

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082265.D
 Acq On : 22 May 2024 01:57
 Operator : JC\MD
 Sample : P2494-05 40X
 Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 5

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: VN082265.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	1047	1056	1061	rBV	142300	343294	4.91%	1.300%
2	8.224	1061	1066	1081	rVB	262219	602245	8.61%	2.280%
3	8.582	1118	1127	1138	rBV2	176677	458062	6.55%	1.734%
4	9.100	1207	1215	1226	rBV	398491	811366	11.60%	3.072%
5	10.571	1456	1465	1471	rBV	620937	1168977	16.71%	4.426%
6	10.629	1471	1475	1485	rVB	127899	234004	3.35%	0.886%
7	11.865	1678	1685	1695	rBV	579762	1042320	14.90%	3.946%
8	11.965	1695	1702	1708	rVV	52539	87283	1.25%	0.330%
9	12.070	1712	1720	1733	rVV	283275	534454	7.64%	2.024%
10	12.400	1766	1776	1784	rBV	274493	520086	7.43%	1.969%
11	12.623	1796	1814	1819	rBV8	39354	202955	2.90%	0.768%
12	12.847	1846	1852	1863	rVB	468584	844104	12.07%	3.196%
13	13.100	1889	1895	1901	rBV	106833	227652	3.25%	0.862%
14	13.170	1901	1907	1914	rVB2	244923	473163	6.76%	1.792%
15	13.335	1920	1935	1942	rBV4	126865	439094	6.28%	1.663%
16	13.482	1953	1960	1965	rBV	396816	635757	9.09%	2.407%
17	13.529	1965	1968	1973	rVB3	54343	83258	1.19%	0.315%
18	13.676	1973	1993	2007	rBV5	209146	1142805	16.34%	4.327%
19	13.794	2007	2013	2022	rBV2	593112	1287719	18.41%	4.876%
20	14.017	2034	2051	2060	rBV6	356329	1347078	19.26%	5.100%
21	14.106	2060	2066	2073	rVV3	263519	638732	9.13%	2.418%
22	14.176	2073	2078	2084	rVB2	304096	541709	7.74%	2.051%
23	14.247	2085	2090	2092	rBV2	52721	87933	1.26%	0.333%
24	14.329	2100	2104	2108	rVB	58935	88181	1.26%	0.334%
25	14.441	2118	2123	2127	rBV3	72597	143918	2.06%	0.545%
26	14.570	2142	2145	2151	rVB6	91206	165180	2.36%	0.625%
27	14.629	2151	2155	2157	rBV3	72458	109571	1.57%	0.415%
28	14.659	2157	2160	2163	rVV3	80629	129882	1.86%	0.492%
29	14.694	2163	2166	2170	rVB	112520	143709	2.05%	0.544%
30	14.794	2177	2183	2187	rBV6	50258	111583	1.60%	0.422%
31	14.847	2187	2192	2202	rVB7	60652	186665	2.67%	0.707%
32	14.959	2202	2211	2218	rBV6	127520	260333	3.72%	0.986%
33	15.035	2218	2224	2233	rBV3	172101	526244	7.52%	1.992%
34	15.211	2248	2254	2260	rVB3	85405	166536	2.38%	0.631%
35	15.317	2267	2272	2286	rVV9	77870	229216	3.28%	0.868%
36	15.435	2286	2292	2298	rVB6	66303	154237	2.20%	0.584%

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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
Title : SW846 8260

37	15.641	2315	2327	2338	rBV	3613029	6995227	100.00%	26.486%
38	15.747	2340	2345	2351	rVB	91633	171849	2.46%	0.651%
39	15.947	2370	2379	2386	rBV6	52664	168270	2.41%	0.637%
40	16.711	2503	2509	2513	rBV2	48548	105081	1.50%	0.398%
41	16.782	2513	2521	2522	rBV	1808193	2801756	40.05%	10.608%

