

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
 Data File : VN074310.D
 Acq On : 03 Sep 2022 01:27
 Operator : JC\MD
 Sample : N4355-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-23

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\82N090222W.M
 Title : SW846 8260

Signal : TIC: VN074310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.405	79	88	97	rBV	2339246	3541553	1.36%	0.355%
2	3.087	194	204	234	rVB	17052850	35672321	13.73%	3.574%
3	3.457	257	267	290	rBV	2704195	6480267	2.49%	0.649%
4	5.075	533	542	575	rVB5	1771032	10268502	3.95%	1.029%
5	5.534	604	620	637	rBV	1370370	4699945	1.81%	0.471%
6	6.040	692	706	722	rBV	905473	2766075	1.06%	0.277%
7	7.069	869	881	906	rVB	6933736	20393890	7.85%	2.043%
8	8.022	1034	1043	1052	rBV2	5485493	13993428	5.38%	1.402%
9	8.392	1095	1106	1114	rBV3	1058232	2791554	1.07%	0.280%
10	8.510	1114	1126	1132	rBV7	935445	2909511	1.12%	0.292%
11	8.904	1183	1193	1199	rBV2	1164174	2814681	1.08%	0.282%
12	9.392	1260	1276	1294	rBV	3244737	8476968	3.26%	0.849%
13	10.445	1449	1455	1460	rBV	3966024	6696720	2.58%	0.671%
14	11.786	1674	1683	1693	rBV2	58666584	90236957	34.72%	9.041%
15	11.898	1693	1702	1713	rVV3	133285076	259893165	100.00%	26.041%
16	12.222	1745	1757	1774	rVB	30536244	46917123	18.05%	4.701%
17	12.516	1796	1807	1816	rVB	3117586	5176540	1.99%	0.519%
18	12.857	1857	1865	1870	rBV	9130506	14050397	5.41%	1.408%
19	12.921	1870	1876	1879	rVV2	32982999	49795303	19.16%	4.989%
20	12.957	1879	1882	1886	rVV	17960698	27275259	10.49%	2.733%
21	12.998	1886	1889	1899	rVB	13806129	19781793	7.61%	1.982%
22	13.157	1909	1916	1927	rBV	19739736	30678787	11.80%	3.074%
23	13.310	1928	1942	1949	rBV2	107793324	154375591	59.40%	15.468%
24	13.645	1988	1999	2008	rBV	22566900	37510329	14.43%	3.758%
25	13.816	2022	2028	2032	rVV	18129425	27915903	10.74%	2.797%
26	14.004	2053	2060	2065	rBV2	1774696	3080927	1.19%	0.309%
27	14.068	2065	2071	2074	rVV	3146984	5282000	2.03%	0.529%
28	14.098	2074	2076	2081	rVV	2709832	3353381	1.29%	0.336%
29	14.157	2081	2086	2091	rVV	5117211	7599926	2.92%	0.761%
30	14.263	2100	2104	2114	rVB2	4859625	7850237	3.02%	0.787%
31	14.474	2133	2140	2143	rBV	3066341	4778537	1.84%	0.479%
32	14.516	2143	2147	2152	rVB	4502100	6508291	2.50%	0.652%
33	14.745	2181	2186	2192	rBV	4219386	6480221	2.49%	0.649%
34	14.868	2198	2207	2213	rBV2	8071885	15823221	6.09%	1.585%
35	15.015	2225	2232	2240	rBV	2096590	3650556	1.40%	0.366%
36	15.127	2240	2251	2255	rBV3	1051198	2656848	1.02%	0.266%

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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\82N090222W.M
Title : SW846 8260

37	15.433	2289	2303	2310	rBV	16597835	29473629	11.34%	2.953%
38	16.527	2481	2489	2502	rVB	4567317	9887910	3.80%	0.991%
39	16.733	2515	2524	2533	rBV	2915006	6495912	2.50%	0.651%

