

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
 Data File : VN076098.D
 Acq On : 04 Jan 2023 21:56
 Operator : JC\MD
 Sample : 01019-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 33885

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN076098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.442	905	916	928	rBV	41188	114775	2.48%	0.313%
2	8.177	1030	1041	1045	rBV2	230360	540213	11.67%	1.475%
3	8.230	1045	1050	1063	rVB	438228	1000209	21.60%	2.731%
4	8.588	1102	1111	1122	rBV2	230458	610293	13.18%	1.666%
5	9.106	1190	1199	1209	rBV	584744	1194504	25.80%	3.261%
6	10.571	1438	1448	1454	rBV	863679	1613124	34.84%	4.404%
7	10.635	1454	1459	1472	rVB	375790	687708	14.85%	1.877%
8	11.871	1661	1669	1678	rBV	753279	1354528	29.25%	3.698%
9	11.965	1678	1685	1695	rVB	162880	286009	6.18%	0.781%
10	12.071	1695	1703	1713	rBV	704243	1342846	29.00%	3.666%
11	12.400	1751	1759	1766	rBV	519312	889007	19.20%	2.427%
12	12.512	1766	1778	1779	rBV6	29904	87241	1.88%	0.238%
13	12.700	1805	1810	1819	rVB	42353	83037	1.79%	0.227%
14	12.853	1823	1836	1844	rVB	630816	1081951	23.37%	2.954%
15	13.041	1861	1868	1872	rBV	208987	346863	7.49%	0.947%
16	13.100	1872	1878	1882	rVV	1282983	2232834	48.22%	6.096%
17	13.135	1882	1884	1887	rVV	566559	698369	15.08%	1.907%
18	13.176	1887	1891	1900	rVB	731897	1162194	25.10%	3.173%
19	13.341	1912	1919	1930	rVB	618653	1049554	22.67%	2.865%
20	13.488	1936	1944	1955	rBV	2792809	4630377	100.00%	12.641%
