

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030421\
 Data File : VX020976.D
 Acq On : 02 Mar 2021 19:51
 Operator : JC/MD
 Sample : M1545-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MH-20A

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_X\Method\82X022421W.M
 Title : SW846 8260

Signal : TIC: VX020976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.417	220	226	237	rVB	44505	74352	3.49%	0.757%
2	2.581	245	254	263	rBV	12126	32658	1.53%	0.333%
3	3.005	317	326	337	rBV2	18641	53029	2.49%	0.540%
4	5.464	732	744	760	rBV2	121794	353074	16.56%	3.596%
5	5.629	760	772	788	rBV2	201511	551881	25.88%	5.621%
6	6.029	827	840	856	rBV	131695	348828	16.36%	3.553%
7	6.829	966	976	993	rBV	335880	784694	36.80%	7.992%
8	8.694	1286	1293	1311	rBV	720715	1134624	53.22%	11.556%
9	10.094	1524	1531	1544	rBV	770501	1011847	47.46%	10.306%
10	11.118	1699	1705	1716	rVB	616197	774509	36.33%	7.889%
11	11.312	1732	1738	1742	rBV	45966	70708	3.32%	0.720%
12	11.377	1742	1749	1759	rVB2	35265	87623	4.11%	0.892%
13	11.465	1759	1764	1767	rBV	31857	47332	2.22%	0.482%
14	11.688	1797	1802	1816	rBV	503006	601391	28.21%	6.125%
15	11.924	1835	1842	1851	rBV5	13288	31835	1.49%	0.324%
16	12.012	1851	1857	1861	rVV	163957	210544	9.88%	2.144%
17	12.059	1861	1865	1873	rVB	800129	980339	45.98%	9.985%
18	12.253	1893	1898	1905	rBV	44651	76203	3.57%	0.776%
19	12.859	1996	2001	2013	rVB	69357	102522	4.81%	1.044%
20	13.236	2060	2065	2086	rVB	1838723	2132075	100.00%	21.716%
21	14.083	2203	2209	2233	rBV	211908	358094	16.80%	3.647%

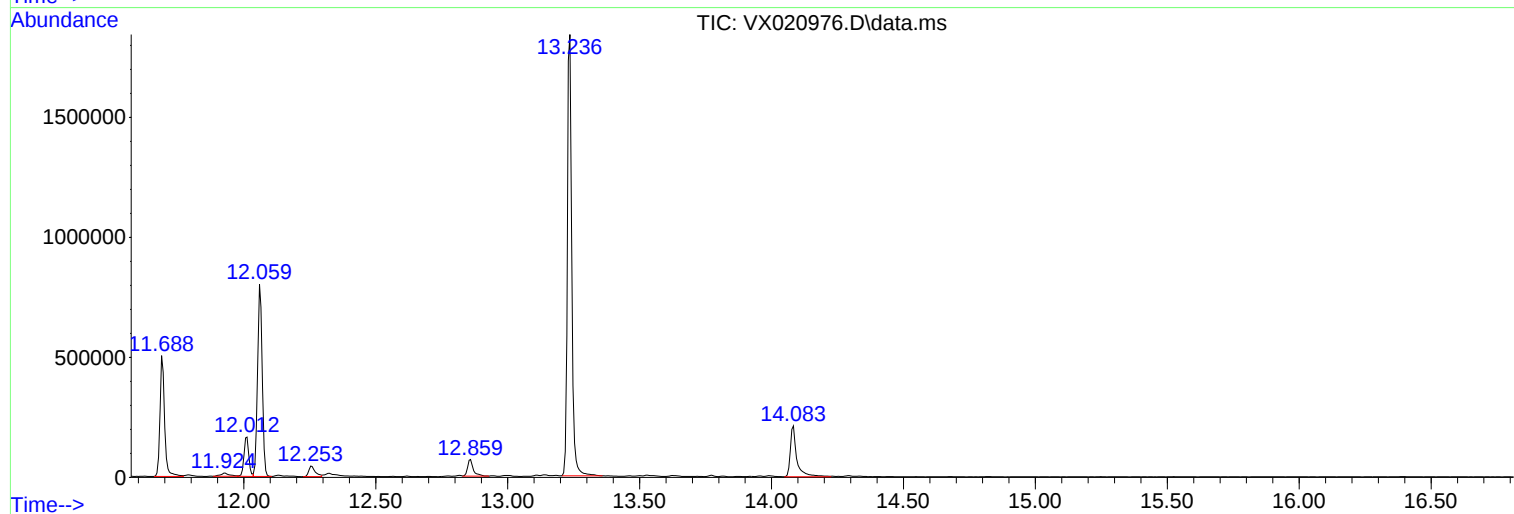