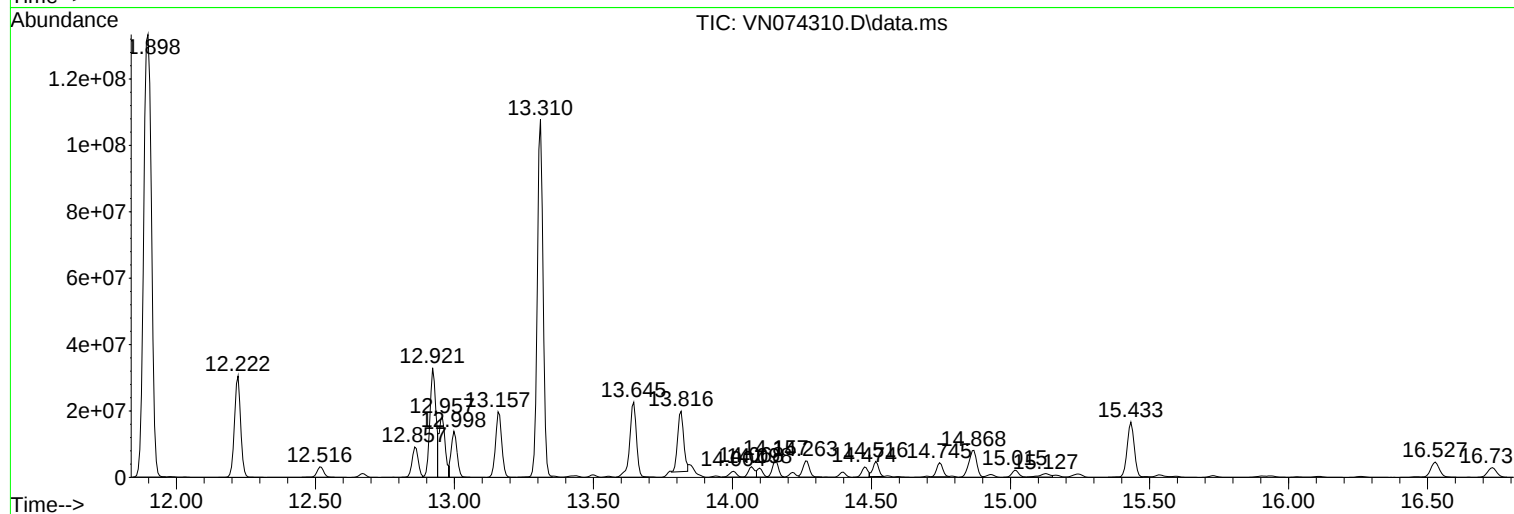
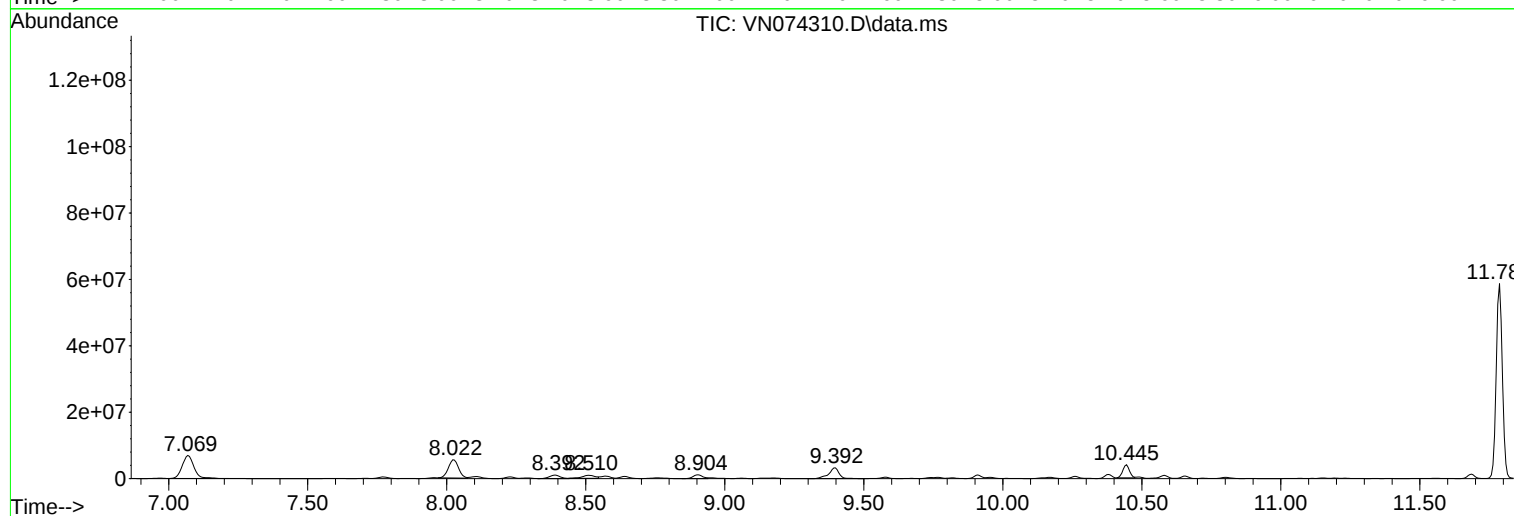
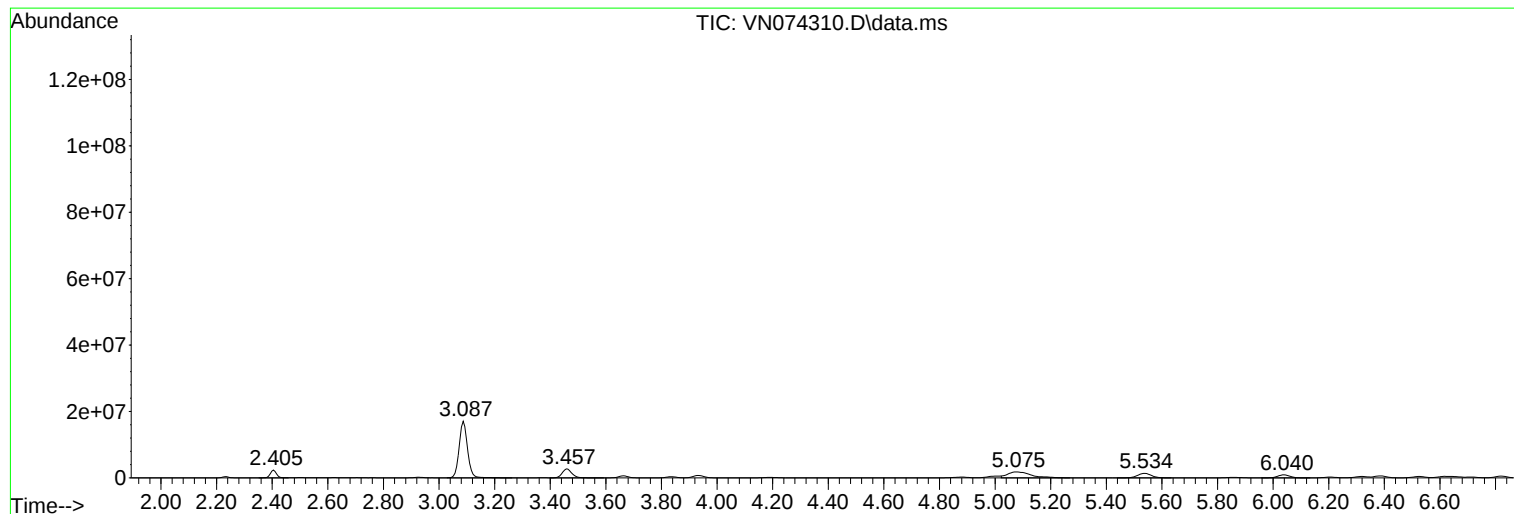
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



