

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
 Data File : VN076320.D
 Acq On : 19 Jan 2023 14:07
 Operator : JC\MD
 Sample : 01221-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-12-0118

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\82N011623W.M
 Title : SW846 8260

Signal : TIC: VN076320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.259	194	205	215	rVB	66137	163637	2.44%	0.301%
2	4.447	395	407	421	rBV2	103393	316522	4.72%	0.582%
3	5.542	582	593	606	rVB2	39667	139511	2.08%	0.256%
4	5.812	626	639	656	rVB4	172327	630460	9.41%	1.158%
5	7.336	888	898	909	rBV	80175	222758	3.32%	0.409%
6	8.177	1031	1041	1045	rBV	295313	723265	10.79%	1.329%
7	8.230	1045	1050	1063	rVV	594826	1446321	21.59%	2.657%
8	8.335	1063	1068	1079	rVB3	43582	104902	1.57%	0.193%
9	8.588	1102	1111	1121	rBV	289173	682150	10.18%	1.253%
10	8.735	1125	1136	1138	rBV6	45735	106072	1.58%	0.195%
11	9.106	1190	1199	1212	rBV	827002	1776508	26.51%	3.264%
12	9.571	1264	1278	1280	rBV4	57598	129047	1.93%	0.237%
13	9.606	1280	1284	1293	rVB	77577	154972	2.31%	0.285%
14	10.018	1348	1354	1362	rVB2	45667	99277	1.48%	0.182%
15	10.106	1362	1369	1372	rBV2	42525	80958	1.21%	0.149%
16	10.153	1372	1377	1383	rVB2	66307	127929	1.91%	0.235%
17	10.453	1421	1428	1433	rBV2	61585	116284	1.74%	0.214%
18	10.571	1440	1448	1454	rBV	1195300	2174786	32.46%	3.995%
19	10.635	1454	1459	1467	rVB	165871	322252	4.81%	0.592%
20	10.759	1472	1480	1486	rVB5	25606	68563	1.02%	0.126%
21	10.982	1512	1518	1527	rBV5	50931	143573	2.14%	0.264%
22	11.065	1527	1532	1543	rVB2	38311	82390	1.23%	0.151%
23	11.871	1660	1669	1677	rBV	1009214	1821097	27.18%	3.346%
24	11.965	1677	1685	1695	rVV	1888953	3194619	47.68%	5.869%
25	12.076	1695	1704	1716	rVB	1419068	2610757	38.96%	4.796%
26	12.400	1747	1759	1767	rBV	1689707	2896413	43.23%	5.321%
27	12.700	1800	1810	1816	rBV	309440	512290	7.65%	0.941%
28	12.853	1827	1836	1845	rBV	802637	1392211	20.78%	2.558%
29	13.035	1861	1867	1873	rBV	676000	1106873	16.52%	2.033%
30	13.100	1873	1878	1880	rVV	432379	679964	10.15%	1.249%
31	13.135	1880	1884	1889	rVV	768568	1276443	19.05%	2.345%
32	13.176	1889	1891	1897	rVB	79780	96321	1.44%	0.177%
33	13.341	1911	1919	1929	rVB	1671158	2795808	41.73%	5.136%
34	13.482	1936	1943	1951	rBV	4123896	6700435	100.00%	12.310%
35	13.617	1957	1966	1971	rBV3	101126	235037	3.51%	0.432%
36	13.676	1971	1976	1981	rVB	65600	99529	1.49%	0.183%

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37	13.729	1981	1985	1989	rBV2	44372	67787	1.01%	0.125%
38	13.794	1989	1996	1998	rBV	1022785	1694520	25.29%	3.113%
39	13.953	2017	2023	2026	rBV	502973	829469	12.38%	1.524%
40	13.994	2026	2030	2035	rVV2	1090704	2060973	30.76%	3.786%
41	14.035	2035	2037	2046	rVB2	396612	618712	9.23%	1.137%
42	14.117	2046	2051	2057	rVB	107648	174658	2.61%	0.321%
43	14.188	2057	2063	2068	rBV	245510	410463	6.13%	0.754%
44	14.247	2068	2073	2076	rVV	605857	1002598	14.96%	1.842%
45	14.276	2076	2078	2082	rVV	337195	424423	6.33%	0.780%
46	14.335	2082	2088	2094	rVB	909875	1434565	21.41%	2.636%
47	14.400	2094	2099	2102	rBV	211926	347587	5.19%	0.639%
48	14.447	2102	2107	2114	rVB2	787048	1339263	19.99%	2.460%
49	14.576	2123	2129	2135	rVB2	211621	344902	5.15%	0.634%
50	14.659	2135	2143	2146	rBV	665440	1141603	17.04%	2.097%
51	14.694	2146	2149	2154	rVV	680619	1047531	15.63%	1.924%
52	14.735	2154	2156	2160	rVB	61965	76014	1.13%	0.140%
53	14.882	2171	2181	2184	rBV2	68106	130866	1.95%	0.240%
54	14.929	2184	2189	2194	rVV	628169	1064754	15.89%	1.956%
55	14.970	2194	2196	2201	rVV	86943	115327	1.72%	0.212%
56	15.053	2201	2210	2216	rVV2	969527	2061788	30.77%	3.788%
57	15.117	2216	2221	2227	rVB5	60673	147082	2.20%	0.270%
58	15.211	2232	2237	2245	rBV3	79858	152499	2.28%	0.280%
59	15.323	2245	2256	2261	rBV3	261099	699776	10.44%	1.286%
60	15.441	2269	2276	2285	rVB2	219485	549876	8.21%	1.010%
61	15.641	2303	2310	2317	rVB	352571	668440	9.98%	1.228%
62	15.753	2323	2329	2334	rBV3	59742	119691	1.79%	0.220%
63	15.811	2334	2339	2350	rVB2	46626	111678	1.67%	0.205%
64	15.947	2355	2362	2371	rBV2	66138	132968	1.98%	0.244%
65	16.129	2383	2393	2404	rBV4	35207	131206	1.96%	0.241%
66	16.341	2421	2429	2444	rVB5	30150	101028	1.51%	0.186%

