

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039601.D
 Acq On : 03 Jan 2024 14:51
 Operator : JC/MD
 Sample : P1002-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1213

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	20	rBV	28474	29855	4.94%	0.465%
2	1.240	21	25	32	rBV	15943	29820	4.94%	0.464%
3	1.355	41	44	50	rBV2	5936	7705	1.28%	0.120%
4	1.453	56	60	64	rBV	21494	25292	4.19%	0.394%
5	1.599	70	84	88	rBV8	7630	25563	4.23%	0.398%
6	2.063	154	160	168	rBV	11518	20942	3.47%	0.326%
7	2.294	192	198	206	rBV	12262	22993	3.81%	0.358%
8	2.373	206	211	225	rVB	41599	72018	11.92%	1.121%
9	2.538	230	238	247	rBV	13641	31522	5.22%	0.491%
10	2.703	259	265	273	rBV	6298	12005	1.99%	0.187%
11	2.959	299	307	321	rVB2	6209	16524	2.74%	0.257%
12	3.331	359	368	378	rBV3	4730	13130	2.17%	0.204%
13	4.227	505	515	535	rBV2	74881	234782	38.87%	3.654%
14	4.568	563	571	581	rBV2	6670	21018	3.48%	0.327%
15	5.385	694	705	721	rVB2	65259	189793	31.42%	2.954%
16	5.550	721	732	746	rBV	95835	270117	44.72%	4.204%
17	5.952	787	798	817	rBV2	75101	201983	33.44%	3.144%
18	6.123	817	826	840	rVV2	10766	30768	5.09%	0.479%
19	6.757	922	930	943	rBV	178915	430364	71.24%	6.699%
20	7.208	996	1004	1026	rBV	71724	173090	28.65%	2.694%
21	7.580	1060	1065	1075	rVB	13380	28905	4.79%	0.450%
22	8.580	1222	1229	1234	rBV	4197	7749	1.28%	0.121%
23	8.647	1234	1240	1249	rVV	391612	604070	100.00%	9.402%
24	8.714	1249	1251	1257	rVV2	3779	7674	1.27%	0.119%
25	8.775	1257	1261	1270	rVB	5821	10942	1.81%	0.170%
26	9.238	1332	1337	1347	rBV	11497	23181	3.84%	0.361%
27	9.525	1381	1384	1390	rVB3	4778	7114	1.18%	0.111%
28	10.055	1463	1471	1483	rBV	406663	588584	97.44%	9.161%
29	10.153	1483	1487	1492	rBV	9104	12844	2.13%	0.200%
30	10.305	1507	1512	1518	rVB2	4357	6863	1.14%	0.107%
31	10.506	1541	1545	1554	rVB	10697	13907	2.30%	0.216%
32	10.683	1570	1574	1580	rVB	18838	23705	3.92%	0.369%
33	10.750	1580	1585	1594	rBV3	44854	78981	13.07%	1.229%
34	11.079	1634	1639	1645	rBV	358964	445475	73.75%	6.934%
35	11.134	1645	1648	1653	rVB	9028	11830	1.96%	0.184%
36	11.280	1668	1672	1676	rBV2	5774	8672	1.44%	0.135%

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	11.390	1686	1690	1694	rBV2	18765	27916	4.62%	0.435%
38	11.567	1714	1719	1724	rBV	351951	443610	73.44%	6.905%
39	11.604	1724	1725	1733	rVV	23184	24806	4.11%	0.386%
40	11.683	1733	1738	1747	rVB	277963	329781	54.59%	5.133%
41	11.823	1755	1761	1767	rBV	54313	76443	12.65%	1.190%
42	11.884	1767	1771	1776	rVV4	16270	23878	3.95%	0.372%
43	11.988	1780	1788	1790	rVV2	48242	79673	13.19%	1.240%
44	12.018	1790	1793	1802	rVV	415170	543688	90.00%	8.463%
45	12.097	1802	1806	1812	rVB4	11085	16203	2.68%	0.252%
46	12.219	1820	1826	1836	rBV	376823	547693	90.67%	8.525%
47	12.305	1836	1840	1850	rVB5	18724	39591	6.55%	0.616%
48	12.591	1884	1887	1895	rVB8	5318	7973	1.32%	0.124%
49	12.805	1916	1922	1927	rVB5	6225	10436	1.73%	0.162%
50	13.140	1971	1977	1986	rBV	86208	125610	20.79%	1.955%
51	13.603	2050	2053	2058	rVB6	6163	9342	1.55%	0.145%
52	13.676	2060	2065	2070	rBV	70704	84017	13.91%	1.308%
53	13.750	2070	2077	2080	rBV4	10318	24354	4.03%	0.379%
54	13.841	2090	2092	2100	rVB6	6791	11574	1.92%	0.180%
55	13.914	2100	2104	2111	rVB	6651	9698	1.61%	0.151%
56	14.030	2119	2123	2128	rVB2	21857	25896	4.29%	0.403%
57	14.140	2136	2141	2145	rBV	26705	32396	5.36%	0.504%
58	14.268	2158	2162	2167	rVB	16330	20621	3.41%	0.321%
59	14.377	2175	2180	2186	rVB2	9696	11992	1.99%	0.187%
60	14.993	2277	2281	2293	rVB5	10109	16905	2.80%	0.263%
61	15.133	2297	2304	2309	rBV3	11510	19526	3.23%	0.304%
62	15.304	2327	2332	2335	rBV2	8235	11103	1.84%	0.173%
63	15.377	2340	2344	2349	rVB	4618	7616	1.26%	0.119%
64	15.487	2357	2362	2370	rBV4	8857	15802	2.62%	0.246%
65	15.670	2386	2392	2398	rBV3	7285	13518	2.24%	0.210%
66	15.969	2435	2441	2452	rBV2	38455	73188	12.12%	1.139%

