

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
 Data File : VN084861.D
 Acq On : 14 Nov 2024 18:58
 Operator : JC\MD
 Sample : P4770-01 500X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1046	1056	1060	rBV	130770	315659	6.52%	1.001%
2	8.218	1060	1065	1078	rVB	240305	529507	10.93%	1.680%
3	8.577	1116	1126	1135	rBV	140877	338163	6.98%	1.073%
4	8.753	1143	1156	1179	rVB4	58721	290786	6.00%	0.922%
5	9.100	1206	1215	1228	rBV	340374	719218	14.85%	2.282%
6	10.012	1362	1370	1379	rVB2	34969	69457	1.43%	0.220%
7	10.141	1379	1392	1399	rBV2	61476	133129	2.75%	0.422%
8	10.565	1456	1464	1469	rVV	509141	934585	19.29%	2.965%
9	10.629	1469	1475	1487	rVV	322036	608802	12.57%	1.931%
10	11.865	1673	1685	1693	rBV	481572	857774	17.71%	2.721%
11	11.959	1694	1701	1710	rVV	450832	773439	15.97%	2.454%
12	12.065	1710	1719	1730	rVB	1972422	3748092	77.37%	11.890%
13	12.394	1765	1775	1785	rBV	994693	1665944	34.39%	5.285%
14	12.694	1818	1826	1833	rBV	317047	518561	10.70%	1.645%
15	12.847	1840	1852	1860	rVB	429532	740803	15.29%	2.350%
16	13.035	1877	1884	1888	rBV	521989	830656	17.15%	2.635%
17	13.094	1888	1894	1898	rVV	1774098	3039903	62.75%	9.643%
18	13.129	1898	1900	1903	rVV	751088	934042	19.28%	2.963%
19	13.170	1903	1907	1917	rVB	932769	1483689	30.63%	4.707%
20	13.335	1928	1935	1942	rBV	644217	1061368	21.91%	3.367%
21	13.482	1952	1960	1967	rBV	2940723	4844369	100.00%	15.367%
22	13.612	1973	1982	1987	rBV3	48461	119624	2.47%	0.379%
23	13.670	1987	1992	1997	rVB	59197	89016	1.84%	0.282%
24	13.794	2006	2013	2014	rBV	540012	858182	17.72%	2.722%
25	13.817	2014	2017	2027	rVB	672860	1059996	21.88%	3.363%
26	13.947	2034	2039	2040	rBV	110376	134296	2.77%	0.426%
27	13.988	2040	2046	2049	rBV2	403949	794511	16.40%	2.520%
28	14.176	2073	2078	2084	rBV	104645	174201	3.60%	0.553%
29	14.241	2084	2089	2092	rVV	209007	361192	7.46%	1.146%
30	14.270	2092	2094	2099	rVV	195578	255114	5.27%	0.809%
31	14.329	2099	2104	2110	rVV	342102	534913	11.04%	1.697%
32	14.441	2118	2123	2132	rVB2	106756	193506	3.99%	0.614%
33	14.570	2140	2145	2151	rVB2	69731	112192	2.32%	0.356%
34	14.653	2151	2159	2162	rBV	202724	356178	7.35%	1.130%
35	14.688	2162	2165	2170	rVV	304778	458960	9.47%	1.456%
36	14.923	2200	2205	2210	rBV	116820	208801	4.31%	0.662%

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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

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37	15.047	2216	2226	2232	rVV4	195684	536000	11.06%	1.700%
38	15.100	2232	2235	2246	rVB3	30131	68362	1.41%	0.217%
39	15.206	2246	2253	2260	rBV5	22957	49521	1.02%	0.157%
40	15.317	2261	2272	2284	rVV3	56554	176775	3.65%	0.561%
41	15.429	2284	2291	2301	rVB4	36926	92756	1.91%	0.294%
42	15.635	2319	2326	2334	rVB	183664	347718	7.18%	1.103%
43	16.776	2513	2520	2522	rBV2	59122	103725	2.14%	0.329%