21	13.618	1958	1966	1971	rBV3	51579	124750	2.69%	0.341%
22	13.676	1971	1976	1981	rBV	101201	160376	3.46%	0.438%
23	13.729	1981	1985	1990	rVB2	35294	58411	1.26%	0.159%
24	13.794	1990	1996	1998	rBV	792454	1304960	28.18%	3.563%
25	13.823	1998	2001	2007	rVB	1066421	1610014	34.77%	4.395%
26	13.876	2007	2010	2017	rVB2	64047	106974	2.31%	0.292%
27	13.953	2017	2023	2025	rBV	148388	230634	4.98%	0.630%
28	13.994	2025	2030	2033	rBV3	641640	1185635	25.61%	3.237%
29	14.123	2047	2052	2056	rBV3	43450	77043	1.66%	0.210%
30	14.188	2056	2063	2068	rVB2	173337	310007	6.70%	0.846%
31	14.247	2068	2073	2076	rBV	298879	510566	11.03%	1.394%
32	14.276	2076	2078	2083	rVV	248800	321426	6.94%	0.878%
33	14.335	2083	2088	2094	rVB	440687	677725	14.64%	1.850%
34	14.400	2094	2099	2101	rBV2	35863	52434	1.13%	0.143%
35	14.447	2101	2107	2112	rVB2	170426	301908	6.52%	0.824%
36	14.576	2123	2129	2135	rVB	161101	257380	5.56%	0.703%

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Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	14.659	2135	2143	2146	rVV	315208	541395	11.69%	1.478%
38	14.694	2146	2149	2154	rVV	501886	774808	16.73%	2.115%
39	14.741	2154	2157	2160	rVV	62889	83117	1.80%	0.227%
40	14.776	2160	2163	2167	rVV	36320	55838	1.21%	0.152%
41	14.882	2171	2181	2184	rBV4	41792	83712	1.81%	0.229%
42	14.929	2184	2189	2194	rVV	299870	522657	11.29%	1.427%
43	14.970	2194	2196	2201	rVB	74958	96921	2.09%	0.265%
44	15.053	2201	2210	2216	rBV3	565477	1394311	30.11%	3.807%
