

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
 Data File : VN074795.D
 Acq On : 06 Oct 2022 19:53
 Operator : JC\MD
 Sample : N4968-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 CLI-0620

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\82N100522W.M
 Title : SW846 8260

Signal : TIC: VN074795.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	53	rBV	236845	426058	1.05%	0.226%
2	2.836	126	133	143	rVB3	166858	637478	1.57%	0.338%
3	4.453	399	408	431	rBV	480161	1432331	3.53%	0.759%
4	8.183	1031	1042	1046	rBV	334402	820341	2.02%	0.435%
5	8.235	1046	1051	1064	rVB	355381	818135	2.02%	0.434%
6	8.612	1101	1115	1130	rBV2	1830022	4860896	11.98%	2.577%
7	9.106	1189	1199	1208	rBV	521218	1089235	2.68%	0.577%
8	10.571	1439	1448	1452	rBV	1527561	2736237	6.74%	1.450%
9	10.635	1452	1459	1483	rVB	22783252	40567986	100.00%	21.503%
10	11.871	1659	1669	1677	rBV	882060	1577568	3.89%	0.836%
11	11.965	1677	1685	1694	rVV	2186036	3749193	9.24%	1.987%
12	12.076	1695	1704	1720	rVV	17450618	34120543	84.11%	18.086%
13	12.400	1750	1759	1774	rBV	12010178	20108586	49.57%	10.659%
14	12.853	1828	1836	1846	rVB	1037567	1813265	4.47%	0.961%
15	13.100	1871	1878	1882	rBV	3858403	6768692	16.68%	3.588%
16	13.135	1882	1884	1887	rVV	1721451	2133284	5.26%	1.131%
17	13.176	1887	1891	1898	rVB	2181672	3494417	8.61%	1.852%
18	13.341	1911	1919	1929	rBV	2459728	4132713	10.19%	2.191%
19	13.482	1933	1943	1950	rBV	7791279	12817360	31.59%	6.794%
20	13.823	1989	2001	2007	rBV2	4507163	9427230	23.24%	4.997%
21	13.959	2017	2024	2025	rVV2	289337	449140	1.11%	0.238%
22	13.994	2025	2030	2046	rVB3	2930643	7067524	17.42%	3.746%
23	14.182	2056	2062	2067	rBV2	420015	705659	1.74%	0.374%
24	14.247	2067	2073	2075	rVV	722206	1120567	2.76%	0.594%
25	14.276	2075	2078	2082	rVV	646713	1005841	2.48%	0.533%
26	14.335	2082	2088	2094	rVV	1249069	1984197	4.89%	1.052%
27	14.447	2102	2107	2116	rVB2	772856	1368589	3.37%	0.725%
28	14.576	2123	2129	2135	rVB	457181	740249	1.82%	0.392%
29	14.653	2135	2142	2145	rBV	965970	1569885	3.87%	0.832%
30	14.694	2145	2149	2154	rVB	1639794	2455420	6.05%	1.301%
31	14.929	2183	2189	2194	rBV	992660	1604671	3.96%	0.851%
32	15.053	2200	2210	2216	rBV3	1938196	4416081	10.89%	2.341%
33	15.212	2228	2237	2244	rBV3	385470	730860	1.80%	0.387%
34	15.323	2244	2256	2268	rVV3	367410	1306555	3.22%	0.693%
35	15.435	2268	2275	2286	rVB5	324958	822882	2.03%	0.436%
36	15.641	2303	2310	2318	rBV	3575918	6818929	16.81%	3.614%

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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\82N100522W.M
Title : SW846 8260

37	15.947	2353	2362	2370	rBV	257524	533226	1.31%	0.283%
38	16.347	2423	2430	2443	rVB4	147058	429244	1.06%	0.228%