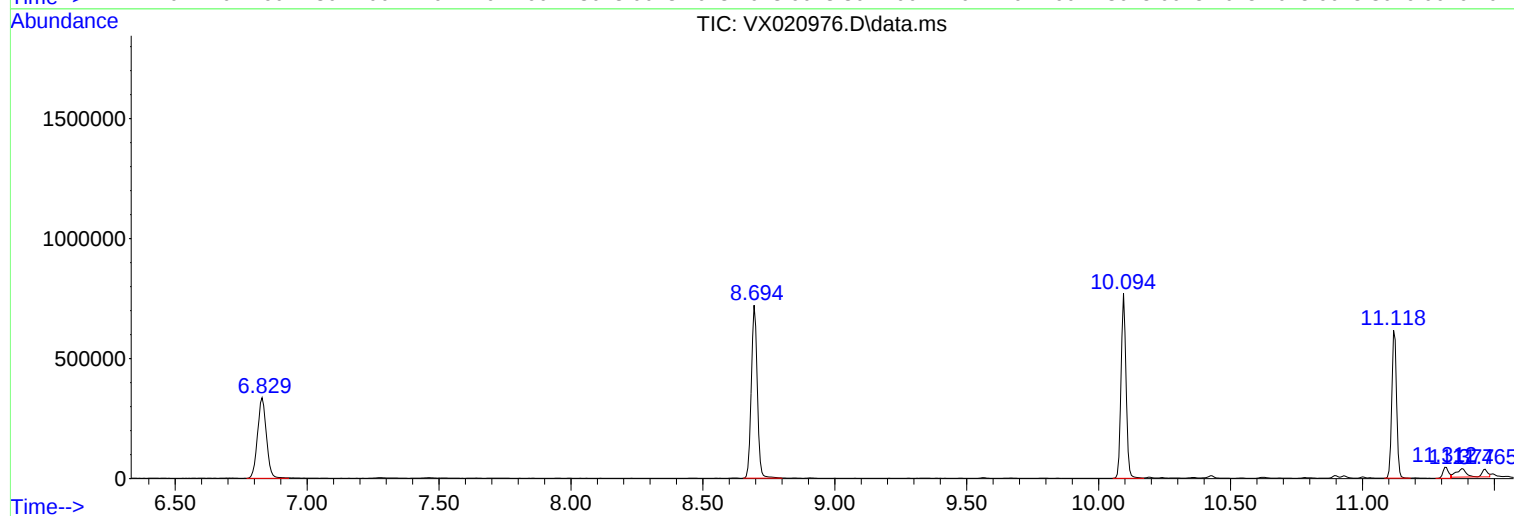
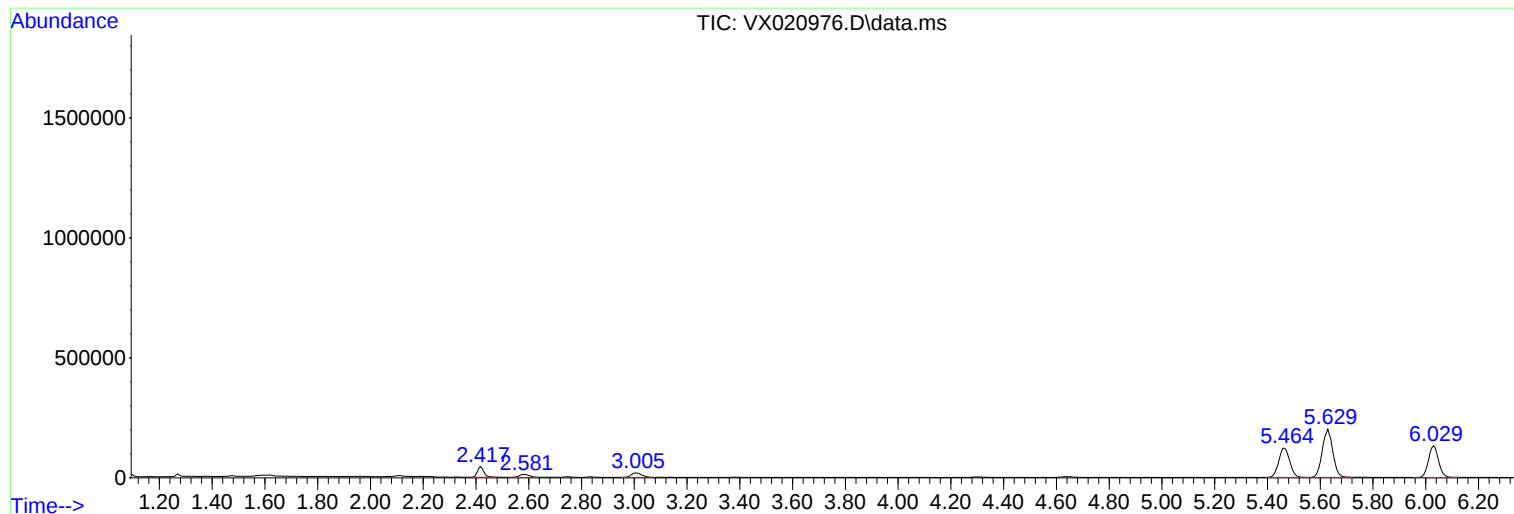
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Quant Title : SW846 8260

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



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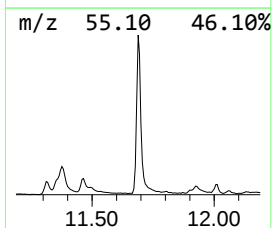
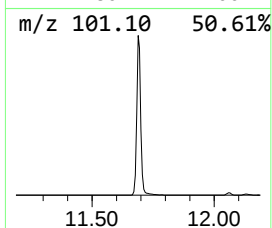
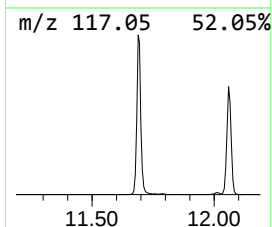
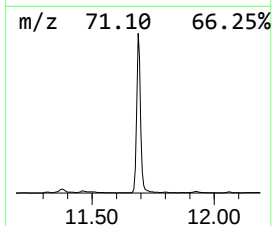
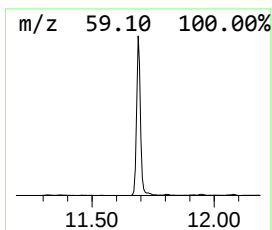
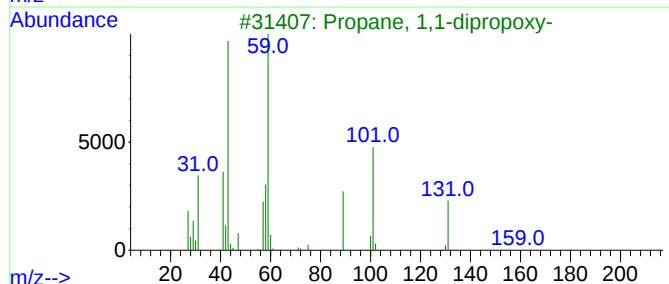
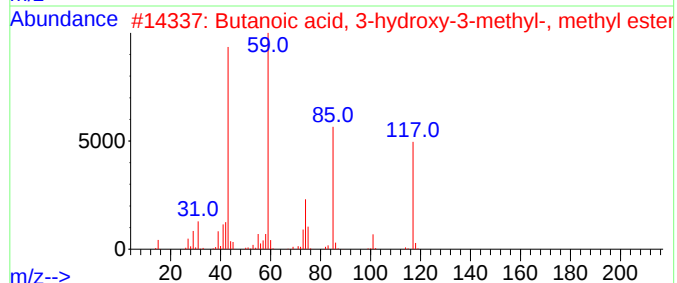
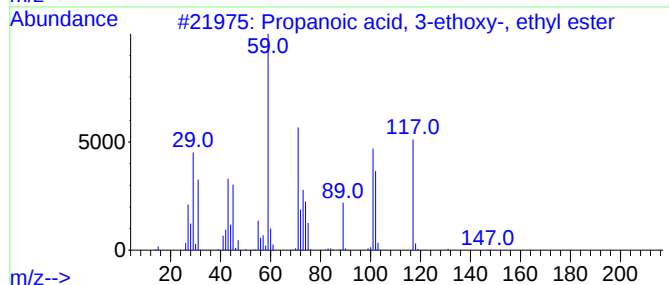
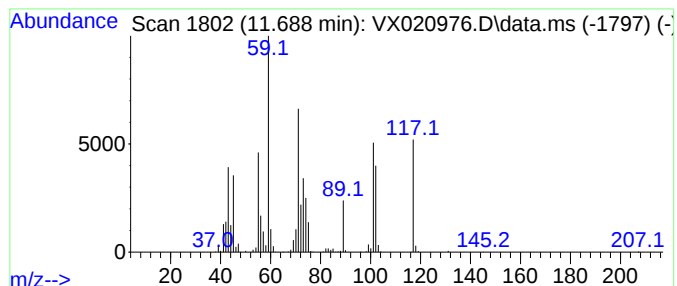
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.688	30.67 ug/l	601391	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 3-ethoxy-, ethyl...	146	C7H14O3	000763-69-9	91