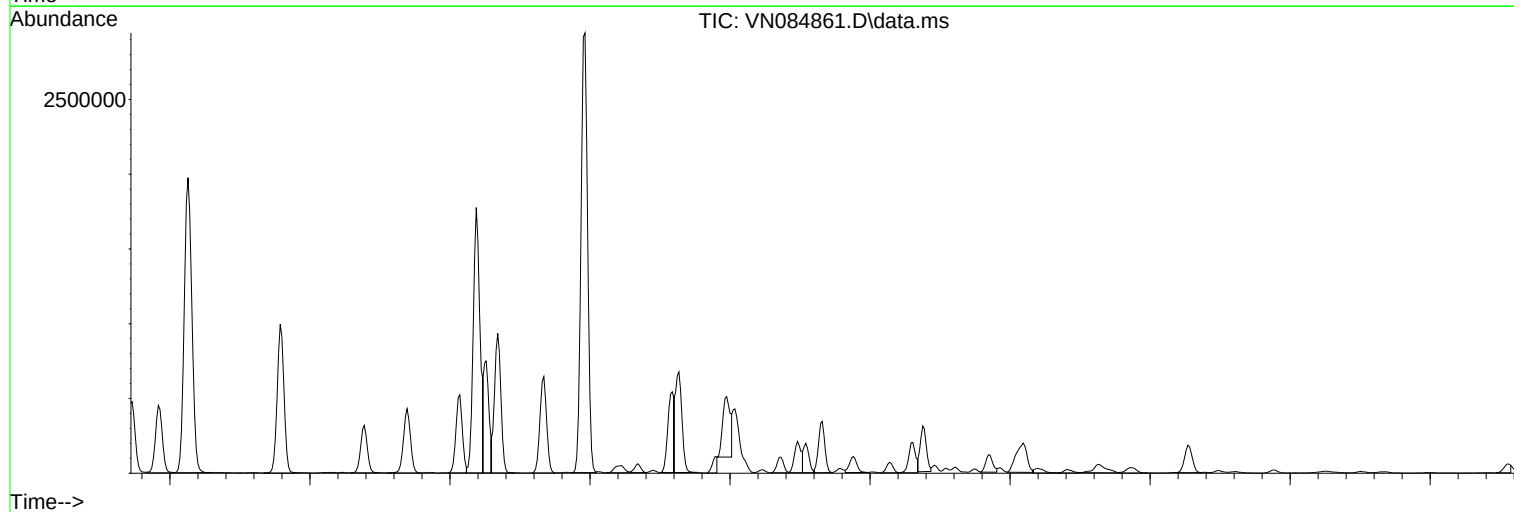
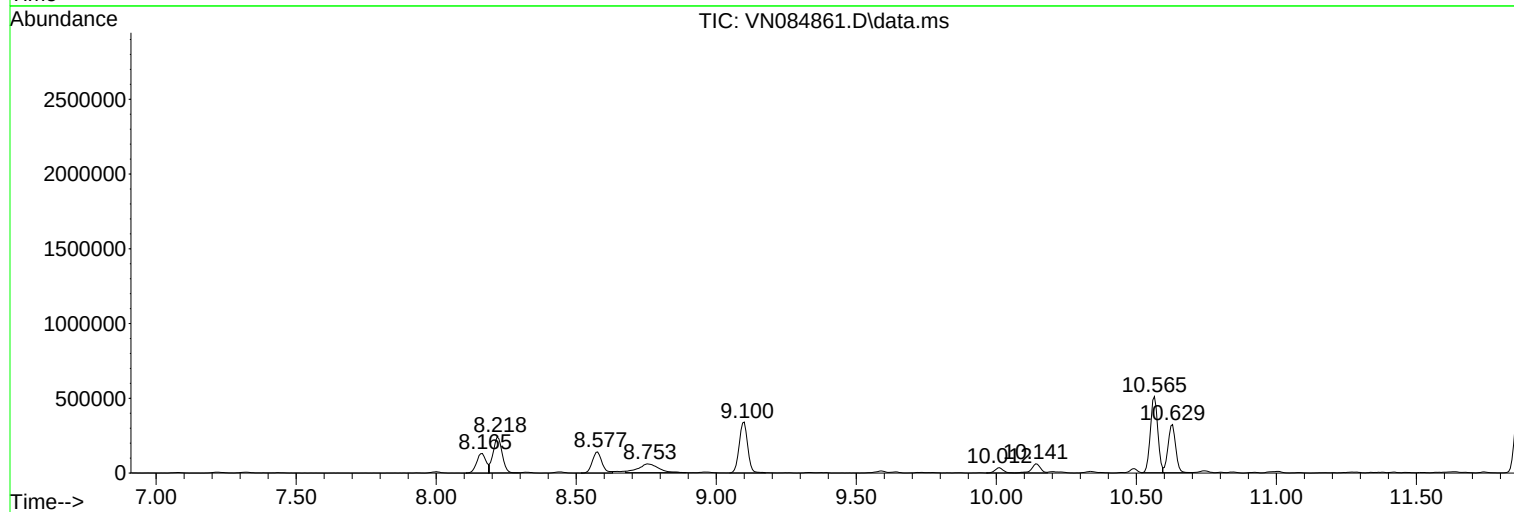
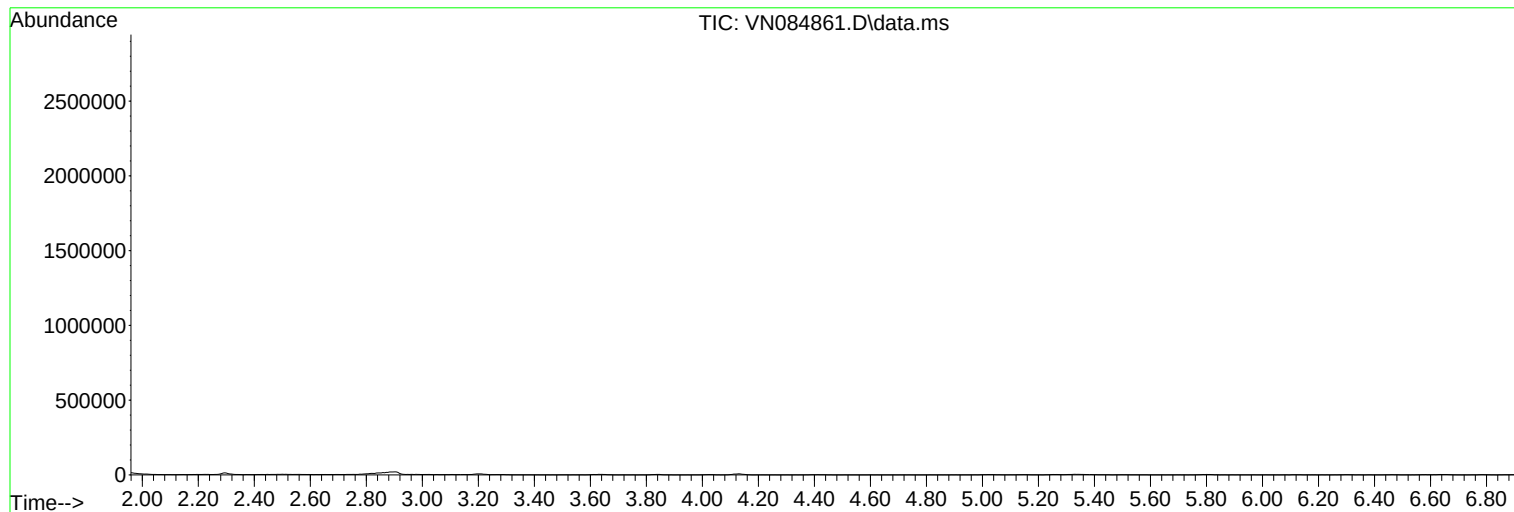
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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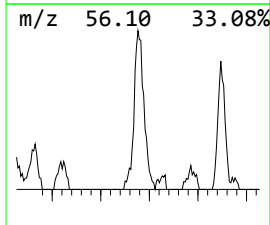
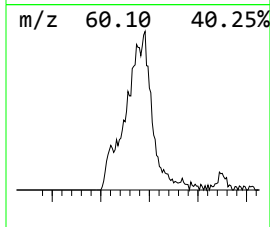
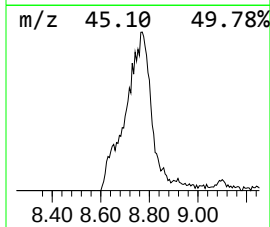
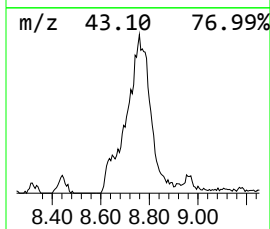
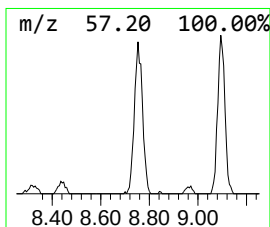
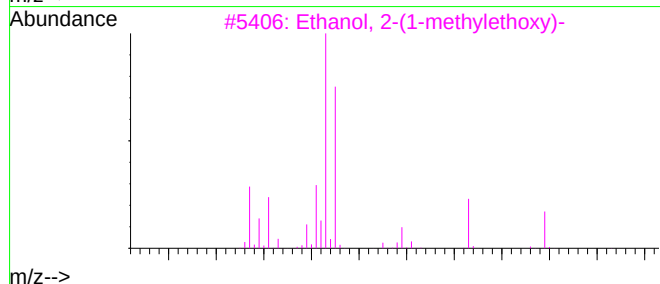
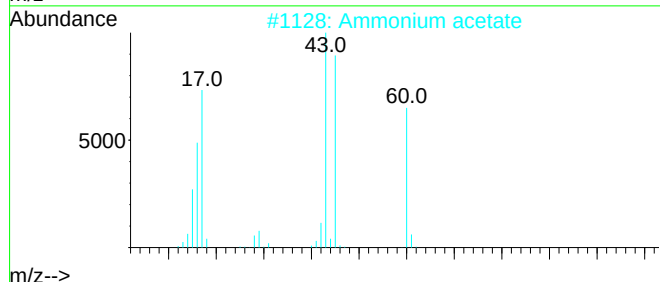
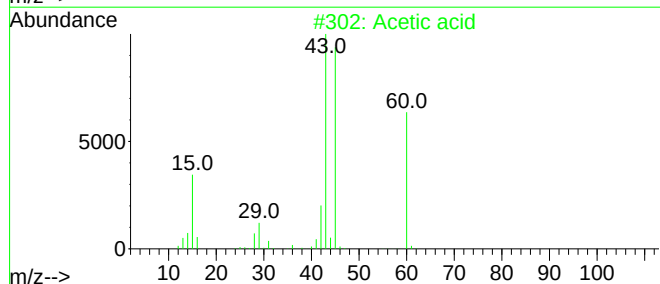
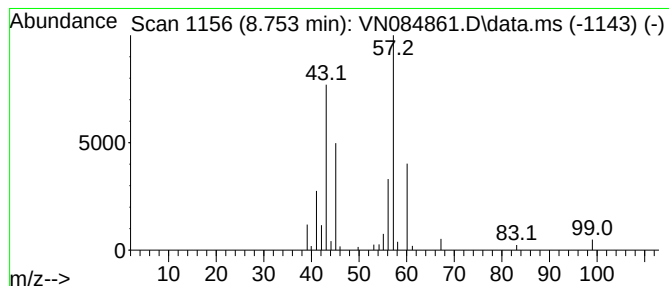
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	20.22 ug/l	290786	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	52
2	Ammonium acetate	77	C2H7NO2	000631-61-8	33
3	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	17
4	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	14
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	10



