

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073688.D
 Acq On : 02 Aug 2022 15:36
 Operator : JC\MD
 Sample : N3971-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-22R

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073688.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	75	87	94	rBV	364808	569394	9.59%	2.033%
2	3.081	195	203	214	rVB	281321	623508	10.50%	2.226%
3	3.457	258	267	283	rVB3	31363	84413	1.42%	0.301%
4	3.928	337	347	359	rBV	148073	390344	6.57%	1.394%
5	4.228	389	398	409	rBV2	22137	64563	1.09%	0.231%
6	4.510	434	446	460	rBV	84406	271066	4.56%	0.968%
7	4.875	499	508	519	rBV2	21394	67013	1.13%	0.239%
8	5.110	535	548	565	rVB	107597	396821	6.68%	1.417%
9	7.063	869	880	889	rBV2	62823	191235	3.22%	0.683%
10	7.340	919	927	940	rVB2	57647	147828	2.49%	0.528%
11	7.951	1020	1031	1036	rBV	260321	621321	10.46%	2.219%
12	8.016	1036	1042	1056	rVB	510037	1208529	20.35%	4.315%
13	8.392	1091	1106	1116	rBV	2476296	5938460	100.00%	21.204%
14	8.522	1123	1128	1142	rVB2	41254	102247	1.72%	0.365%
15	8.904	1184	1193	1213	rVB	653649	1342259	22.60%	4.793%
16	10.380	1437	1444	1451	rBV	925997	1695398	28.55%	6.054%
17	10.445	1451	1455	1461	rVB	109329	185156	3.12%	0.661%
18	10.580	1469	1478	1484	rBV2	48138	87280	1.47%	0.312%
19	10.657	1484	1491	1498	rVB	53131	92860	1.56%	0.332%