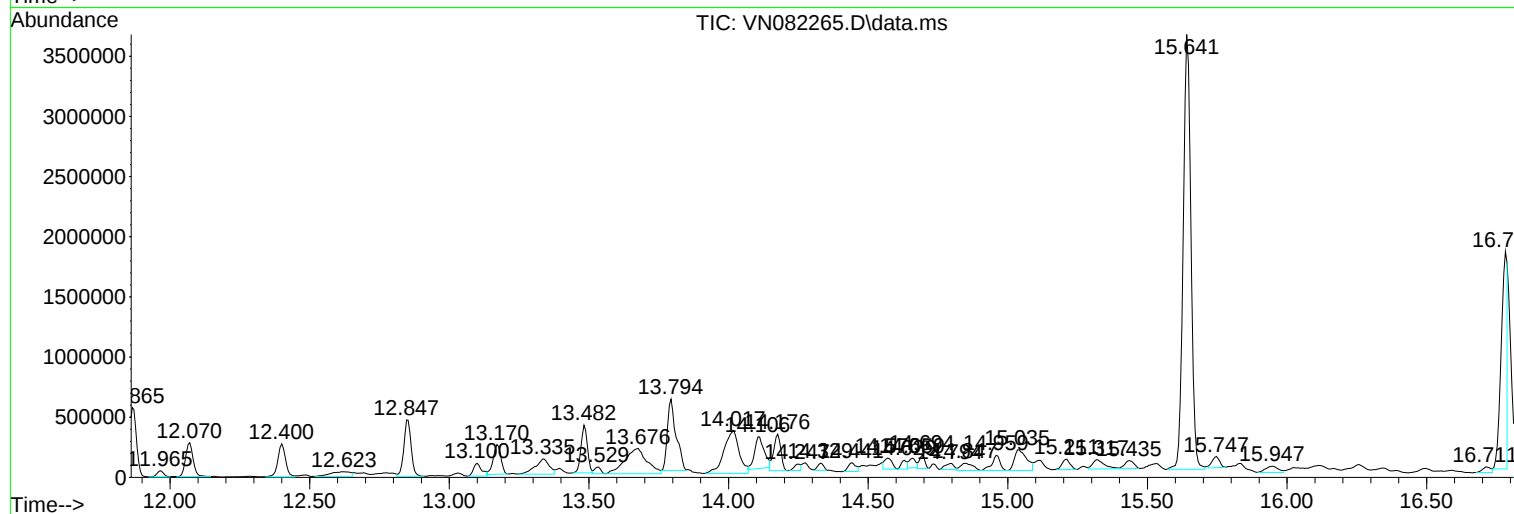
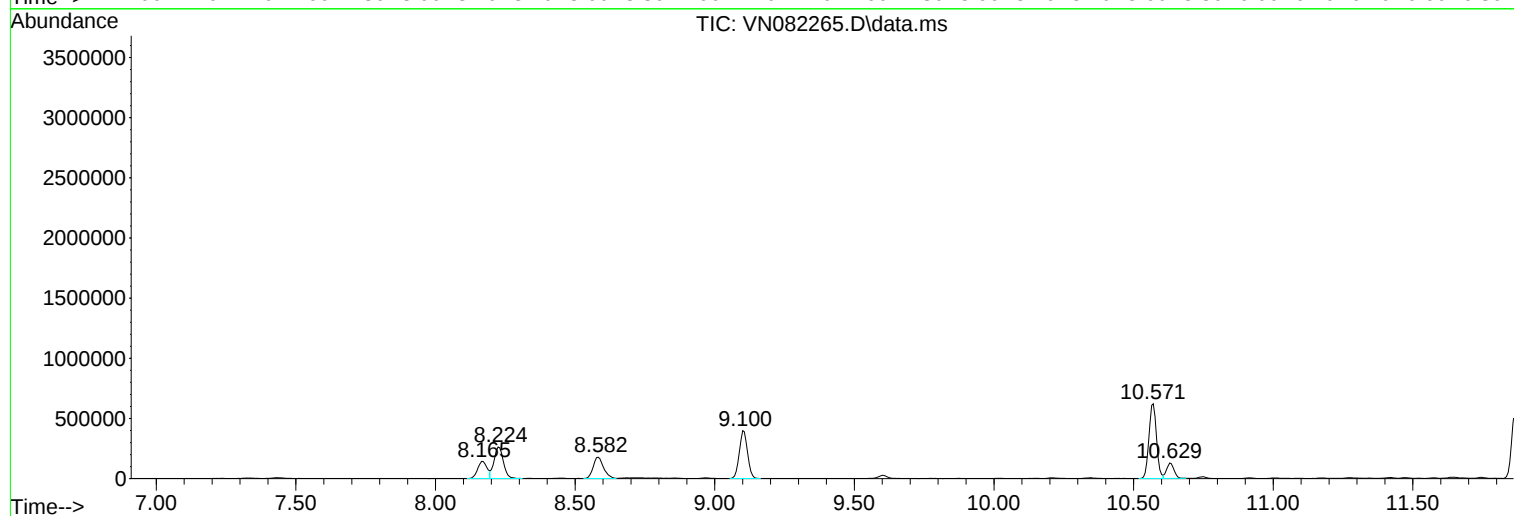
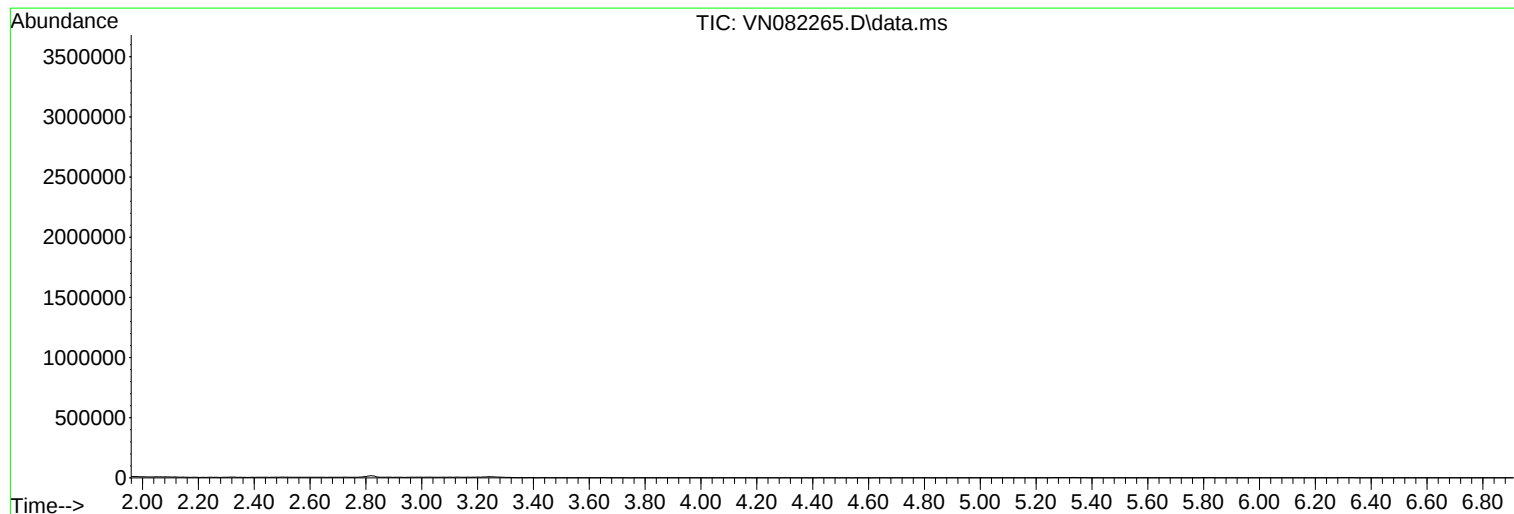
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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ALS Vial : 40 Sample Multiplier: 1