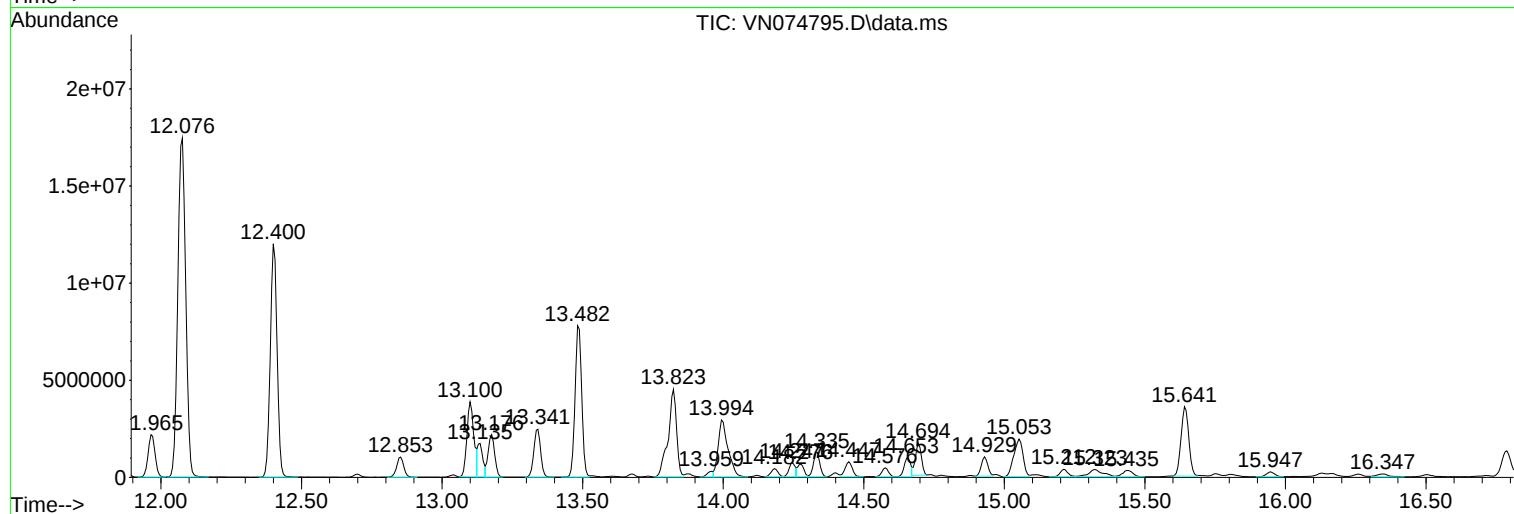
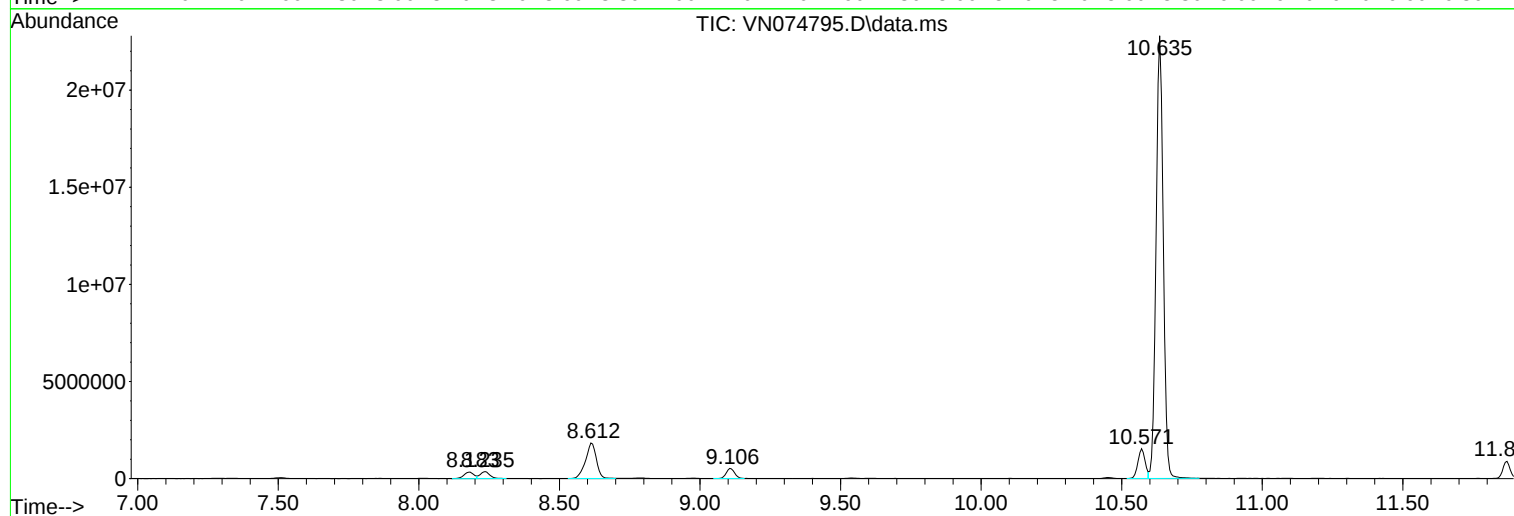
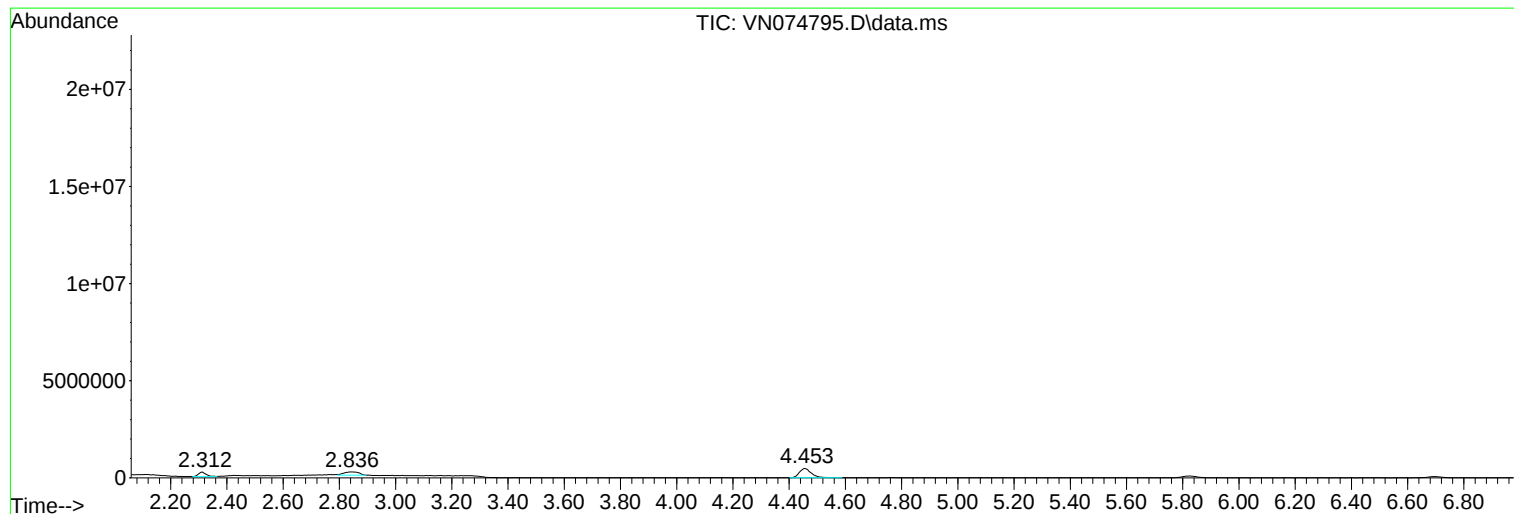
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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Instrument :
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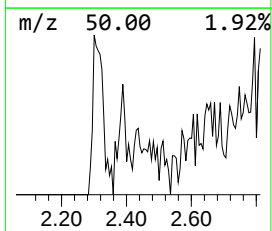
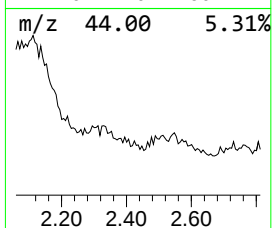
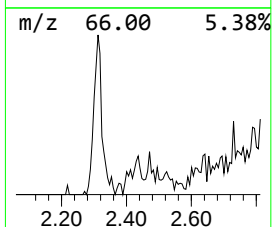
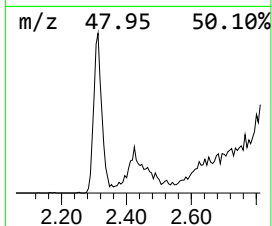
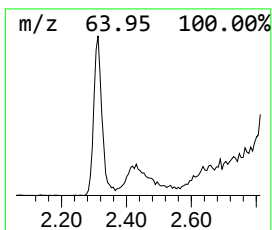
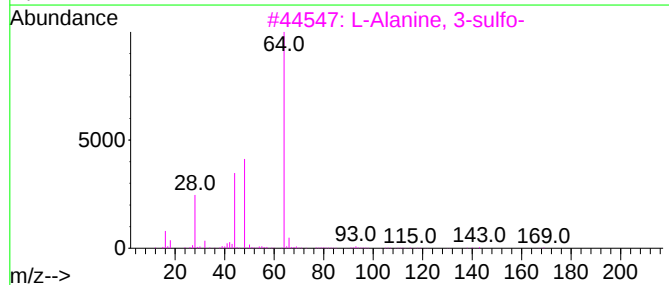
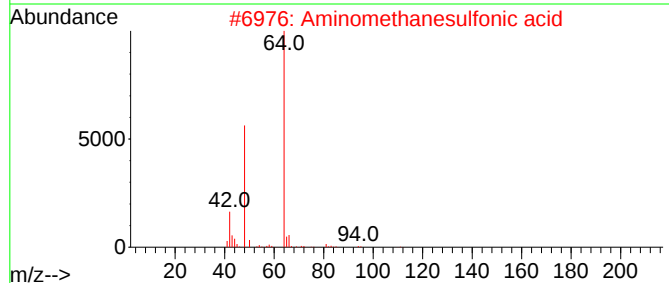
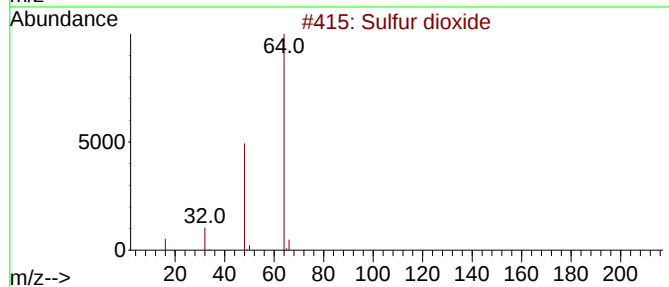
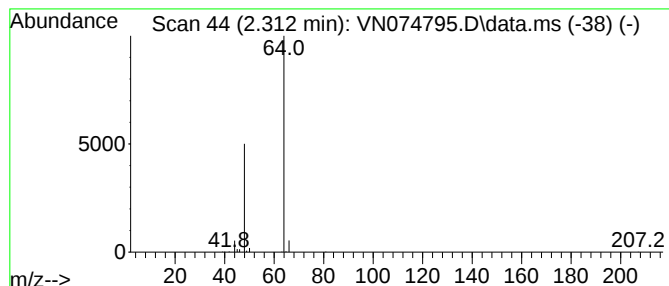
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	26.04 ug/l	426058	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

