

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041422\
 Data File : VX028110.D
 Acq On : 14 Apr 2022 16:24
 Operator : JC/MD
 Sample : N2403-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-49

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\82X041222W.M
 Title : SW846 8260

Signal : TIC: VX028110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.953	297	306	320	rBV	519289	1122133	21.10%	7.019%
2	3.117	322	333	349	rVB	2348122	5318763	100.00%	33.271%
3	5.391	692	706	722	rBV	162306	472050	8.88%	2.953%
4	5.556	722	733	747	rVB	248305	698510	13.13%	4.369%
5	5.958	787	799	807	rBV	170219	442826	8.33%	2.770%
6	6.044	807	813	826	rVB2	54058	144733	2.72%	0.905%
7	6.233	831	844	855	rBV	188656	512416	9.63%	3.205%
8	6.763	921	931	944	rBV	397831	949602	17.85%	5.940%
9	8.427	1196	1204	1210	rBV	68836	120897	2.27%	0.756%
10	8.507	1210	1217	1229	rVB	203809	335889	6.32%	2.101%
11	8.653	1234	1241	1249	rVV	858554	1321574	24.85%	8.267%
12	8.842	1263	1272	1283	rBV	227713	363428	6.83%	2.273%
13	9.445	1365	1371	1380	rBV2	66742	102627	1.93%	0.642%
14	10.025	1458	1466	1467	rBV	115084	181969	3.42%	1.138%
15	10.055	1467	1471	1476	rVV	875217	1196524	22.50%	7.485%
16	10.104	1476	1479	1482	rVV	68457	89976	1.69%	0.563%
17	10.146	1482	1486	1491	rVB	277626	355267	6.68%	2.222%
18	10.793	1586	1592	1599	rBV3	32714	64729	1.22%	0.405%
19	11.085	1634	1640	1645	rBV	706093	927321	17.43%	5.801%
20	11.152	1648	1651	1661	rVV2	35448	61849	1.16%	0.387%
21	11.274	1661	1671	1674	rVV	64053	91881	1.73%	0.575%
22	12.024	1788	1794	1801	rBV	913061	1111350	20.89%	6.952%

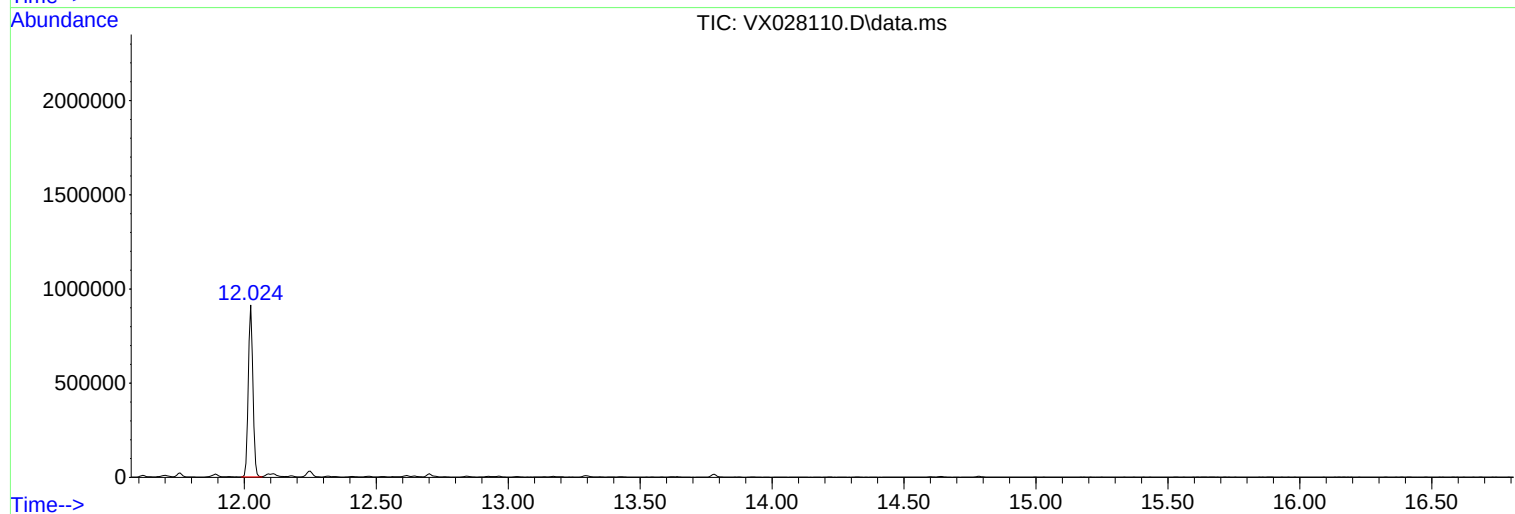
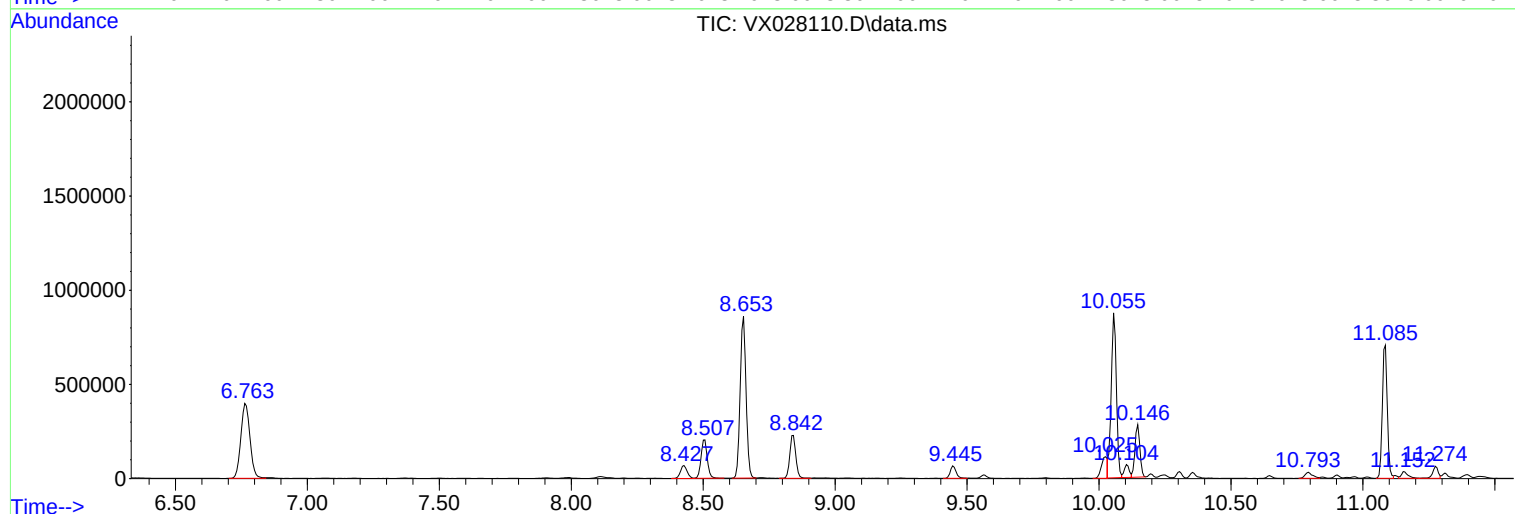
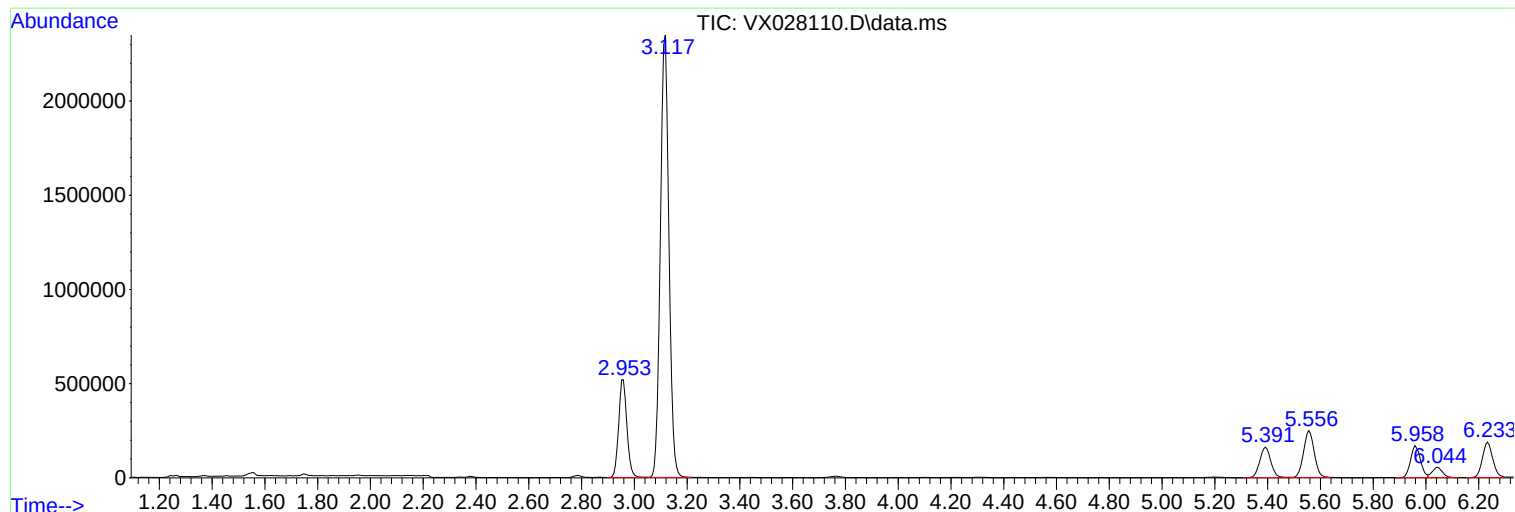
