

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020425\
 Data File : VN085650.D
 Acq On : 04 Feb 2025 14:27
 Operator : JC\MD
 Sample : Q1241-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 JPP-3.5-013025

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\82N011425W.M
 Title : SW846 8260

Signal : TIC: VN085650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.436	411	422	435	rBV2	13858	42784	3.47%	0.524%
2	4.724	462	471	479	rBV3	6446	19181	1.56%	0.235%
3	6.735	805	813	822	rVB7	4203	13313	1.08%	0.163%
4	8.165	1046	1056	1061	rBV	176693	428662	34.81%	5.250%
5	8.224	1061	1066	1080	rVB	271482	594572	48.28%	7.283%
6	8.577	1110	1126	1136	rBV	198428	455745	37.01%	5.582%
7	8.688	1136	1145	1149	rBV5	10418	28473	2.31%	0.349%
8	8.777	1151	1160	1168	rVB2	14425	55504	4.51%	0.680%
9	9.100	1204	1215	1226	rBV	439128	874487	71.01%	10.711%
10	9.671	1303	1312	1320	rBV	48349	100080	8.13%	1.226%
11	10.359	1421	1429	1438	rBV	136462	239651	19.46%	2.935%
12	10.447	1438	1444	1453	rVB2	8180	17665	1.43%	0.216%
13	10.565	1455	1464	1473	rBV	686579	1231530	100.00%	15.084%
14	10.982	1528	1535	1544	rBV	260145	439614	35.70%	5.385%
15	11.082	1544	1552	1558	rVV3	31570	59318	4.82%	0.727%
16	11.170	1559	1567	1579	rVB2	120143	271129	22.02%	3.321%
17	11.600	1633	1640	1652	rBV	479056	754412	61.26%	9.240%
18	11.765	1663	1668	1673	rBV3	12883	20909	1.70%	0.256%
19	11.865	1677	1685	1695	rBV	609562	1057190	85.84%	12.949%
20	12.212	1736	1744	1749	rBV	7683	14029	1.14%	0.172%
21	12.847	1845	1852	1862	rBV	411748	693185	56.29%	8.490%
22	13.788	2005	2012	2023	rBV	441498	752853	61.13%	9.221%

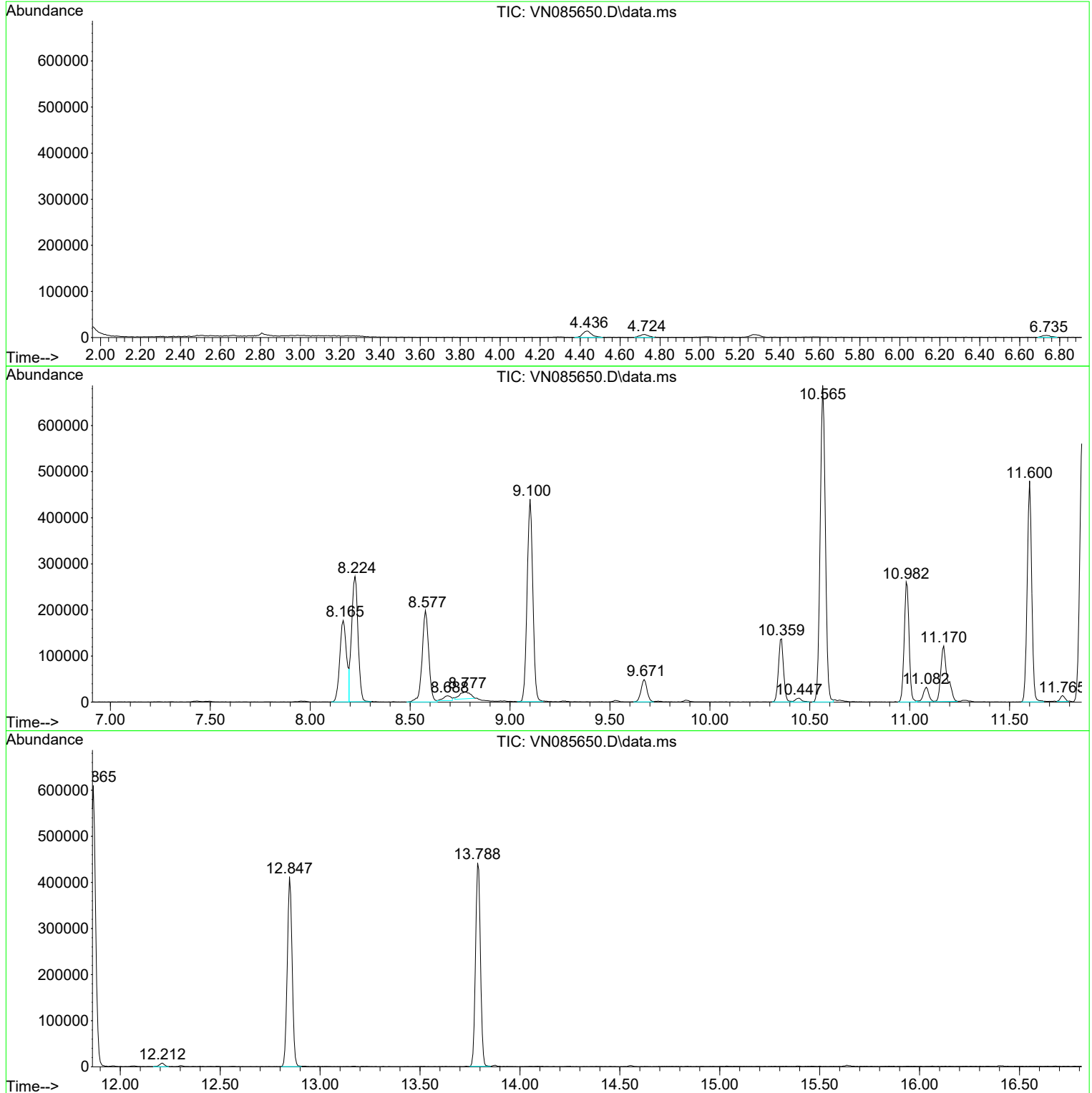
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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



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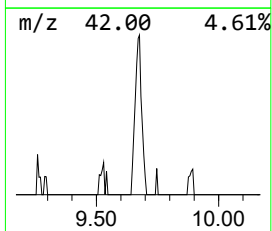
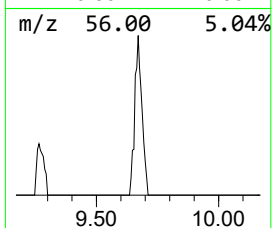
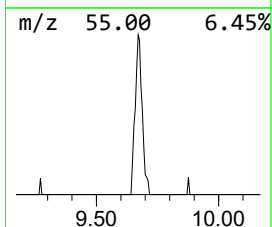
