

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
 Data File : VX033043.D
 Acq On : 24 Nov 2022 06:50
 Operator : JC/MD
 Sample : N5741-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-35

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033043.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	42	rBV	138247	228617	14.18%	3.757%
2	1.374	42	47	54	rVB	19265	23009	1.43%	0.378%
3	1.752	105	109	121	rVB	29312	39375	2.44%	0.647%
4	2.221	180	186	194	rVB	20638	32310	2.00%	0.531%
5	2.752	264	273	283	rBV2	9422	28833	1.79%	0.474%
6	2.867	284	292	302	rVV	23783	53923	3.34%	0.886%
7	2.989	302	312	325	rVV2	24702	97996	6.08%	1.610%
8	3.111	325	332	342	rVB	42411	97822	6.07%	1.608%
9	3.758	426	438	447	rBV4	11492	35592	2.21%	0.585%
10	4.306	518	528	539	rBV3	21185	62159	3.86%	1.022%
11	5.385	693	705	714	rBV2	62440	184517	11.44%	3.032%
12	5.471	714	719	724	rVV3	11033	29599	1.84%	0.486%
13	5.556	724	733	745	rVB	131855	374964	23.26%	6.162%
14	5.958	787	799	804	rBV	69295	179200	11.11%	2.945%
15	6.038	804	812	828	rVB	609228	1612364	100.00%	26.497%
16	6.202	830	839	844	rBV4	7029	19943	1.24%	0.328%
17	6.763	919	931	941	rBV	204494	484736	30.06%	7.966%
18	8.647	1234	1240	1248	rBV	326453	505580	31.36%	8.309%
19	8.720	1248	1252	1260	rVB	12117	19223	1.19%	0.316%
20	8.958	1282	1291	1299	rVB	16690	26928	1.67%	0.443%
21	9.049	1299	1306	1313	rBV	17713	28080	1.74%	0.461%
22	9.458	1364	1373	1385	rVB2	20637	34407	2.13%	0.565%
23	10.055	1465	1471	1483	rVB	407782	564737	35.03%	9.281%
24	10.195	1489	1494	1503	rBV	104655	136183	8.45%	2.238%
25	10.964	1613	1620	1625	rBV	33529	42688	2.65%	0.702%
26	11.079	1634	1639	1649	rBV	275610	353601	21.93%	5.811%