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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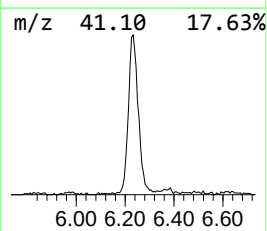
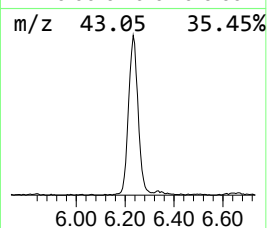
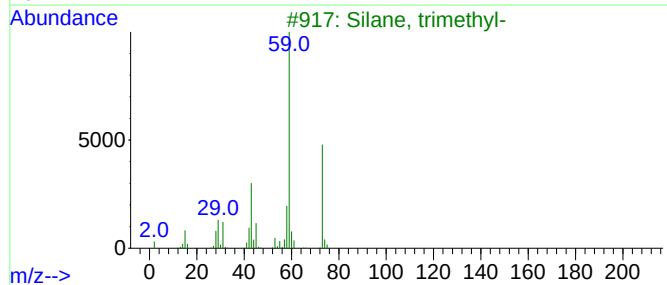
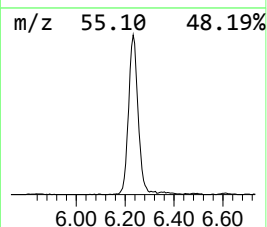
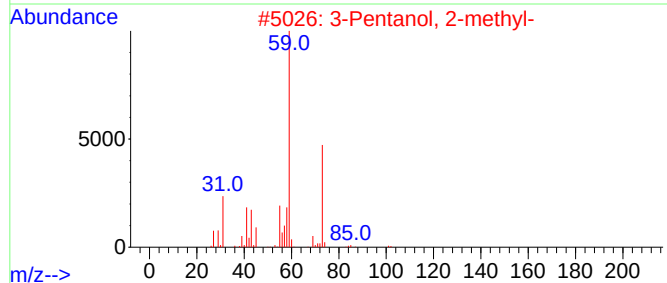
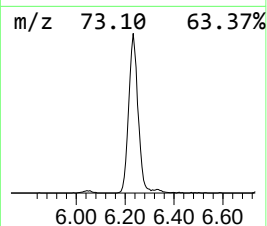
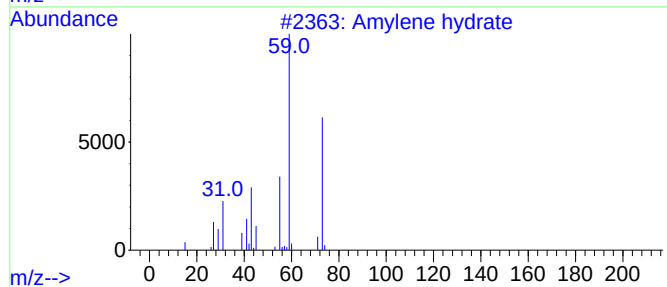
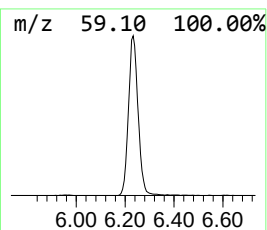
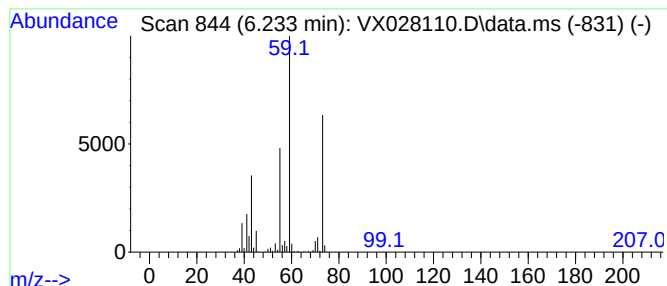
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	26.98 ug/l	512416	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	78
2			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
3			Silane, trimethyl-	74	C3H10Si	000993-07-7	39
4			3-Hexanol	102	C6H14O	000623-37-0	38
5			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	36



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Instrument :
