

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
 Data File : VX032289.D
 Acq On : 21 Oct 2022 15:25
 Operator : JC/MD
 Sample : N5185-21
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RW-01

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: VX032289.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	26	29	43	rBV	454990	511541	4.41%	1.202%
2	1.368	43	46	65	rVV	2315943	2902492	25.03%	6.821%
3	1.752	103	109	127	rVB	8982936	11595384	100.00%	27.248%
4	1.953	137	142	154	rVB	1120939	1671002	14.41%	3.927%
5	2.215	180	185	195	rVB	300512	444543	3.83%	1.045%
6	2.343	198	206	220	rVB	145153	298926	2.58%	0.702%
7	2.782	260	278	281	rBV	397626	907725	7.83%	2.133%
8	2.825	281	285	289	rVV	657173	1392755	12.01%	3.273%
9	2.867	289	292	304	rVB	582474	1146380	9.89%	2.694%
10	3.105	320	331	347	rVB2	590990	1347733	11.62%	3.167%
11	3.446	378	387	401	rBV	83969	185061	1.60%	0.435%
12	3.733	426	434	443	rVB	84337	200457	1.73%	0.471%
13	3.837	443	451	457	rBV	54073	134045	1.16%	0.315%
14	4.105	485	495	504	rVB2	56379	143309	1.24%	0.337%
15	4.306	518	528	540	rVB	904351	2558219	22.06%	6.012%
16	5.196	647	674	688	rBV	46998	182070	1.57%	0.428%
17	5.385	694	705	712	rBV	83777	253518	2.19%	0.596%
18	5.477	712	720	727	rVV2	172180	577164	4.98%	1.356%
19	5.556	727	733	739	rVV	157477	461213	3.98%	1.084%
20	5.623	740	744	764	rVB3	71345	210515	1.82%	0.495%
21	5.824	766	777	790	rBV5	42448	138112	1.19%	0.325%
22	5.958	790	799	804	rVV	90793	229979	1.98%	0.540%
23	6.037	804	812	824	rVV	516108	1392479	12.01%	3.272%
24	6.165	824	833	841	rVV3	63363	260217	2.24%	0.611%
25	6.257	842	848	857	rVV3	85922	260272	2.24%	0.612%
26	6.361	857	865	878	rVB3	48738	141683	1.22%	0.333%
27	6.763	921	931	939	rBV	224291	550189	4.74%	1.293%
28	7.379	1019	1032	1044	rBV3	141565	393836	3.40%	0.925%
29	8.647	1235	1240	1247	rVB	433645	687918	5.93%	1.617%
30	10.055	1460	1471	1476	rBV	452832	621487	5.36%	1.460%
31	10.195	1488	1494	1500	rVB	1487144	1891404	16.31%	4.445%
32	10.305	1506	1512	1518	rVB	494206	656546	5.66%	1.543%
33	10.963	1613	1620	1626	rBV	313399	378061	3.26%	0.888%
34	11.079	1634	1639	1645	rBV	375315	482419	4.16%	1.134%
35	11.305	1671	1676	1683	rVB	611254	744938	6.42%	1.751%
36	11.402	1686	1692	1696	rVV	143655	180494	1.56%	0.424%

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37	11.451	1696	1700	1707	rVB	154616	183990	1.59%	0.432%
38	11.616	1721	1727	1734	rVB	550200	699338	6.03%	1.643%
39	11.750	1745	1749	1755	rVB	147786	179389	1.55%	0.422%
40	12.024	1789	1794	1800	rVB	479597	600500	5.18%	1.411%
41	12.091	1800	1805	1810	rBV	146016	189105	1.63%	0.444%
42	12.244	1824	1830	1837	rBV	1691623	2067900	17.83%	4.859%
43	12.311	1837	1841	1852	rVB3	104194	174690	1.51%	0.411%
44	12.463	1861	1866	1872	rVB	123371	150896	1.30%	0.355%
45	12.615	1885	1891	1894	rBV	206138	244507	2.11%	0.575%
46	12.701	1900	1905	1913	rVB2	240845	343953	2.97%	0.808%
47	12.920	1934	1941	1945	rBV	199209	237310	2.05%	0.558%
48	13.170	1978	1982	1992	rVB	179637	211846	1.83%	0.498%
49	13.292	1992	2002	2007	rBV2	434453	565677	4.88%	1.329%
50	13.774	2076	2081	2091	rBV	454784	571370	4.93%	1.343%