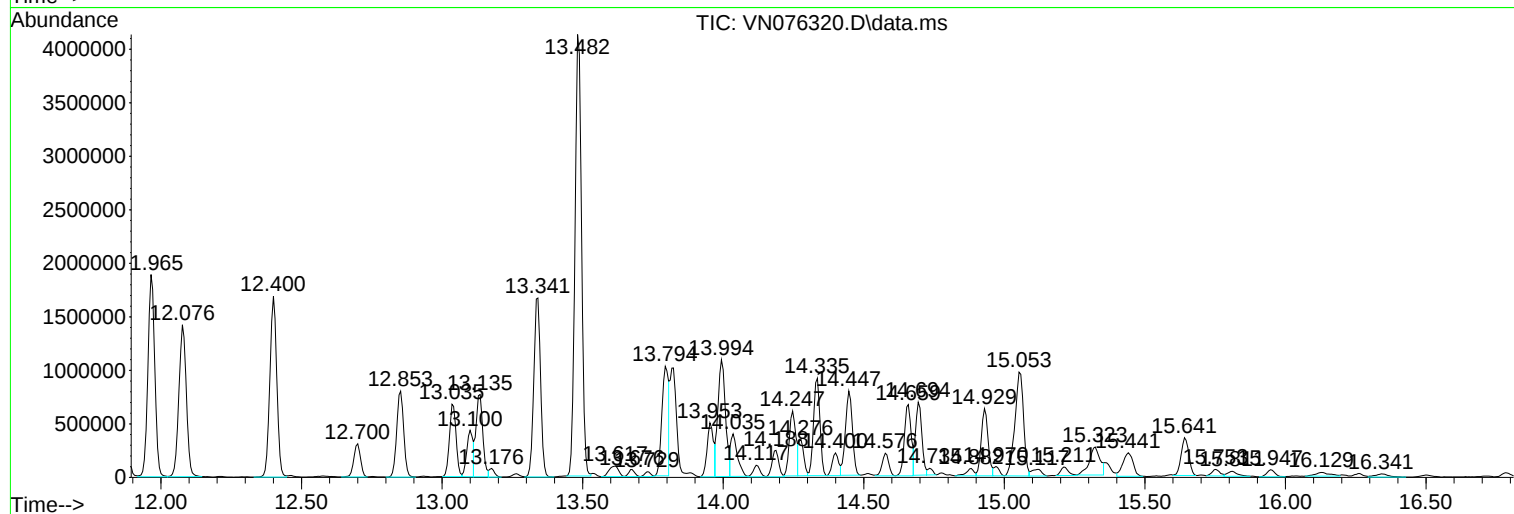
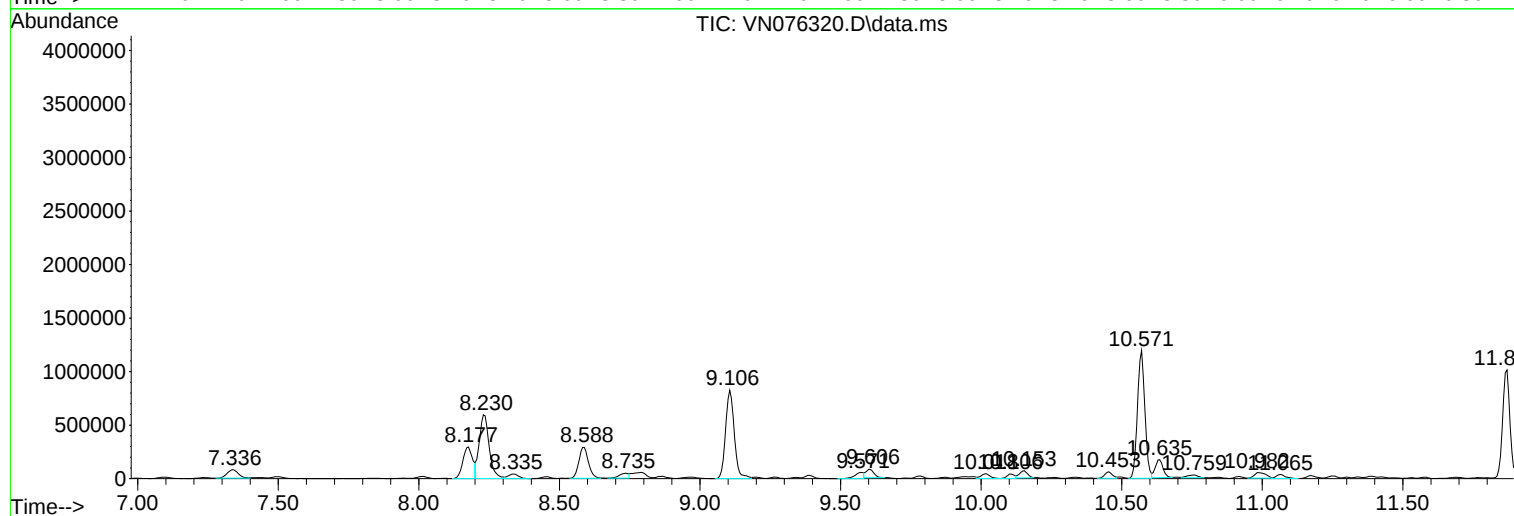
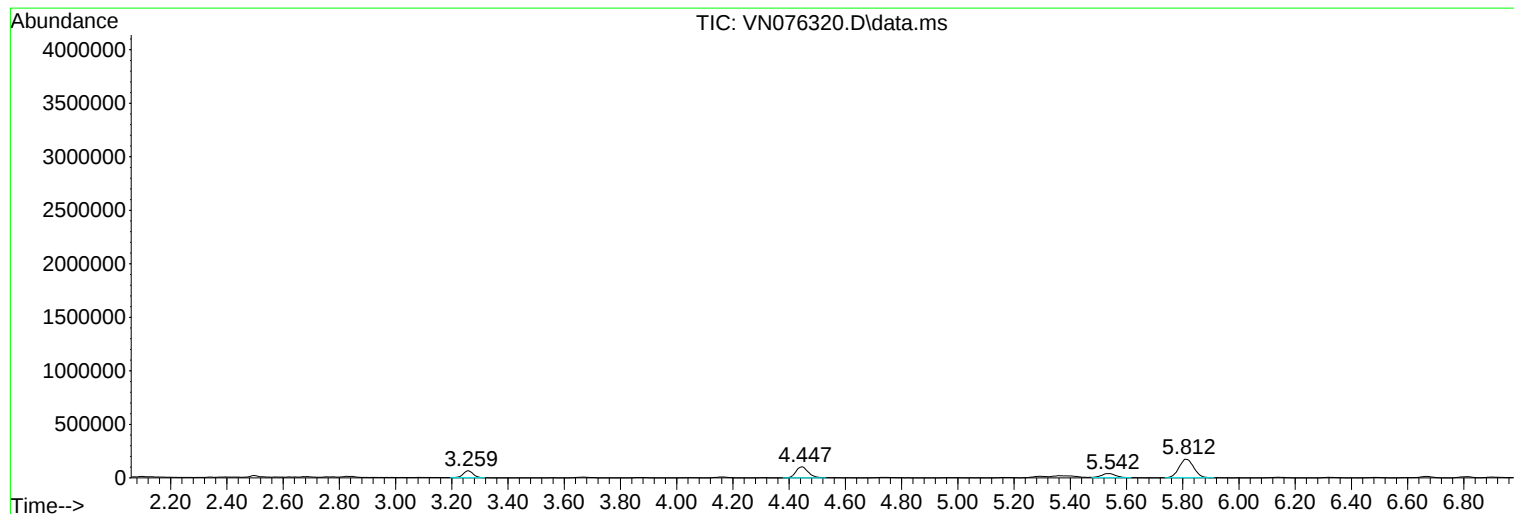
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ClientSampleId :
MW-12-0118

