

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
 Data File : VN072994.D
 Acq On : 21 Jun 2022 19:34
 Operator : JC\MD
 Sample : N3381-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-8

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_N\methods\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN072994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	48	58	62	rBV	41261	63691	2.82%	0.358%
2	2.328	62	75	76	rBV3	18908	69871	3.09%	0.393%
3	2.405	83	88	92	rBV	78596	120371	5.32%	0.677%
4	3.087	195	204	216	rVB	149101	344976	15.26%	1.941%
5	3.457	258	267	279	rVB3	42372	108899	4.82%	0.613%
6	3.657	293	301	312	rVB4	16284	42701	1.89%	0.240%
7	3.928	338	347	358	rBV	23921	63734	2.82%	0.359%
8	4.228	389	398	415	rVB2	24596	76545	3.39%	0.431%
9	4.516	438	447	457	rBV	19383	60277	2.67%	0.339%
10	4.998	519	529	533	rBV5	8692	24678	1.09%	0.139%
11	5.104	541	547	556	rVV4	15461	49597	2.19%	0.279%
12	6.387	756	765	776	rVB3	17267	48079	2.13%	0.270%
13	6.534	778	790	796	rBV6	13545	42063	1.86%	0.237%
14	6.616	796	804	809	rBV3	10366	26688	1.18%	0.150%
15	6.822	829	839	848	rBV6	11702	36047	1.59%	0.203%
16	7.069	869	881	889	rBV2	64037	191065	8.45%	1.075%
17	7.140	889	893	904	rVB6	10117	26454	1.17%	0.149%
18	7.769	992	1000	1010	rVB4	22648	62042	2.74%	0.349%
19	7.951	1021	1031	1036	rBV	205611	483359	21.38%	2.719%
20	8.016	1036	1042	1053	rVB	408724	956595	42.31%	5.382%
21	8.369	1093	1102	1113	rBV	208984	482440	21.34%	2.714%
22	8.516	1121	1127	1134	rVB2	15229	32377	1.43%	0.182%
23	8.904	1184	1193	1205	rBV	527541	1119719	49.52%	6.299%
24	9.904	1357	1363	1376	rVB2	24030	47528	2.10%	0.267%
25	10.263	1416	1424	1430	rBV6	19704	41883	1.85%	0.236%
26	10.375	1435	1443	1450	rBV	714812	1307880	57.84%	7.358%
27	10.439	1450	1454	1460	rVV	42964	79575	3.52%	0.448%
28	11.680	1656	1665	1675	rBV	735190	1280824	56.65%	7.206%
29	11.780	1675	1682	1693	rVV	828943	1375496	60.83%	7.738%
30	11.892	1693	1701	1713	rVB	1252805	2261072	100.00%	12.721%
31	12.216	1748	1756	1766	rBV	472028	772121	34.15%	4.344%
32	12.516	1797	1807	1813	rBV2	32278	58005	2.57%	0.326%
33	12.669	1825	1833	1843	rVB	579633	978291	43.27%	5.504%
34	12.857	1859	1865	1870	rBV2	28702	43978	1.95%	0.247%
35	12.922	1870	1876	1878	rVV	113513	181067	8.01%	1.019%
36	12.951	1878	1881	1885	rVV	109928	172092	7.61%	0.968%

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37	12.992	1885	1888	1894	rVB	48677	75409	3.34%	0.424%
38	13.157	1909	1916	1924	rBV	352985	578720	25.59%	3.256%
39	13.304	1932	1941	1949	rBV	900000	1443652	63.85%	8.122%
40	13.610	1986	1993	1997	rBV	720965	1368599	60.53%	7.700%
41	13.704	2005	2009	2017	rVB	42599	73506	3.25%	0.414%
42	13.810	2017	2027	2042	rVB	385581	651142	28.80%	3.663%
43	13.992	2051	2058	2066	rVB3	14852	29325	1.30%	0.165%
44	14.069	2066	2071	2074	rBV4	14114	24573	1.09%	0.138%
45	14.151	2080	2085	2091	rVB	18941	29956	1.32%	0.169%
46	14.263	2099	2104	2111	rVB2	30608	50759	2.24%	0.286%
47	14.863	2198	2206	2211	rBV4	33371	61792	2.73%	0.348%
48	15.427	2294	2302	2310	rBV	132742	255416	11.30%	1.437%