27	11.305	1670	1676	1685	rBV	30759	39448	2.45%	0.648%
28	12.024	1788	1794	1802	rBV	428388	544401	33.76%	8.947%
29	12.244	1825	1830	1836	rBV	98761	124357	7.71%	2.044%
30	12.701	1900	1905	1913	rVB	28540	37308	2.31%	0.613%
31	13.292	1997	2002	2007	rVB2	13481	17653	1.09%	0.290%
32	13.774	2075	2081	2091	rBV	19144	25489	1.58%	0.419%

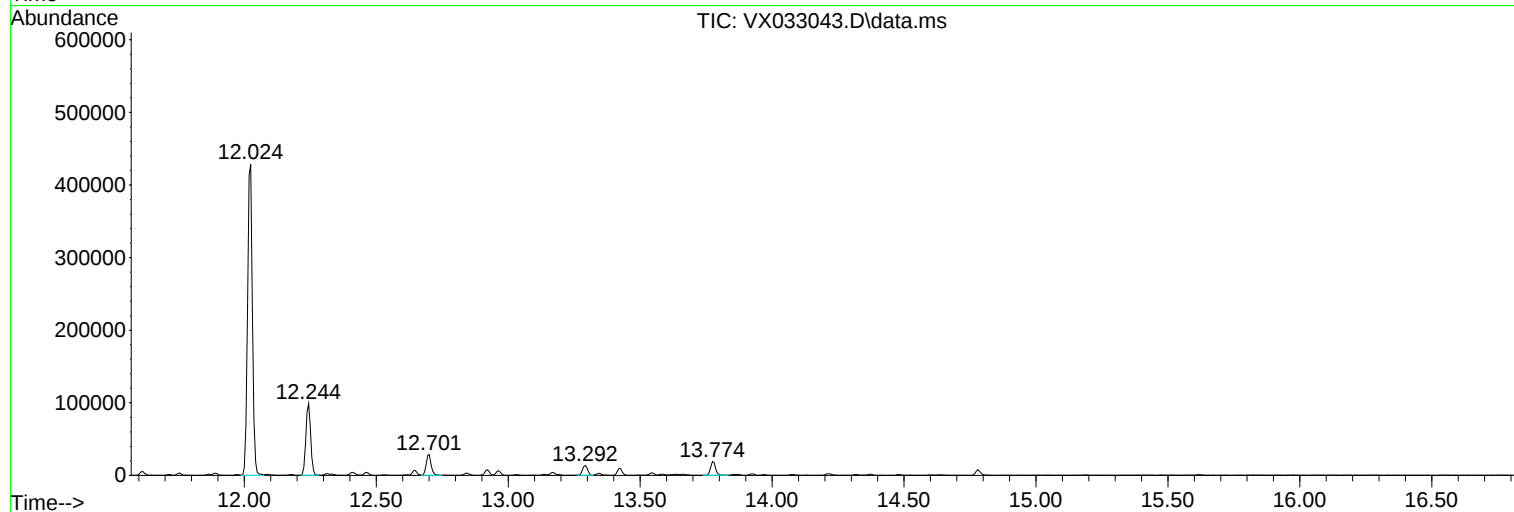
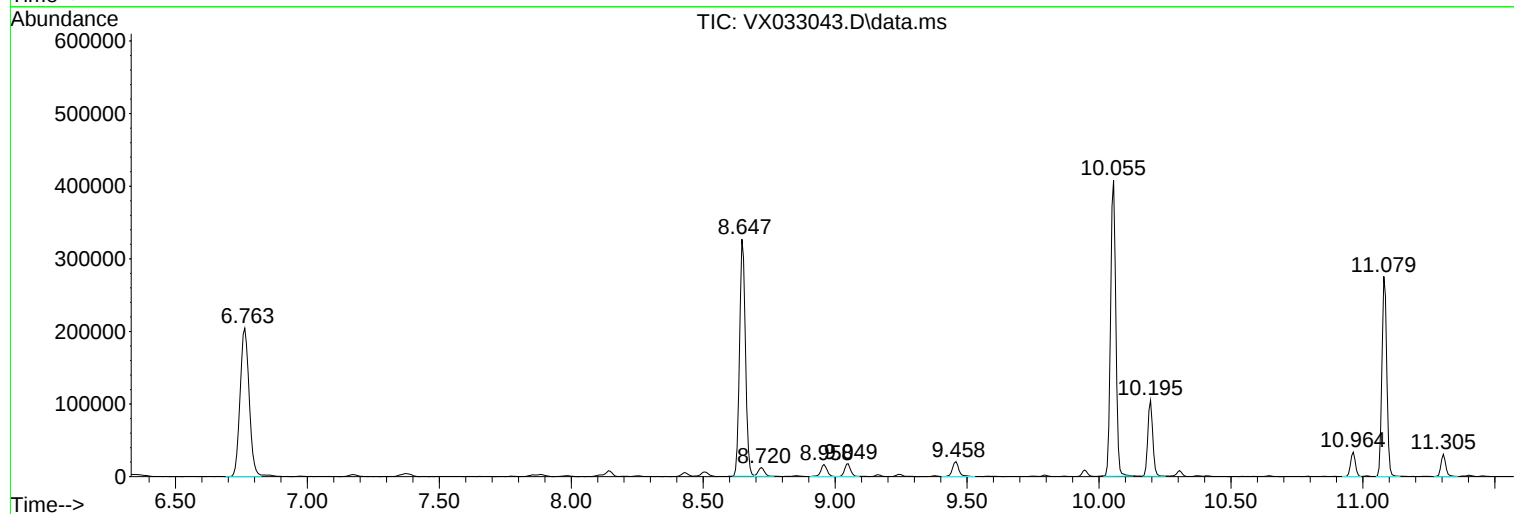
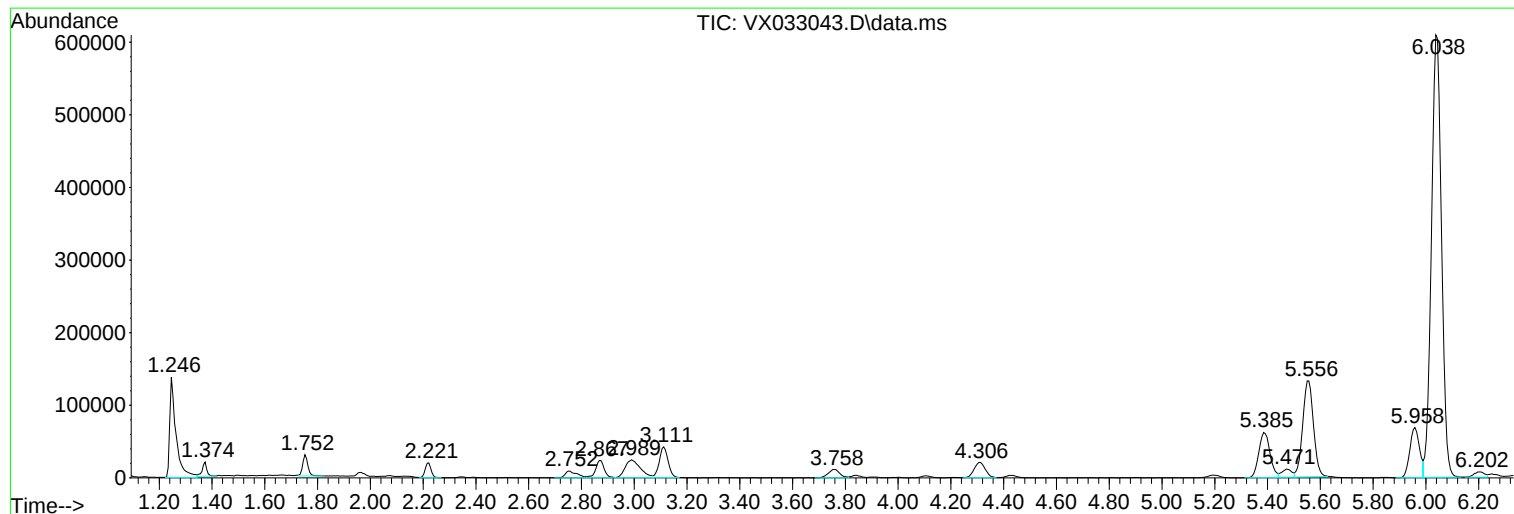
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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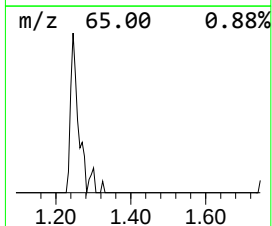
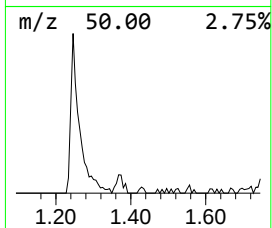
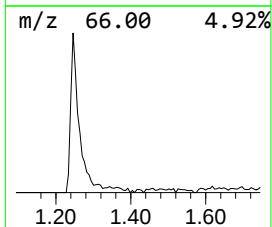
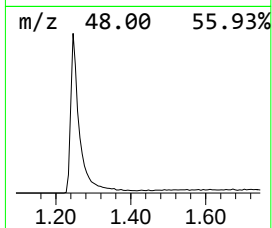
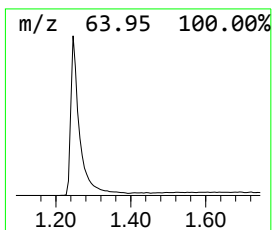
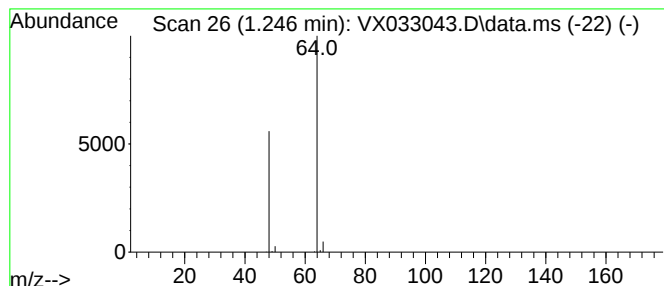