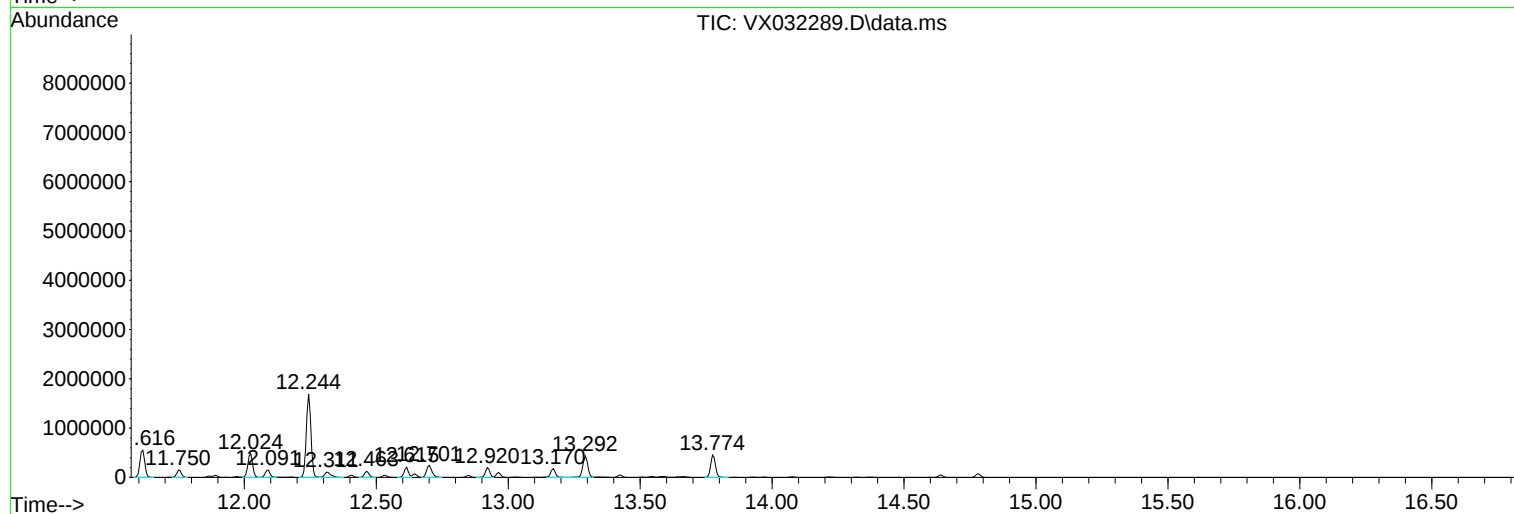
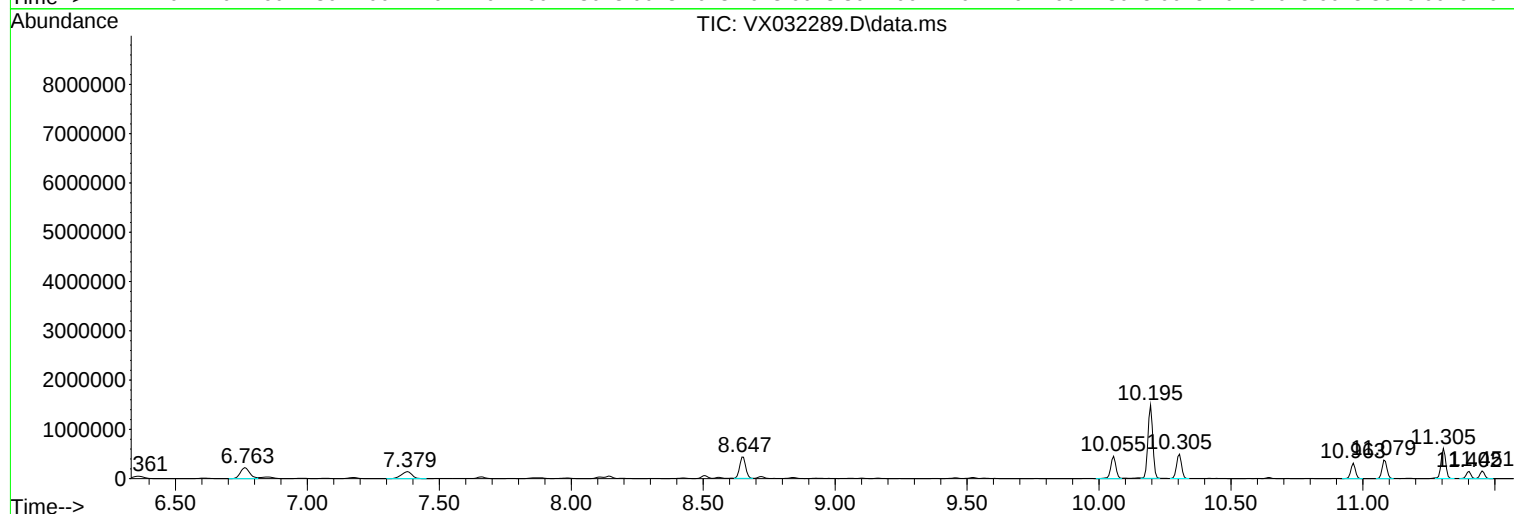
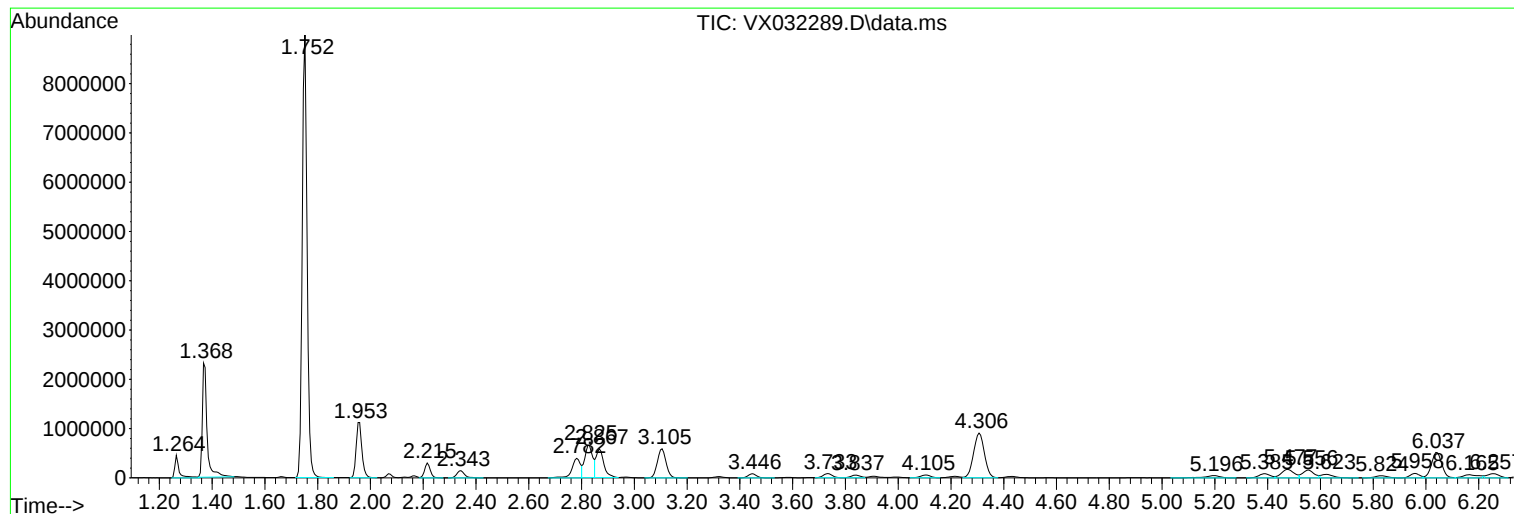
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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