2			Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	35
3			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	35
4			Hydrazine, 1,1-dimethyl-2-propyl-	102	C5H14N2	052728-54-8	27
5			Pentanoic acid, 3-hydroxy-, ethy...	146	C7H14O3	054074-85-0	25



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ClientSampled :
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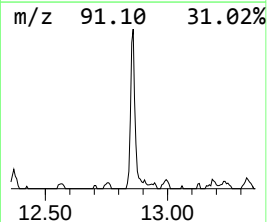
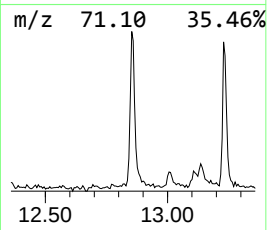
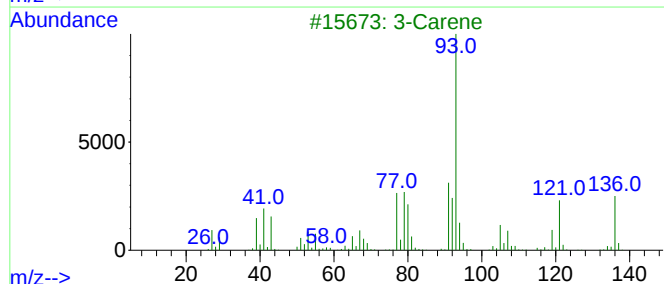
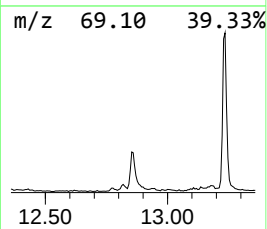
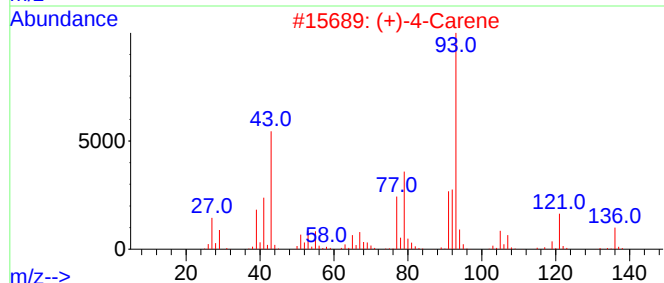
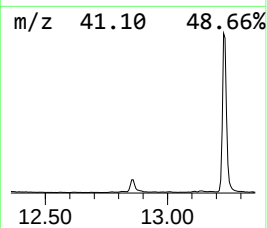
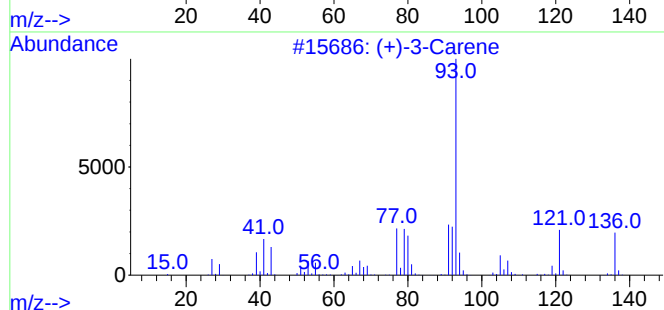
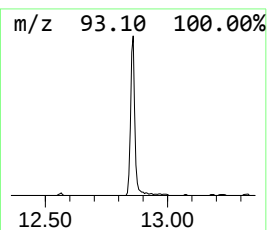
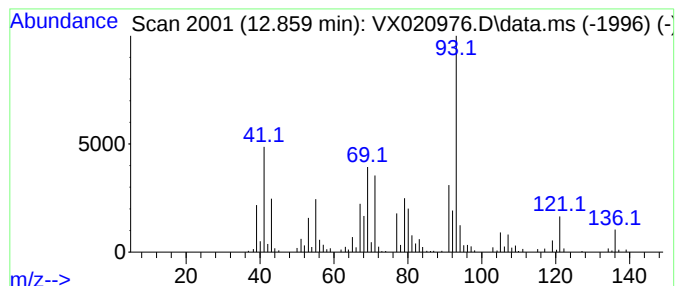