20	11.233	1581	1589	1598	rBV2	34260	63905	1.08%	0.228%
21	11.686	1657	1666	1676	rBV	927707	1626748	27.39%	5.809%
22	11.786	1676	1683	1692	rVV	703082	1202948	20.26%	4.295%
23	11.898	1694	1702	1711	rVB	142154	278203	4.68%	0.993%
24	12.222	1745	1757	1764	rVB2	40731	75978	1.28%	0.271%
25	12.522	1797	1808	1815	rVB	112099	203273	3.42%	0.726%
26	12.674	1826	1834	1845	rVB	758099	1305374	21.98%	4.661%
27	12.863	1860	1866	1875	rVB	136518	221806	3.74%	0.792%
28	12.998	1884	1889	1896	rVB	54777	90345	1.52%	0.323%
29	13.163	1911	1917	1927	rVB	69466	119923	2.02%	0.428%
30	13.310	1936	1942	1956	rVB	61078	111623	1.88%	0.399%
31	13.616	1986	1994	1997	rBV	965842	1770893	29.82%	6.323%
32	13.645	1997	1999	2006	rVV	785454	1024880	17.26%	3.659%
33	13.710	2006	2010	2017	rVV2	71121	124867	2.10%	0.446%
34	13.816	2017	2028	2043	rVB	1549525	2650595	44.63%	9.464%
35	14.157	2079	2086	2092	rBV	185614	285607	4.81%	1.020%
36	14.221	2092	2097	2100	rVV	40519	68467	1.15%	0.244%

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Integrator: RTE

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37	14.268	2100	2105	2111	rVB2	195773	326484	5.50%	1.166%
38	14.480	2132	2141	2145	rBV	113474	185667	3.13%	0.663%
39	14.745	2181	2186	2192	rBV	89287	147952	2.49%	0.528%
