

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Title : SW846 8260

Signal : TIC: VX031523.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.416	52	54	55	rBV	10444490	7523140	31.96%	6.307%
2	2.179	153	179	192	rBV	4346958	23541989	100.00%	19.736%
3	2.294	192	198	208	rVV	3146172	5255516	22.32%	4.406%
4	2.392	208	214	229	rVB	645503	1368540	5.81%	1.147%
5	2.587	238	246	263	rVB	119247	411214	1.75%	0.345%
6	3.934	450	467	497	rBV3	265182	1460406	6.20%	1.224%
7	4.239	504	517	534	rBV	2305477	6146376	26.11%	5.153%
8	5.385	692	705	718	rBV	105751	309162	1.31%	0.259%
9	5.550	722	732	747	rVB	101638	287869	1.22%	0.241%
10	5.958	788	799	804	rBV2	113082	298836	1.27%	0.251%
11	6.038	804	812	824	rVB	664004	1803036	7.66%	1.512%
12	6.623	894	908	923	rBV2	81073	268368	1.14%	0.225%
13	6.763	923	931	941	rVB	156567	381466	1.62%	0.320%
14	7.281	999	1016	1036	rBV	3492531	10859621	46.13%	9.104%
15	8.647	1234	1240	1246	rBV	609824	979801	4.16%	0.821%
16	8.720	1246	1252	1259	rVB	785568	1207465	5.13%	1.012%
17	9.244	1333	1338	1352	rBV	878060	1318921	5.60%	1.106%
18	9.519	1380	1383	1391	rVB	538280	784674	3.33%	0.658%
19	10.055	1456	1471	1476	rBV	402304	578662	2.46%	0.485%
20	10.317	1503	1514	1523	rVB2	1766193	2851008	12.11%	2.390%
21	10.598	1553	1560	1565	rBV	10170490	14545944	61.79%	12.194%
22	10.653	1565	1569	1577	rVB2	887633	1594509	6.77%	1.337%
23	11.079	1634	1639	1645	rBV	804439	1057927	4.49%	0.887%
24	11.750	1745	1749	1754	rVB	455522	564491	2.40%	0.473%
25	11.957	1779	1783	1788	rVB	240967	289962	1.23%	0.243%
26	12.024	1789	1794	1801	rVB2	524223	698242	2.97%	0.585%
27	12.219	1819	1826	1839	rBV	1049715	1557539	6.62%	1.306%
28	12.415	1850	1858	1863	rBV	3621273	4339704	18.43%	3.638%
29	12.585	1879	1886	1902	rBV	1010781	1442689	6.13%	1.209%
30	12.799	1918	1921	1931	rVB2	406216	710644	3.02%	0.596%
31	12.963	1942	1948	1957	rVB2	130226	276427	1.17%	0.232%
32	13.597	2046	2052	2058	rBV3	161500	270268	1.15%	0.227%
33	13.713	2067	2071	2076	rBV	208945	296941	1.26%	0.249%
34	13.780	2076	2082	2088	rVV	16226130	20700000	87.93%	17.353%
35	13.872	2093	2097	2102	rVB	692843	885790	3.76%	0.743%
36	14.195	2146	2150	2159	rBV	155874	325061	1.38%	0.273%

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ClientSampleId :  
ORA-0131

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\82X091922W.M  
Title : SW846 8260

37	14.640	2218	2223	2232	rVB	964080	1282855	5.45%	1.075%
38	14.780	2240	2246	2252	rVB	620281	809737	3.44%	0.679%