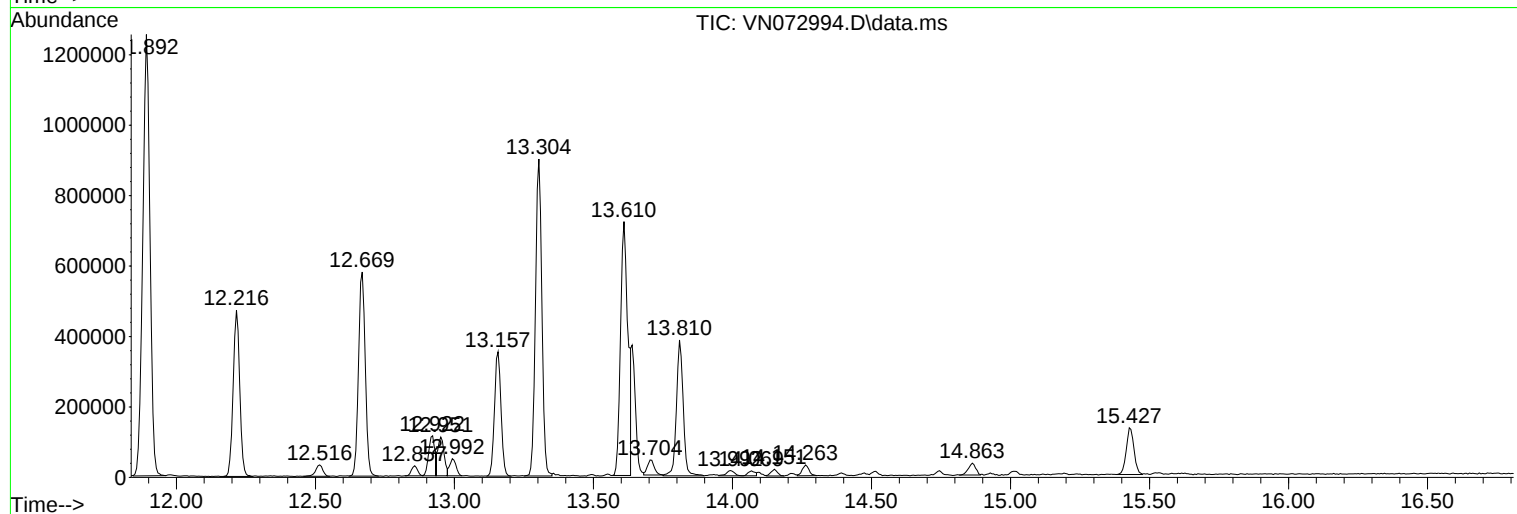
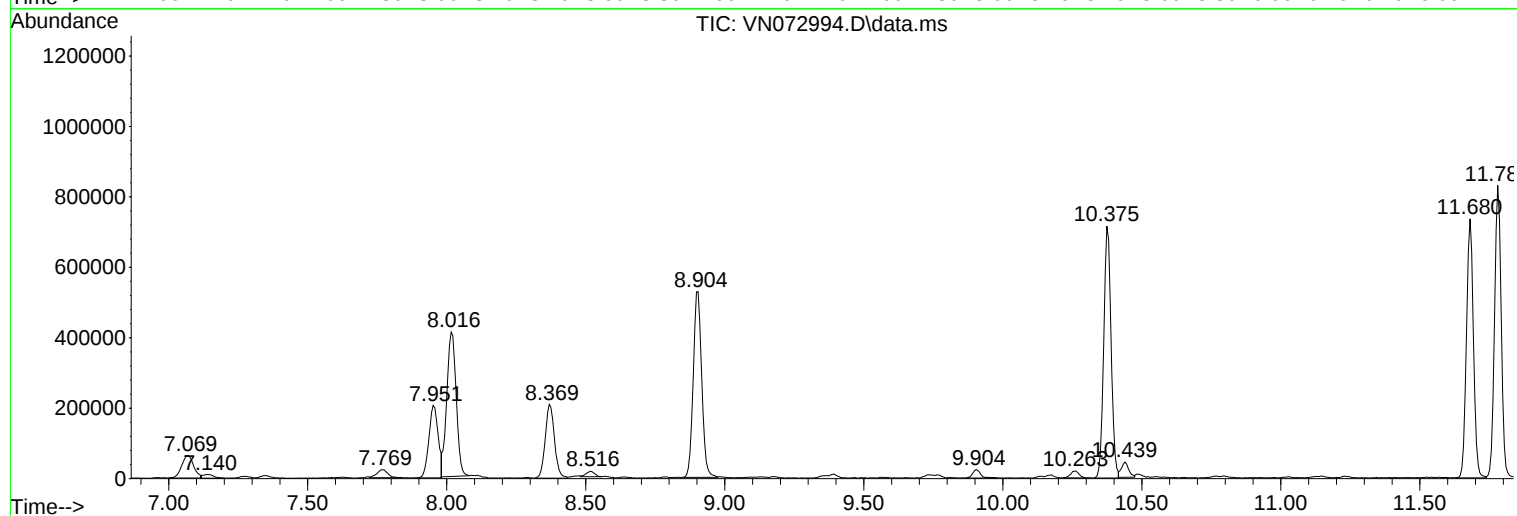
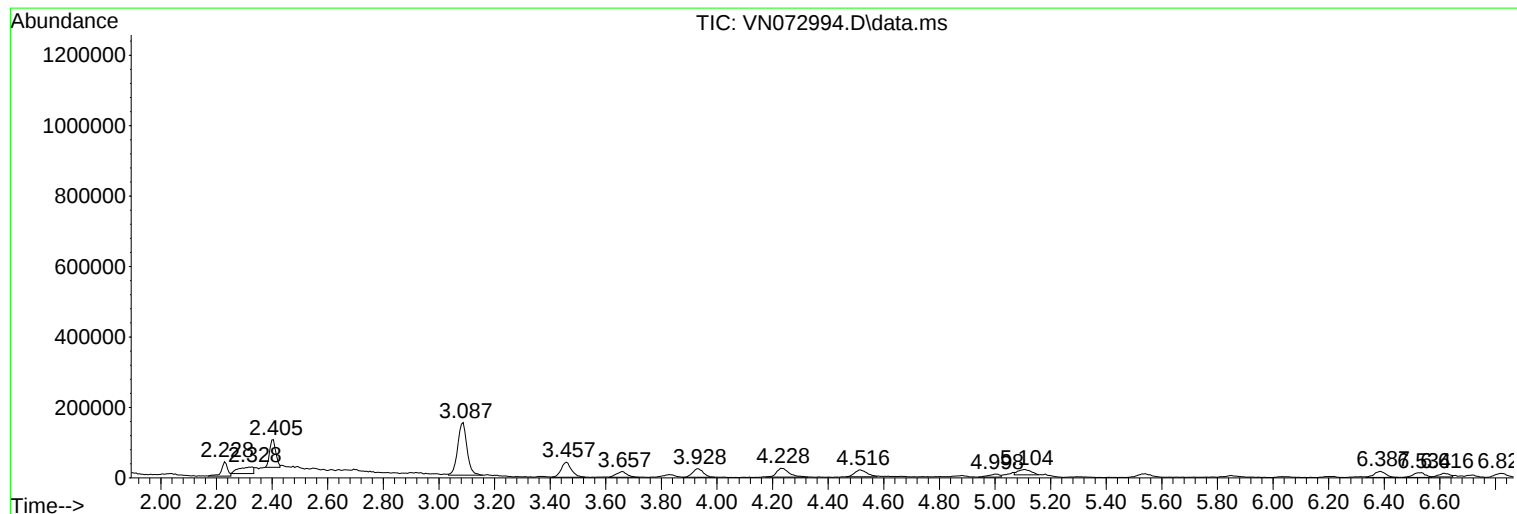
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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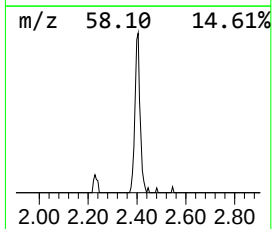
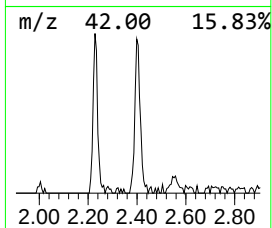
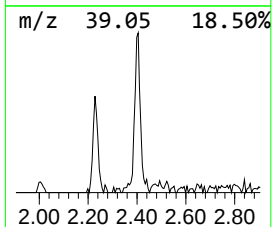
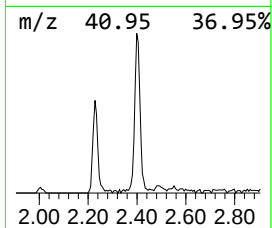
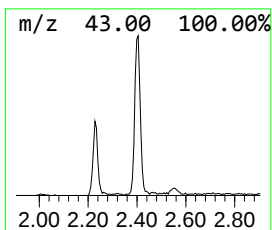
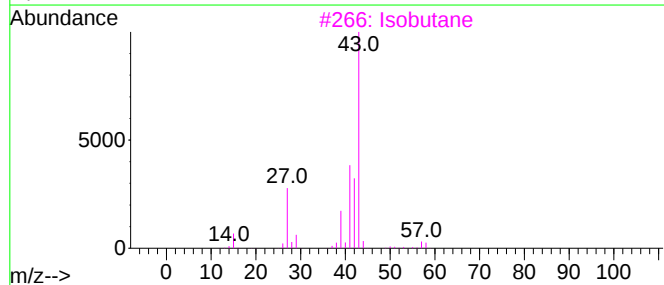