40	14.868	2199	2207	2213	rBV3	264939	505239	8.51%	1.804%
41	15.021	2226	2233	2238	rBV4	45314	82256	1.39%	0.294%
42	15.433	2295	2303	2313	rBV	779356	1453532	24.48%	5.190%

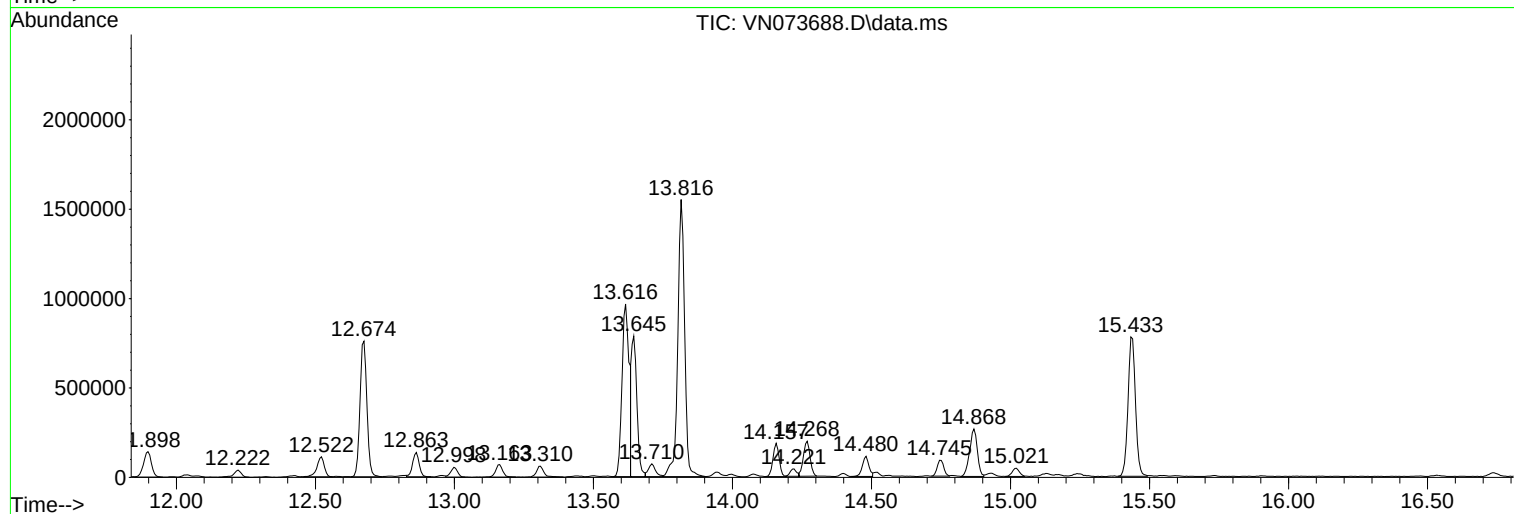
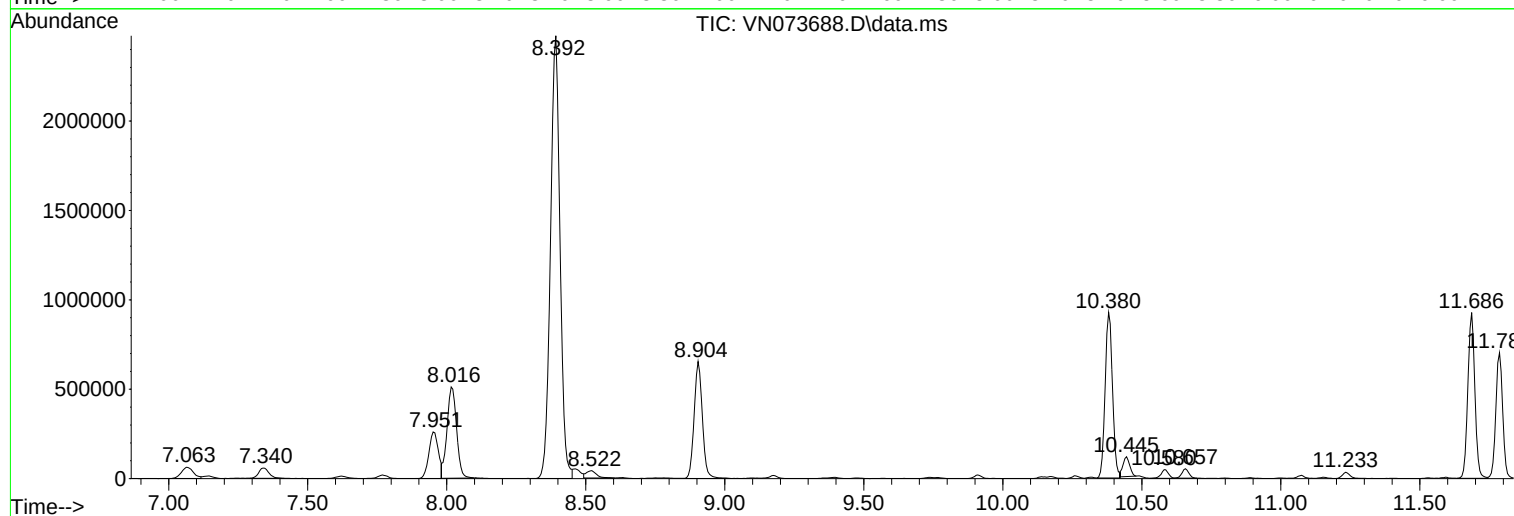
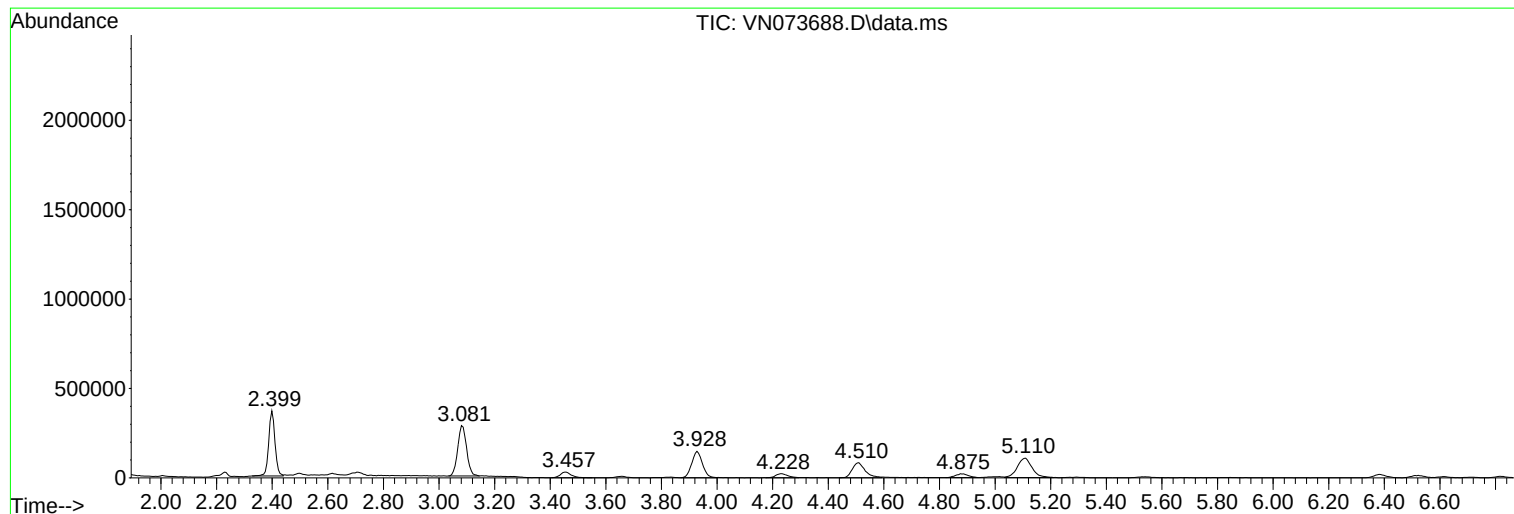
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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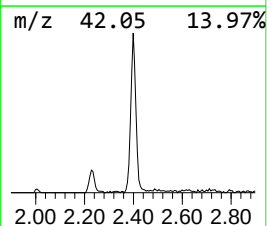
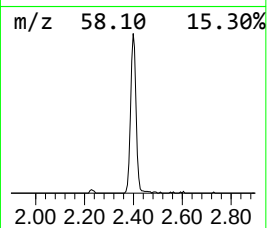
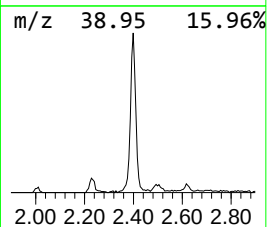
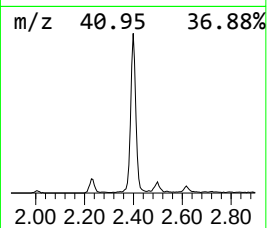
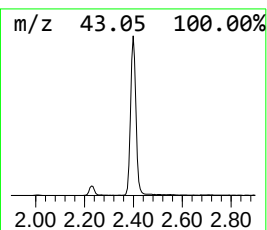
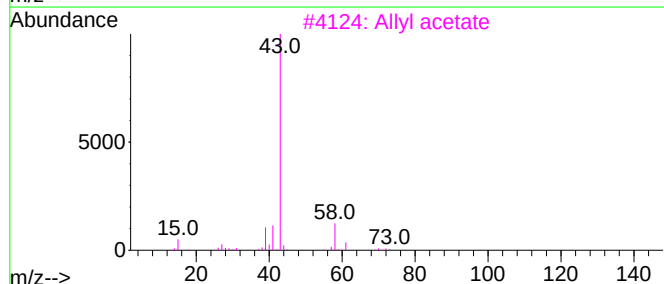
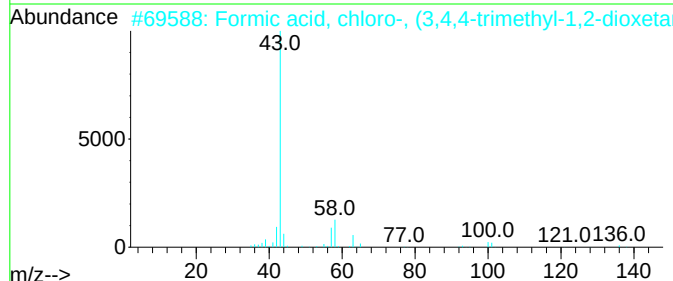
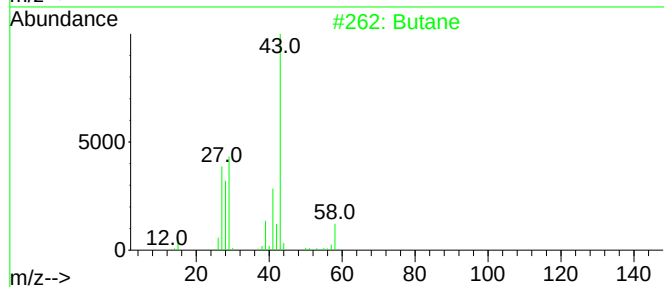
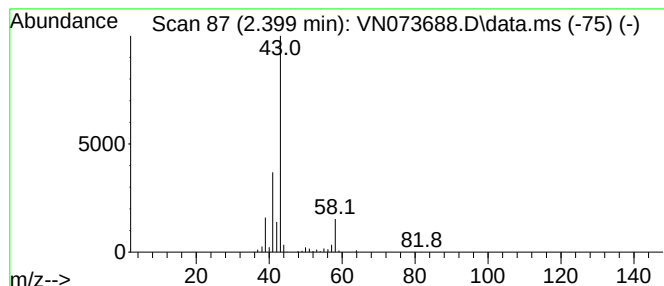
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	23.56 ug/l	569394	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	38
3			Allyl acetate	100	C5H8O2	000591-87-7	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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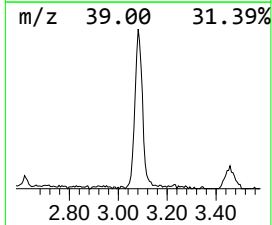
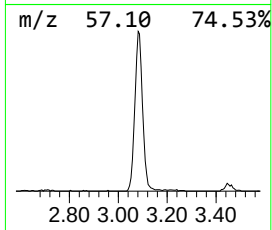
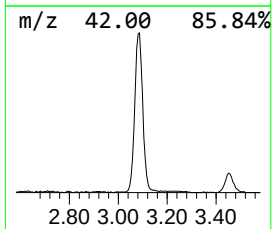
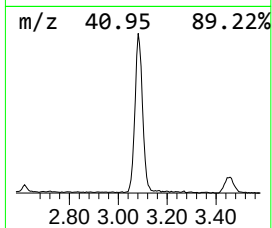
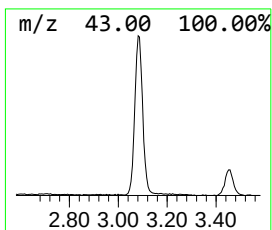
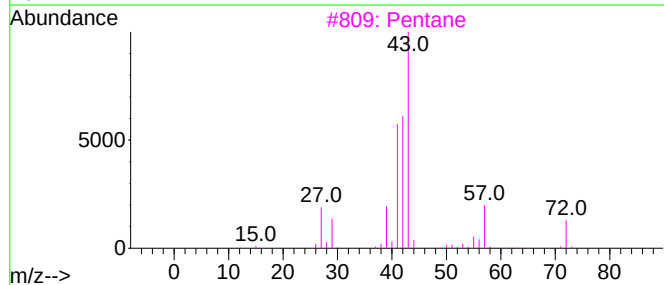