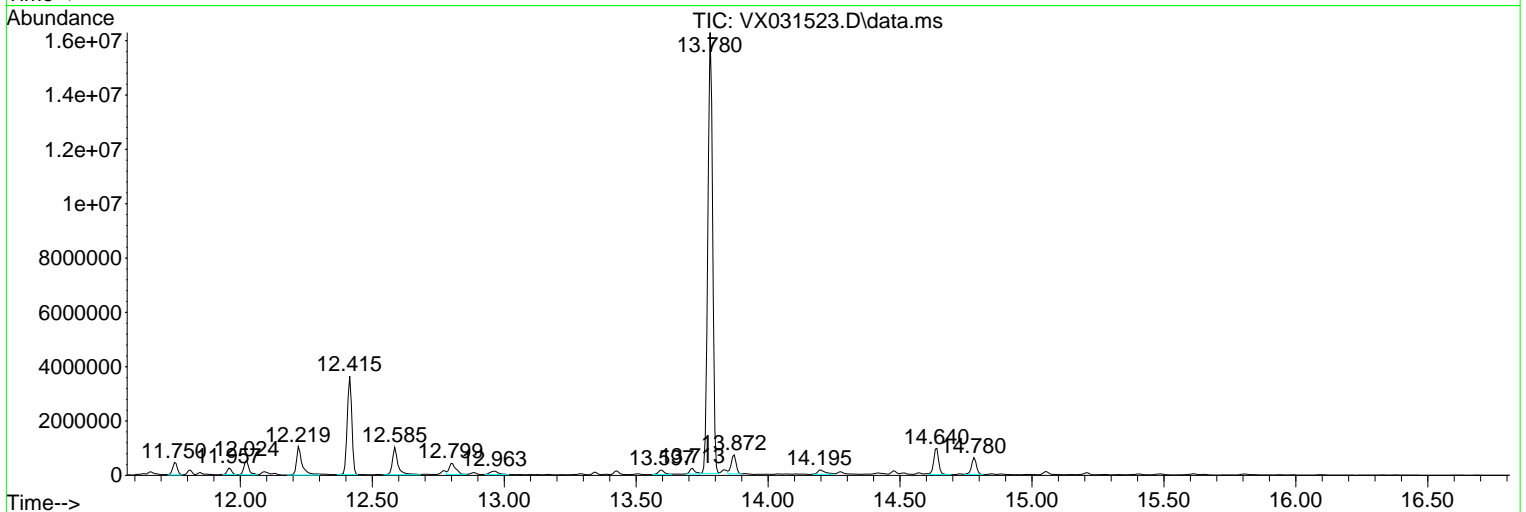
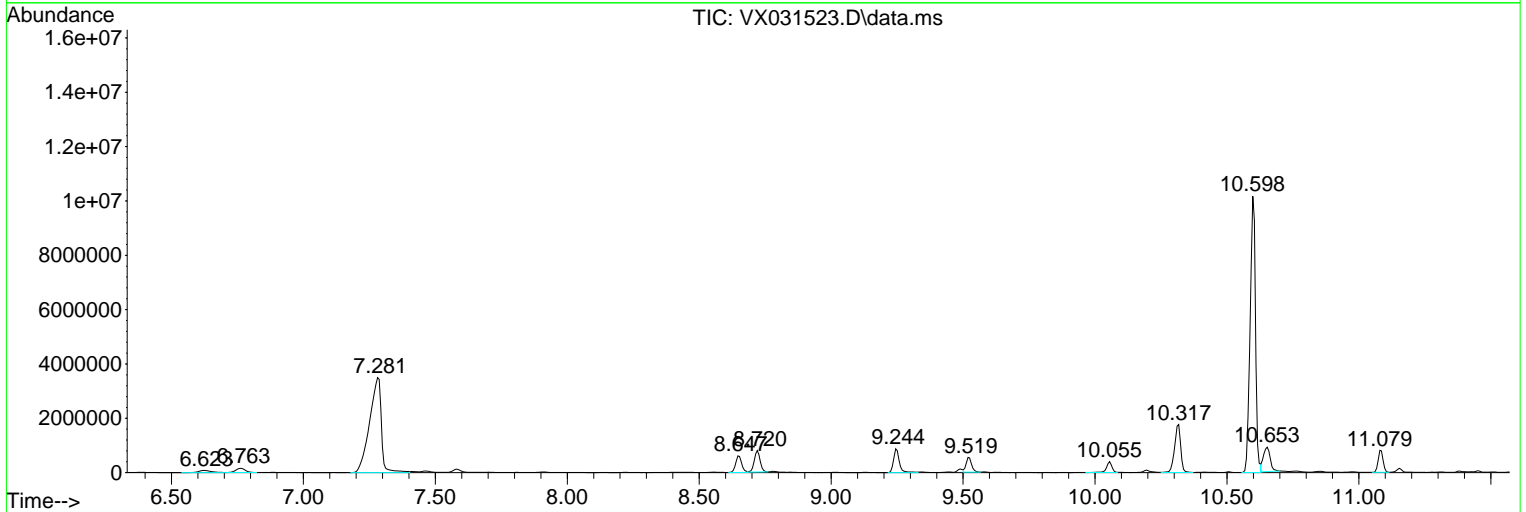
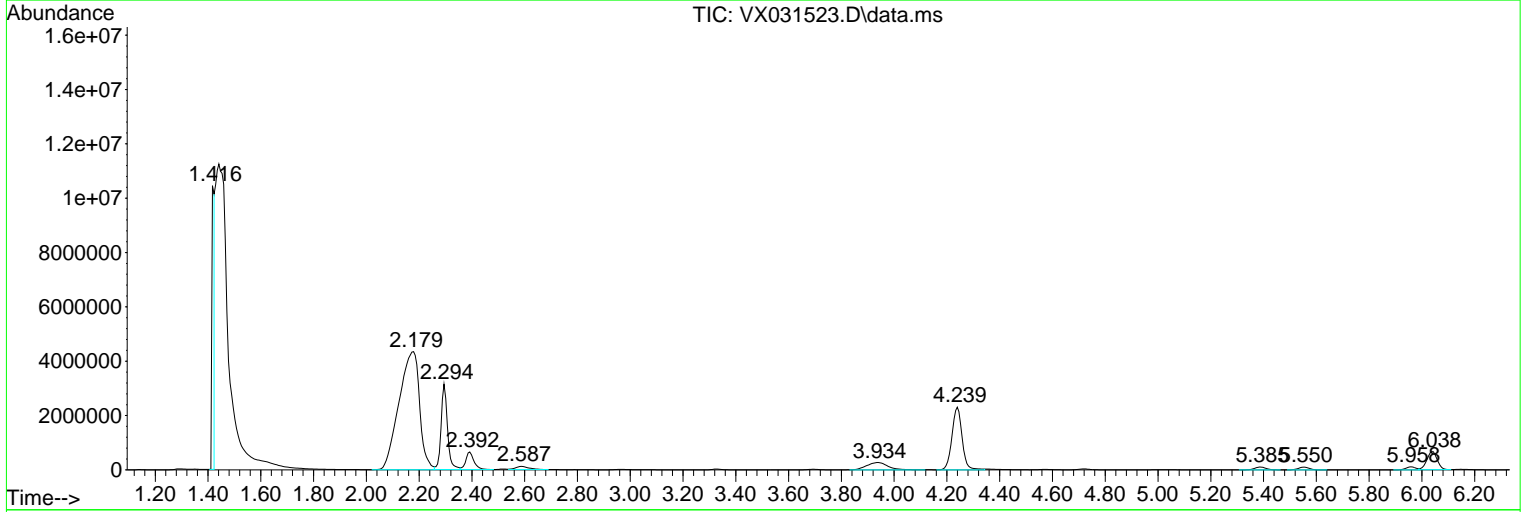
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