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 (+)-3-Carene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	5.23 ug/l	102522	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(+)-3-Carene	136	C10H16	000498-15-7	94
2		(+)-4-Carene	136	C10H16	029050-33-7	93
3		3-Carene	136	C10H16	013466-78-9	90
4		.beta.-Pinene	136	C10H16	000127-91-3	81
5		Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	81



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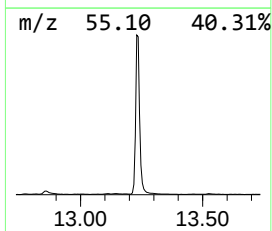
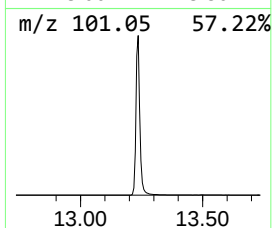
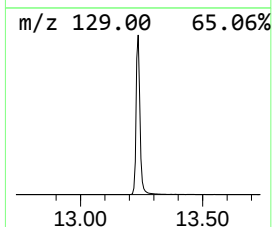
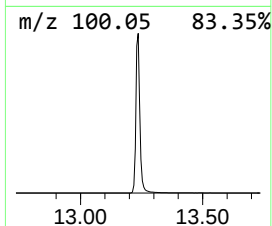
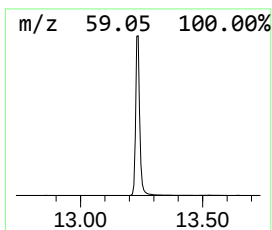
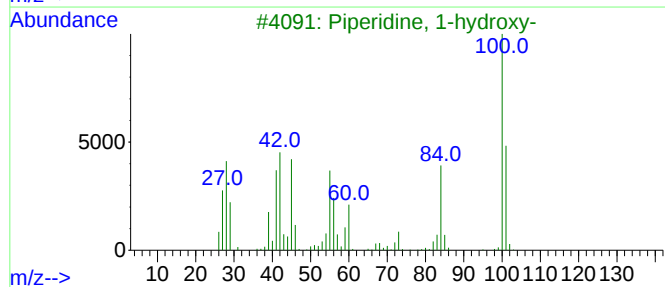
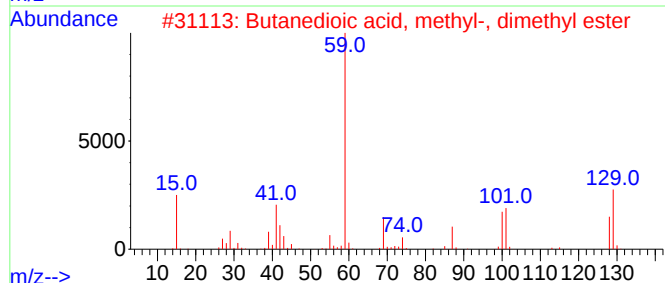
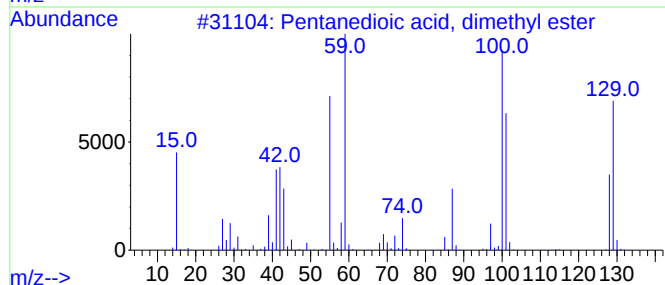
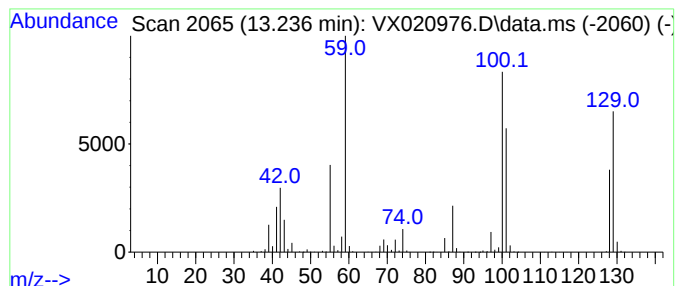