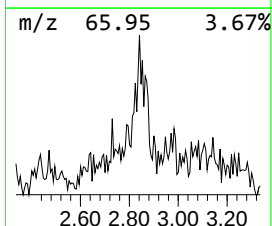
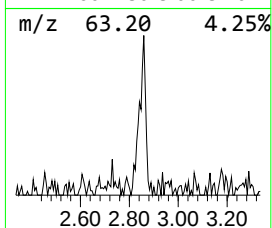
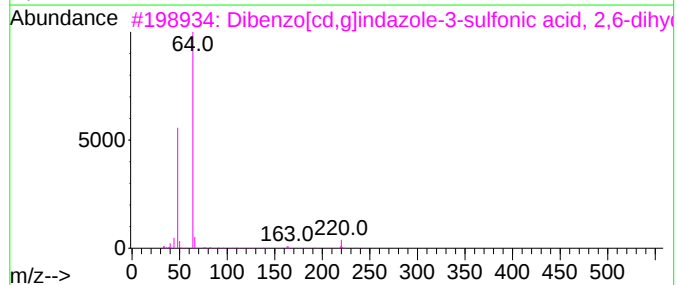
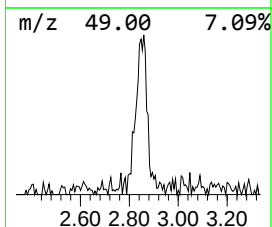
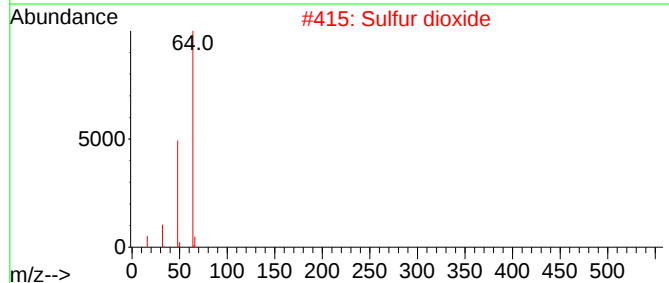
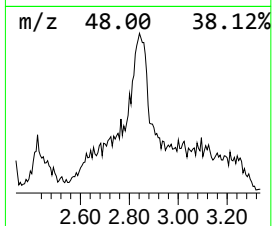
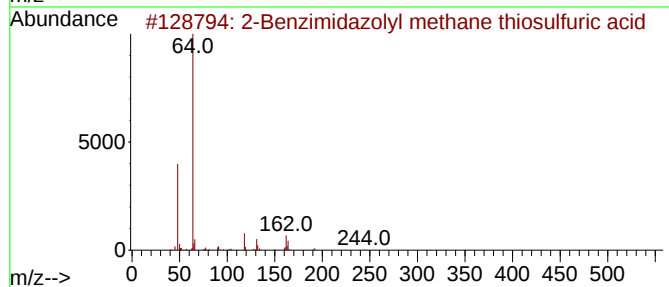
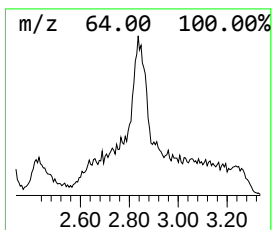
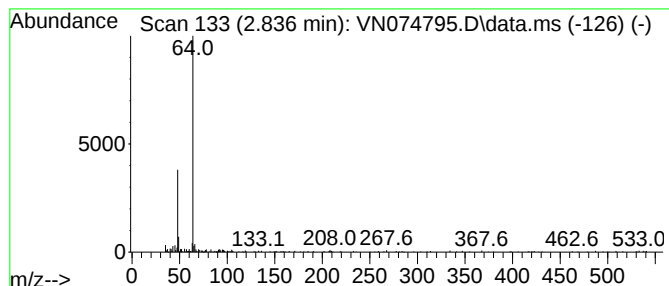
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Benzimidazolyl methane th... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	38.96 ug/l	637478	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	83		
2	Sulfur dioxide	64	O2S	007446-09-5	74		
3	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	74		
4	N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	64		
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64		