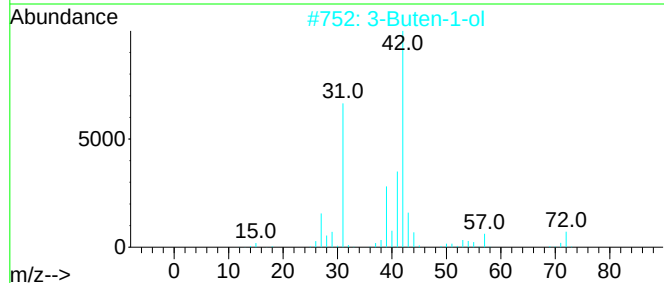
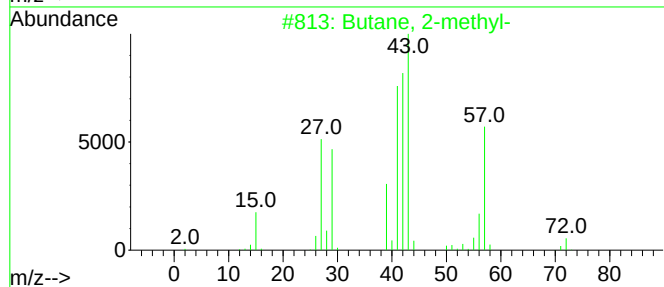
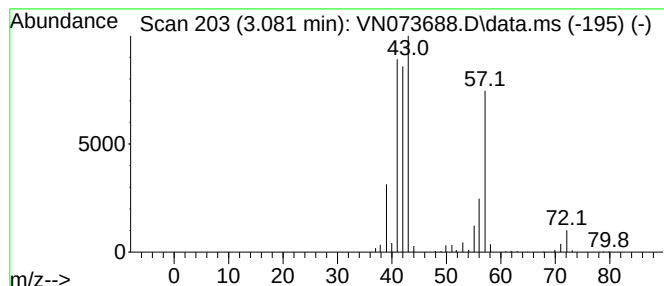
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	25.80 ug/l	623508	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	90
2		3-Buten-1-ol	72	C4H8O	000627-27-0	43
3		Pentane	72	C5H12	000109-66-0	28
4		1-Butene	56	C4H8	000106-98-9	10
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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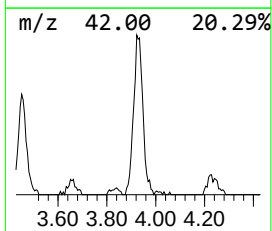
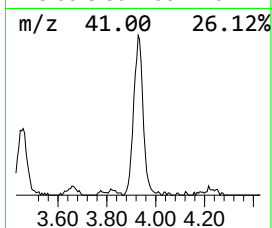
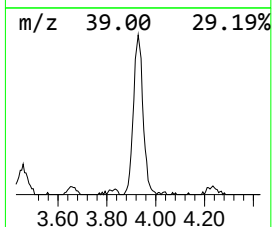
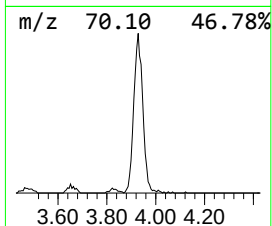
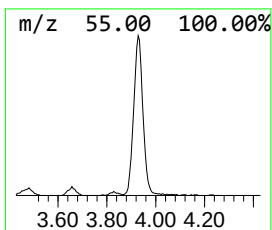
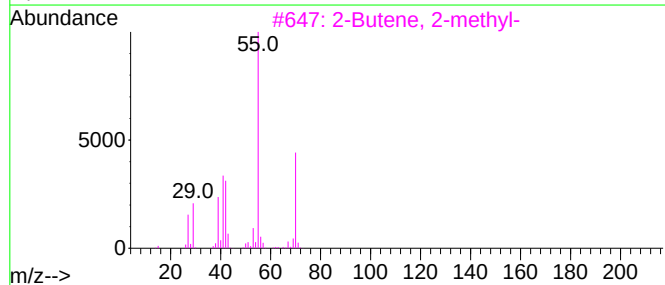
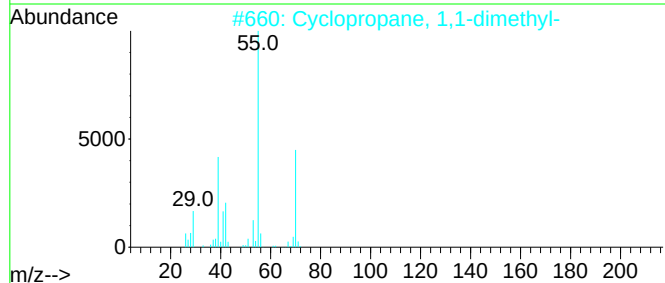
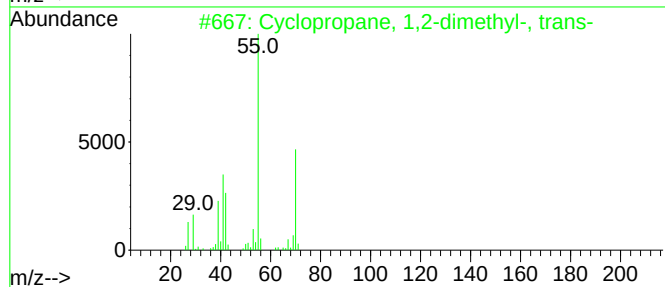
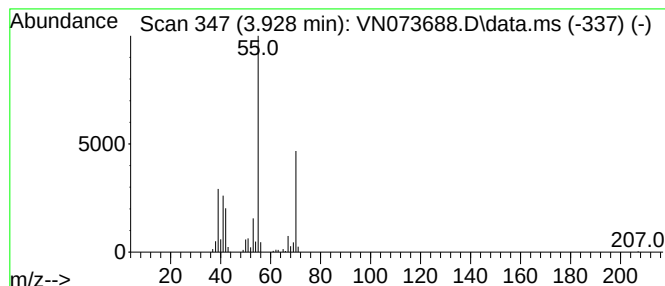
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.928	16.15 ug/l	390344	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
2		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
3		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
4		1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
5		2-Pentene, (E)-	70	C5H10	000646-04-8	64



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ClientSampleId :