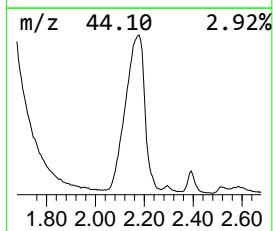
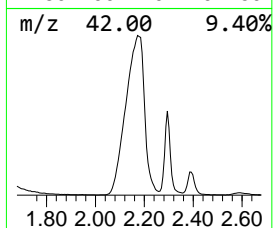
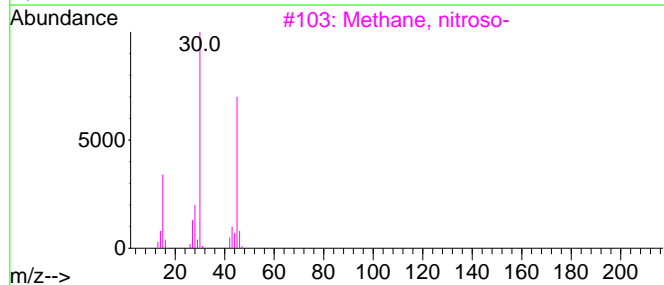
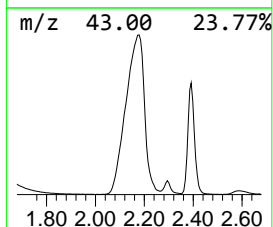
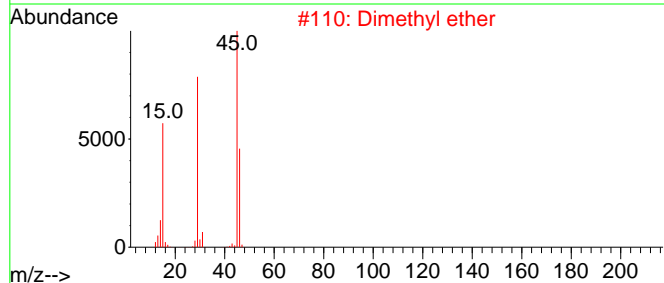
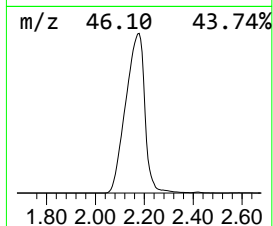
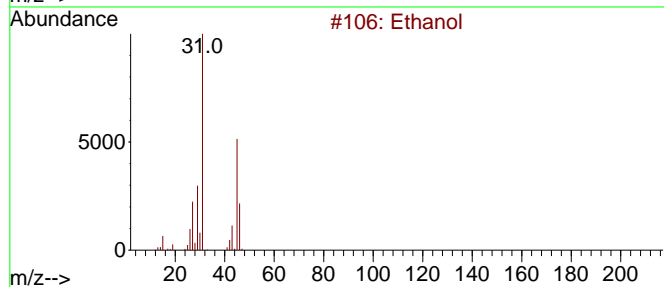
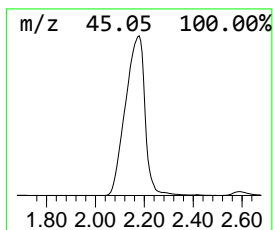
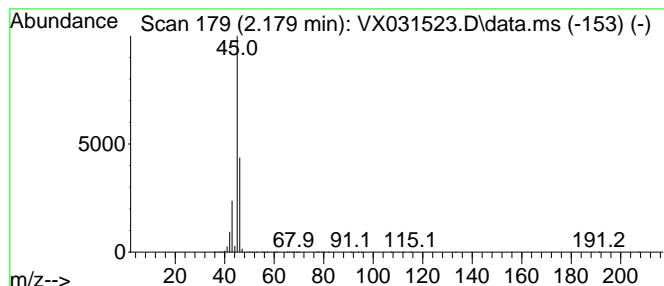
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.179	4089.01 ug/l	23542000	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol	46	C2H6O	000064-17-5	86
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Formic acid	46	CH2O2	000064-18-6	4
5		Oxalic acid	90	C2H2O4	000144-62-7	4



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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

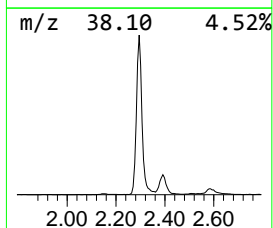
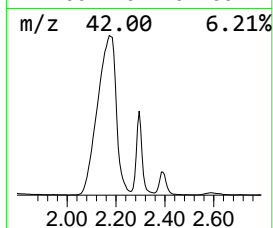
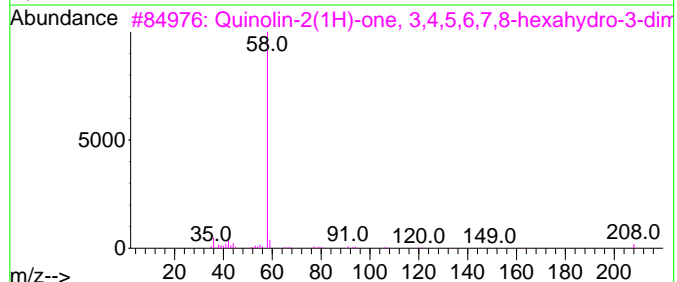
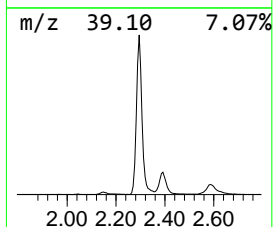
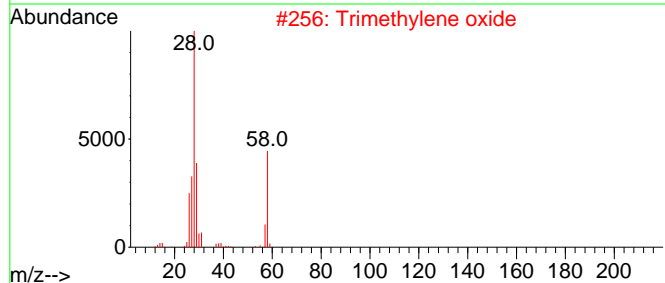
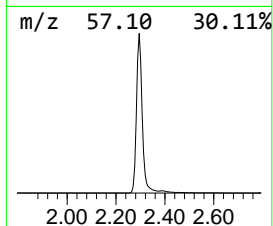
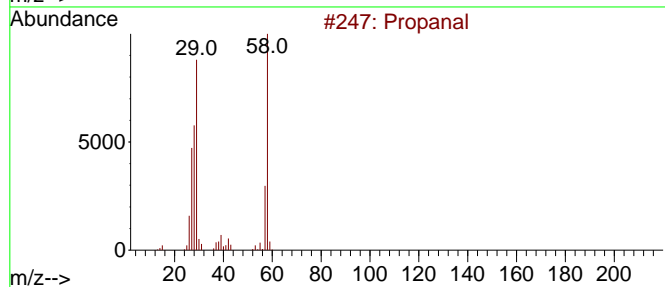
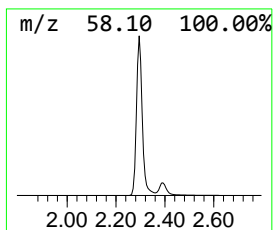
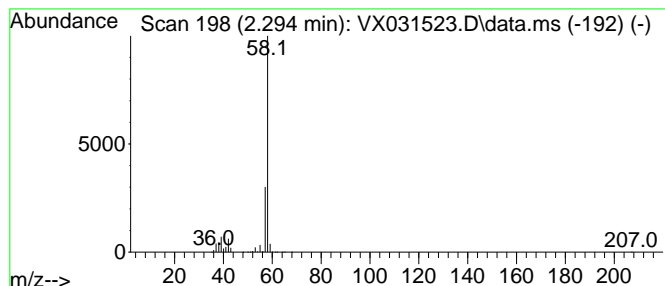
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	912.83 ug/l	5255520	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	7



