

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
 Data File : VN071167.D
 Acq On : 04 Mar 2022 13:40
 Operator : JC\MD
 Sample : N1776-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 INF-03-22

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\82N021522W.M
 Title : SW846 8260

Signal : TIC: VN071167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.446	69	78	88	rVB	945443	1519377	2.67%	0.484%
2	3.140	182	196	215	rBV	4947493	11330470	19.88%	3.608%
3	3.522	250	261	284	rVV2	1953836	5299944	9.30%	1.687%
4	3.722	286	295	307	rVB	281489	703941	1.24%	0.224%
5	3.999	333	342	361	rVB	932003	2509277	4.40%	0.799%
6	4.263	375	387	402	rBV4	179338	659179	1.16%	0.210%
7	4.969	491	507	515	rBV	230849	832387	1.46%	0.265%
8	5.087	515	527	531	rVV	705934	2441731	4.28%	0.777%
9	5.163	532	540	568	rVB5	1396163	8289050	14.54%	2.639%
10	5.622	602	618	639	rBV	980541	3346282	5.87%	1.065%
11	5.934	659	671	685	rVB2	238128	764824	1.34%	0.244%
12	6.122	690	703	719	rBV2	407590	1244078	2.18%	0.396%
13	6.469	752	762	774	rVB	698619	2134658	3.75%	0.680%
14	6.610	774	786	794	rBV	496433	1549517	2.72%	0.493%
15	6.698	794	801	812	rVV3	252168	974139	1.71%	0.310%
16	6.898	826	835	850	rVB	597718	1738286	3.05%	0.553%
17	7.045	850	860	867	rBV2	202750	605894	1.06%	0.193%
18	7.145	867	877	886	rVV	2926632	8692573	15.25%	2.768%
19	7.216	886	889	901	rVB2	336235	798708	1.40%	0.254%
20	7.839	987	995	1005	rVB	1192199	2897861	5.08%	0.923%
21	8.016	1015	1025	1030	rBV	561465	1440436	2.53%	0.459%
22	8.087	1030	1037	1045	rVV4	2207797	5891447	10.34%	1.876%
23	8.175	1045	1052	1064	rVB2	800604	2097998	3.68%	0.668%
24	8.292	1064	1072	1078	rBV	326173	733591	1.29%	0.234%
25	8.457	1088	1100	1112	rBV	10250599	24532905	43.05%	7.811%
26	8.581	1113	1121	1127	rBV4	536333	1618866	2.84%	0.515%
27	8.704	1137	1142	1152	rVB	292013	699600	1.23%	0.223%
28	8.963	1176	1186	1199	rBV3	2234361	5521947	9.69%	1.758%
29	9.239	1228	1233	1243	rVB	377579	811851	1.42%	0.258%
30	9.457	1254	1270	1276	rBV2	835565	2544059	4.46%	0.810%
31	9.969	1349	1357	1361	rBV	765409	1518124	2.66%	0.483%
32	10.010	1361	1364	1372	rVB2	449325	862954	1.51%	0.275%
33	10.316	1409	1416	1422	rBV2	539314	1037650	1.82%	0.330%
34	10.433	1429	1436	1442	rBV	2600574	4842273	8.50%	1.542%
35	10.498	1442	1447	1461	rVV	3977315	7447554	13.07%	2.371%
36	10.633	1461	1470	1476	rVV2	343705	762755	1.34%	0.243%

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37	10.851	1501	1507	1518	rVB5	270658	637243	1.12%	0.203%
38	11.739	1650	1658	1665	rBV	2318328	4100280	7.19%	1.305%
39	11.839	1667	1675	1685	rVV	15474055	26248924	46.06%	8.357%
40	11.951	1685	1694	1706	rVB	29276301	56992473	100.00%	18.146%
41	12.274	1738	1749	1760	rBV	5087986	8492002	14.90%	2.704%
42	12.574	1793	1800	1808	rBV	1605520	2616525	4.59%	0.833%
43	12.727	1818	1826	1836	rVB	1901307	3267803	5.73%	1.040%
44	12.916	1847	1858	1863	rBV	2975206	4841114	8.49%	1.541%
45	12.974	1863	1868	1871	rVV	2167782	3767649	6.61%	1.200%
46	13.010	1871	1874	1878	rVV	3595523	5530358	9.70%	1.761%
47	13.051	1878	1881	1892	rVB	2723155	4170706	7.32%	1.328%
48	13.216	1901	1909	1918	rBV	4060565	6663920	11.69%	2.122%
49	13.363	1926	1934	1948	rVV	13328734	21502759	37.73%	6.846%
50	13.698	1980	1991	2001	rBV2	6196957	13235338	23.22%	4.214%
51	13.833	2007	2014	2015	rBV	656906	892150	1.57%	0.284%
52	13.868	2015	2020	2037	rVB	7152754	13528198	23.74%	4.307%
53	14.063	2046	2053	2058	rBV2	491848	853759	1.50%	0.272%
54	14.121	2058	2063	2067	rBV	602028	1046460	1.84%	0.333%
55	14.210	2073	2078	2084	rVB	1370961	2046708	3.59%	0.652%
56	14.274	2084	2089	2092	rVV	370804	592785	1.04%	0.189%
57	14.321	2092	2097	2105	rVB2	1525245	2469214	4.33%	0.786%
58	14.533	2125	2133	2136	rBV	960163	1497377	2.63%	0.477%
59	14.574	2136	2140	2145	rVB	740038	1149042	2.02%	0.366%
60	14.804	2173	2179	2185	rBV	933533	1443562	2.53%	0.460%
61	14.921	2191	2199	2206	rBV2	1628885	3311605	5.81%	1.054%
62	15.498	2289	2297	2305	rBV	1350444	2486363	4.36%	0.792%