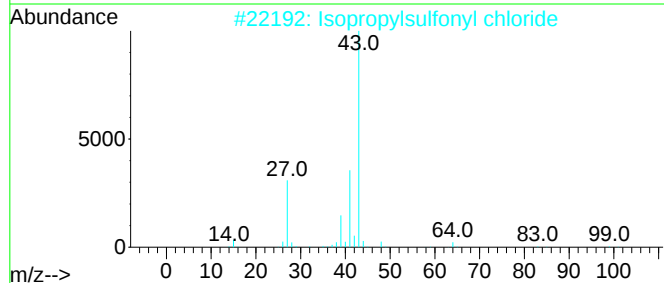
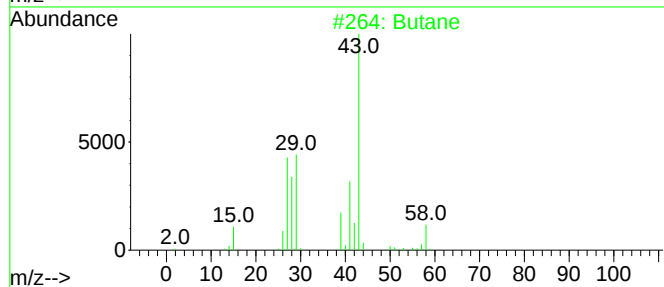
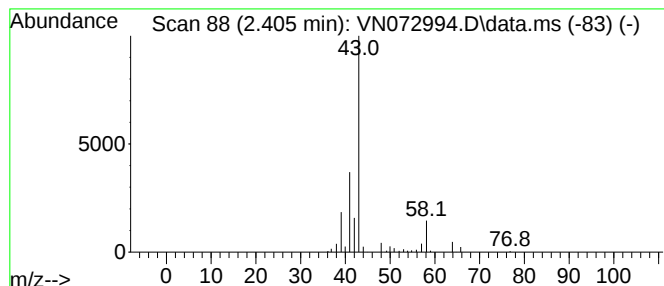
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.405	6.29 ug/l	120371	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	52
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	28
3			Isobutane	58	C4H10	000075-28-5	9
4			1-Propanesulfonyl chloride	142	C3H7ClO2S	010147-36-1	9
5			Acetone	58	C3H6O	000067-64-1	5



