

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082262.D
 Acq On : 22 May 2024 00:44
 Operator : JC\MD
 Sample : P2494-02 40X
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 2

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.283	554	566	576	rBV3	14372	48952	1.36%	0.314%
2	8.171	1047	1057	1061	rBV	143588	338443	9.40%	2.169%
3	8.229	1061	1067	1080	rVB	253371	580484	16.12%	3.720%
4	8.582	1118	1127	1138	rBV	178807	430446	11.96%	2.759%
5	9.106	1207	1216	1228	rBV	384019	794259	22.06%	5.090%
6	9.600	1289	1300	1309	rBV2	17340	40736	1.13%	0.261%
7	10.571	1456	1465	1471	rBV	609827	1133623	31.49%	7.265%
8	10.629	1471	1475	1484	rVB	71817	135779	3.77%	0.870%
9	11.865	1677	1685	1695	rBV	555986	1000505	27.79%	6.412%
10	11.965	1695	1702	1707	rVV2	29350	48495	1.35%	0.311%
11	12.070	1713	1720	1732	rBV	157281	290515	8.07%	1.862%
12	12.400	1765	1776	1784	rBV	144338	278775	7.74%	1.787%
13	12.853	1846	1853	1862	rVB	436251	758777	21.08%	4.863%
14	13.100	1889	1895	1899	rBV	58744	106928	2.97%	0.685%
15	13.170	1902	1907	1914	rVB2	138993	256244	7.12%	1.642%
16	13.335	1925	1935	1942	rBV2	49686	132000	3.67%	0.846%
17	13.482	1951	1960	1965	rBV	214107	357800	9.94%	2.293%
18	13.529	1965	1968	1973	rVB3	32903	50987	1.42%	0.327%
19	13.676	1979	1993	1998	rBV8	49151	168230	4.67%	1.078%
20	13.794	2006	2013	2022	rBV2	537810	1066324	29.62%	6.834%
21	14.017	2033	2051	2058	rBV6	115812	428725	11.91%	2.748%
22	14.106	2061	2066	2073	rVV3	123830	230296	6.40%	1.476%
23	14.176	2073	2078	2084	rVB2	149593	252740	7.02%	1.620%
24	14.247	2084	2090	2092	rBV	29050	48458	1.35%	0.311%
25	14.329	2100	2104	2108	rBV	34506	49867	1.39%	0.320%
26	14.441	2117	2123	2127	rBV5	40421	81916	2.28%	0.525%
27	14.576	2142	2146	2151	rVB5	34004	58412	1.62%	0.374%
28	14.629	2151	2155	2157	rBV5	41722	62606	1.74%	0.401%
29	14.658	2157	2160	2163	rVV2	51555	82720	2.30%	0.530%
30	14.694	2163	2166	2170	rVV	60258	76203	2.12%	0.488%
31	14.788	2177	2182	2188	rVB8	25041	57097	1.59%	0.366%
32	14.958	2202	2211	2218	rBV4	86382	171319	4.76%	1.098%
33	15.035	2218	2224	2232	rBV3	93652	256492	7.12%	1.644%
34	15.206	2248	2253	2260	rVB4	45840	88324	2.45%	0.566%
35	15.323	2268	2273	2284	rVB8	34555	85358	2.37%	0.547%
36	15.435	2287	2292	2298	rVB6	33888	78929	2.19%	0.506%

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Peak Location: TOP

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Peak separation: 5

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37	15.529	2301	2308	2314	rVB6	24752	64727	1.80%	0.415%
38	15.641	2320	2327	2338	rVV	1843847	3599918	100.00%	23.072%
39	15.747	2340	2345	2350	rVB2	46772	85362	2.37%	0.547%
40	15.829	2357	2359	2370	rVB8	42676	82532	2.29%	0.529%
41	15.953	2371	2380	2387	rBV8	25596	77773	2.16%	0.498%
42	16.029	2387	2393	2400	rBV8	13374	37840	1.05%	0.243%
43	16.123	2400	2409	2413	rBV10	16617	42247	1.17%	0.271%
44	16.717	2502	2510	2513	rBV3	24983	56784	1.58%	0.364%
45	16.782	2513	2521	2522	rBV	929920	1428137	39.67%	9.153%