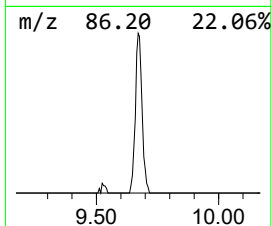
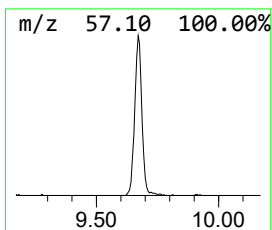
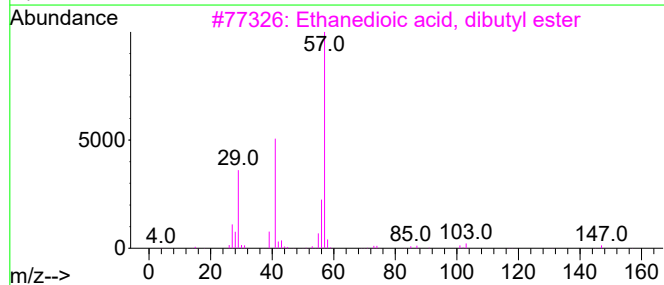
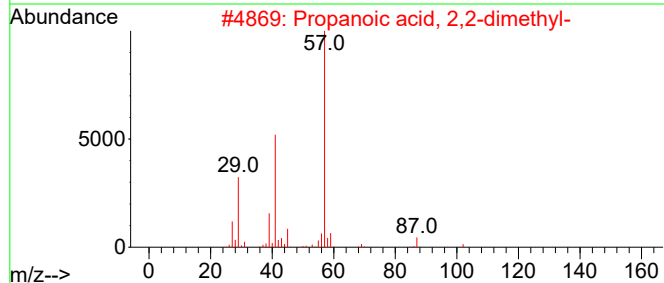
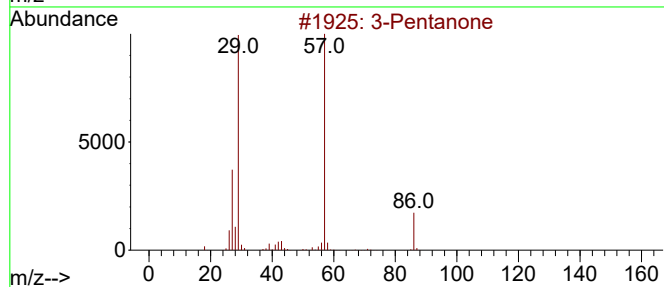
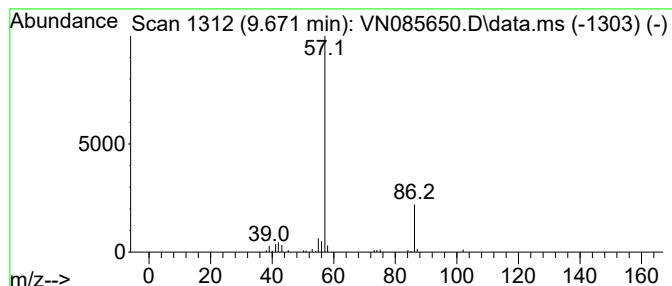
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	5.72 ug/l	100080	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	72
2			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	17
3			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	17
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	9
5			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9



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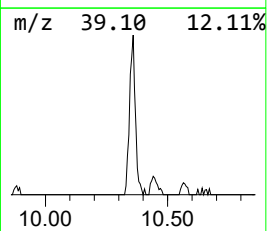
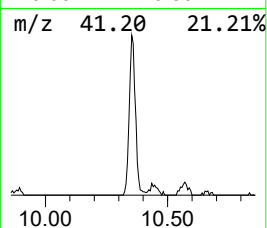
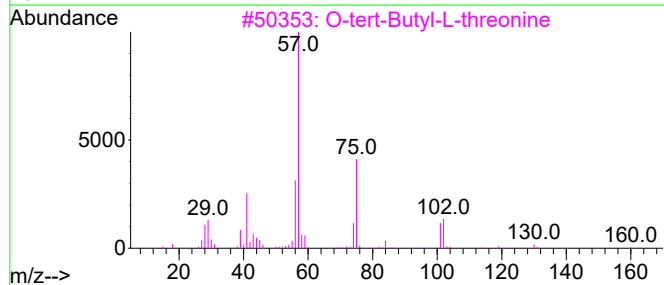
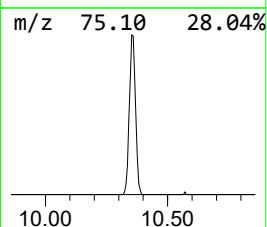
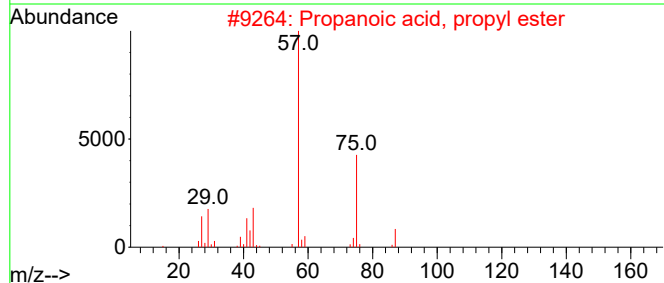
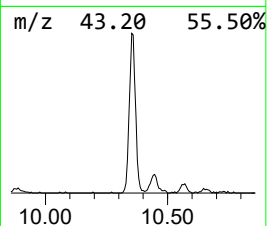