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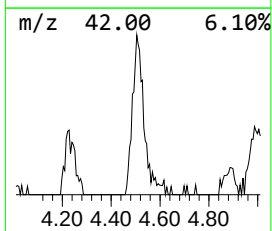
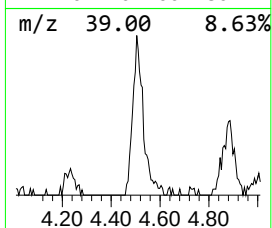
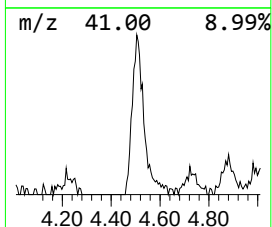
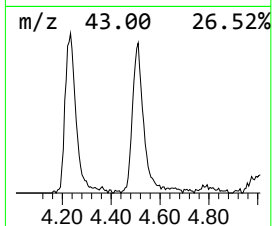
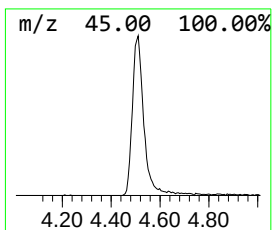
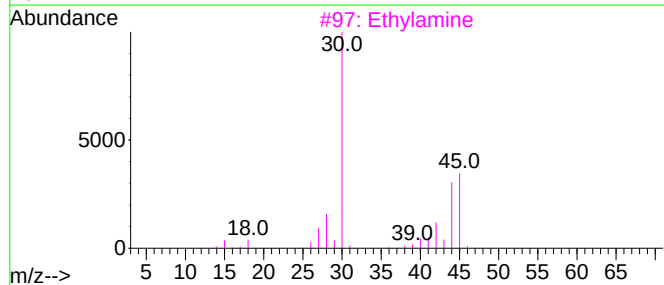
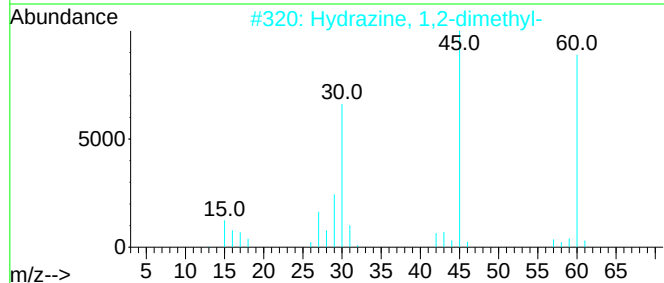
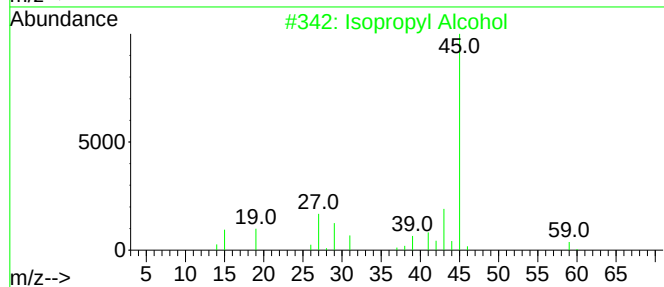
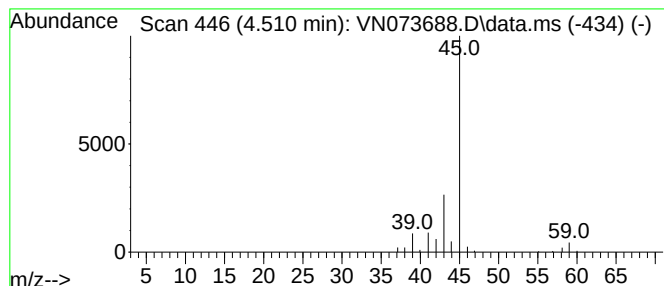
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	11.21 ug/l	271066	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Ethylamine	45	C2H7N	000075-04-7	4
4		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
5		Methoxyacetyl chloride	108	C3H5ClO2	038870-89-2	4



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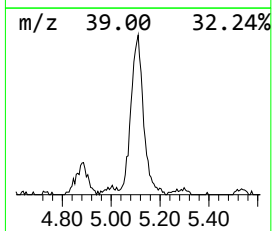
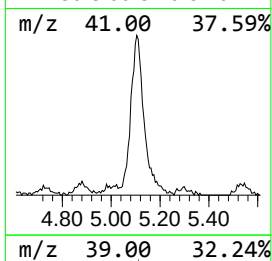
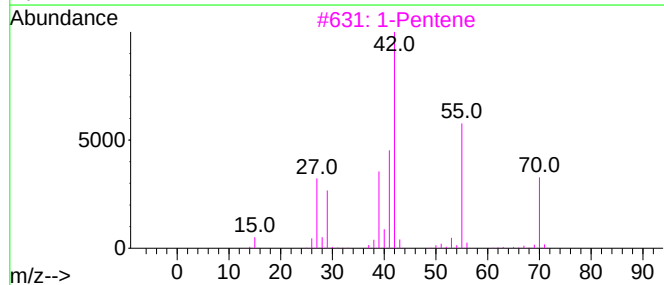
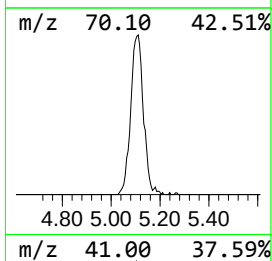
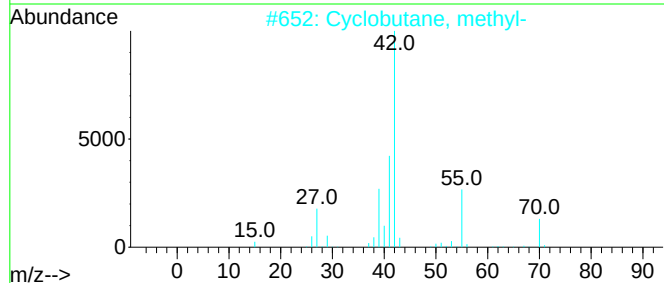
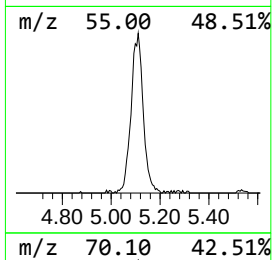
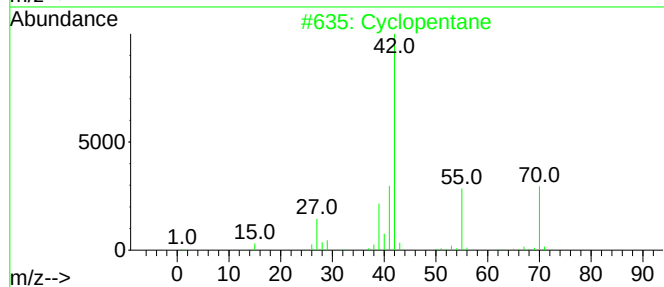
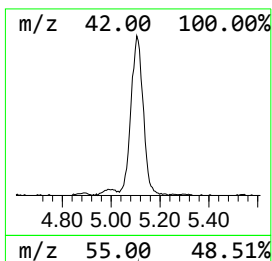
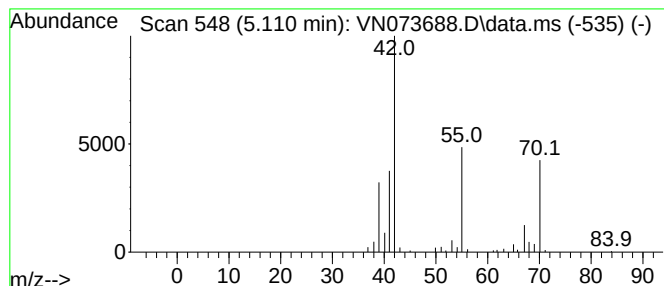
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	16.42 ug/l	396821	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	72
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	1-Pentene	70	C5H10	000109-67-1	59
