

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082267.D
 Acq On : 22 May 2024 02:45
 Operator : JC\MD
 Sample : P2494-07 40X
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 7

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: VN082267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1048	1057	1061	rBV	152149	359421	6.28%	1.585%
2	8.224	1061	1066	1082	rVB	277656	623209	10.89%	2.748%
3	8.582	1117	1127	1140	rBV2	190087	464968	8.12%	2.050%
4	9.100	1206	1215	1229	rBV	405729	847060	14.80%	3.735%
5	10.571	1456	1465	1471	rBV	636784	1206279	21.07%	5.319%
6	10.629	1471	1475	1486	rVB	94524	177859	3.11%	0.784%
7	11.865	1677	1685	1696	rBV	596316	1079731	18.86%	4.761%
8	11.965	1696	1702	1708	rVV	37187	63965	1.12%	0.282%
9	12.070	1713	1720	1731	rVV	214023	395550	6.91%	1.744%
10	12.400	1765	1776	1784	rBV	213255	410881	7.18%	1.812%
11	12.623	1796	1814	1816	rBV9	35706	144165	2.52%	0.636%
12	12.847	1846	1852	1863	rVB	480320	856658	14.96%	3.777%
13	13.094	1889	1894	1901	rBV	76039	168775	2.95%	0.744%
14	13.170	1901	1907	1914	rVB2	183604	352625	6.16%	1.555%
15	13.335	1921	1935	1942	rBV3	106468	387314	6.77%	1.708%
16	13.482	1954	1960	1965	rBV	285946	456804	7.98%	2.014%
17	13.529	1965	1968	1973	rVB2	44594	62213	1.09%	0.274%
18	13.676	1973	1993	2007	rBV4	192930	1037629	18.13%	4.575%
19	13.794	2007	2013	2022	rBV2	563012	1171397	20.46%	5.165%