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

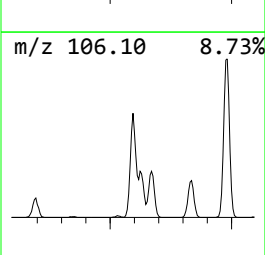
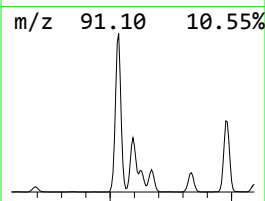
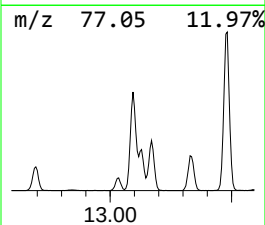
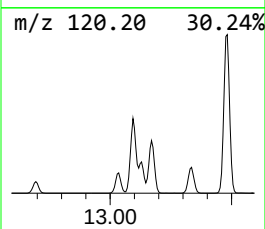
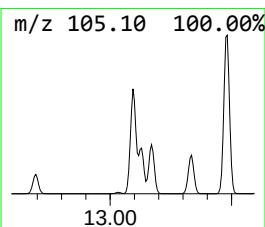
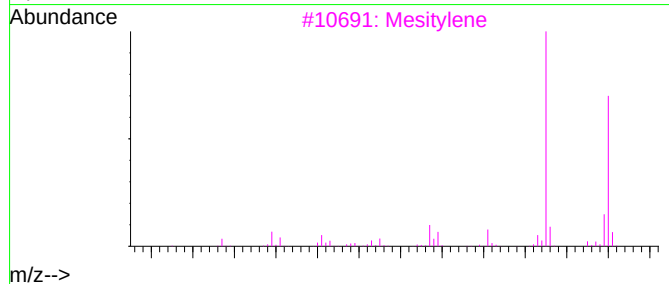
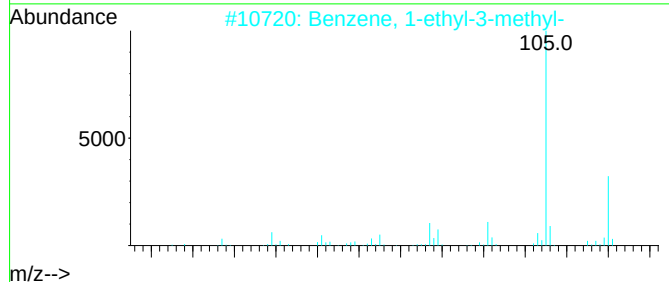
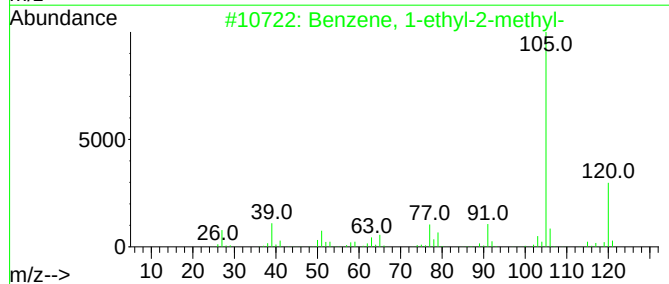
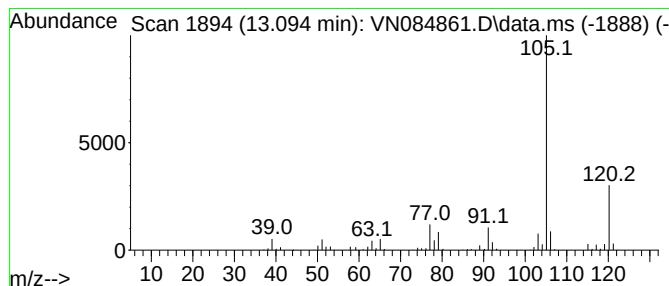
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	177.11 ug/l	3039900	1,4-Dichlorobenzene-d4	13.788

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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