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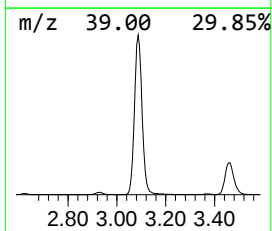
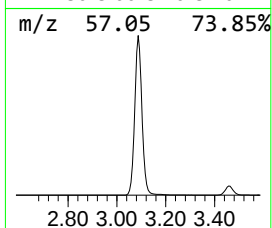
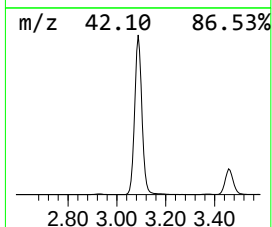
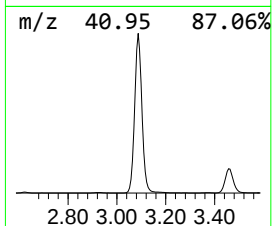
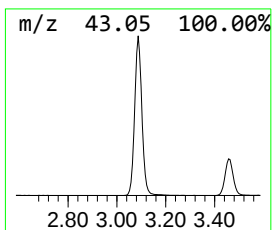
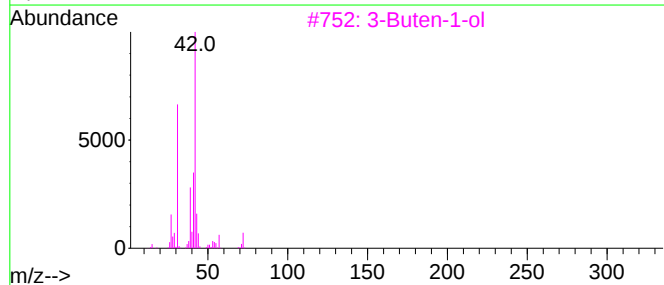
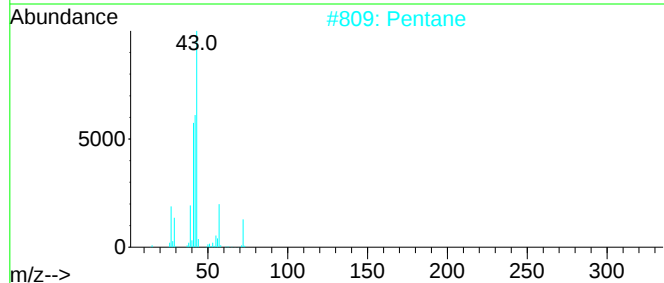
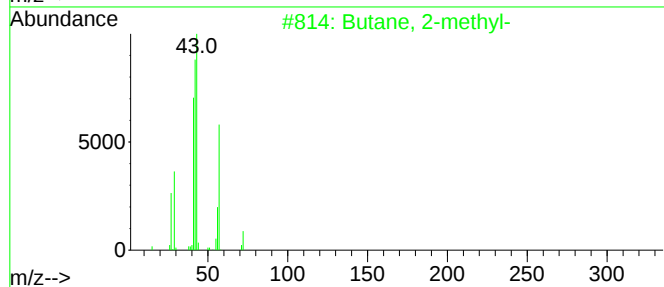
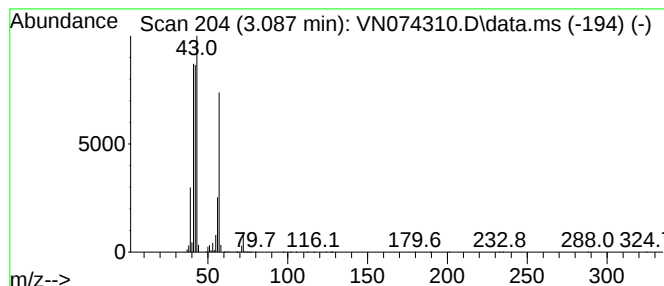
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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.
3.087	127.46 ug/l	35672300	Pentafluorobenzene	8.016

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	43
3	3-Buten-1-ol			72	C4H8O	000627-27-0	28
4	1-Butene			56	C4H8	000106-98-9	10
5	1-Propene, 2-methyl-			56	C4H8	000115-11-7	9



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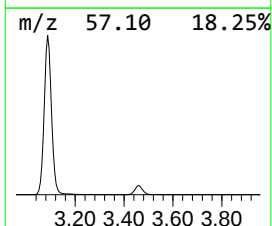
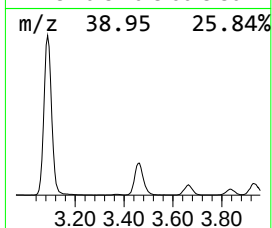
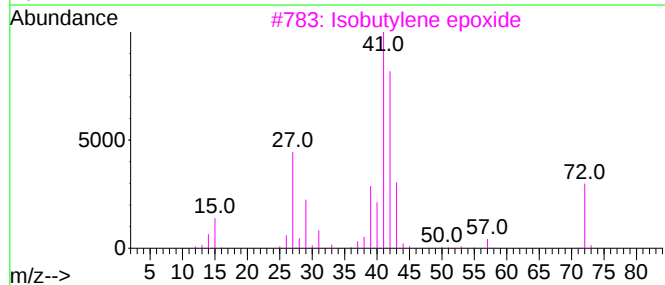
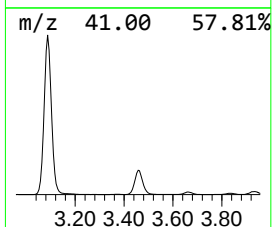
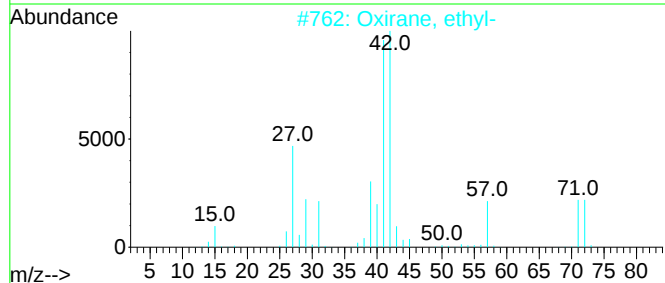
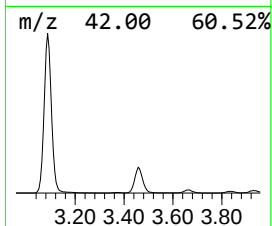
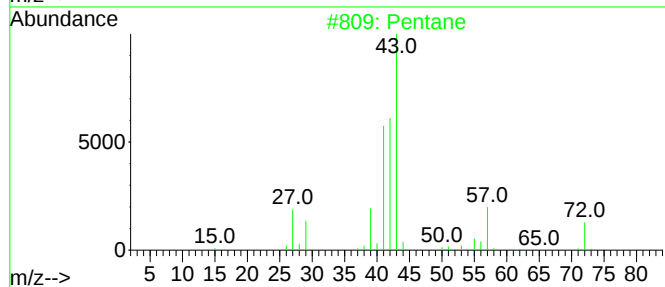
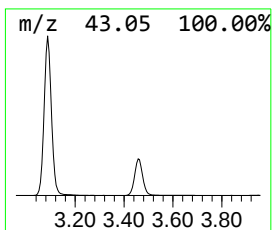
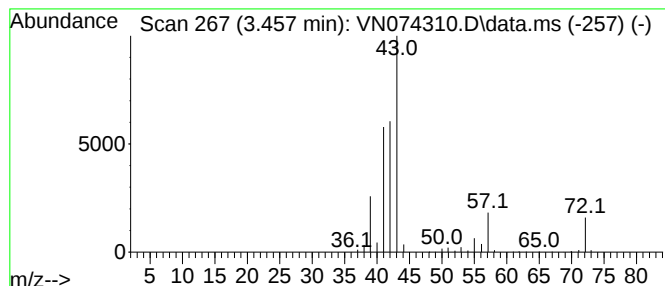
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	23.15 ug/l	6480270	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Isobutylene epoxide	72	C4H8O	000558-30-5	47
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	25