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Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	30.49 ug/l	228617	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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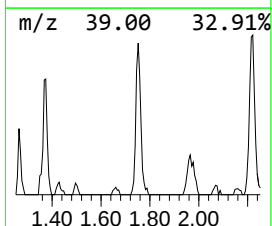
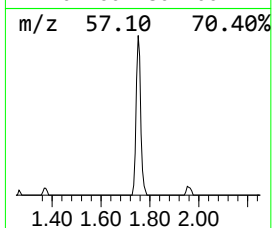
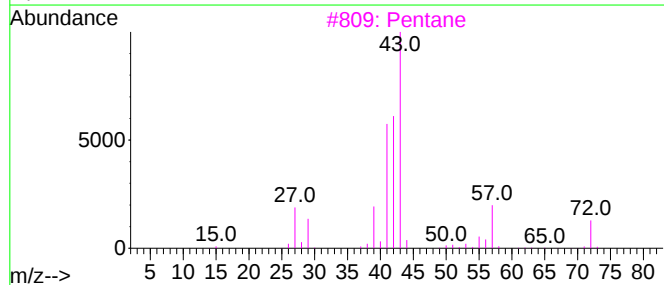
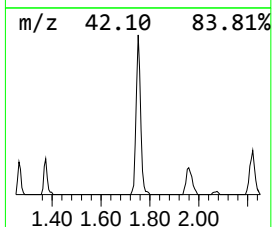
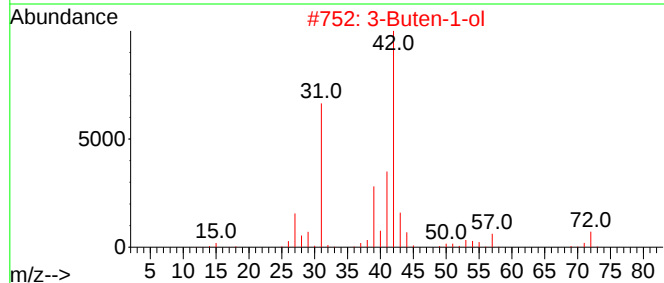
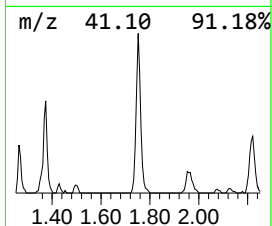
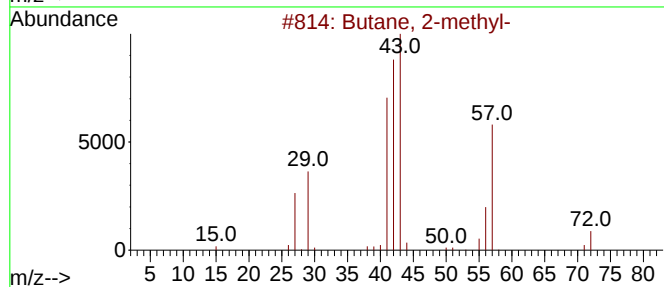
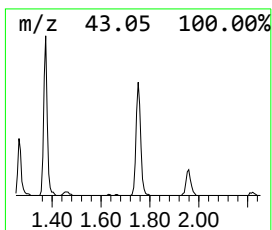
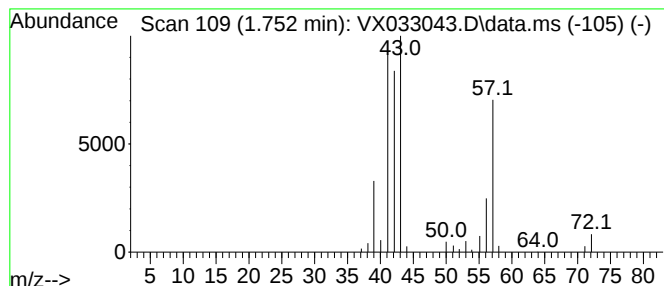
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Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.25 ug/l	39375	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5			1-Butene	56	C4H8	000106-98-9	14