45	15.106	2216	2219	2228	rVV3	58139	130399	2.82%	0.356%
46	15.212	2230	2237	2245	rBV	318937	586330	12.66%	1.601%
47	15.323	2245	2256	2268	rVV3	157935	539432	11.65%	1.473%
48	15.441	2268	2276	2285	rVB4	137025	356251	7.69%	0.973%
49	15.641	2304	2310	2316	rBV	231540	441639	9.54%	1.206%
50	15.700	2316	2320	2325	rVV2	83410	143699	3.10%	0.392%
51	15.759	2325	2330	2332	rVV4	55197	108150	2.34%	0.295%
52	15.788	2332	2335	2353	rVB9	85804	301337	6.51%	0.823%
53	15.947	2353	2362	2370	rBV2	113677	243013	5.25%	0.663%
54	16.129	2384	2393	2394	rBV5	93211	157021	3.39%	0.429%
55	16.170	2395	2400	2410	rVB2	274991	601252	12.98%	1.641%
56	16.259	2410	2415	2422	rBV3	37913	82324	1.78%	0.225%
57	16.347	2422	2430	2445	rVB3	85053	288198	6.22%	0.787%
58	16.506	2445	2457	2470	rBV	209586	531968	11.49%	1.452%
59	16.717	2482	2493	2499	rBV2	102204	269946	5.83%	0.737%

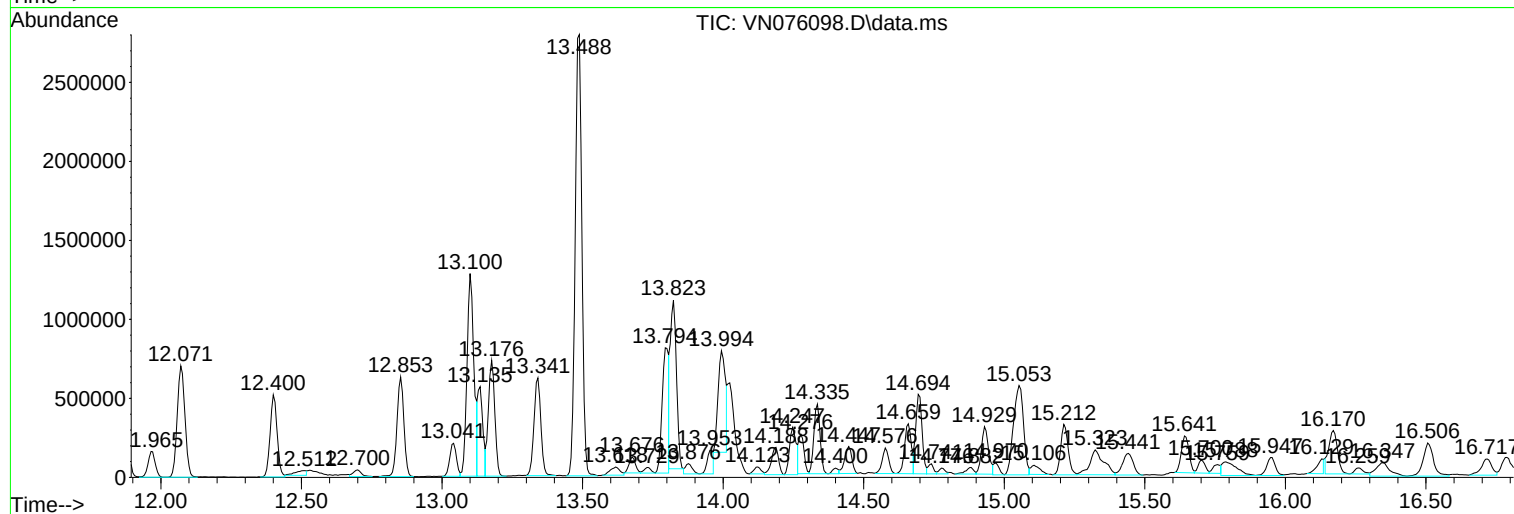
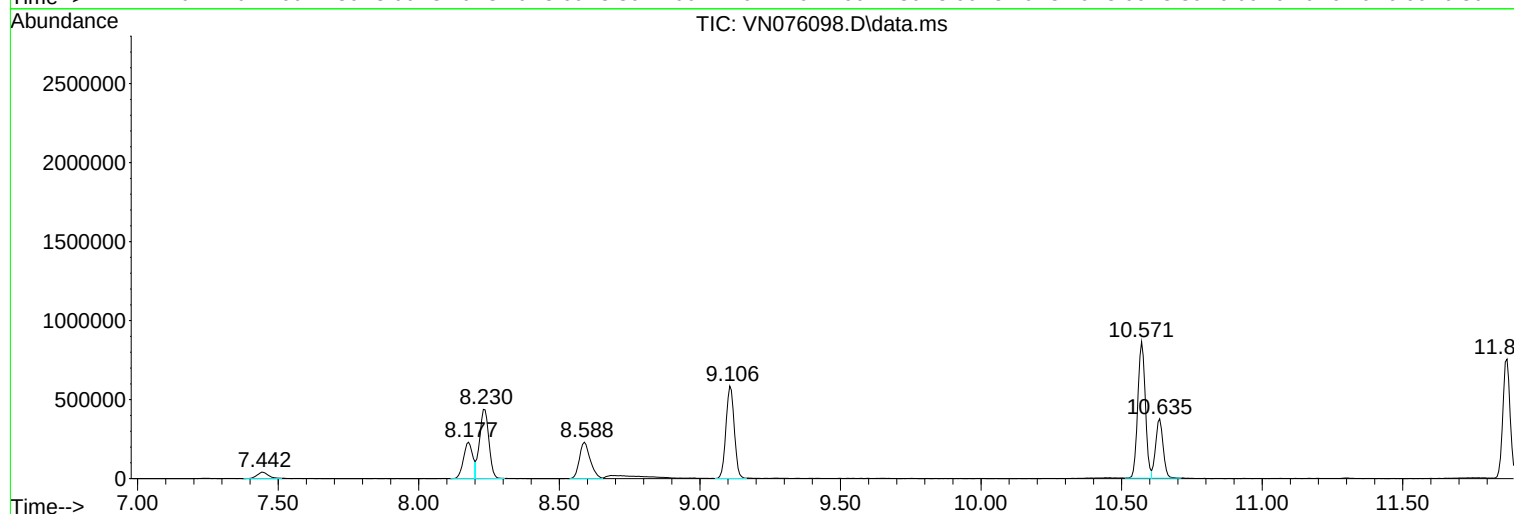
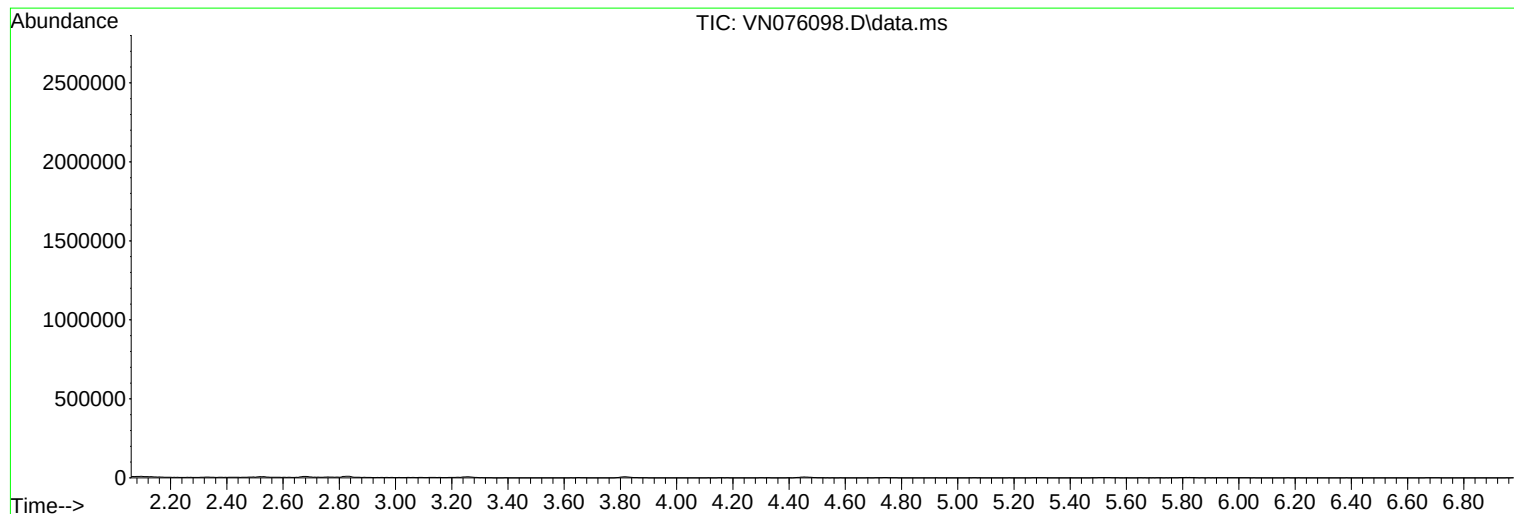
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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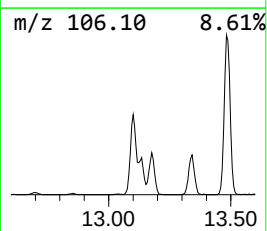
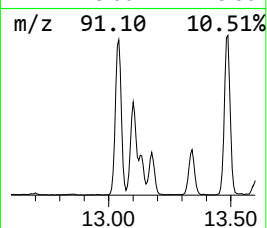
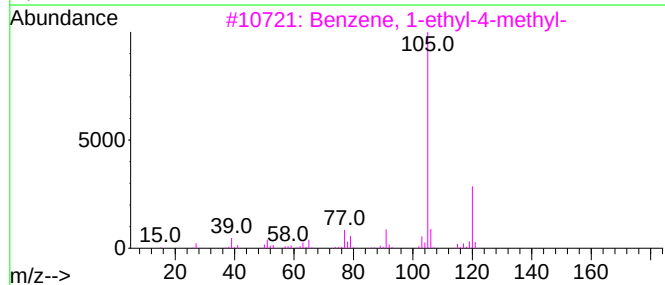
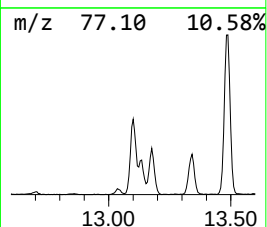
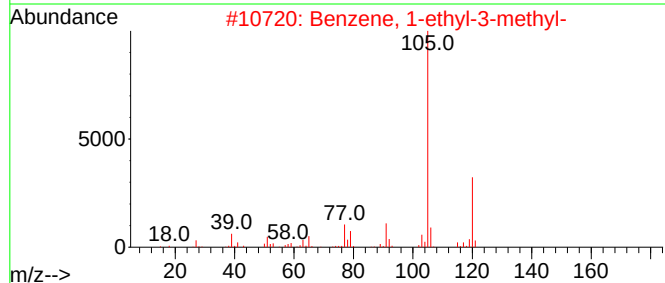
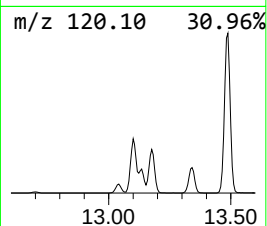
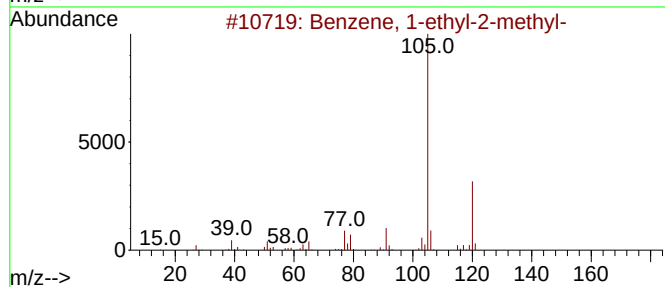
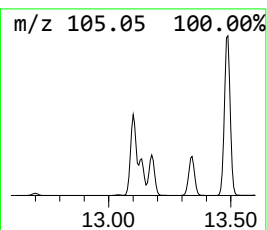
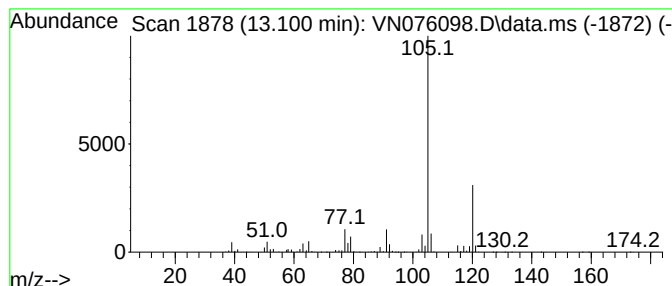