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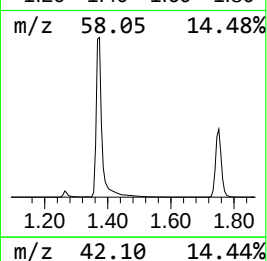
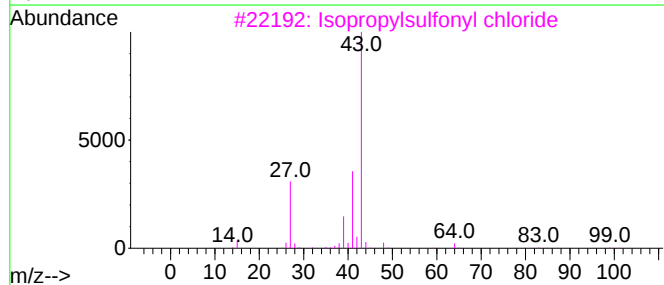
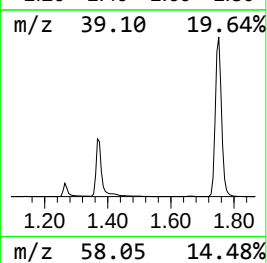
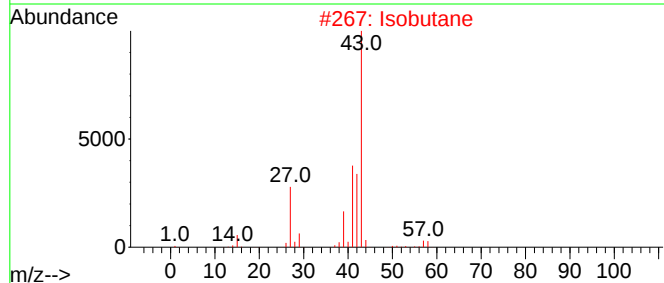
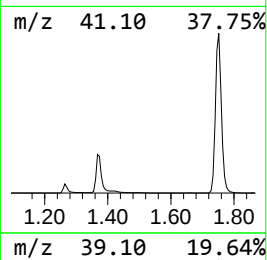
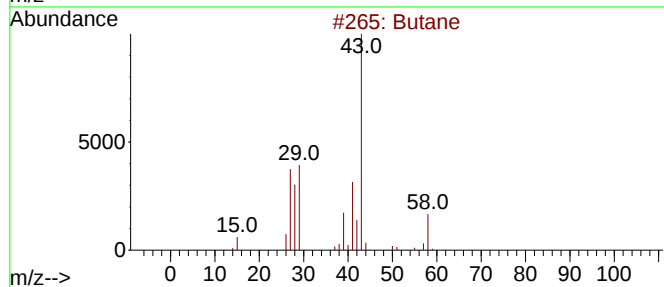
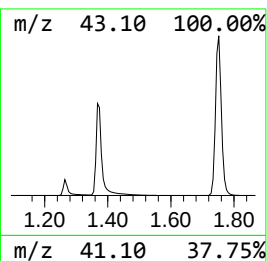
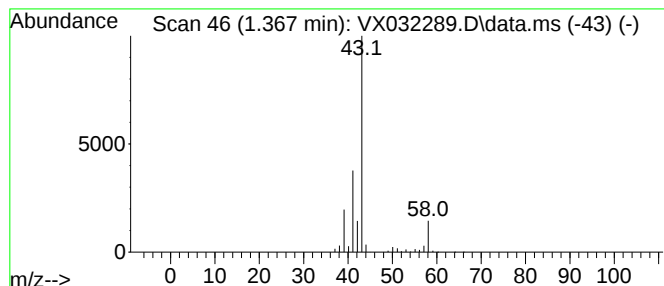
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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.
1.367	314.66 ug/l	2902490	Pentafluorobenzene	5.550

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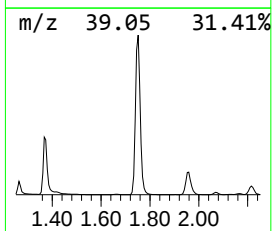
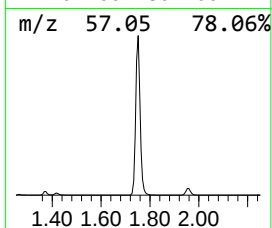
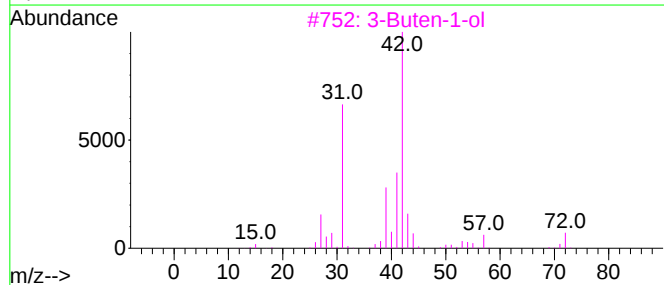
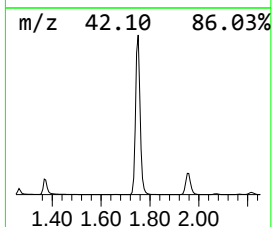
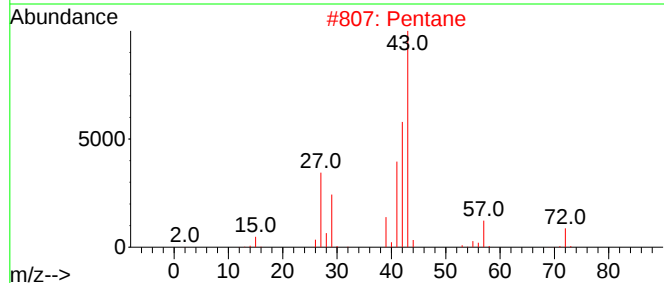
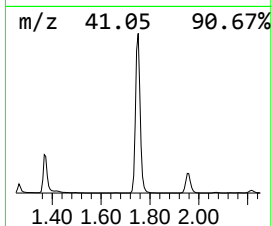
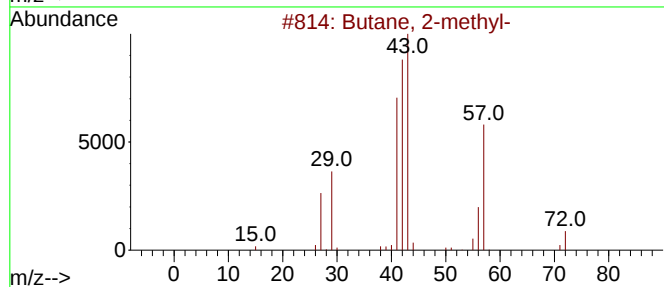
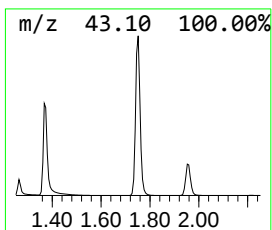
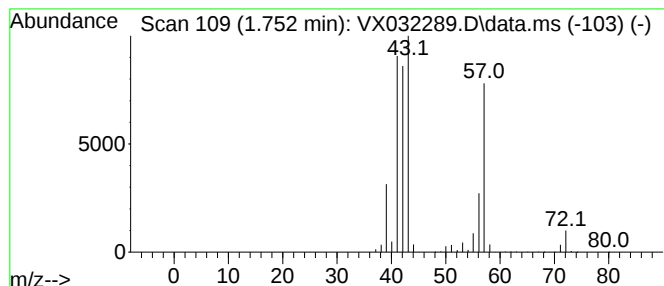
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X101922W.M
Quant Title : SW846 8260