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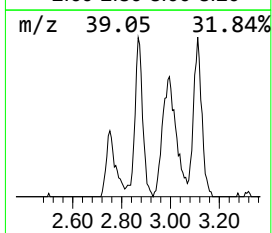
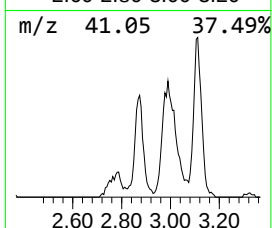
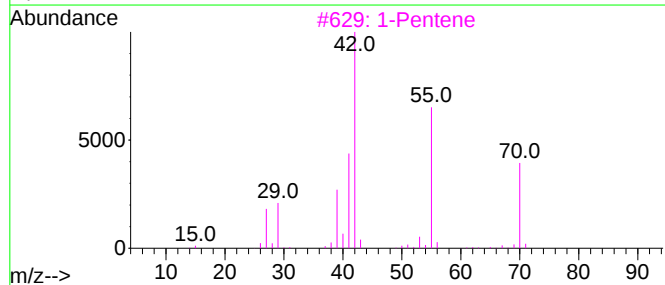
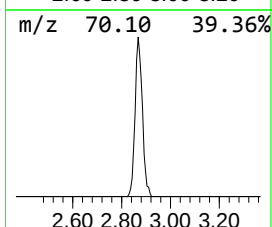
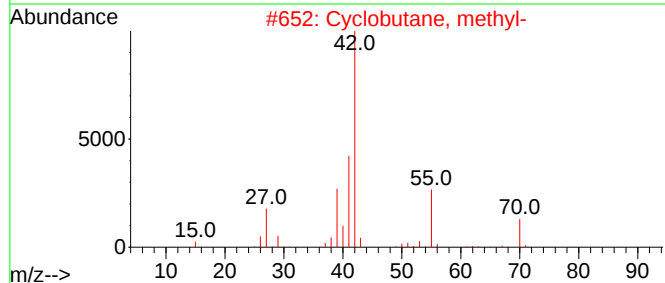
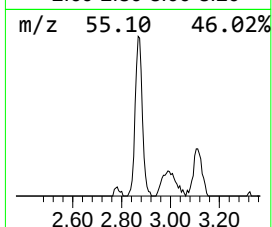
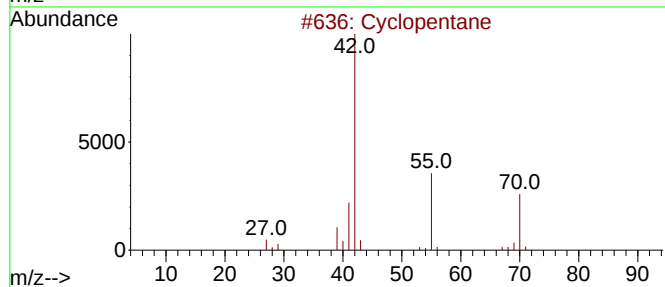
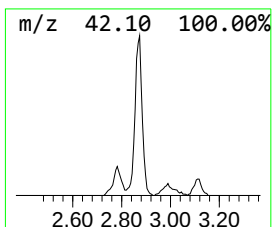
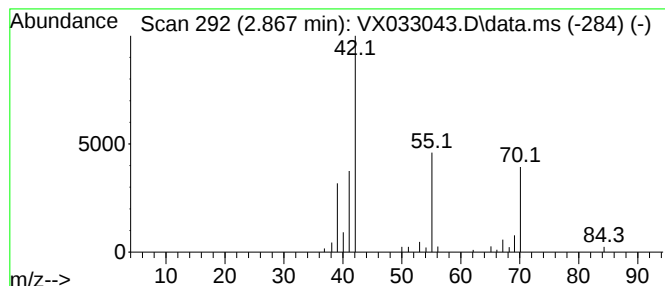
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	7.19 ug/l	53923	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3			1-Pentene	70	C5H10	000109-67-1	80
4			1-Pentanol	88	C5H12O	000071-41-0	40
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	25



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ClientSampleId :
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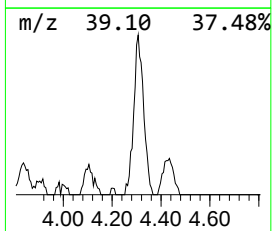