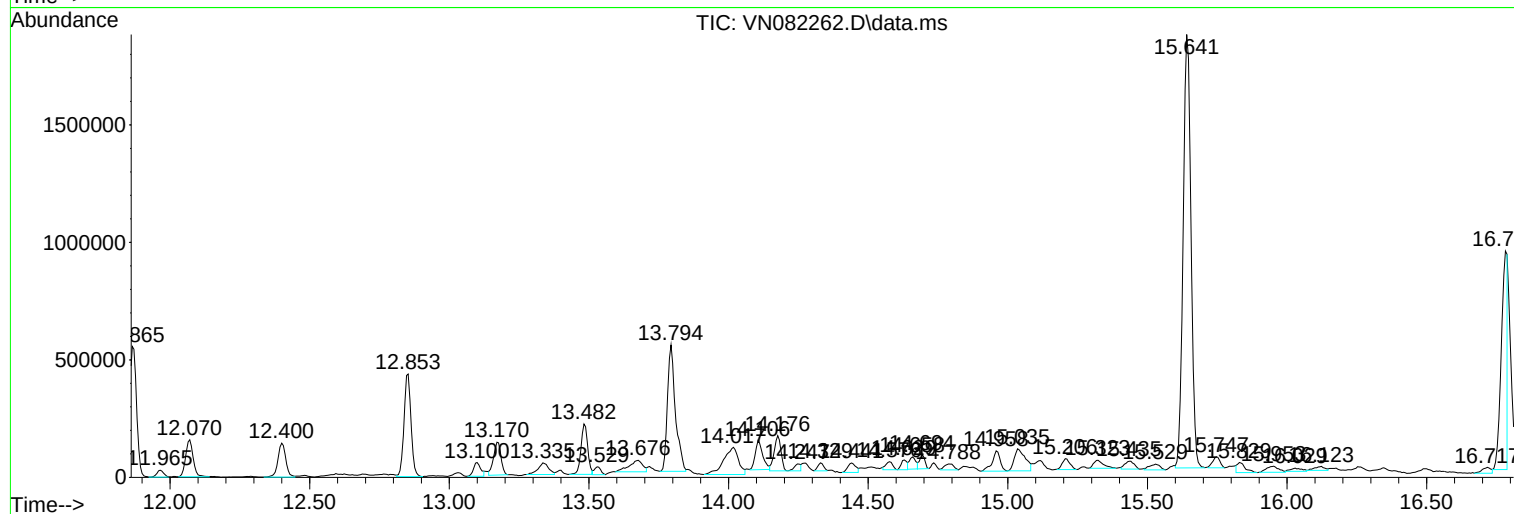
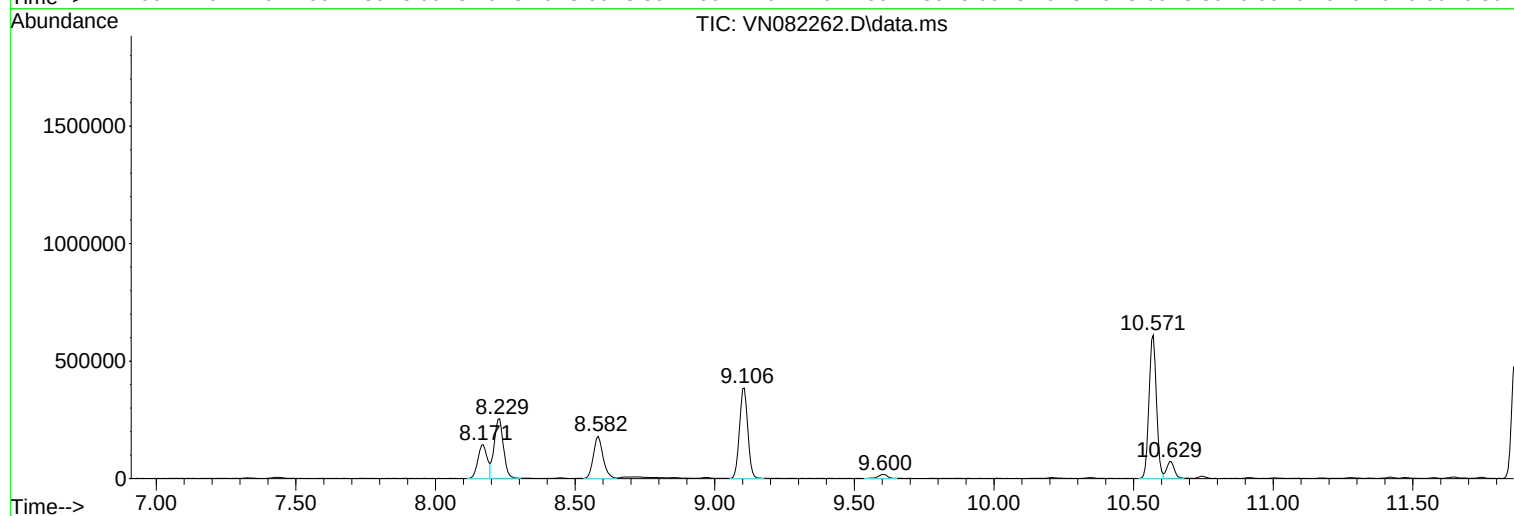
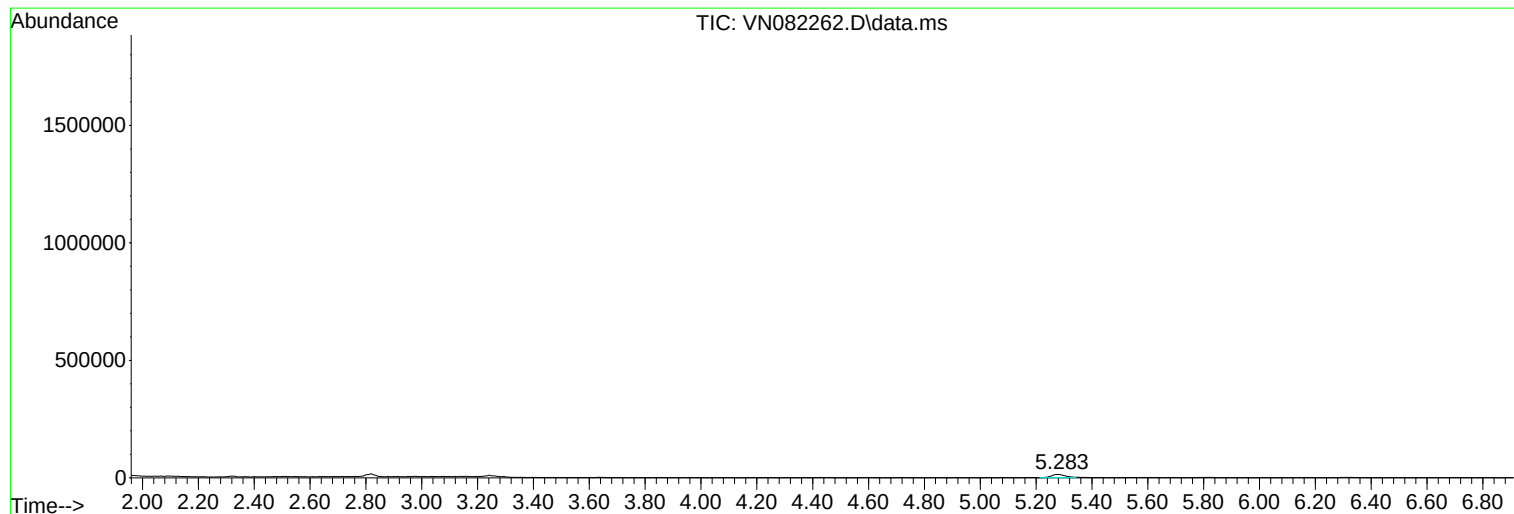
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
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2