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	1257.05 ug/l	11595400	Pentafluorobenzene	5.550

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			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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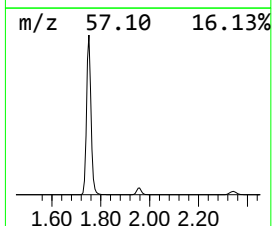
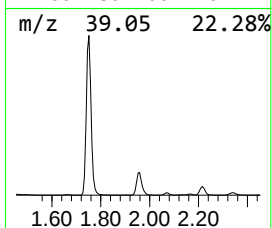
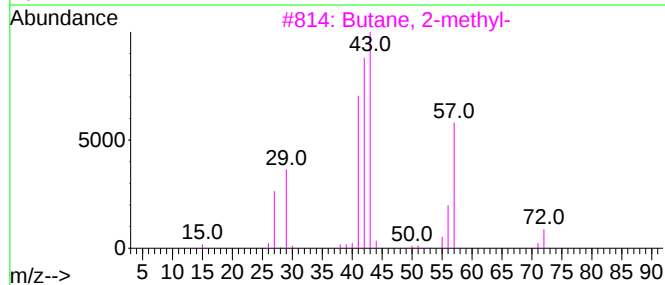
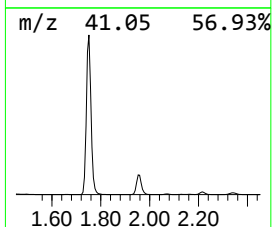
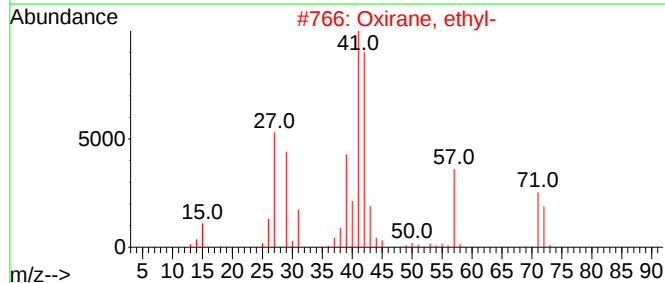
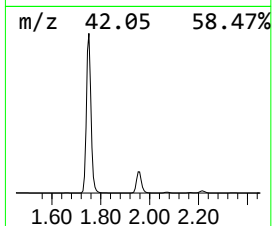
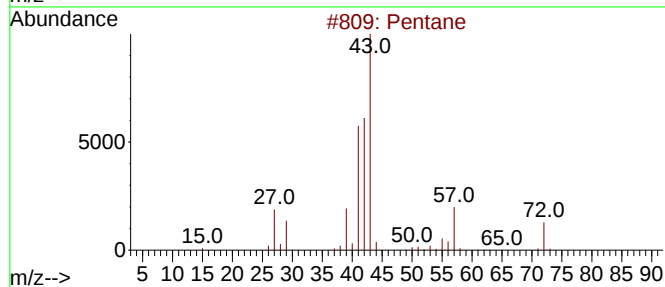
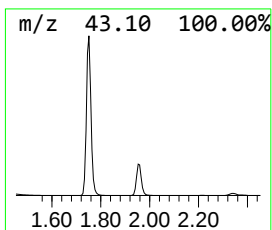
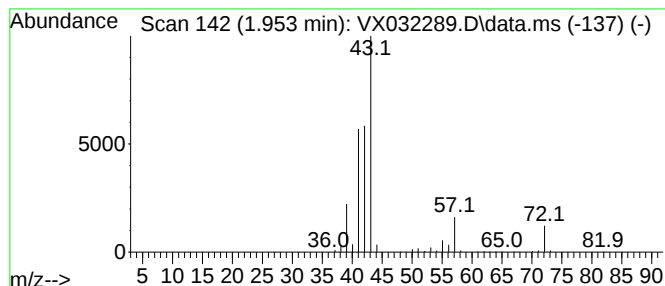
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Quant Title : SW846 8260

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	181.15 ug/l	1671000	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Butane, 2-methyl-	72	C5H12	000078-78-4	38
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	9



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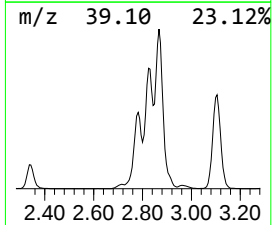
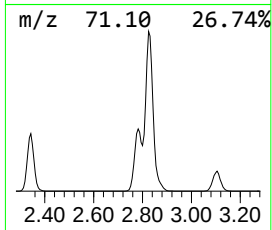
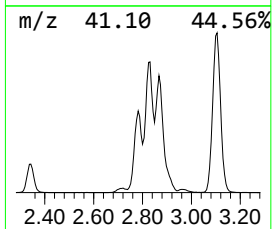
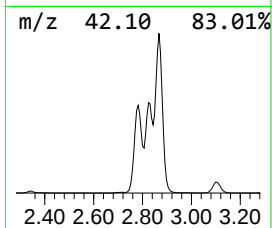
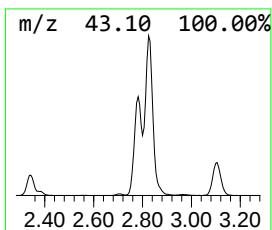
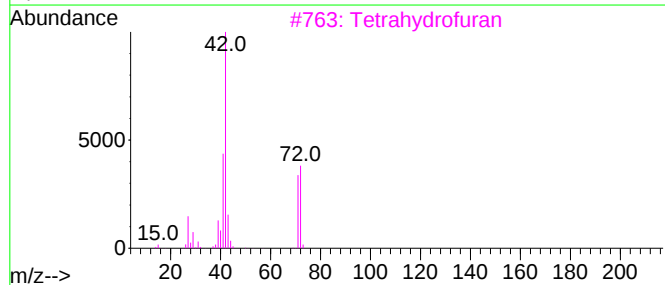
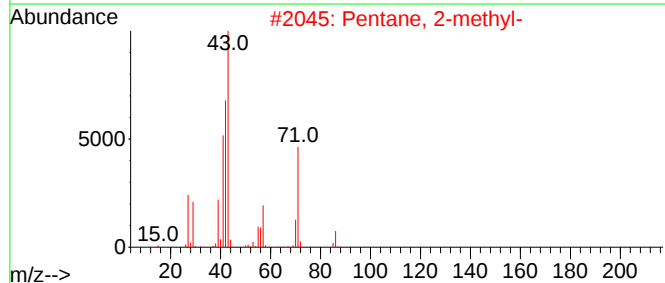
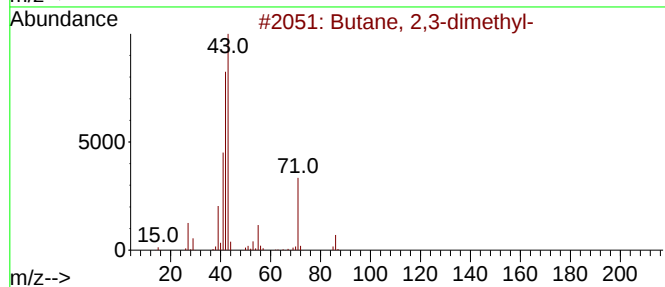
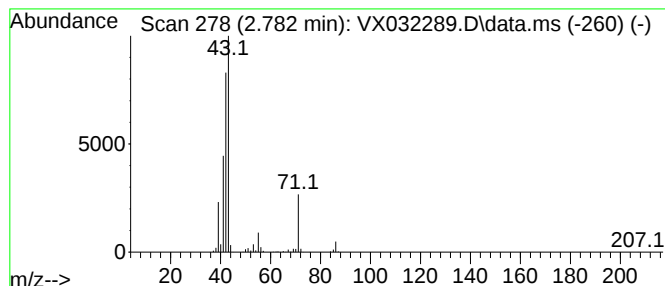
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	98.41 ug/l	907725	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3			Tetrahydrofuran	72	C4H8O	000109-99-9	38
4			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	12
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	10