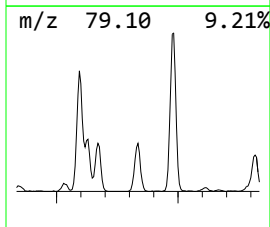
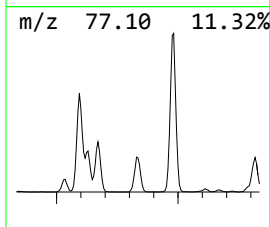
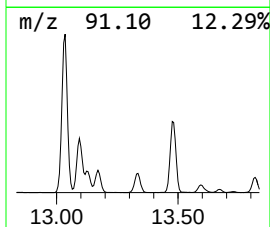
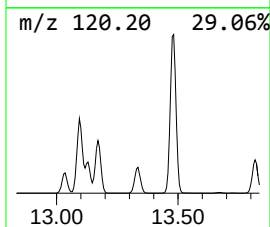
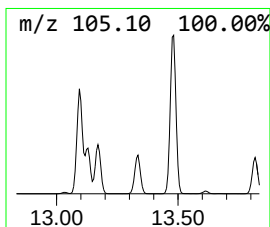
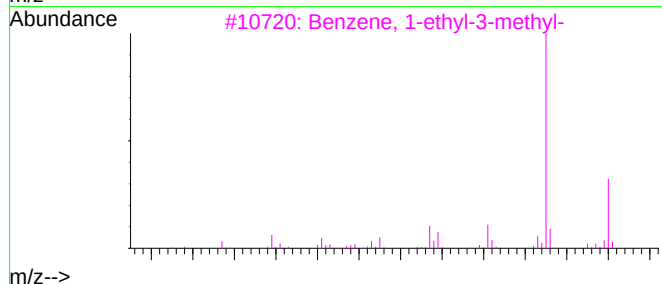
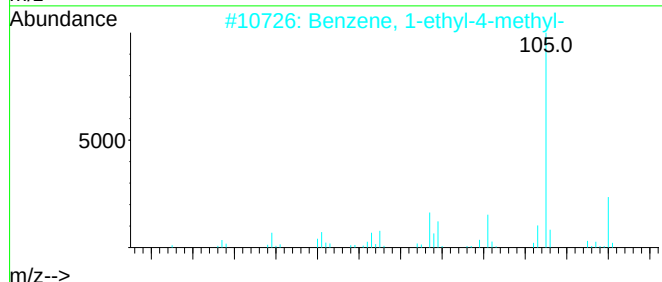
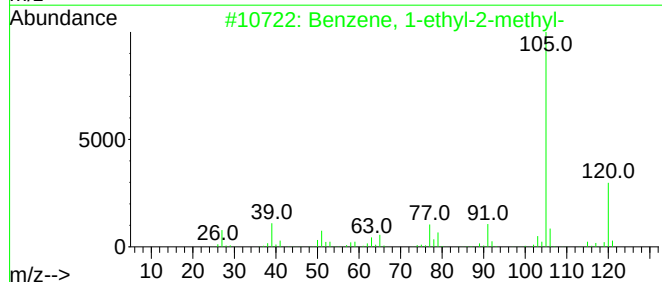
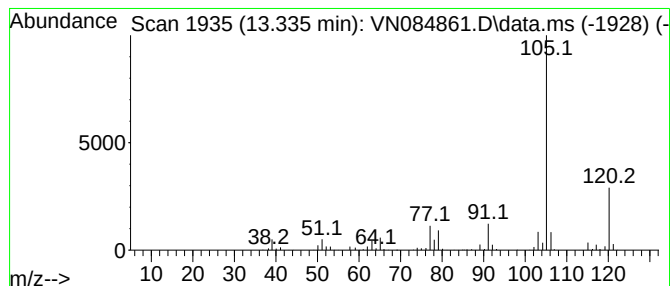
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	61.84 ug/l	1061370	1,4-Dichlorobenzene-d4	13.788

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-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91



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Quant Title : SW846 8260

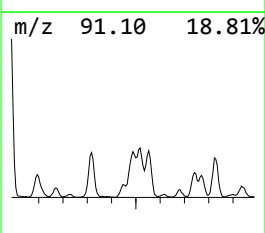
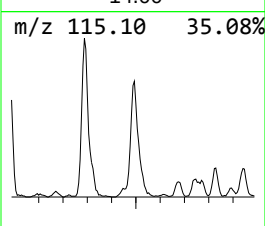
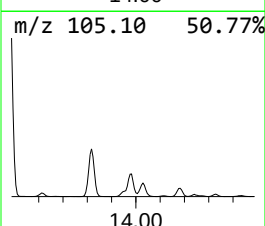
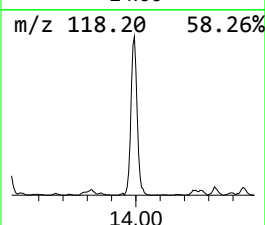
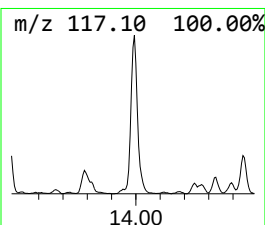
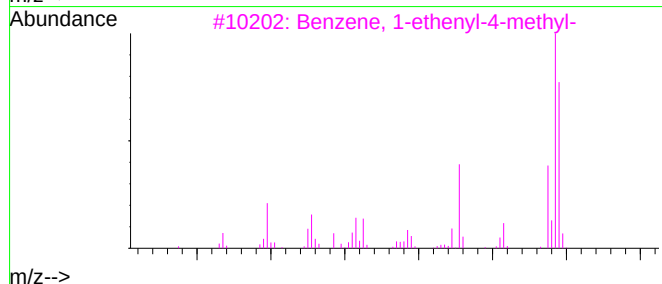
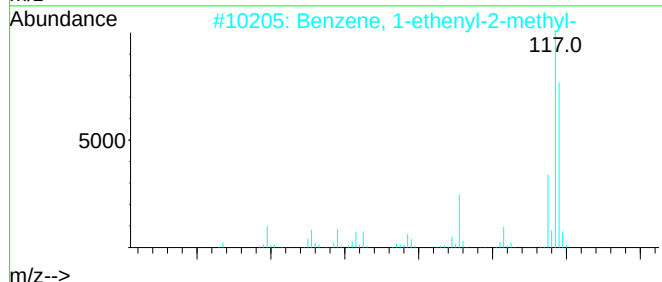
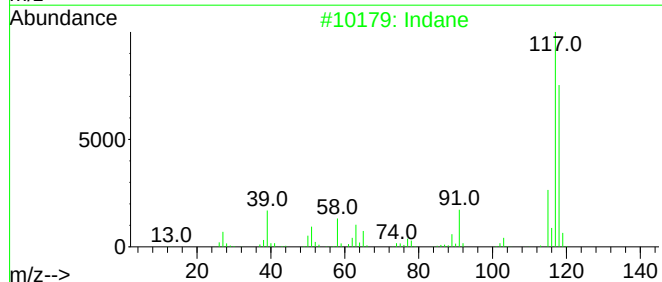
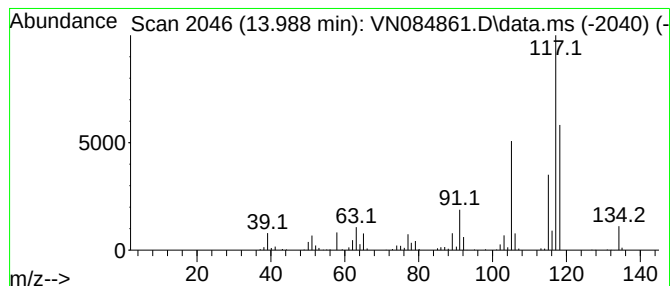
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	46.29 ug/l	794511	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	76
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