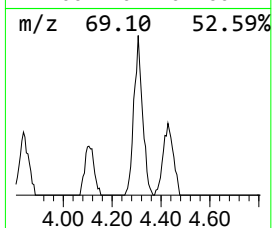
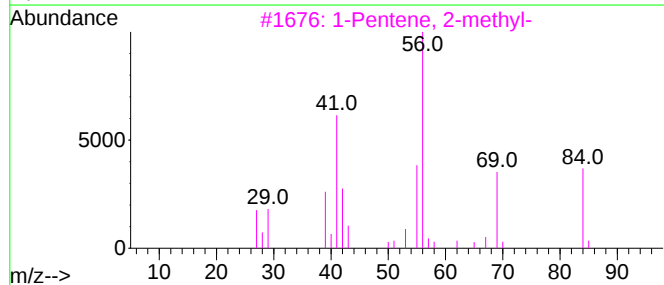
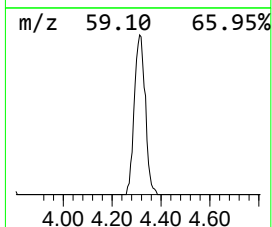
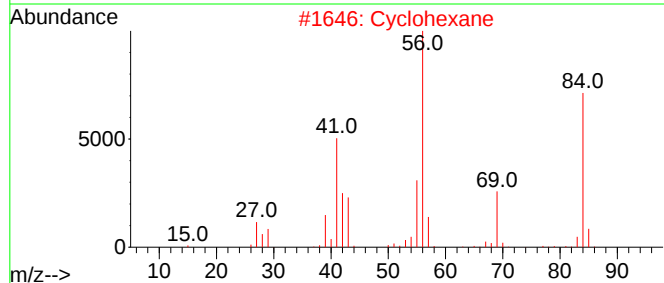
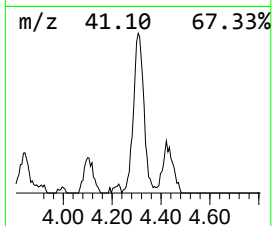
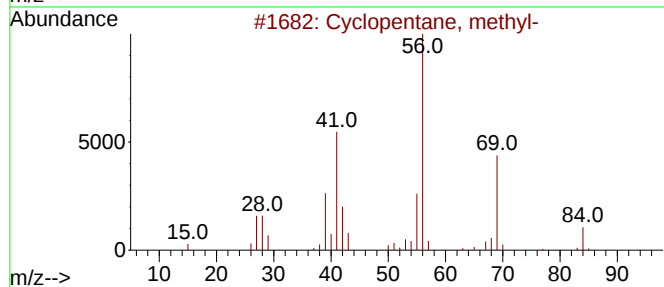
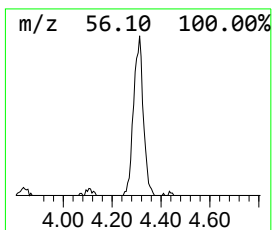
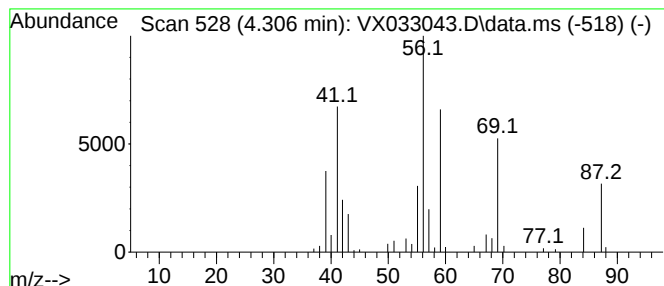
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	8.29 ug/l	62159	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2			Cyclohexane	84	C6H12	000110-82-7	52
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47
4			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	47
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	43



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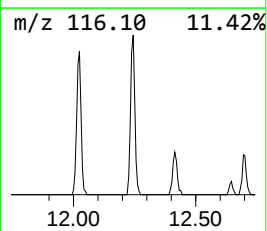
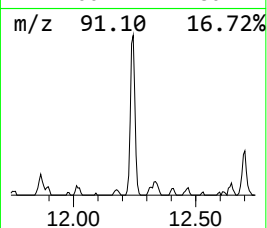
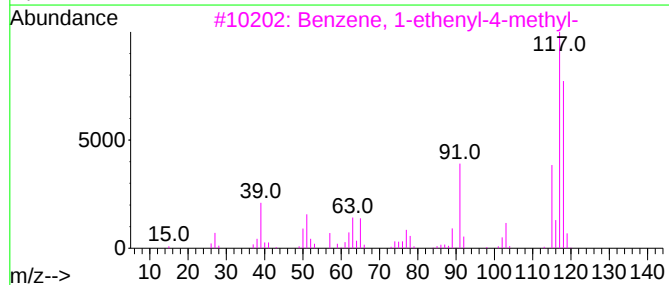
