

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121219\
 Data File : VN059573.D
 Acq On : 12 Dec 2019 14:49
 Operator : JC/SP
 Sample : K5664-04
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 02-03-08-09-10-11-12-COMP

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_N\METHODS\82N120919W.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	3.796	614	629	648	rBV	12269	34305	1.45%	0.282%
2	4.040	688	705	731	rBV3	17821	56912	2.40%	0.468%
3	6.815	1550	1568	1594	rBV2	8043	25946	1.10%	0.213%
4	7.567	1783	1802	1813	rBV2	162886	401185	16.94%	3.298%
5	7.644	1813	1826	1849	rVB	311826	739410	31.22%	6.079%
6	8.005	1922	1938	1963	rBV	200249	466176	19.68%	3.832%
7	8.567	2097	2113	2132	rBV	456957	943069	39.82%	7.753%
8	9.188	2287	2306	2324	rBV	72527	145033	6.12%	1.192%
9	9.976	2538	2551	2568	rBV3	18046	38297	1.62%	0.315%
10	10.078	2568	2583	2598	rBV	706376	1297048	54.76%	10.663%
11	10.271	2630	2643	2661	rBV2	7124	25698	1.08%	0.211%
12	11.403	2978	2995	3016	rBV	625320	1094444	46.21%	8.997%
13	12.400	3292	3305	3325	rBV	456703	778332	32.86%	6.399%
14	12.827	3424	3438	3457	rBV	1577623	2368504	100.00%	19.471%
15	13.072	3498	3514	3541	rBV	307669	587770	24.82%	4.832%
16	13.342	3585	3598	3613	rBV	566485	939384	39.66%	7.723%
17	13.448	3619	3631	3647	rBV	1446683	2222499	93.84%	18.271%

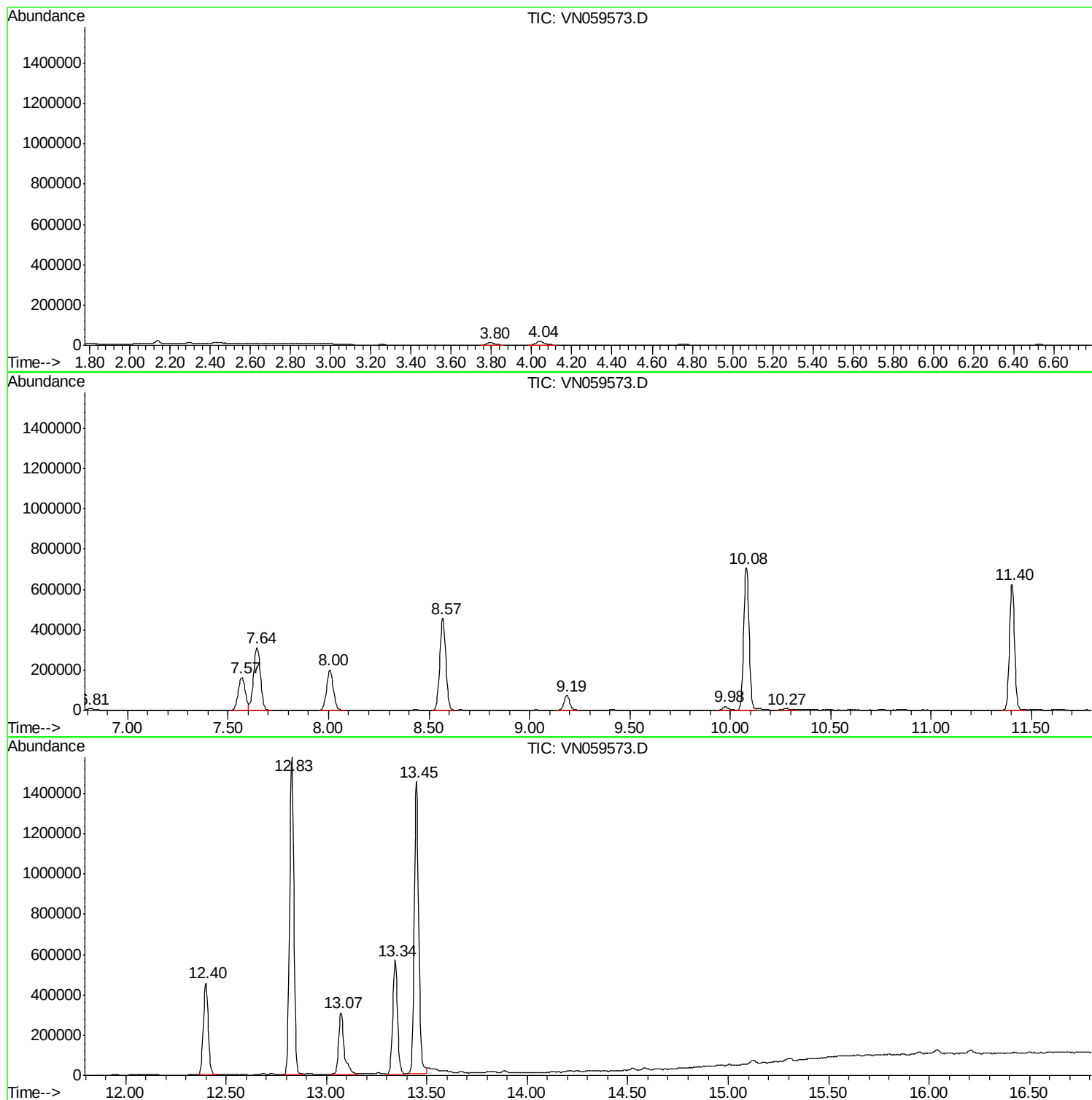
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Quant Title : SW846 8260

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



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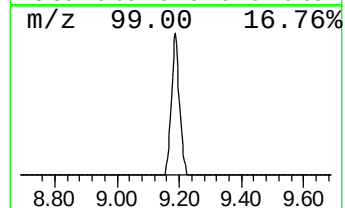
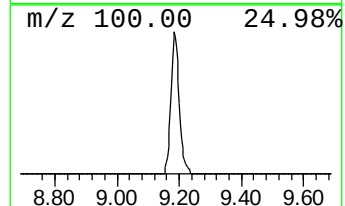
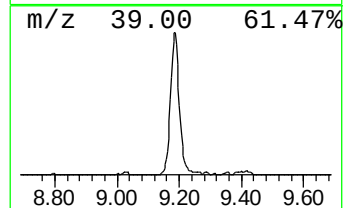
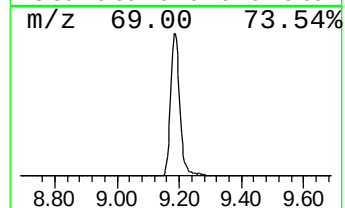