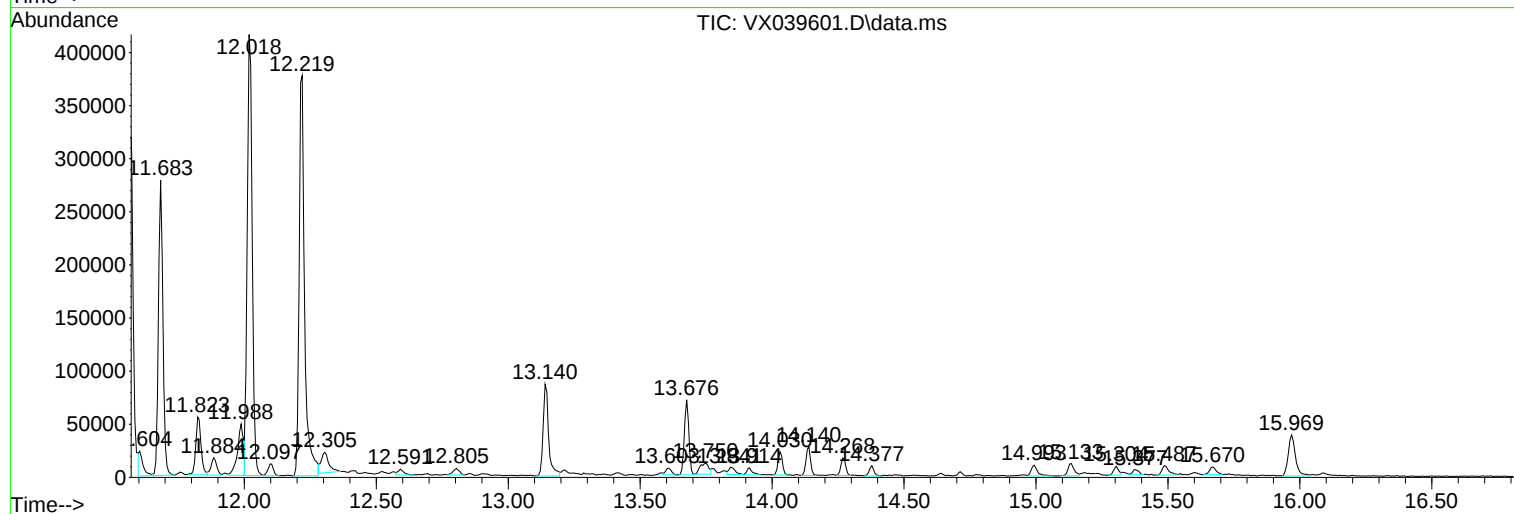
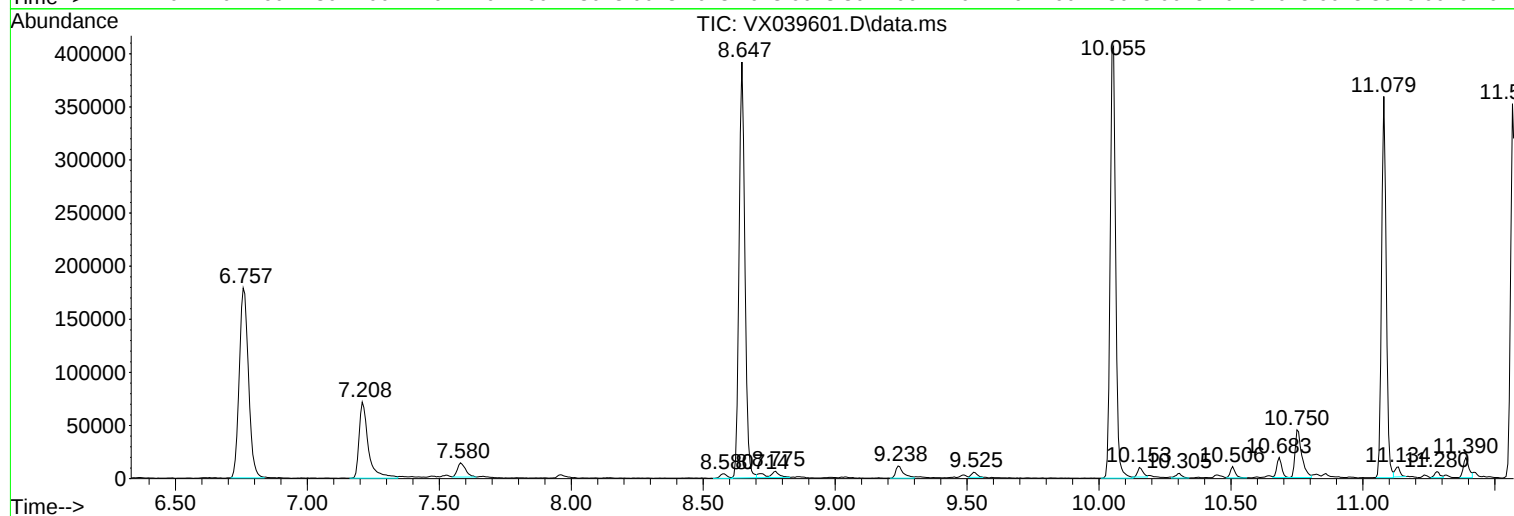
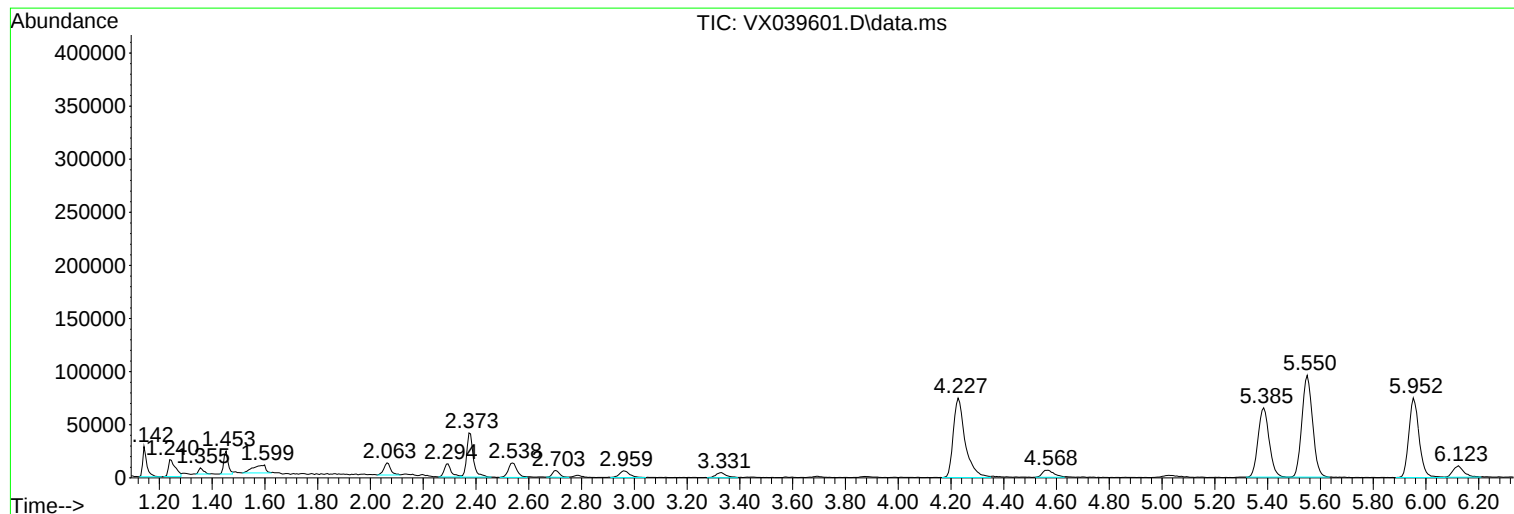
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