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

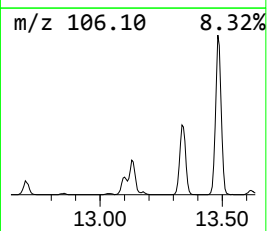
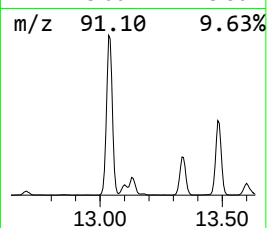
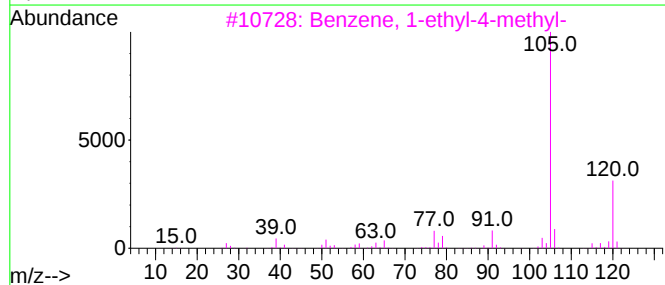
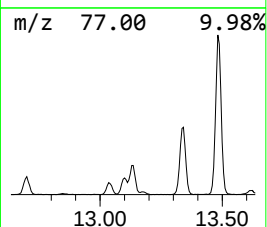
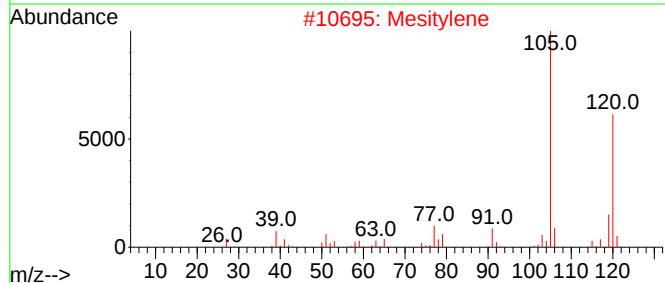
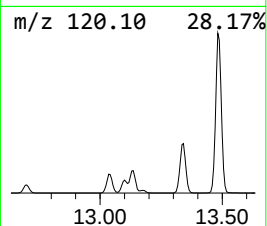
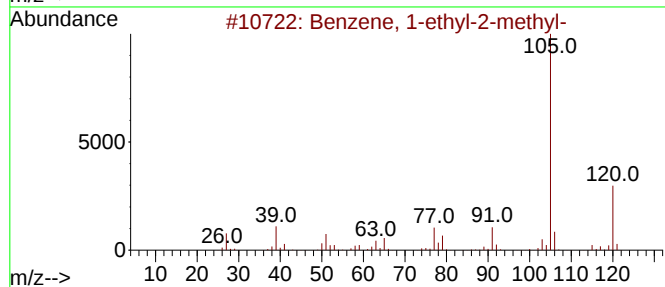
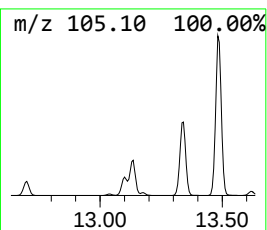
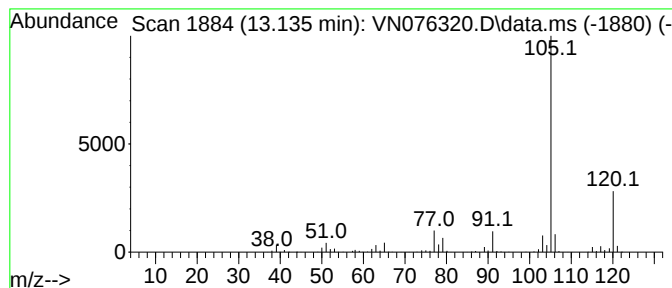
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.135	37.66 ug/l	1276440	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	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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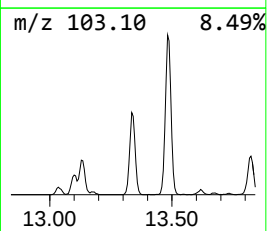
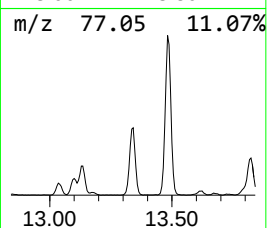
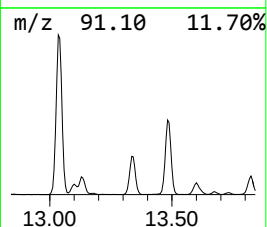
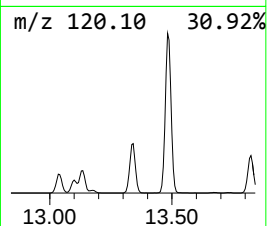
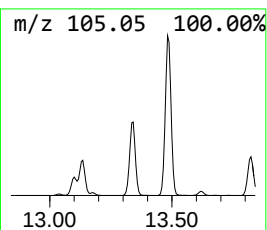
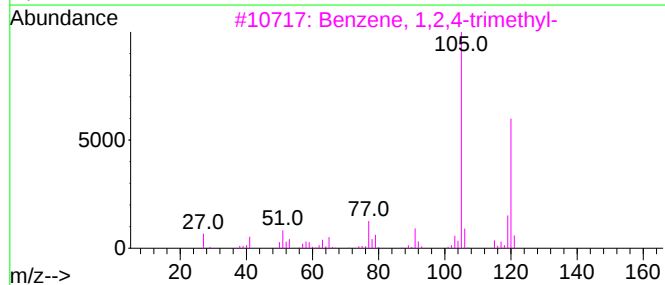
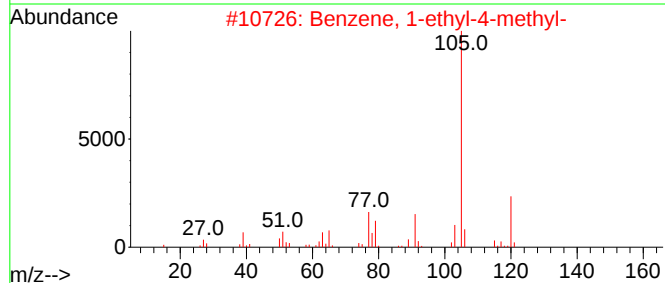
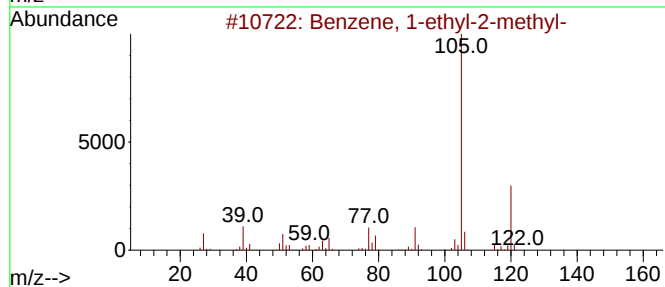
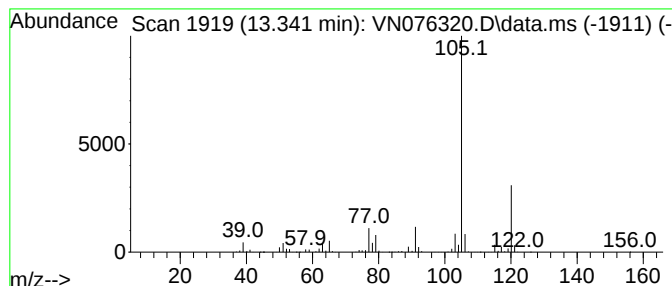
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	82.50 ug/l	2795810	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			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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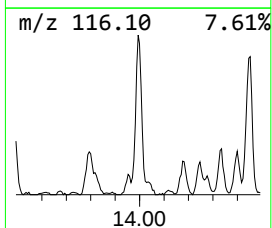
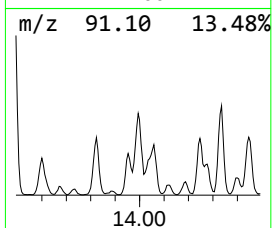
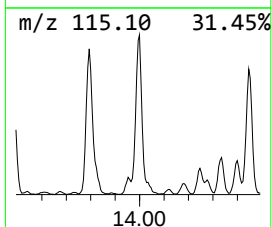
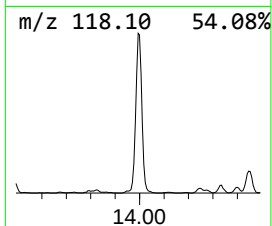
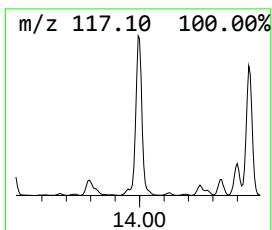
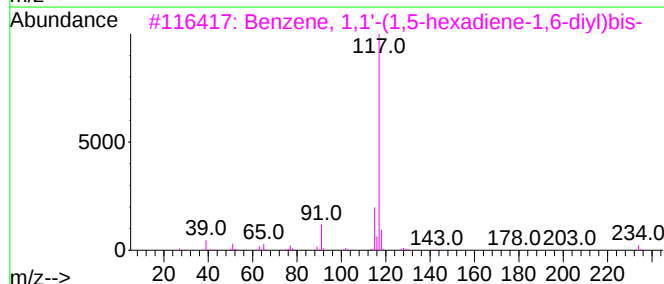
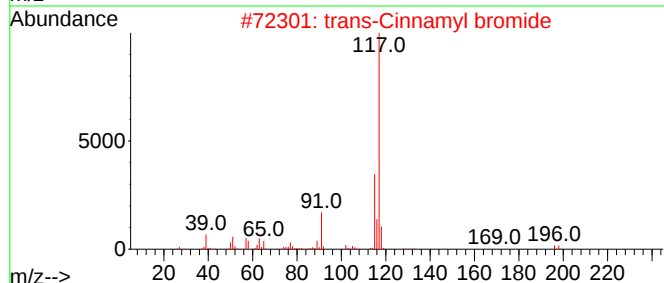
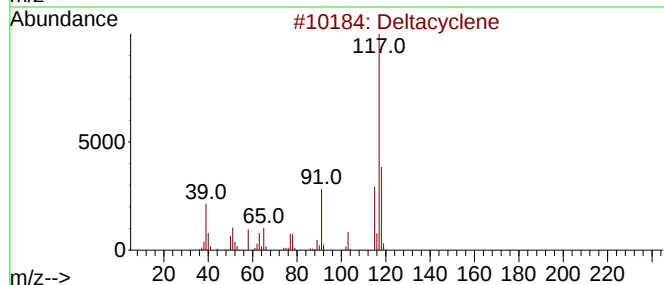
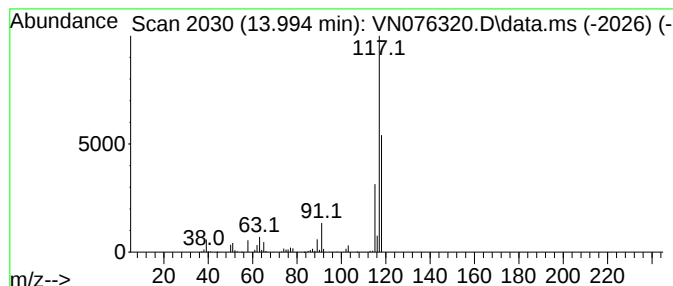
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Peak Number 3 trans-Cinnamyl bromide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	60.81 ug/l	2060970	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Deltacyclene	118	C9H10	007785-10-6	59
2			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
4			Indole	117	C8H7N	000120-72-9	46
5			Benzyl nitrile	117	C8H7N	000140-29-4	37