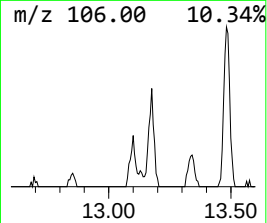
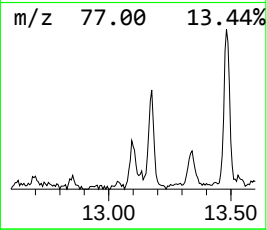
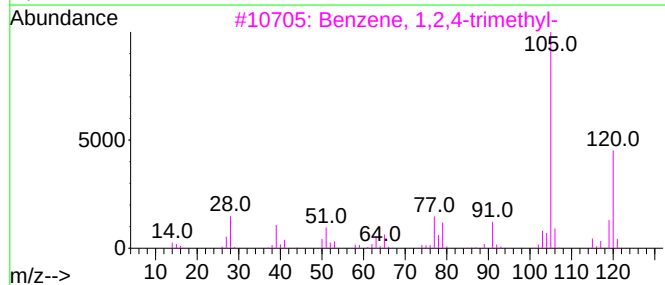
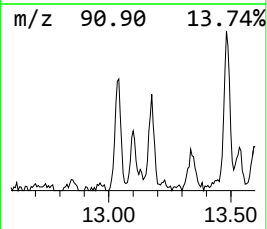
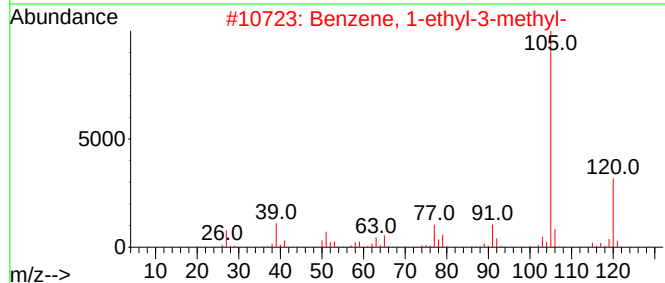
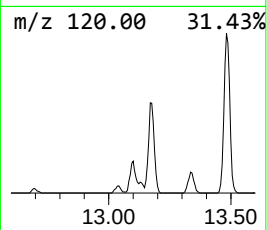
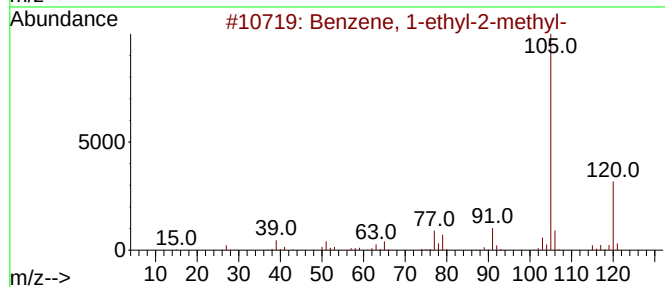
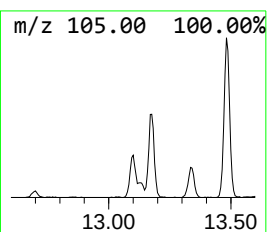
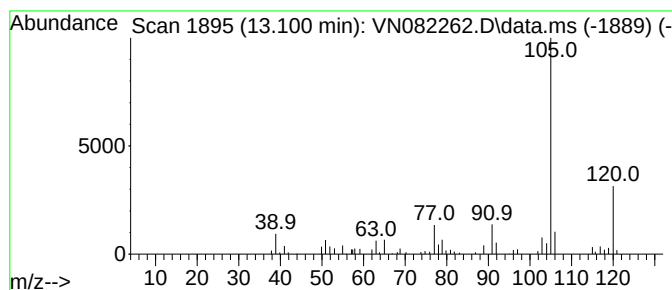
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	5.01 ug/l	106928	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	91
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	90



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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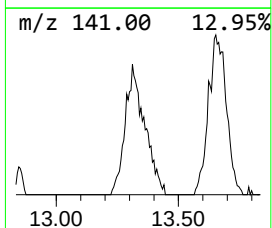
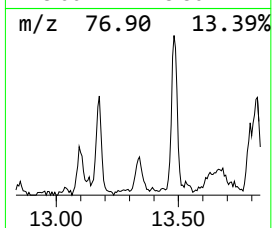
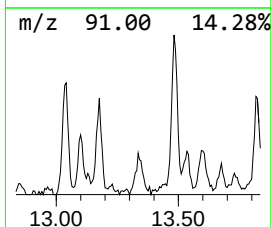
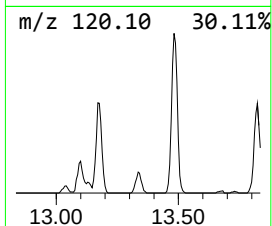
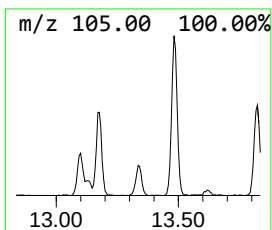
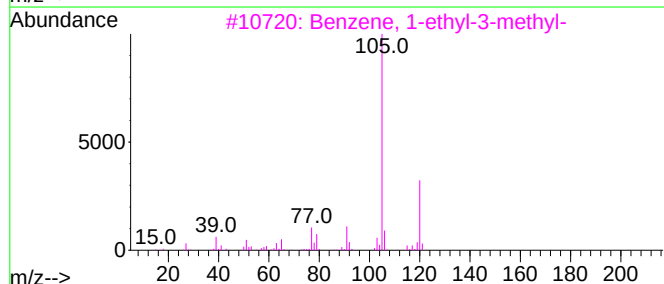
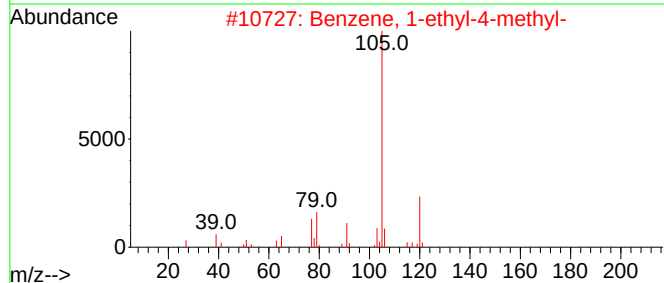
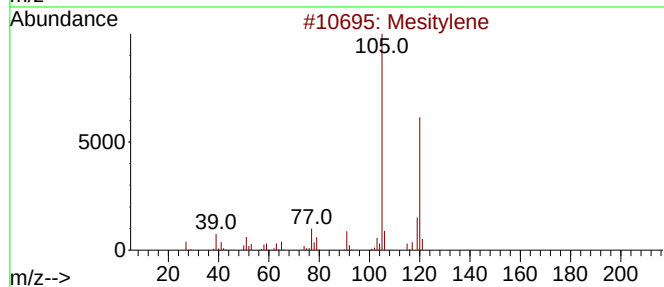
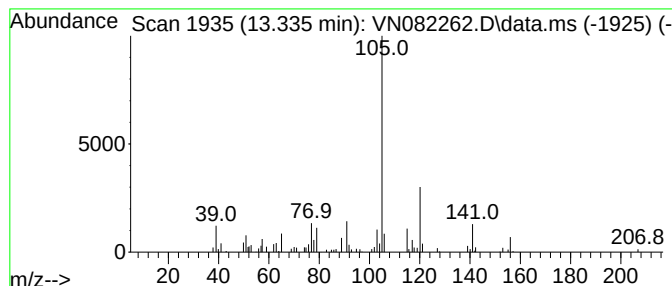
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	6.19 ug/l	132000	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	70
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	70
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	70
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	70
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	70