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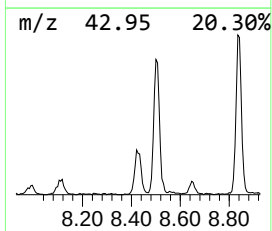
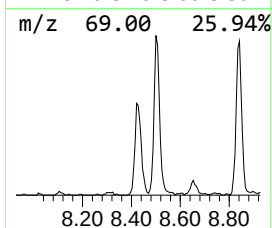
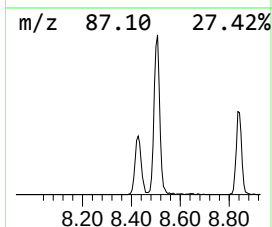
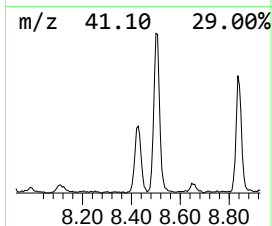
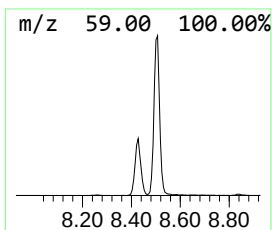
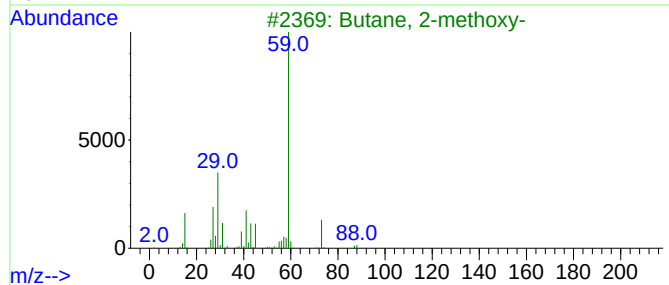
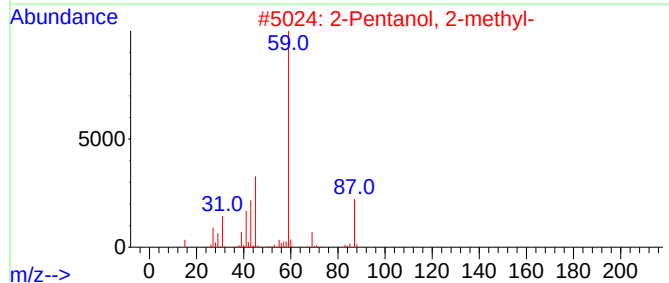
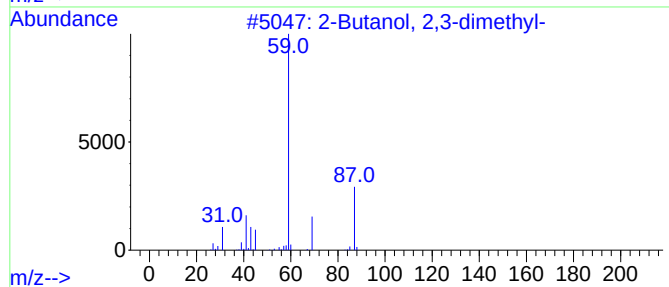
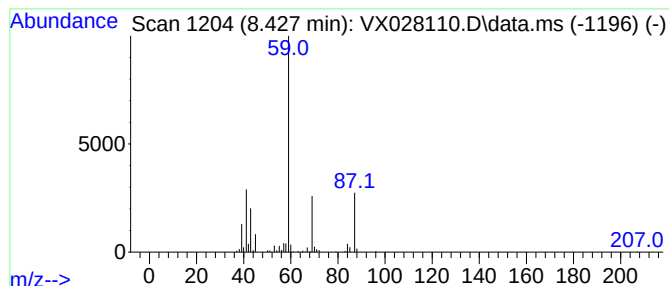
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.427	5.05 ug/l	120897	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	78
3	Butane, 2-methoxy-			88	C5H12O	006795-87-5	59
4	Propane, 2-ethoxy-2-methyl-			102	C6H14O	000637-92-3	50
5	Acetic acid, cyano-, 1,1-dimethyl...			141	C7H11NO2	001116-98-9	40



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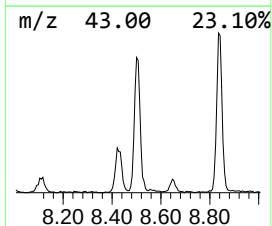