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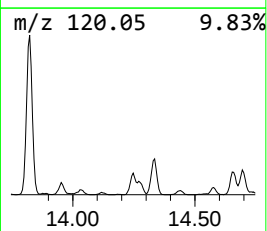
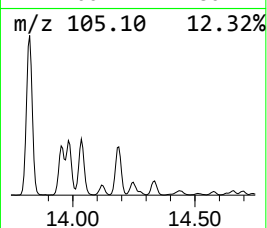
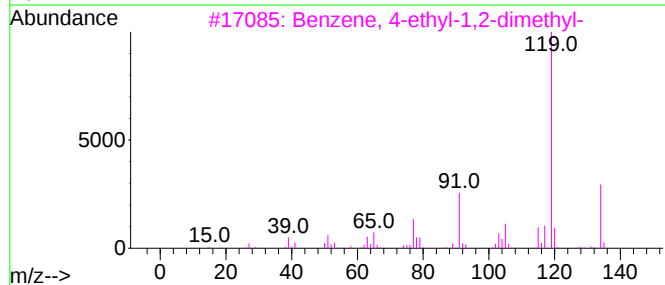
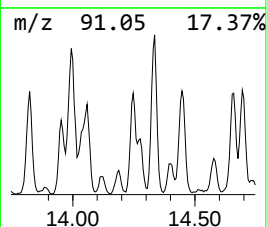
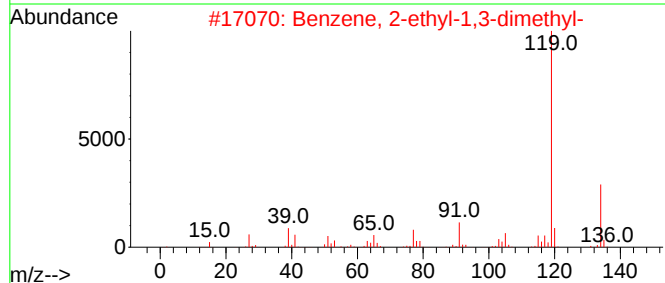
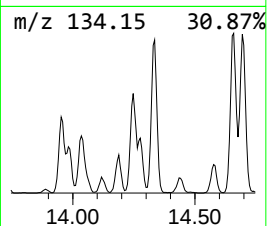
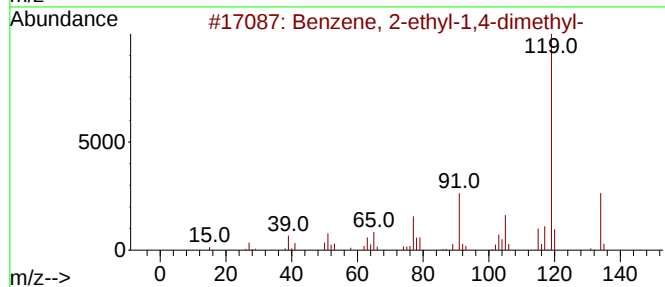
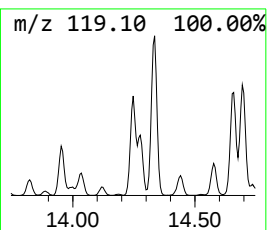
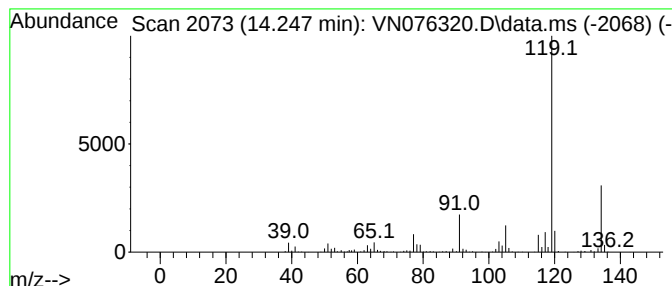
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Peak Number 4 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	29.58 ug/l	1002600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

