

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
 Data File : VX032290.D
 Acq On : 21 Oct 2022 15:49
 Operator : JC/MD
 Sample : N5185-23
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RW-02

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\82X101922W.M
 Title : SW846 8260

Signal : TIC: VX032290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	43	rBV	425563	507932	4.75%	1.269%
2	1.368	43	46	52	rBV	2126845	2424307	22.68%	6.057%
3	1.752	103	109	126	rVB	8143691	10687907	100.00%	26.703%
4	1.953	137	142	156	rVB	1091394	1603584	15.00%	4.006%
5	2.215	180	185	197	rVB	298423	447739	4.19%	1.119%
6	2.343	197	206	222	rVB	140716	280189	2.62%	0.700%
7	2.782	257	278	281	rBV	387676	879469	8.23%	2.197%
8	2.825	281	285	289	rVV	647721	1351865	12.65%	3.378%
9	2.867	289	292	304	rVB	532067	1045017	9.78%	2.611%
10	3.105	320	331	351	rVB2	576553	1315101	12.30%	3.286%
11	3.446	378	387	401	rVB	82926	182433	1.71%	0.456%
12	3.733	426	434	443	rVB	84433	199428	1.87%	0.498%
13	3.837	443	451	458	rBV	55399	140251	1.31%	0.350%
14	4.105	485	495	504	rVB2	54436	138392	1.29%	0.346%
15	4.306	518	528	540	rVV	838531	2379986	22.27%	5.946%
16	5.196	649	674	688	rBV2	46846	182010	1.70%	0.455%
17	5.385	692	705	712	rBV	82197	250619	2.34%	0.626%
18	5.477	712	720	726	rVV3	160684	517569	4.84%	1.293%
19	5.550	727	732	739	rVV	155860	455274	4.26%	1.137%
20	5.623	740	744	763	rVB2	72418	211373	1.98%	0.528%
21	5.830	767	778	790	rBV3	42536	136310	1.28%	0.341%
22	5.958	790	799	804	rVV	90331	229587	2.15%	0.574%
23	6.037	804	812	824	rVV	469168	1267377	11.86%	3.166%
24	6.159	824	832	839	rVV3	62427	221890	2.08%	0.554%
25	6.257	842	848	857	rVV4	84785	253458	2.37%	0.633%
26	6.354	857	864	878	rVB2	47840	137841	1.29%	0.344%
27	6.763	921	931	939	rBV	220031	546653	5.11%	1.366%
28	7.379	1019	1032	1043	rBV4	140226	377094	3.53%	0.942%
29	8.647	1235	1240	1247	rVB	437756	684477	6.40%	1.710%
30	10.055	1460	1471	1476	rBV	450595	610674	5.71%	1.526%
31	10.195	1489	1494	1500	rVB	1508868	1874322	17.54%	4.683%
32	10.305	1506	1512	1518	rVB	447992	586743	5.49%	1.466%
33	10.963	1613	1620	1627	rBV	296992	366207	3.43%	0.915%
34	11.079	1634	1639	1646	rBV	368441	475685	4.45%	1.188%
35	11.305	1671	1676	1683	rVB	589907	715654	6.70%	1.788%
36	11.402	1685	1692	1696	rVV	127119	161418	1.51%	0.403%

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37	11.451	1696	1700	1707	rVB	133070	157833	1.48%	0.394%
38	11.616	1721	1727	1736	rVB	517238	657060	6.15%	1.642%
39	11.750	1745	1749	1755	rVB	128405	158040	1.48%	0.395%
40	12.024	1789	1794	1800	rVB	470877	588920	5.51%	1.471%
41	12.085	1800	1804	1809	rBV	139751	170696	1.60%	0.426%
42	12.244	1824	1830	1837	rBV	1600644	1934893	18.10%	4.834%
43	12.311	1837	1841	1852	rVB3	100177	167256	1.56%	0.418%
44	12.463	1861	1866	1872	rVB	124117	147294	1.38%	0.368%
45	12.616	1885	1891	1894	rBV	195339	246571	2.31%	0.616%
46	12.701	1900	1905	1913	rVB2	234855	329915	3.09%	0.824%
47	12.920	1934	1941	1945	rBV	192452	233066	2.18%	0.582%
48	12.963	1945	1948	1954	rVB	93146	107389	1.00%	0.268%
49	13.170	1978	1982	1992	rVB	173679	211232	1.98%	0.528%
50	13.292	1992	2002	2007	rBV2	421019	549986	5.15%	1.374%
51	13.774	2076	2081	2091	rBV	414381	518930	4.86%	1.297%