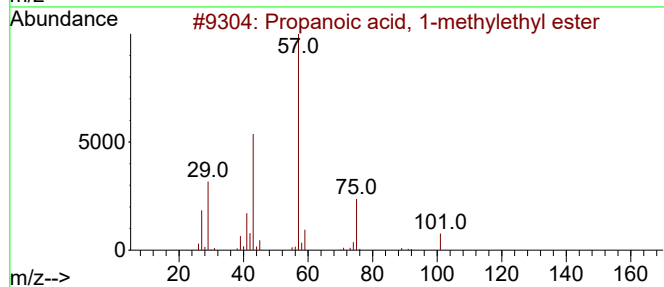
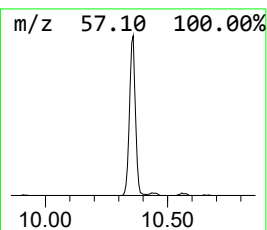
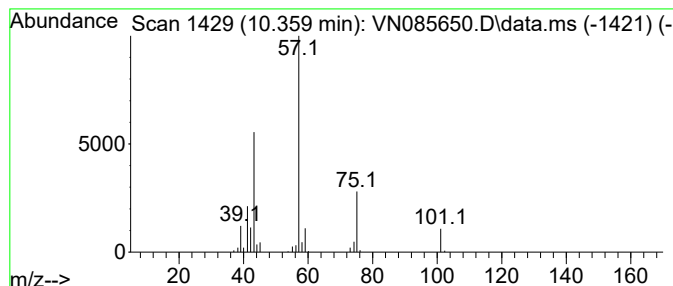
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	13.70 ug/l	239651	1,4-Difluorobenzene	9.100

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	38
3			O-tert-Butyl-L-threonine	175	C8H17NO3	004378-13-6	33
4			Diethyl 2-(N-(tert-butoxycarbony...	275	C12H21NO6	102831-44-7	28
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28



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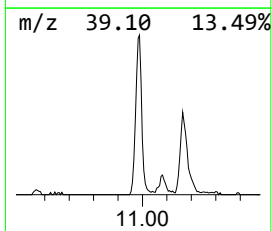
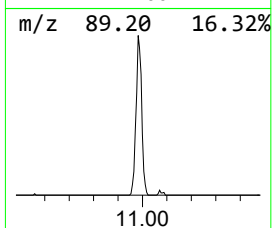
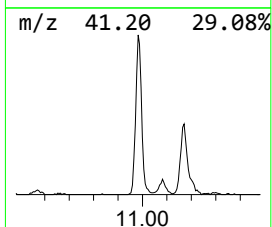
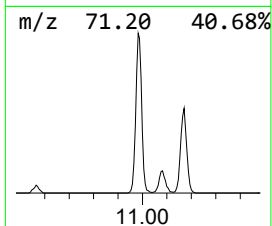
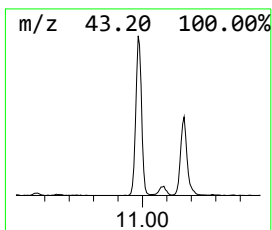
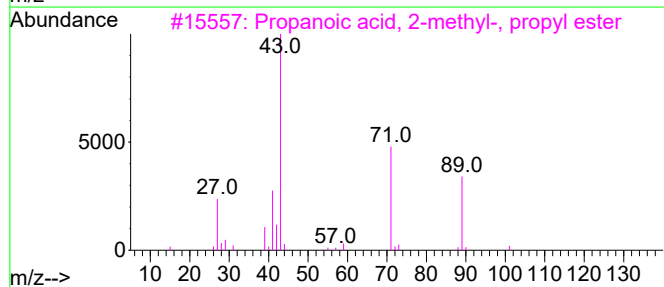
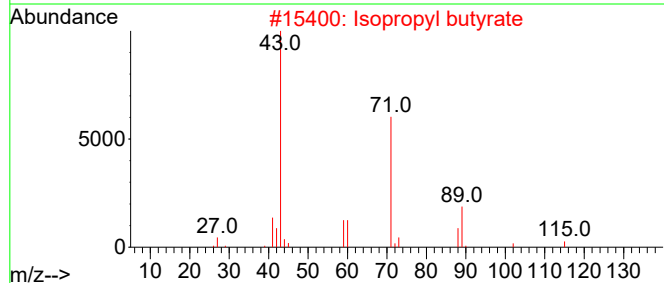
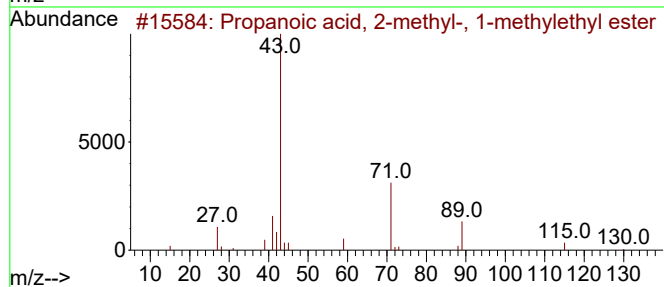
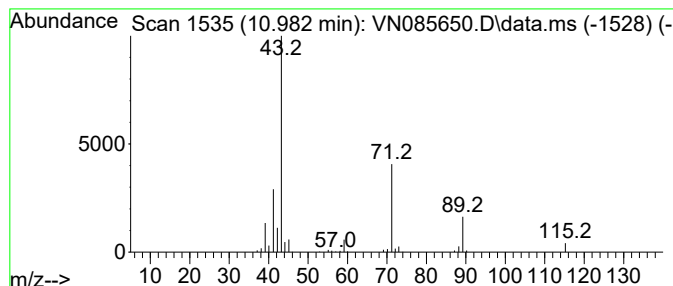
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.982	20.79 ug/l	439614	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	56