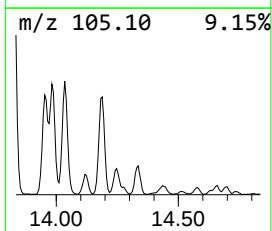
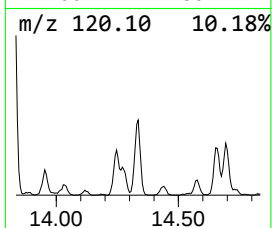
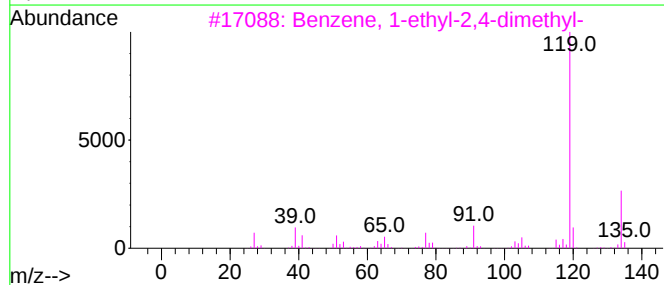
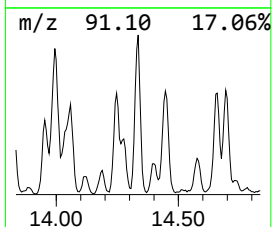
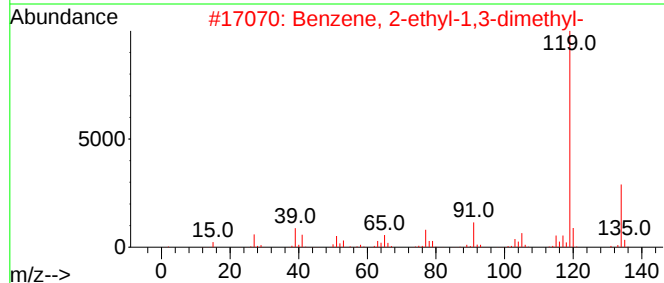
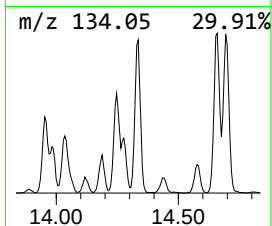
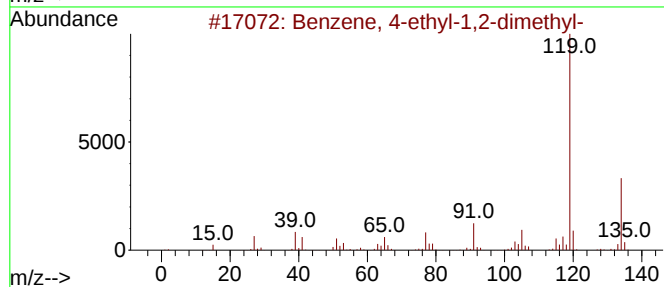
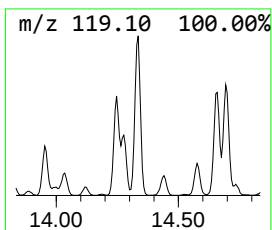
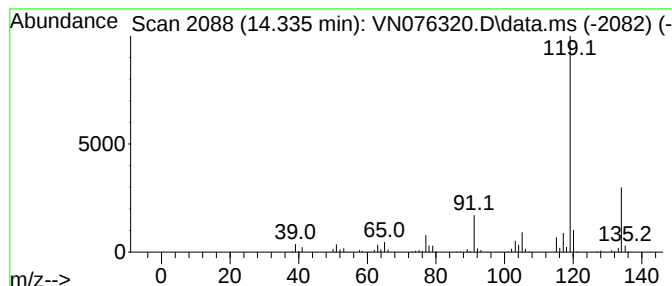
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.335	42.33 ug/l	1434570	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	95
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