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Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.236	108.74 ug/l	2132080	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	50
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	12
4			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	12
5			Pyrrolidine, 1-nitroso-	100	C4H8N2O	000930-55-2	10



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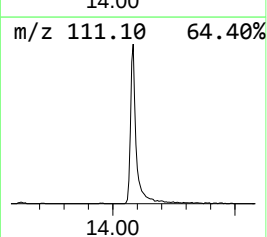
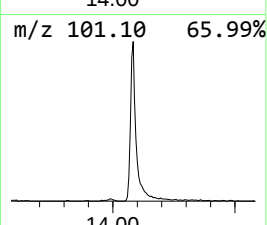
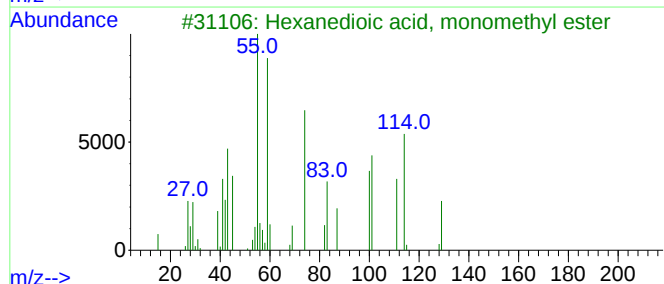
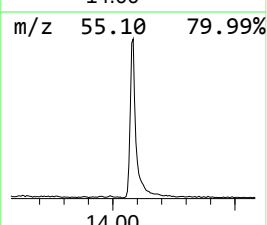
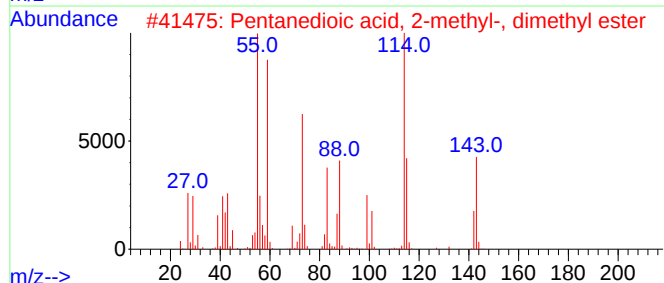
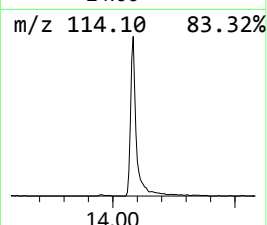
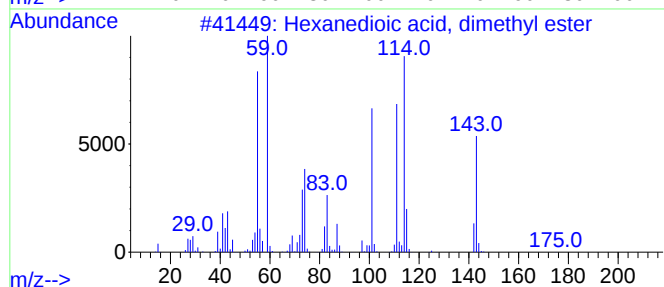
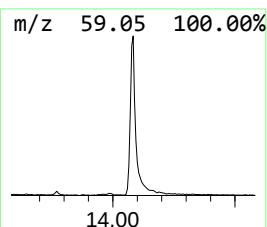
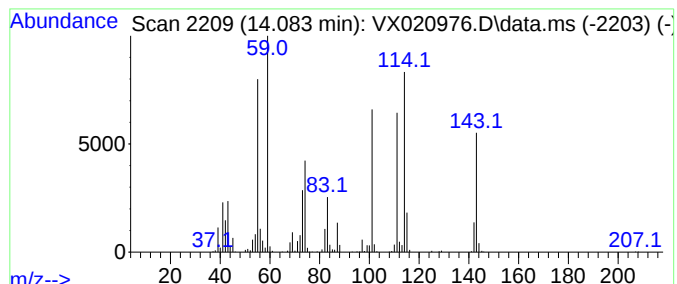
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Peak Number 4 Hexanedioic acid, dimethyl ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.083	18.26 ug/l	358094	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dimethyl ester	174	C8H14O4	000627-93-0	91
2			Pentanedioic acid, 2-methyl-, di...	174	C8H14O4	014035-94-0	32
3			Hexanedioic acid, monomethyl ester	160	C7H12O4	000627-91-8	25
4			4-Ethyl-4-heptanol	144	C9H20O	000597-90-0	14
5			3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	12



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	11.688	30.7	ug/l	601391	4	12.059	980339	50.0
(+)-3-Carene	12.859	5.2	ug/l	102522	4	12.059	980339	50.0
Pentanedioic ac...	13.236	108.7	ug/l	2132080	4	12.059	980339	50.0
Hexanedioic aci...	14.083	18.3	ug/l	358094	4	12.059	980339	50.0