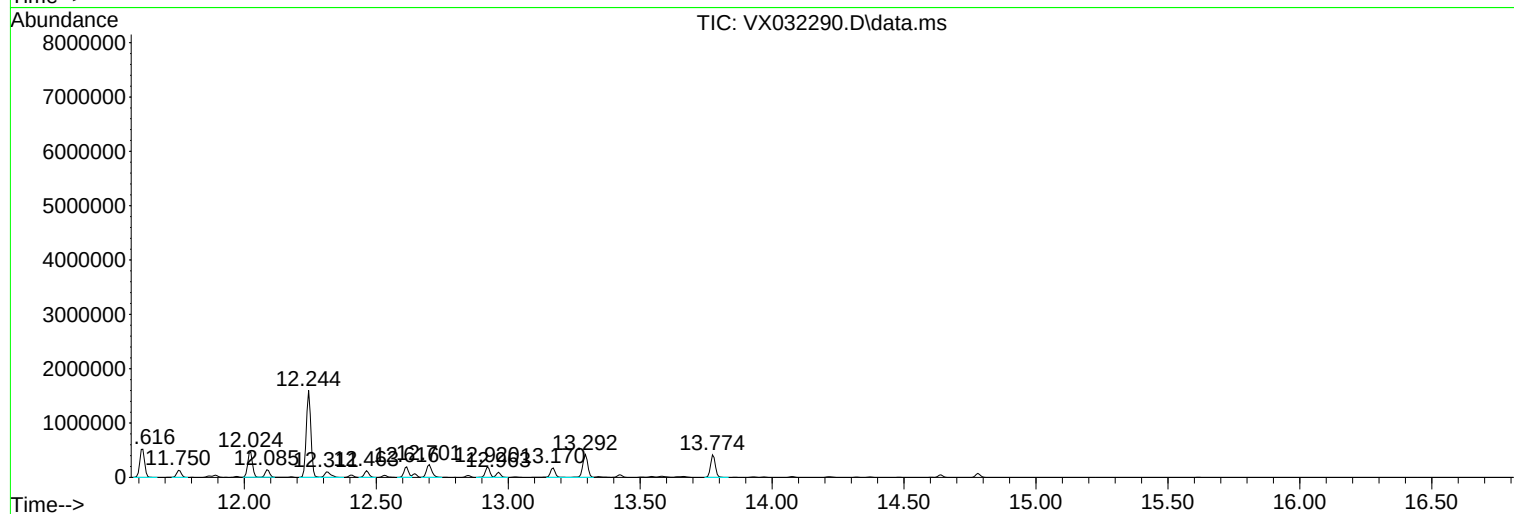
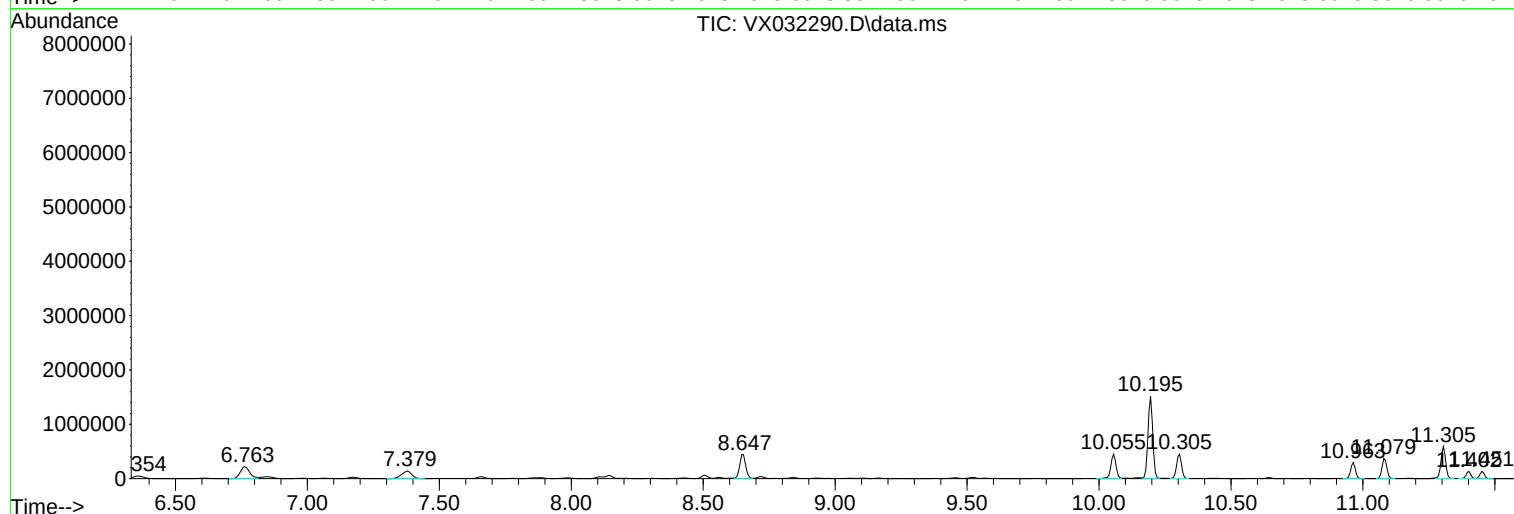
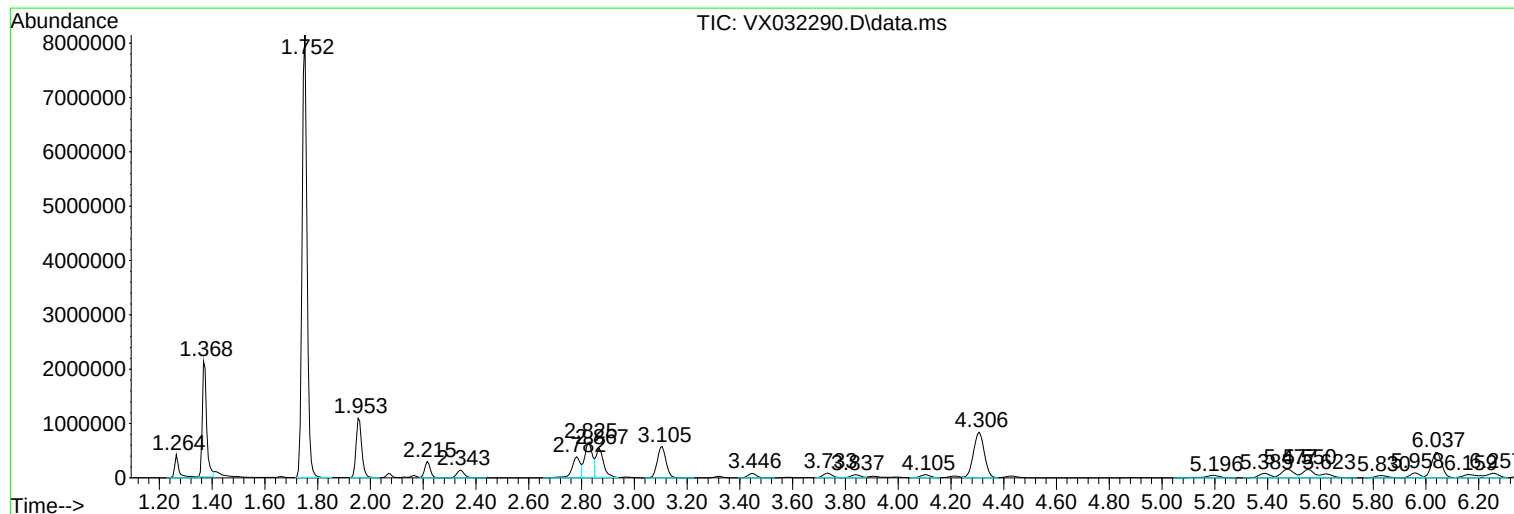
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