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	85.55 ug/l	2232830	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			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



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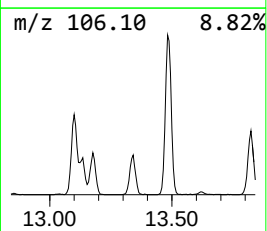
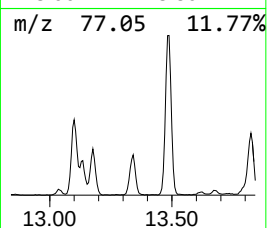
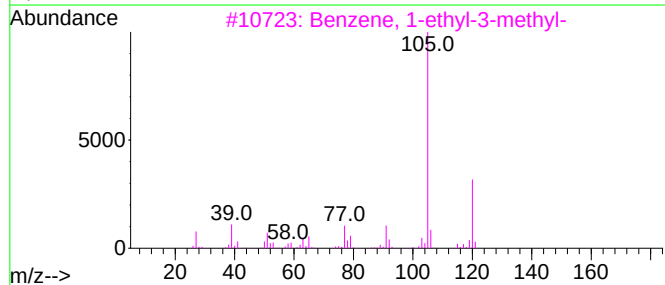
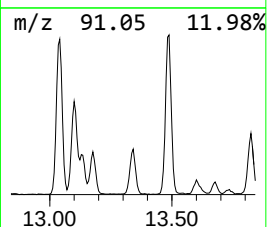
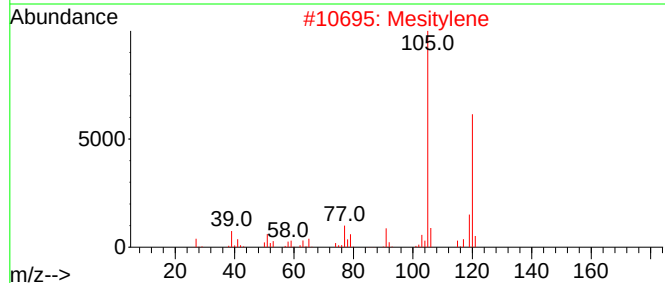
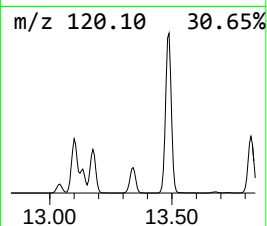
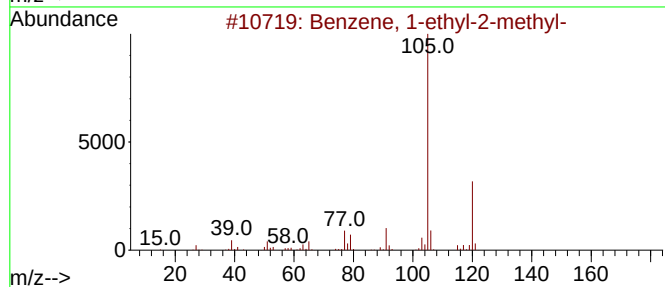
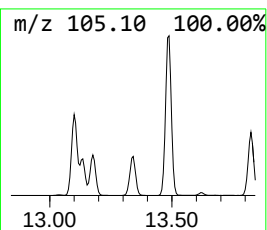
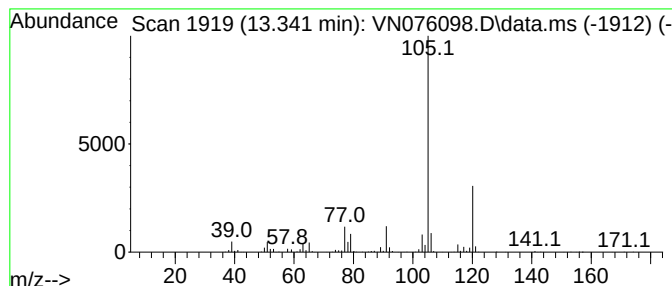
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	40.21 ug/l	1049550	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	94
2			Mesitylene	120	C9H12	000108-67-8	90
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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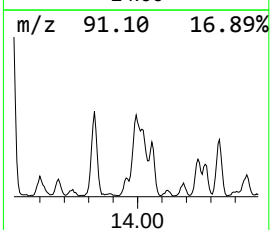
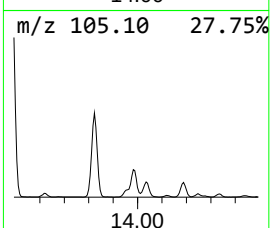
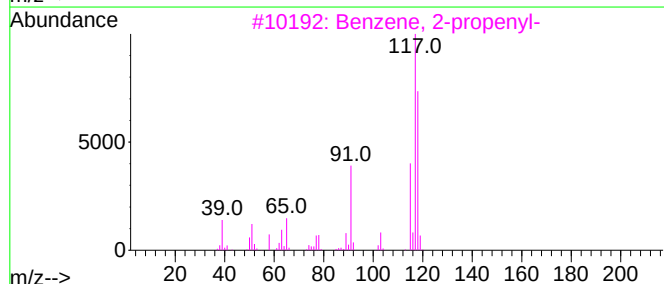
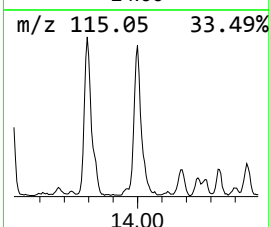
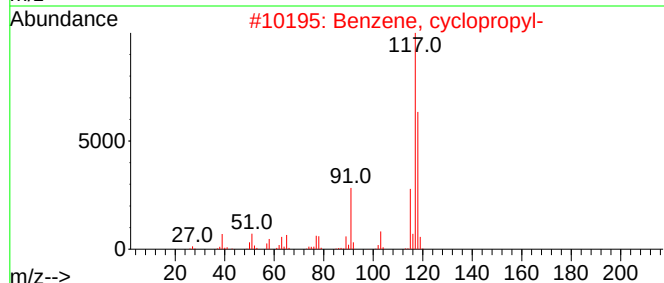
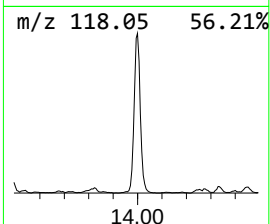
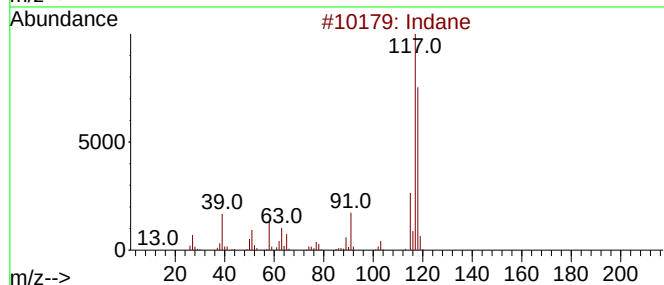
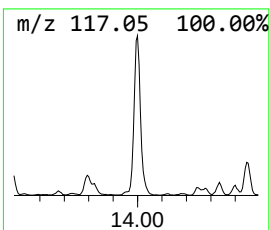
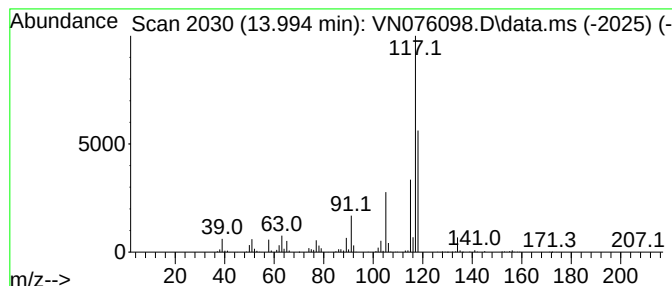
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	45.43 ug/l	1185640	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	53
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	50