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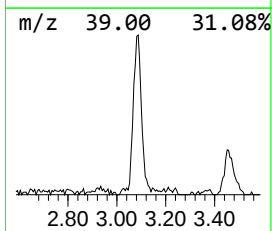
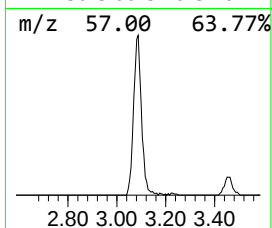
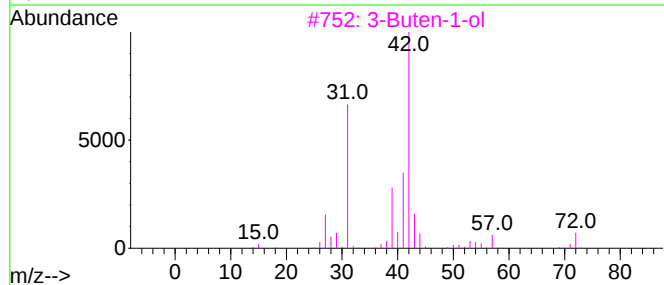
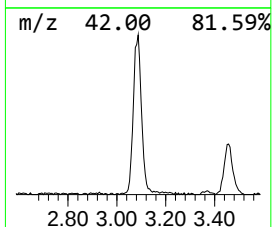
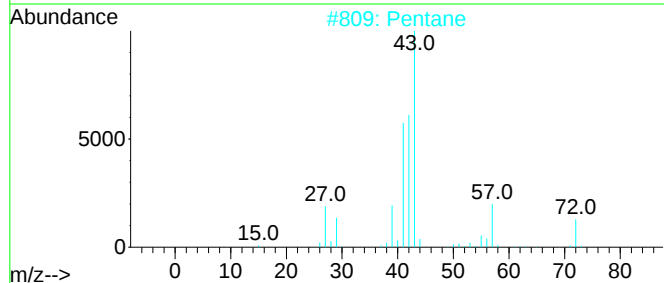
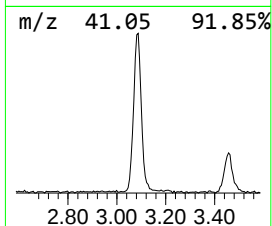
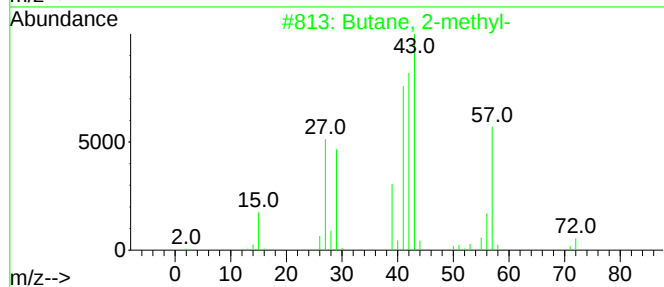
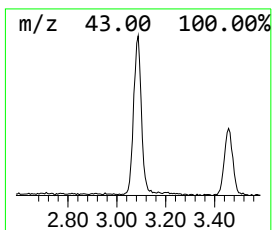
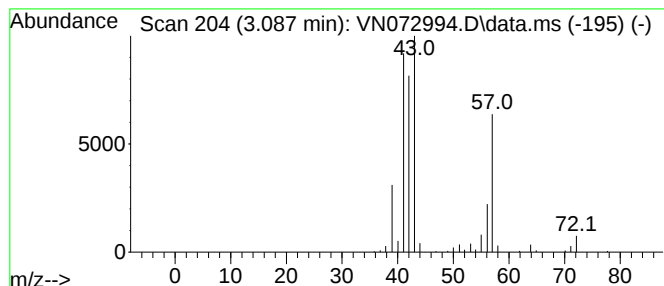
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	18.03 ug/l	344976	Pentafluorobenzene	8.016