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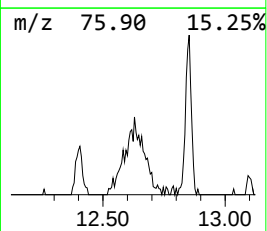
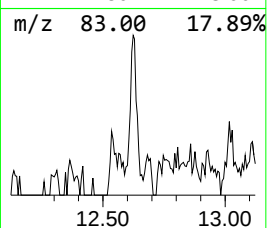
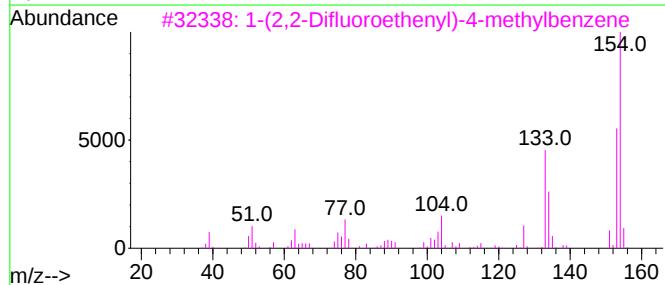
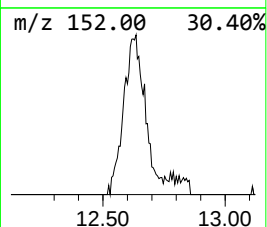
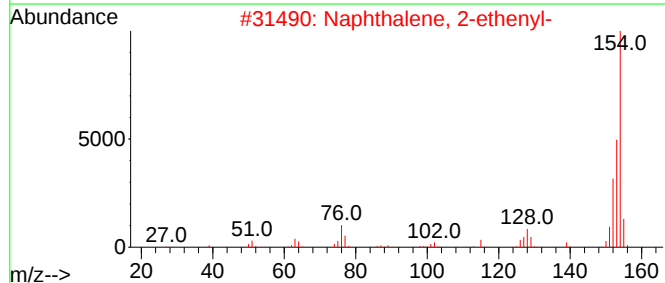
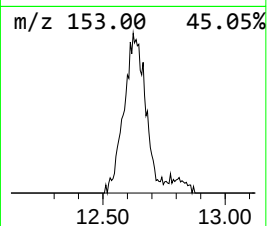
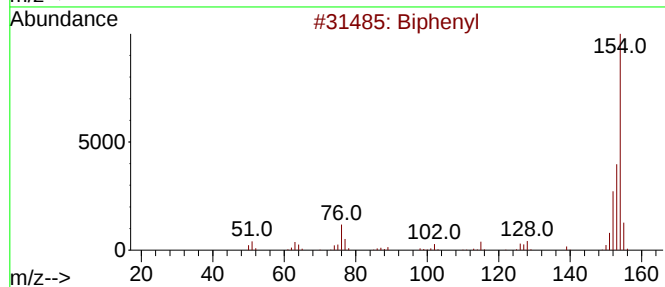
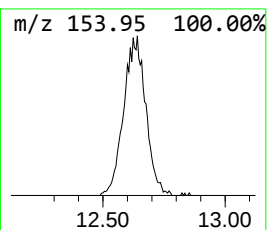
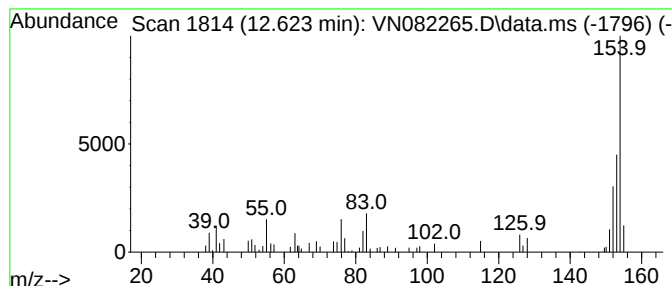
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Biphenyl Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.623	9.74 ug/l	202955	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	93
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	81
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	59
4			Propanedinitrile, (phenylmethyle...	154	C10H6N2	002700-22-3	47
5			Acenaphthene	154	C12H10	000083-32-9	46



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Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
5

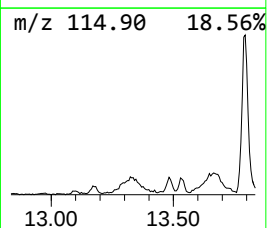
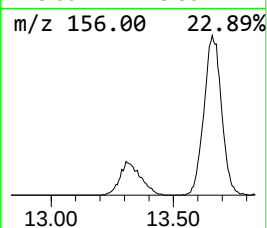
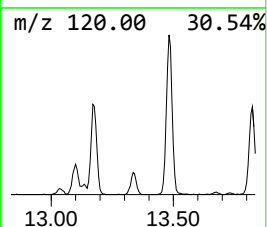
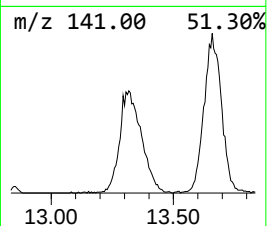
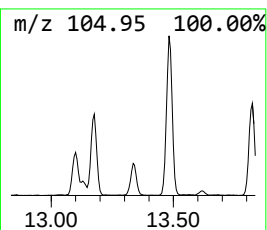
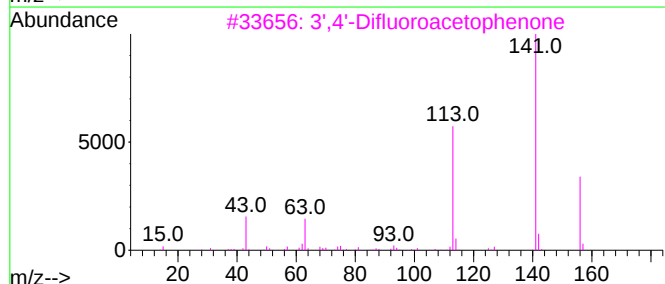
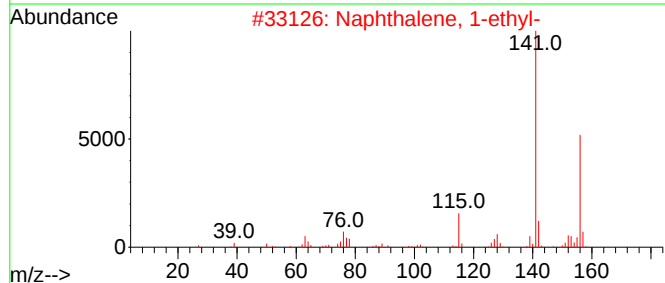
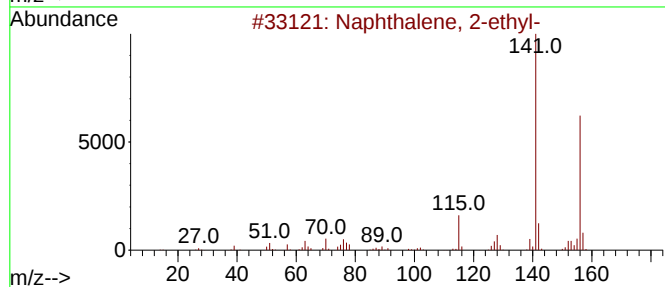
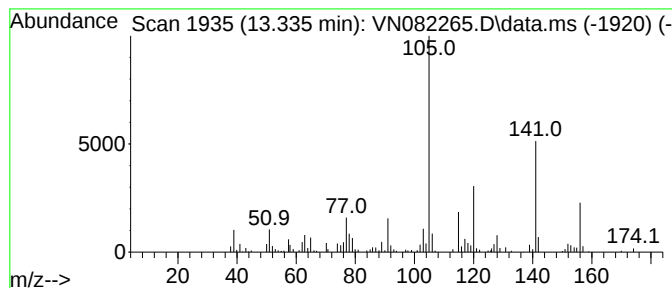
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	17.05 ug/l	439094	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	55
2			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	55
3			3',4'-Difluoroacetophenone	156	C8H6F2O	000369-33-5	38
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	38
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	38