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	47
5	Cyclobutanone	70	C4H6O	001191-95-3	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22R

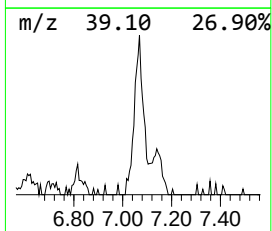
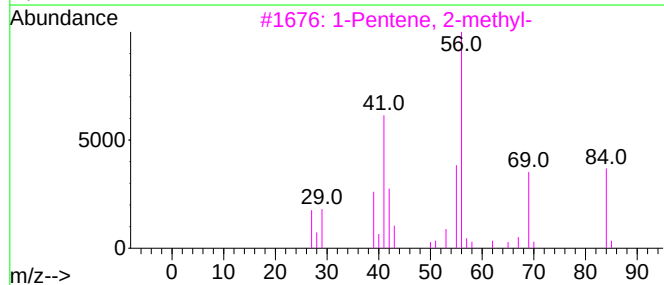
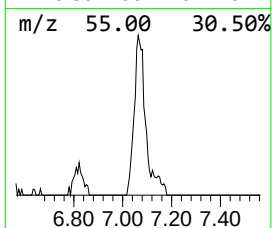
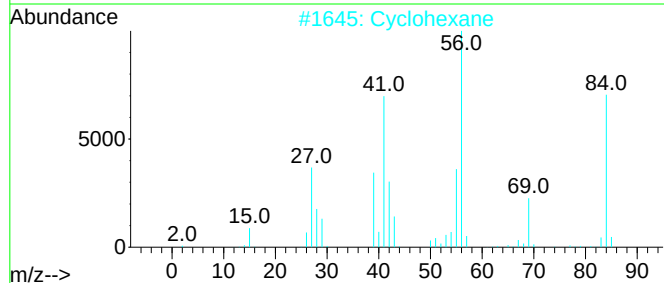
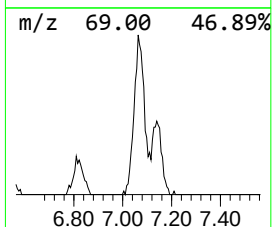
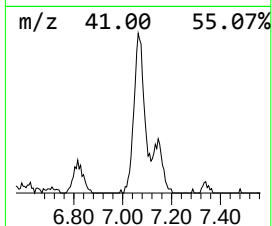
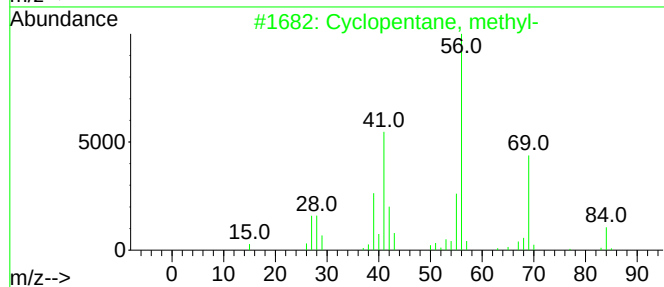
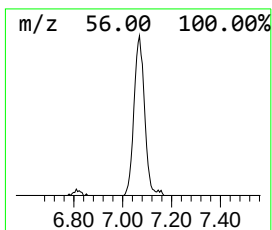
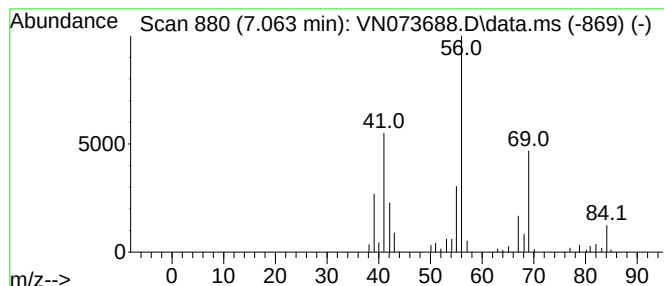
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	7.91 ug/l	191235	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclohexane	84	C6H12	000110-82-7	83
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22R

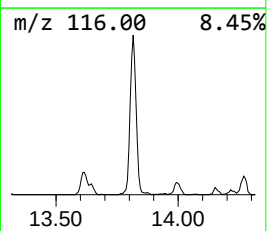
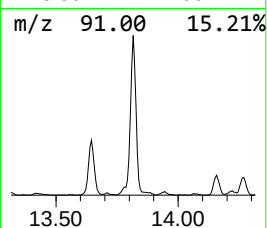
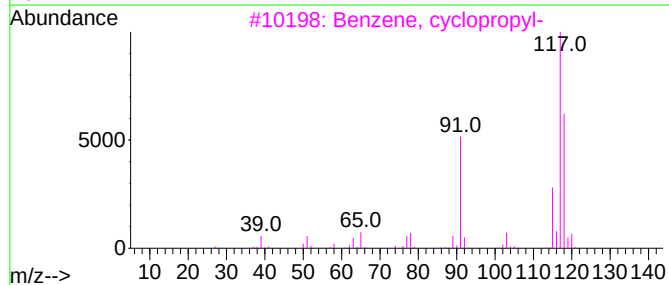
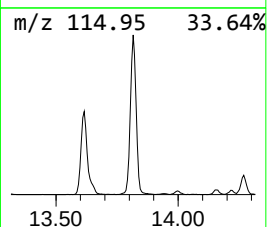
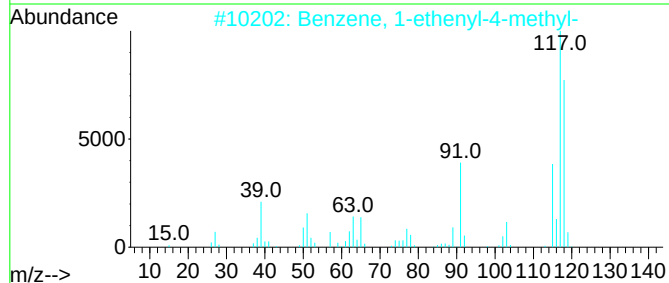
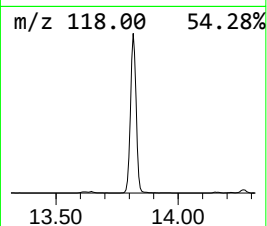
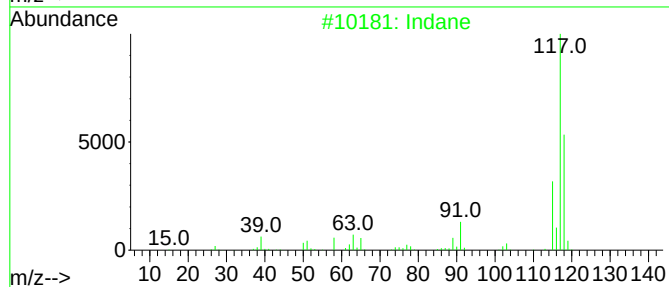
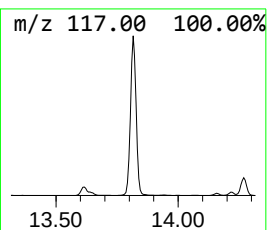
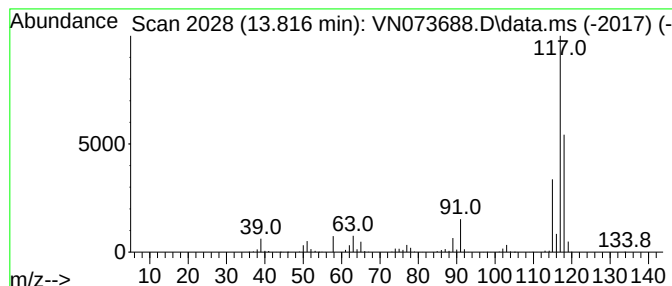
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Quant Title : SW846 8260

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.