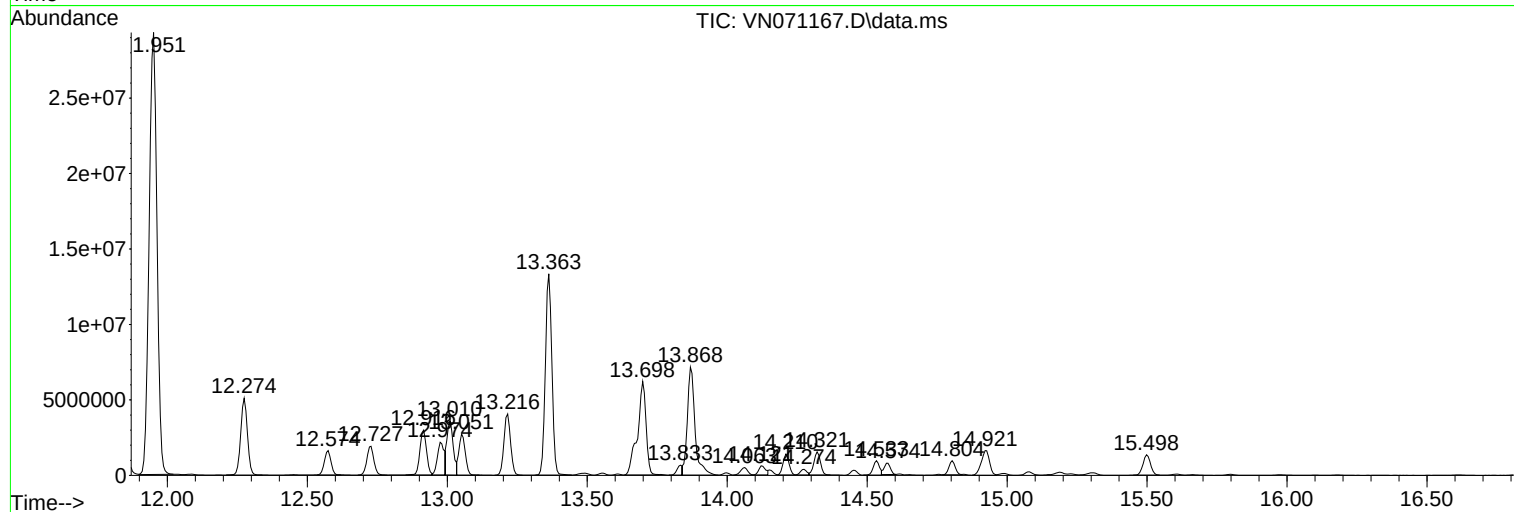
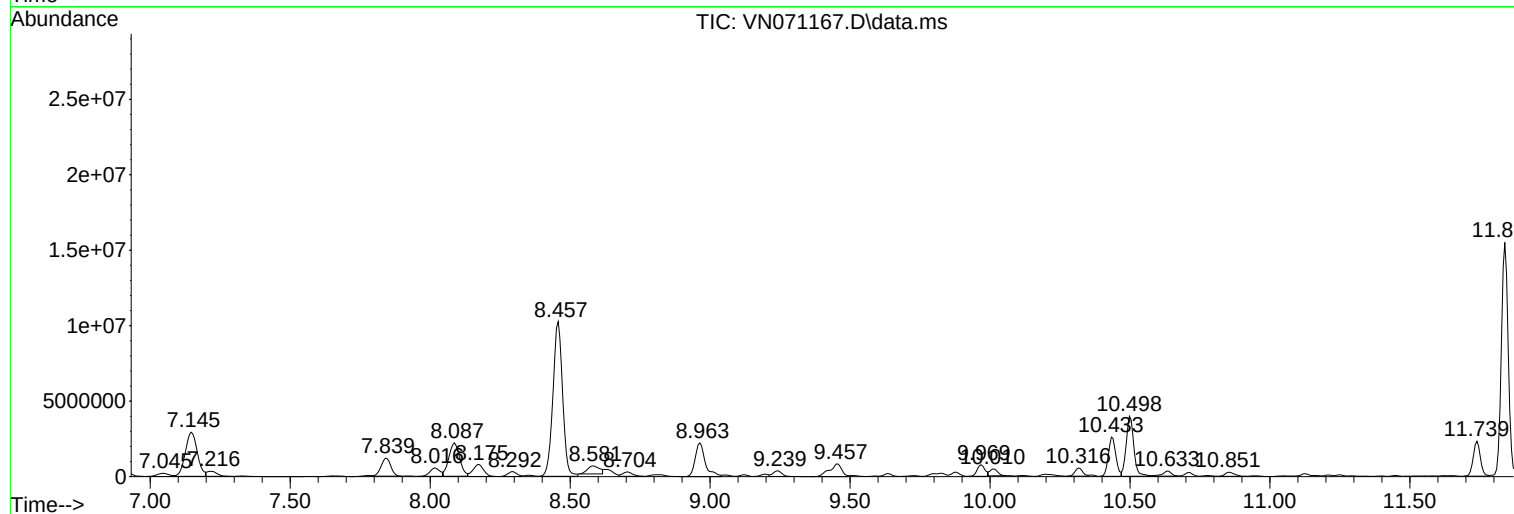
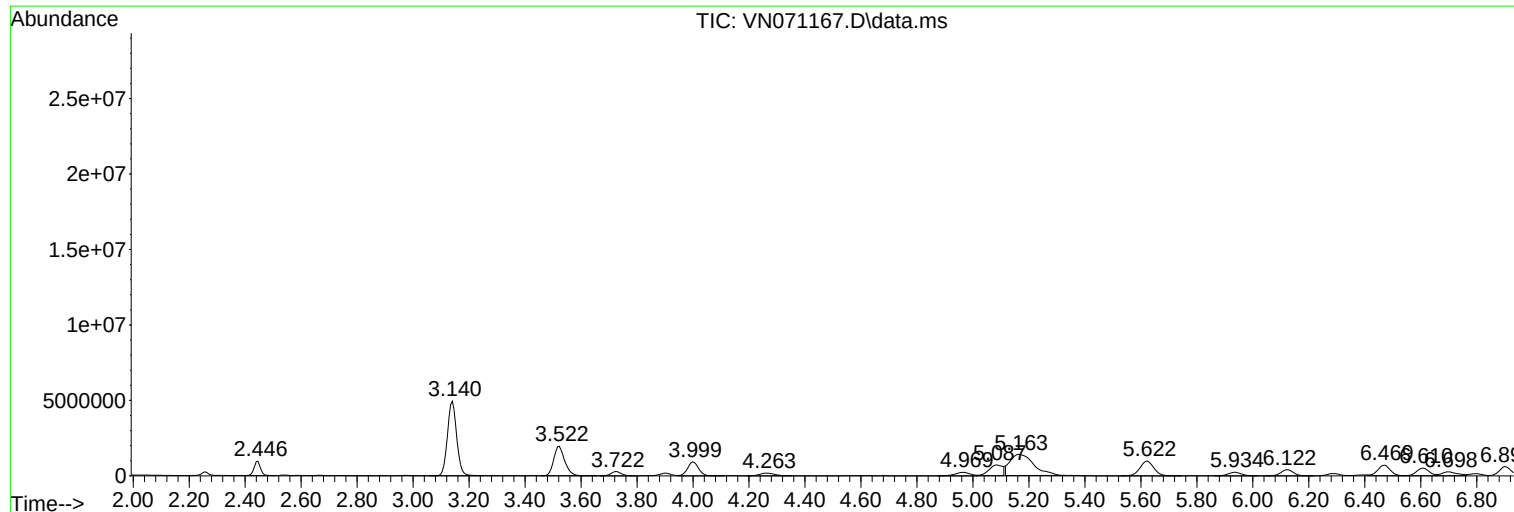
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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