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	64
3			3-Buten-1-ol	72	C4H8O	000627-27-0	43
4			1-Butene	56	C4H8	000106-98-9	9
5			Azetidine	57	C3H7N	000503-29-7	9



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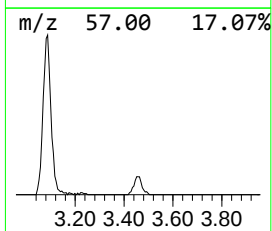
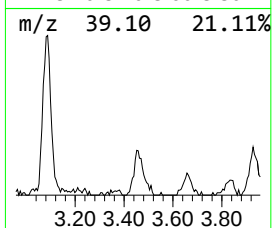
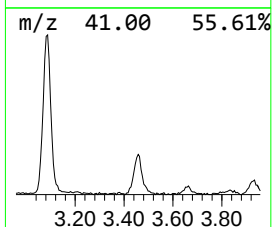
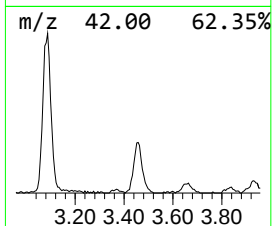
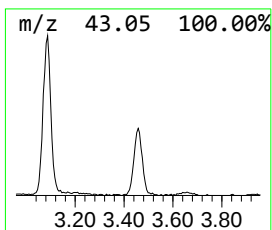
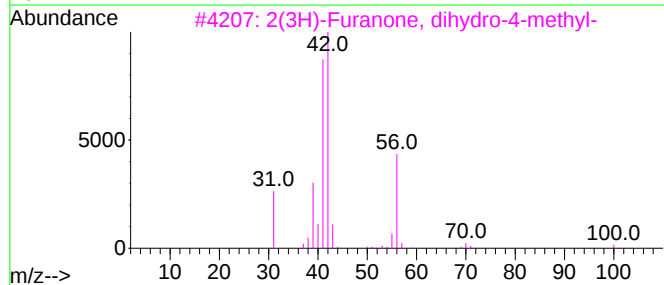
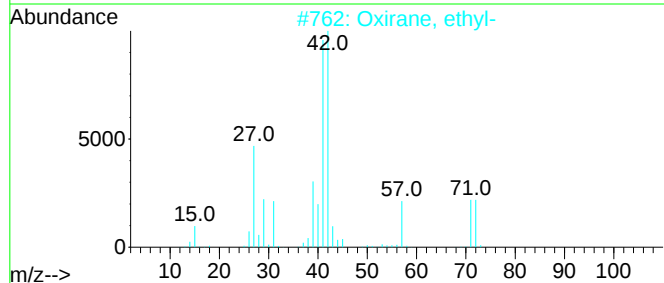
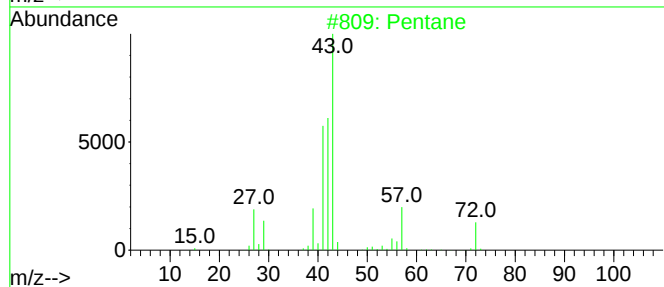
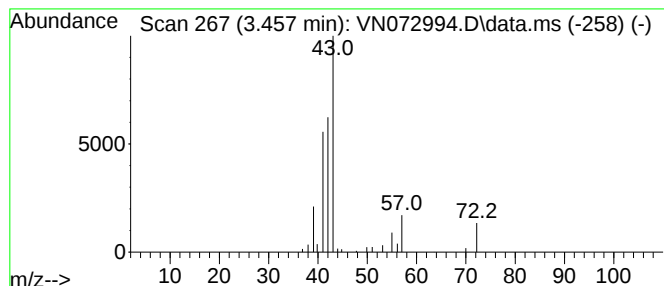
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Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	5.69 ug/l	108899	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	38
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	23
5			Borane, ethyldimethyl-	70	C4H11B	001113-22-0	9