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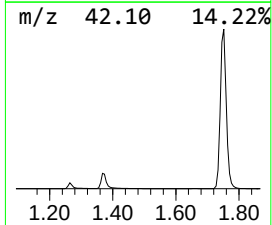
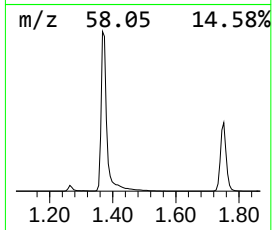
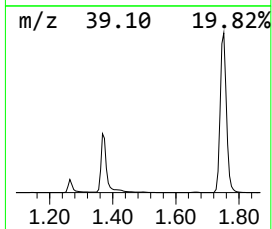
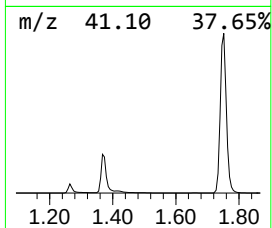
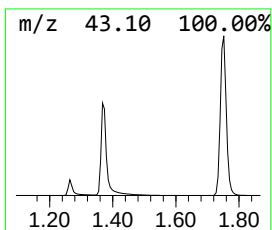
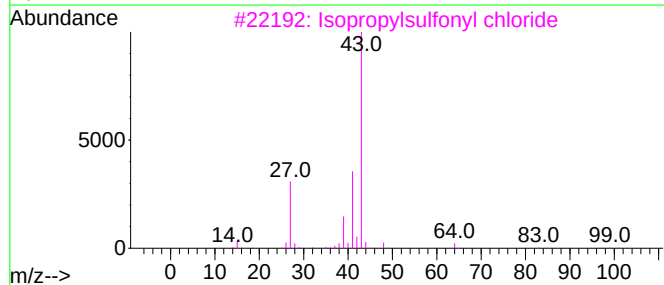
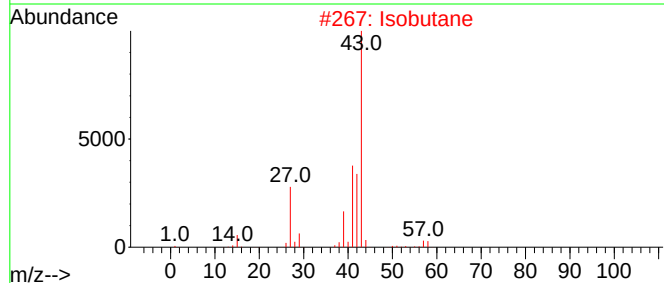
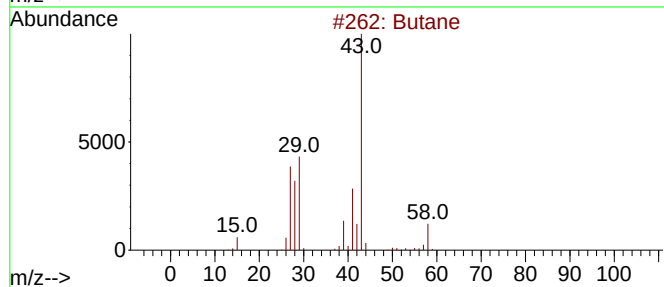
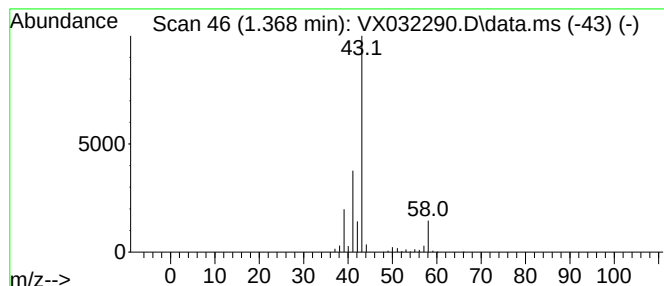
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	266.25 ug/l	2424310	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	80
2	Isobutane			58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-			58	C2H6N2	000503-28-6	5



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Instrument :
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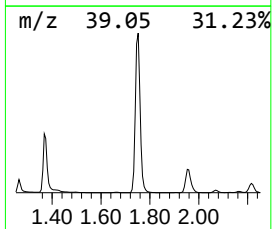
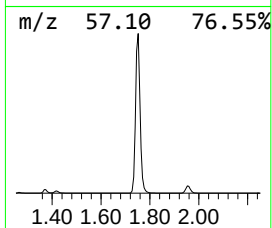
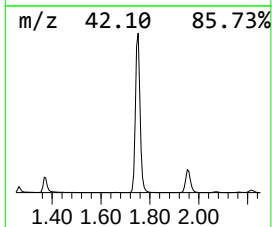
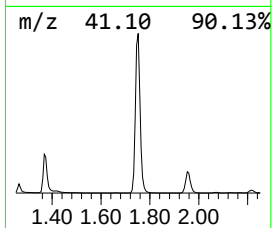
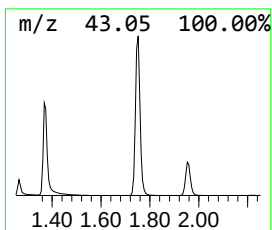
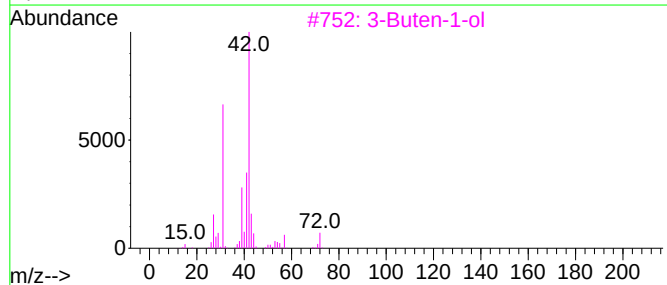
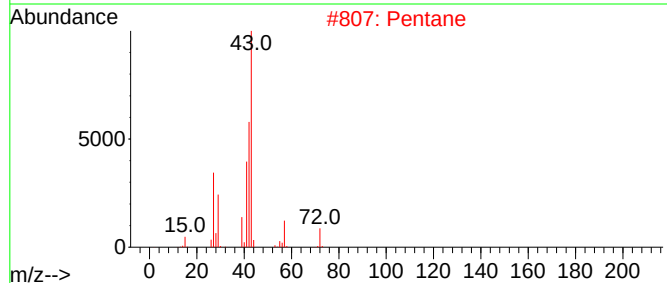
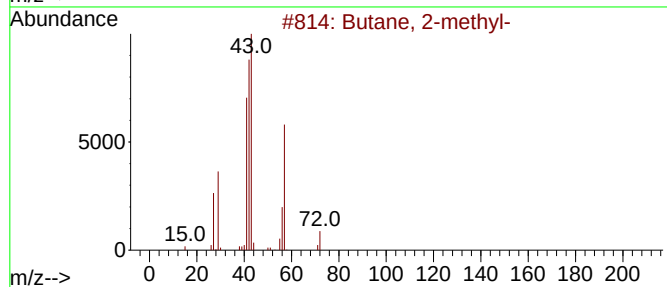
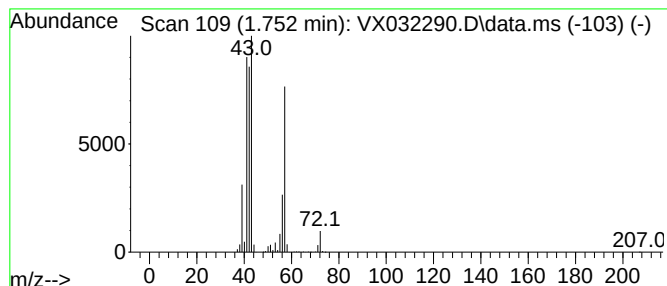
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	1173.79 ug/l	10687900	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	42
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5			1-Butene	56	C4H8	000106-98-9	10