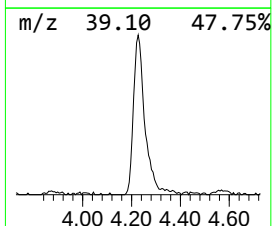
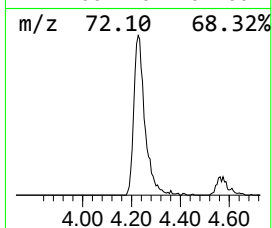
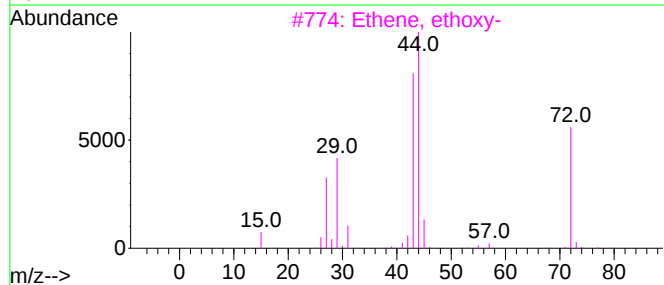
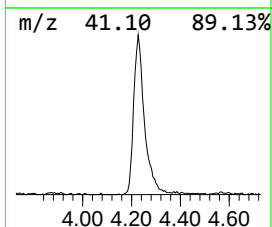
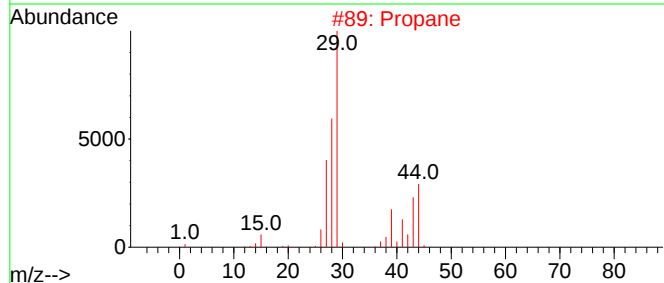
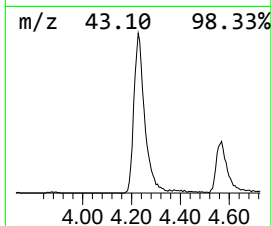
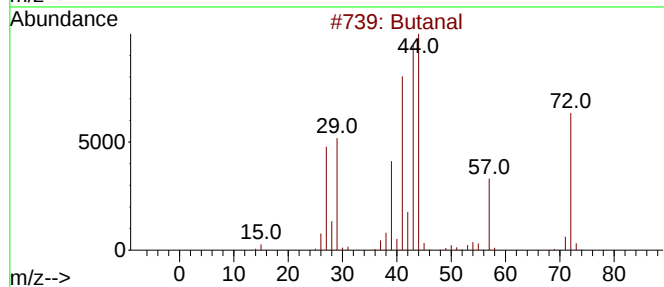
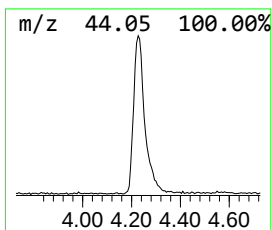
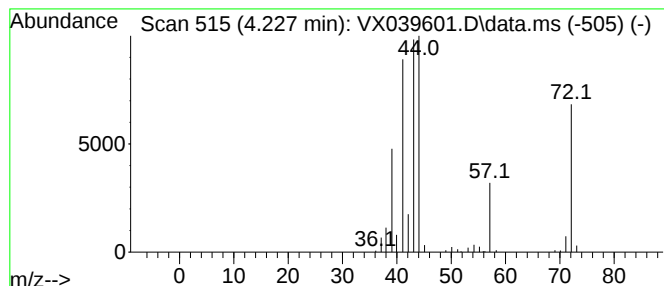
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	43.46 ug/l	234782	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propane	44	C3H8	000074-98-6	53
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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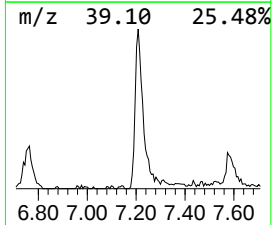
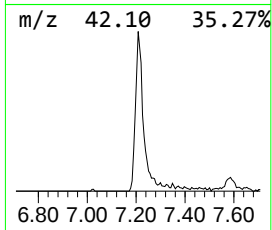
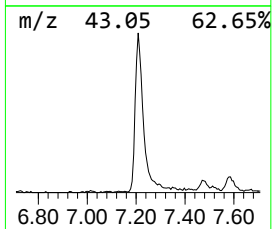
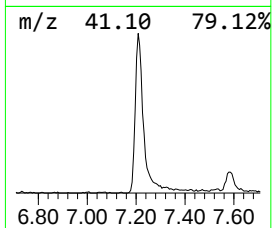
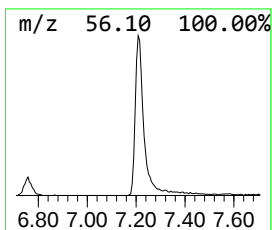
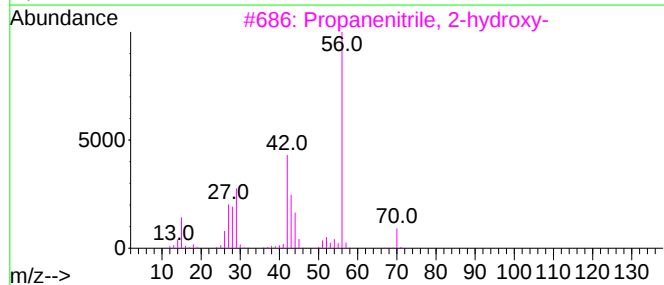
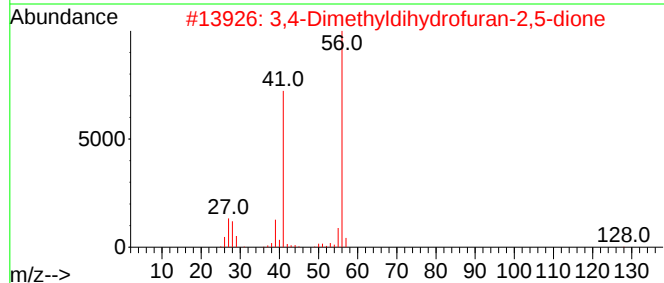
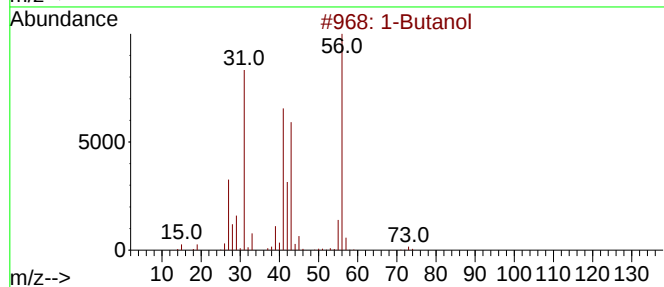
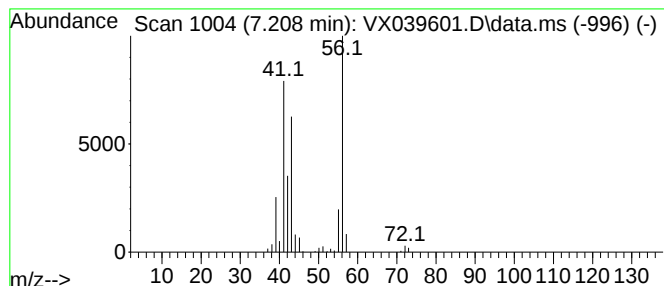
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	20.11 ug/l	173090	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	83
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	45
3	Propanenitrile, 2-hydroxy-			71	C3H5NO	000078-97-7	9
4	Formic acid, butyl ester			102	C5H10O2	000592-84-7	9
5	Oxirane, (1-methylethyl)-			86	C5H10O	001438-14-8	9