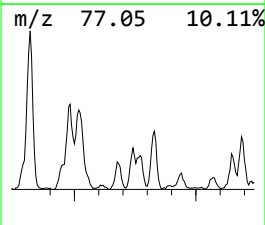
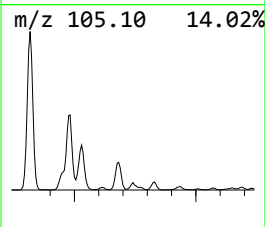
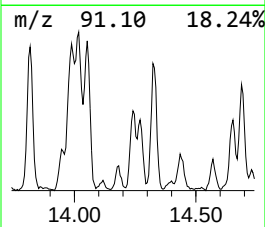
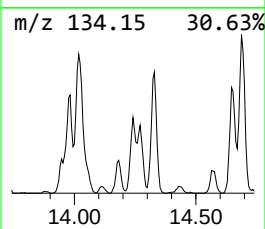
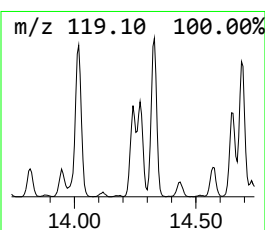
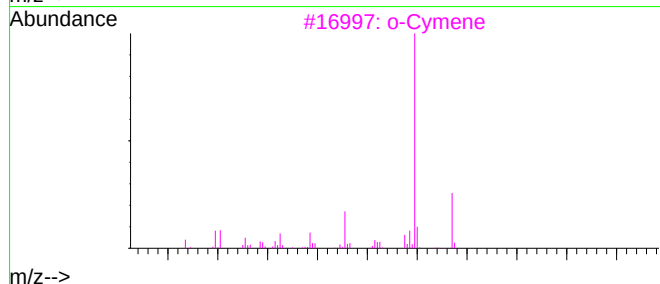
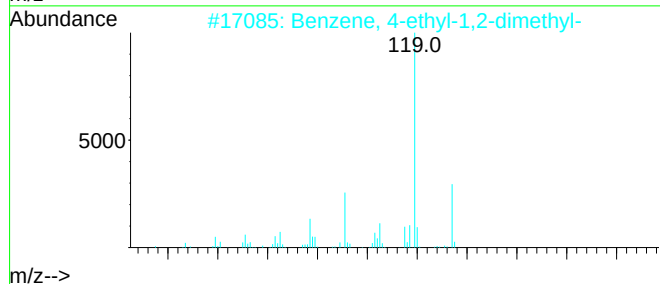
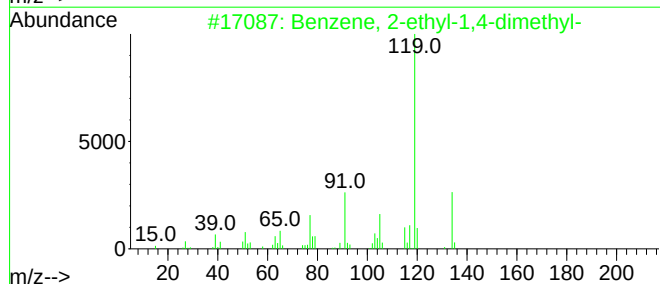
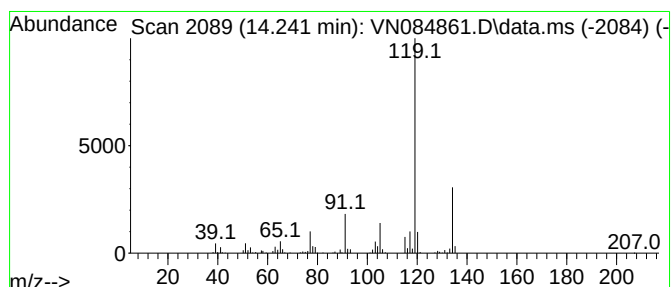
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	21.04 ug/l	361192	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