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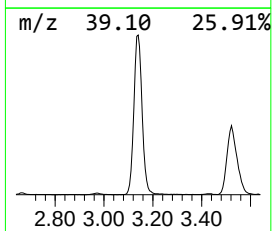
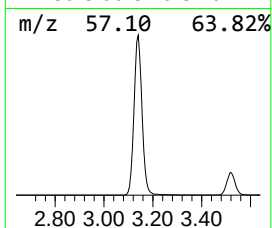
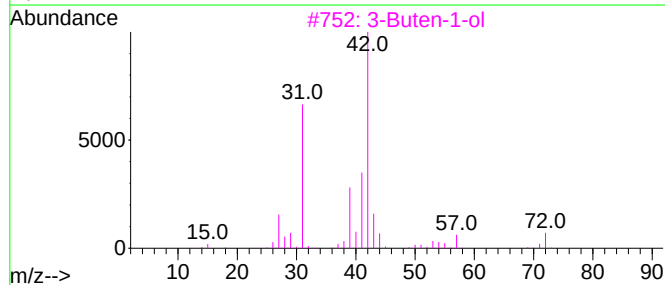
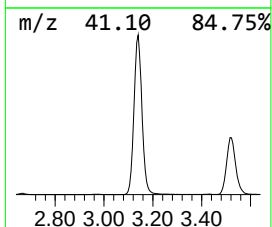
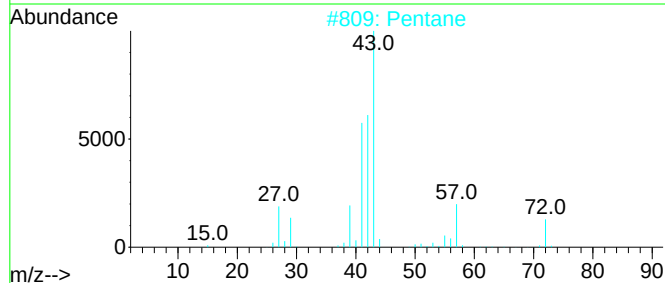
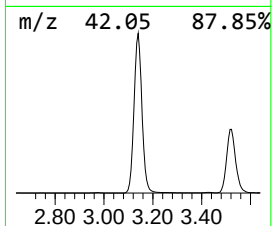
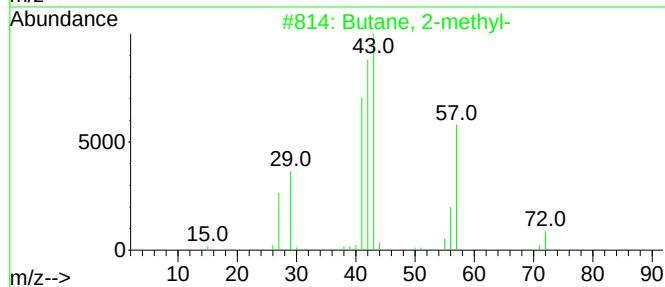
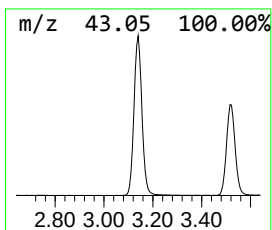
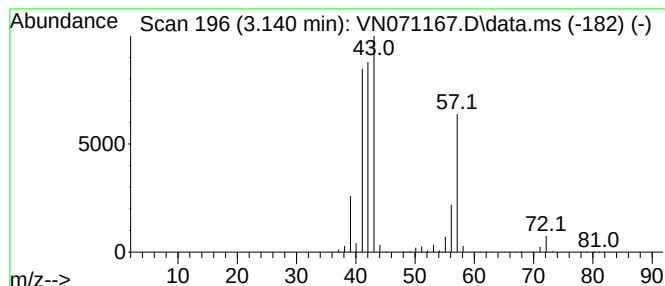
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	96.16 ug/l	11330500	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	91
2	Pentane			72	C5H12	000109-66-0	33
3	3-Buten-1-ol			72	C4H8O	000627-27-0	28
4	Methane, isocyanato-			57	C2H3NO	000624-83-9	9
5	1-Butene			56	C4H8	000106-98-9	9



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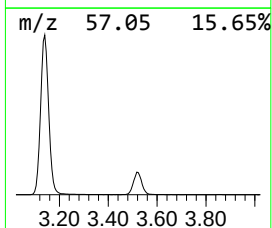
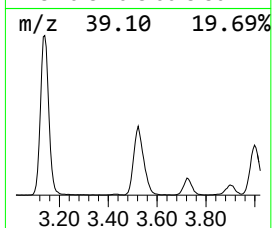
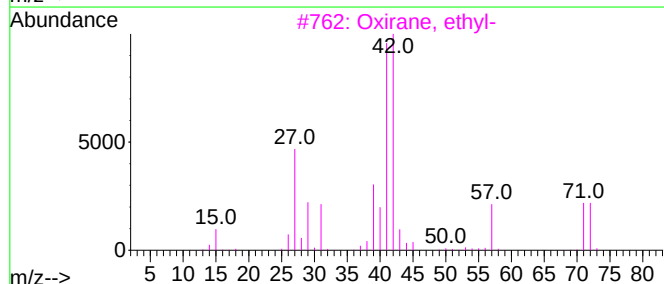
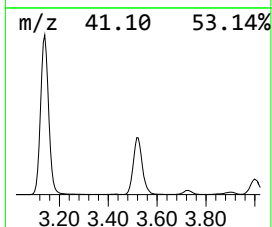
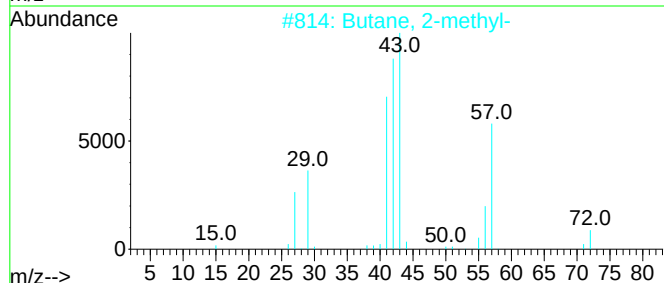
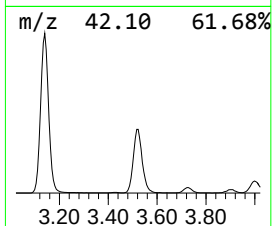
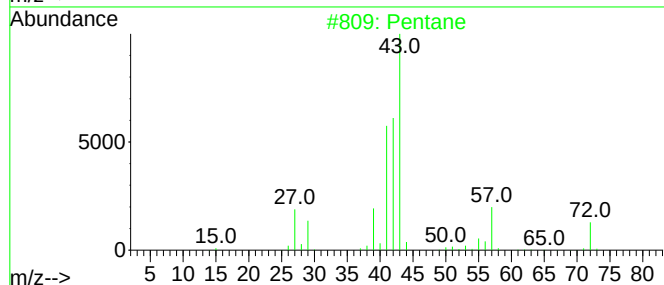
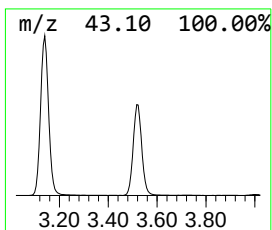
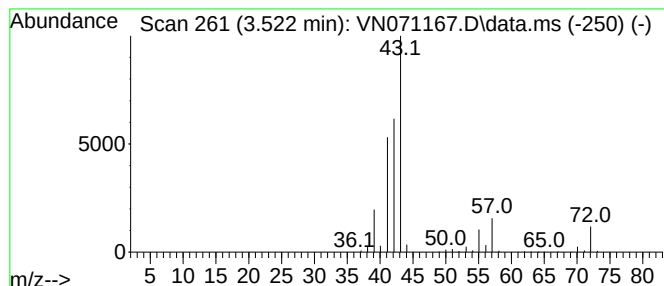
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.522	44.98 ug/l	5299940	Pentafluorobenzene	8.081

