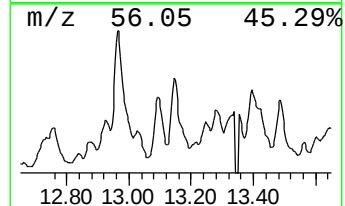
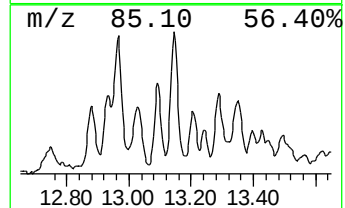
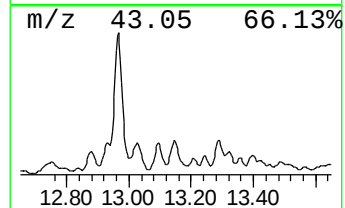
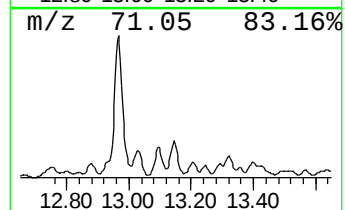
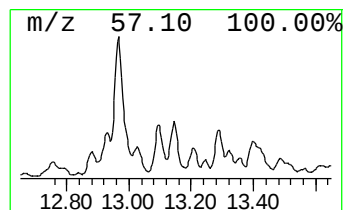
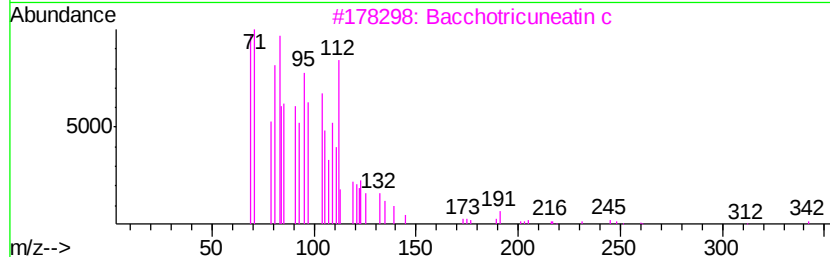
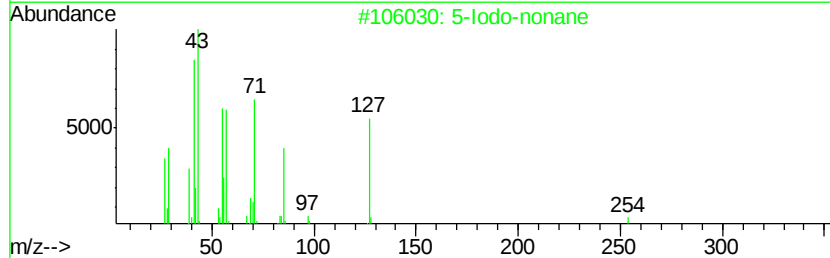
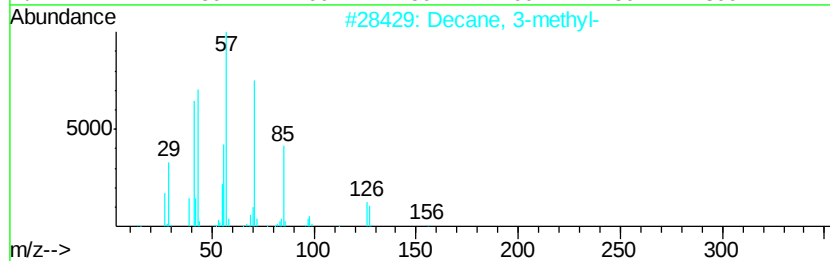
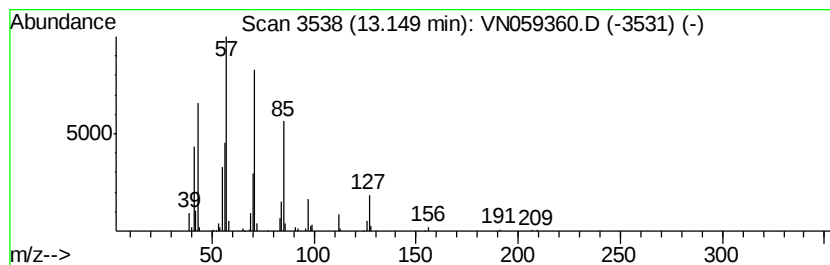
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Quant Title : SW846 8260

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

Peak Number 5 Decane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	6.49 ug/l	132511	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3-methyl-	156	C11H24	013151-34-3	86
2		5-Iodo-nonane	254	C9H19I	059456-19-8	78
3		Bacchotricuneatin c	342	C20H22O5	066563-30-2	72
4		Tetradecane	198	C14H30	000629-59-4	59
5		Undecane, 3-methyl-	170	C12H26	001002-43-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, butyl-	12.56	5.1	ug/l	104583	4	13.35	1021270	50.0
1-Dodecanol, 3,7,...	12.73	5.8	ug/l	118682	4	13.35	1021270	50.0
Decane, 4-methyl-	12.97	26.1	ug/l	532150	4	13.35	1021270	50.0
Dodecane, 2,7,10-...	13.09	6.0	ug/l	121662	4	13.35	1021270	50.0
Decane, 3-methyl-	13.15	6.5	ug/l	132511	4	13.35	1021270	50.0