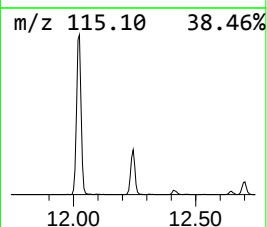
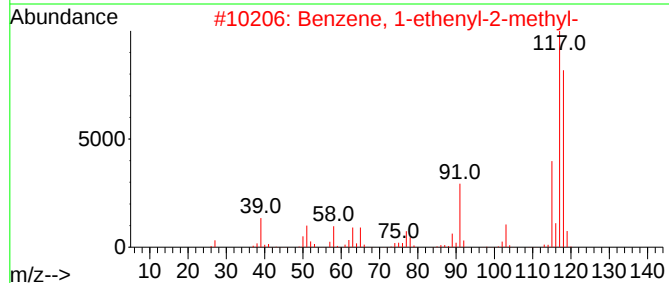
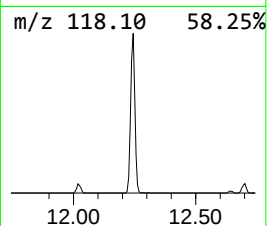
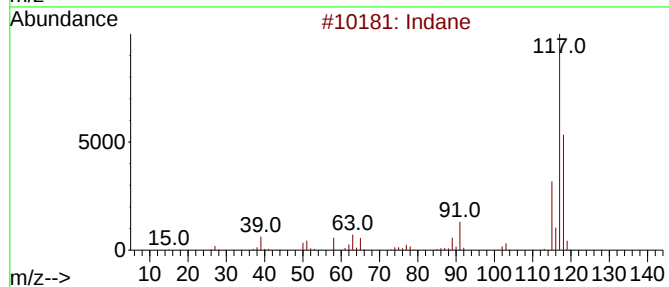
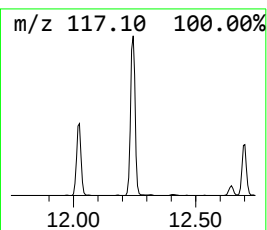
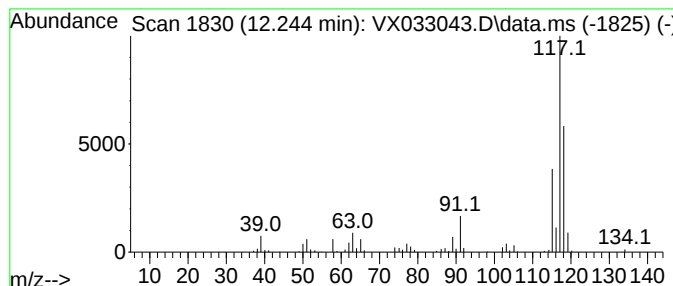
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	11.42 ug/l	124357	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	68
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	62



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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
Sulfur dioxide	1.246	30.5	ug/l	228617	1	5.556	374964	50.0
Butane, 2-methyl-	1.752	5.3	ug/l	39375	1	5.556	374964	50.0
Cyclopentane	2.867	7.2	ug/l	53923	1	5.556	374964	50.0
Cyclopentane, m...	4.306	8.3	ug/l	62159	1	5.556	374964	50.0
Indane	12.244	11.4	ug/l	124357	4	12.024	544401	50.0