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	64
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	16



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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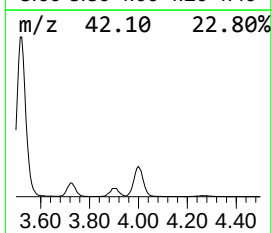
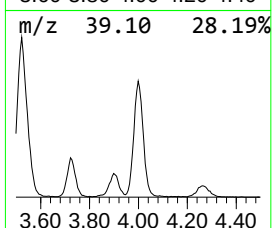
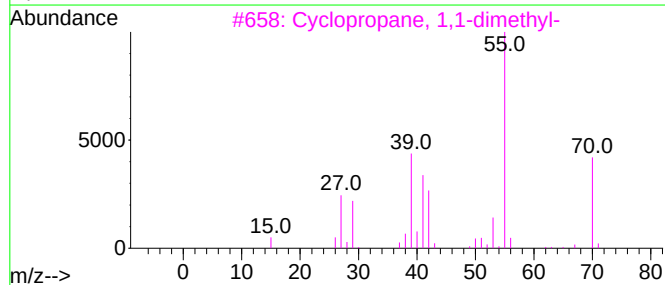
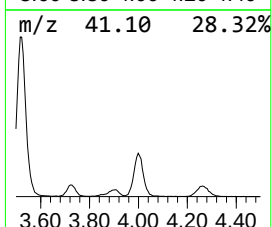
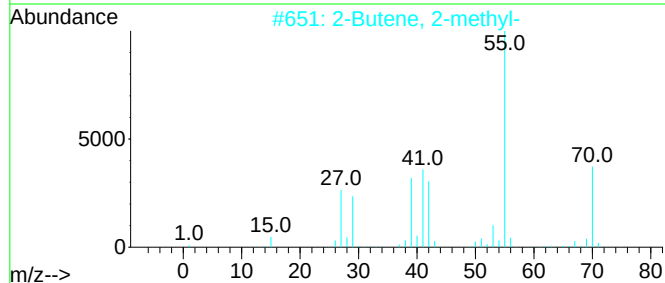
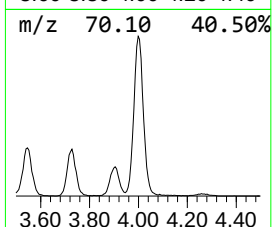
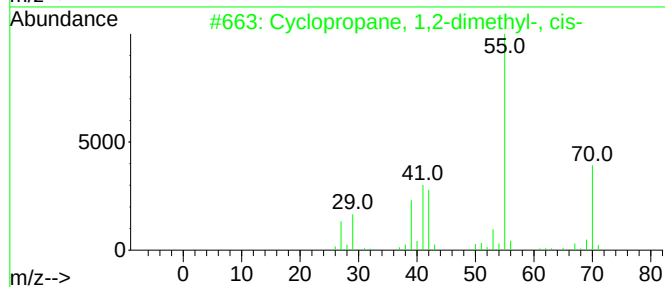
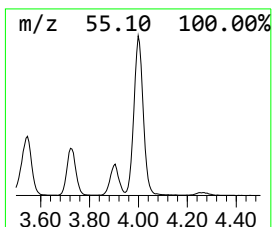
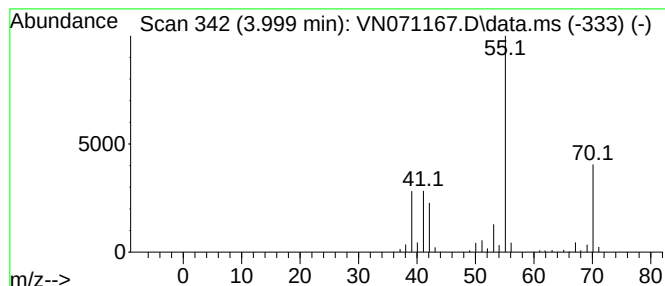
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.999	21.30 ug/l	2509280	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80