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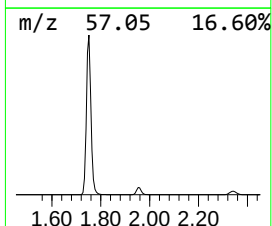
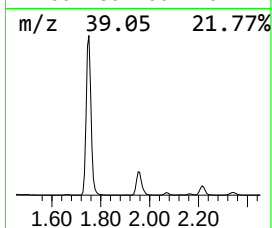
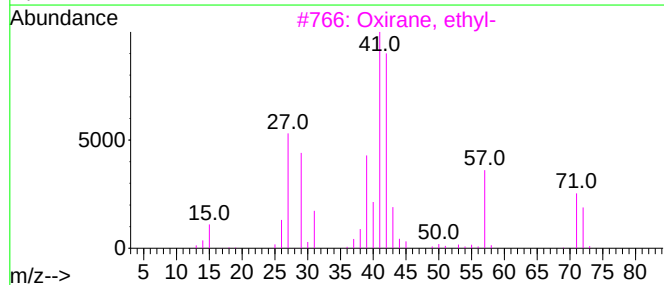
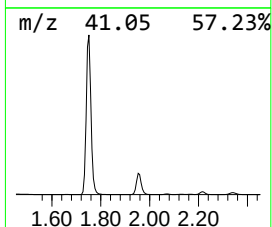
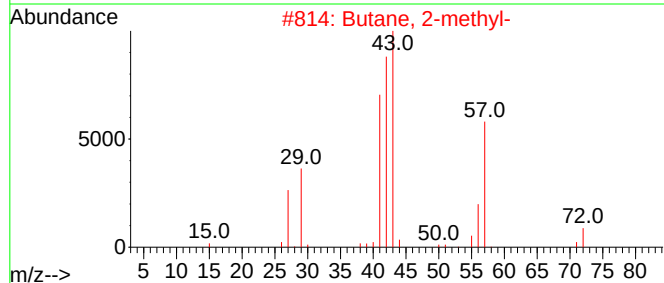
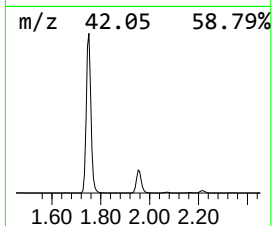
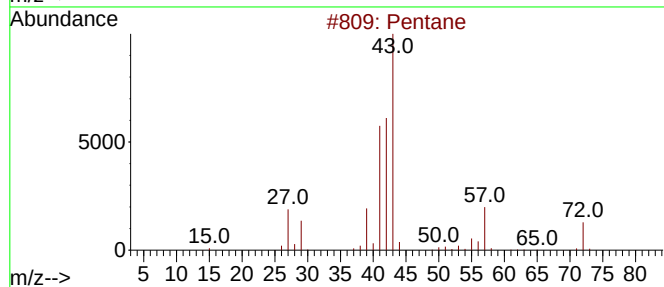
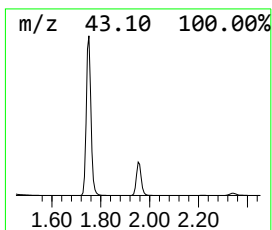
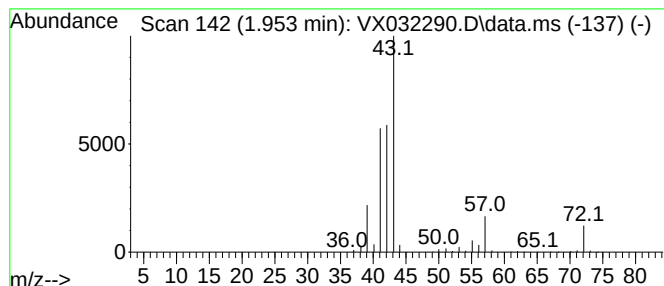
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Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	176.11 ug/l	1603580	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	53
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Cyclobutylamine	71	C4H9N	002516-34-9	9



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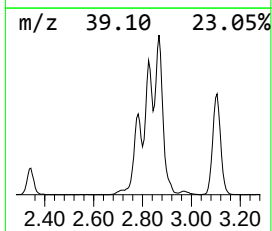
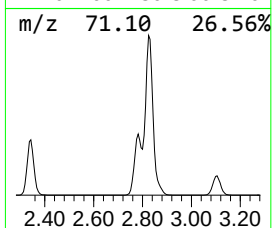
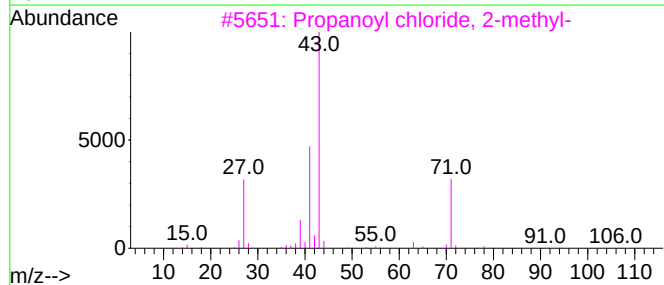
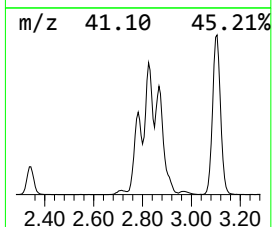
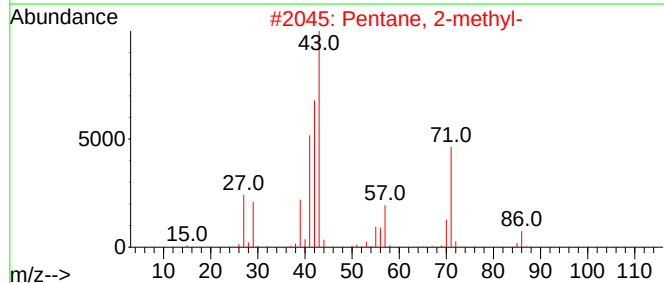
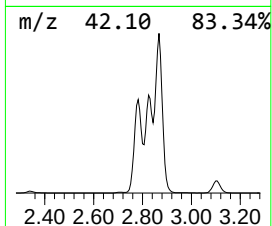
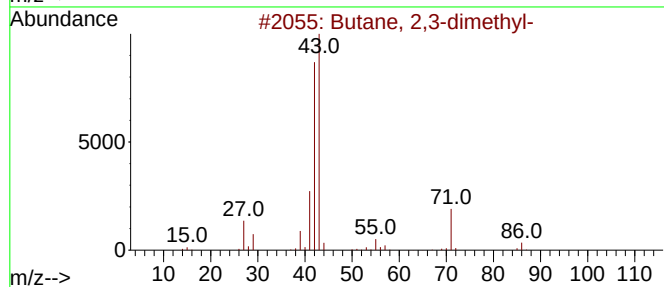
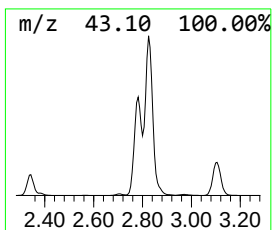
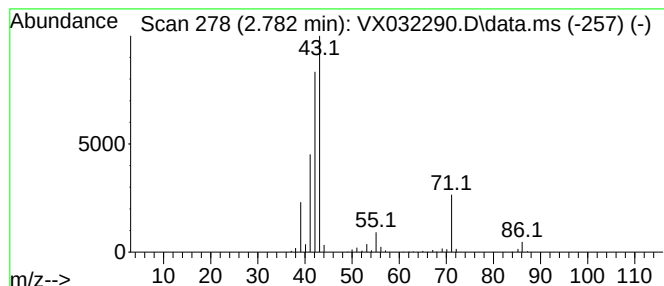
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	96.59 ug/l	879469	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5			Pyrrolidine	71	C4H9N	000123-75-1	9