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 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

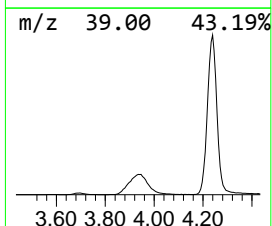
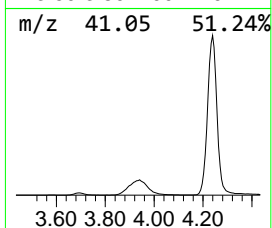
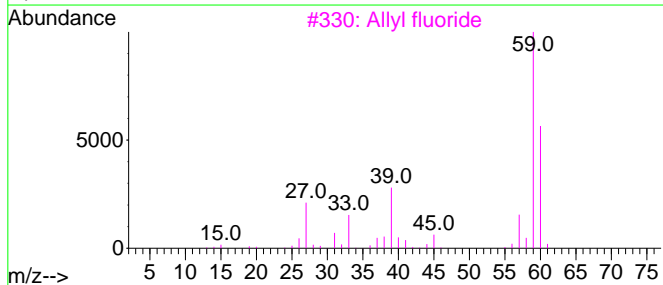
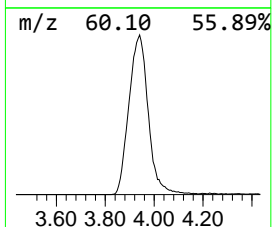
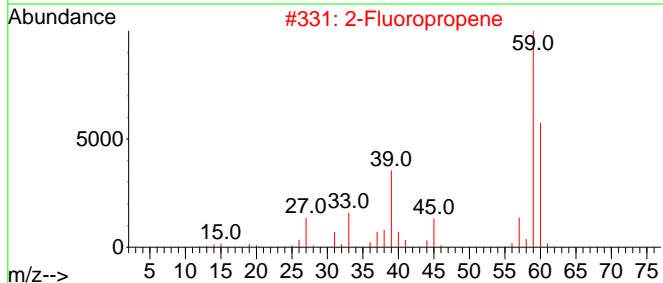
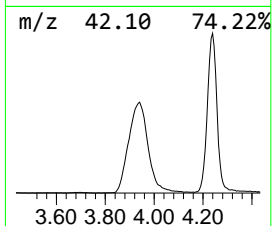
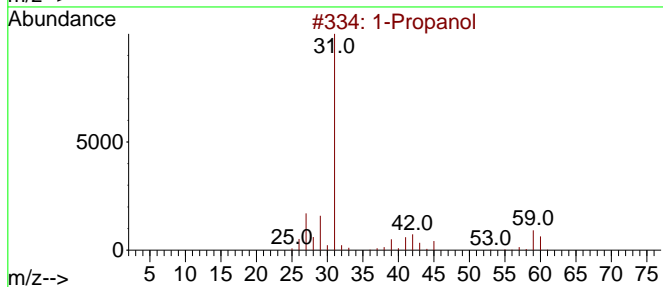
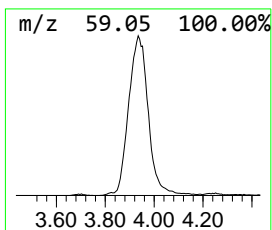
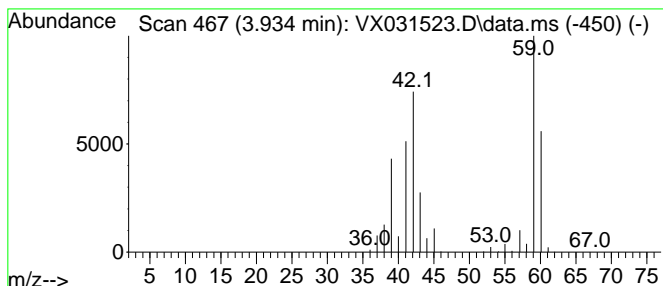
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 1-Propanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.934	253.66 ug/l	1460410	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	59
2		2-Fluoropropene	60	C3H5F	001184-60-7	43
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	25
5		Propene	42	C3H6	000115-07-1	25



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 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