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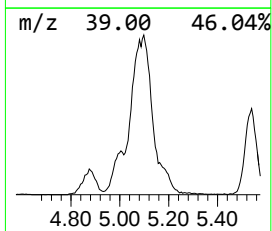
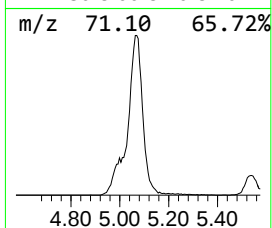
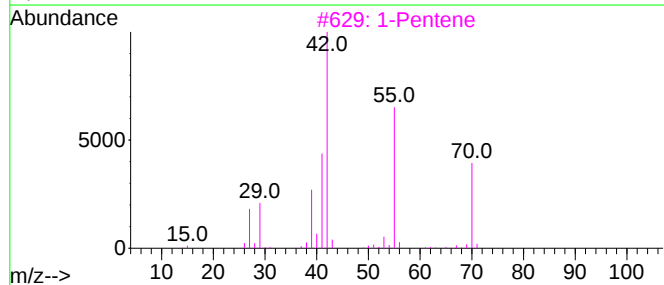
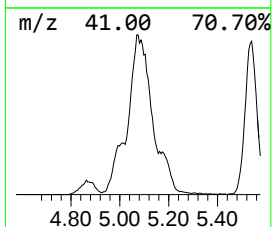
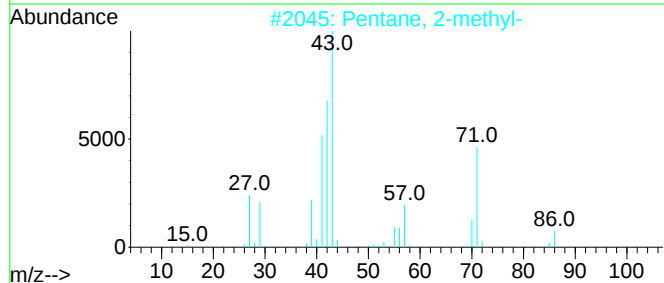
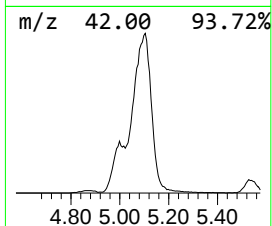
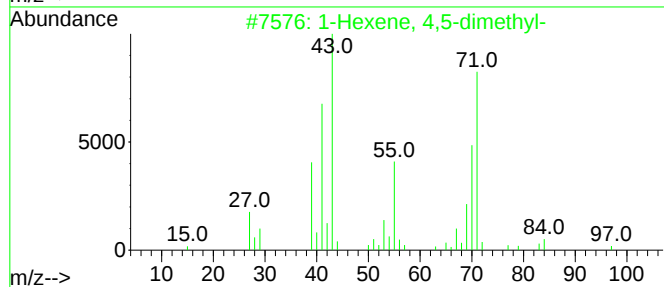
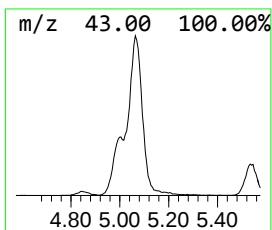
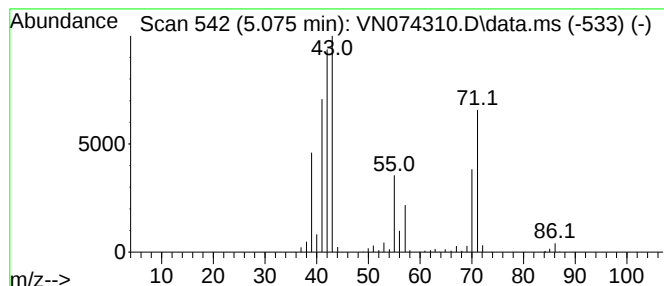
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown5.075 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	36.69 ug/l	10268500	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	47
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	46
3		1-Pentene	70	C5H10	000109-67-1	43
4		Cyclopentane	70	C5H10	000287-92-3	32
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	28



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Instrument :
MSVOA_N
ClientSampleId :
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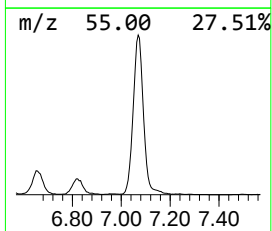
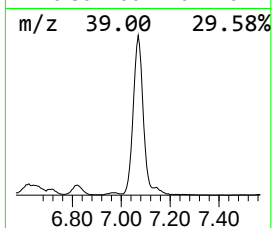
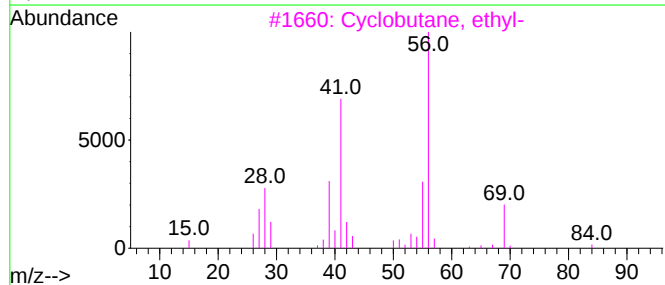
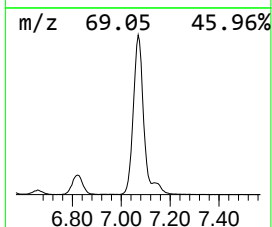
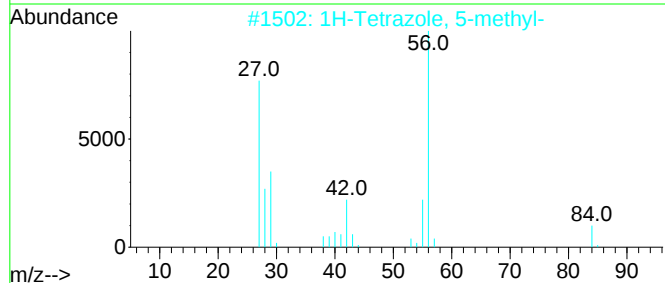
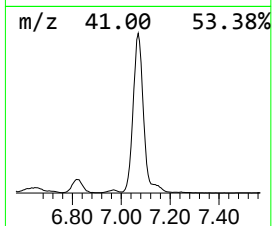
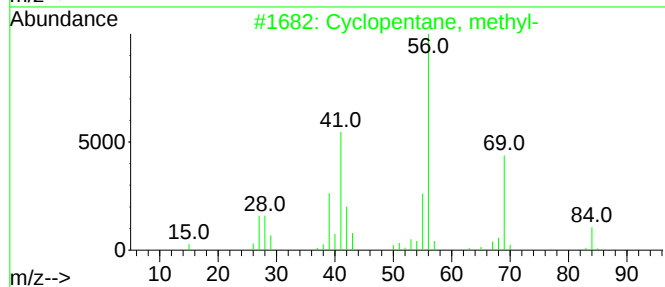
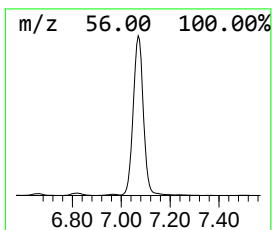
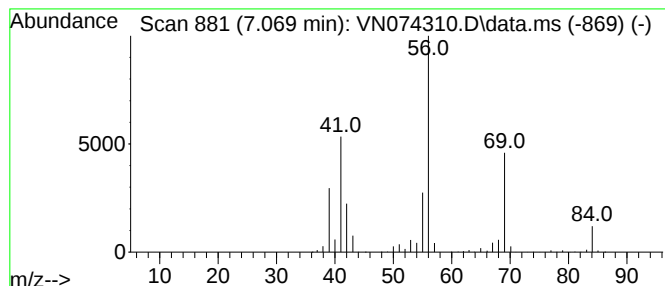
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	72.87 ug/l	20393900	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4		Cyclobutane	56	C4H8	000287-23-0	53
5		Cyclohexane	84	C6H12	000110-82-7	50