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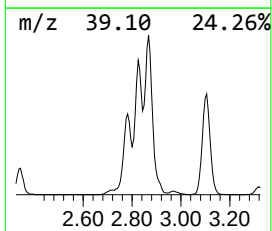
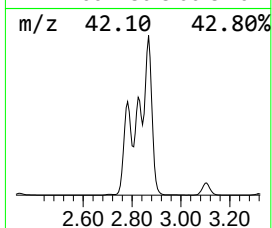
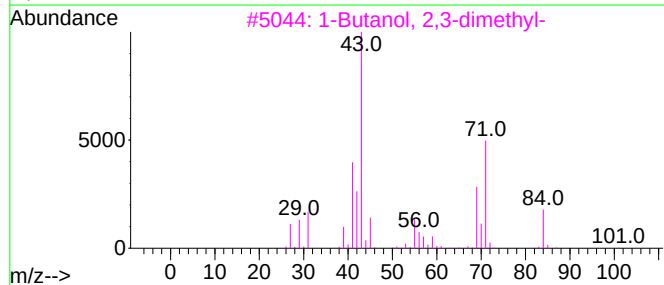
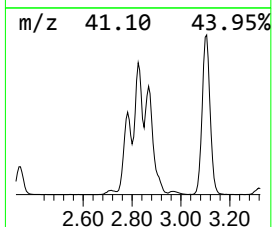
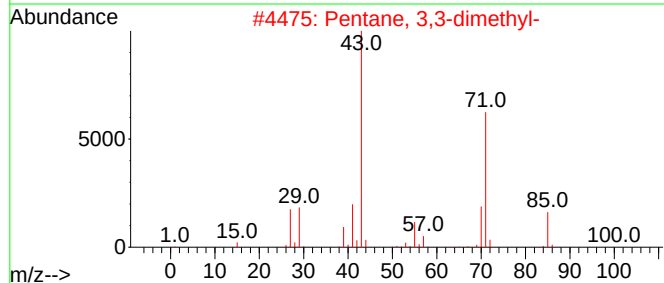
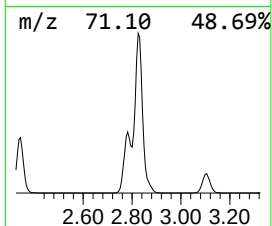
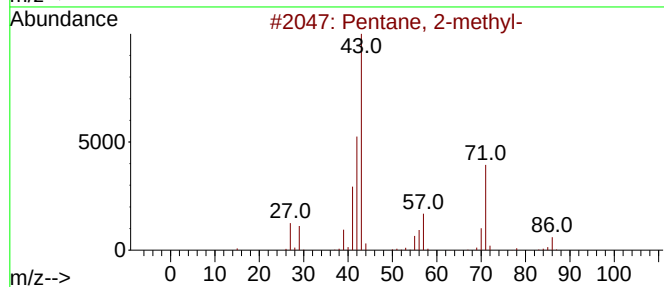
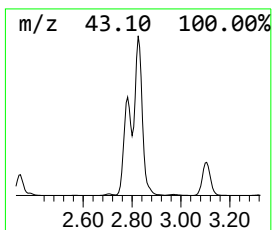
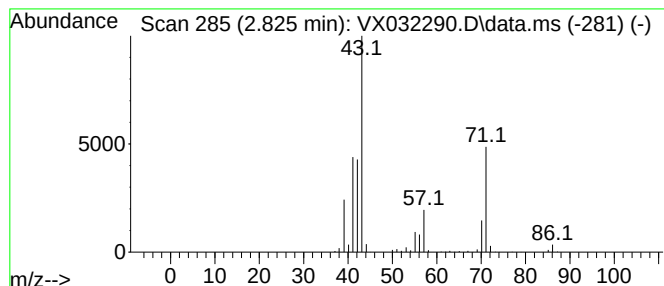
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	148.47 ug/l	1351870	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	39
4			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