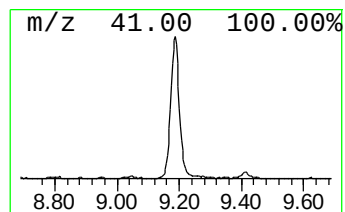
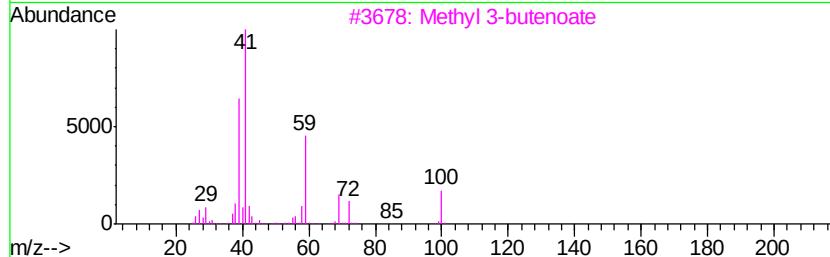
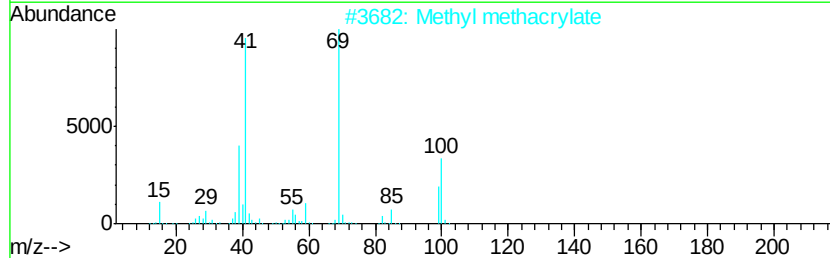
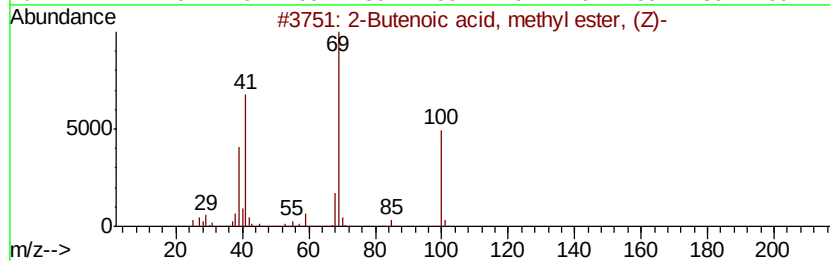
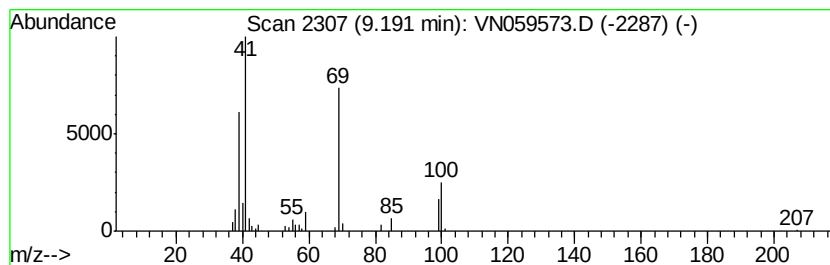
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Quant Title : SW846 8260

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

Peak Number 1 2-Butenoic acid, methyl est... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	7.69 ug/l	145033	1,4-Difluorobenzene	8.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	87
2		Methyl methacrylate	100	C5H8O2	000080-62-6	60
3		Methyl 3-butenate	100	C5H8O2	003724-55-8	50
4		2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	50
5		2-Butenoic acid, 2-methylpropyl ...	142	C8H14O2	000589-66-2	43



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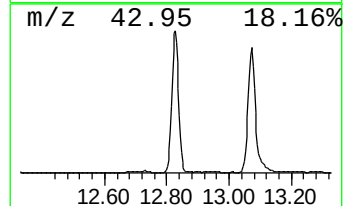