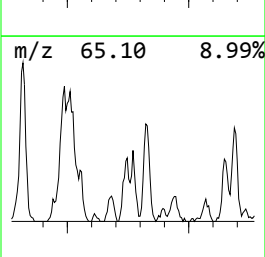
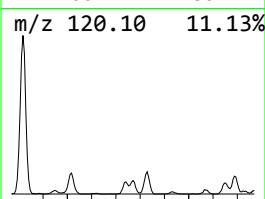
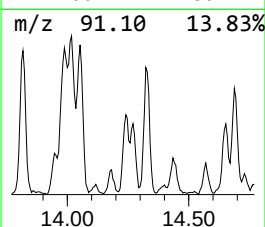
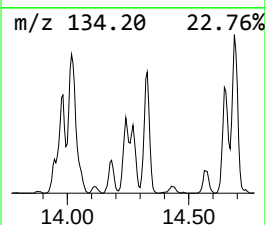
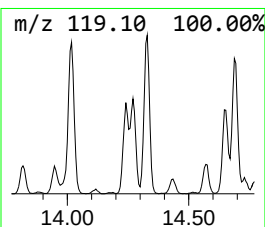
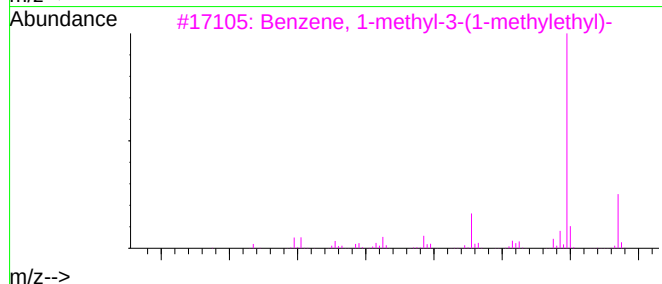
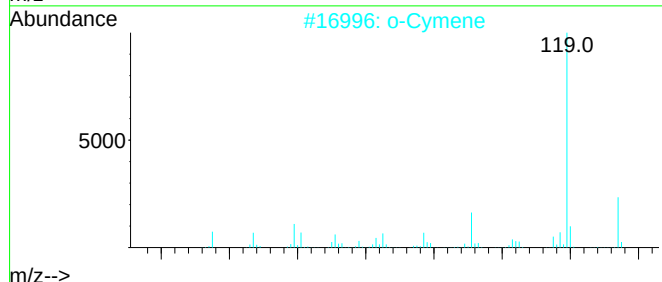
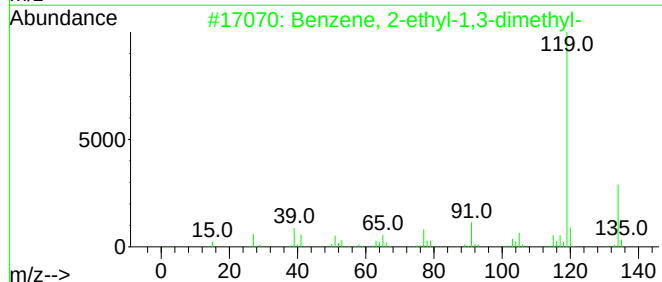
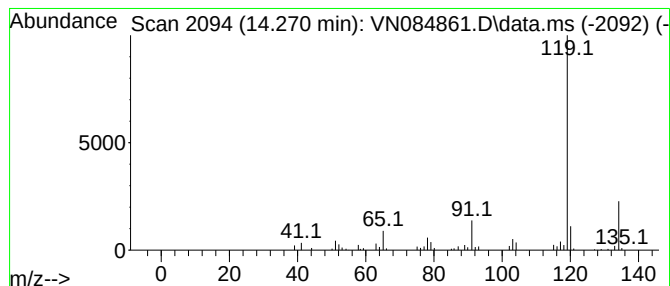
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.270	14.86 ug/l	255114	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91
2	o-Cymene	134	C10H14	000527-84-4	91
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5	p-Cymene	134	C10H14	000099-87-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

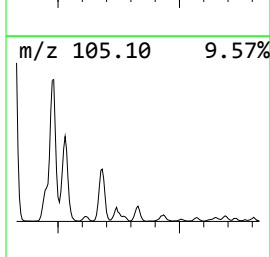
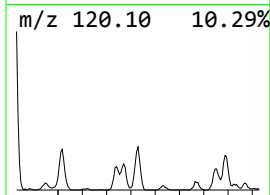
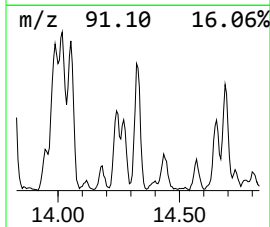
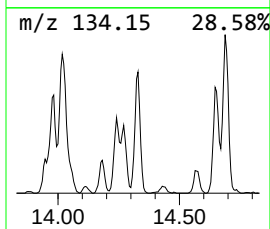
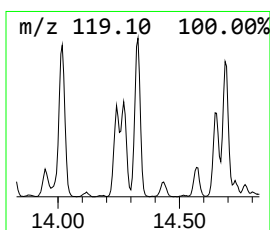
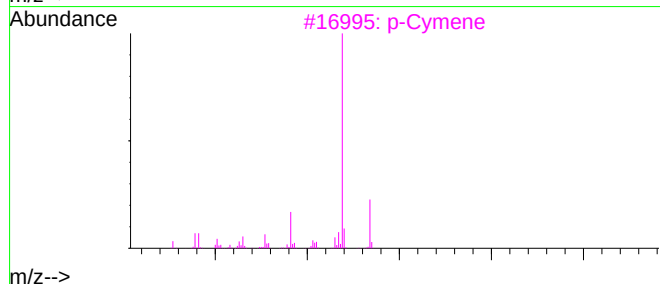
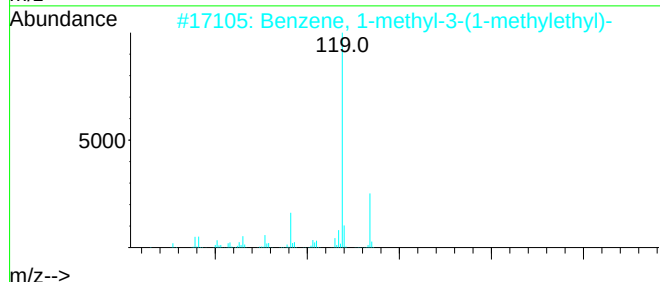
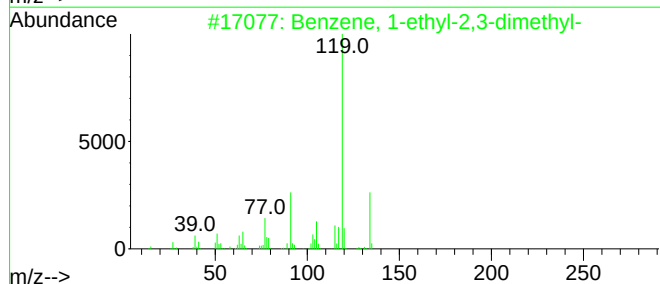
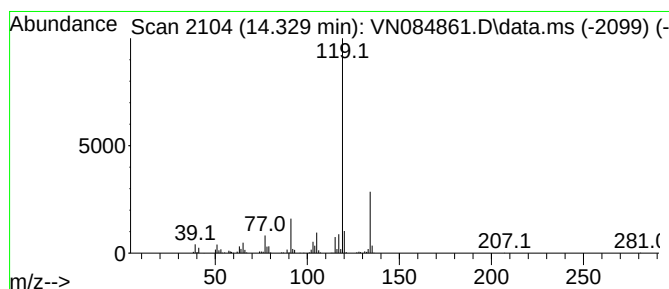
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.329	31.17 ug/l	534913	1,4-Dichlorobenzene-d4		13.788	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	95
2	Benzene, 1-methyl-3-(1-methyleth...		134	C10H14	000535-77-3	95
3	p-Cymene		134	C10H14	000099-87-6	95
4	o-Cymene		134	C10H14	000527-84-4	95
5	Benzene, 4-ethyl-1,2-dimethyl-		134	C10H14	000934-80-5	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