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ALS Vial : 15 Sample Multiplier: 1

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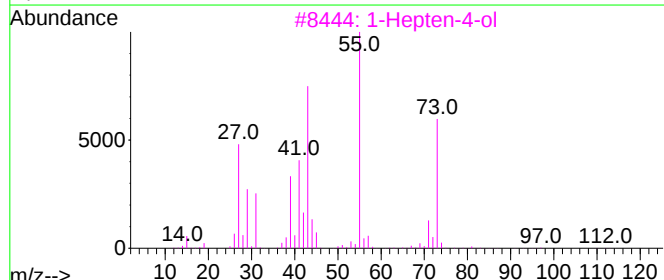
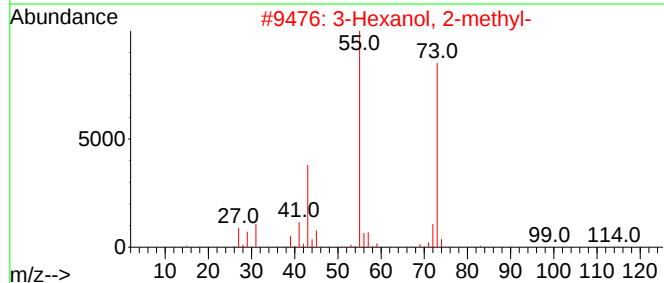
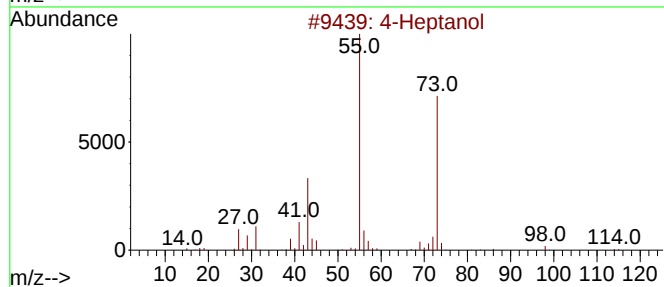
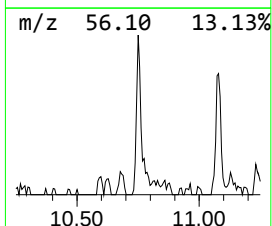
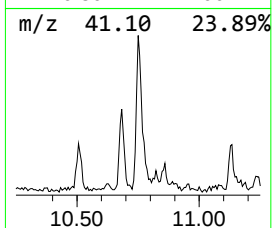
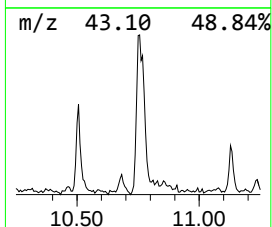
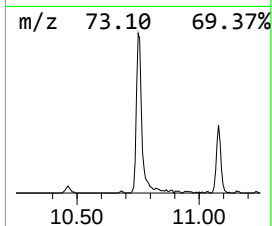
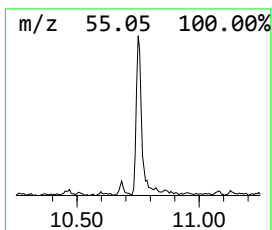
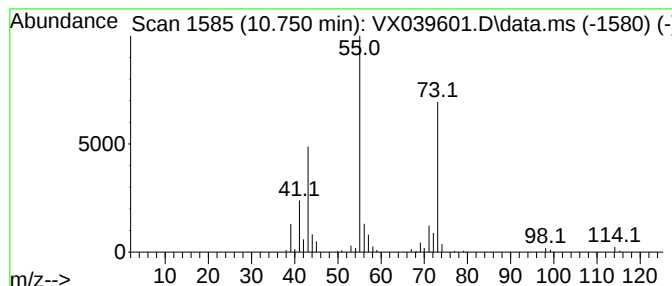
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 4-Heptanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	6.71 ug/l	78981	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	64
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	45
3			1-Hepten-4-ol	114	C7H14O	003521-91-3	40
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
5			Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	38