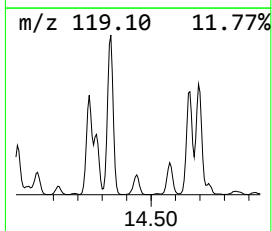
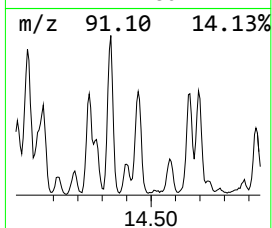
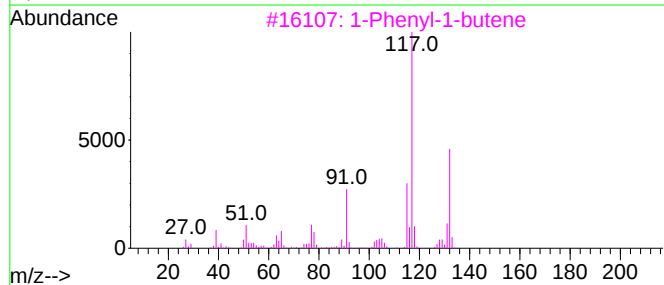
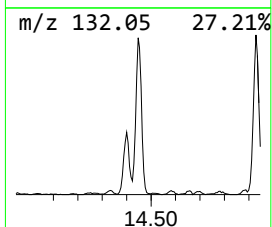
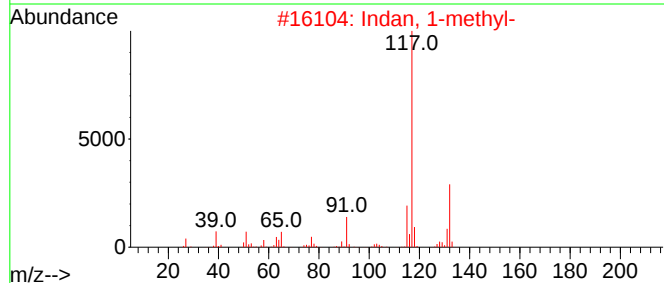
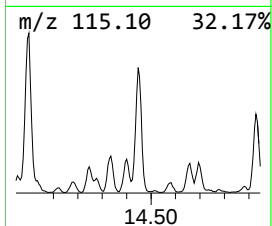
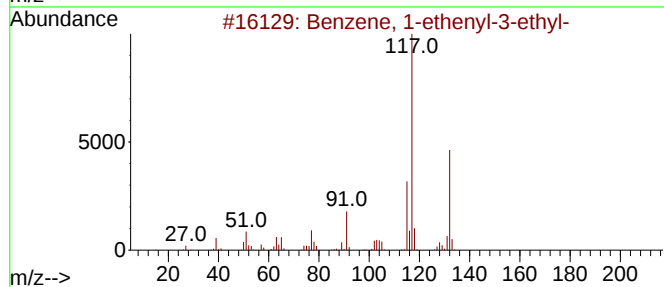
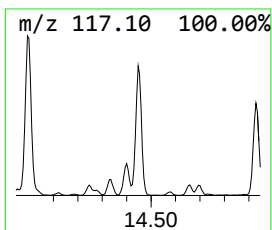
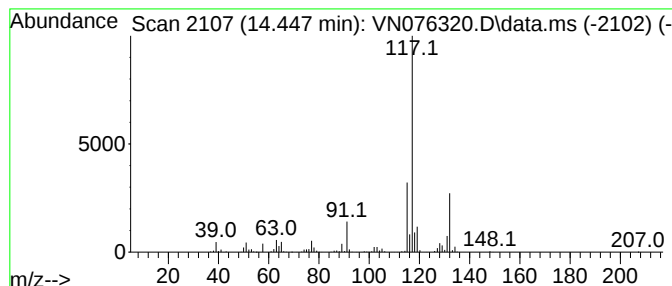
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	39.52 ug/l	1339260	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	83
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

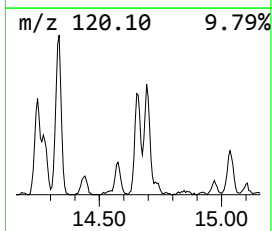
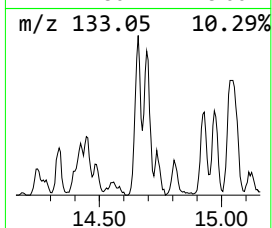
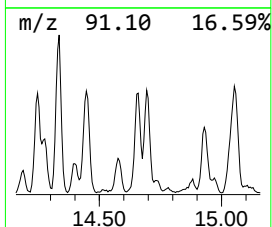
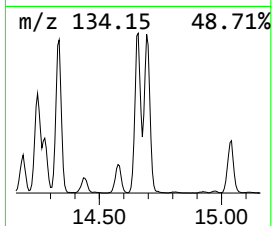
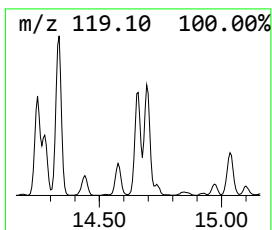
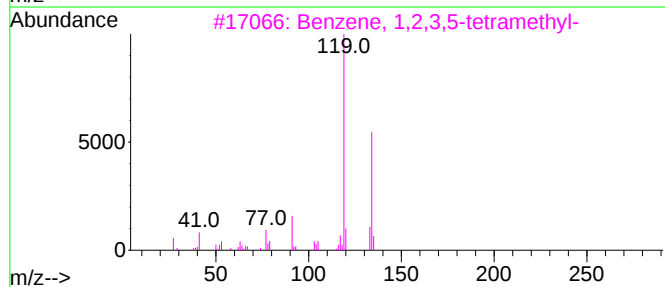
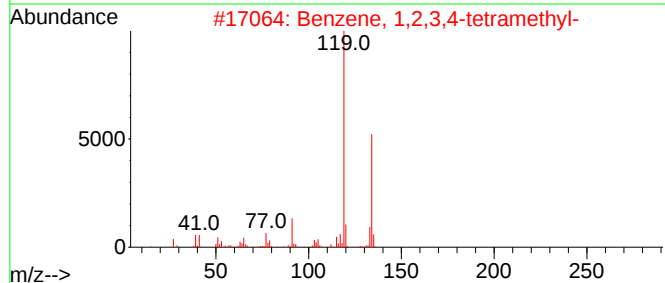
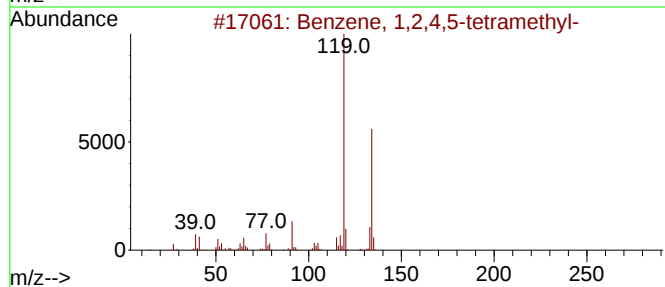
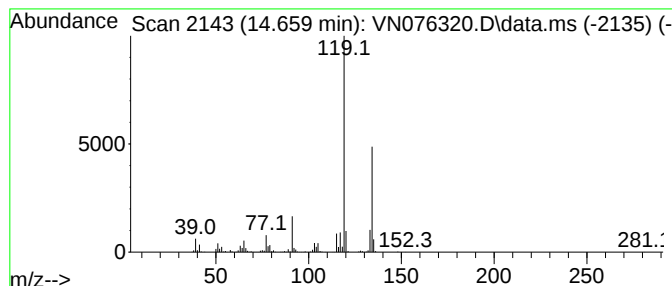
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	33.69 ug/l	1141600	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	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5			o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