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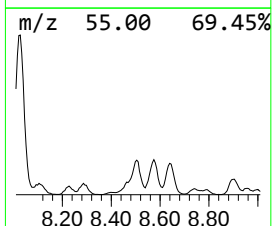
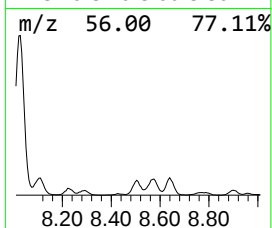
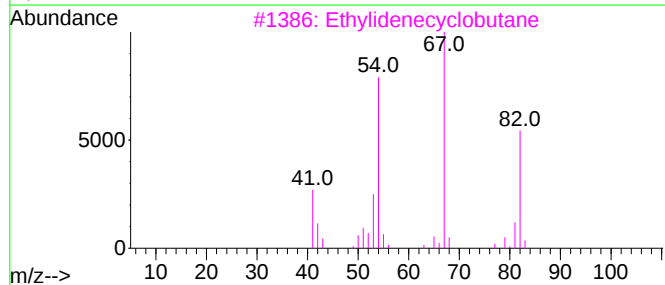
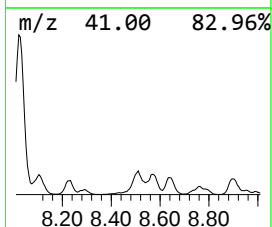
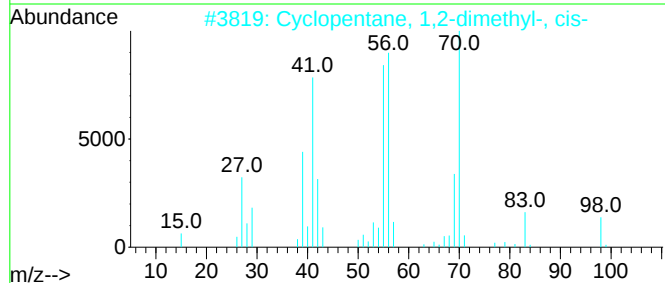
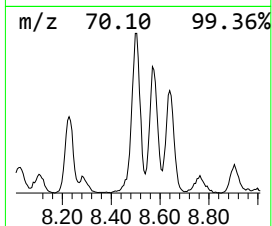
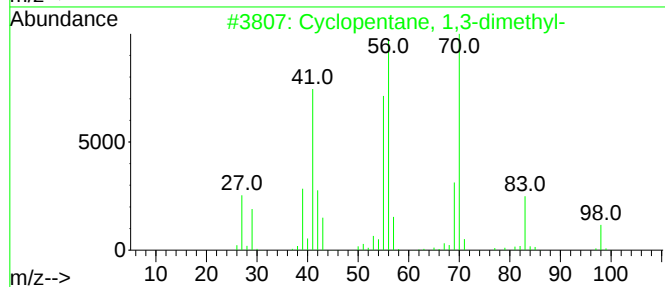
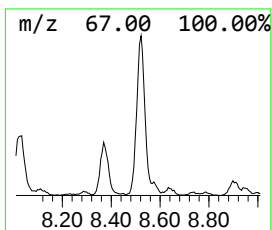
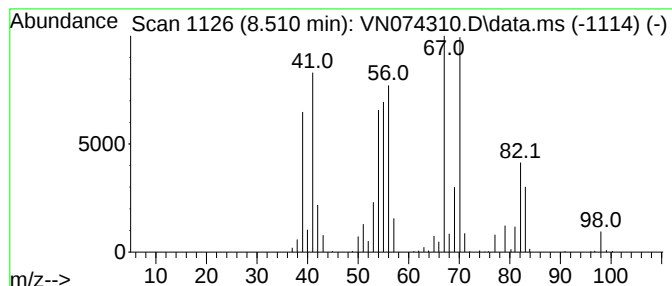
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	51.68 ug/l	2909510	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	50
2			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	46
3			Ethylidenecyclobutane	82	C6H10	001528-21-8	46
4			Cyclopropane, (1-methylethylidene)-	82	C6H10	004741-86-0	45
5			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