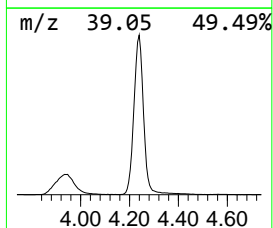
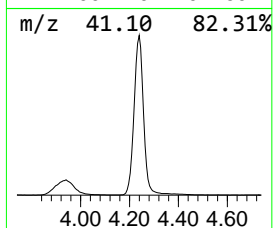
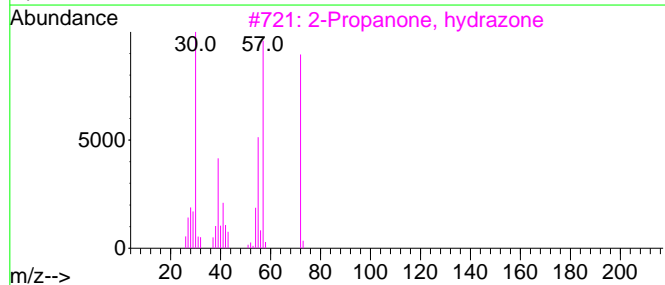
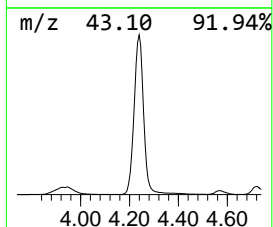
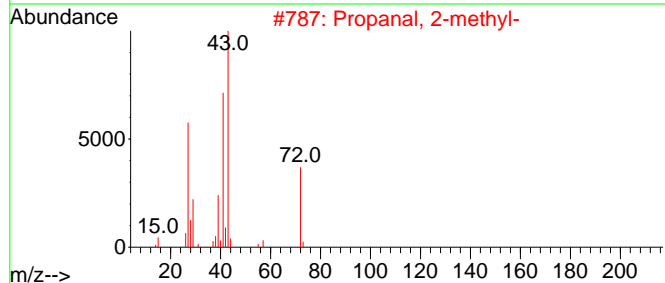
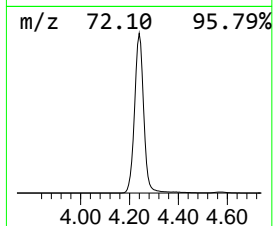
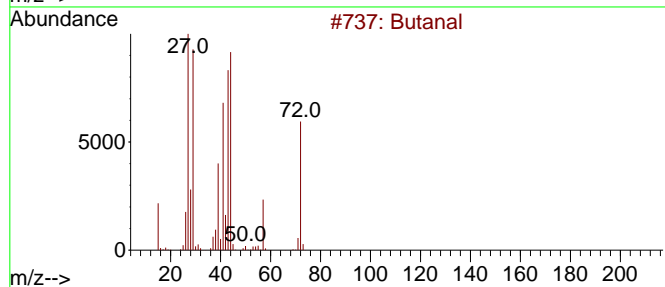
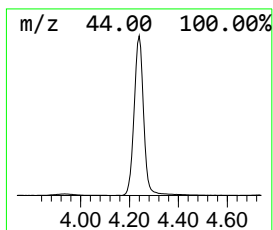
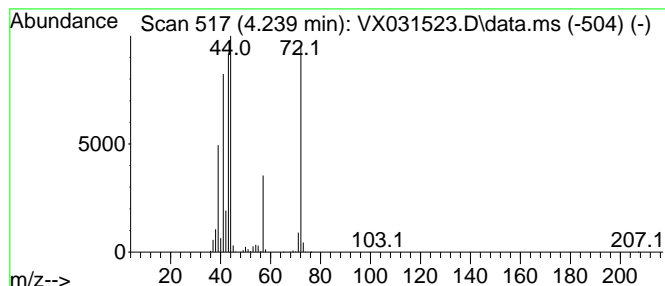
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.239	1067.56 ug/l	6146380	Pentafluorobenzene	5.550

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	91
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5		Isobutylene epoxide	72	C4H8O	000558-30-5	27



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 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

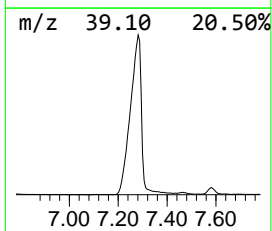
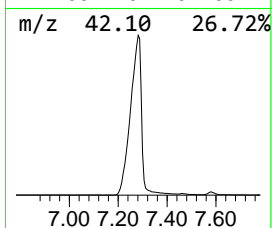
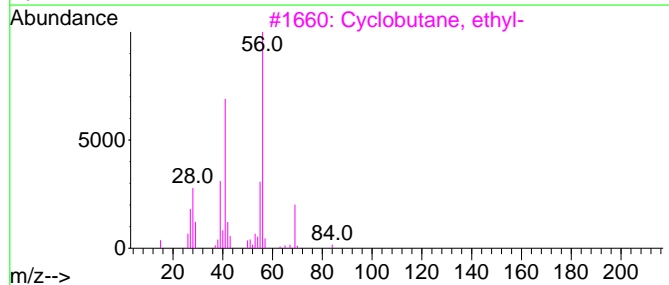
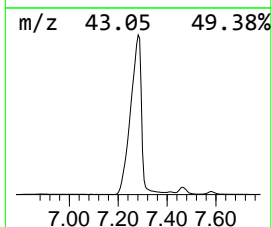
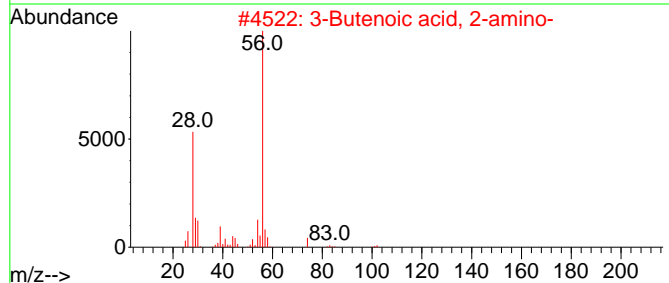
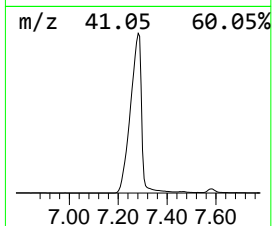
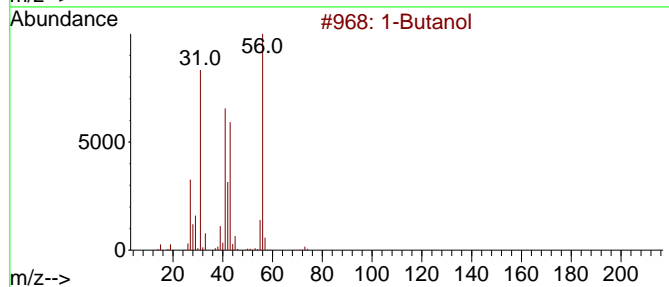
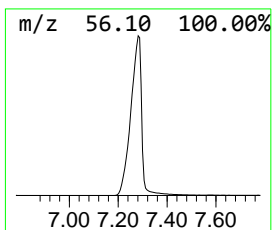
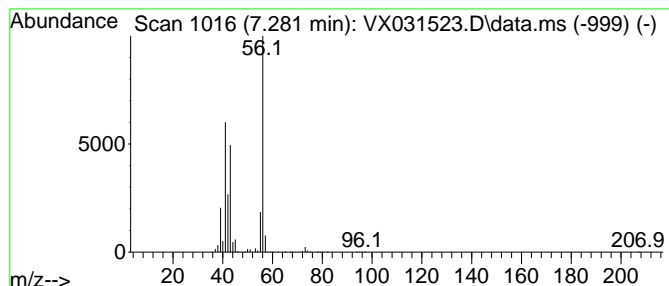
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.281	1423.41 ug/l	10859600	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol	74	C4H10O	000071-36-3	90
2		3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
4		Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
5		Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