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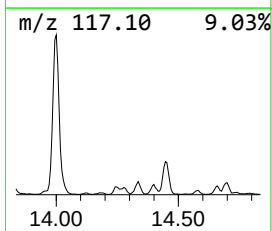
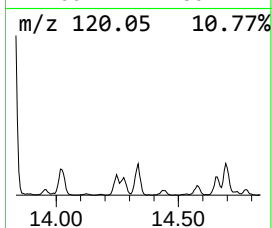
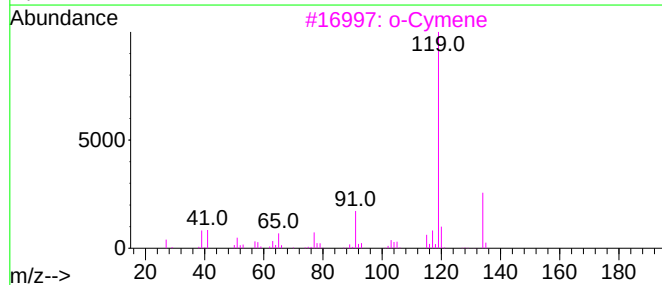
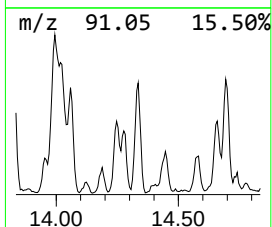
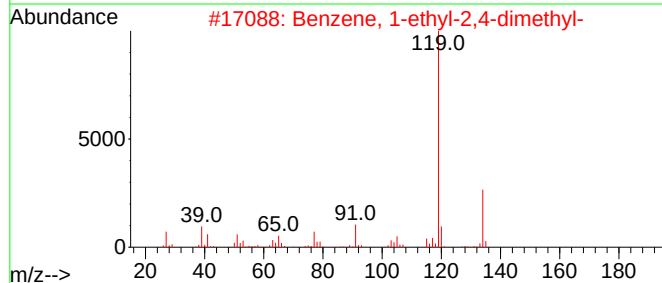
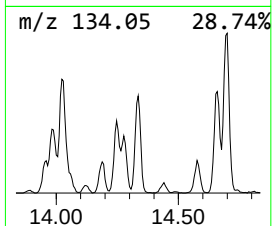
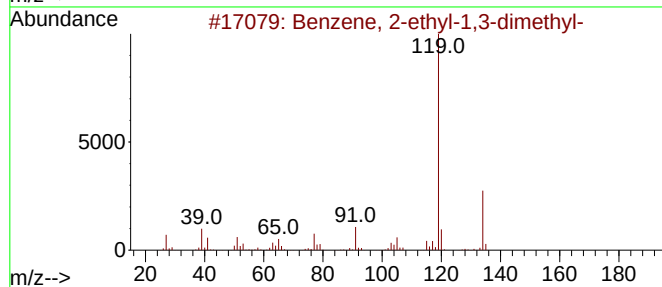
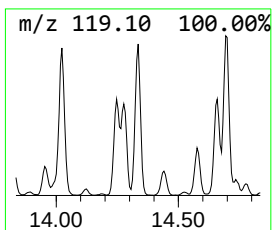
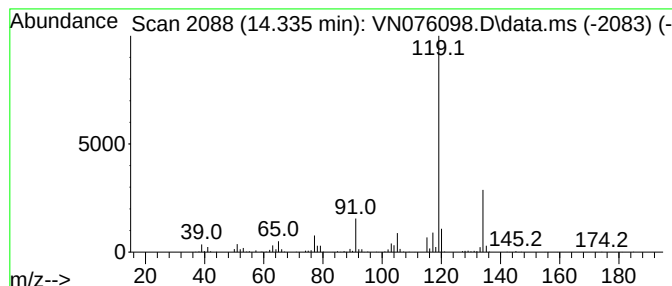
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	25.97 ug/l	677725	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



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33885

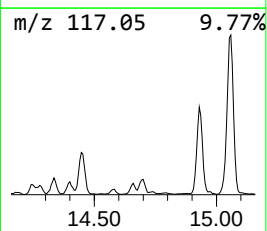
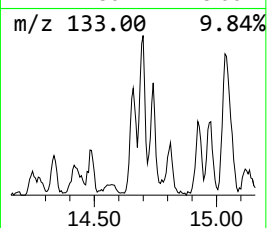
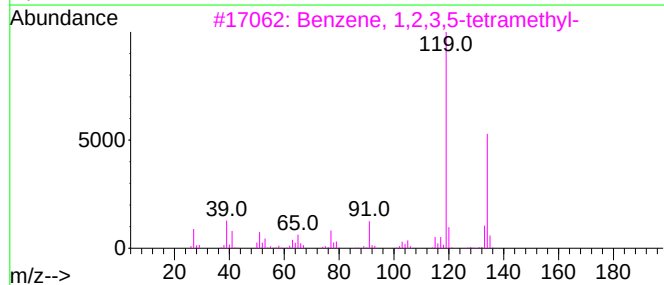
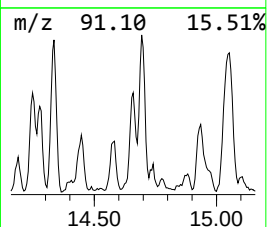
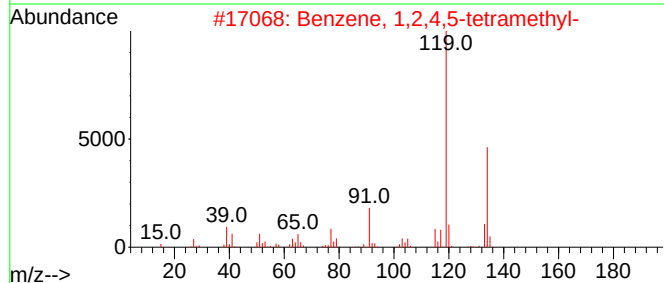
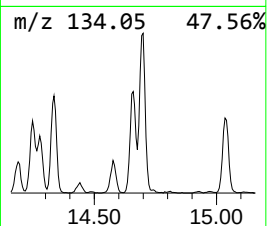
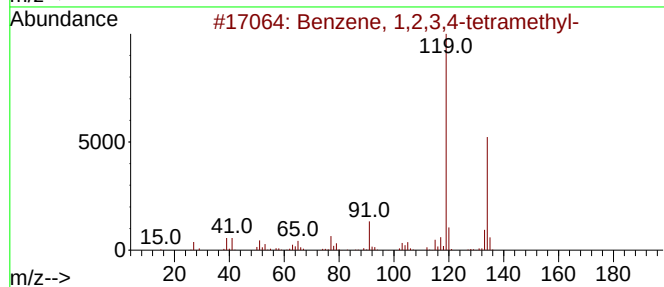
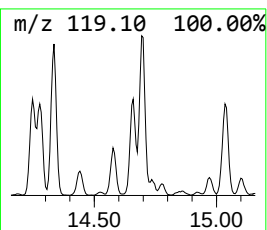
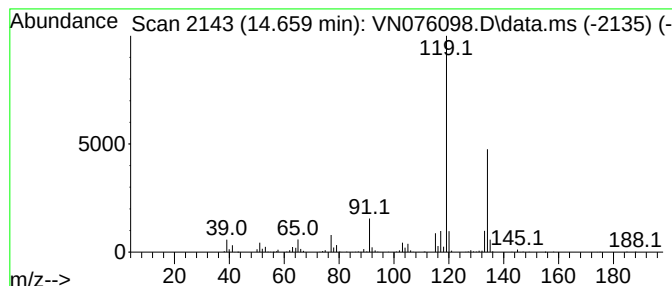
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	20.74 ug/l	541395	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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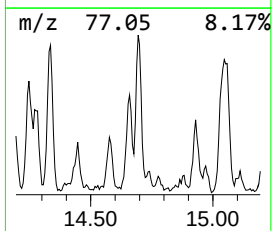
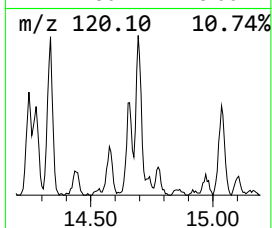
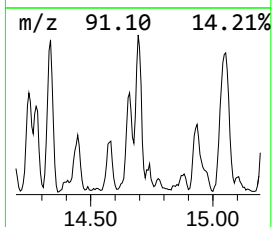
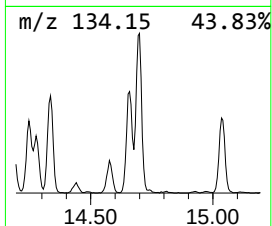
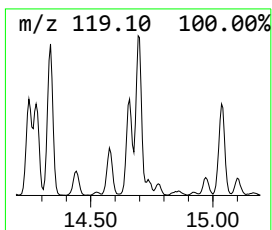
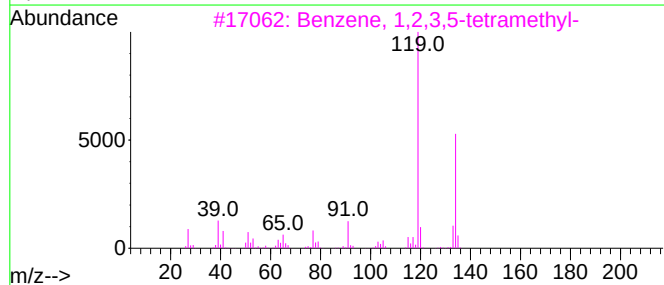
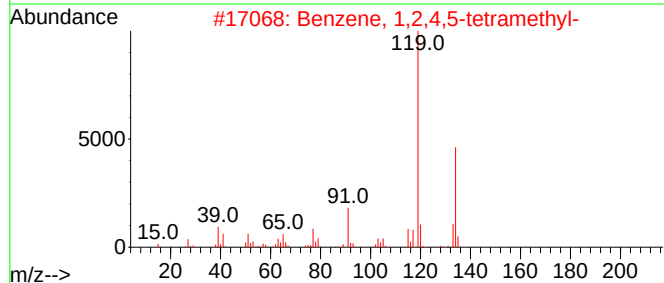