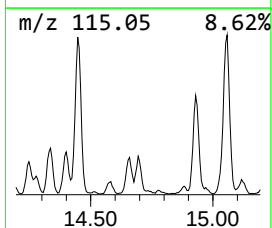
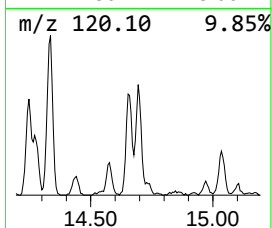
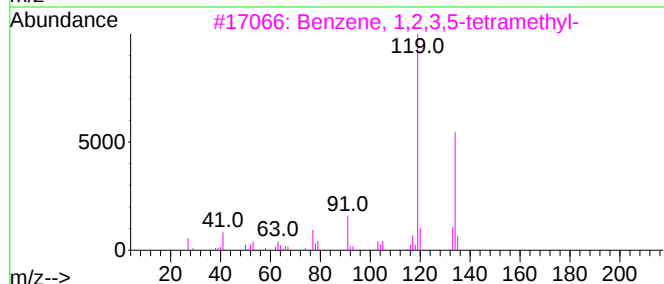
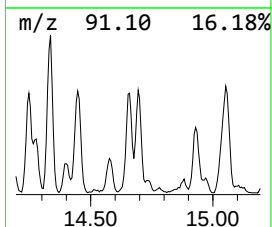
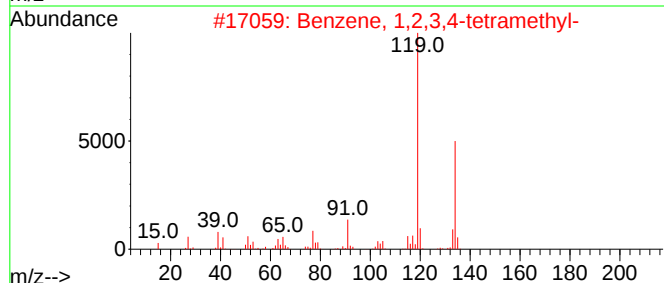
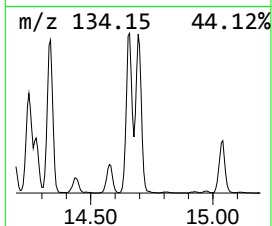
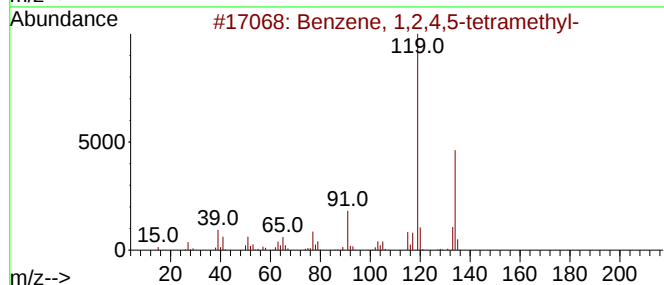
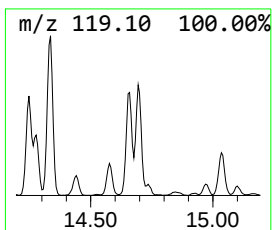
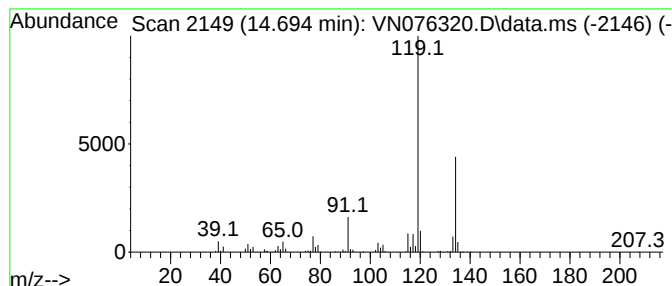
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	30.91 ug/l	1047530	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	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

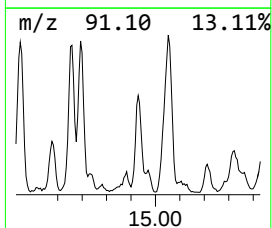
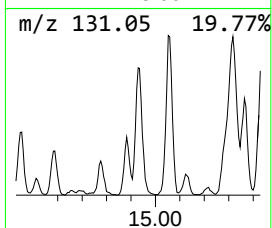
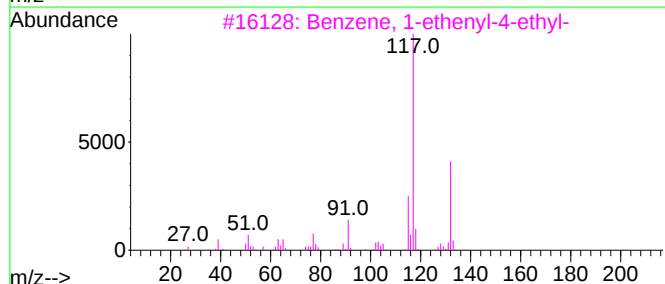
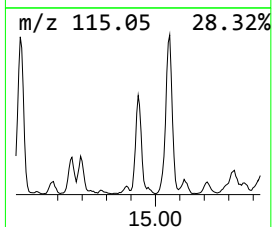
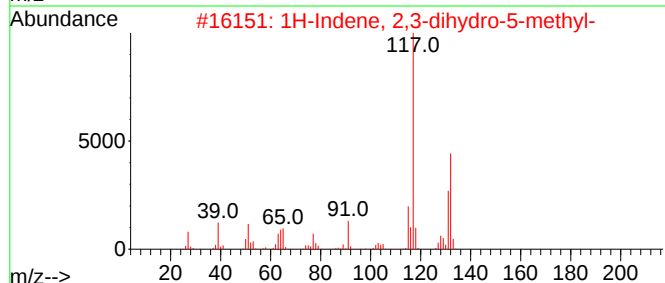
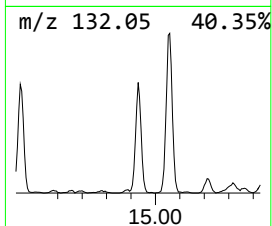
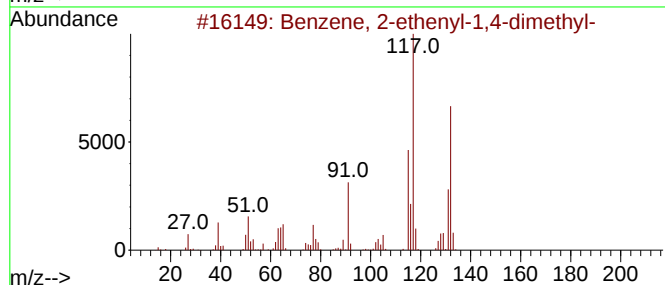
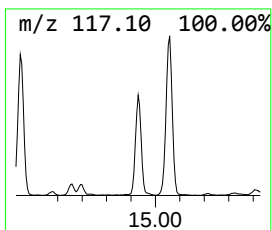
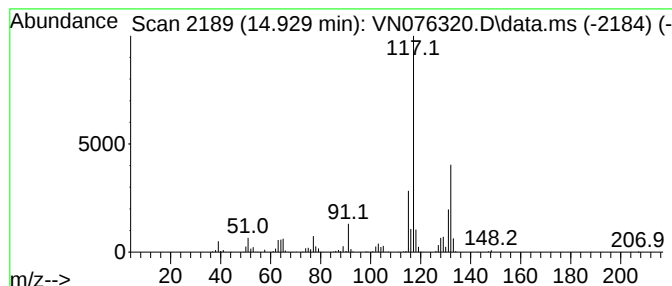
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.929	31.42 ug/l	1064750	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			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