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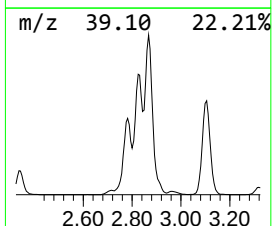
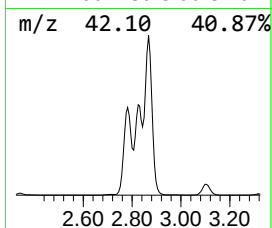
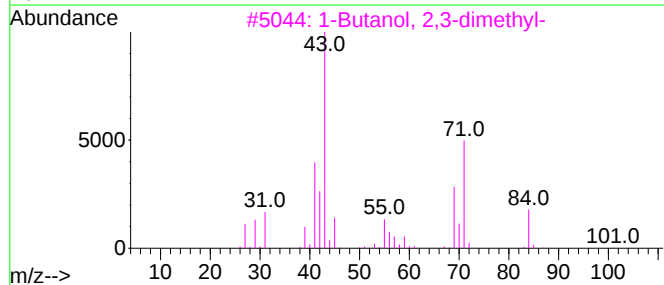
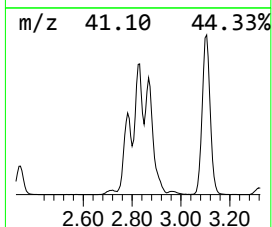
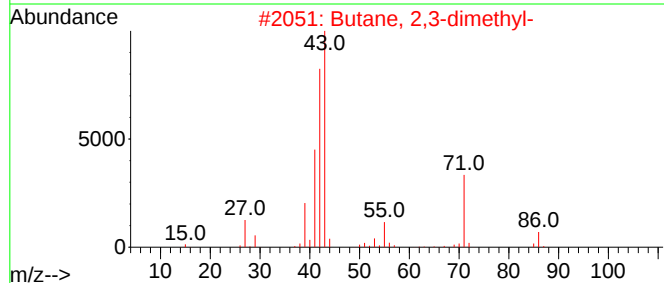
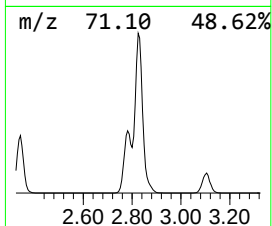
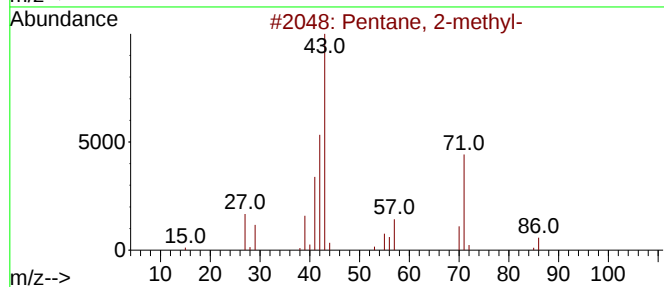
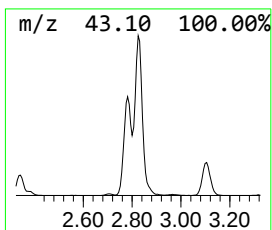
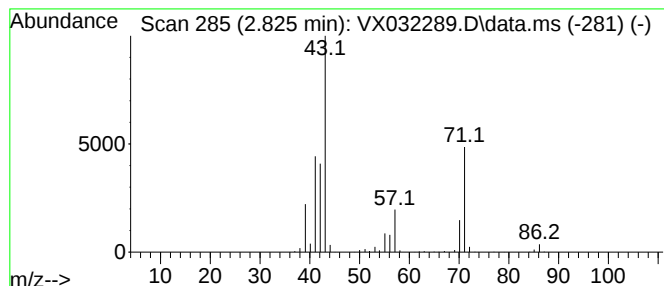
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	150.99 ug/l	1392760	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