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Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

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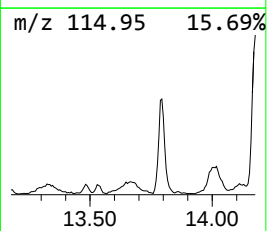
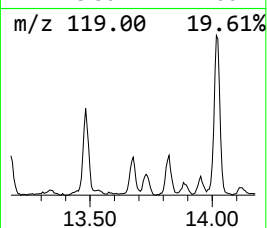
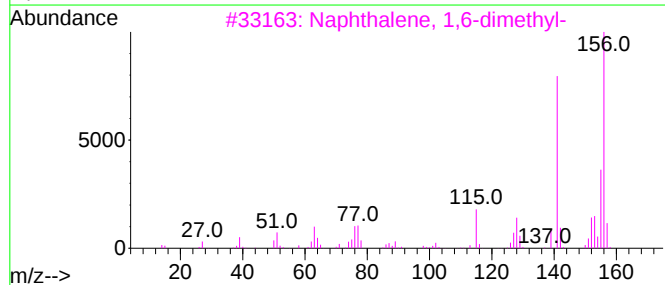
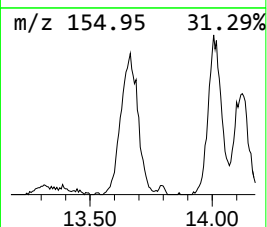
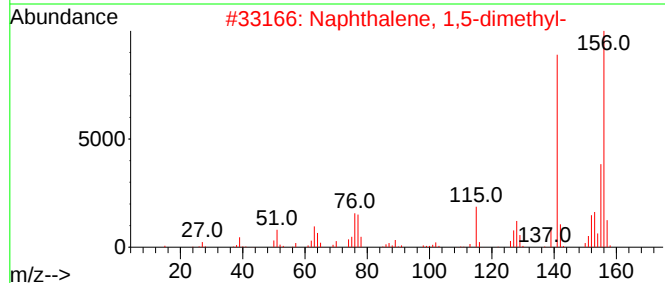
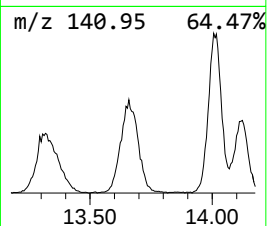
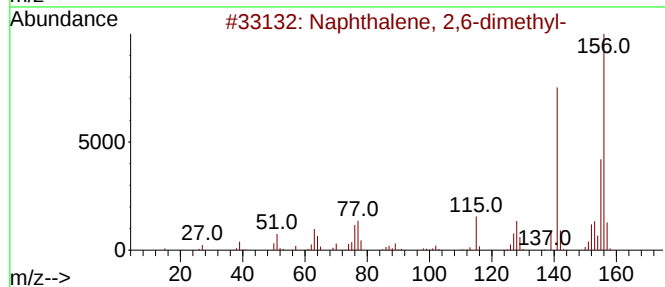
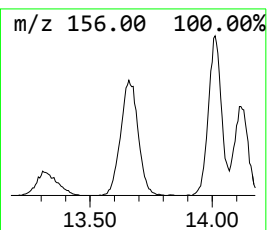
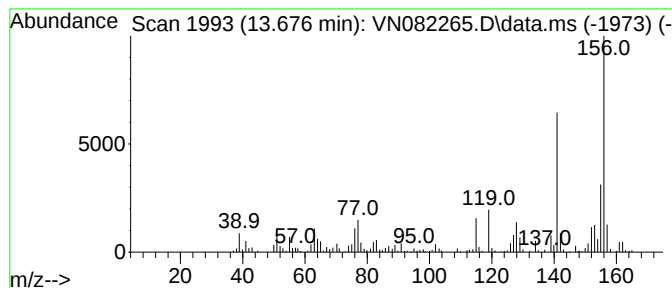
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	44.37 ug/l	1142810	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	98
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	97



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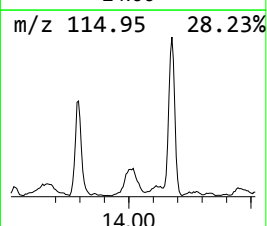
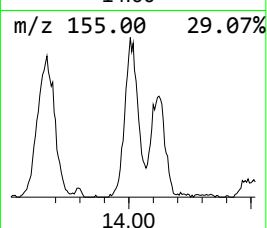
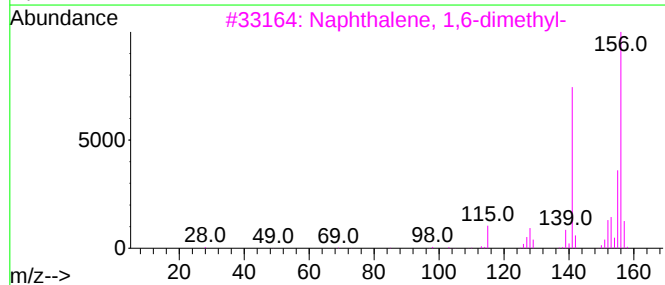
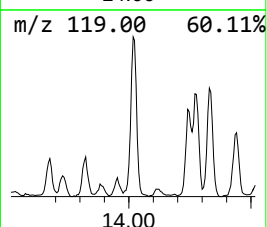
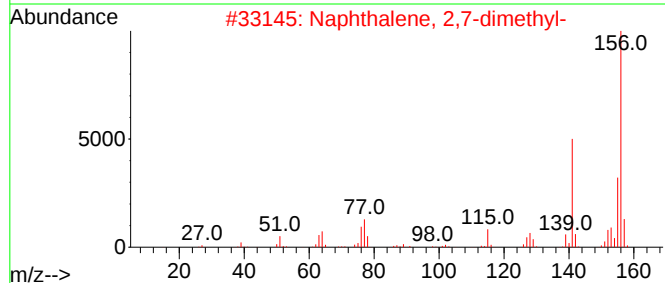
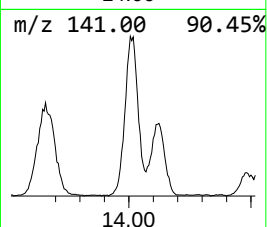
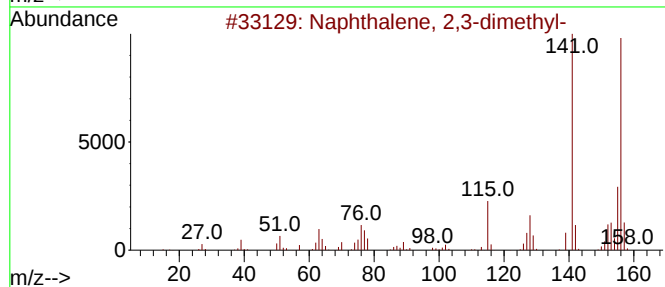
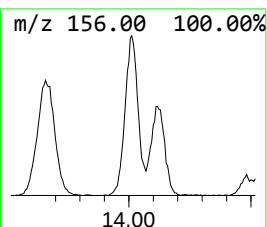
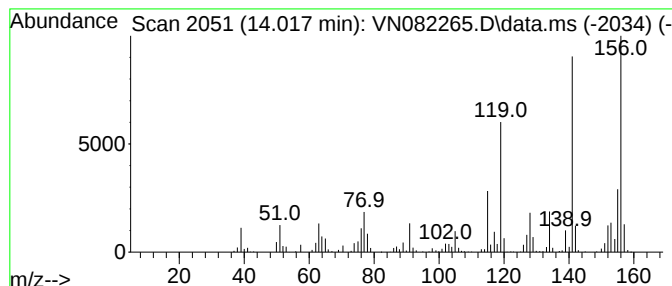
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	52.30 ug/l	1347080	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	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96