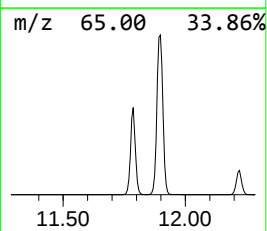
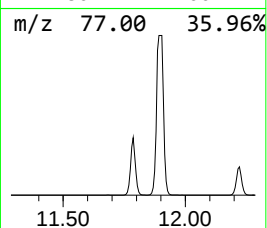
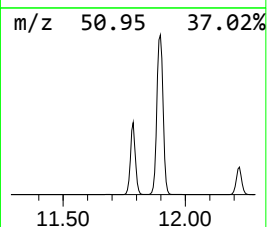
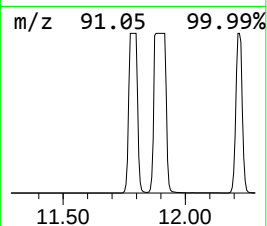
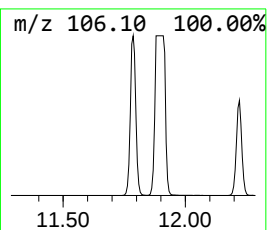
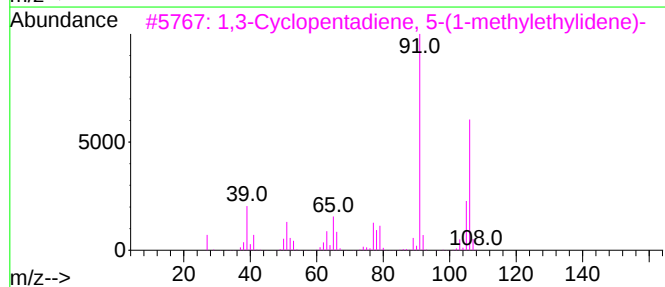
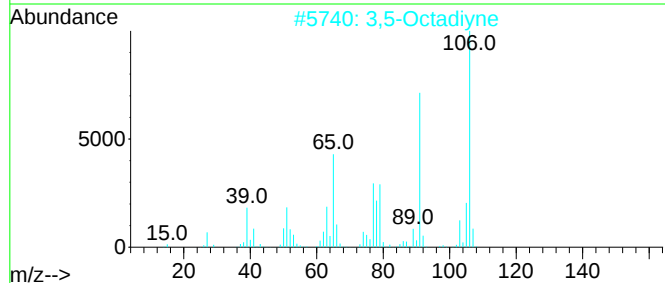
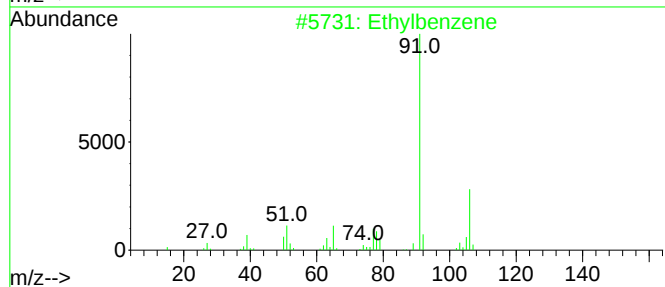
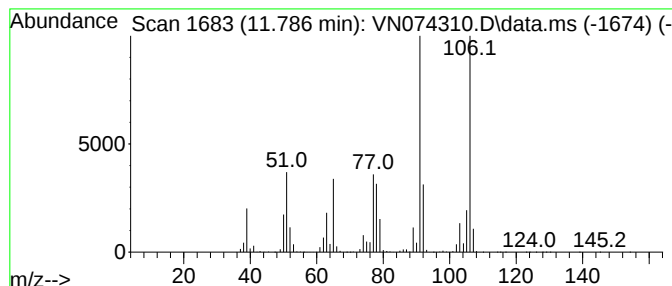
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 6 3,5-Octadiyne Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.786	50.00 ug/l	90237000	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylbenzene	106	C8H10	000100-41-4	93
2	3,5-Octadiyne	106	C8H10	016387-70-5	90
3	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	68
4	o-Xylene	106	C8H10	000095-47-6	62
5	p-Xylene	106	C8H10	000106-42-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23

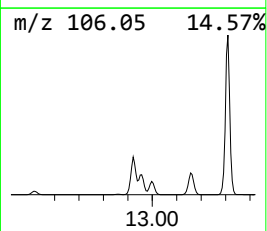
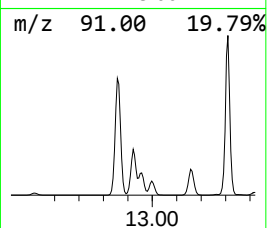
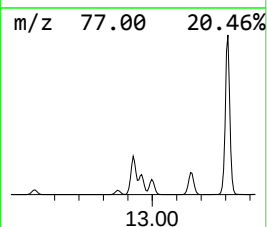
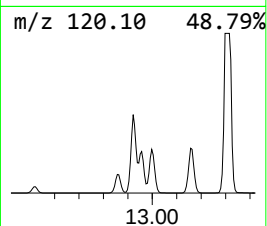
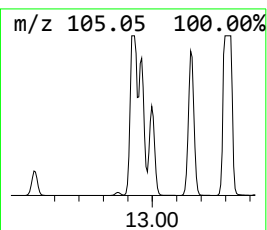
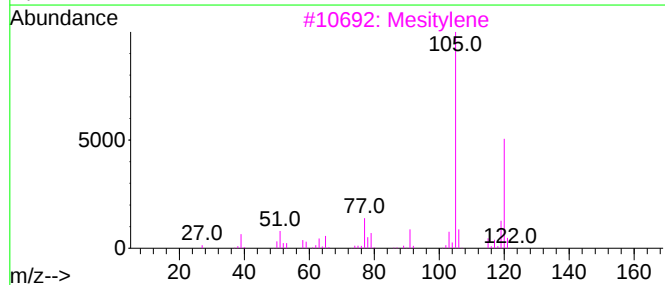
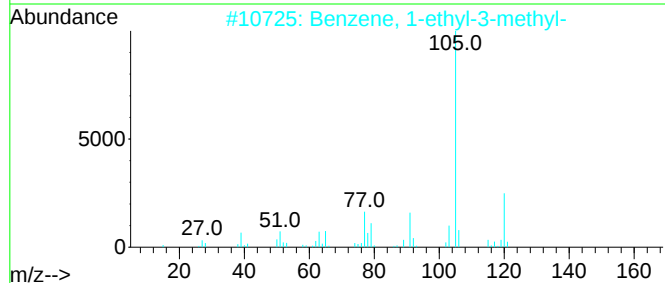
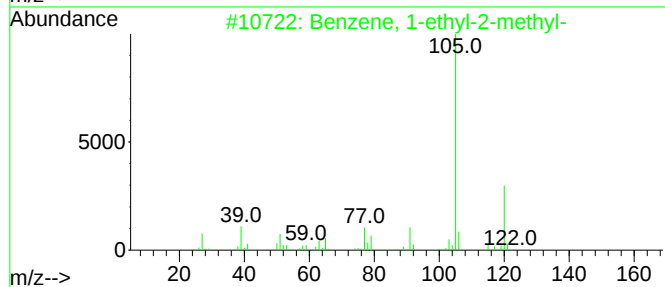
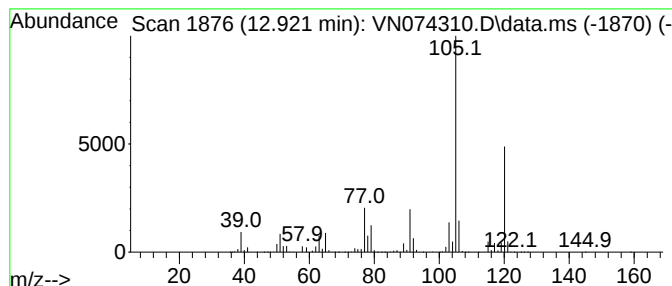
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	66.38 ug/l	49795300	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	90
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
3			Mesitylene	120	C9H12	000108-67-8	87
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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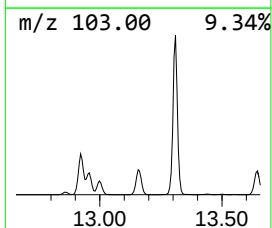
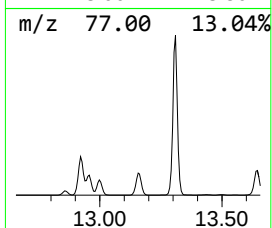
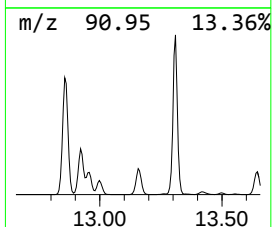
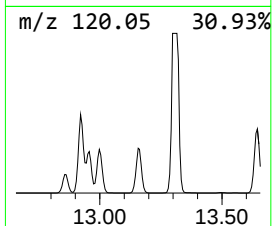
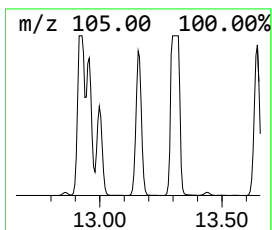
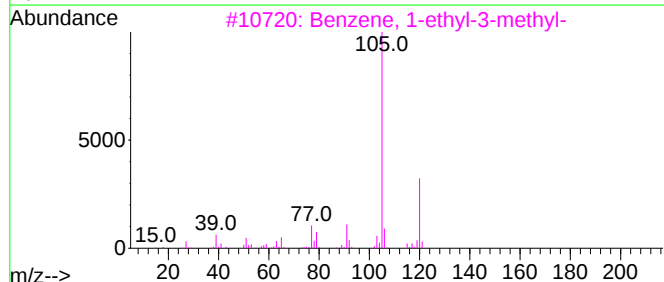
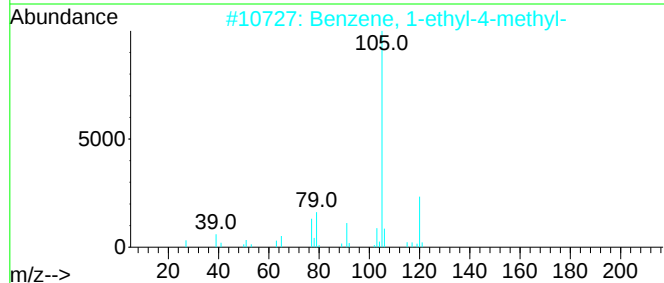
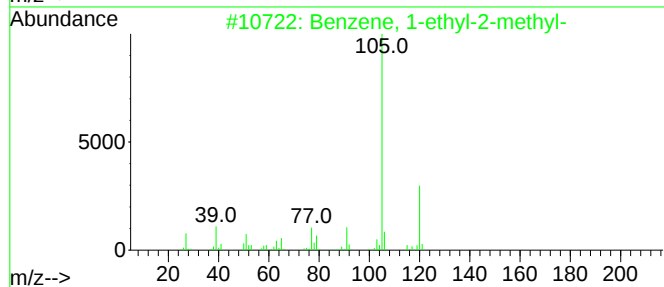
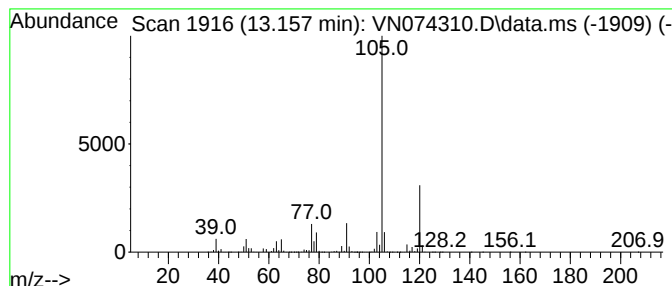
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	40.89 ug/l	30678800	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	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