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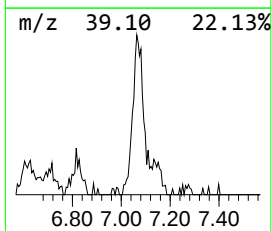
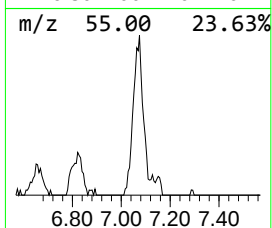
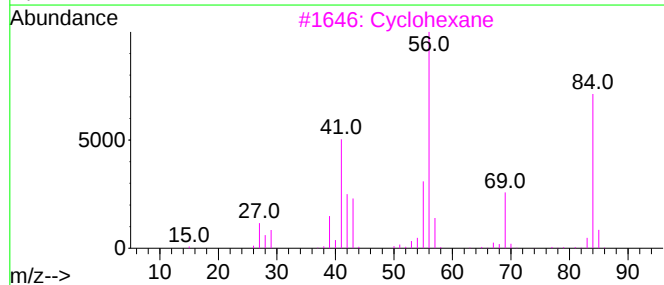
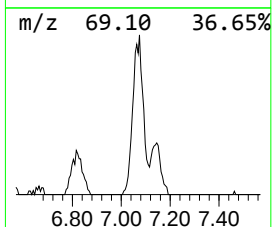
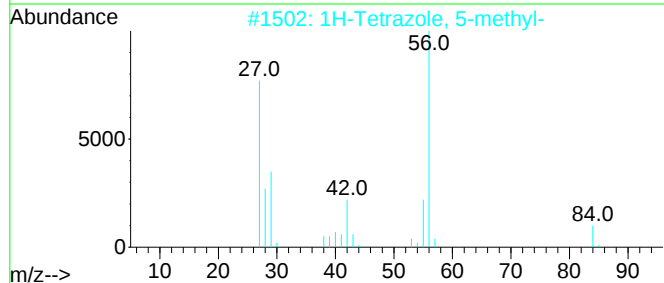
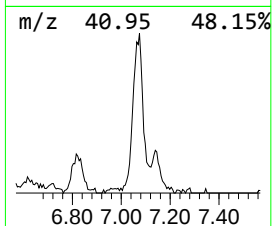
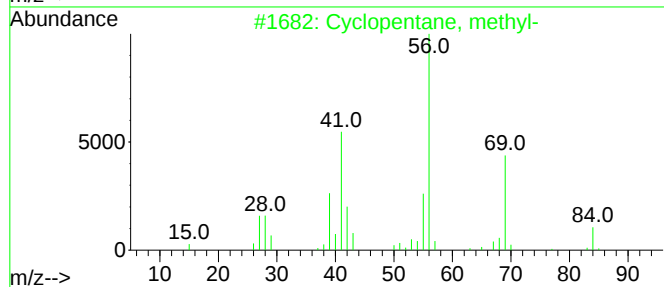
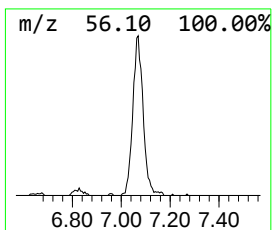
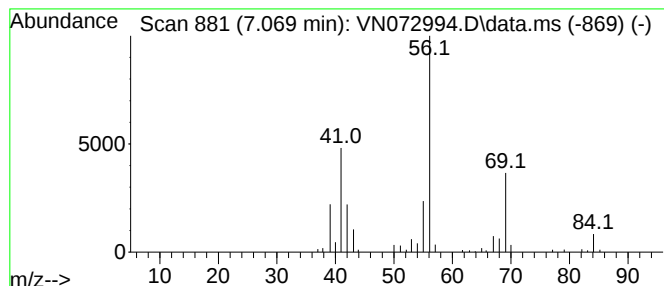
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	9.99 ug/l	191065	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3		Cyclohexane	84	C6H12	000110-82-7	74
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		Cyclopropane, propyl-	84	C6H12	002415-72-7	56



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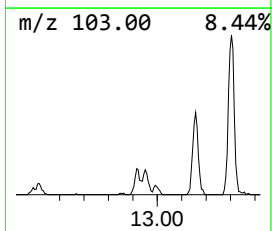
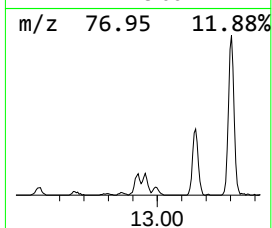
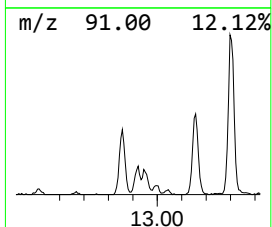
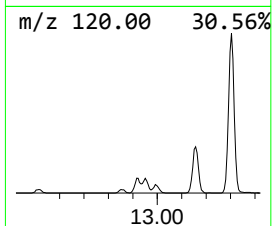
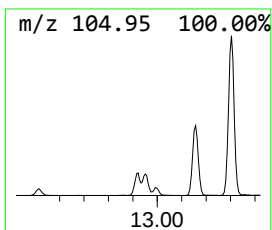
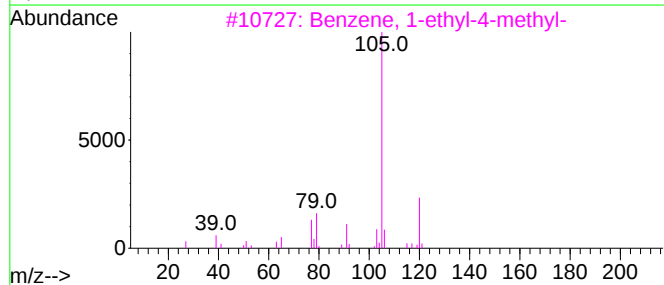
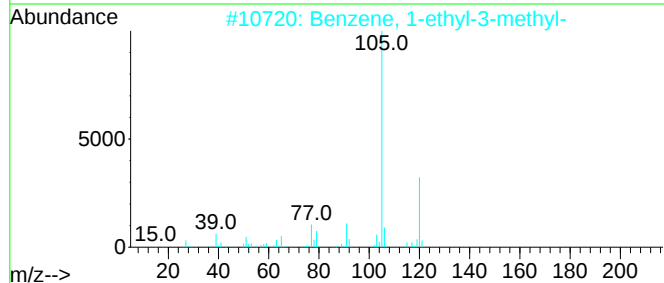
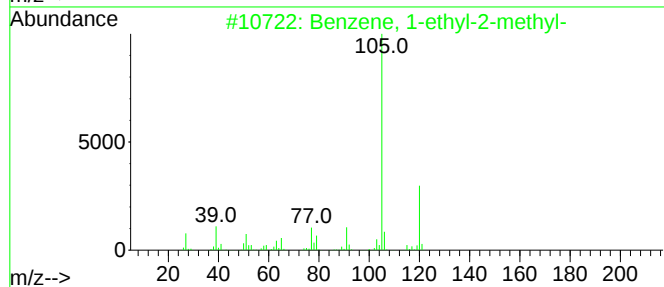
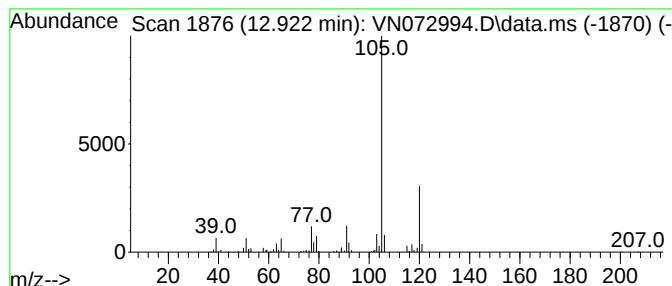
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	6.62 ug/l	181067	1,4-Dichlorobenzene-d4	13.610