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Instrument :
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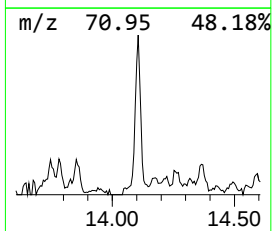
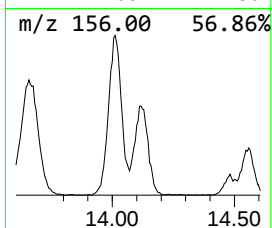
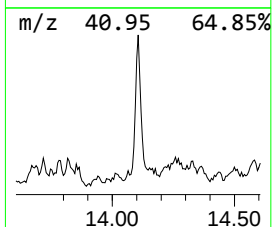
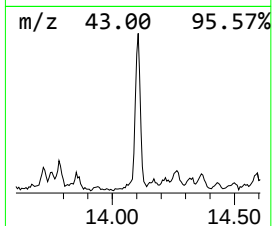
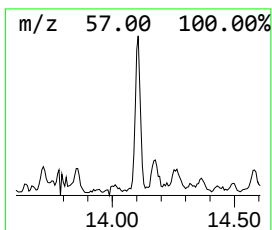
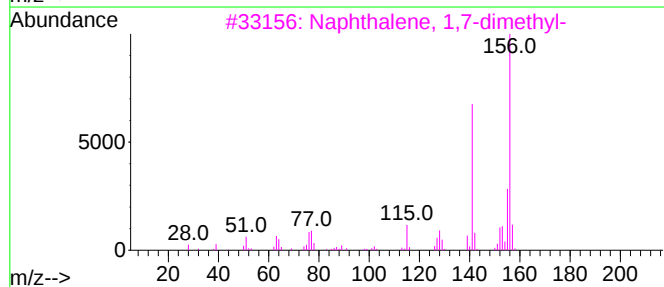
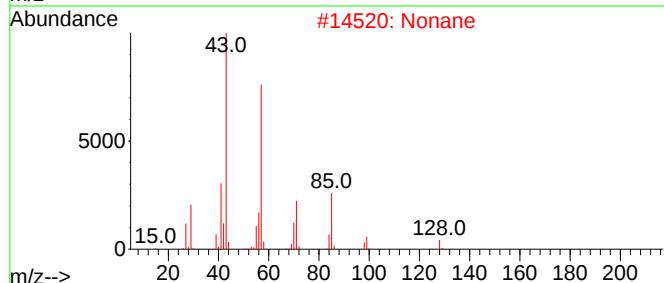
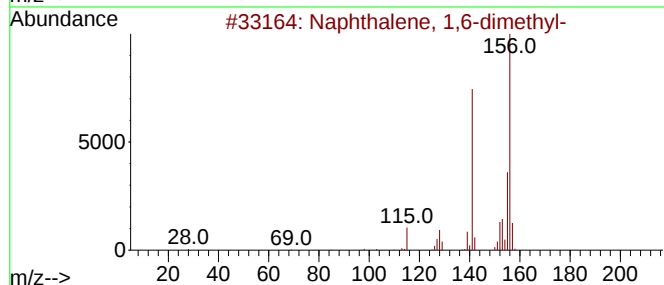
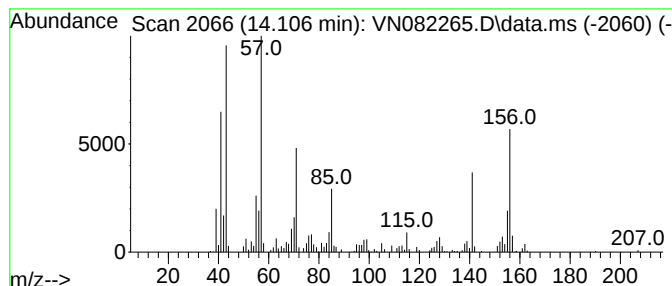
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	24.80 ug/l	638732	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
2			Nonane	128	C9H20	000111-84-2	83
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	59
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	56
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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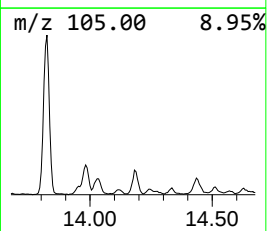
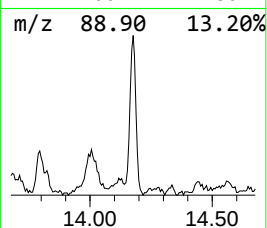
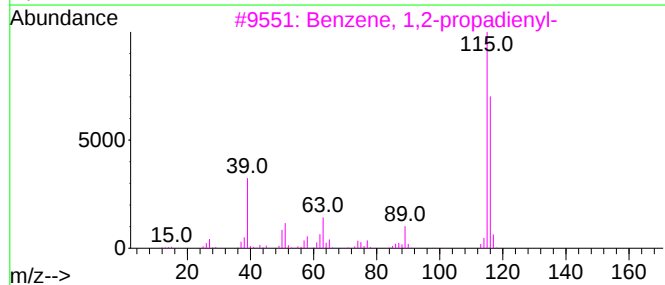
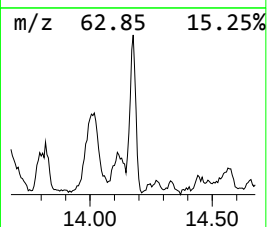
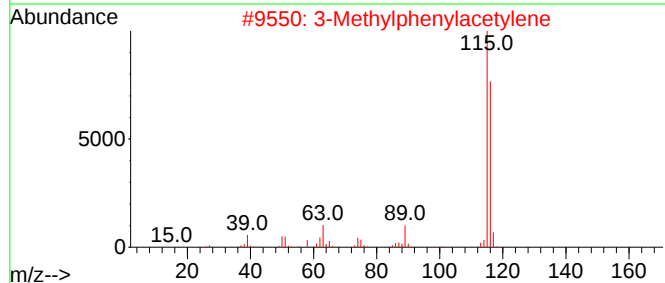
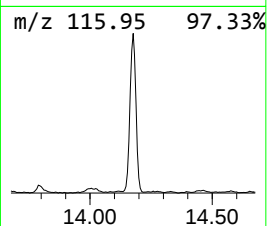
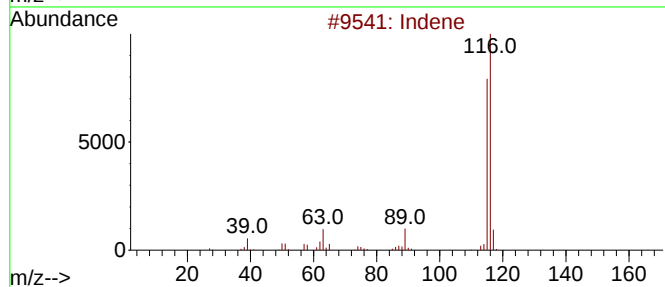
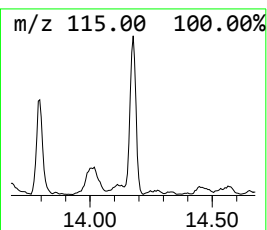
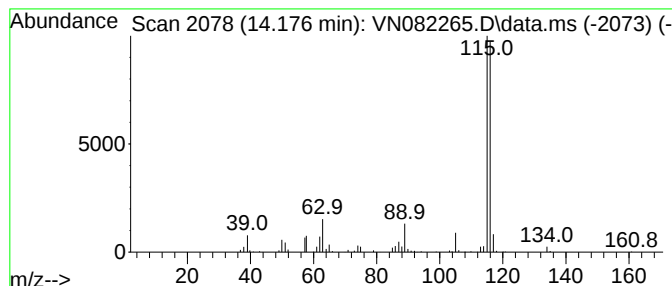
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Quant Title : SW846 8260