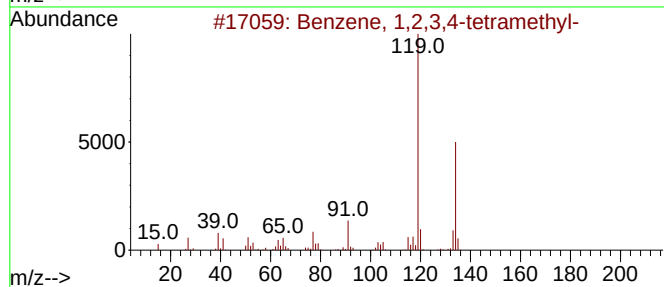
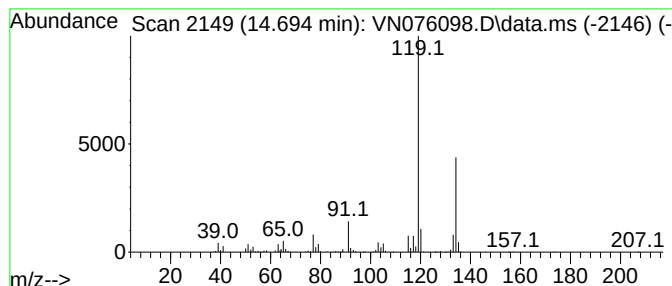
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	29.69 ug/l	774808	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
4			o-Cymene	134	C10H14	000527-84-4	96
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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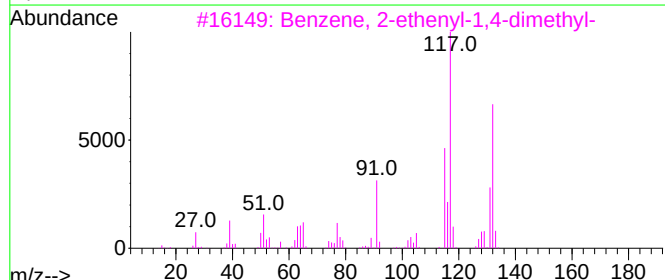
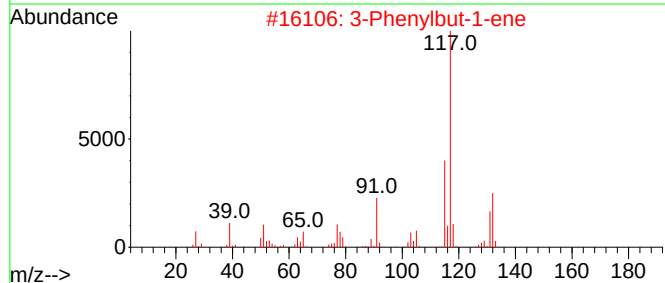
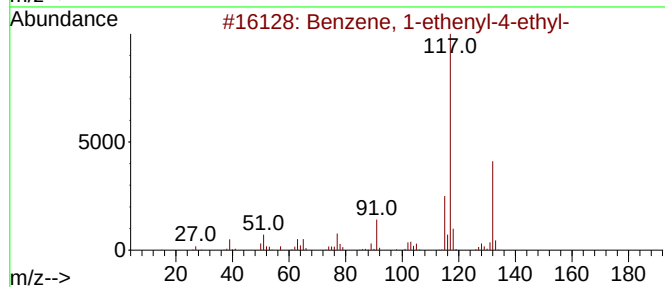
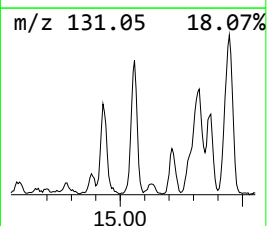
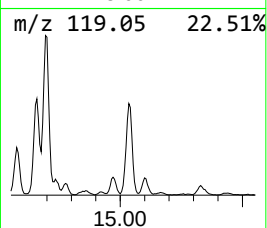
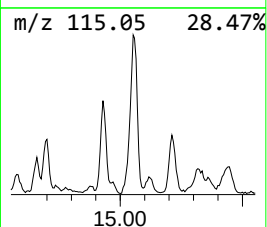
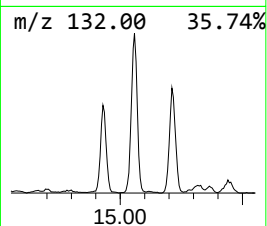
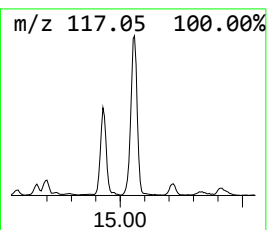
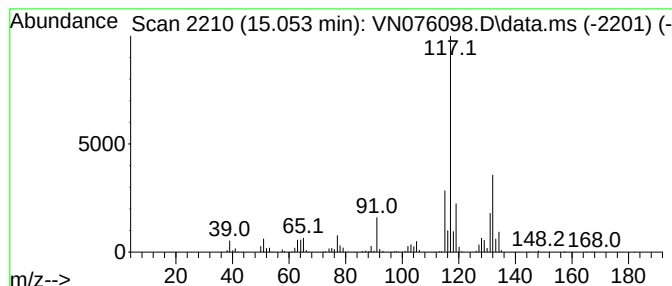
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	53.42 ug/l	1394310	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
4			Indan, 1-methyl-	132	C10H12	000767-58-8	81
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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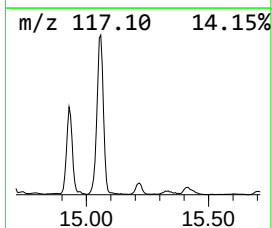
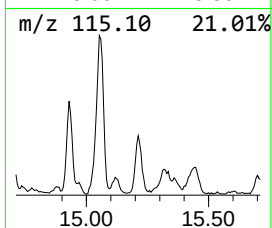
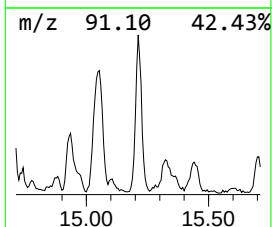
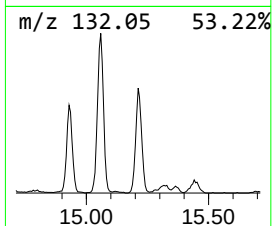
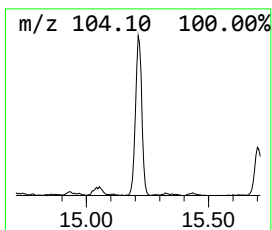
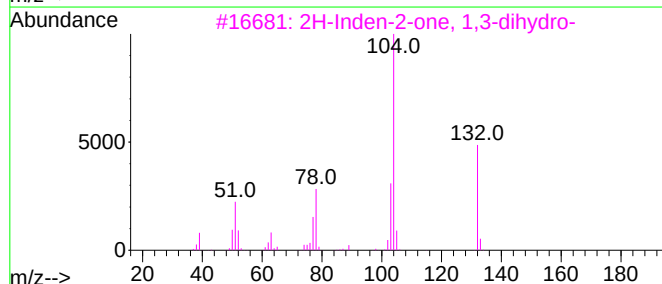
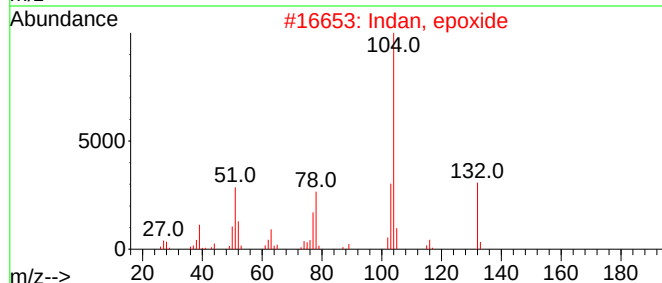
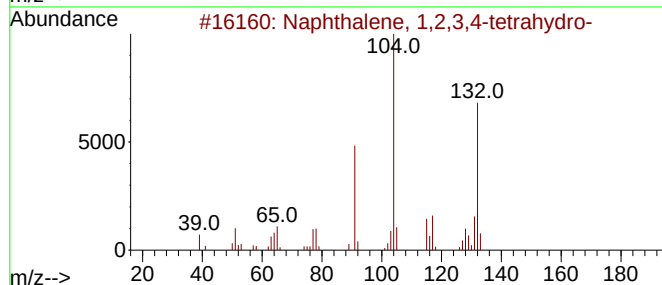
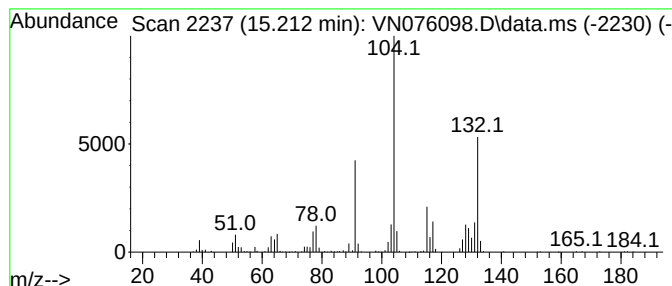
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	22.47 ug/l	586330	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	95