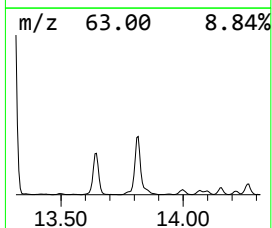
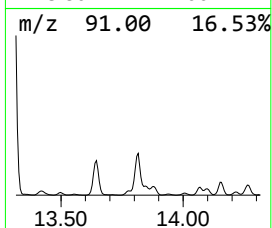
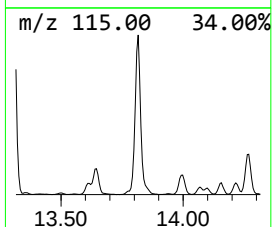
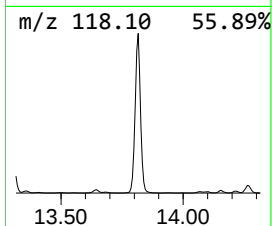
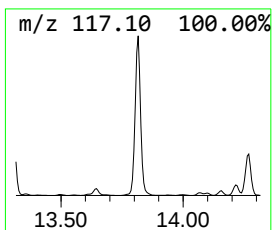
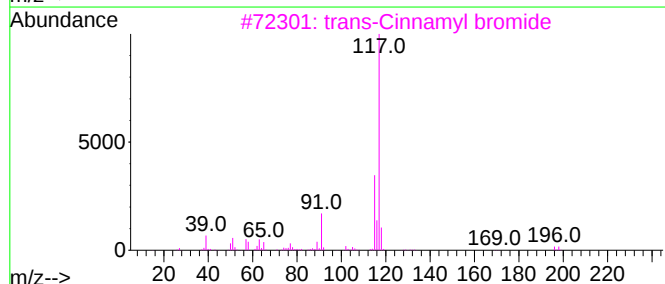
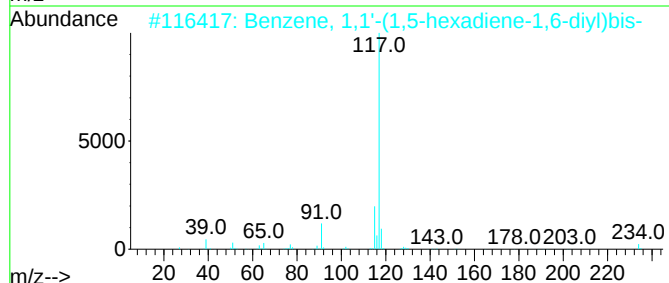
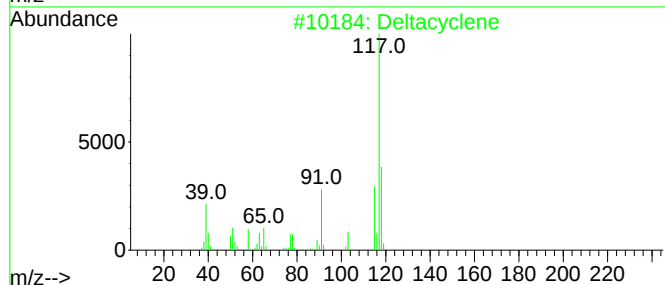
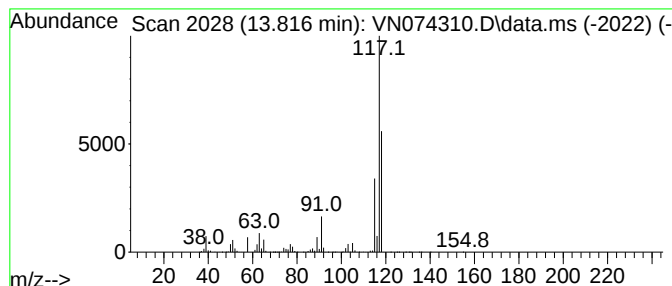
Instrument :
MSVOA_N
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.816	37.21 ug/l	27915900	1,4-Dichlorobenzene-d4			13.610
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Deltacyclene		118	C9H10	007785-10-6	64
2	Benzene, 1,1'-(1,5-hexadiene-1,6...		234	C18H18	004439-45-6	53
3	trans-Cinnamyl bromide		196	C9H9Br	026146-77-0	53
4	Benzaldehyde, 4-(1-phenyl-2-prop...		238	C16H14O2	1000277-56-1	50
5	Benzyl nitrile		117	C8H7N	000140-29-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23