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

Peak Number 6 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	21.03 ug/l	541709	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	94
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
4			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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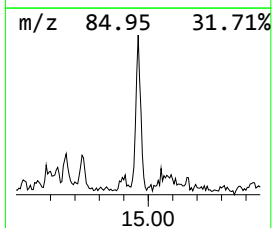
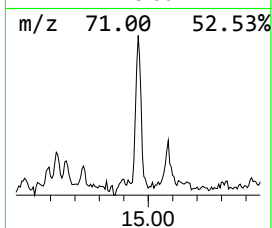
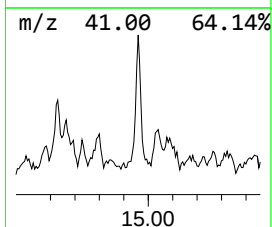
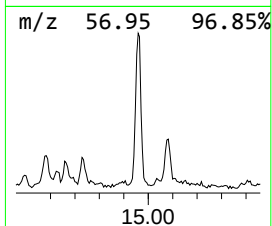
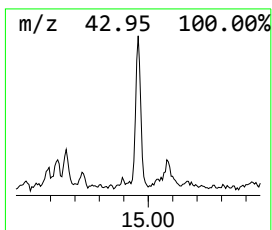
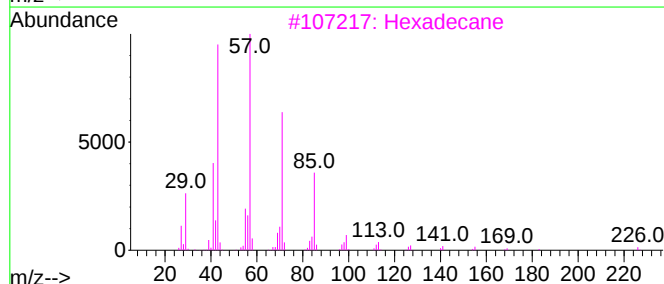
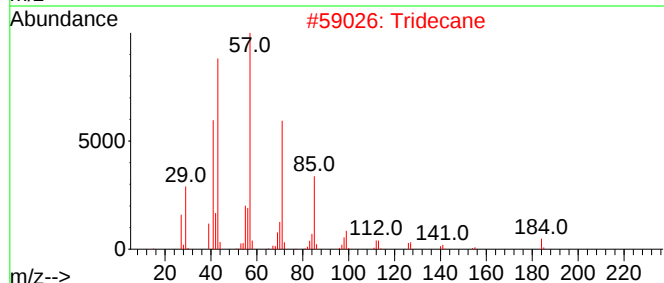
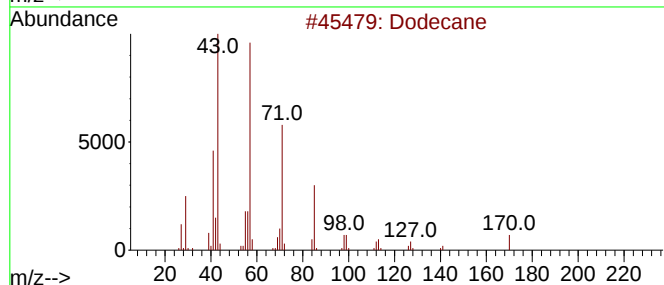
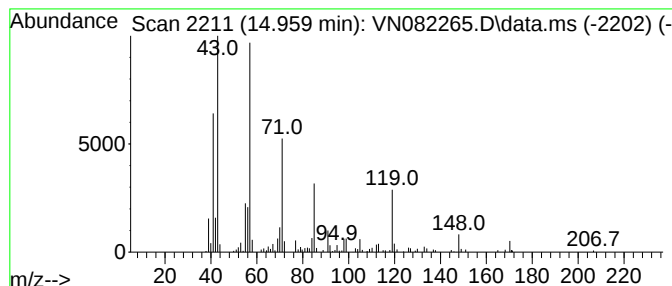
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Quant Title : SW846 8260