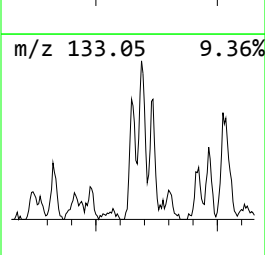
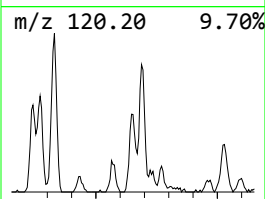
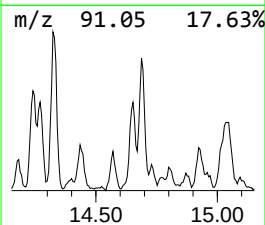
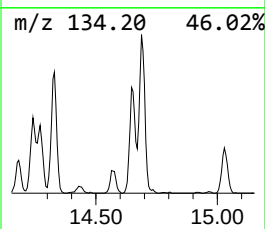
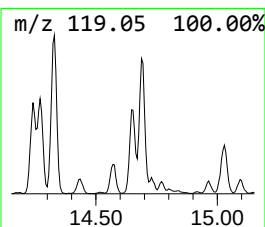
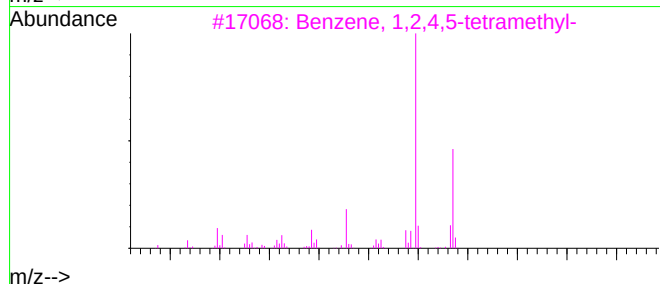
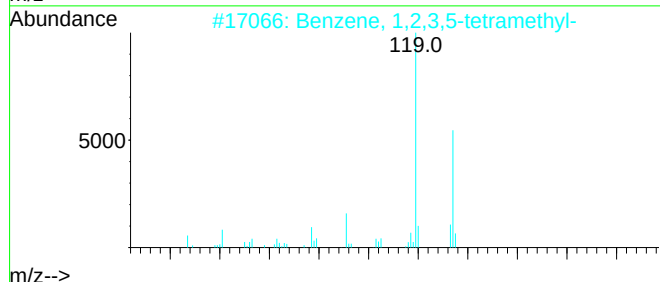
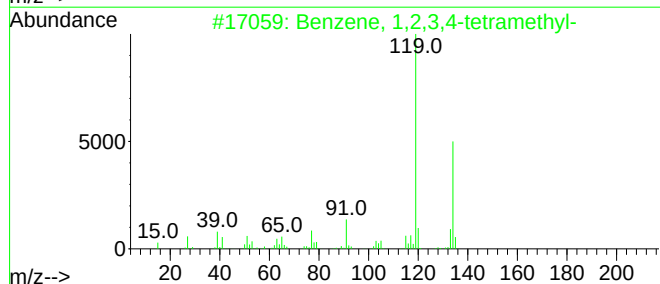
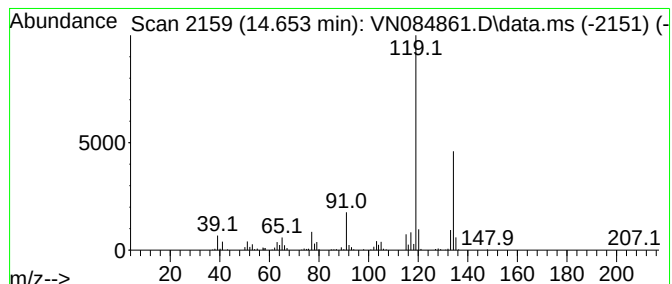
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.653	20.75 ug/l	356178	1,4-Dichlorobenzene-d4		13.788	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-		134	C10H14	000488-23-3	97
2	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	96
3	Benzene, 1,2,4,5-tetramethyl-		134	C10H14	000095-93-2	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\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

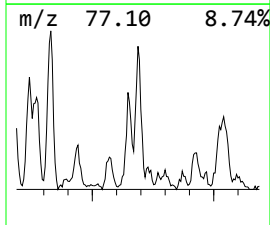
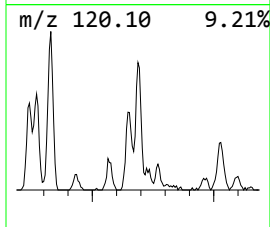
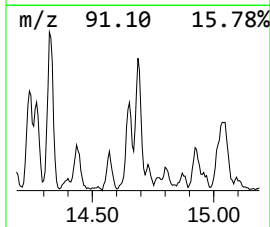
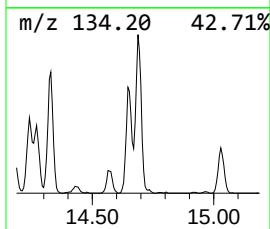
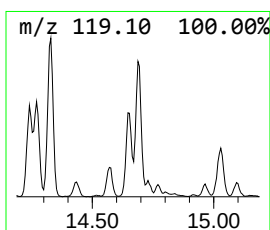
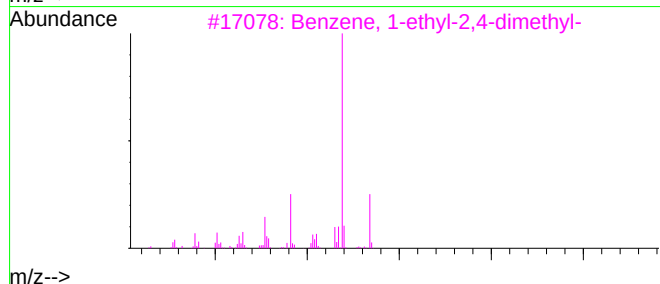
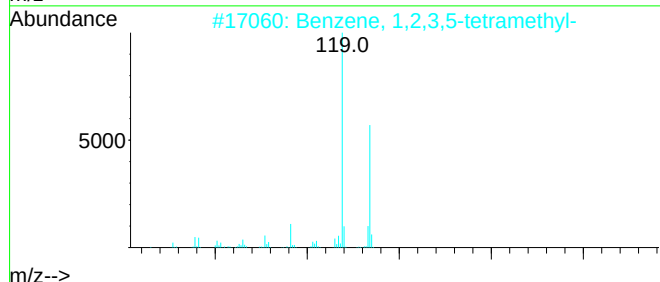
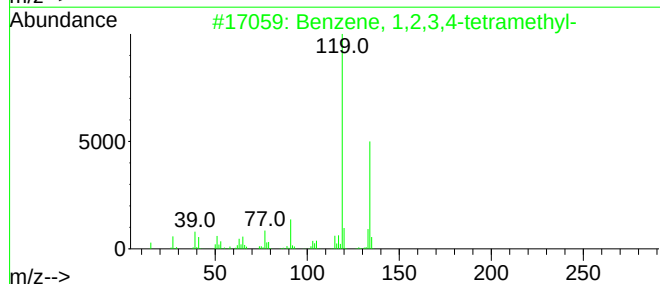
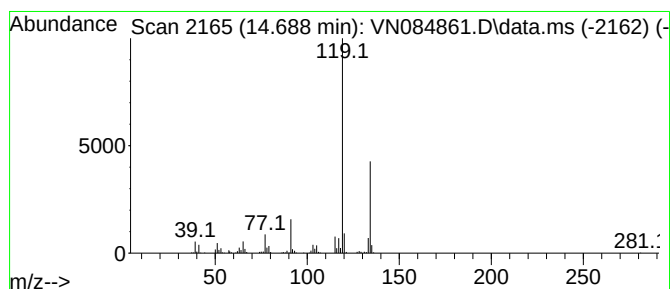
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.688	26.74 ug/l	458960	1,4-Dichlorobenzene-d4		13.788	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-		134	C10H14	000488-23-3	95
2	Benzene, 1,2,3,5-tetramethyl-		134	C10H14	000527-53-7	95
3	Benzene, 1-ethyl-2,4-dimethyl-		134	C10H14	000874-41-9	94
4	o-Cymene		134	C10H14	000527-84-4	94
5	Benzene, 2-ethyl-1,3-dimethyl-		134	C10H14	002870-04-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