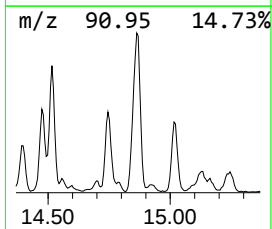
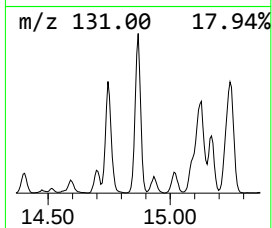
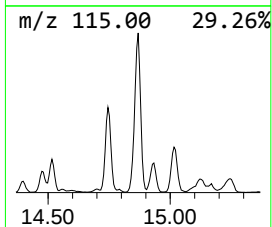
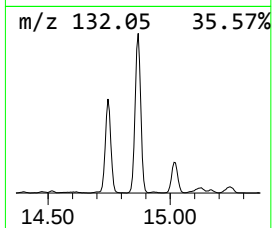
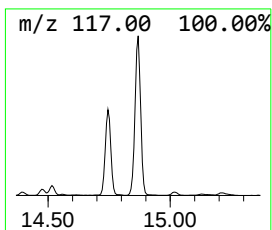
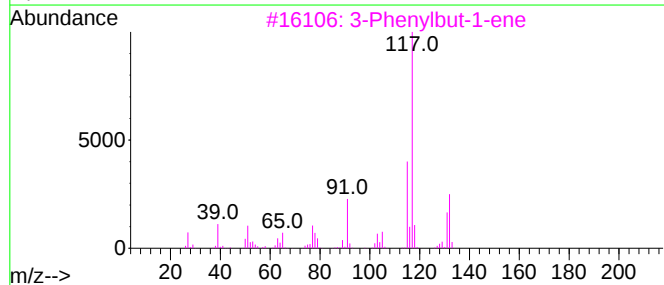
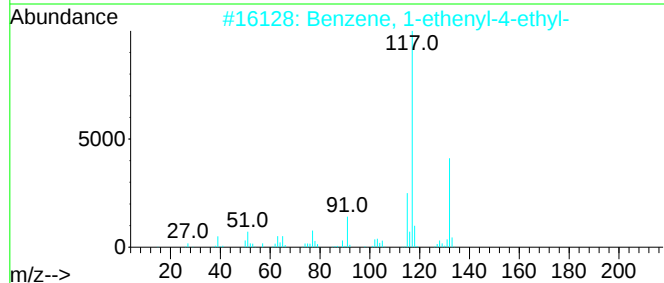
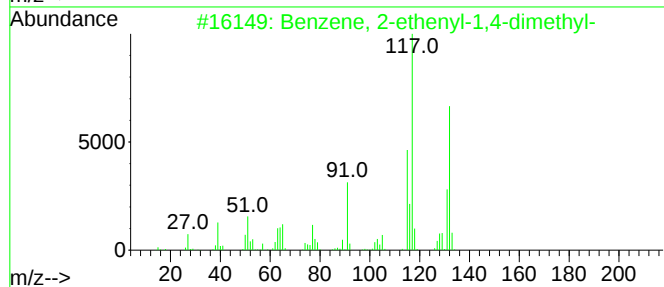
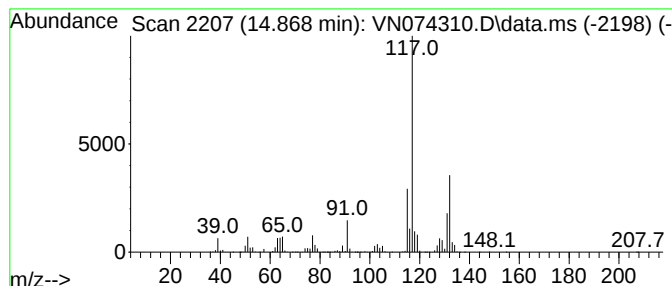
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	21.09 ug/l	15823200	1,4-Dichlorobenzene-d4	13.610

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	91
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074310.D
Acq On : 03 Sep 2022 01:27
Operator : JC\MD
Sample : N4355-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.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-methyl-	3.087	127.5	ug/l	35672300	1	8.016	13993400	50.0
Pentane	3.457	23.1	ug/l	6480270	1	8.016	13993400	50.0
unknown5.075	5.075	36.7	ug/l	10268500	1	8.016	13993400	50.0
Cyclopentane, m...	7.069	72.9	ug/l	20393900	1	8.016	13993400	50.0
Cyclopentane, 1...	8.510	51.7	ug/l	2909510	2	8.904	2814680	50.0
3,5-Octadiyne	11.786	50.0	ug/l	90237000	3	11.686	90237000	50.0
Benzene, 1-ethy...	12.922	66.4	ug/l	49795300	4	13.610	37510300	50.0
Benzene, 1-ethy...	13.157	40.9	ug/l	30678800	4	13.610	37510300	50.0
Benzene, 1,1'-(...	13.816	37.2	ug/l	27915900	4	13.610	37510300	50.0
Benzene, 2-ethe...	14.868	21.1	ug/l	15823200	4	13.610	37510300	50.0