20	14.012	2035	2050	2059	rBV5	308810	1118896	19.55%	4.933%
21	14.106	2060	2066	2073	rVV3	231895	562155	9.82%	2.479%
22	14.176	2073	2078	2084	rVB2	239401	443492	7.75%	1.955%
23	14.253	2086	2091	2092	rBV2	39662	60559	1.06%	0.267%
24	14.329	2100	2104	2108	rVB	50581	70256	1.23%	0.310%
25	14.441	2118	2123	2126	rBV5	53835	100108	1.75%	0.441%
26	14.629	2151	2155	2157	rBV3	62083	88216	1.54%	0.389%
27	14.659	2158	2160	2163	rVV3	66212	86253	1.51%	0.380%
28	14.694	2163	2166	2170	rVB	82469	112292	1.96%	0.495%
29	14.794	2177	2183	2187	rBV5	38636	77380	1.35%	0.341%
30	14.841	2187	2191	2202	rVB8	50285	154308	2.70%	0.680%
31	14.959	2203	2211	2217	rVB3	112913	218732	3.82%	0.964%
32	15.035	2218	2224	2234	rBV4	136980	466054	8.14%	2.055%
33	15.206	2248	2253	2260	rVB6	70425	143090	2.50%	0.631%
34	15.317	2267	2272	2281	rBV6	54454	124321	2.17%	0.548%
35	15.441	2287	2293	2298	rVB4	51807	115877	2.02%	0.511%
36	15.529	2300	2308	2315	rVB4	43357	127173	2.22%	0.561%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
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37	15.641	2315	2327	2339	rBV	2932682	5724490	100.00%	25.240%
38	15.747	2340	2345	2351	rVB2	76321	140079	2.45%	0.618%
39	15.953	2371	2380	2386	rBV7	40099	127404	2.23%	0.562%
40	16.711	2504	2509	2512	rBV2	36577	69371	1.21%	0.306%
41	16.782	2513	2521	2522	rBV	1481119	2283410	39.89%	10.068%

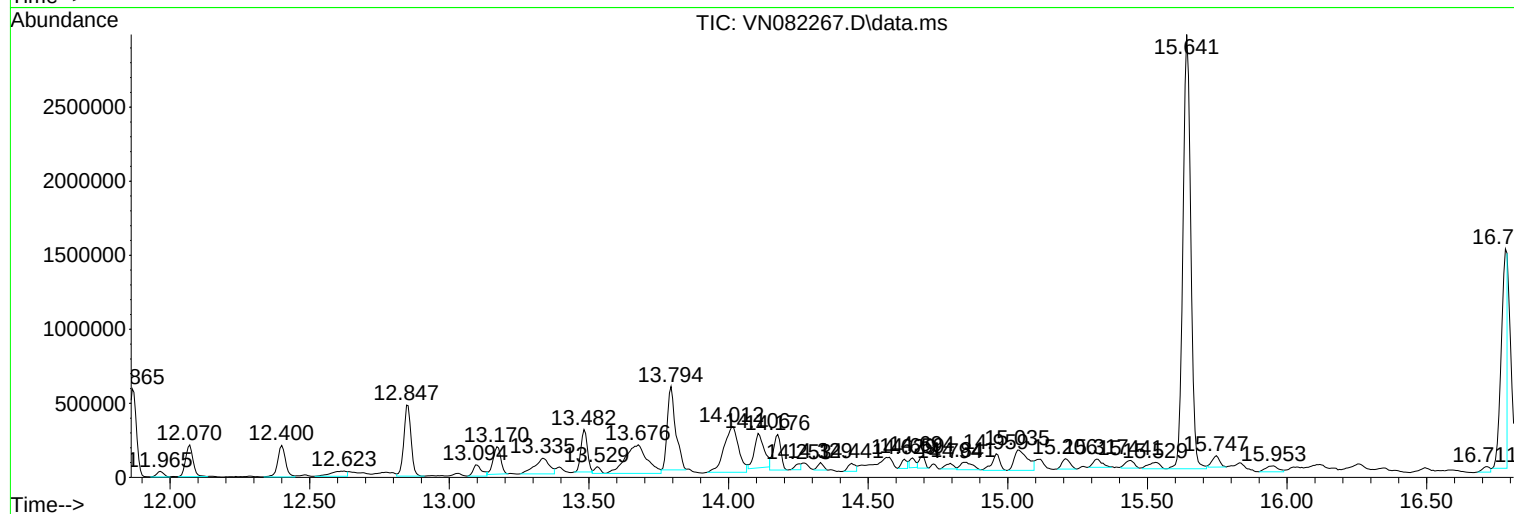