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Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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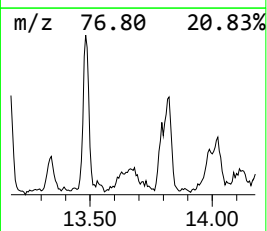
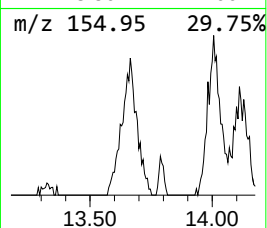
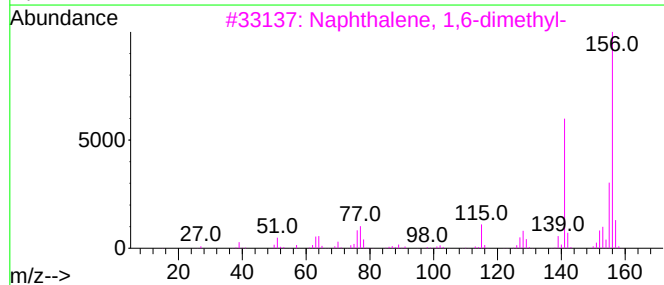
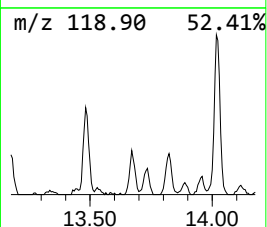
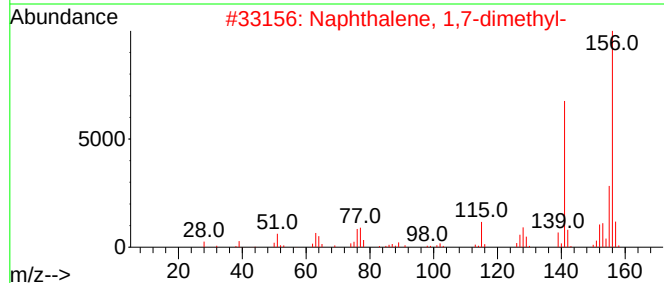
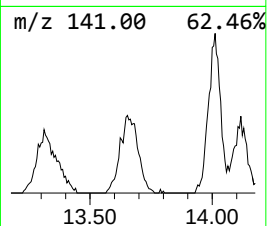
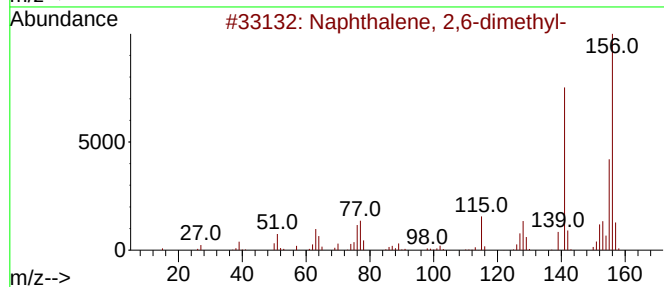
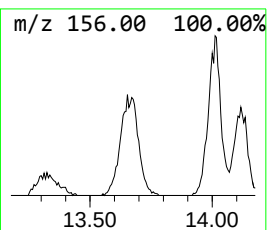
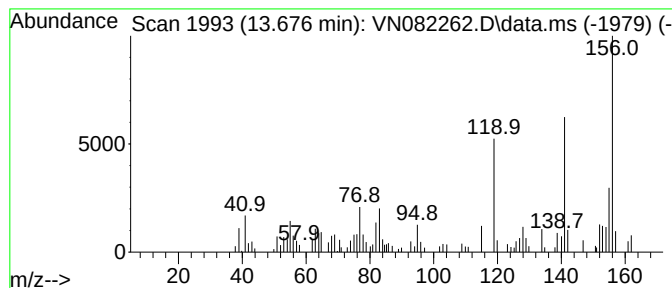
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	7.89 ug/l	168230	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93