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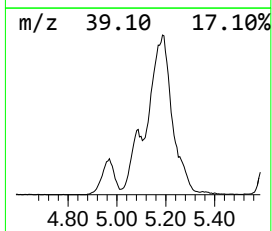
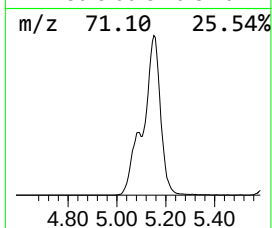
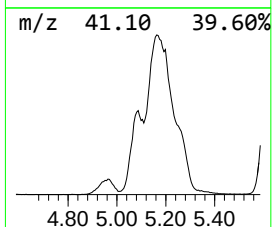
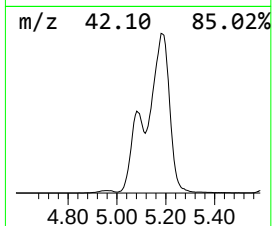
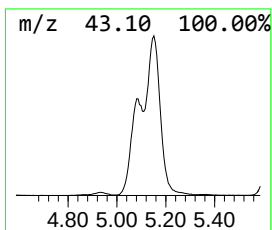
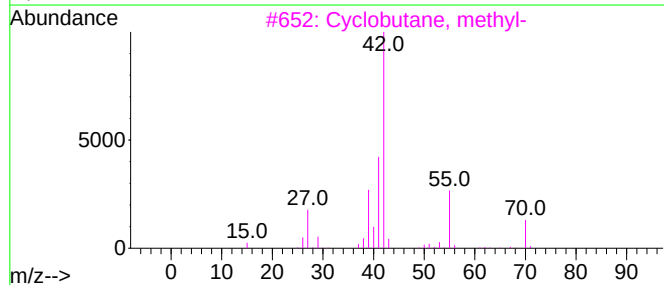
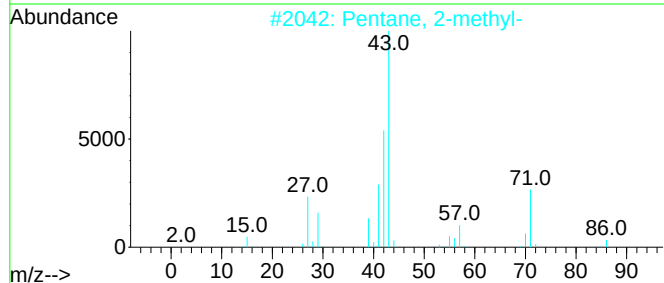
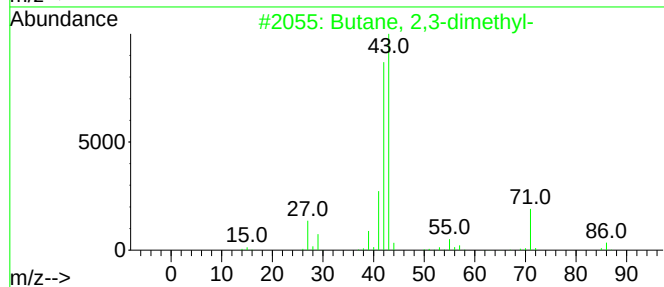
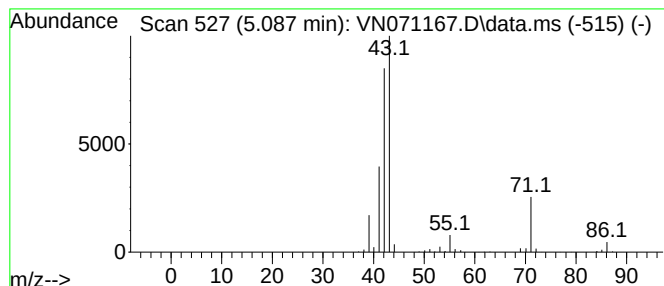
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	20.72 ug/l	2441730	Pentafluorobenzene	8.081

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	53
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	38
4			C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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ClientSampleId :
INF-03-22

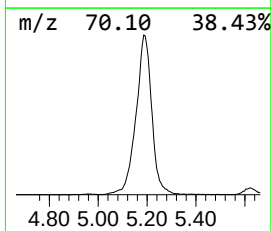
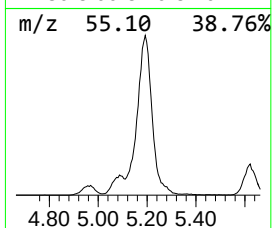
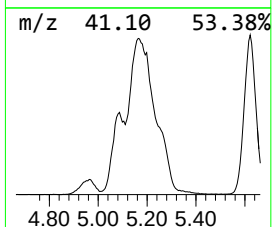
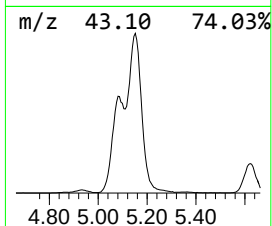
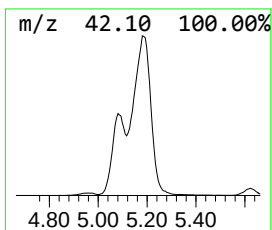
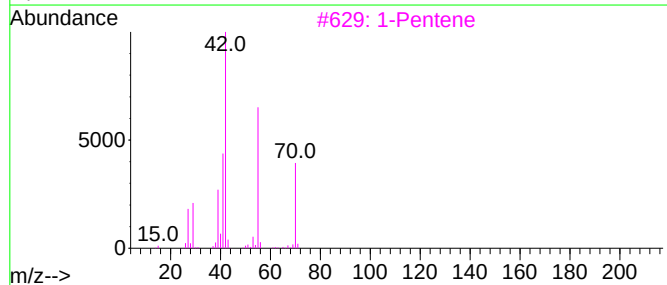
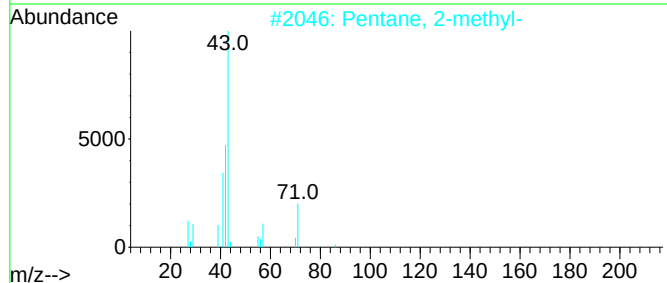
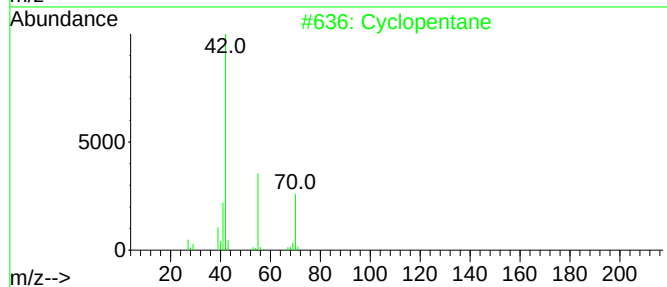
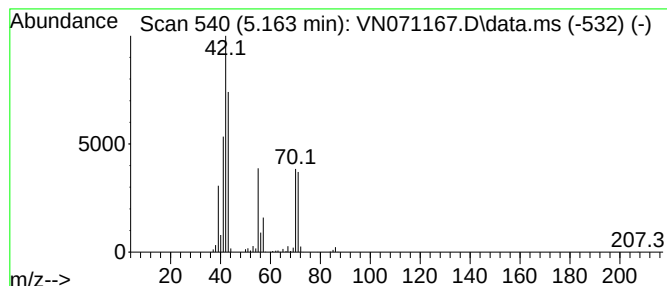
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	70.35 ug/l	8289050	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	53
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			1-Pentene	70	C5H10	000109-67-1	50
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	40
5			Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