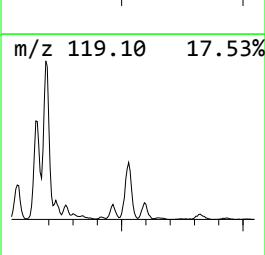
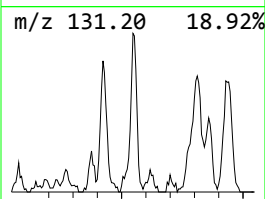
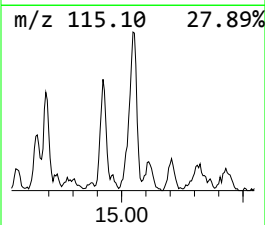
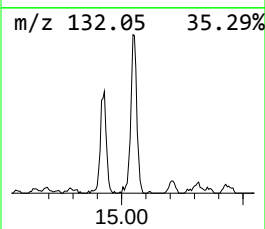
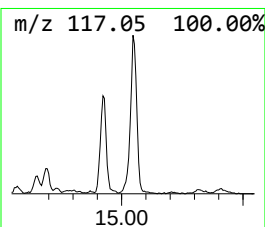
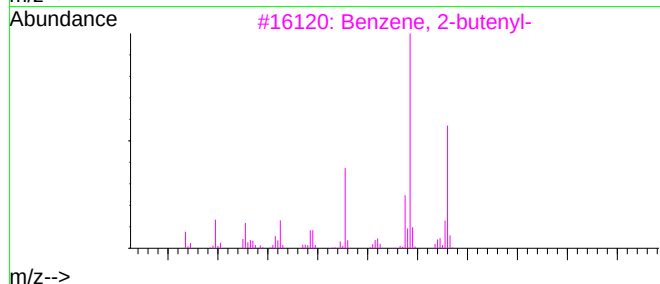
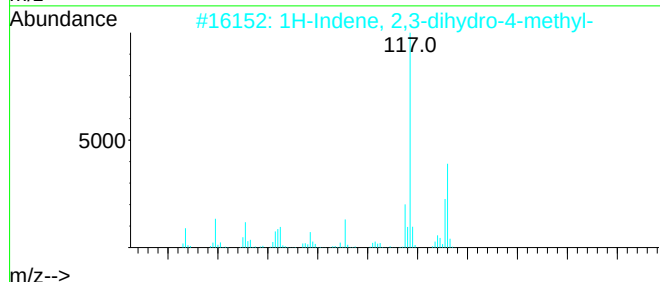
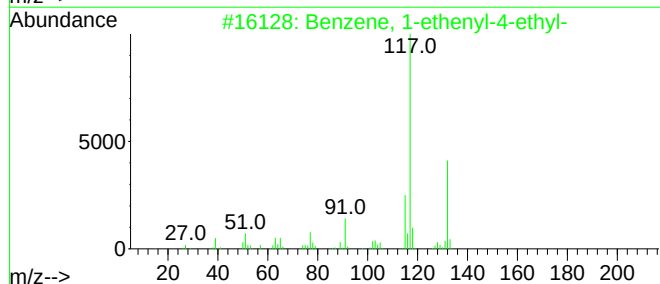
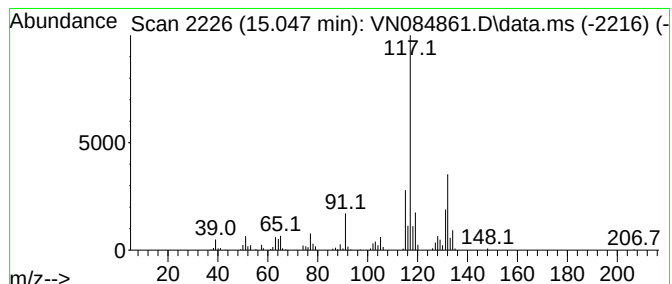
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.047	31.23 ug/l	536000	1,4-Dichlorobenzene-d4	13.788	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111424\
Data File : VN084861.D
Acq On : 14 Nov 2024 18:58
Operator : JC\MD
Sample : P4770-01 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
Acetic acid	8.753	20.2	ug/l	290786	2	9.100	719218	50.0
Benzene, 1-ethy...	13.094	177.1	ug/l	3039900	4	13.788	858182	50.0
Benzene, 1-ethy...	13.335	61.8	ug/l	1061370	4	13.788	858182	50.0
Indane	13.988	46.3	ug/l	794511	4	13.788	858182	50.0
Benzene, 2-ethy...	14.241	21.0	ug/l	361192	4	13.788	858182	50.0
Benzene, 2-ethy...	14.270	14.9	ug/l	255114	4	13.788	858182	50.0
Benzene, 1-ethy...	14.329	31.2	ug/l	534913	4	13.788	858182	50.0
Benzene, 1,2,3,...	14.653	20.8	ug/l	356178	4	13.788	858182	50.0
Benzene, 1,2,3,...	14.688	26.7	ug/l	458960	4	13.788	858182	50.0
Benzene, 1-ethe...	15.047	31.2	ug/l	536000	4	13.788	858182	50.0