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	42



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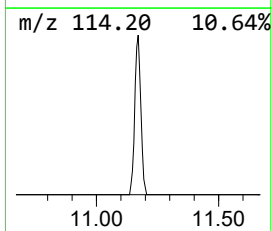
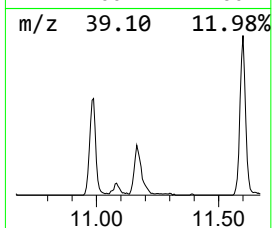
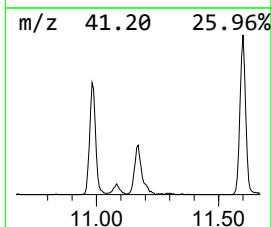
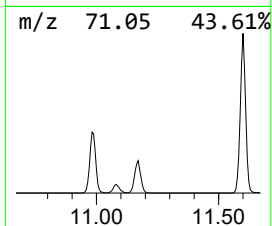
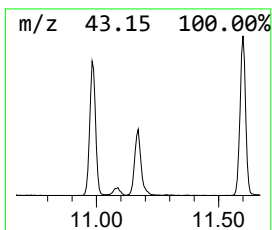
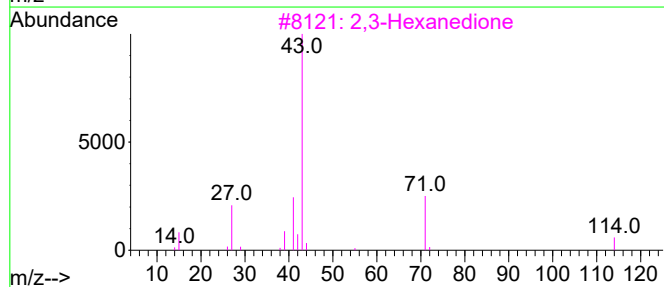
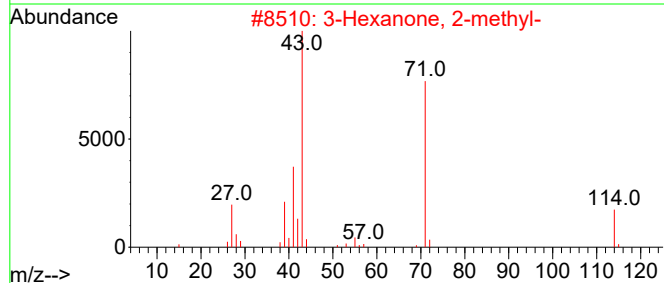
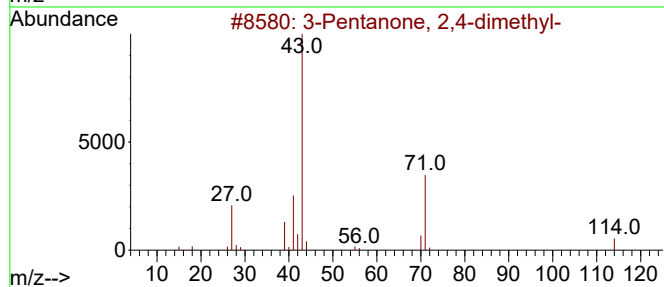
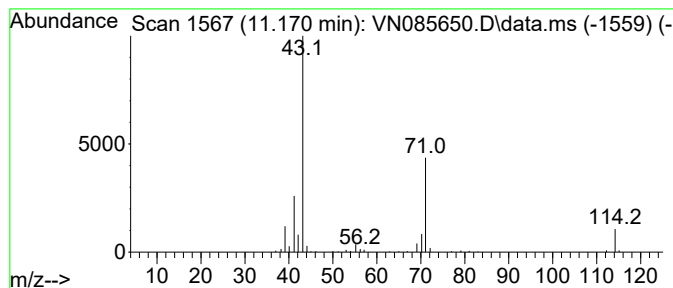
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Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	12.82 ug/l	271129	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80		
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	76		
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	72		
4	4-Heptanone	114	C7H14O	000123-19-3	59		
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38		