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

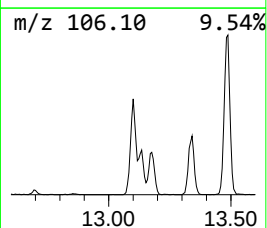
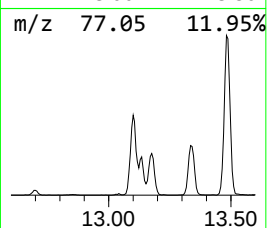
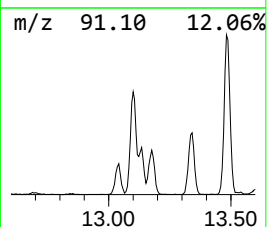
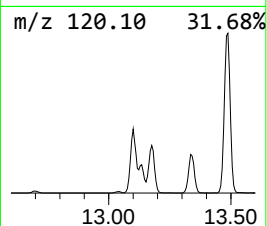
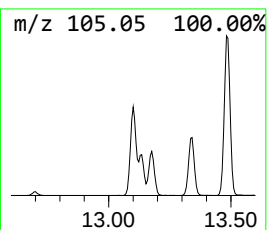
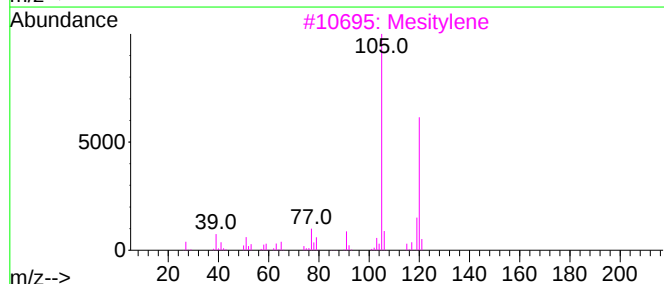
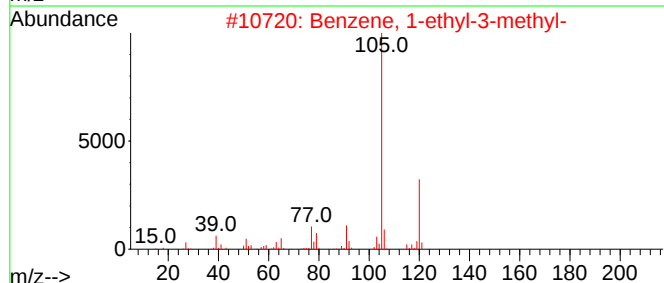
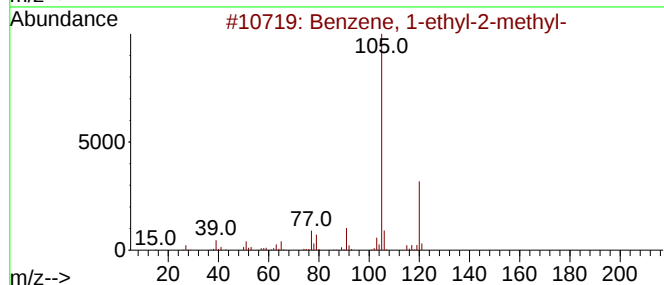
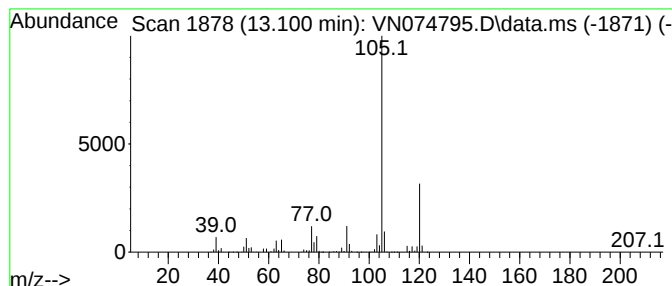
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	35.90 ug/l	6768690	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CLI-0620