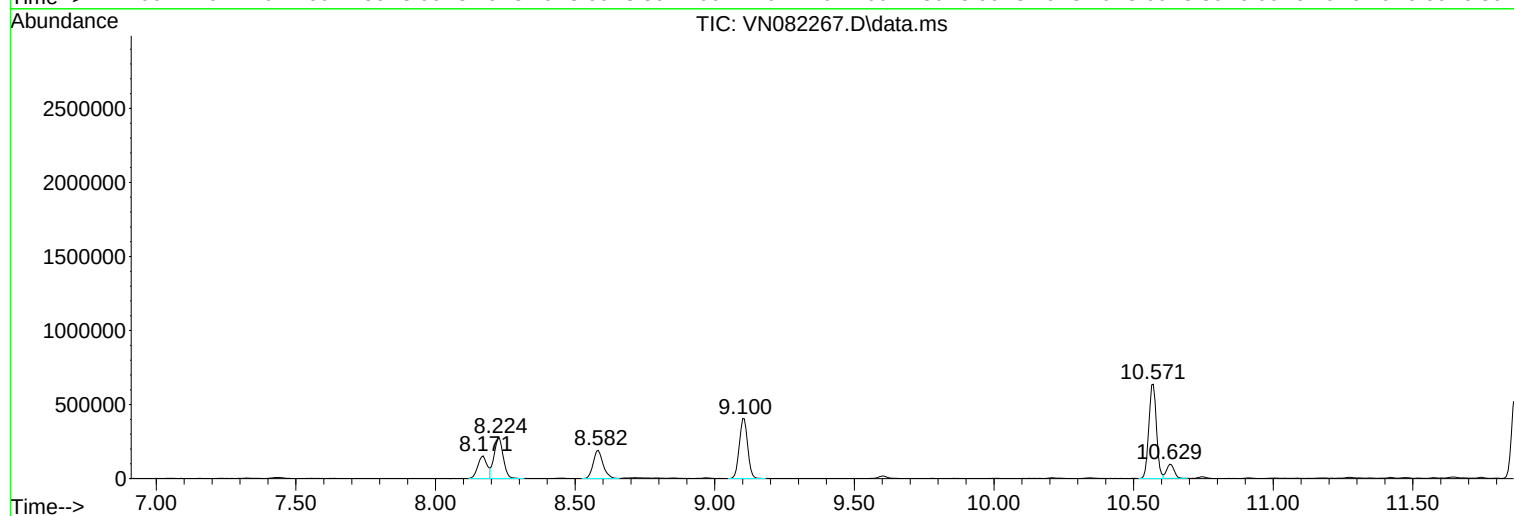
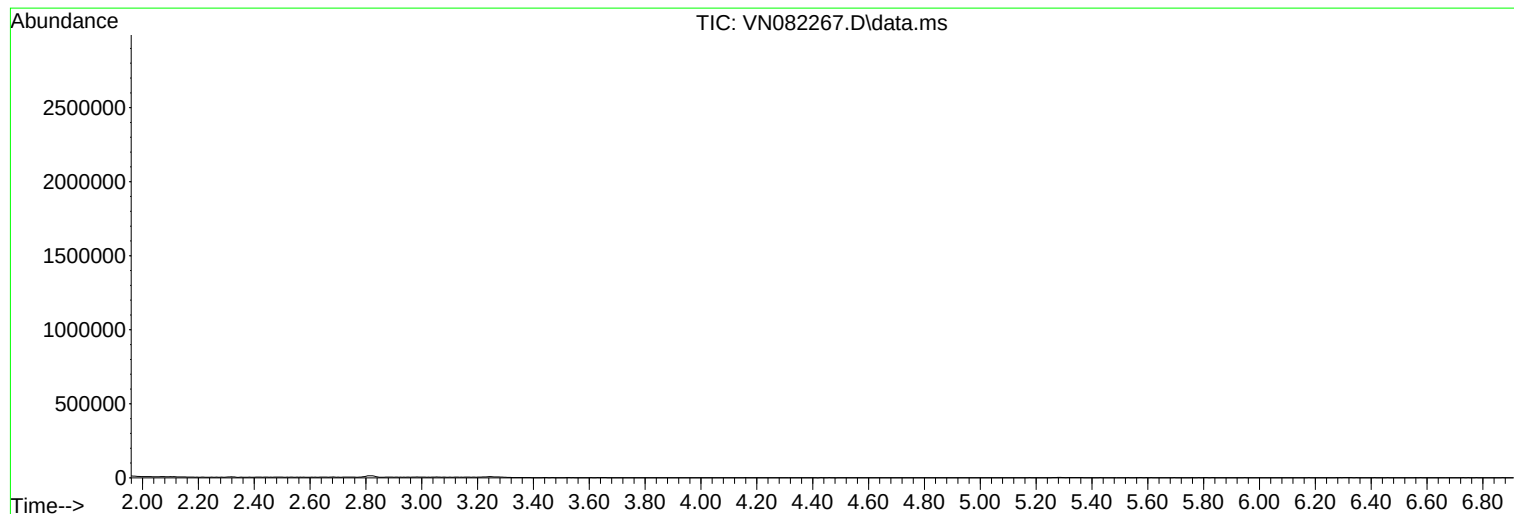
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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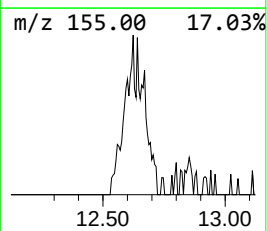
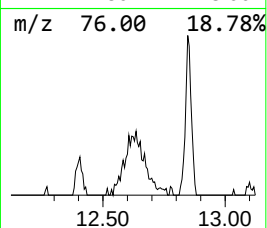
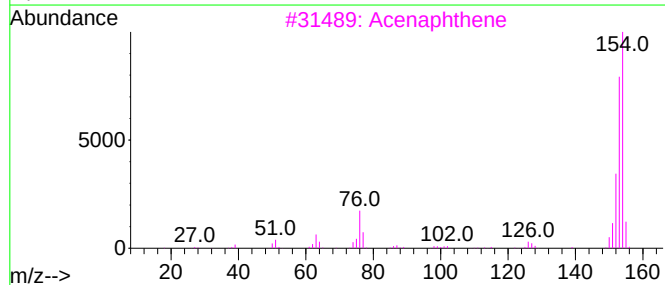
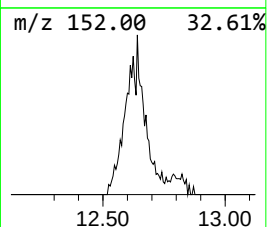
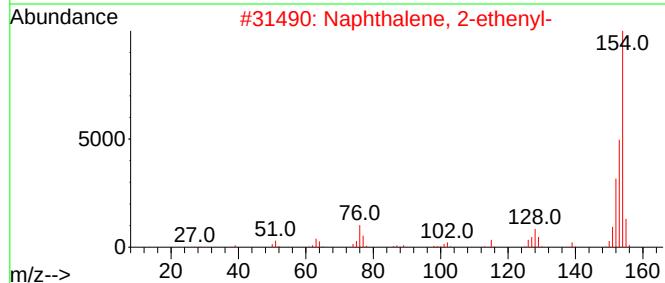
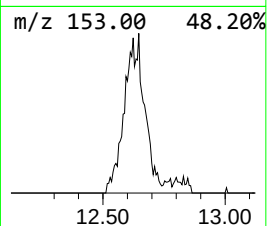
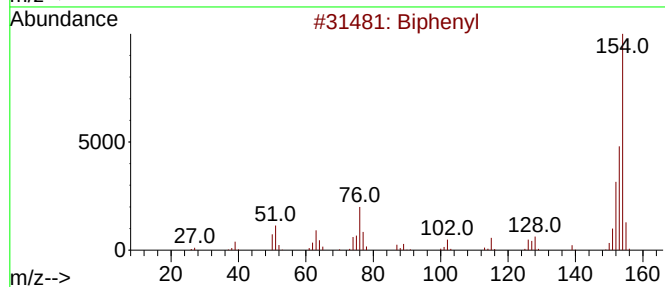
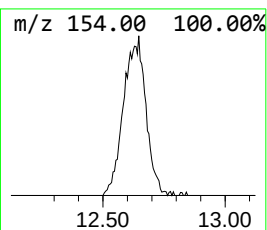
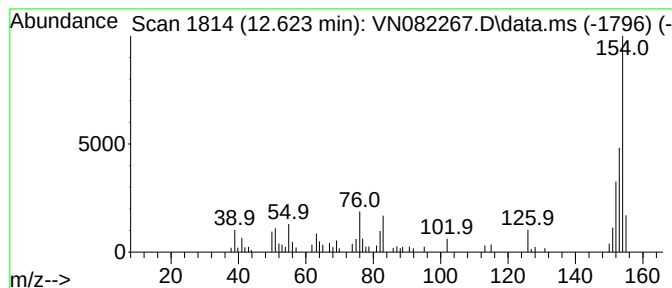
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Biphenyl Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.623	6.68 ug/l	144165	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	90
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	72
3			Acenaphthene	154	C12H10	000083-32-9	43
4			Propanedinitrile, (phenylmethyle...	154	C10H6N2	002700-22-3	37
5			Glutaric acid, dodec-2-en-1-yl 2...	434	C25H38O6	1000392-01-1	35



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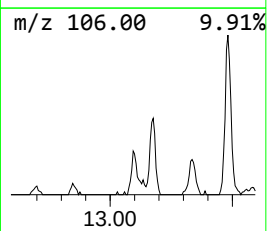
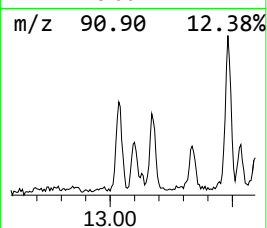
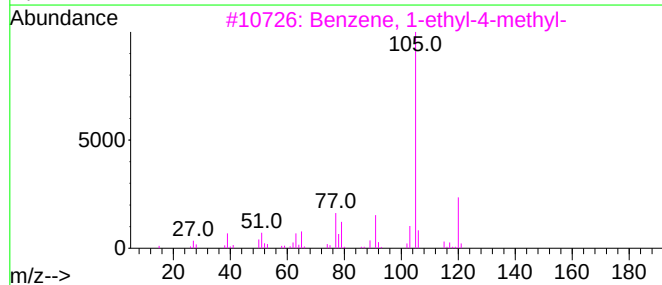
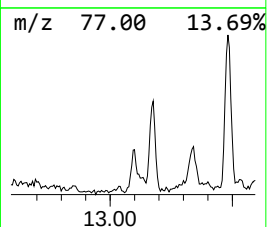
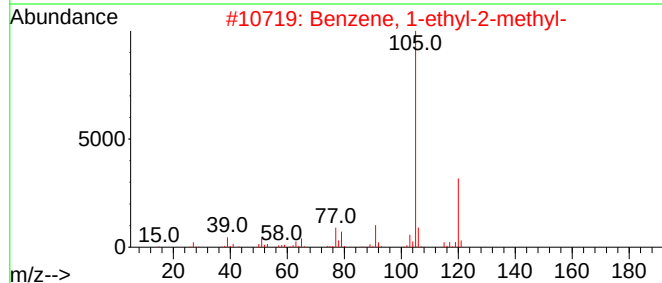
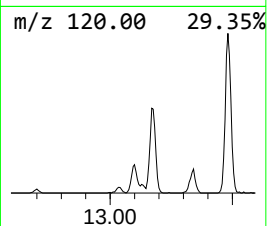
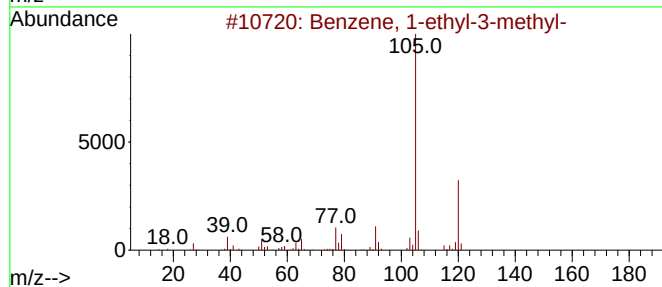
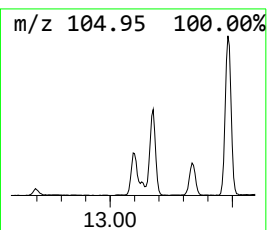
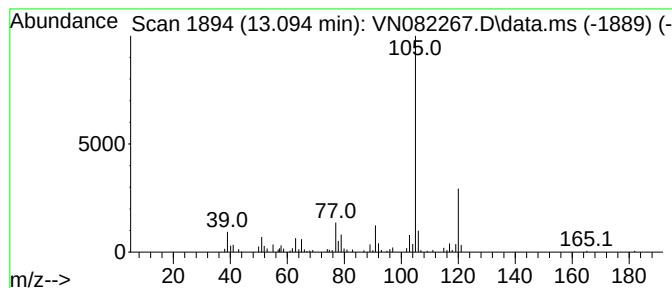