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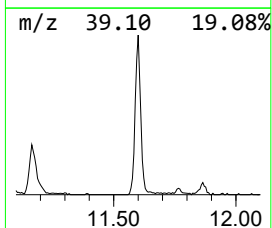
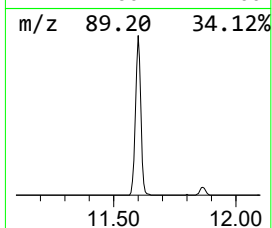
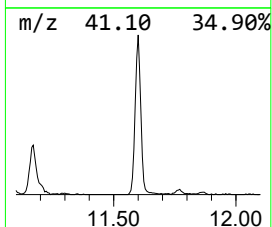
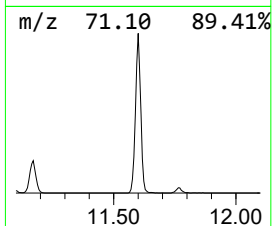
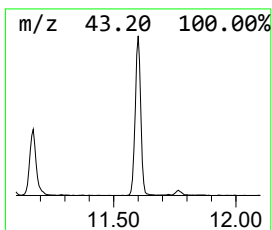
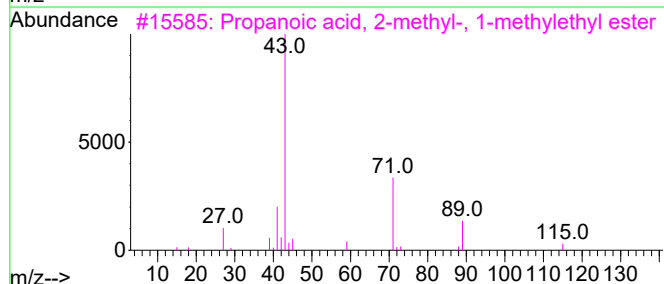
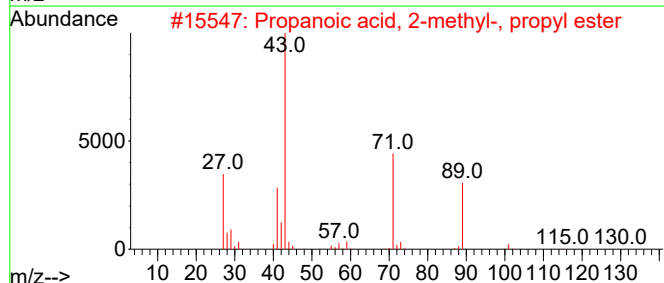
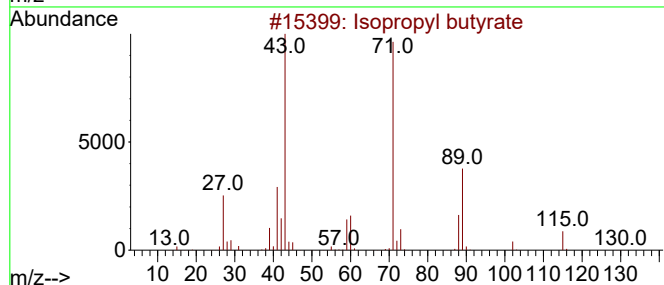
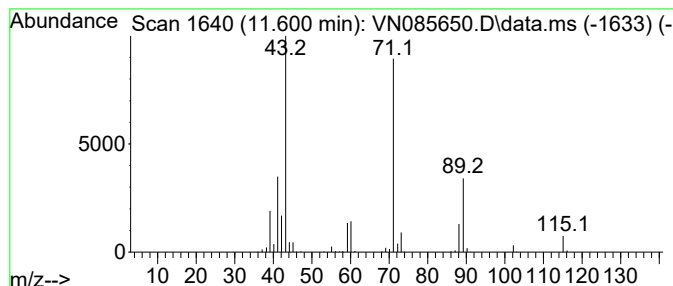
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.600	35.68 ug/l	754412	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, 1-methylethyl ester	130	C7H14O2	000617-50-5	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone	9.671	5.7	ug/l	100080	2	9.100	874487	50.0
Propanoic acid,...	10.359	13.7	ug/l	239651	2	9.100	874487	50.0
Propanoic acid,...	10.982	20.8	ug/l	439614	3	11.865	1057190	50.0
3-Pentanone, 2,...	11.171	12.8	ug/l	271129	3	11.865	1057190	50.0
Isopropyl butyrate	11.600	35.7	ug/l	754412	3	11.865	1057190	50.0