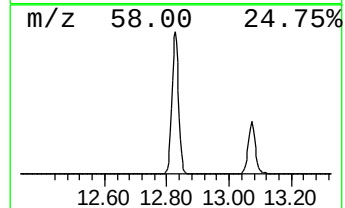
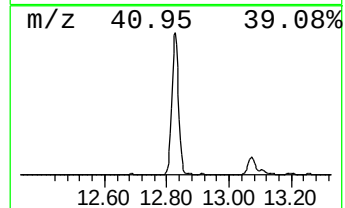
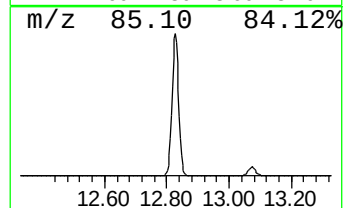
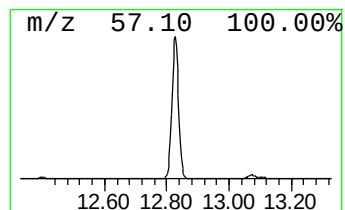
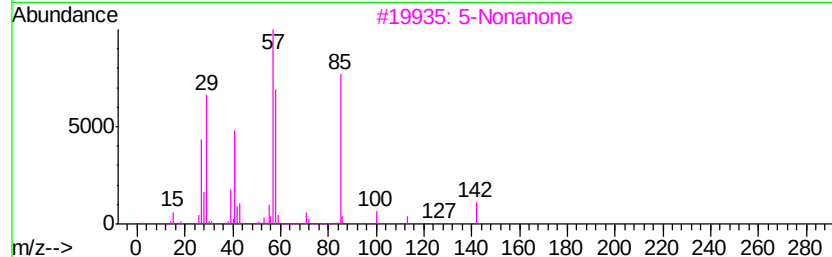
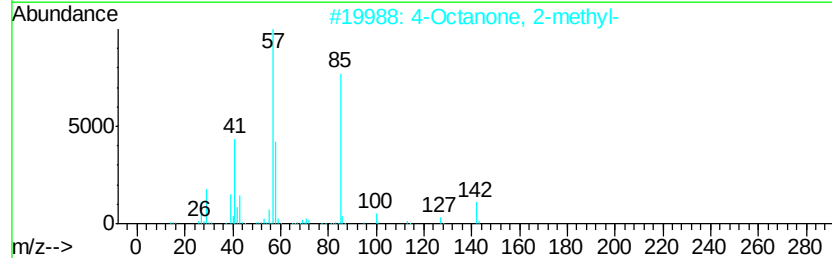
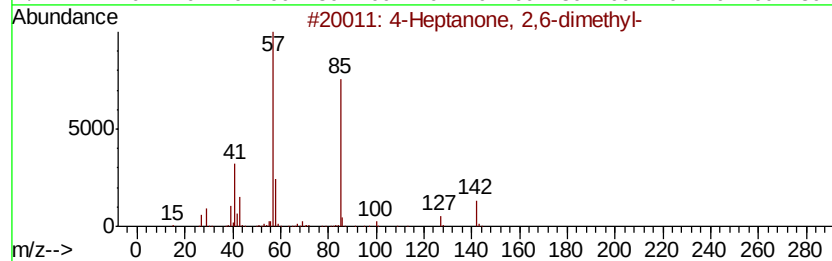
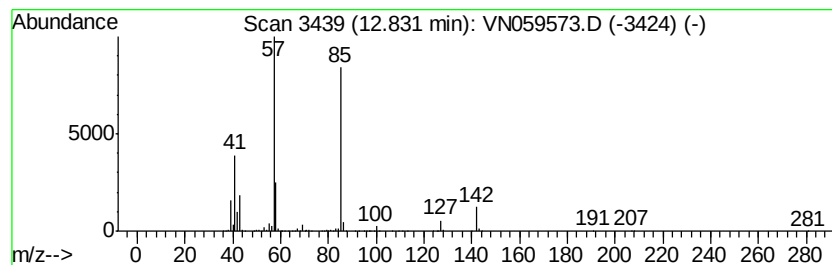
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	126.07 ug/l	2368500	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2		4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3		5-Nonanone	142	C9H18O	000502-56-7	64
4		t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5		3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50



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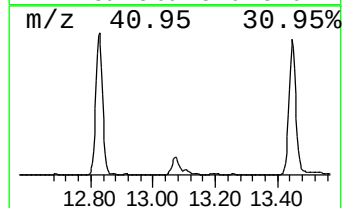
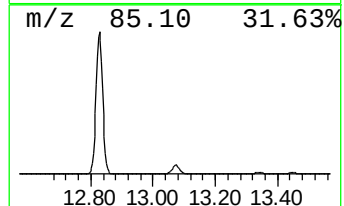