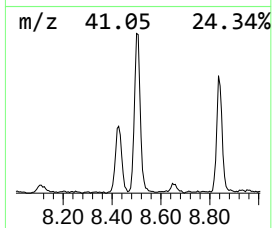
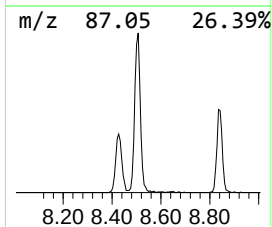
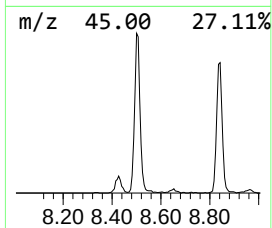
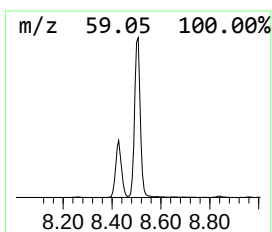
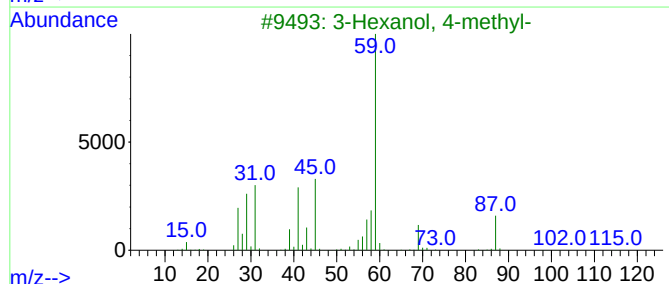
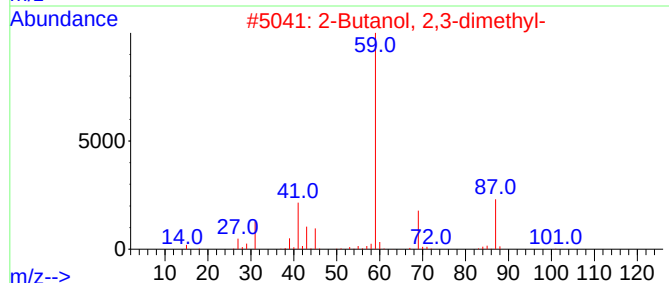
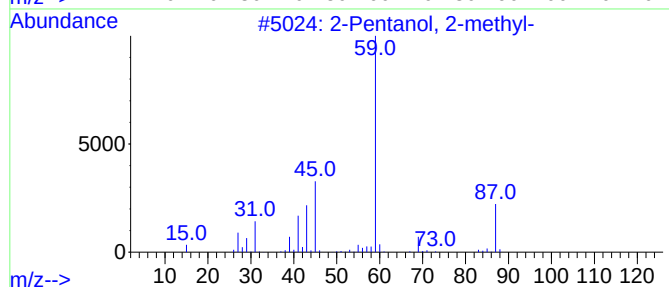
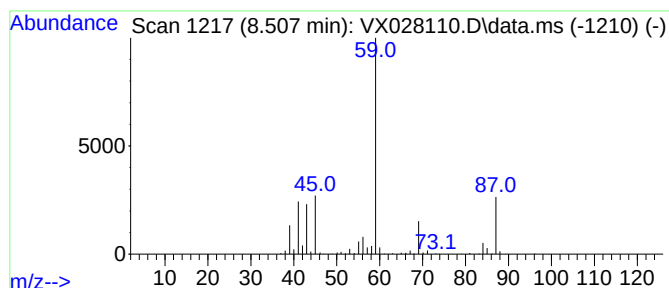
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Quant Title : SW846 8260

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

Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.507	14.04 ug/l	335889	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	78
2	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	72
3	3-Hexanol, 4-methyl-			116	C7H16O	000615-29-2	64
4	3-Pentanol, 2,2-dimethyl-			116	C7H16O	003970-62-5	56
5	Propane, 2-ethoxy-2-methyl-			102	C6H14O	000637-92-3	53