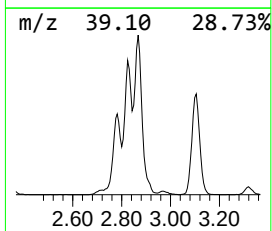
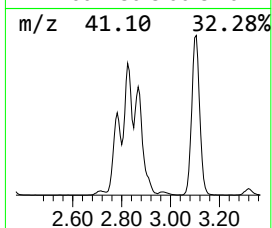
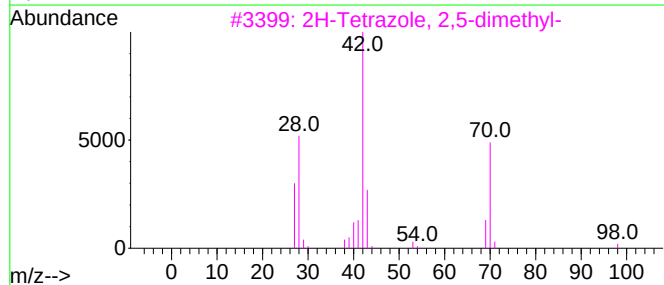
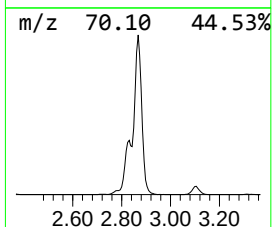
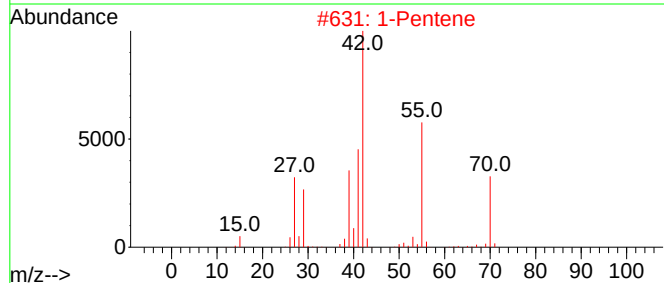
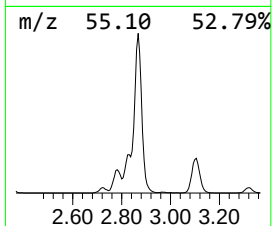
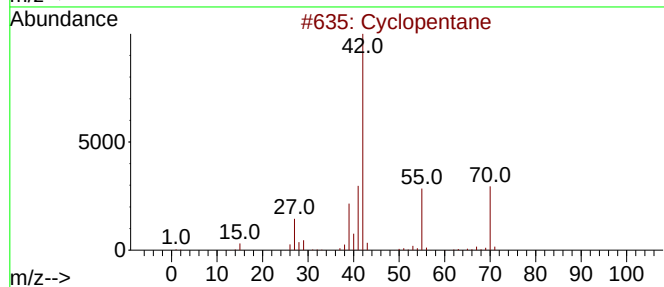
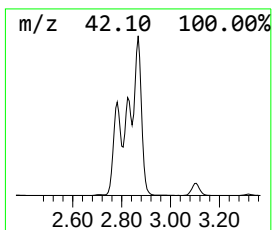
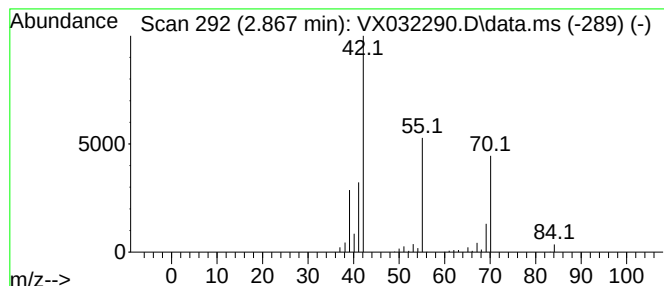
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	114.77 ug/l	1045020	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			1-Pentene	70	C5H10	000109-67-1	72
3			2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	40
4			2-Pentene	70	C5H10	000109-68-2	37
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

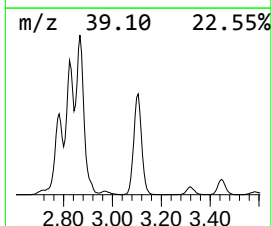
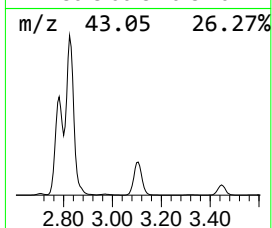
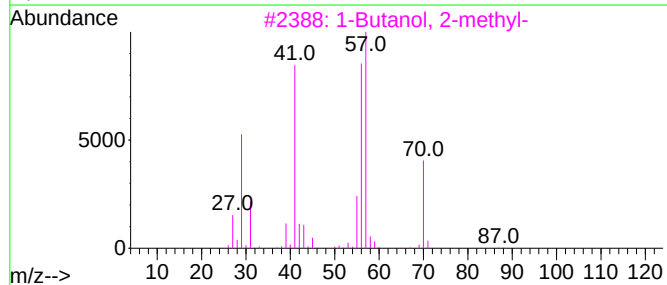
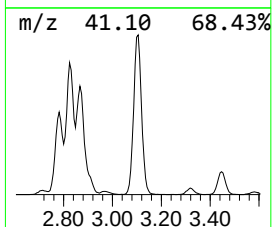
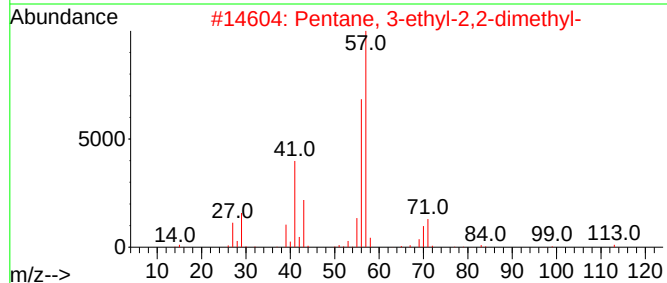
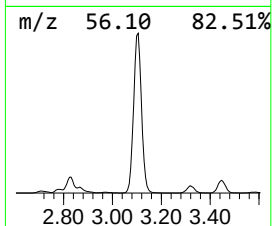
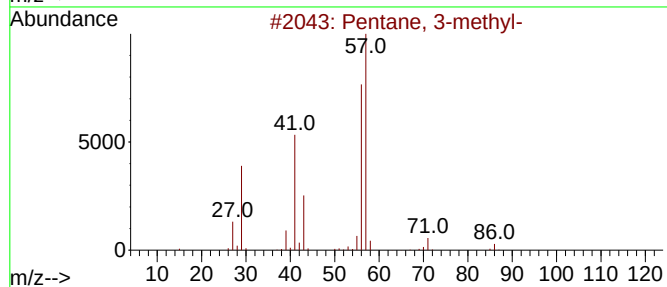
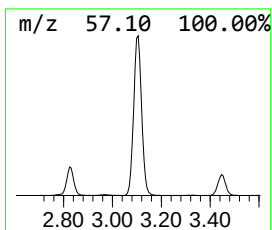
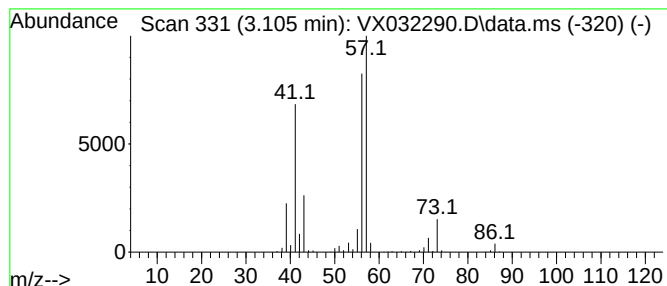
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	144.43 ug/l	1315100	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
3			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	39
4			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	39
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