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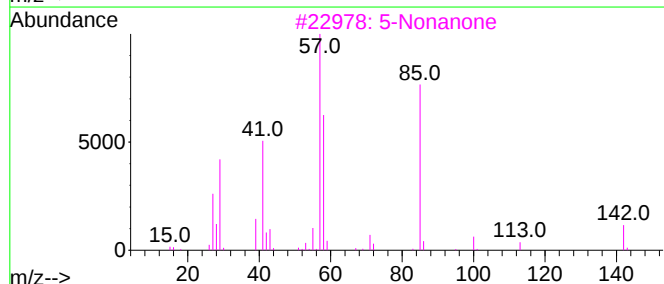
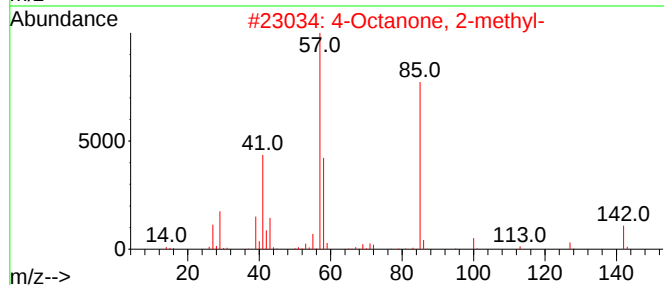
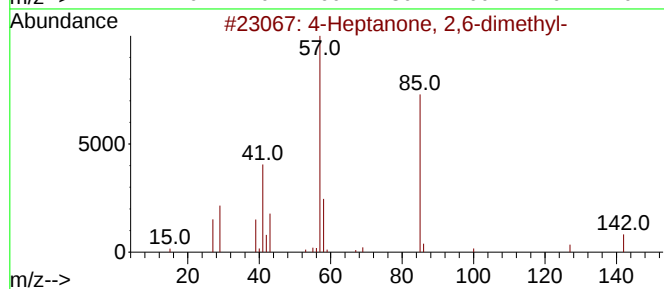
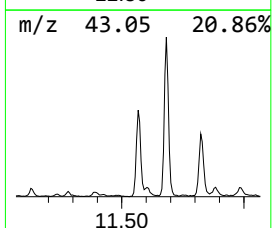
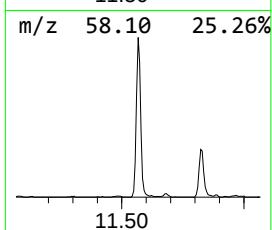
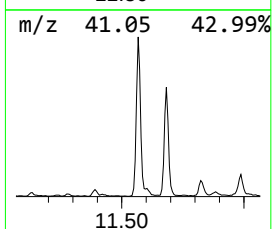
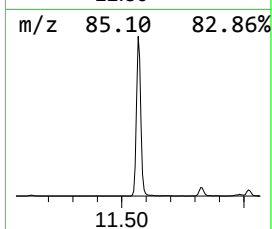
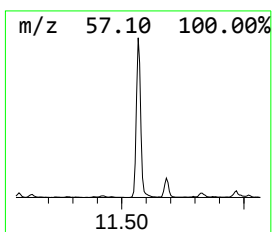
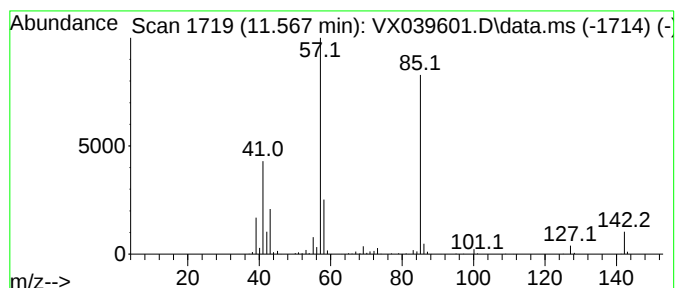
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.567	40.80 ug/l	443610	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	59
5			2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

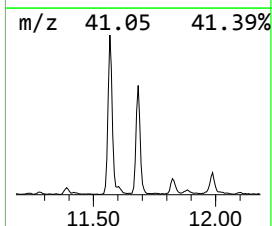
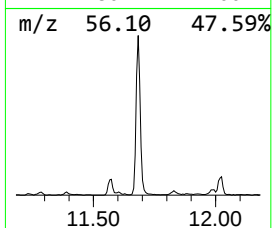
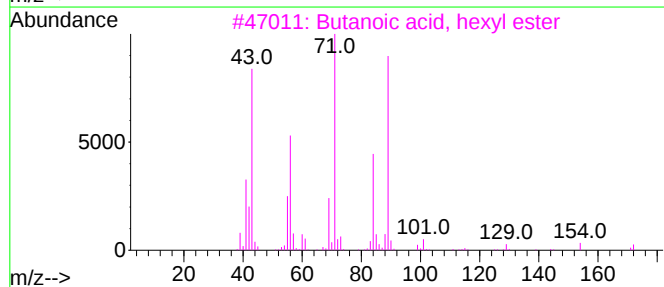
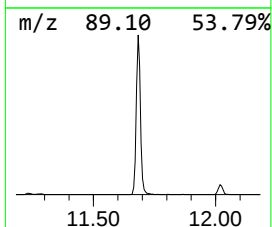
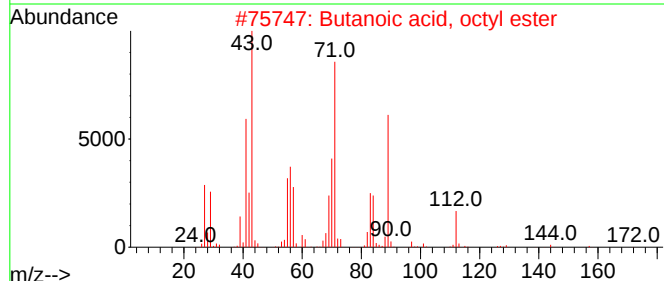
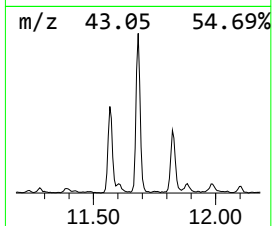
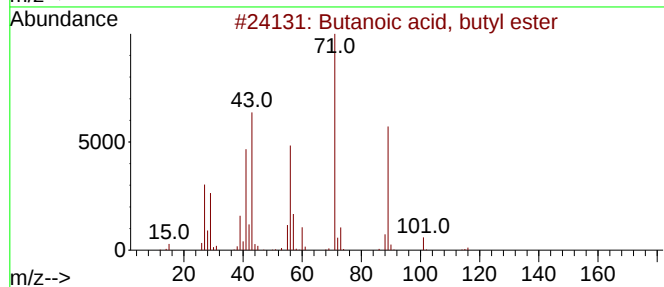
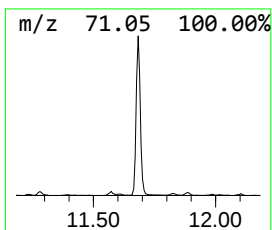
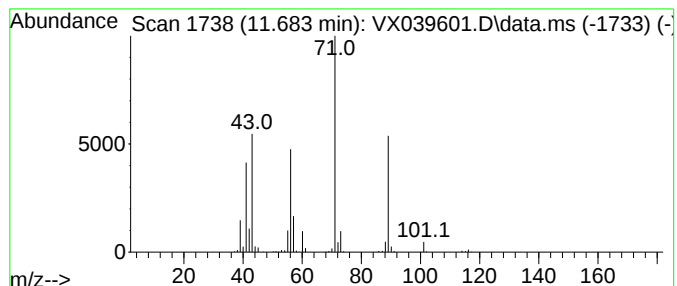
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Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	30.33 ug/l	329781	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