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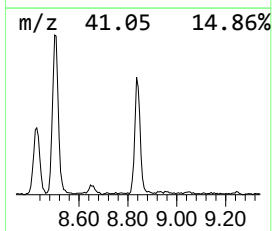
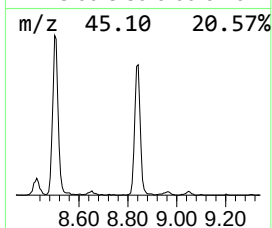
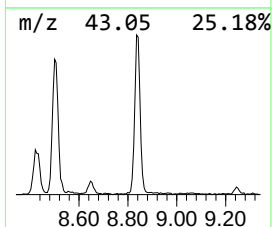
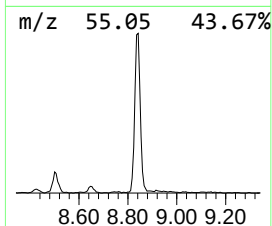
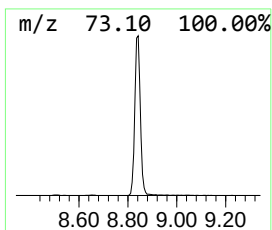
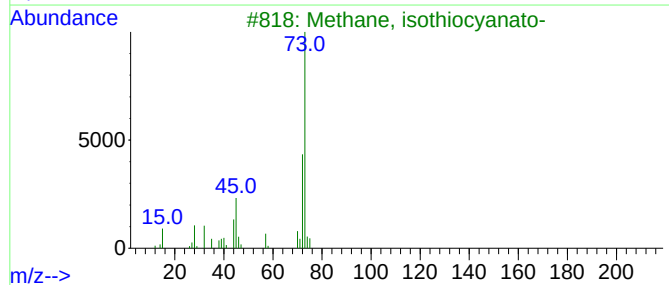
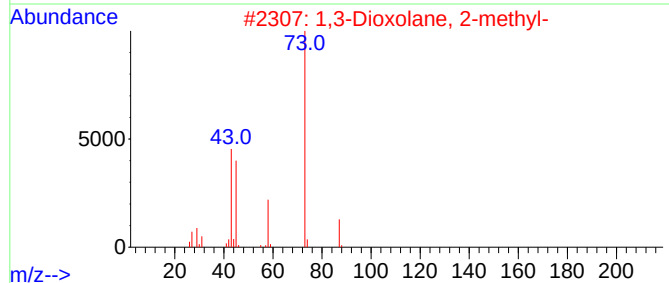
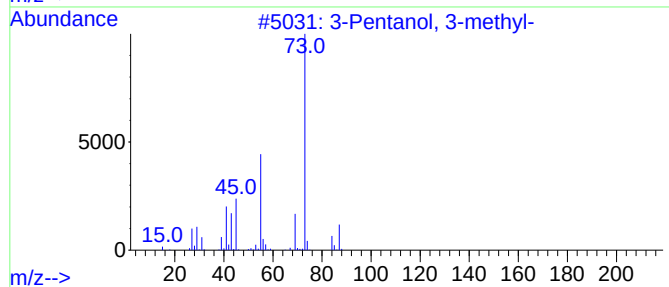
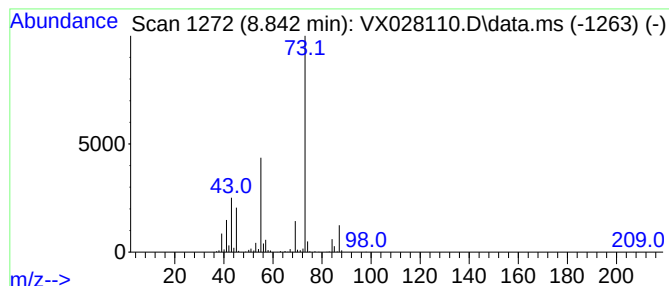
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	15.19 ug/l	363428	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
5			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	25



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.233	27.0	ug/l	512416	2	6.763	949602	50.0
2-Butanol, 2,3-...	8.427	5.0	ug/l	120897	3	10.055	1196520	50.0
2-Pentanol, 2-m...	8.507	14.0	ug/l	335889	3	10.055	1196520	50.0
3-Pentanol, 3-m...	8.842	15.2	ug/l	363428	3	10.055	1196520	50.0