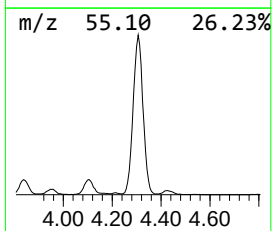
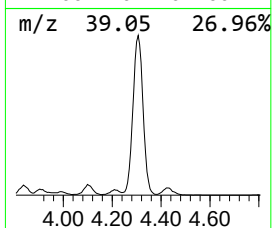
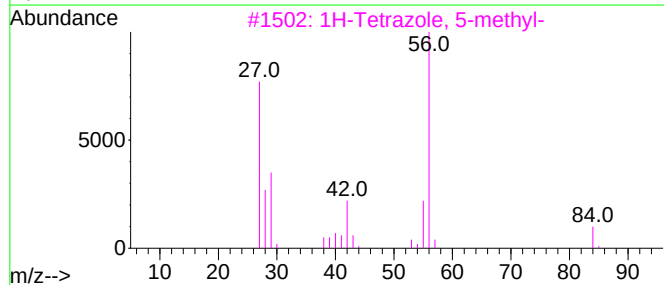
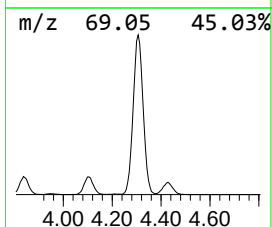
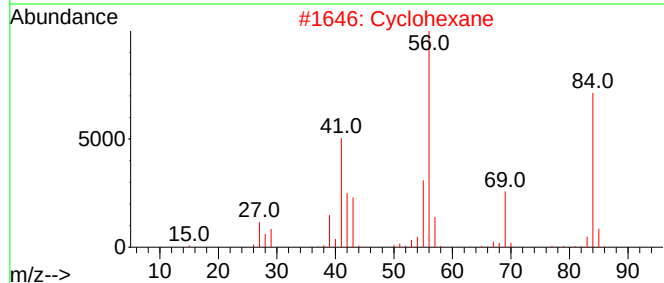
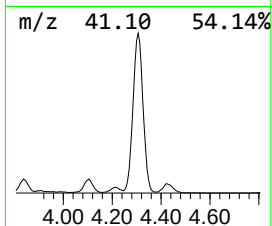
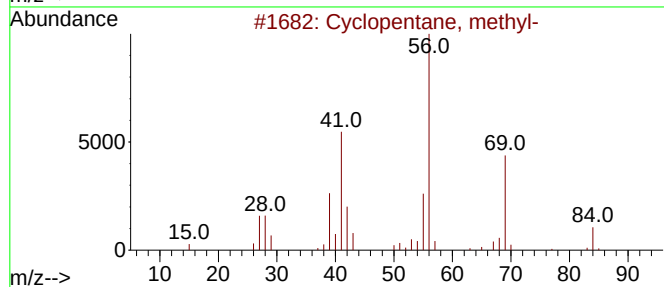
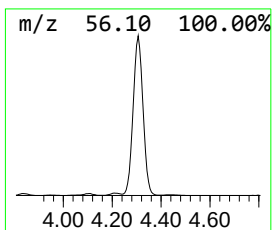
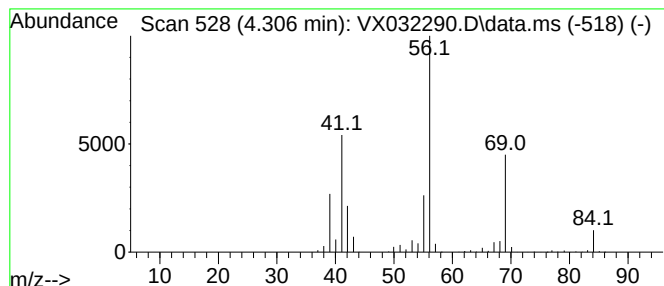
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	261.38 ug/l	2379990	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

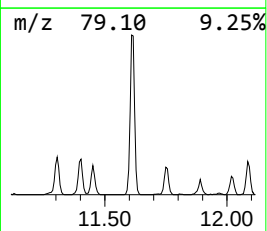
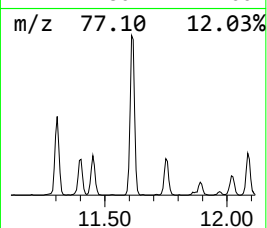
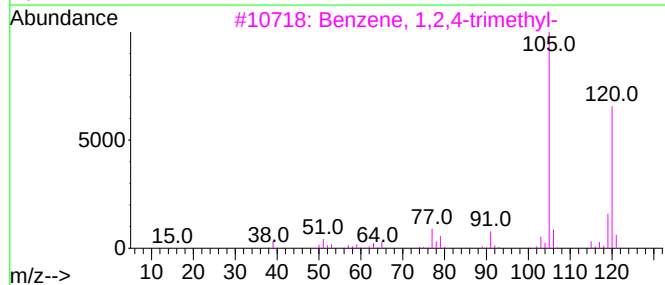
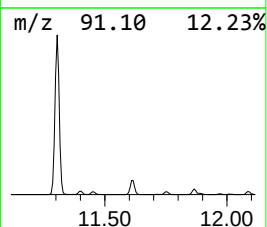
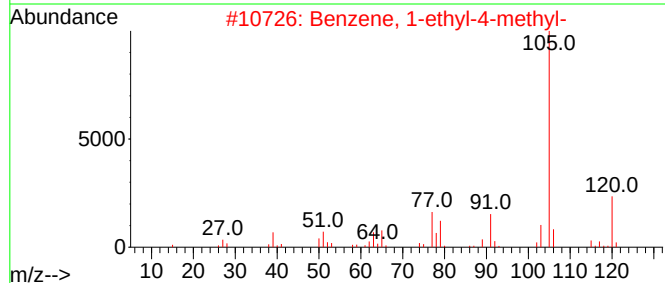
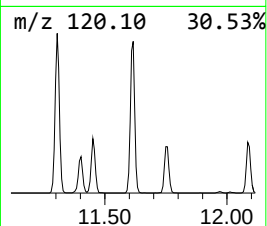
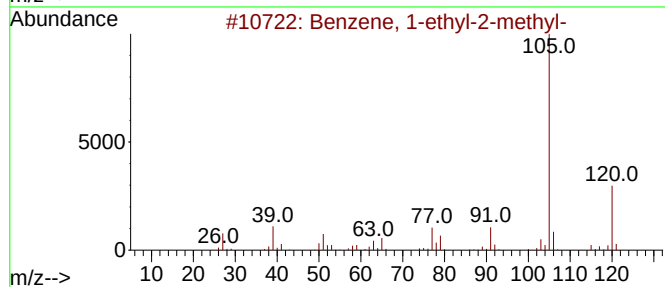
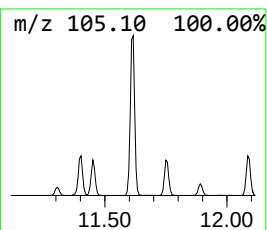
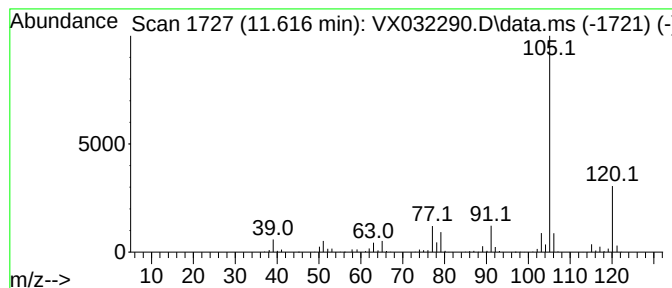
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	55.79 ug/l	657060	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