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MSVOA_N
ClientSampleId :
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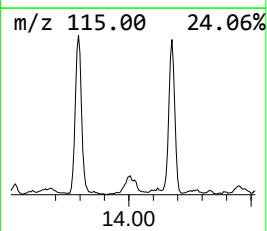
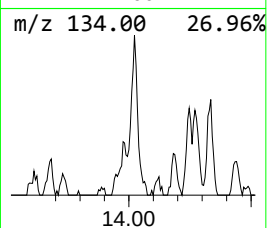
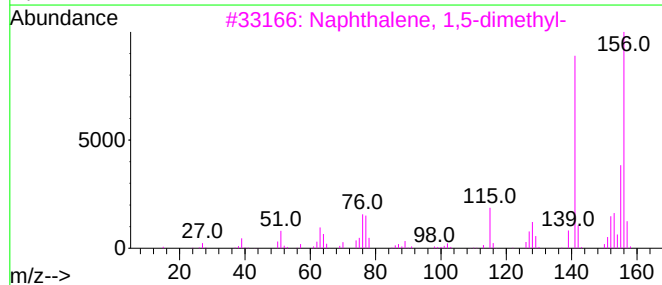
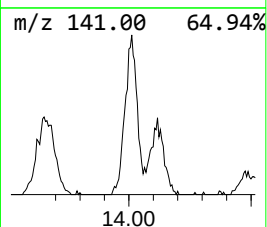
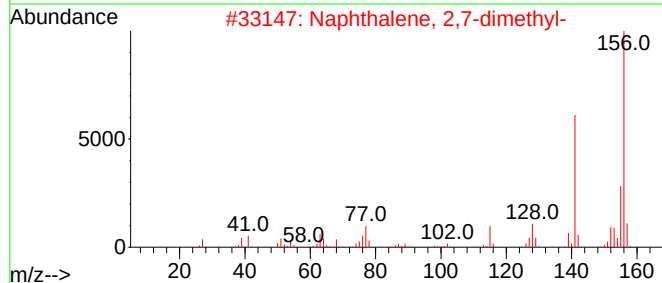
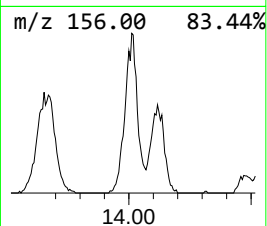
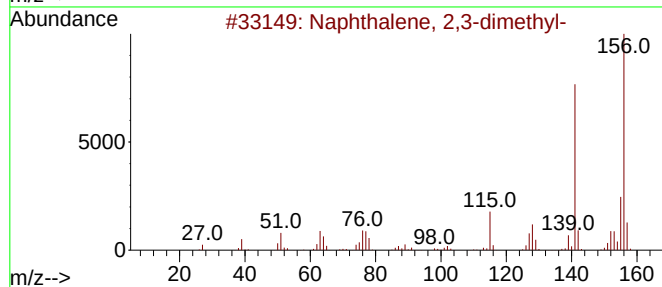
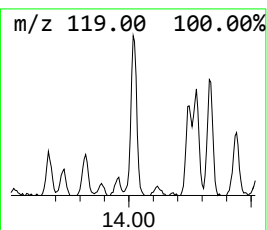
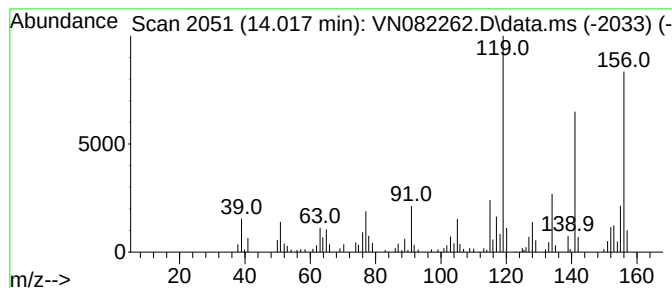
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	20.10 ug/l	428725	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95



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Instrument :
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ClientSampleId :
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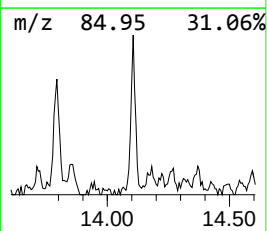
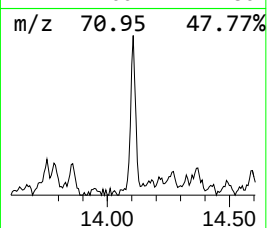
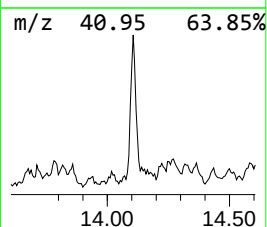
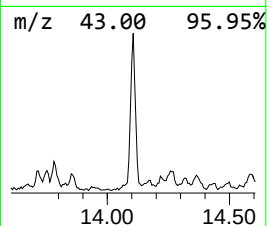
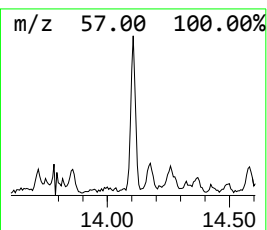
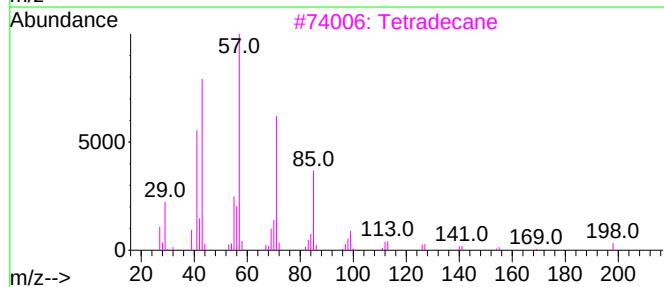
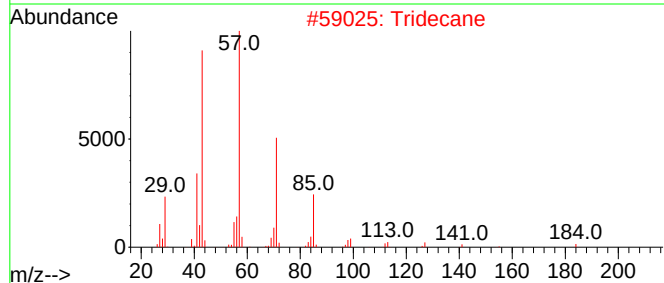
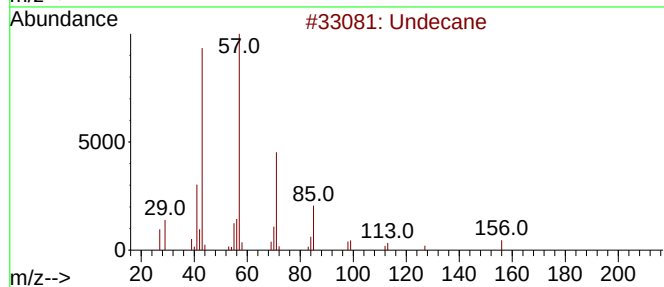
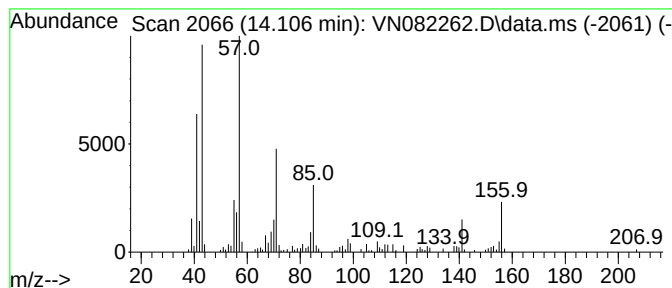
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Quant Title : SW846 8260