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	7.20 ug/l	168775	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Mesitylene	120	C9H12	000108-67-8	87
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	83



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Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

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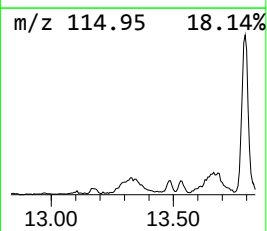
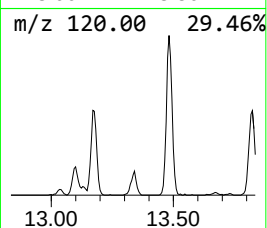
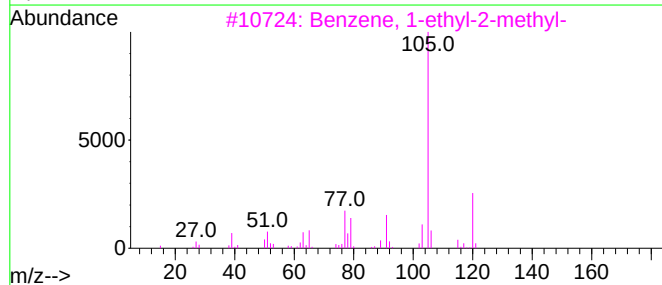
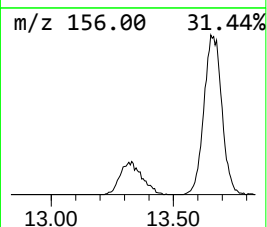
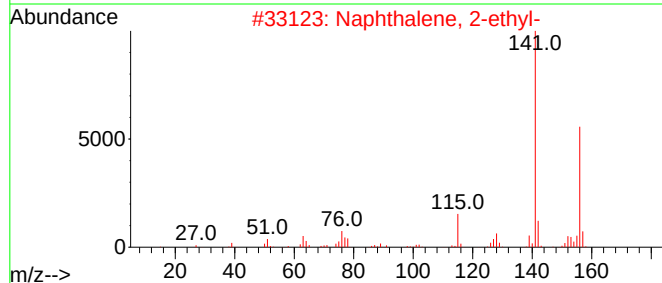
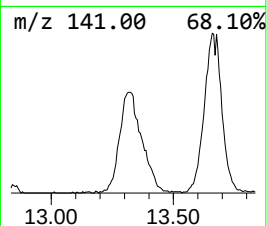
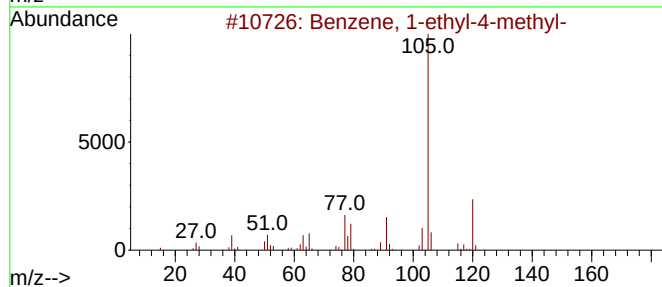
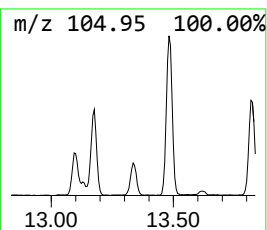
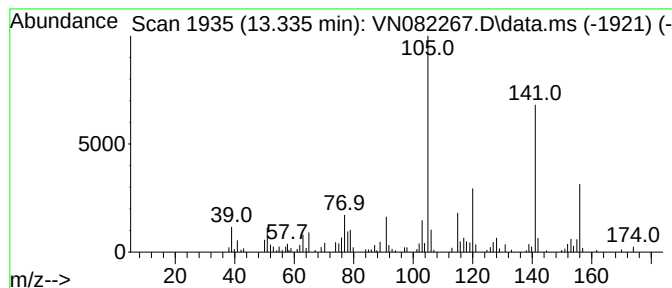
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	16.53 ug/l	387314	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	83
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	50
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	42
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	42
5			2,4-Nonadiyne	120	C9H12	063621-15-8	42



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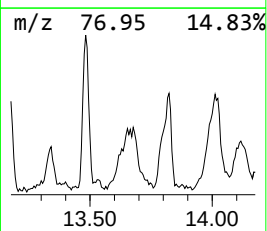
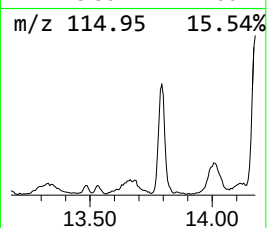
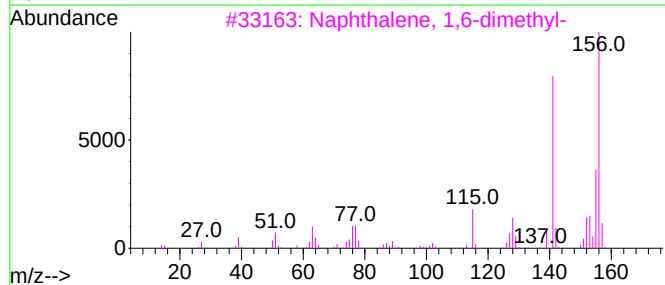
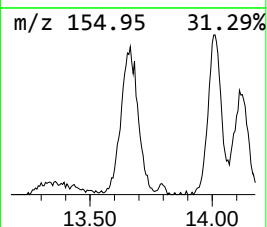
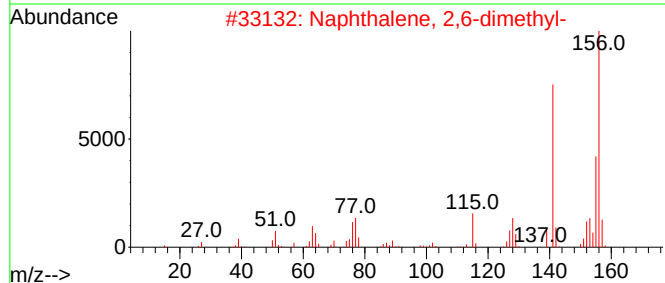