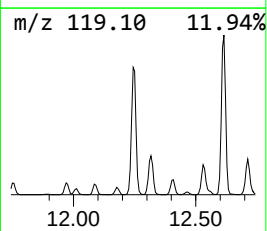
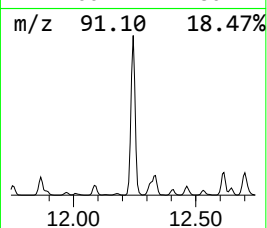
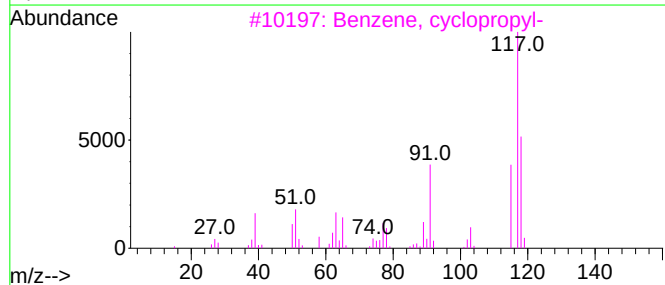
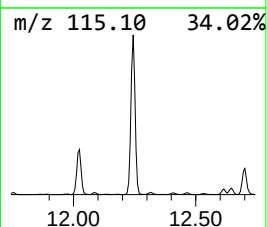
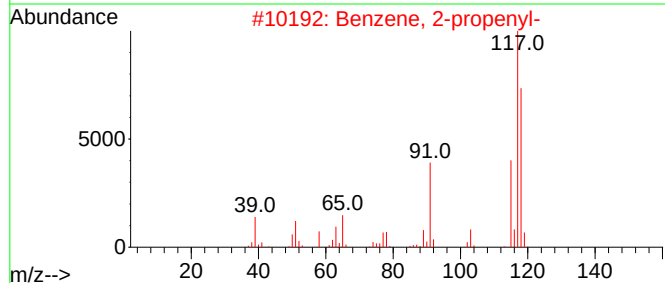
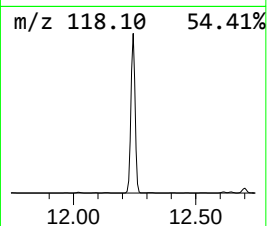
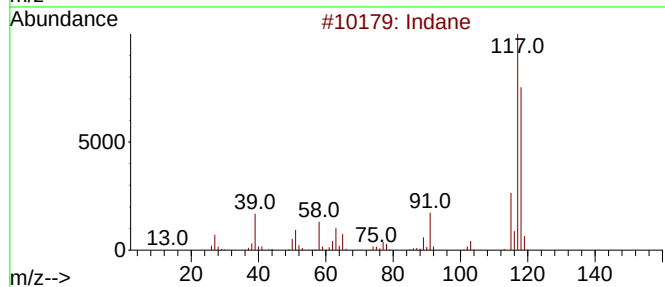
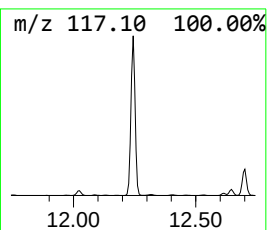
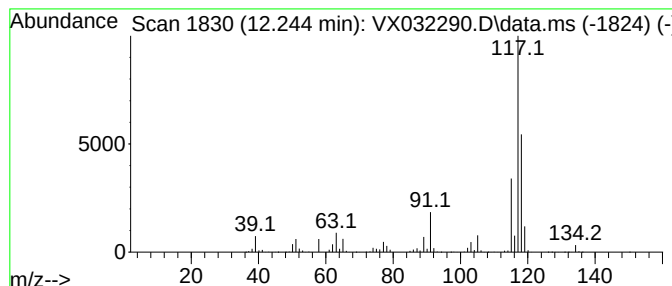
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	164.28 ug/l	1934890	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Deltacyclene	118	C9H10	007785-10-6	68
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032290.D
Acq On : 21 Oct 2022 15:49
Operator : JC/MD
Sample : N5185-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.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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Butane, 2-methyl-	1.752	1173.8	ug/l	10687900	1	5.556	455274	50.0
Pentane	1.953	176.1	ug/l	1603580	1	5.556	455274	50.0
Butane, 2,3-dim...	2.782	96.6	ug/l	879469	1	5.556	455274	50.0
Pentane, 2-methyl-	2.825	148.5	ug/l	1351870	1	5.556	455274	50.0
Cyclopentane	2.867	114.8	ug/l	1045020	1	5.556	455274	50.0
Pentane, 3-methyl-	3.105	144.4	ug/l	1315100	1	5.556	455274	50.0
Cyclopentane, m...	4.306	261.4	ug/l	2379990	1	5.556	455274	50.0
Benzene, 1-ethy...	11.616	55.8	ug/l	657060	4	12.024	588920	50.0
Indane	12.244	164.3	ug/l	1934890	4	12.024	588920	50.0