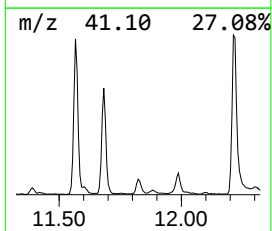
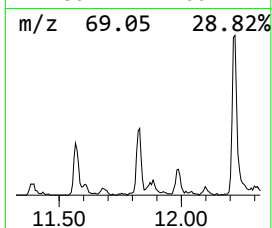
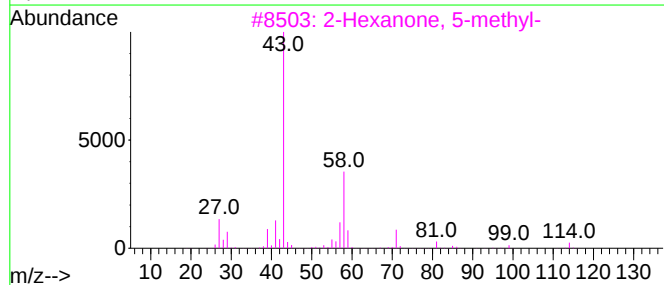
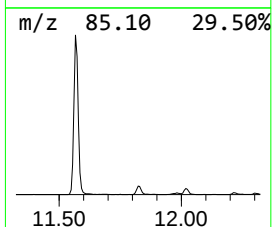
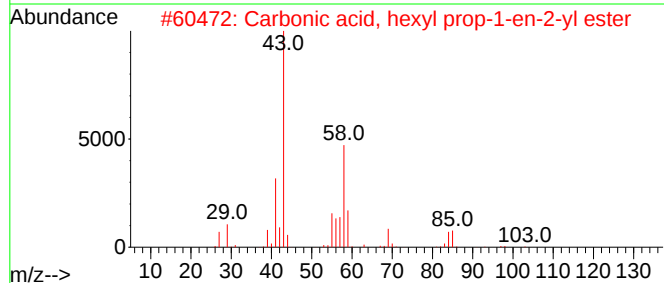
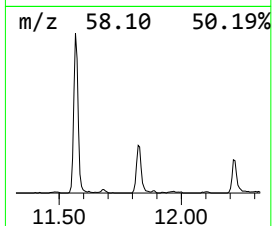
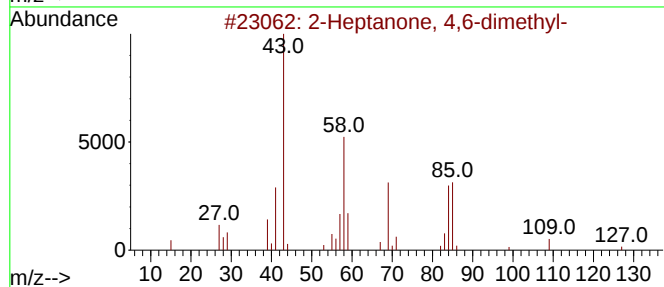
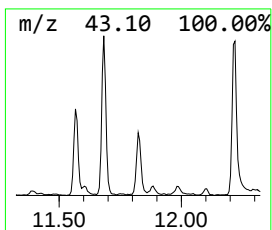
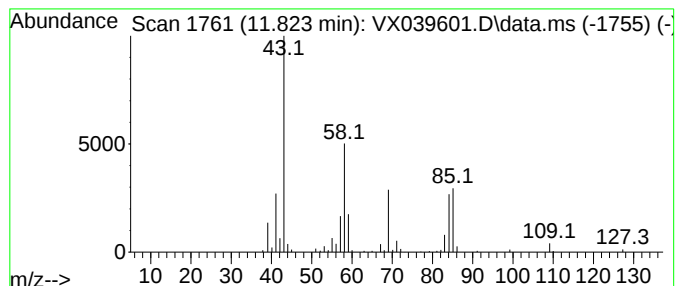
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Quant Title : SW846 8260

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

Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.823	7.03 ug/l	76443	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	74
2			Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	59
3			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
4			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43
5			Hexane, 3-ethyl-	114	C8H18	000619-99-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

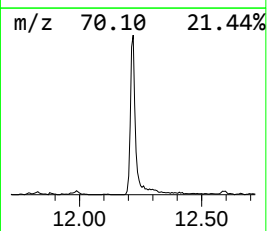
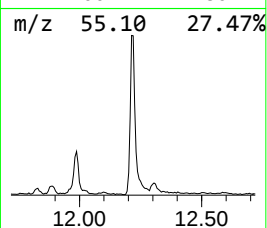
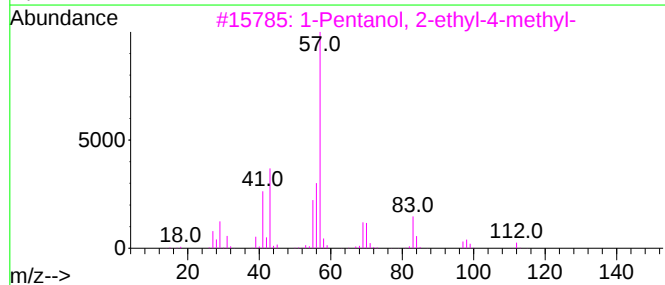
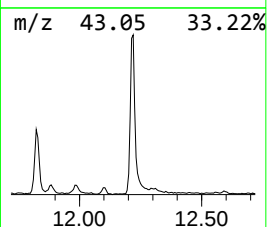
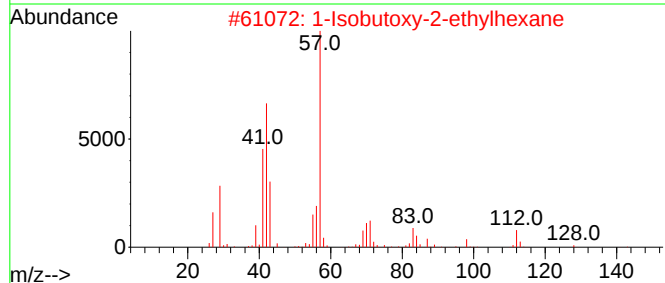
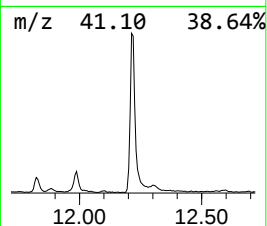
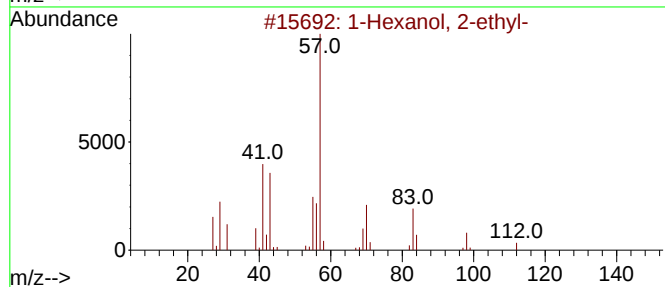
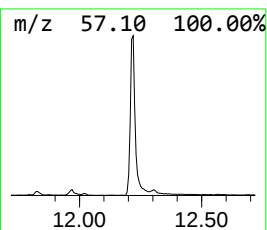
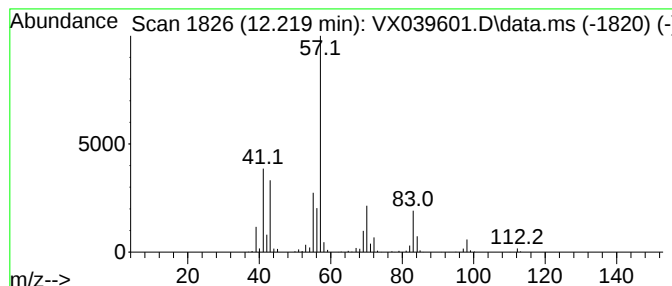
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	50.37 ug/l	547693	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