2			Indan, epoxide	132	C9H8O	000768-22-9	53
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	49
4			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	43
5			Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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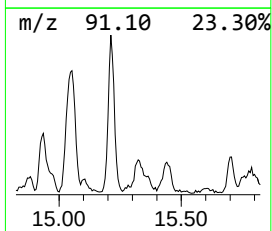
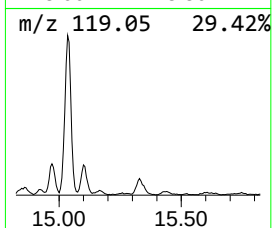
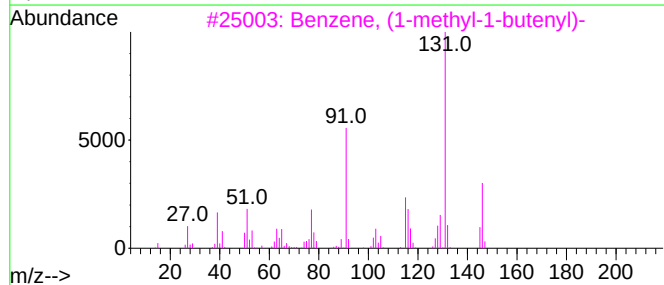
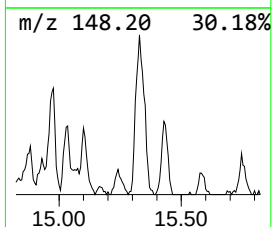
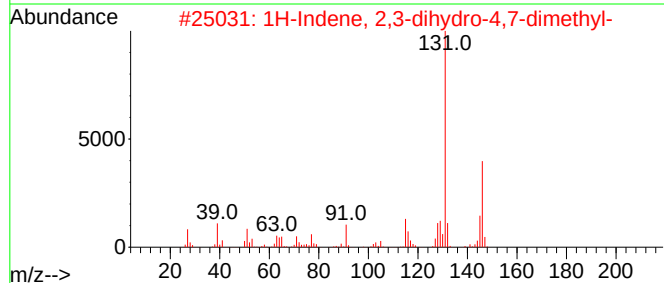
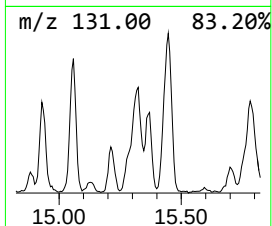
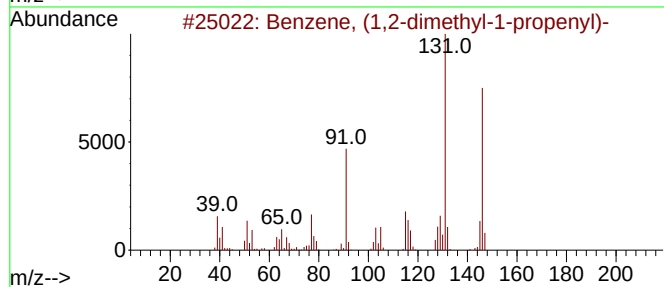
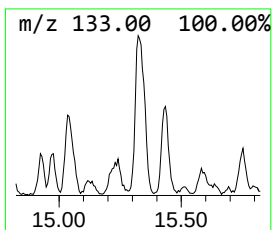
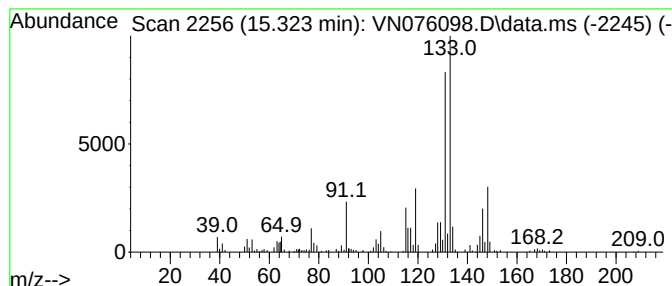
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1,2-dimethyl-1-propenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	20.67 ug/l	539432	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	90
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	83
3			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	56
4			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	50
5			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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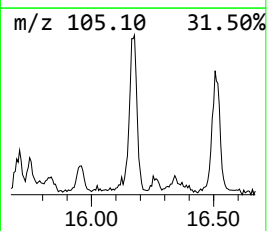
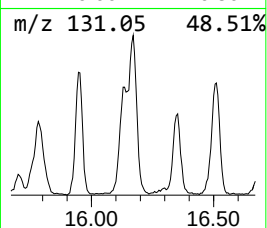
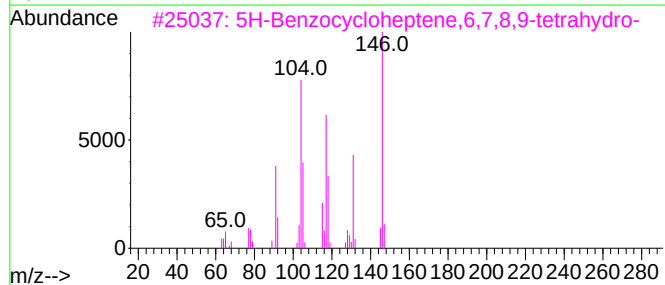
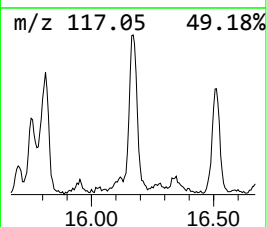
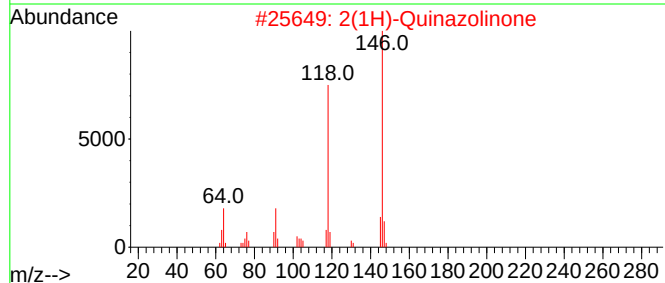
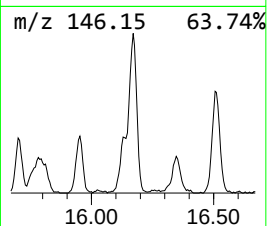
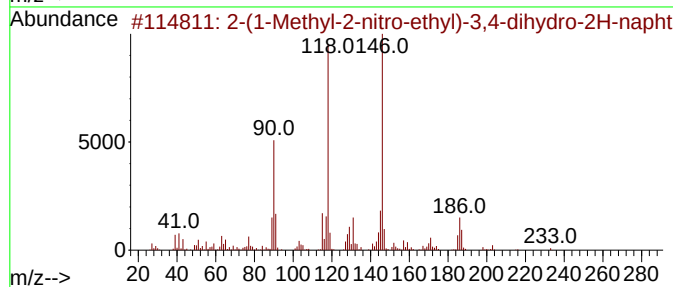