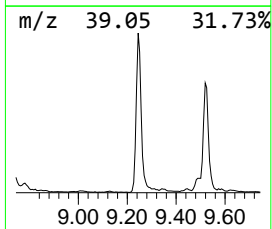
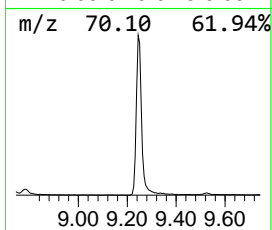
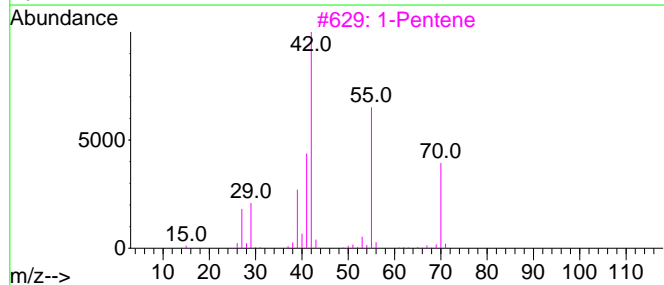
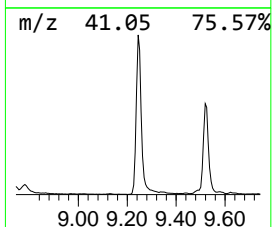
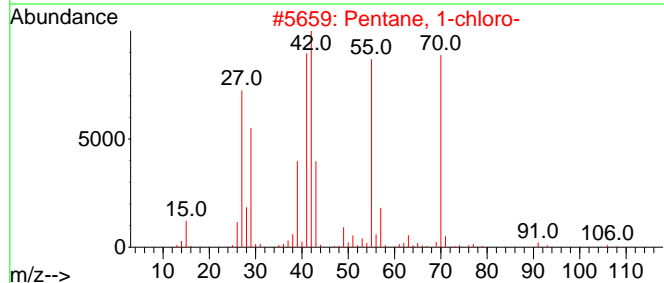
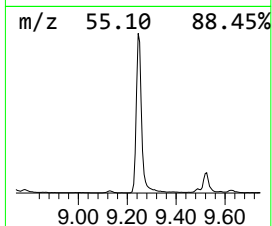
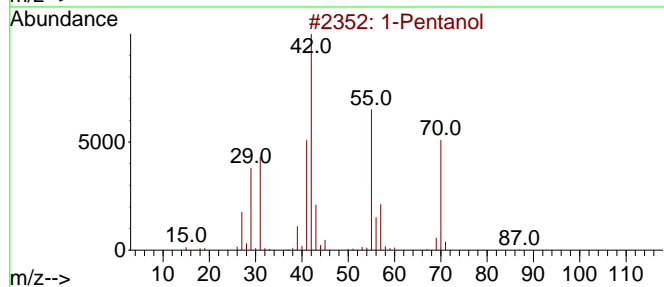
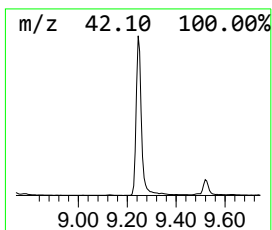
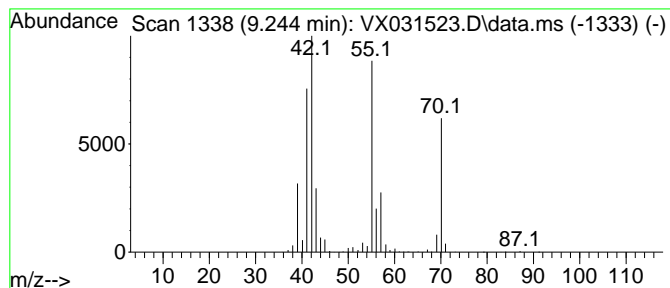
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 1-Pentanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	113.96 ug/l	1318920	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentanol	88	C5H12O	000071-41-0	90
2		Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	72
3		1-Pentene	70	C5H10	000109-67-1	64
4		1-Butanol, 3-methyl-, formate	116	C6H12O2	000110-45-2	59
5		Cyclopentane	70	C5H10	000287-92-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
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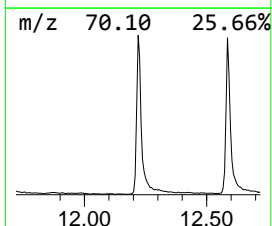
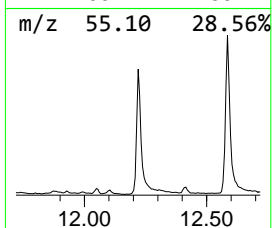
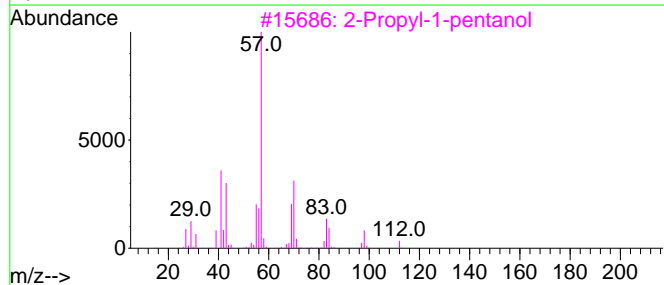
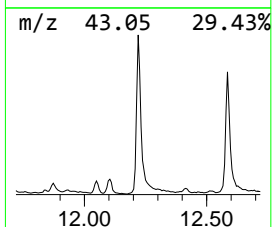
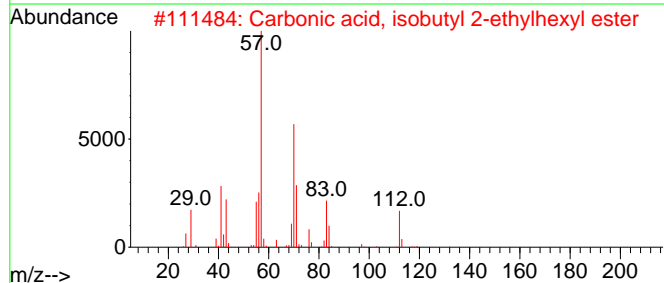
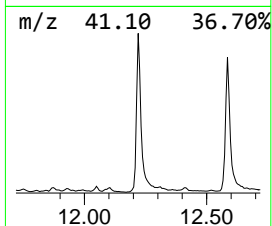
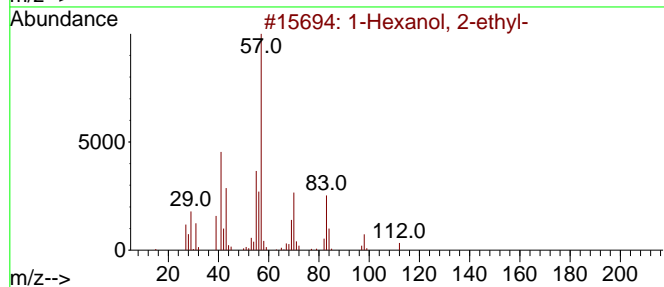
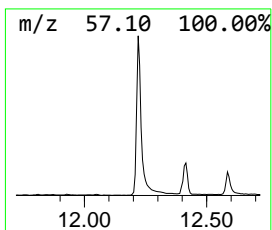
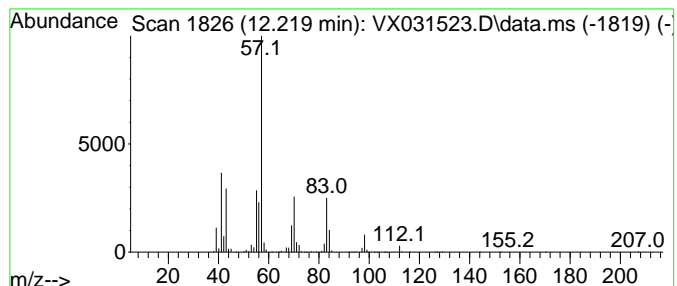
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	111.53 ug/l	1557540	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	Carbonic acid, isobutyl 2-ethylh...			230	C13H26O3	1000383-13-3	53
3	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether			144	C9H20O	1000365-10-2	50
5	2-Decene, 5-methyl-, (Z)-			154	C11H22	074645-86-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