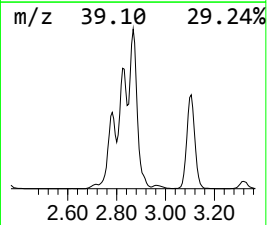
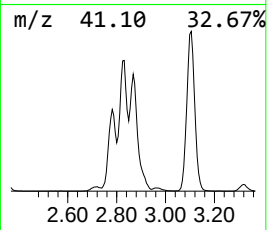
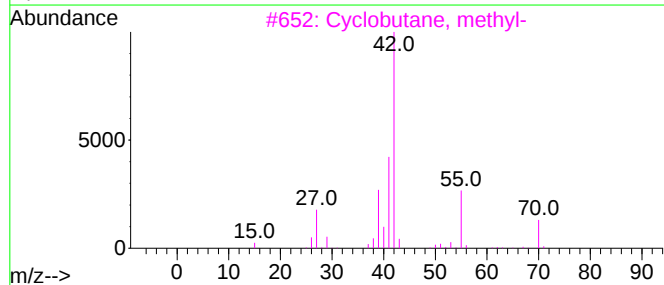
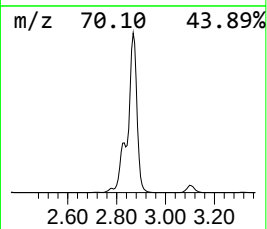
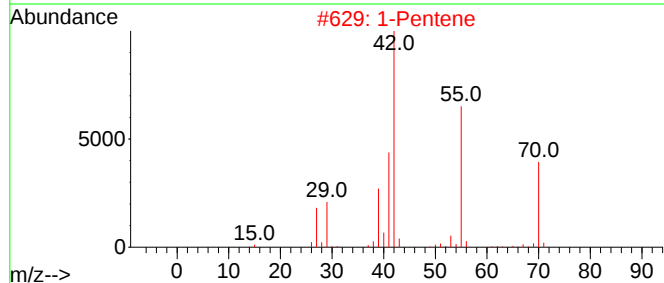
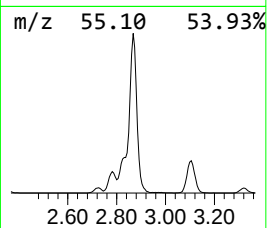
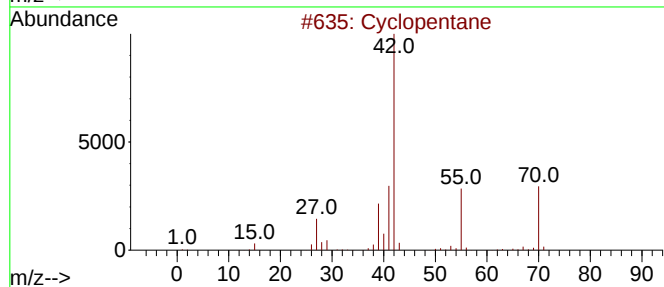
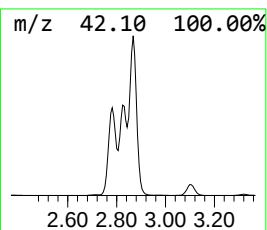
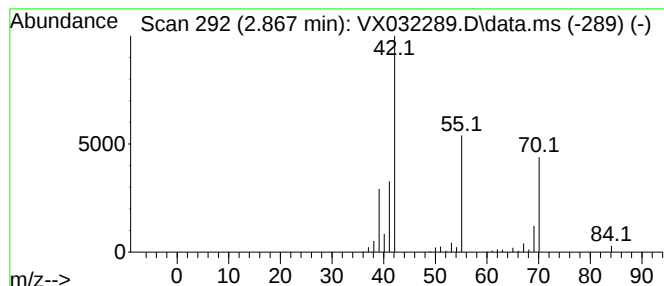
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Quant Title : SW846 8260

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	124.28 ug/l	1146380	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			1-Pentene	70	C5H10	000109-67-1	80
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	50
4			2-Pentene	70	C5H10	000109-68-2	43
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

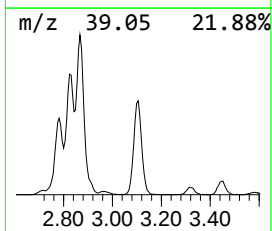
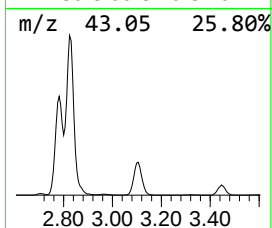
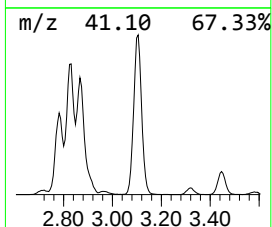
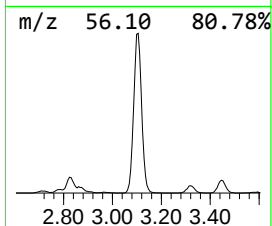
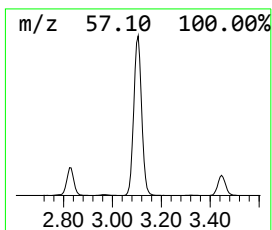
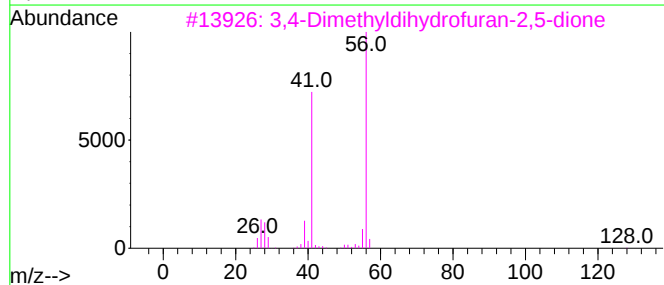
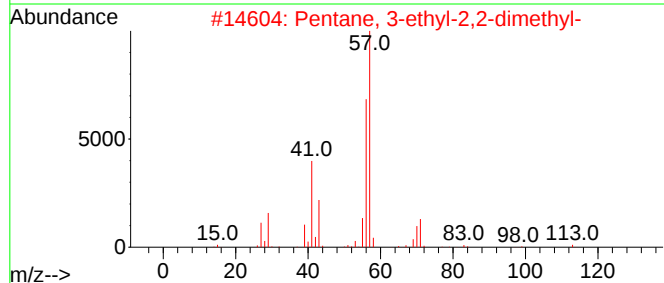
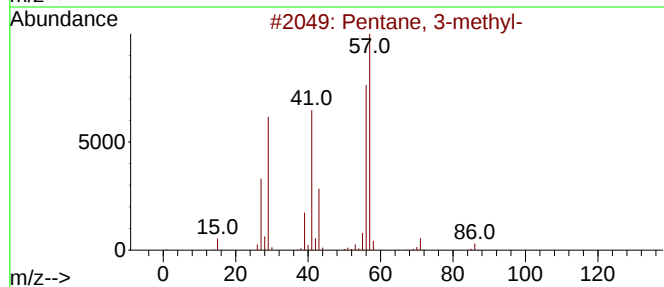
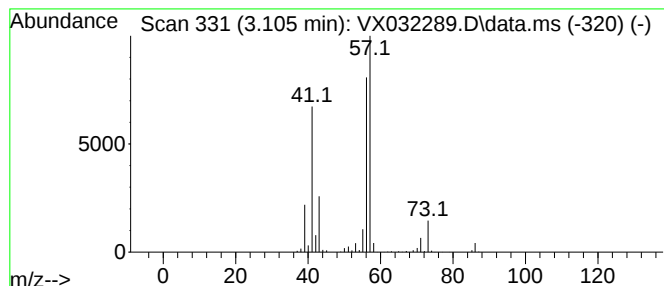
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Quant Title : SW846 8260