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

Peak Number 7 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	10.11 ug/l	260333	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Tridecane	184	C13H28	000629-50-5	64
3			Hexadecane	226	C16H34	000544-76-3	52
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	50
5			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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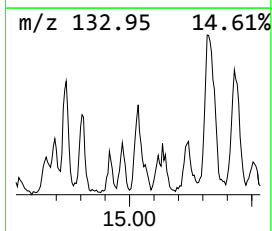
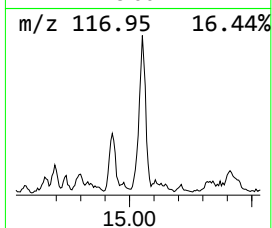
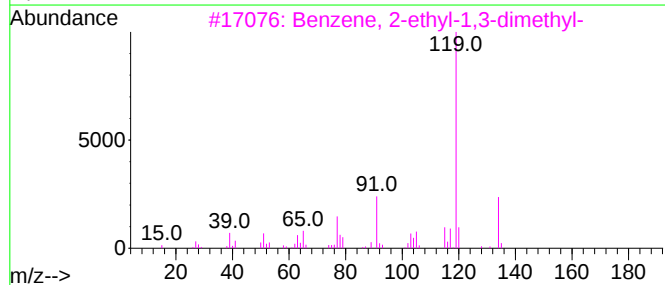
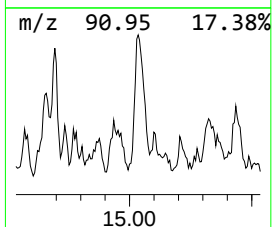
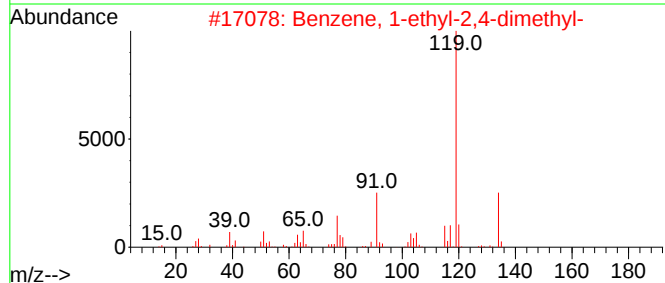
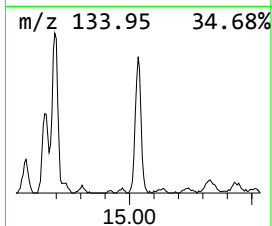
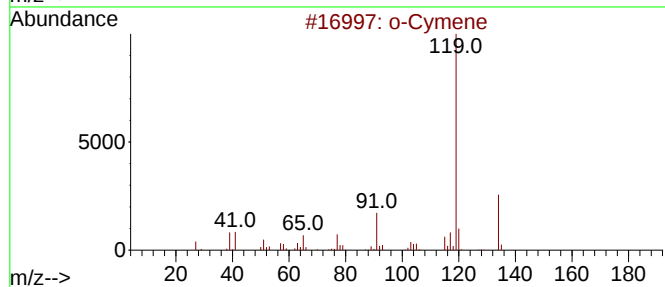
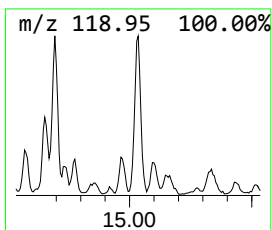
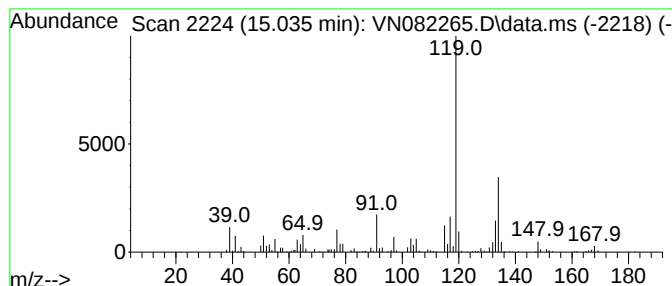
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Quant Title : SW846 8260