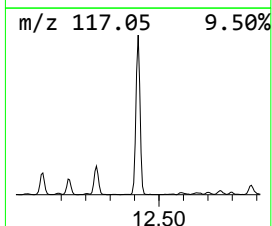
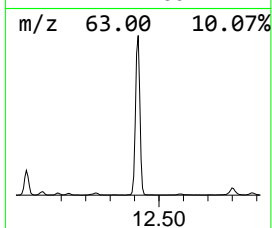
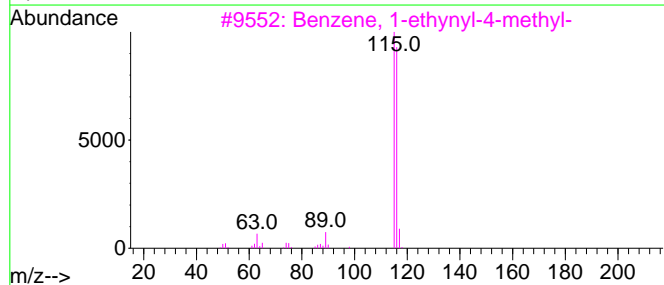
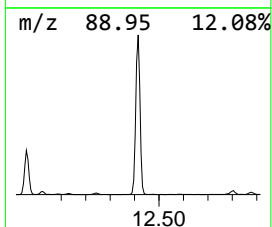
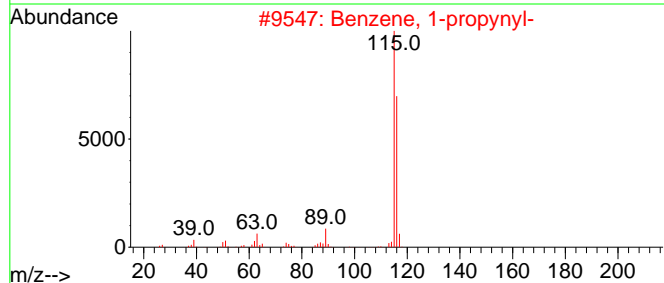
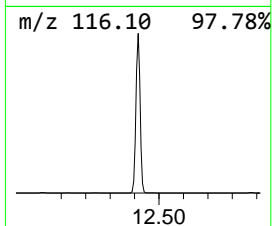
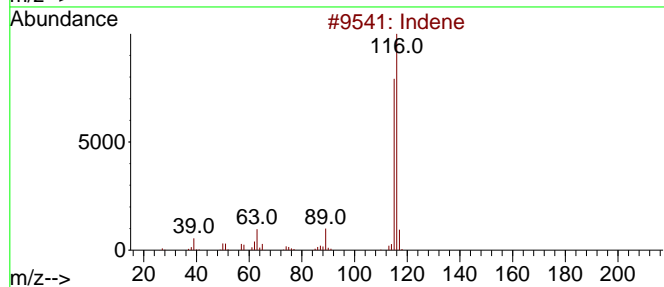
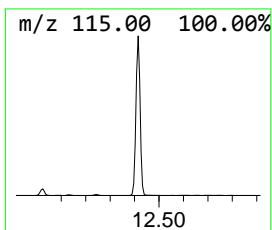
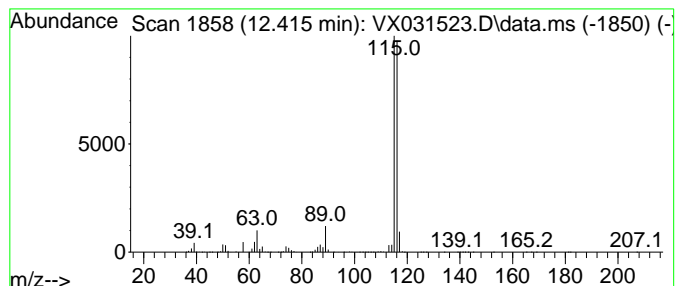
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 Quant Title : SW846 8260