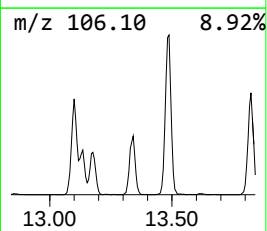
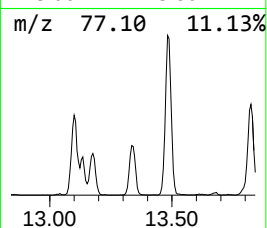
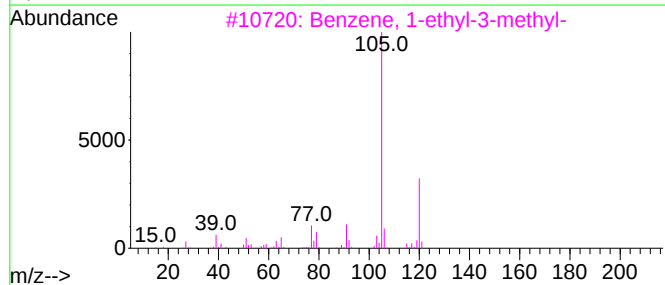
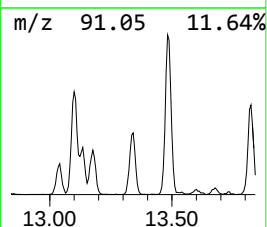
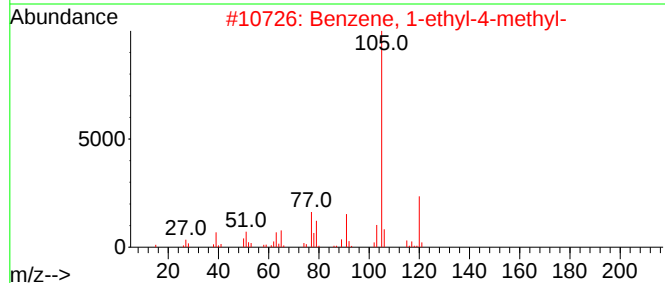
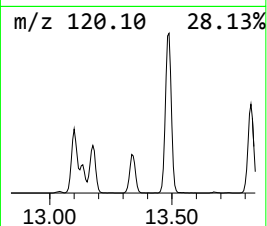
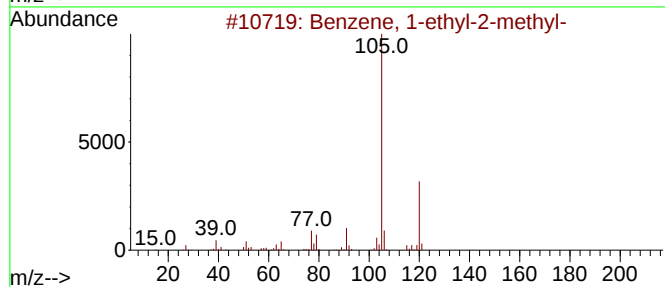
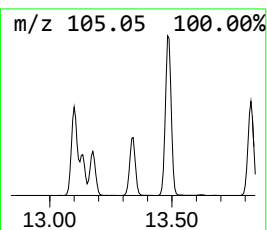
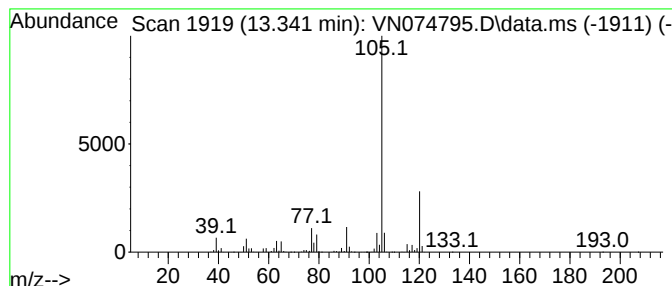
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	21.92 ug/l	4132710	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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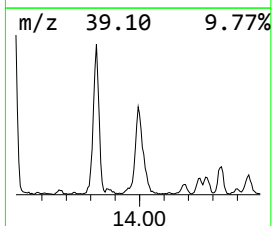
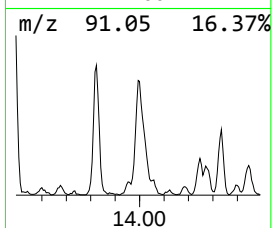
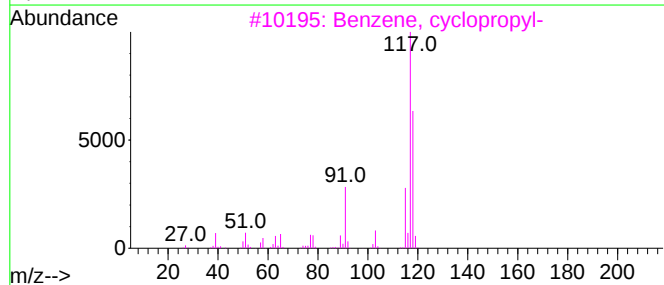
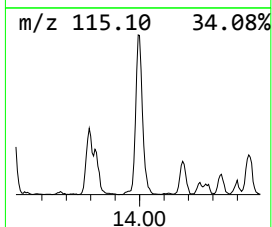
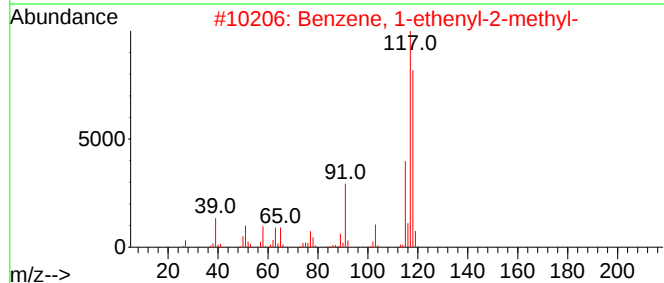
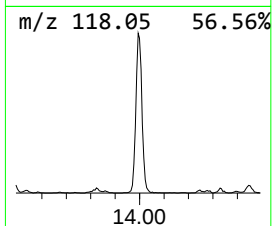
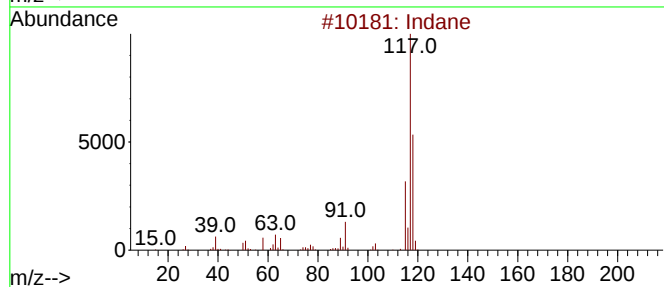
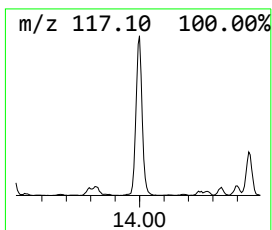
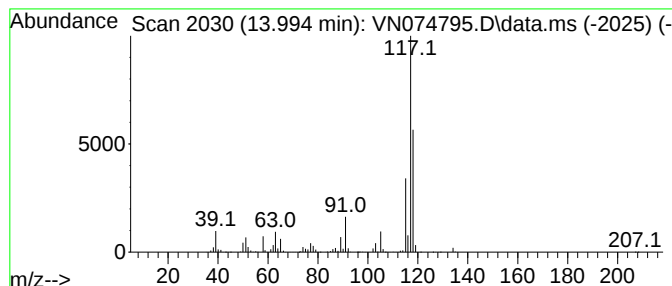
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Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	37.48 ug/l	7067520	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