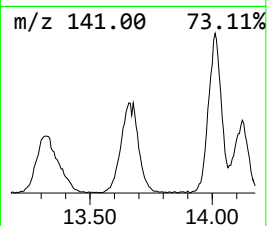
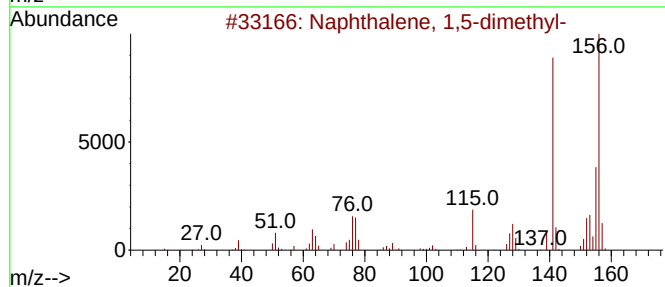
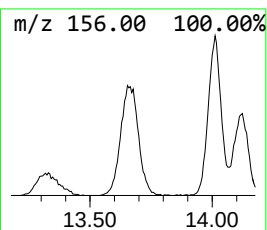
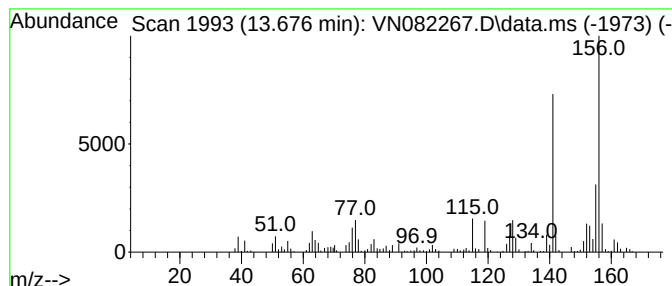
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	44.29 ug/l	1037630	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



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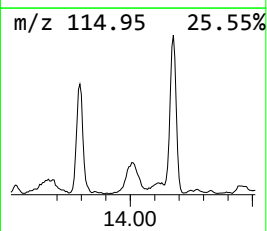
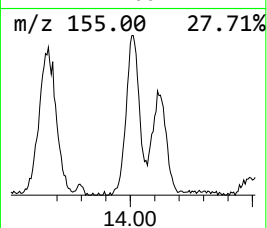
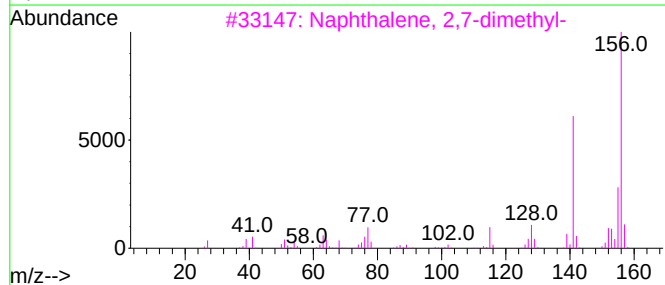
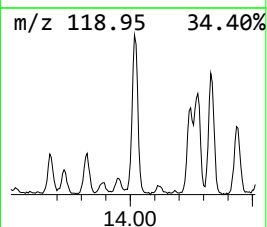
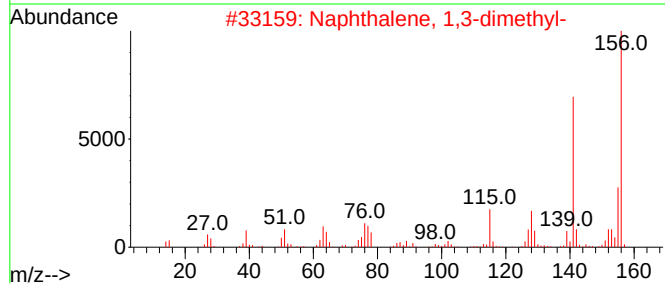
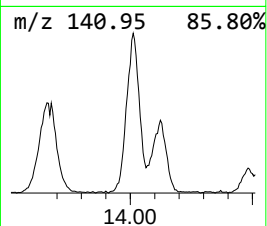
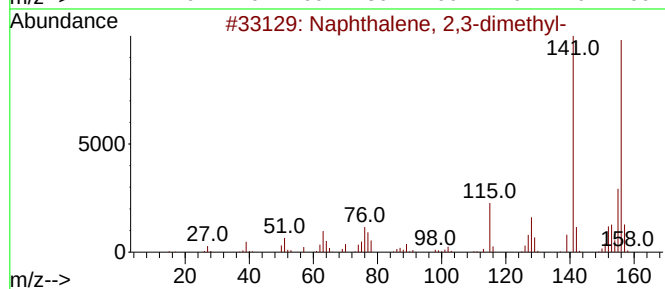
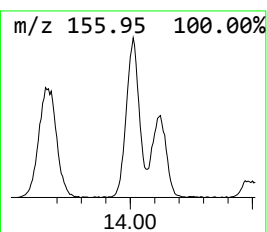
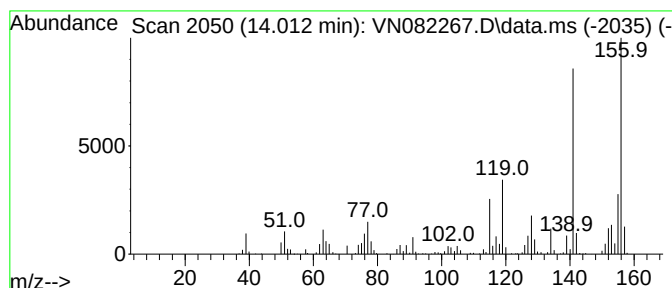
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.012	47.76 ug/l	1118900	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	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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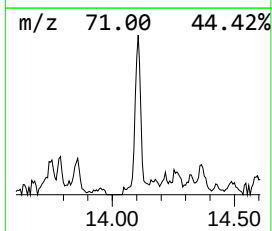
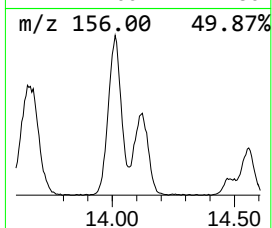
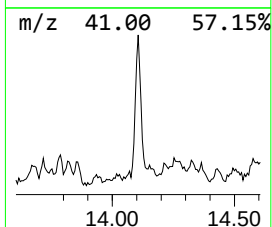
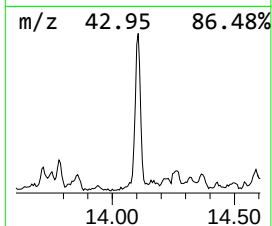
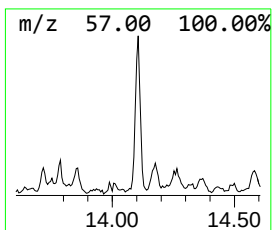
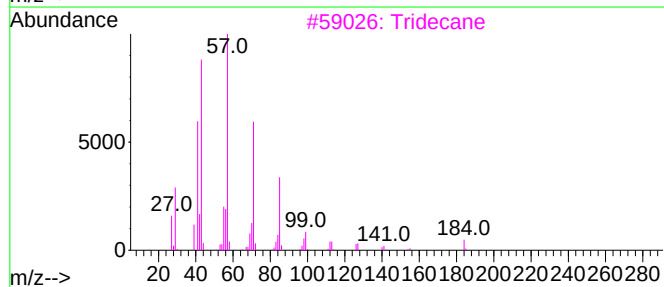
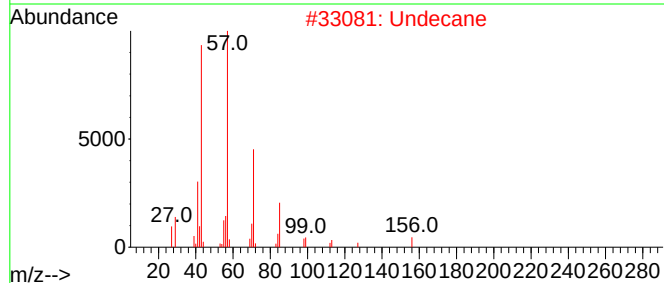
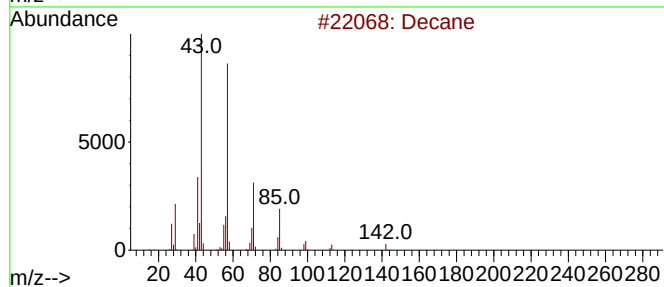
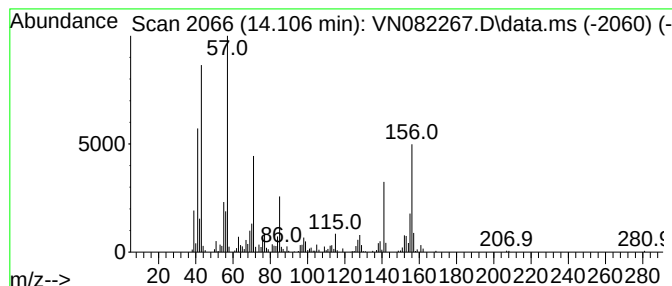
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Quant Title : SW846 8260