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

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 Peak Number 9 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	310.76 ug/l	4339700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

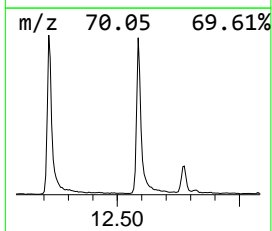
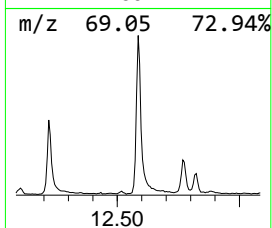
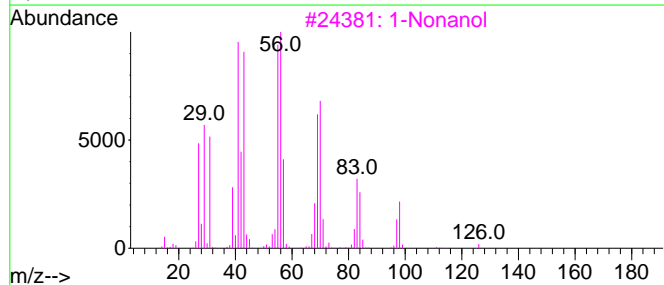
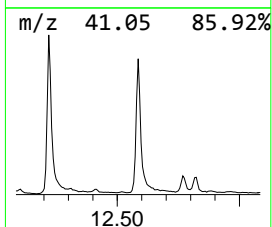
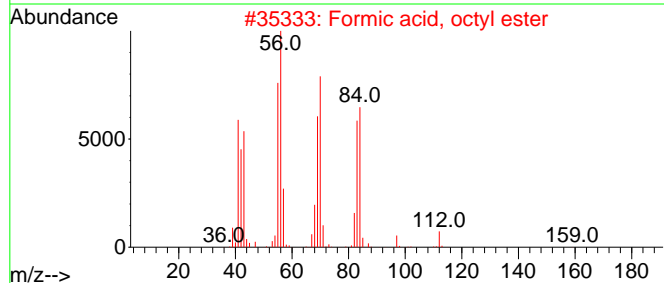
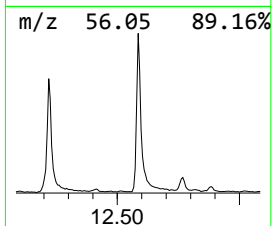
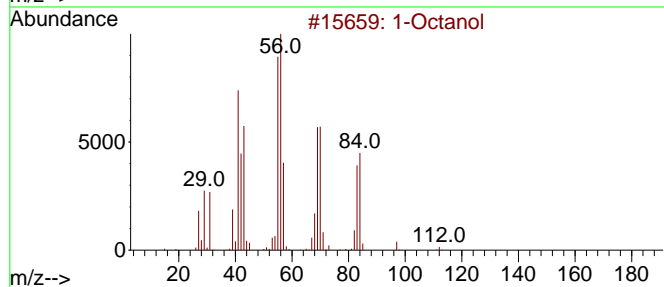
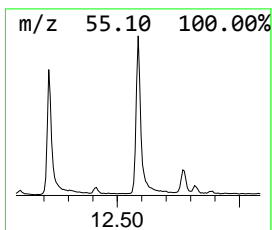
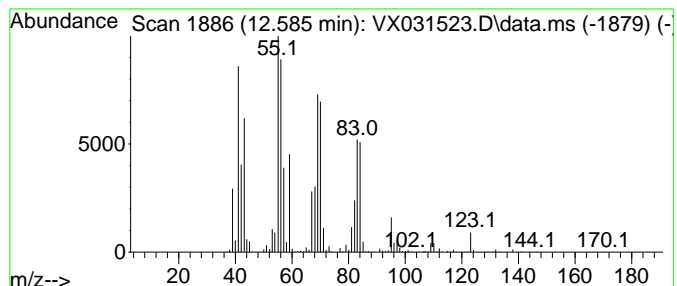
TIC Library : C:\Database\NIST20.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 10 1-Octanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	103.31 ug/l	1442690	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol	130	C8H18O	000111-87-5	64
2		Formic acid, octyl ester	158	C9H18O2	000112-32-3	59
3		1-Nonanol	144	C9H20O	000143-08-8	47
4		1-Octene	112	C8H16	000111-66-0	43
5		Cyanoacetic acid, heptyl ester	183	C10H17NO2	1000406-22-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX092122\  
 Data File : VX031523.D  
 Acq On : 21 Sep 2022 14:42  
 Operator : JC/MD  
 Sample : N4720-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ORA-0131

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091922W.M  
 Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.179	4089.0	ug/l	23542000	1	5.550	287869	50.0
Propanal	2.294	912.8	ug/l	5255520	1	5.550	287869	50.0
1-Propanol	3.934	253.7	ug/l	1460410	1	5.550	287869	50.0
Butanal	4.239	1067.6	ug/l	6146380	1	5.550	287869	50.0
1-Butanol	7.281	1423.4	ug/l	10859600	2	6.763	381466	50.0
1-Pentanol	9.244	114.0	ug/l	1318920	3	10.055	578662	50.0
1-Hexanol, 2-et...	12.219	111.5	ug/l	1557540	4	12.024	698242	50.0
Indene	12.415	310.8	ug/l	4339700	4	12.024	698242	50.0
1-Octanol	12.585	103.3	ug/l	1442690	4	12.024	698242	50.0