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-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072994.D
Acq On : 21 Jun 2022 19:34
Operator : JC\MD
Sample : N3381-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-8

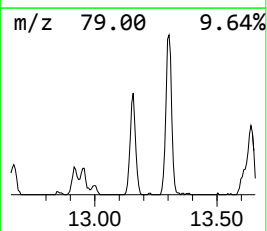
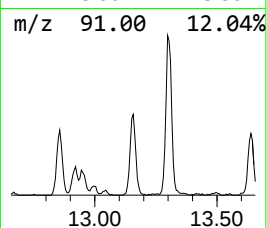
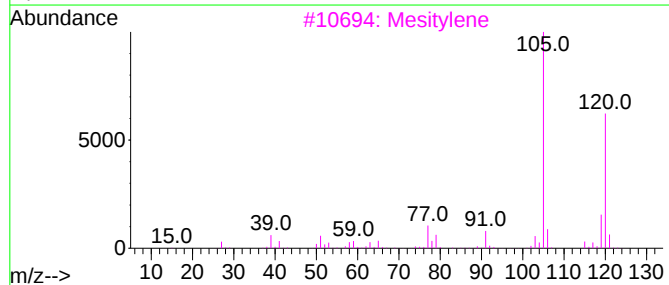
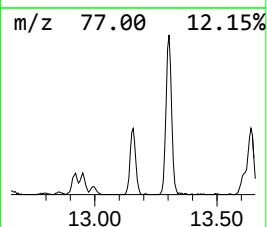
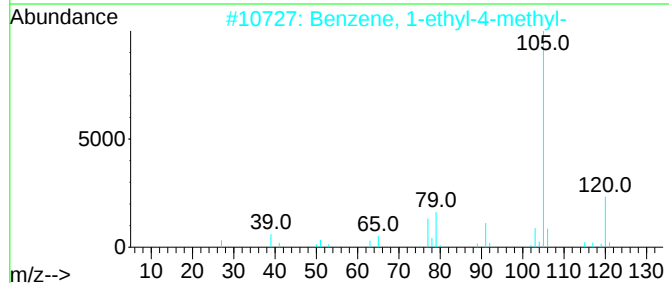
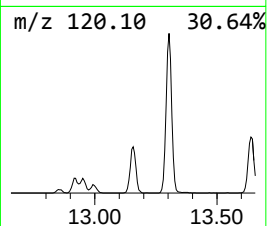
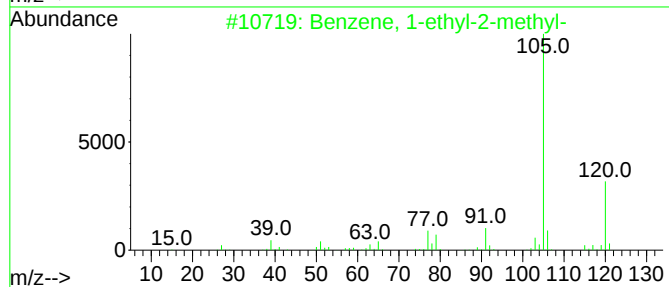
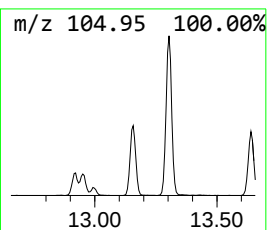
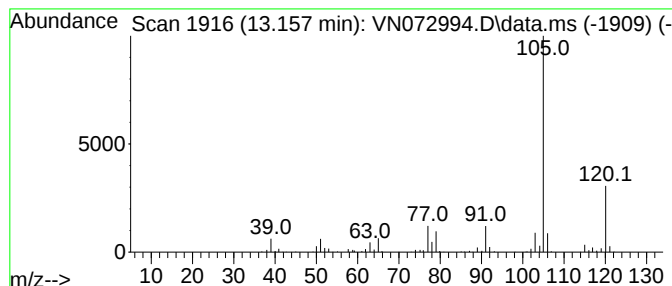
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	21.14 ug/l	578720	1,4-Dichlorobenzene-d4	13.610