13.816	74.84 ug/l	2650600	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	80
4			Deltacyclene	118	C9H10	007785-10-6	80
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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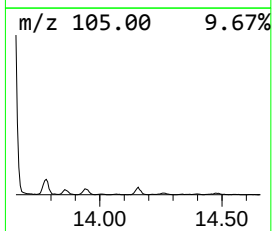
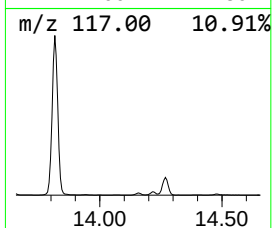
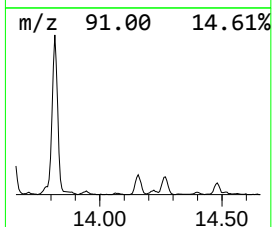
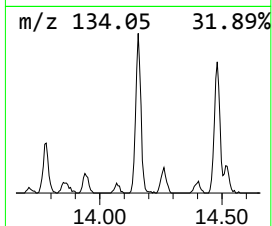
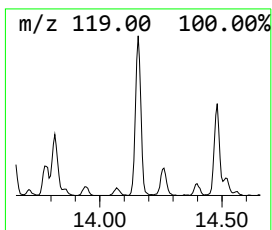
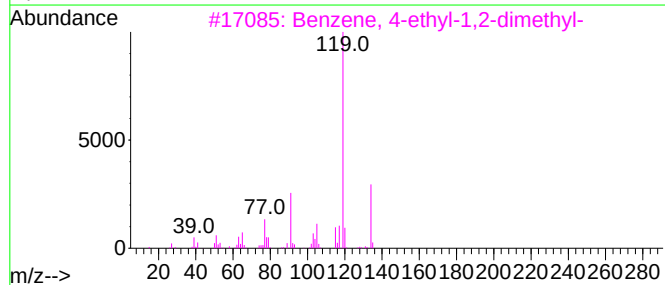
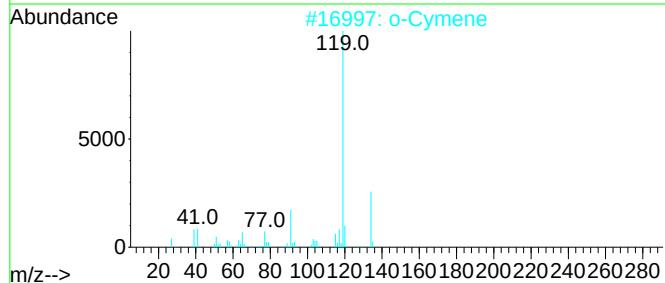
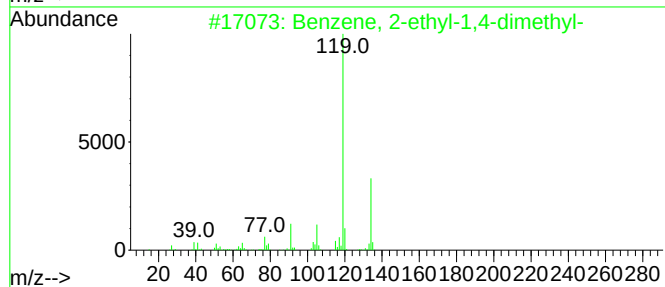
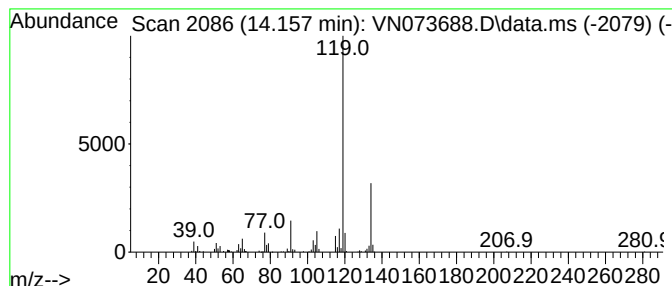
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	8.06 ug/l	285607	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
2			o-Cymene	134	C10H14	000527-84-4	94
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22R

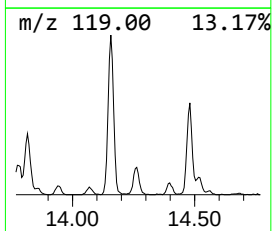
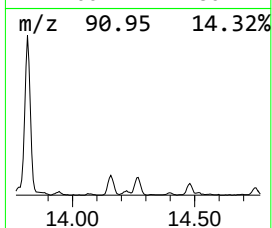
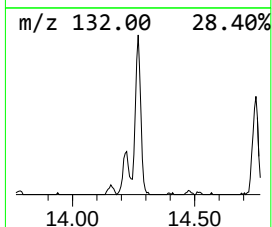
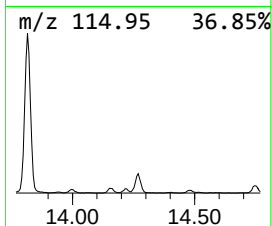
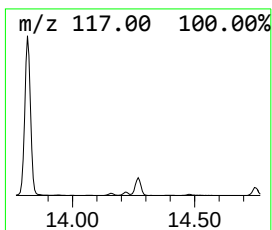
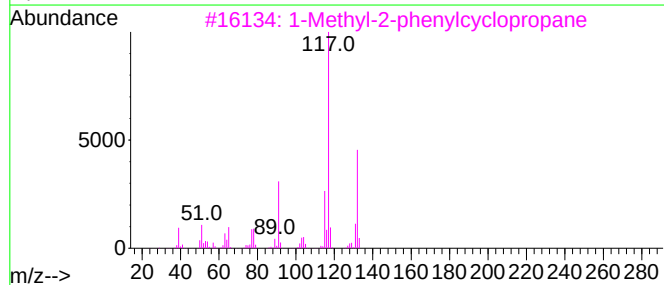
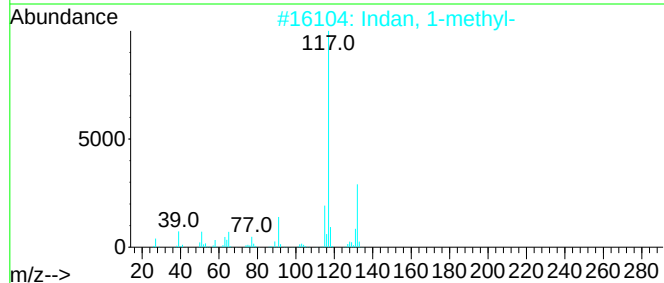
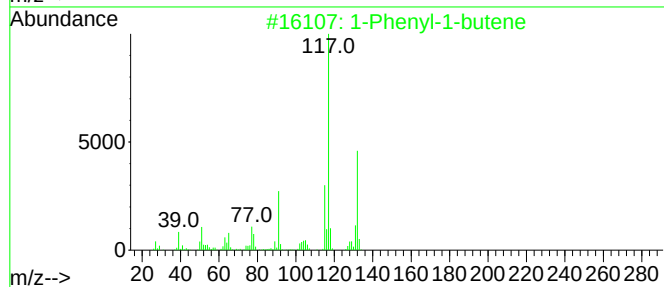
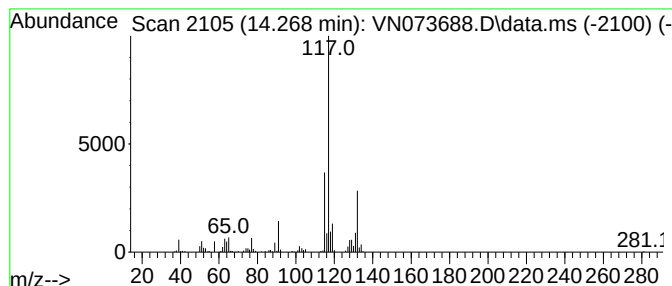
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Quant Title : SW846 8260

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

Peak Number 9 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	9.22 ug/l	326484	1,4-Dichlorobenzene-d4	13.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	83
2		Indan, 1-methyl-	132	C10H12	000767-58-8	81