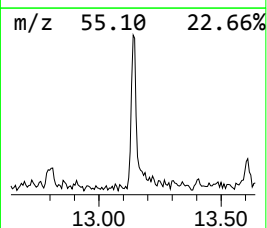
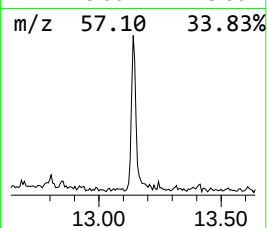
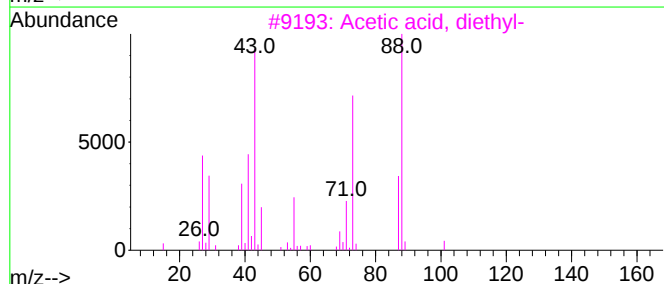
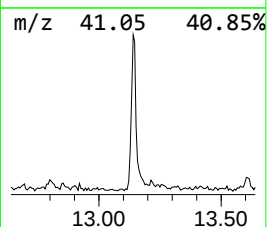
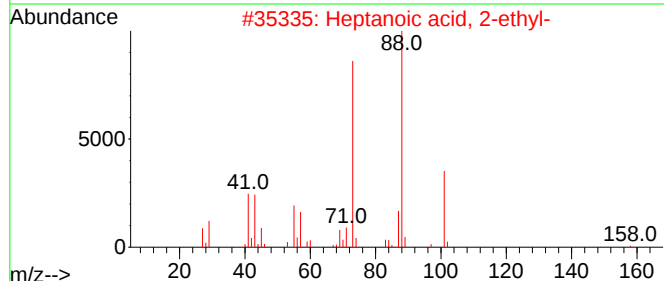
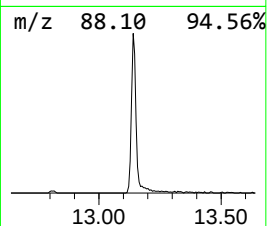
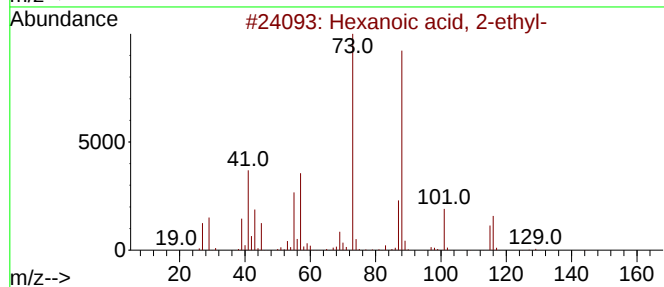
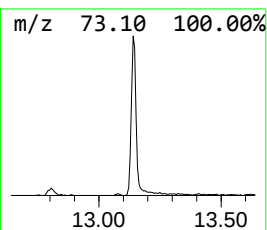
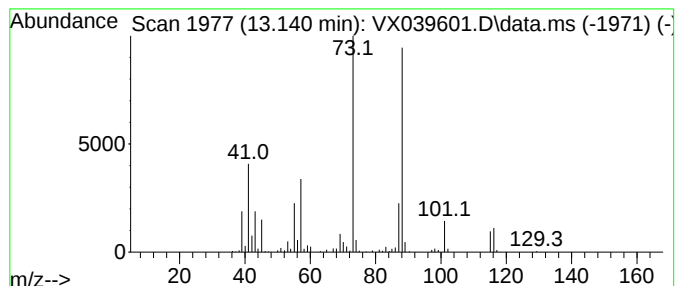
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Quant Title : SW846 8260

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

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	11.55 ug/l	125610	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42
4			Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	42
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

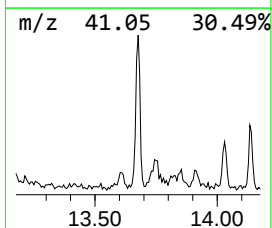
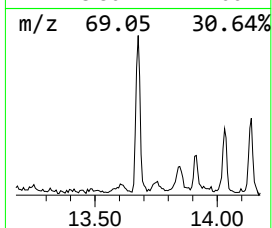
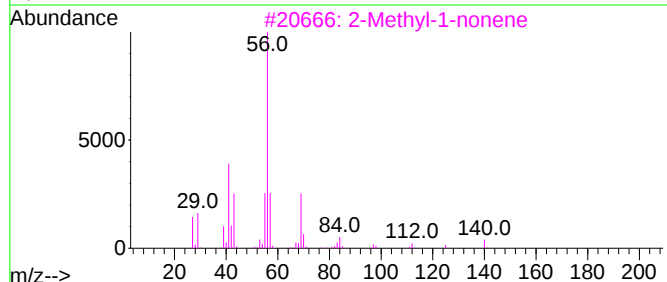
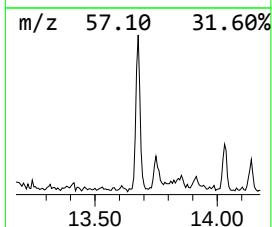
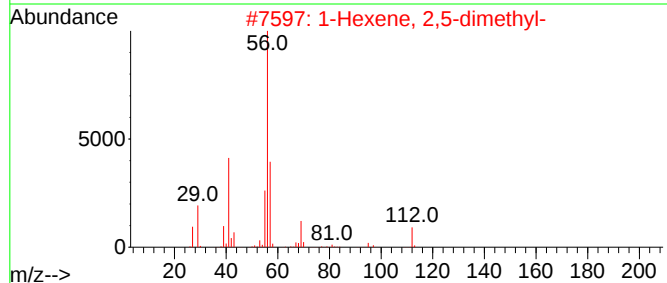
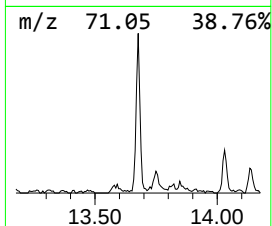
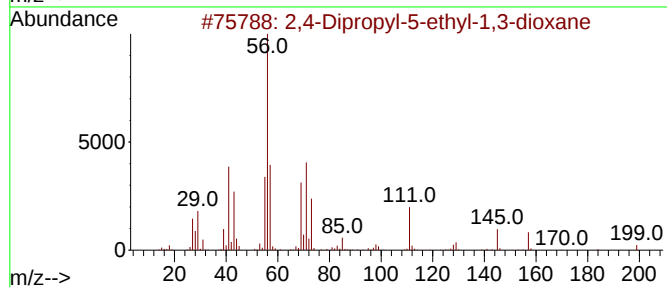
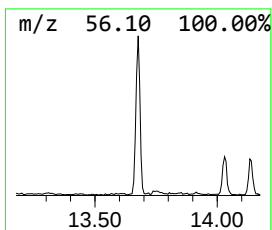
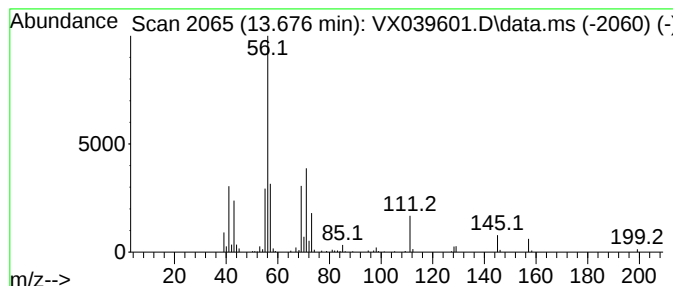
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.676 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	7.73 ug/l	84017	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
2		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
3		2-Methyl-1-nonene	140	C10H20	002980-71-4	32
4		Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	32
5		Tridecane, 7-methylene-	196	C14H28	019780-80-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