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	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072994.D
Acq On : 21 Jun 2022 19:34
Operator : JC\MD
Sample : N3381-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-8

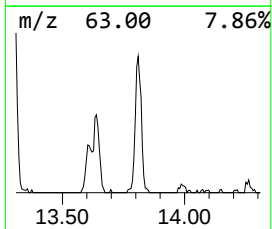
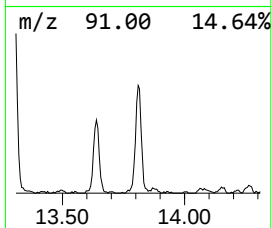
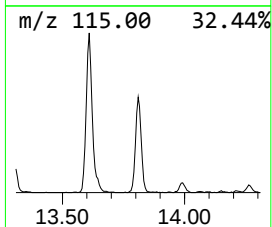
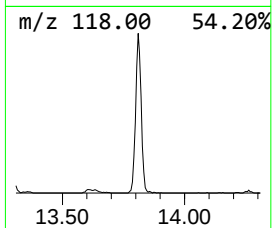
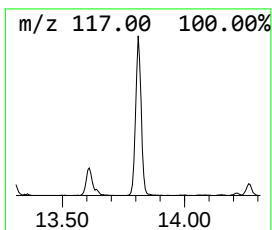
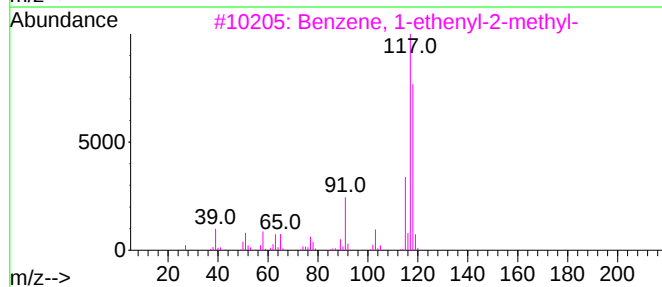
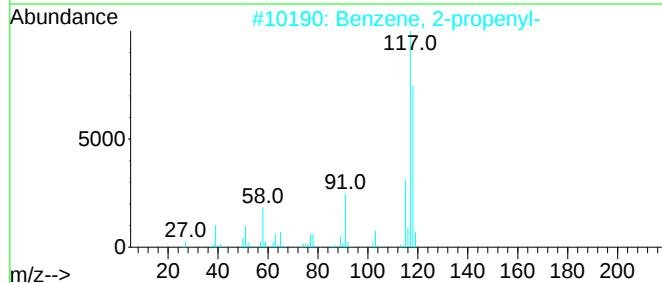
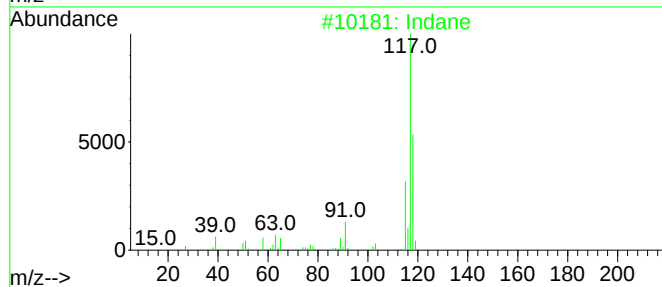
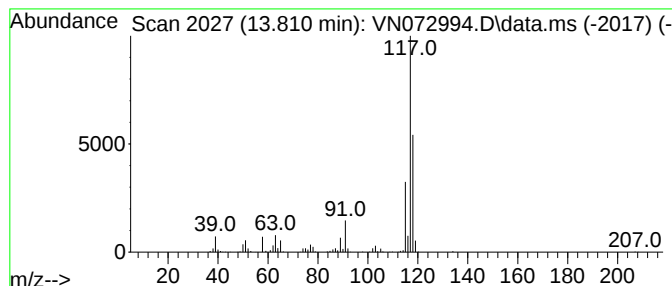
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Quant Title : SW846 8260

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

Peak Number 7 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	23.79 ug/l	651142	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072994.D
Acq On : 21 Jun 2022 19:34
Operator : JC\MD
Sample : N3381-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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
Butane	2.405	6.3	ug/l	120371	1	8.016	956595	50.0
Butane, 2-methyl-	3.087	18.0	ug/l	344976	1	8.016	956595	50.0
Pentane	3.457	5.7	ug/l	108899	1	8.016	956595	50.0
Cyclopentane, m...	7.069	10.0	ug/l	191065	1	8.016	956595	50.0
Benzene, 1-ethy...	12.922	6.6	ug/l	181067	4	13.610	1368600	50.0
Benzene, 1-ethy...	13.157	21.1	ug/l	578720	4	13.610	1368600	50.0
Indane	13.810	23.8	ug/l	651142	4	13.610	1368600	50.0