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

Peak Number 5 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	10.80 ug/l	230296	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	74
2			Tridecane	184	C13H28	000629-50-5	58
3			Tetradecane	198	C14H30	000629-59-4	58
4			Dodecane	170	C12H26	000112-40-3	53
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082262.D
Acq On : 22 May 2024 00:44
Operator : JC\MD
Sample : P2494-02 40X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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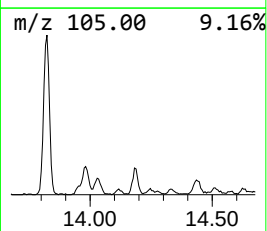
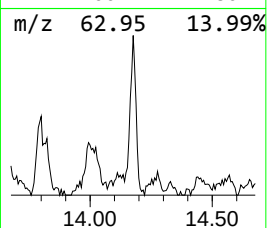
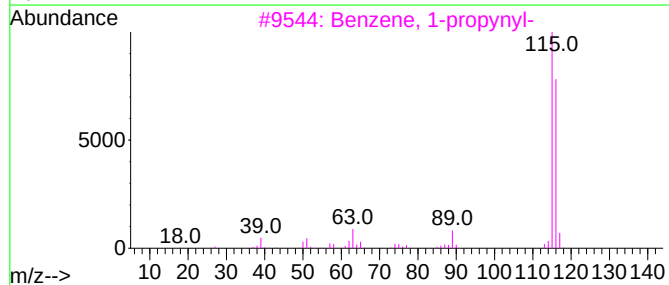
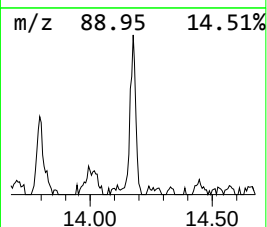
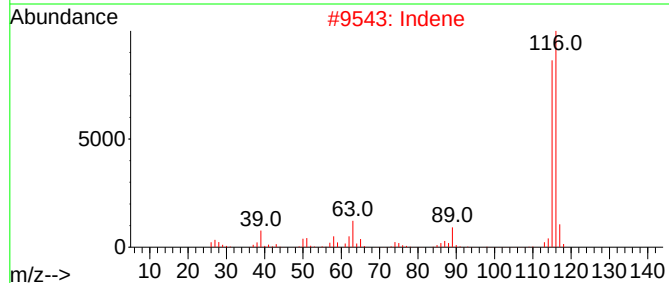
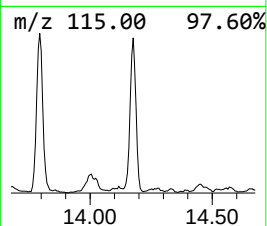
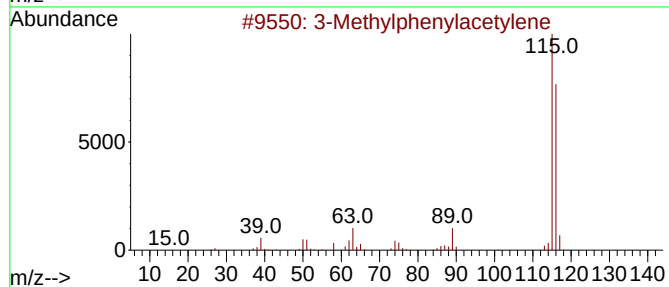
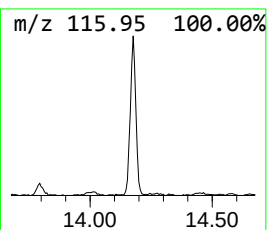
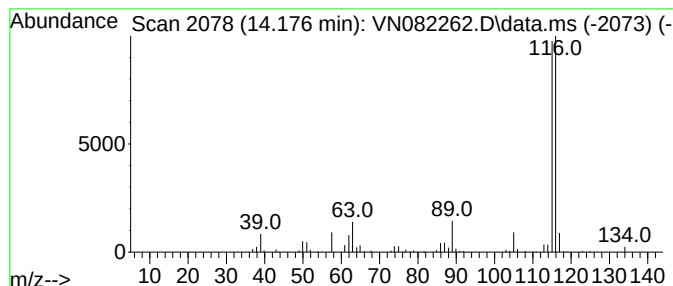
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Quant Title : SW846 8260