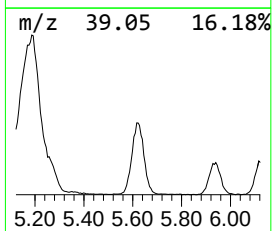
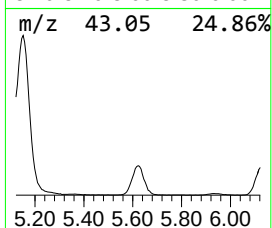
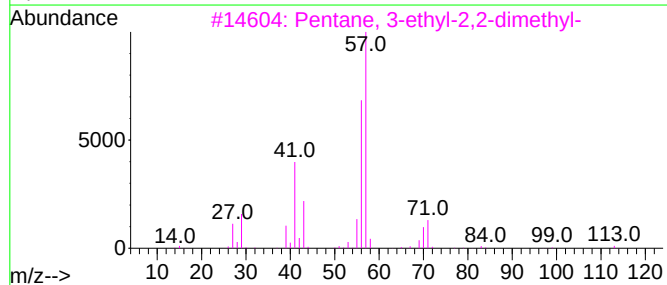
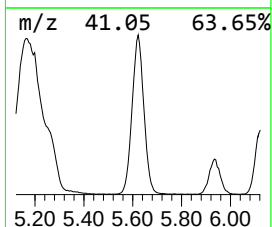
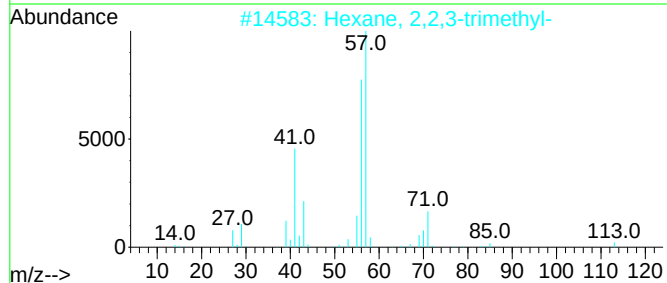
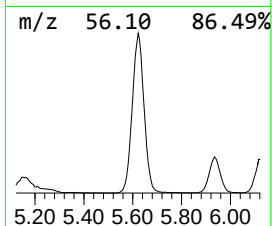
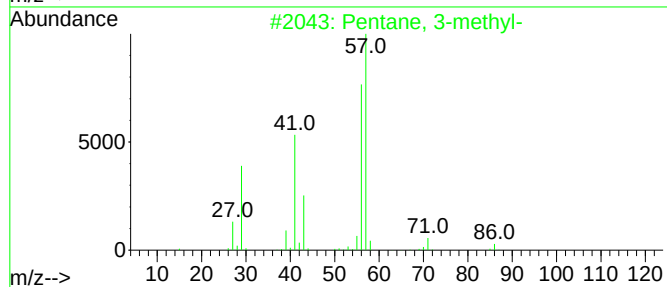
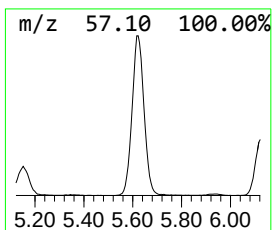
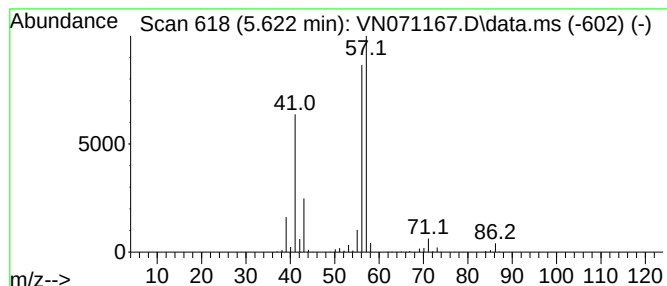
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	28.40 ug/l	3346280	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
5			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

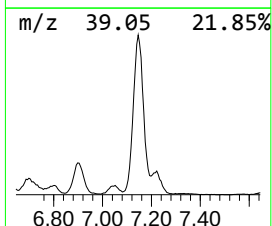
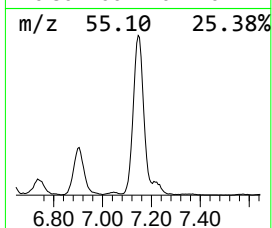
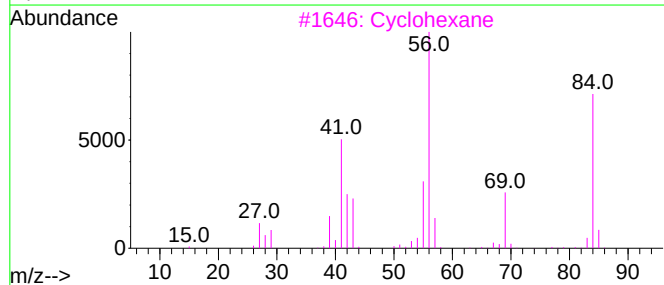
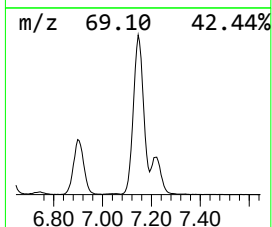
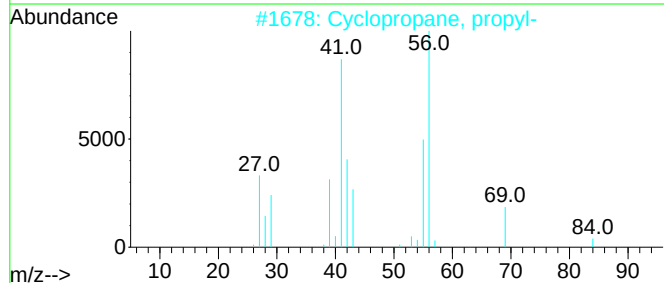
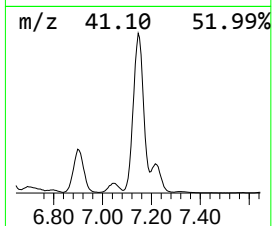
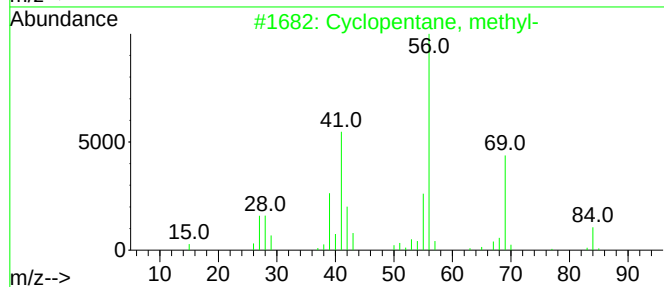
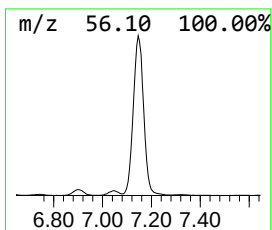
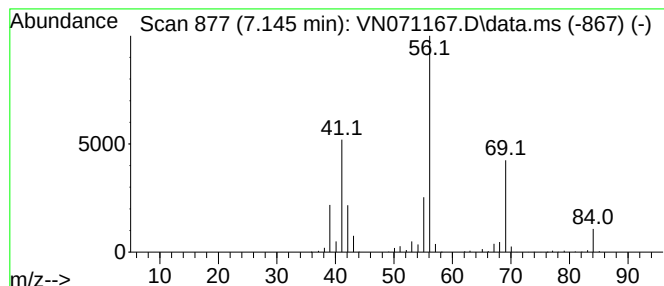
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	73.77 ug/l	8692570	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclopropane, propyl-	84	C6H12	002415-72-7	78
3			Cyclohexane	84	C6H12	000110-82-7	78
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