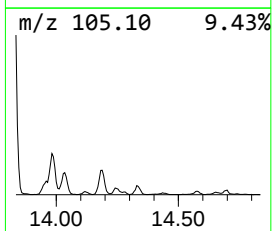
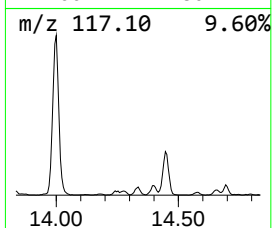
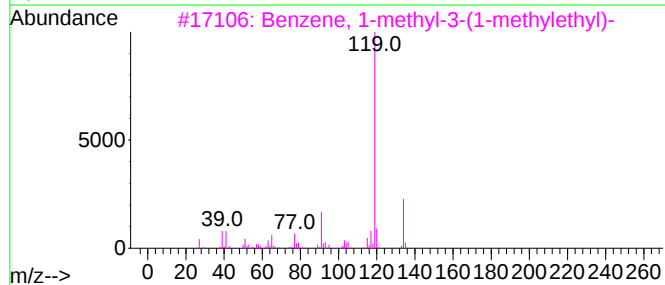
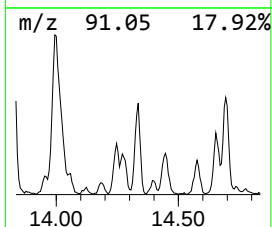
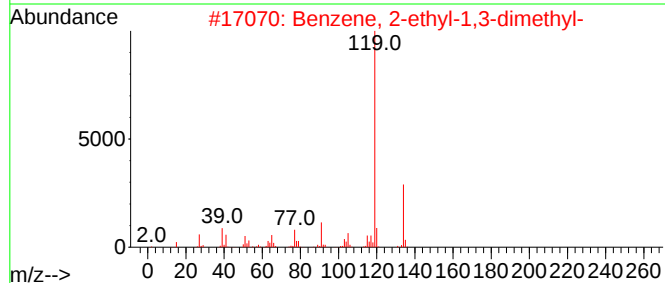
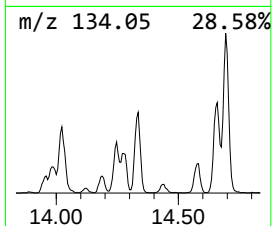
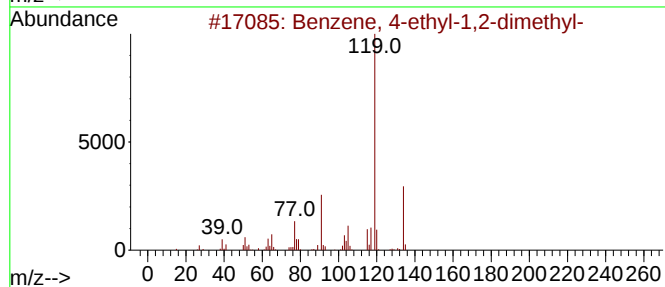
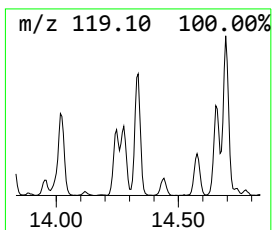
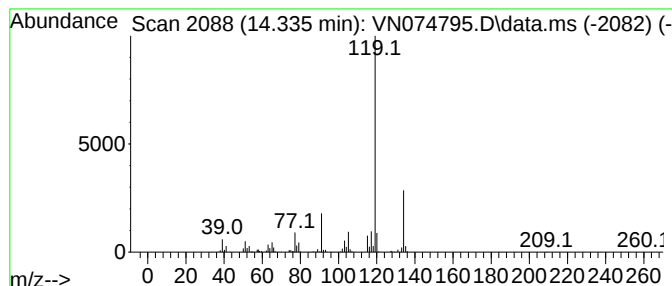
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	10.52 ug/l	1984200	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	93
4			o-Cymene	134	C10H14	000527-84-4	93
5			p-Cymene	134	C10H14	000099-87-6	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

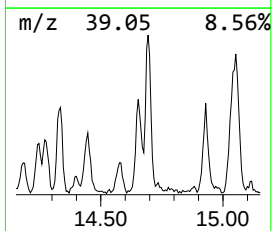
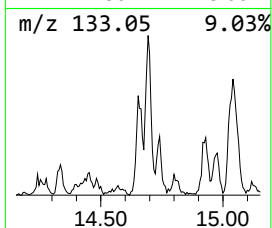
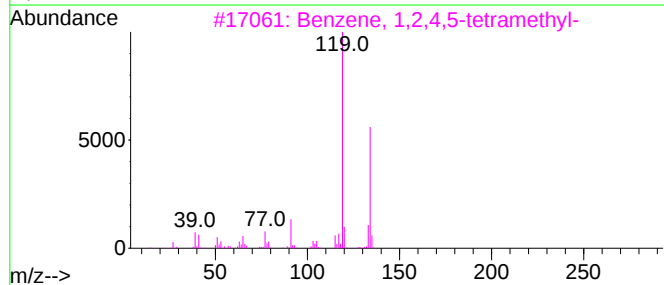
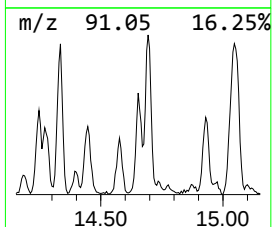
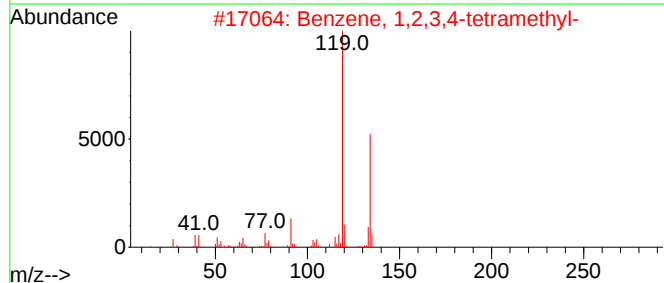
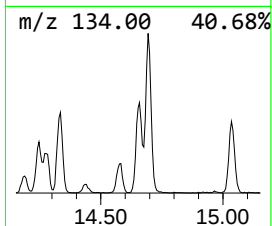
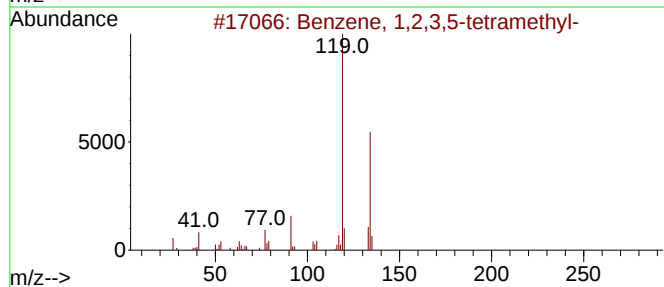
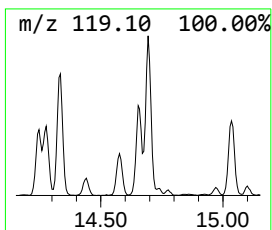
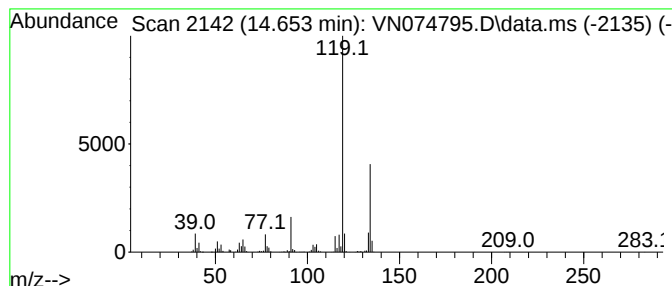
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.653	8.33 ug/l	1569890	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93
5			o-Cymene	134	C10H14	000527-84-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