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

Peak Number 6 3-Methylphenylacetylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	11.85 ug/l	252740	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
2			Indene	116	C9H8	000095-13-6	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	87
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082262.D
Acq On : 22 May 2024 00:44
Operator : JC\MD
Sample : P2494-02 40X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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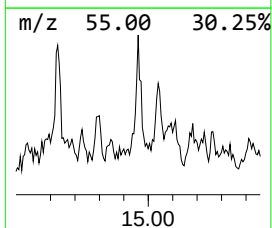
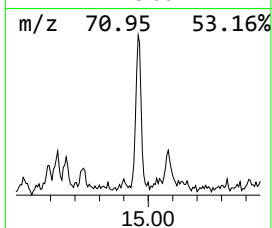
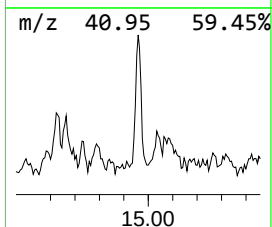
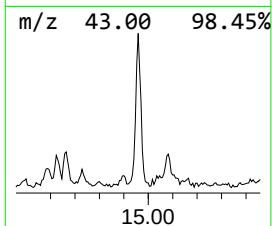
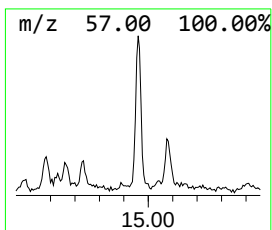
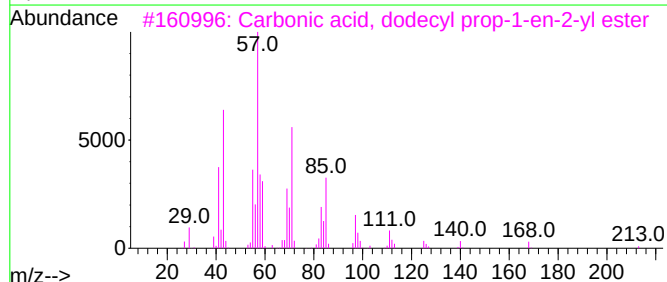
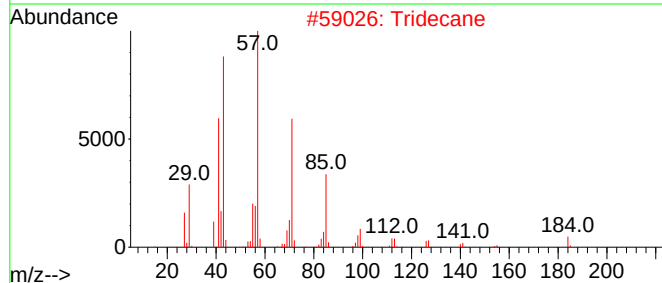
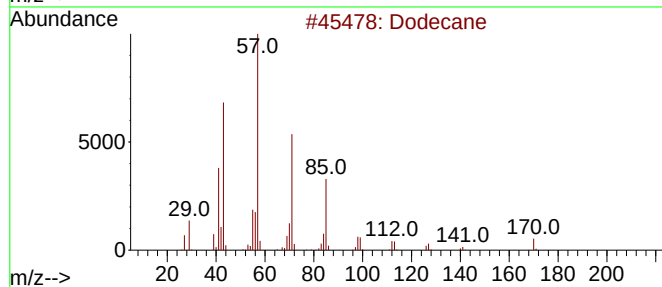
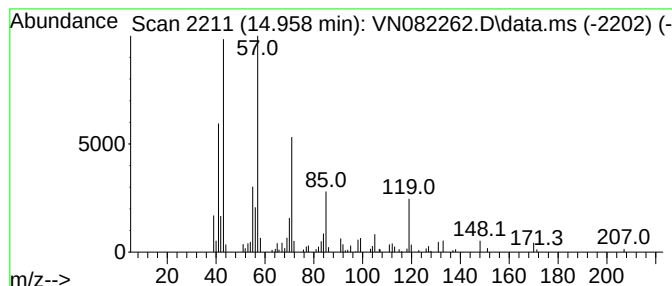
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Quant Title : SW846 8260