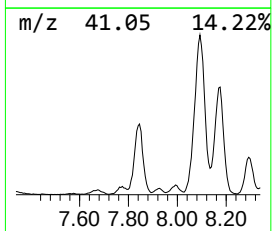
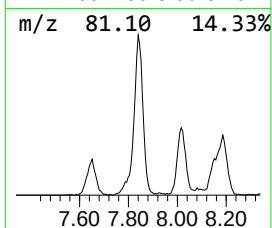
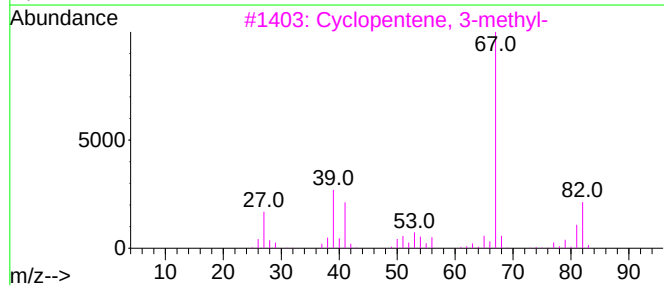
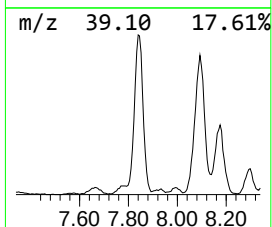
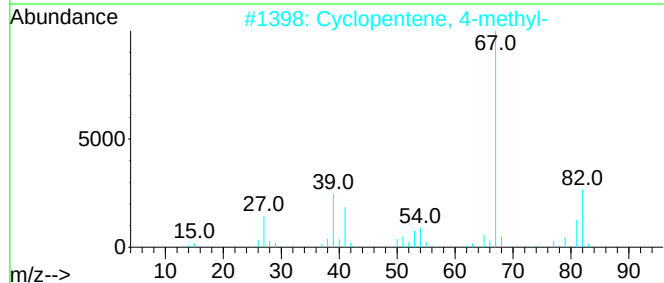
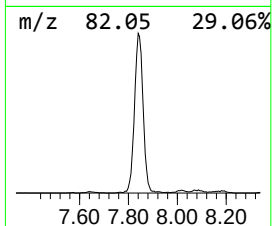
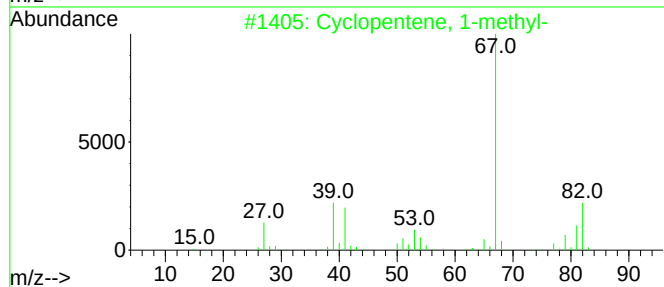
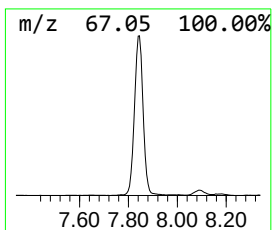
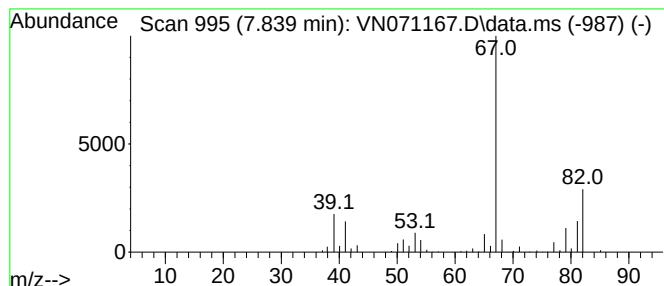
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.839	24.59 ug/l	2897860	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	90
3			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	83
5			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

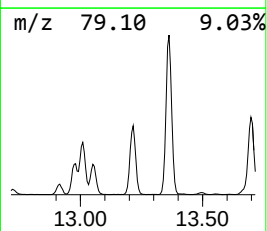
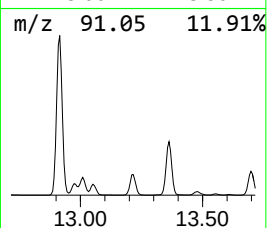
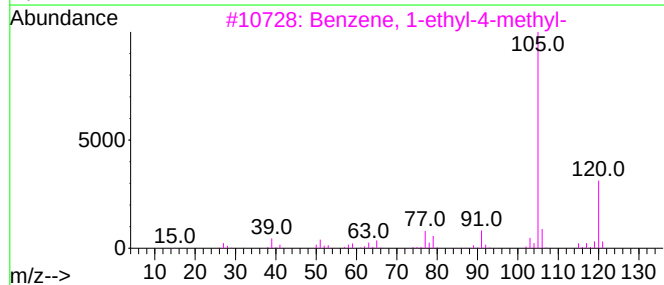
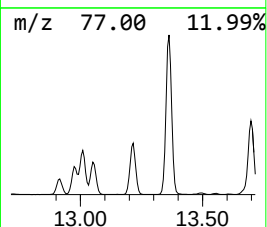
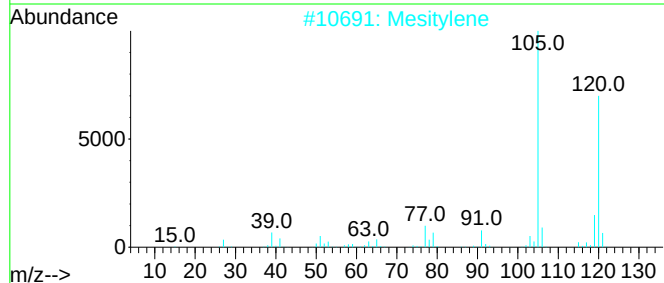
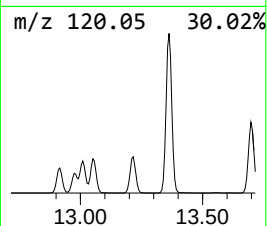
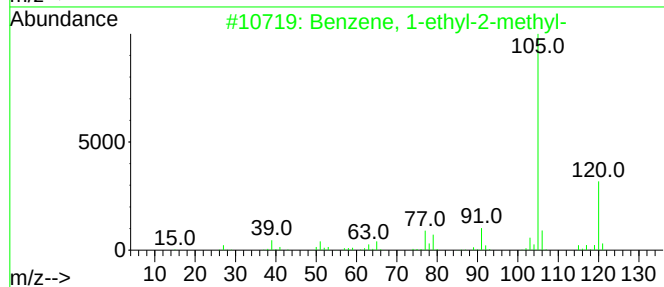
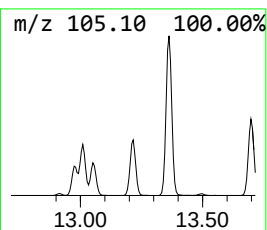
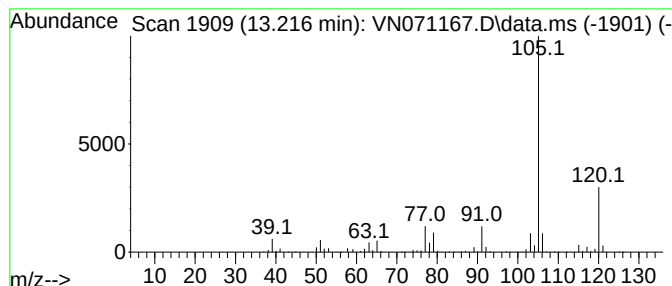
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	25.17 ug/l	6663920	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Mesitylene	120	C9H12	000108-67-8	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