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	146.11 ug/l	1347730	Pentafluorobenzene	5.550

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			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
4			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	40
5			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

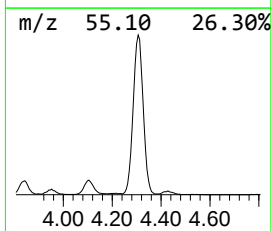
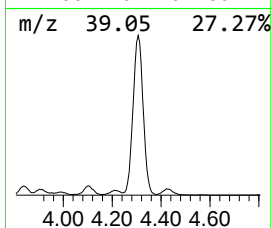
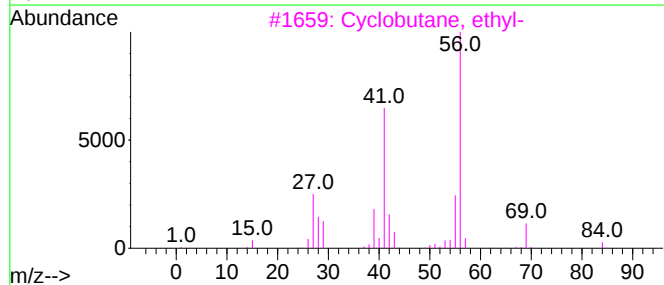
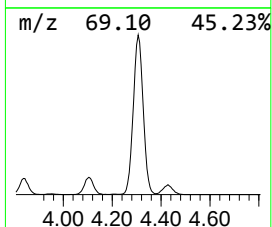
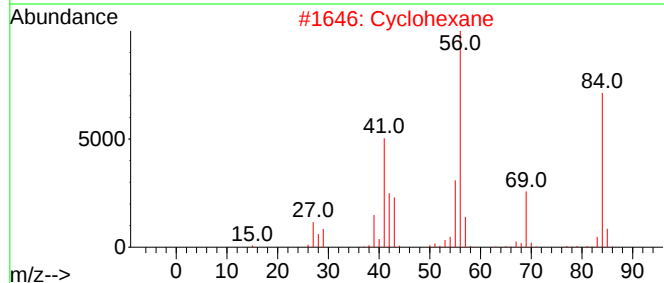
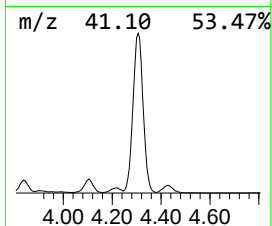
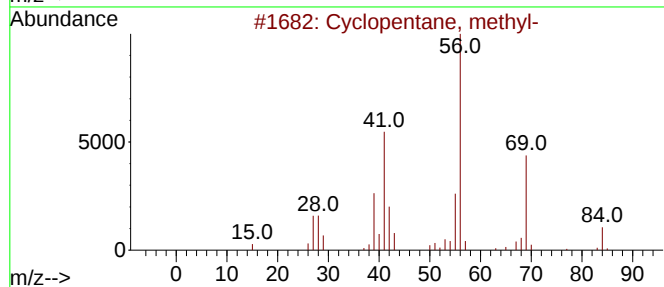
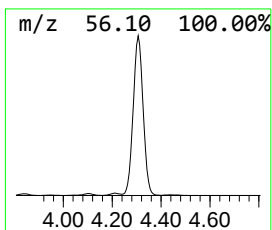
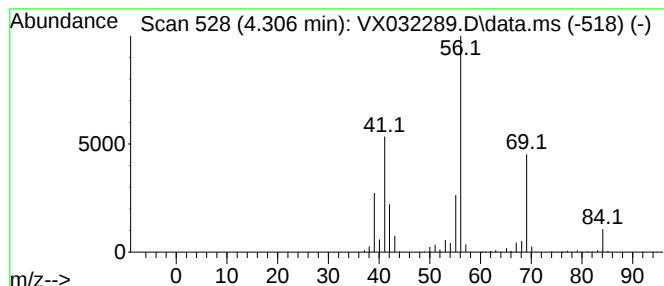
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Quant Title : SW846 8260

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	277.34 ug/l	2558220	Pentafluorobenzene	5.550

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			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclobutane	56	C4H8	000287-23-0	53
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

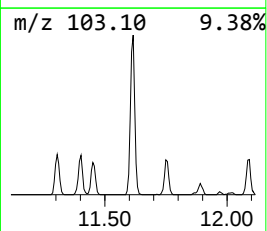
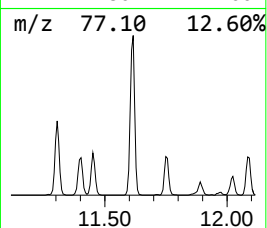
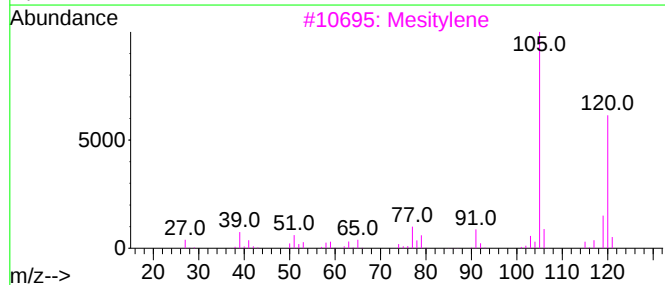
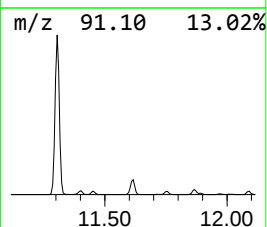
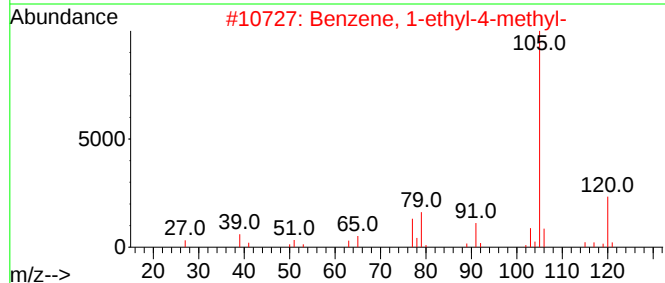
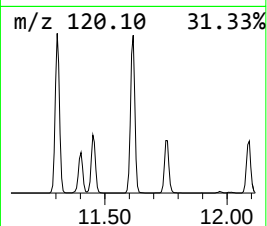
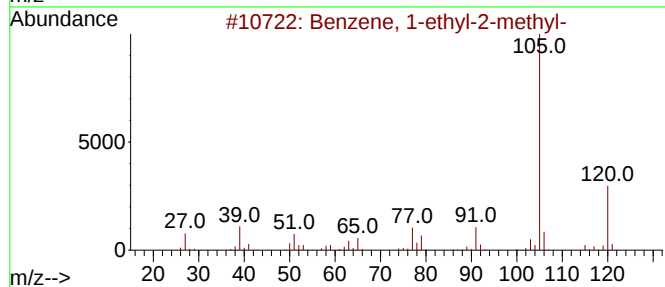
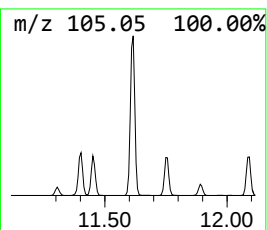
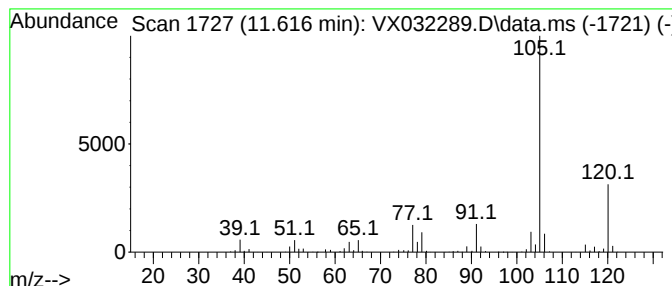
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Quant Title : SW846 8260