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

Peak Number 8 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	20.43 ug/l	526244	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	94
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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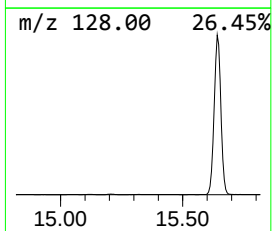
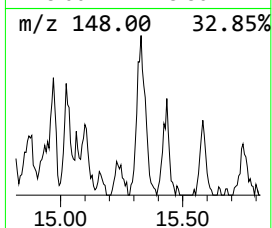
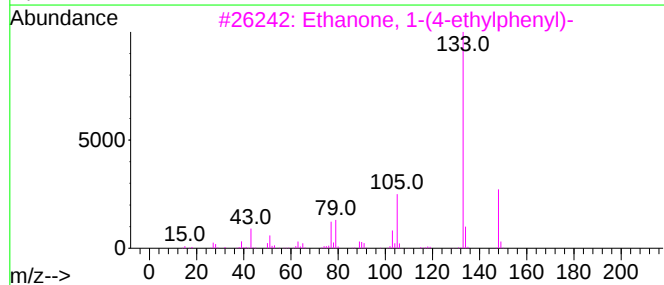
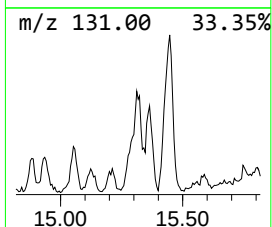
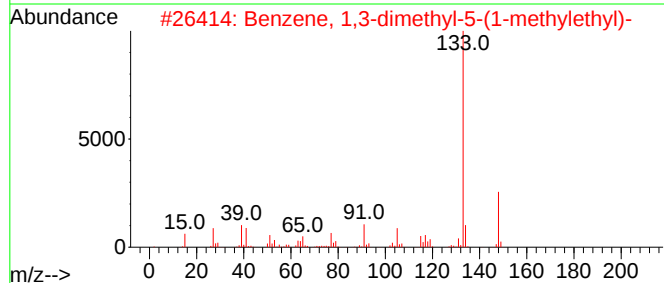
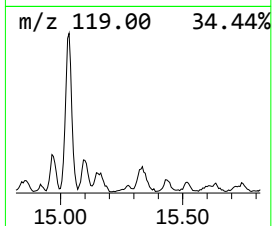
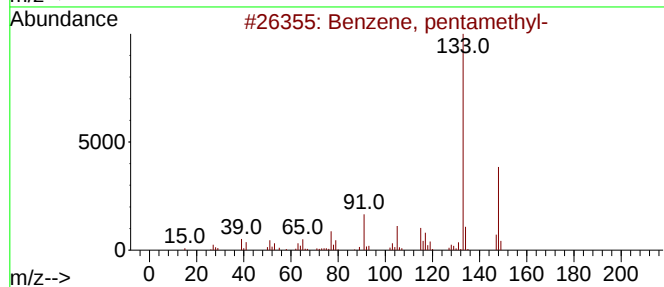
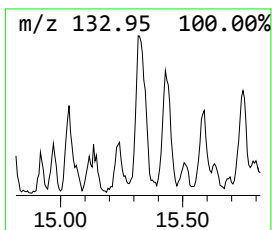
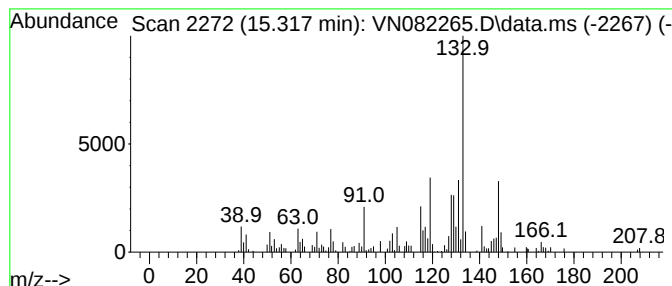
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.317 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	8.90 ug/l	229216	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, pentamethyl-	148	C11H16	000700-12-9	46
2			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	46
3			Ethanone, 1-(4-ethylphenyl)-	148	C10H12O	000937-30-4	45
4			m-Ethylacetophenone	148	C10H12O	022699-70-3	43
5			Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	020944-88-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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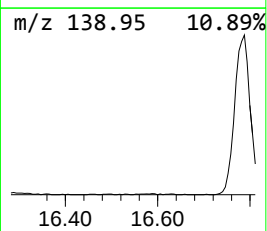
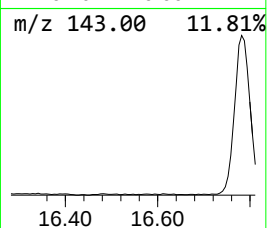
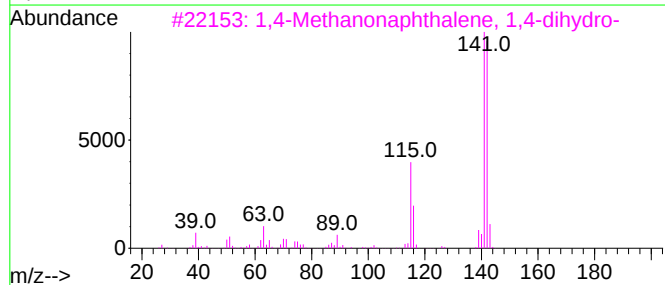
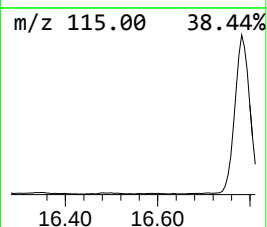
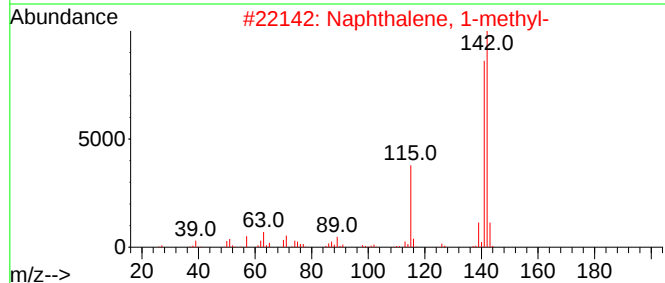
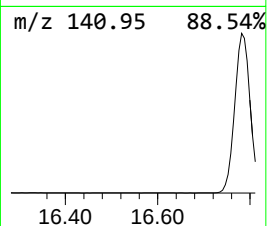
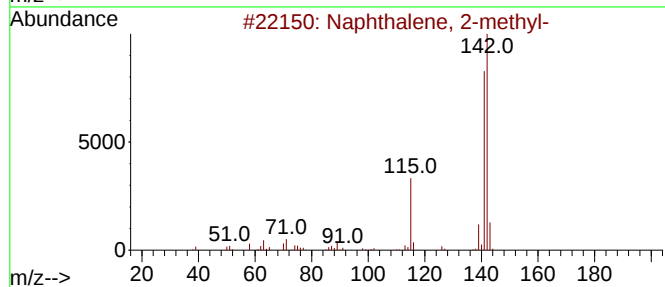
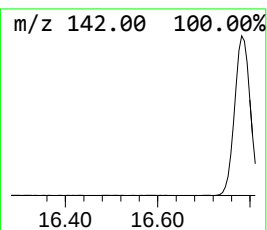
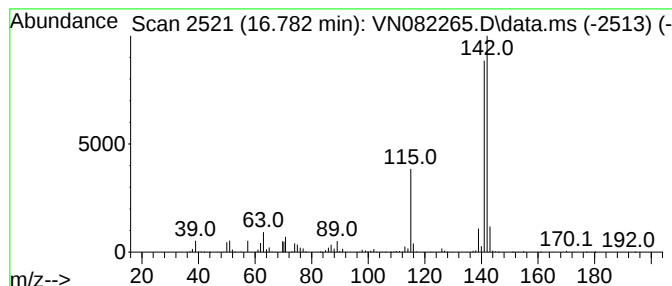
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Quant Title : SW846 8260

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	108.79 ug/l	2801760	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	94
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 : VN082265.D
Acq On : 22 May 2024 01:57
Operator : JC\MD
Sample : P2494-05 40X
Misc : 5.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 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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Naphthalene, 2-...	13.335	17.1	ug/l	439094	4	13.794	1287720	50.0
Naphthalene, 2,...	13.676	44.4	ug/l	1142810	4	13.794	1287720	50.0
Naphthalene, 2,...	14.017	52.3	ug/l	1347080	4	13.794	1287720	50.0
Naphthalene, 1,...	14.106	24.8	ug/l	638732	4	13.794	1287720	50.0
Indene	14.176	21.0	ug/l	541709	4	13.794	1287720	50.0
Dodecane	14.959	10.1	ug/l	260333	4	13.794	1287720	50.0
o-Cymene	15.035	20.4	ug/l	526244	4	13.794	1287720	50.0
unknown15.317	15.317	8.9	ug/l	229216	4	13.794	1287720	50.0
Naphthalene, 2-...	16.782	108.8	ug/l	2801760	4	13.794	1287720	50.0