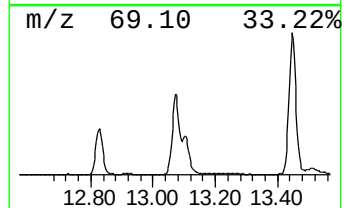
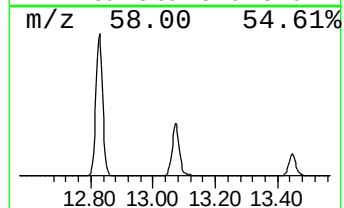
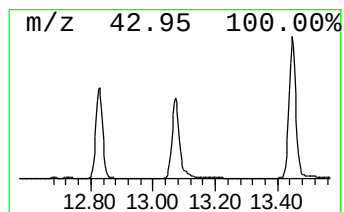
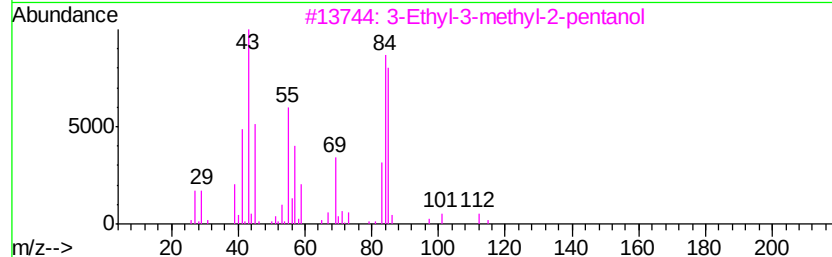
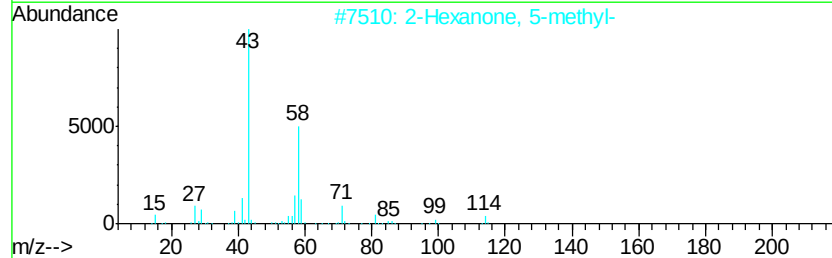
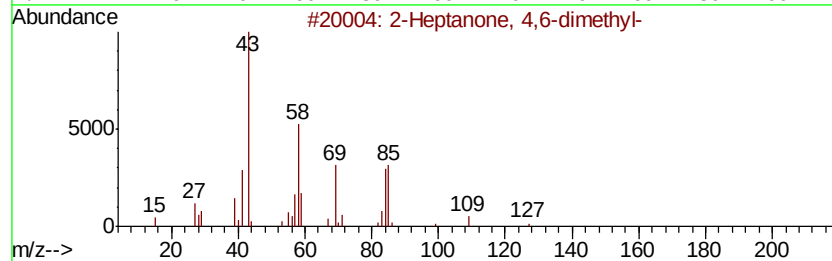
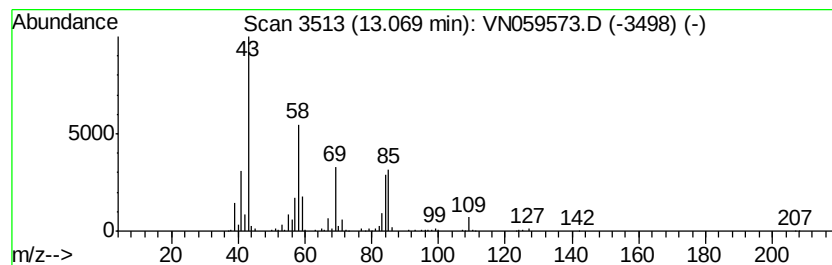
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Peak Number 3 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	31.28 ug/l	587770	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	47
3		3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	47
4		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	40
5		Hexane, 3-ethyl-	114	C8H18	000619-99-8	38



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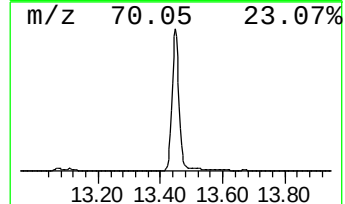
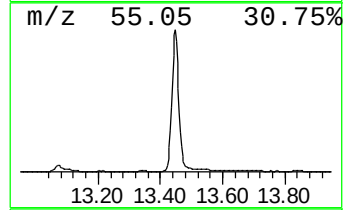
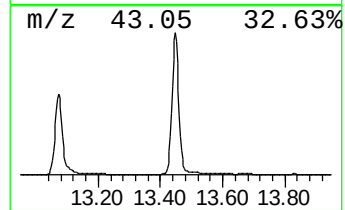