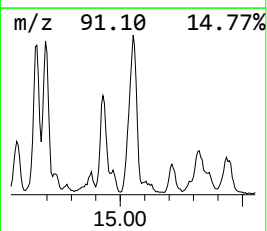
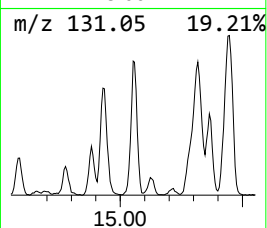
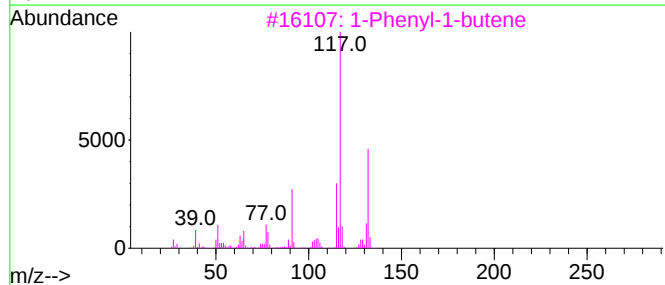
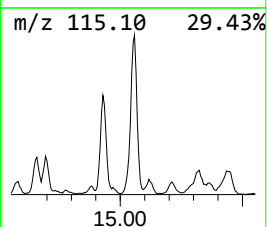
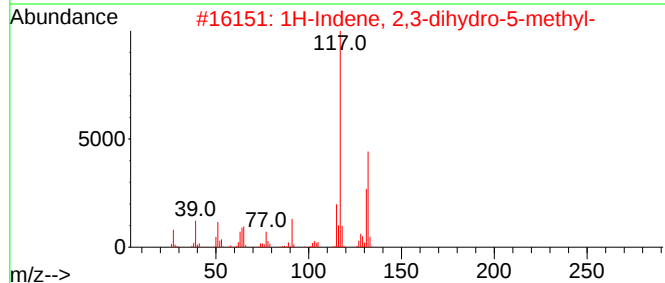
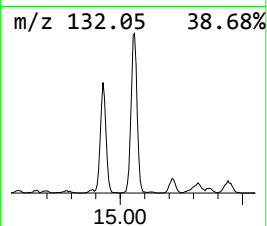
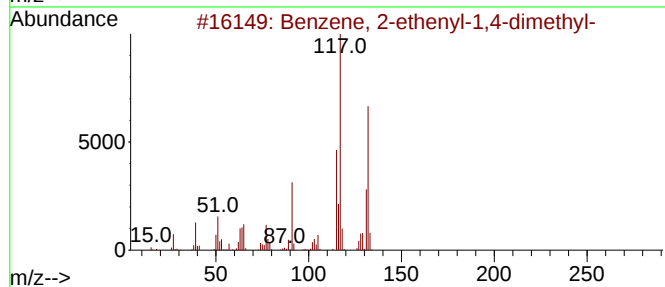
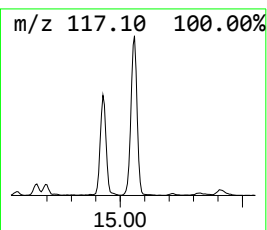
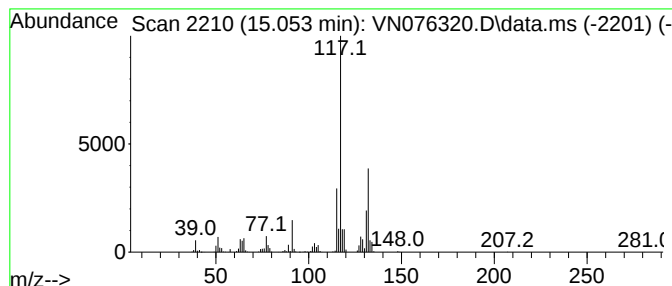
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	60.84 ug/l	2061790	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	92
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3		1-Phenyl-1-butene	132	C10H12	000824-90-8	90
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
5		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011923\
Data File : VN076320.D
Acq On : 19 Jan 2023 14:07
Operator : JC\MD
Sample : 01221-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12-0118

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011623W.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	82.5	ug/l	2795810	4	13.794	1694520	50.0
trans-Cinnamyl ...	13.994	60.8	ug/l	2060970	4	13.794	1694520	50.0
Benzene, 2-ethy...	14.247	29.6	ug/l	1002600	4	13.794	1694520	50.0
Benzene, 4-ethy...	14.335	42.3	ug/l	1434570	4	13.794	1694520	50.0
Benzene, 1-ethe...	14.447	39.5	ug/l	1339260	4	13.794	1694520	50.0
Benzene, 1,2,4,...	14.659	33.7	ug/l	1141600	4	13.794	1694520	50.0
Benzene, 1,2,3,...	14.694	30.9	ug/l	1047530	4	13.794	1694520	50.0
Benzene, 2-ethe...	14.929	31.4	ug/l	1064750	4	13.794	1694520	50.0
1H-Indene, 2,3-...	15.053	60.8	ug/l	2061790	4	13.794	1694520	50.0