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

Peak Number 6 Decane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	24.00 ug/l	562155	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	60
2			Undecane	156	C11H24	001120-21-4	43
3			Tridecane	184	C13H28	000629-50-5	38
4			Dodecane	170	C12H26	000112-40-3	38
5			Hexadecane	226	C16H34	000544-76-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

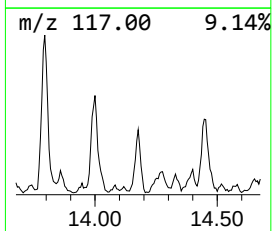
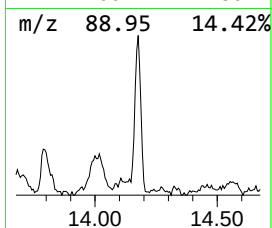
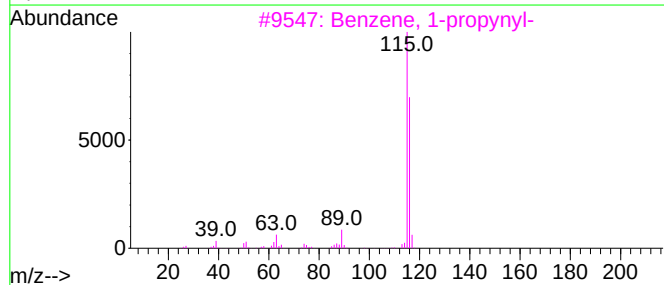
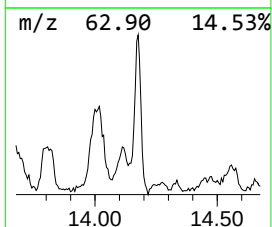
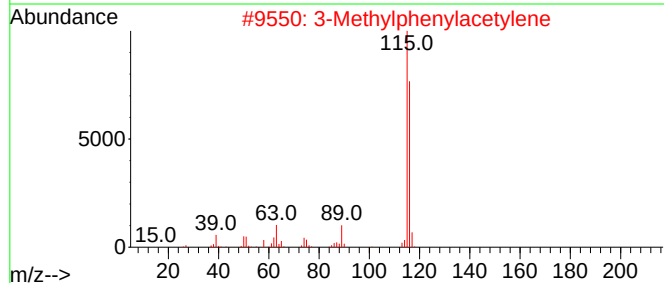
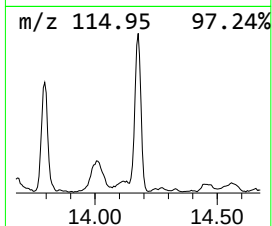
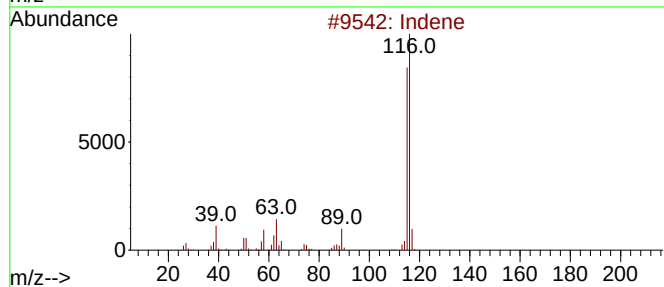
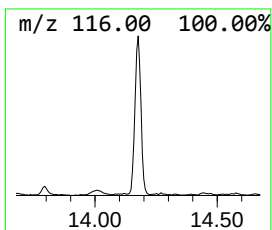
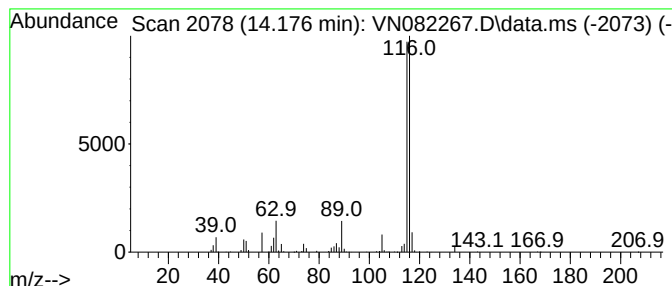
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.176	18.93 ug/l	443492	1,4-Dichlorobenzene-d4			13.794
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Indene		116	C9H8	000095-13-6	95
2	3-Methylphenylacetylene		116	C9H8	000766-82-5	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	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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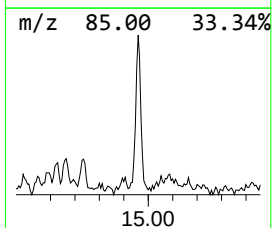
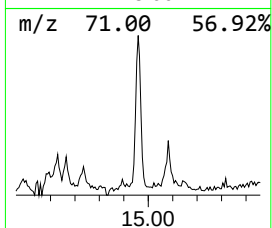
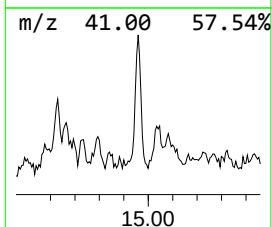
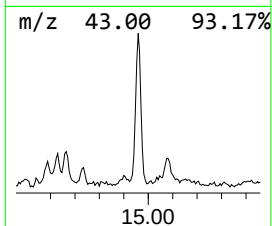
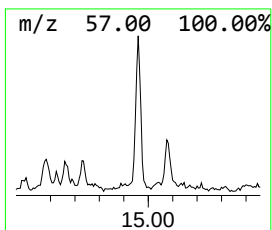