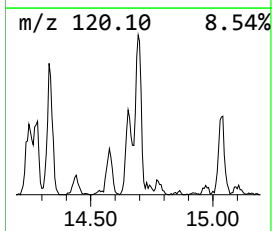
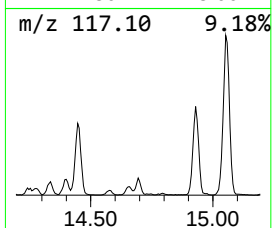
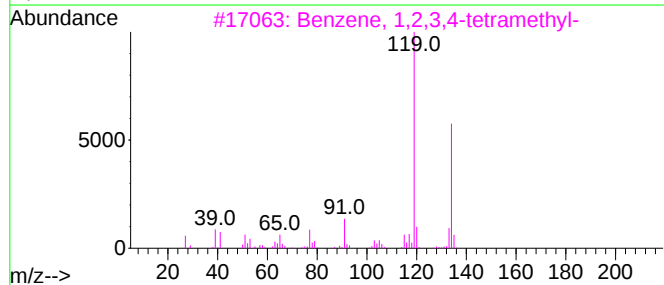
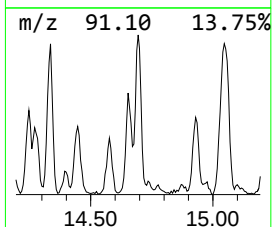
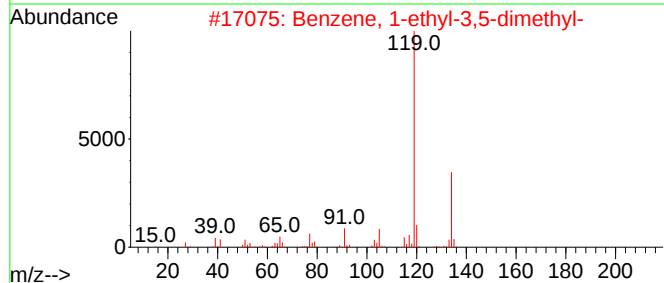
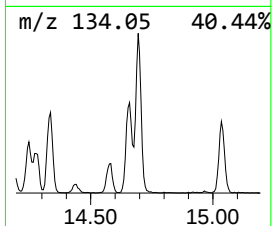
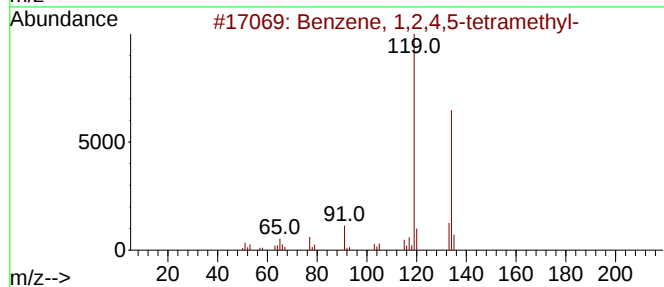
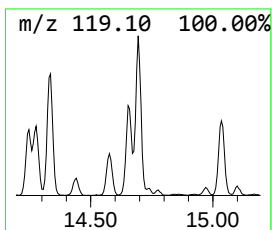
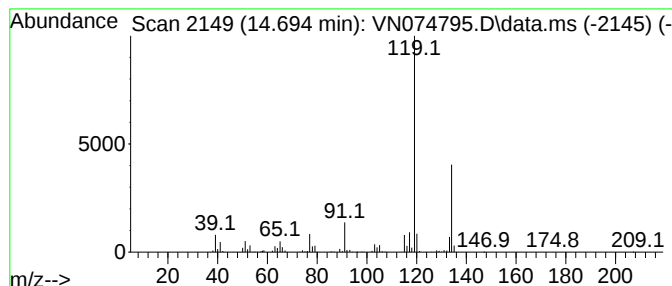
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	13.02 ug/l	2455420	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
2			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

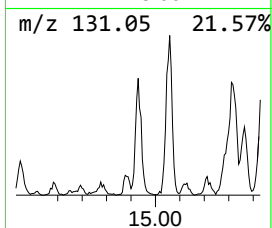
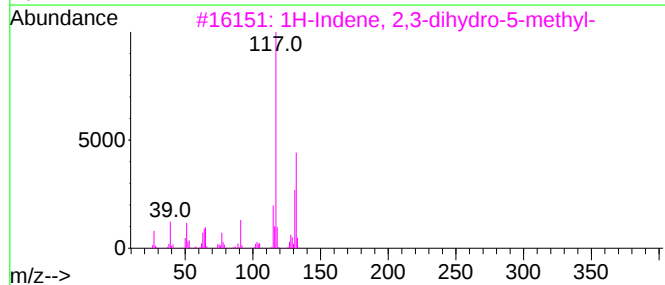
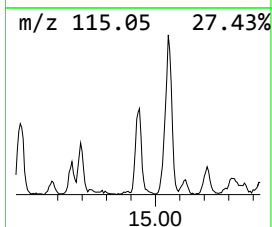
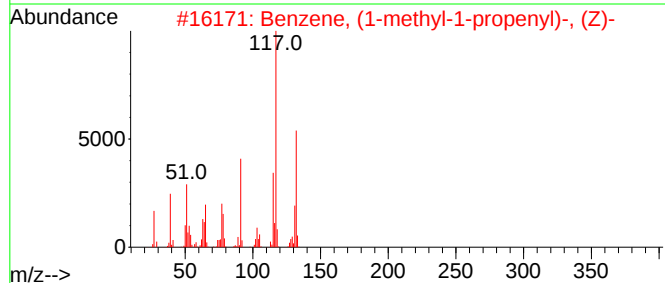
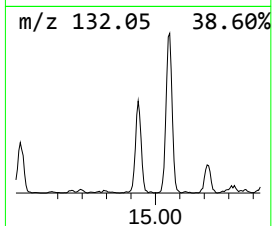
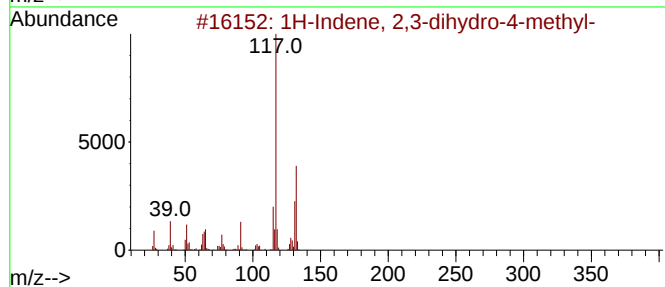
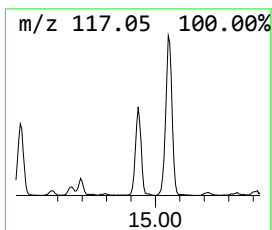
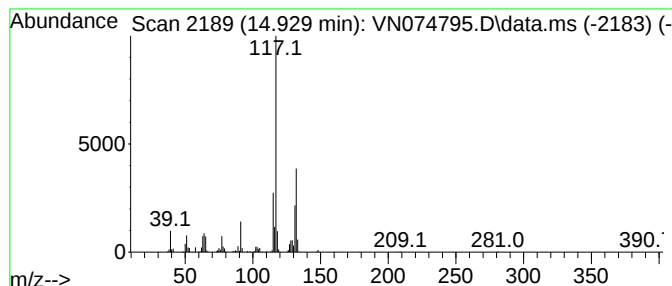
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	8.51 ug/l	1604670	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	90
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4			Indan, 1-methyl-	132	C10H12	000767-58-8	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