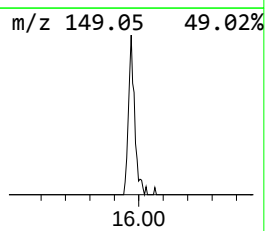
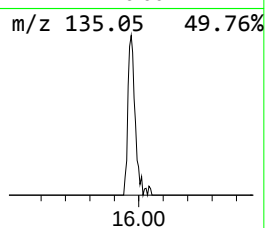
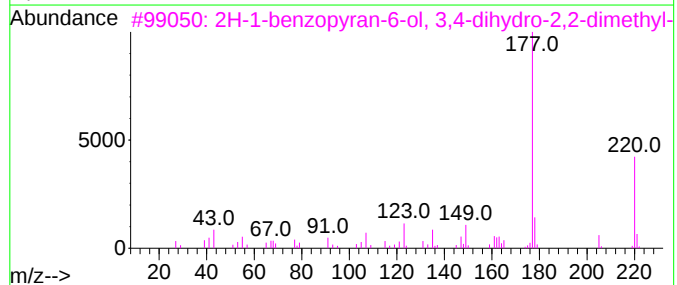
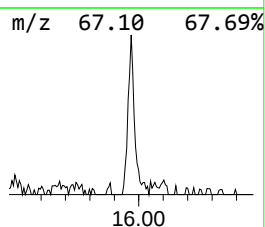
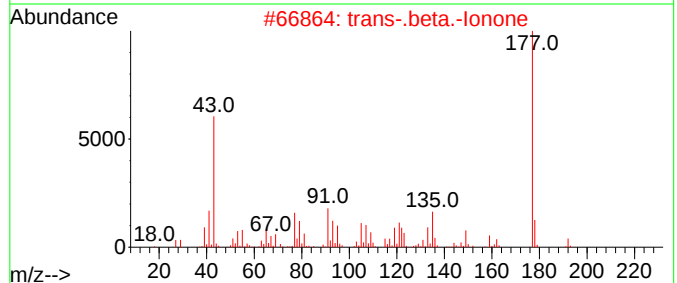
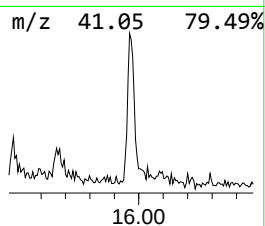
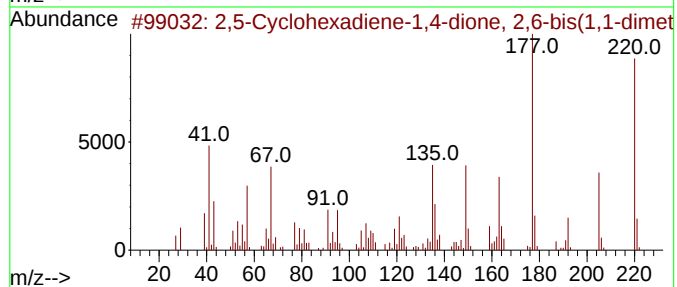
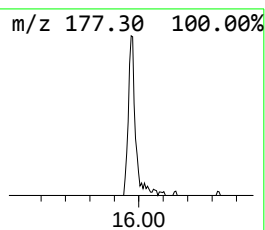
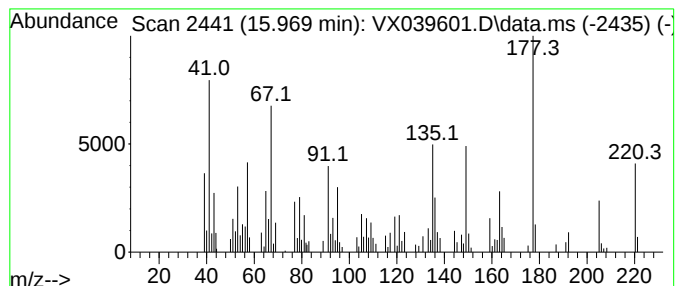
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Quant Title : SW846 8260

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

Peak Number 10 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.969	6.73 ug/l	73188	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2			trans-.beta.-Ionone	192	C13H20O	000079-77-6	42
3			2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	38
4			2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	35
5			1-(4-Fluorophenyl)-1H-pyrazol-5-...	177	C9H8FN3	727967-95-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039601.D
Acq On : 03 Jan 2024 14:51
Operator : JC/MD
Sample : P1002-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1-Butanol	7.208	20.1	ug/l	173090	2	6.757	430364	50.0
4-Heptanol	10.750	6.7	ug/l	78981	3	10.055	588584	50.0
4-Heptanone, 2,...	11.567	40.8	ug/l	443610	4	12.018	543688	50.0
Butanoic acid, ...	11.683	30.3	ug/l	329781	4	12.018	543688	50.0
2-Heptanone, 4,...	11.823	7.0	ug/l	76443	4	12.018	543688	50.0
1-Hexanol, 2-et...	12.219	50.4	ug/l	547693	4	12.018	543688	50.0
Hexanoic acid, ...	13.140	11.6	ug/l	125610	4	12.018	543688	50.0
unknown13.676	13.676	7.7	ug/l	84017	4	12.018	543688	50.0
2,5-Cyclohexadi...	15.969	6.7	ug/l	73188	4	12.018	543688	50.0