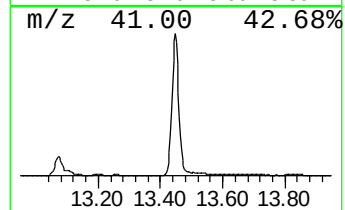
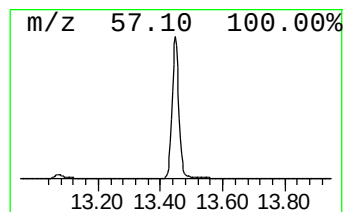
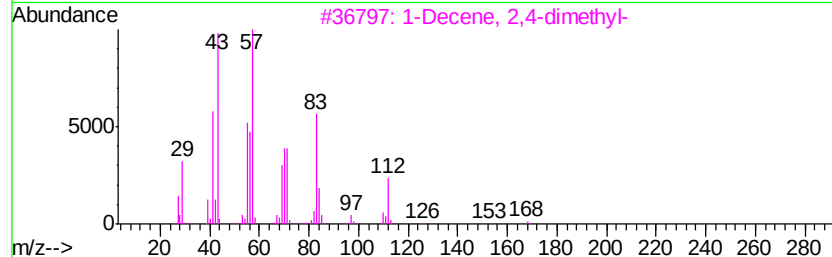
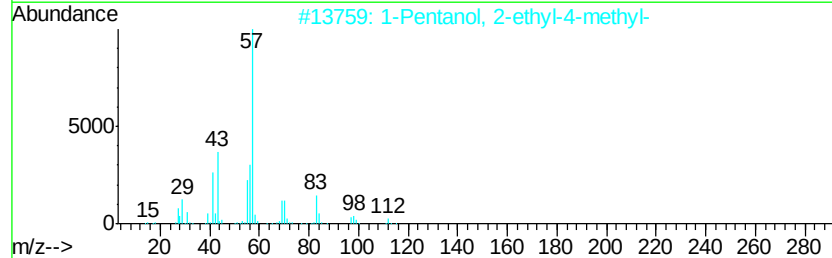
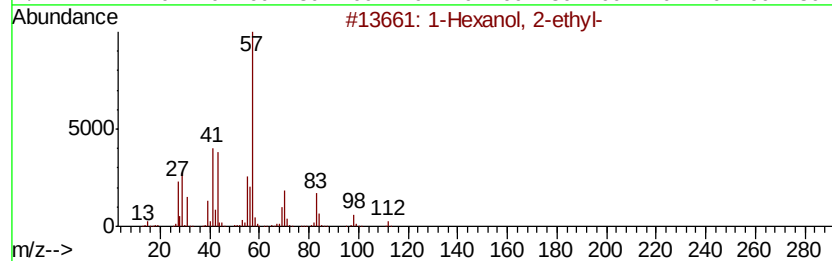
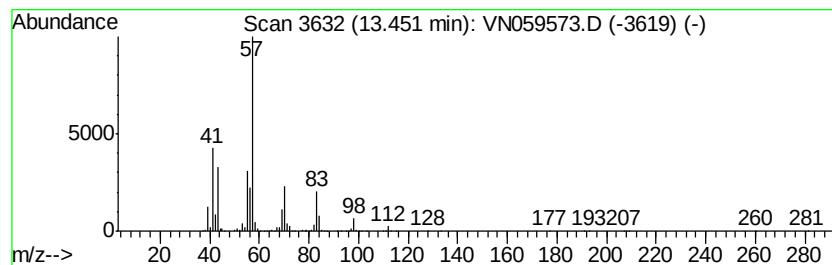
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	118.30 ug/l	2222500	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	72
3	1-Decene, 2,4-dimethyl-	168 C12H24	055170-80-4	53
4	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50
5	Carbonic acid, isobutyl 2-ethylh...	230 C13H26O3	1000357-82-9	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butenoic acid, ...	9.19	7.7	ug/l	145033	2	8.57	943069	50.0
4-Heptanone, 2,6-...	12.83	126.1	ug/l	2368500	4	13.34	939384	50.0
2-Heptanone, 4,6-...	13.07	31.3	ug/l	587770	4	13.34	939384	50.0
1-Hexanol, 2-ethyl-	13.45	118.3	ug/l	2222500	4	13.34	939384	50.0