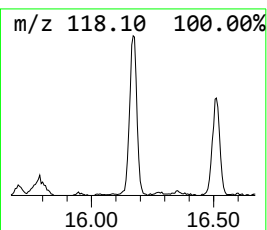
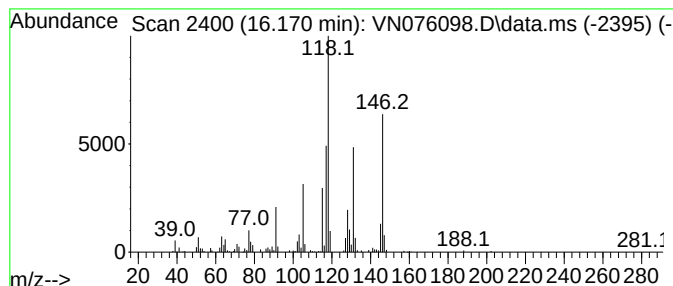
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.170 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	23.04 ug/l	601252	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Methyl-2-nitro-ethyl)-3,4-d...	233	C13H15NO3	1000190-31-3	43		
2	2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	43		
3	5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	43		
4	.alpha.-Methylstyrene	118	C9H10	000098-83-9	35		
5	3-Chloropropionic acid, 3-phenyl...	226	C12H15ClO2	078987-69-6	35		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010423\
Data File : VN076098.D
Acq On : 04 Jan 2023 21:56
Operator : JC\MD
Sample : 01019-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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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Benzene, 1-ethy...	13.341	40.2	ug/l	1049550	4	13.794	1304960	50.0
Indane	13.994	45.4	ug/l	1185640	4	13.794	1304960	50.0
Benzene, 2-ethy...	14.335	26.0	ug/l	677725	4	13.794	1304960	50.0
Benzene, 1,2,3,...	14.659	20.7	ug/l	541395	4	13.794	1304960	50.0
Benzene, 1,2,4,...	14.694	29.7	ug/l	774808	4	13.794	1304960	50.0
Benzene, 1-ethe...	15.053	53.4	ug/l	1394310	4	13.794	1304960	50.0
Naphthalene, 1,...	15.212	22.5	ug/l	586330	4	13.794	1304960	50.0
Benzene, (1,2-d...	15.323	20.7	ug/l	539432	4	13.794	1304960	50.0
unknown16.170	16.170	23.0	ug/l	601252	4	13.794	1304960	50.0