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

Peak Number 7 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	8.03 ug/l	171319	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	86
2			Tridecane	184	C13H28	000629-50-5	52
3			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	50
4			Undecane	156	C11H24	001120-21-4	50
5			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082262.D
Acq On : 22 May 2024 00:44
Operator : JC\MD
Sample : P2494-02 40X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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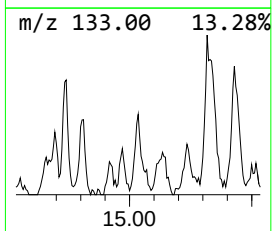
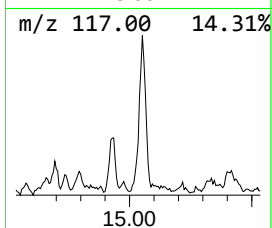
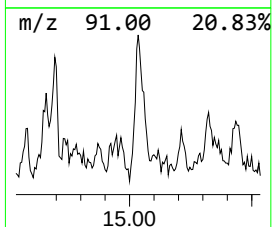
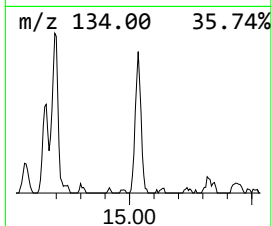
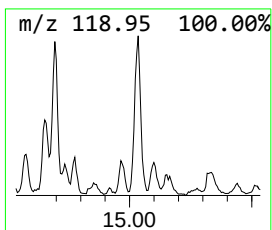
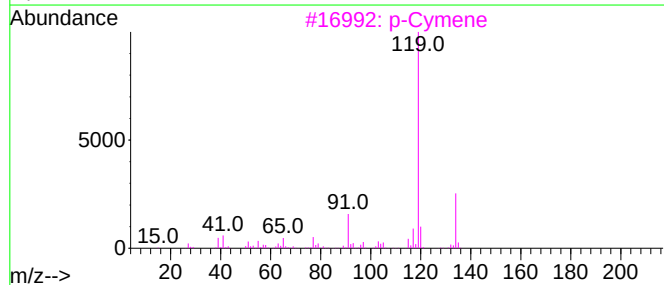
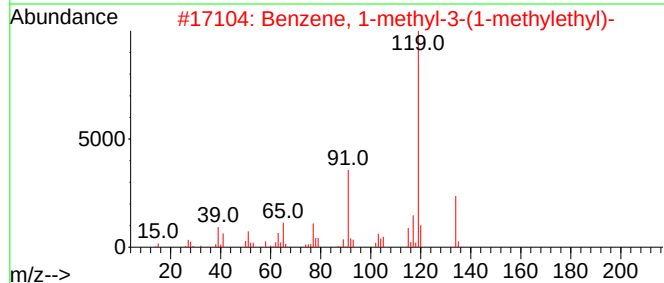
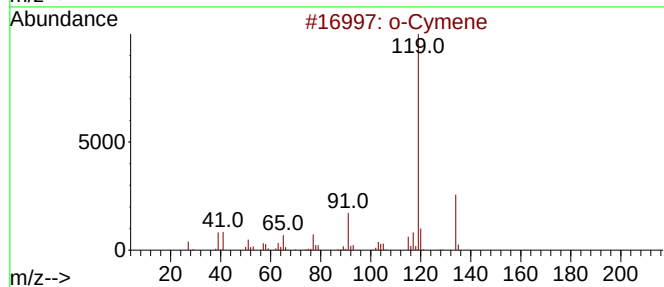
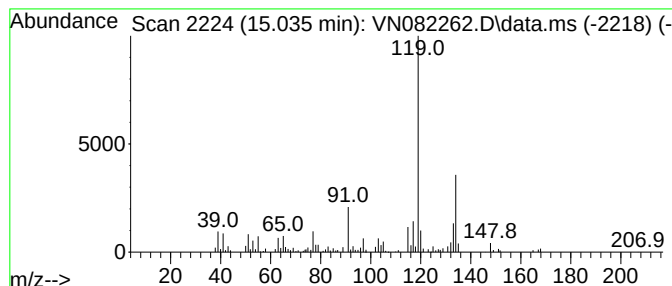
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Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	12.03 ug/l	256492	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	93
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	93
3			p-Cymene	134	C10H14	000099-87-6	90
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	90
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082262.D
Acq On : 22 May 2024 00:44
Operator : JC\MD
Sample : P2494-02 40X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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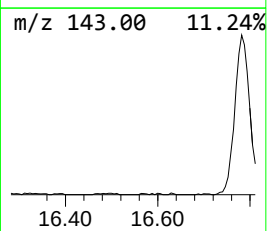
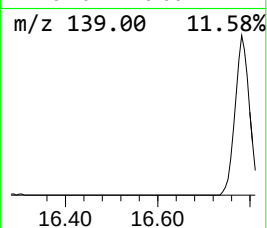
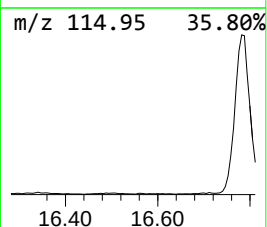
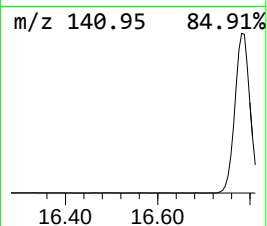
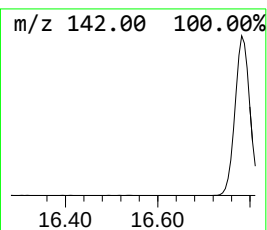
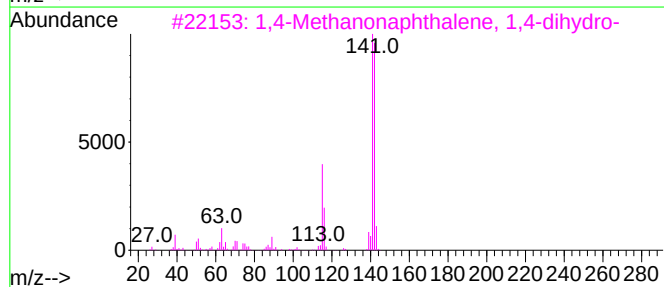
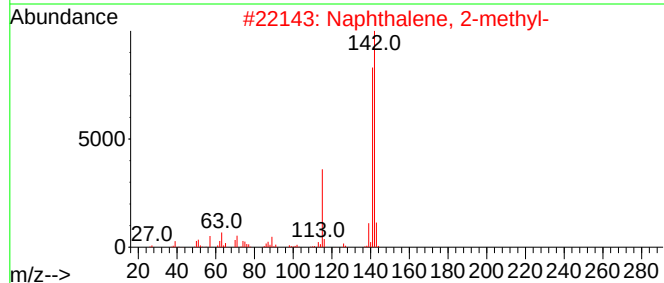
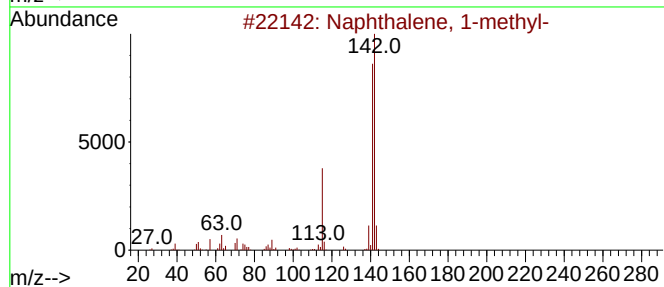
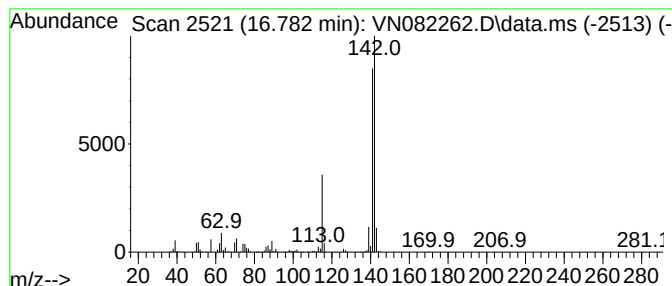
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	66.97 ug/l	1428140	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082262.D
Acq On : 22 May 2024 00:44
Operator : JC\MD
Sample : P2494-02 40X
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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
Benzene, 1-ethy...	13.100	5.0	ug/l	106928	4	13.794	1066320	50.0
Benzene, 1-ethy...	13.335	6.2	ug/l	132000	4	13.794	1066320	50.0
Naphthalene, 2,...	13.676	7.9	ug/l	168230	4	13.794	1066320	50.0
Naphthalene, 2,...	14.017	20.1	ug/l	428725	4	13.794	1066320	50.0
Undecane	14.106	10.8	ug/l	230296	4	13.794	1066320	50.0
3-Methylphenyla...	14.176	11.9	ug/l	252740	4	13.794	1066320	50.0
Dodecane	14.959	8.0	ug/l	171319	4	13.794	1066320	50.0
o-Cymene	15.035	12.0	ug/l	256492	4	13.794	1066320	50.0
Naphthalene, 1-...	16.782	67.0	ug/l	1428140	4	13.794	1066320	50.0