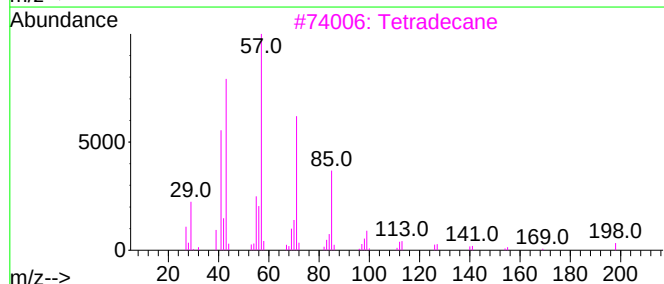
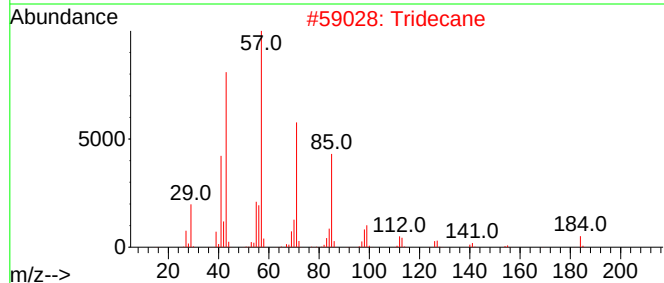
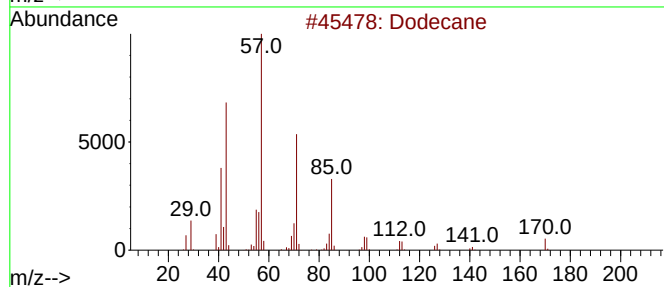
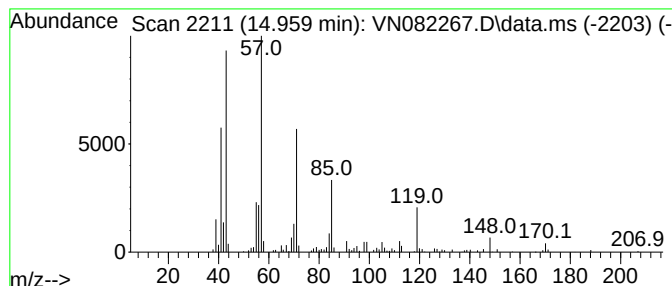
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	9.34 ug/l	218732	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	76
2			Tridecane	184	C13H28	000629-50-5	59
3			Tetradecane	198	C14H30	000629-59-4	59
4			Bacchotricuneatin c	342	C20H22O5	066563-30-2	53
5			Hexadecane	226	C16H34	000544-76-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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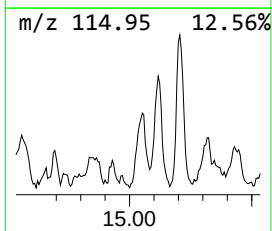
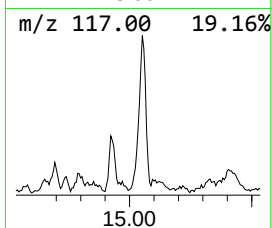
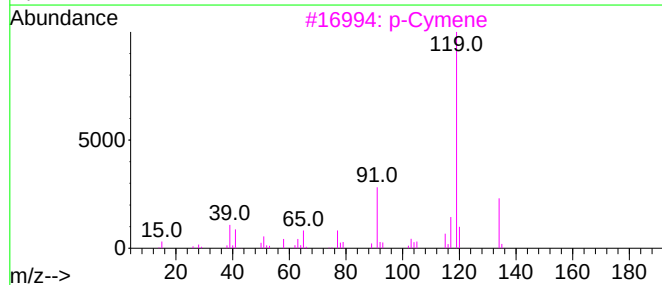
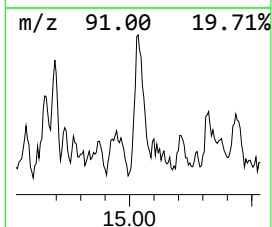
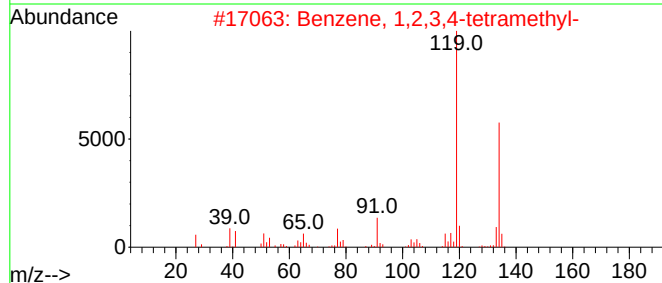
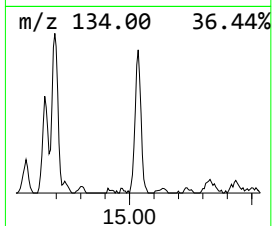
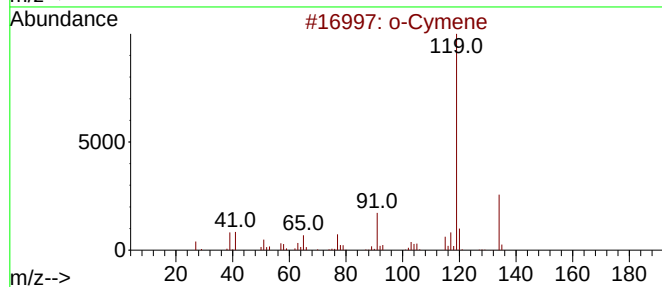
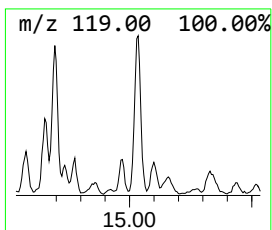
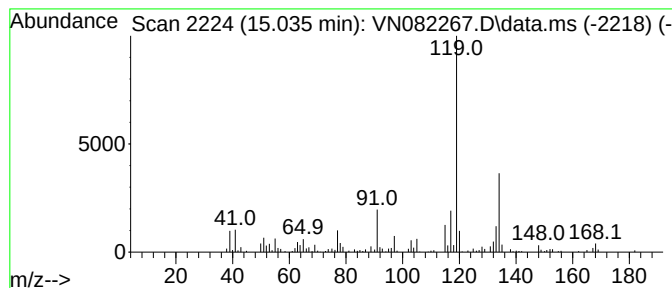
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Quant Title : SW846 8260

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

Peak Number 9 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	19.89 ug/l	466054	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, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	87
3			p-Cymene	134	C10H14	000099-87-6	87
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	87