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	58.23 ug/l	699338	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			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

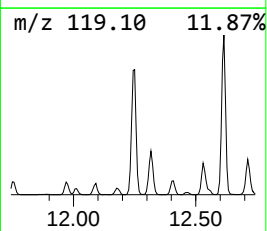
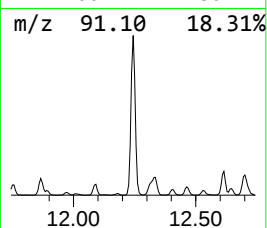
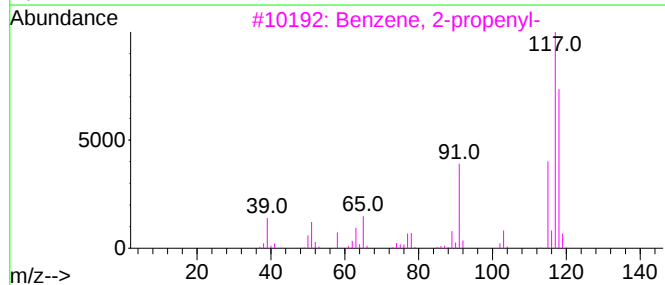
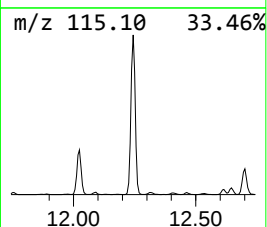
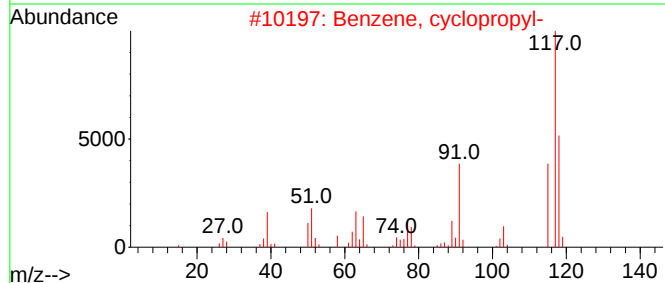
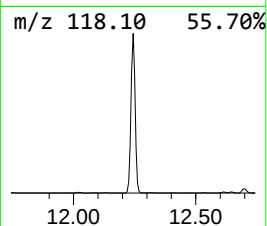
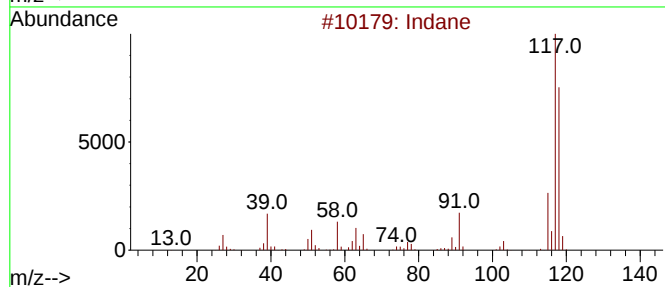
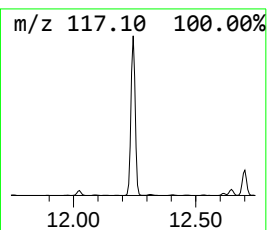
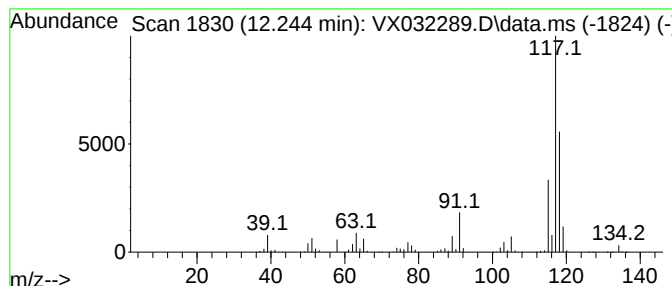
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Quant Title : SW846 8260

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	172.18 ug/l	2067900	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, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4			Delta-cyclene	118	C9H10	007785-10-6	68
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102122\
Data File : VX032289.D
Acq On : 21 Oct 2022 15:25
Operator : JC/MD
Sample : N5185-21
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-01

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	1257.1	ug/l	11595400	1	5.550	461213	50.0
Pentane	1.953	181.2	ug/l	1671000	1	5.550	461213	50.0
Butane, 2,3-dim...	2.782	98.4	ug/l	907725	1	5.550	461213	50.0
Pentane, 2-methyl-	2.825	151.0	ug/l	1392760	1	5.550	461213	50.0
Cyclopentane	2.867	124.3	ug/l	1146380	1	5.550	461213	50.0
Pentane, 3-methyl-	3.105	146.1	ug/l	1347730	1	5.550	461213	50.0
Cyclopentane, m...	4.306	277.3	ug/l	2558220	1	5.550	461213	50.0
Benzene, 1-ethy...	11.616	58.2	ug/l	699338	4	12.024	600500	50.0
Indane	12.244	172.2	ug/l	2067900	4	12.024	600500	50.0