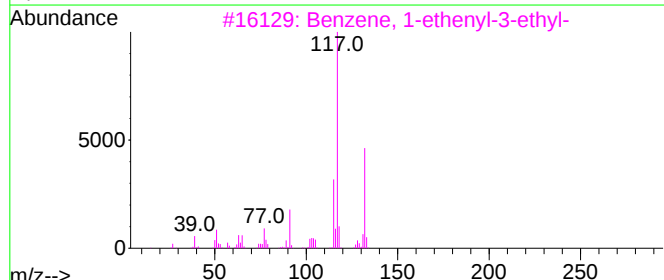
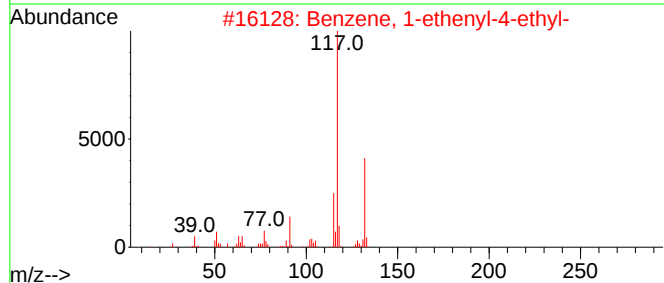
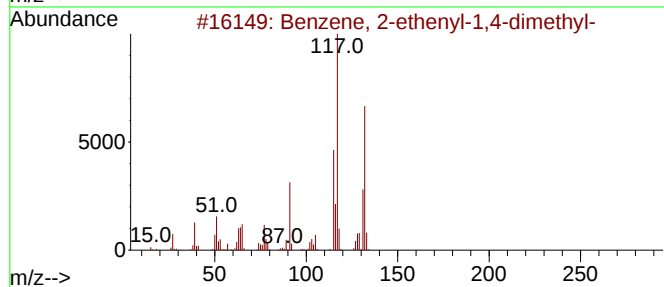
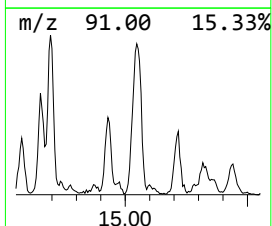
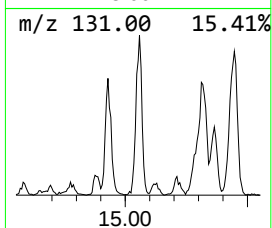
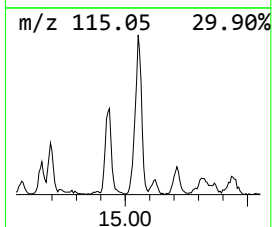
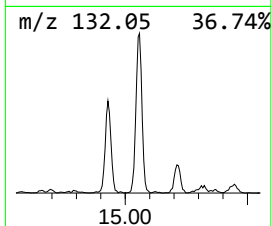
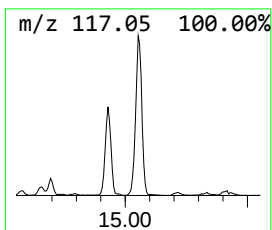
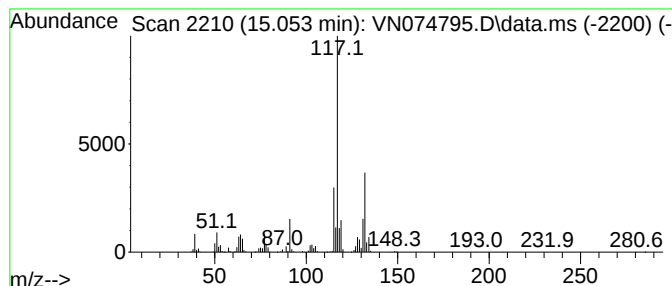
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	23.42 ug/l	4416080	1,4-Dichlorobenzene-d4	13.794

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			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100622\
Data File : VN074795.D
Acq On : 06 Oct 2022 19:53
Operator : JC\MD
Sample : N4968-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0620

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.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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2-Benzimidazoly...	2.836	39.0	ug/l	637478	1	8.235	818135	50.0
Benzene, 1-ethy...	13.100	35.9	ug/l	6768690	4	13.794	9427230	50.0
Benzene, 1-ethy...	13.341	21.9	ug/l	4132710	4	13.794	9427230	50.0
Indane	13.994	37.5	ug/l	7067520	4	13.794	9427230	50.0
Benzene, 4-ethy...	14.335	10.5	ug/l	1984200	4	13.794	9427230	50.0
Benzene, 1,2,3,...	14.653	8.3	ug/l	1569890	4	13.794	9427230	50.0
Benzene, 1,2,4,...	14.694	13.0	ug/l	2455420	4	13.794	9427230	50.0
1H-Indene, 2,3-...	14.929	8.5	ug/l	1604670	4	13.794	9427230	50.0
Benzene, 2-ethe...	15.053	23.4	ug/l	4416080	4	13.794	9427230	50.0