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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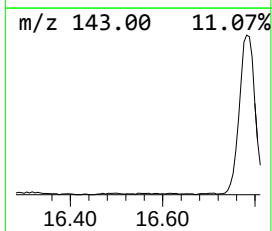
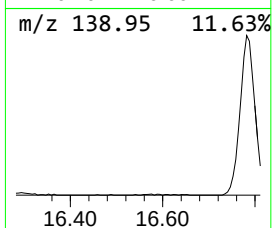
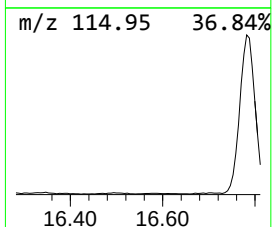
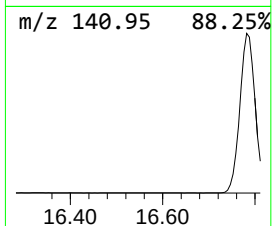
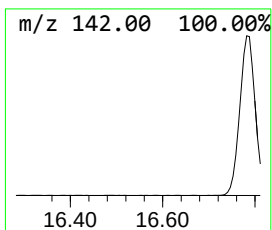
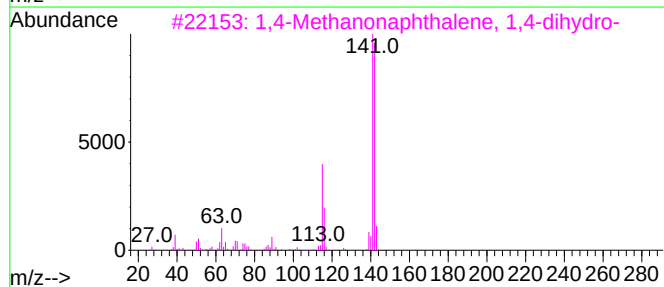
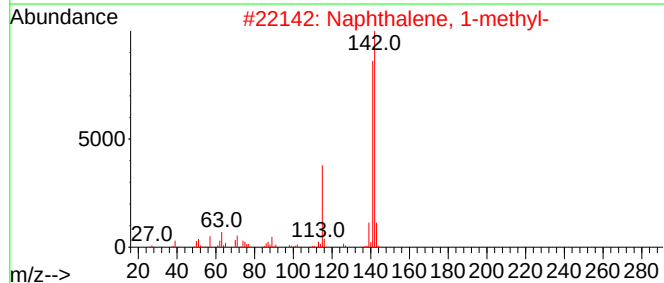
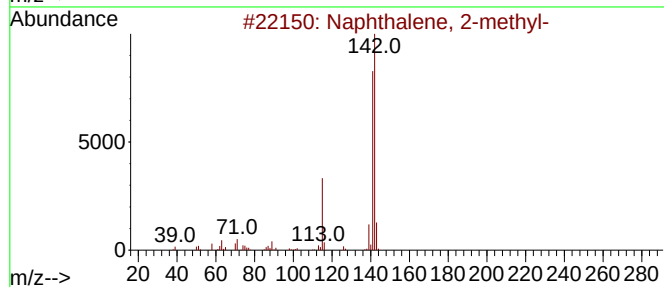
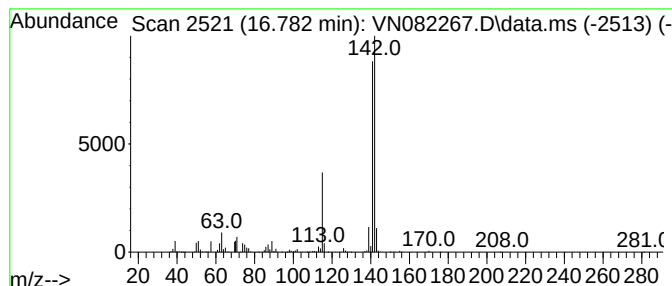
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.782	97.47 ug/l	2283410	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082267.D
Acq On : 22 May 2024 02:45
Operator : JC\MD
Sample : P2494-07 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 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
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Benzene, 1-ethy...	13.094	7.2	ug/l	168775	4	13.794	1171400	50.0
Benzene, 1-ethy...	13.335	16.5	ug/l	387314	4	13.794	1171400	50.0
Naphthalene, 1,...	13.676	44.3	ug/l	1037630	4	13.794	1171400	50.0
Naphthalene, 2,...	14.012	47.8	ug/l	1118900	4	13.794	1171400	50.0
Decane	14.106	24.0	ug/l	562155	4	13.794	1171400	50.0
Indene	14.176	18.9	ug/l	443492	4	13.794	1171400	50.0
Dodecane	14.959	9.3	ug/l	218732	4	13.794	1171400	50.0
o-Cymene	15.035	19.9	ug/l	466054	4	13.794	1171400	50.0
Naphthalene, 2-...	16.782	97.5	ug/l	2283410	4	13.794	1171400	50.0