3		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72
5		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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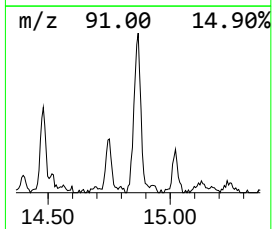
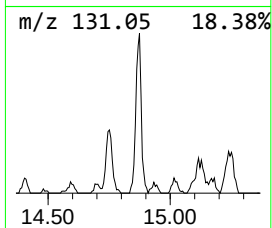
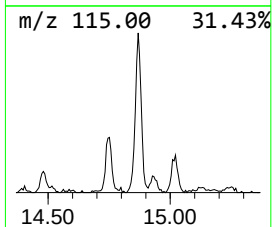
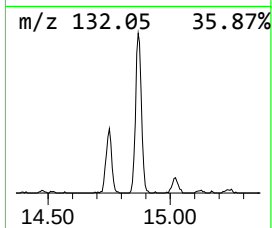
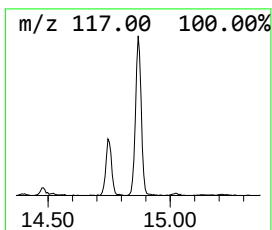
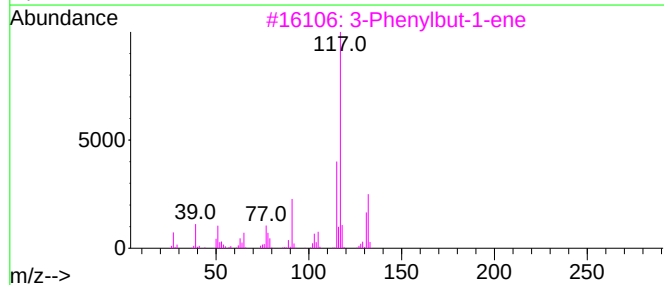
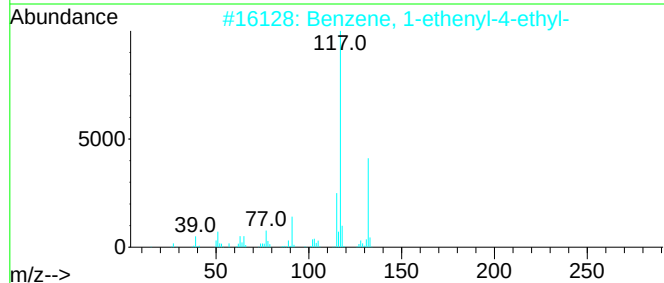
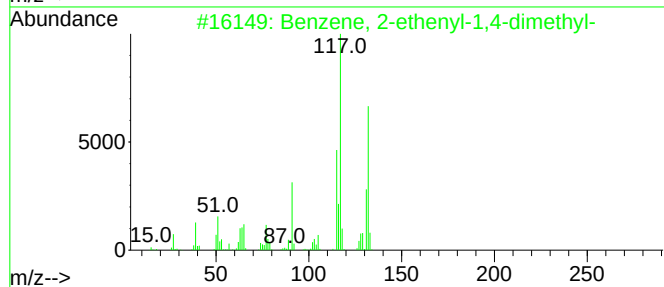
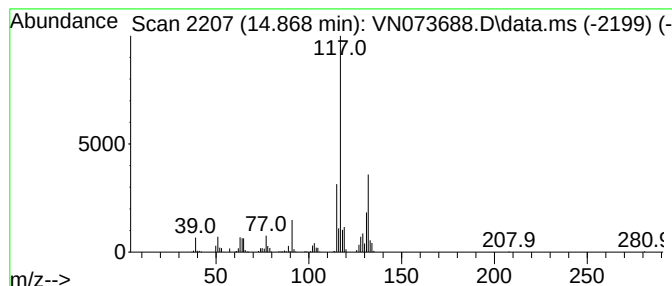
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	14.27 ug/l	505239	1,4-Dichlorobenzene-d4	13.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5		Indan, 1-methyl-	132	C10H12	000767-58-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
Data File : VN073688.D
Acq On : 02 Aug 2022 15:36
Operator : JC\MD
Sample : N3971-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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-	3.081	25.8	ug/l	623508	1	8.016	1208530	50.0
Cyclopropane, 1...	3.928	16.1	ug/l	390344	1	8.016	1208530	50.0
Isopropyl Alcohol	4.510	11.2	ug/l	271066	1	8.016	1208530	50.0
Cyclopentane	5.110	16.4	ug/l	396821	1	8.016	1208530	50.0
Cyclopentane, m...	7.063	7.9	ug/l	191235	1	8.016	1208530	50.0
Indane	13.816	74.8	ug/l	2650600	4	13.616	1770890	50.0
Benzene, 2-ethy...	14.157	8.1	ug/l	285607	4	13.616	1770890	50.0
1-Phenyl-1-butene	14.269	9.2	ug/l	326484	4	13.616	1770890	50.0
Benzene, 2-ethe...	14.868	14.3	ug/l	505239	4	13.616	1770890	50.0