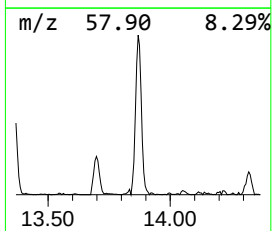
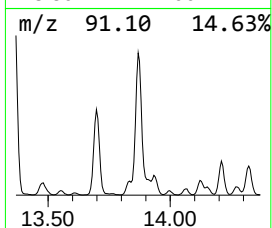
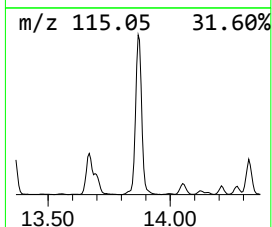
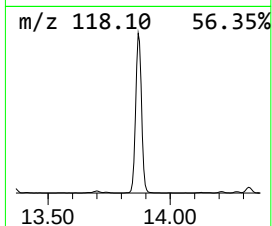
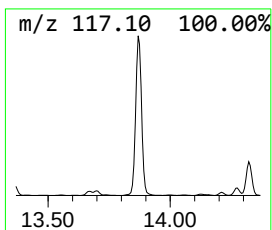
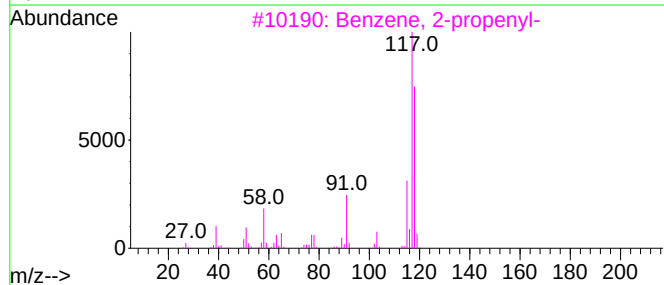
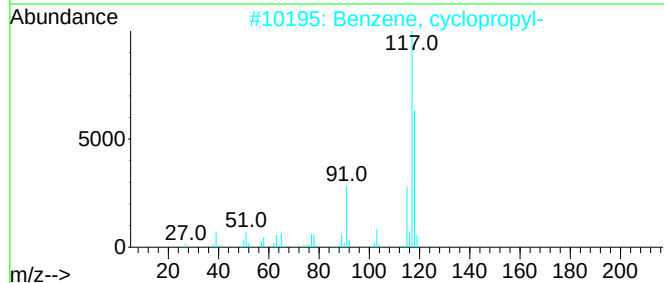
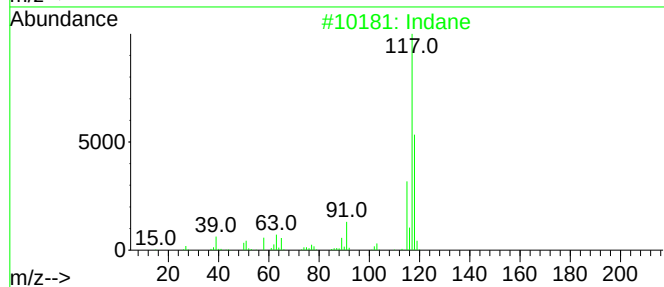
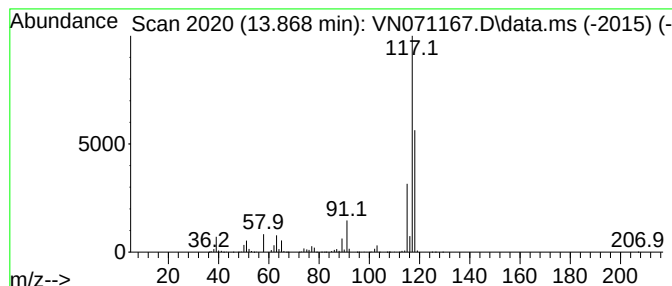
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	51.11 ug/l	13528200	1,4-Dichlorobenzene-d4	13.669

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	64
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030422\
Data File : VN071167.D
Acq On : 04 Mar 2022 13:40
Operator : JC\MD
Sample : N1776-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF-03-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021522W.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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Pentane	3.522	45.0	ug/l	5299940	1	8.081	5891450	50.0
Cyclopropane, 1...	3.999	21.3	ug/l	2509280	1	8.081	5891450	50.0
Butane, 2,3-dim...	5.087	20.7	ug/l	2441730	1	8.081	5891450	50.0
Cyclopentane	5.163	70.3	ug/l	8289050	1	8.081	5891450	50.0
Pentane, 3-methyl-	5.622	28.4	ug/l	3346280	1	8.081	5891450	50.0
Cyclopentane, m...	7.145	73.8	ug/l	8692570	1	8.081	5891450	50.0
Cyclopentene, 1...	7.839	24.6	ug/l	2897860	1	8.081	5891450	50.0
Benzene, 1-ethy...	13.216	25.2	ug/l	6663920	4	13.669	13235300	50.0
Indane	13.868	51.1	ug/l	13528200	4	13.669	13235300	50.0