

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
 Data File : VN082271.D
 Acq On : 22 May 2024 04:21
 Operator : JC\MD
 Sample : P2494-11 40X
 Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 11

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: VN082271.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	1045	1056	1061	rBV	150899	364701	7.70%	1.791%
2	8.224	1061	1066	1078	rVB	284024	633461	13.37%	3.112%
3	8.582	1116	1127	1140	rBV2	190193	469278	9.90%	2.305%
4	9.100	1207	1215	1227	rBV	418181	851964	17.98%	4.185%
5	10.571	1455	1465	1471	rBV	651446	1226858	25.89%	6.026%
6	10.629	1471	1475	1489	rVB	100592	187738	3.96%	0.922%
7	11.865	1677	1685	1696	rBV	620185	1108416	23.39%	5.444%
8	11.965	1696	1702	1708	rVV	38410	65764	1.39%	0.323%
9	12.070	1711	1720	1732	rVB	212717	407574	8.60%	2.002%
10	12.400	1765	1776	1784	rBV	208065	392095	8.27%	1.926%
11	12.623	1796	1814	1817	rBV10	27140	120994	2.55%	0.594%
12	12.847	1846	1852	1863	rVB	508430	892090	18.82%	4.382%
13	13.100	1889	1895	1899	rBV	80092	148042	3.12%	0.727%
14	13.170	1902	1907	1915	rVB2	175643	323146	6.82%	1.587%
15	13.335	1921	1935	1942	rBV3	89163	292731	6.18%	1.438%
16	13.482	1954	1960	1965	rVV	296296	461096	9.73%	2.265%
17	13.529	1965	1968	1973	rVB3	33672	52791	1.11%	0.259%
18	13.670	1973	1992	2007	rBV5	153867	799130	16.86%	3.925%
19	13.794	2007	2013	2022	rBV2	609438	1247435	26.32%	6.127%
20	14.011	2034	2050	2060	rBV6	240358	915934	19.33%	4.499%
21	14.106	2060	2066	2073	rVV4	183756	438377	9.25%	2.153%
22	14.176	2073	2078	2084	rVB2	193872	355370	7.50%	1.746%
23	14.247	2085	2090	2091	rBV2	34678	48697	1.03%	0.239%
24	14.329	2100	2104	2109	rVB	45461	61867	1.31%	0.304%
25	14.435	2117	2122	2126	rBV3	45780	87246	1.84%	0.429%
26	14.629	2151	2155	2157	rBV4	46114	68744	1.45%	0.338%
27	14.653	2157	2159	2163	rVV3	56385	89231	1.88%	0.438%
28	14.694	2163	2166	2170	rVB	76231	97527	2.06%	0.479%
29	14.788	2176	2182	2187	rBV5	28416	72575	1.53%	0.356%
30	14.847	2187	2192	2202	rVB8	39881	126369	2.67%	0.621%
31	14.958	2202	2211	2218	rVB4	99642	199796	4.22%	0.981%
32	15.035	2218	2224	2234	rBV4	112045	381297	8.05%	1.873%
33	15.206	2248	2253	2260	rVB3	47417	92554	1.95%	0.455%
34	15.317	2268	2272	2282	rVB4	43925	92596	1.95%	0.455%
35	15.429	2287	2291	2298	rVB4	41853	94829	2.00%	0.466%
36	15.641	2314	2327	2338	rBV	2411195	4739328	100.00%	23.279%

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37	15.747	2339	2345	2351	rVB	61297	123139	2.60%	0.605%
38	15.835	2357	2360	2365	rVB4	41728	65712	1.39%	0.323%
39	15.941	2371	2378	2386	rBV8	31682	98528	2.08%	0.484%
40	16.494	2463	2472	2479	rBV8	25745	79131	1.67%	0.389%
41	16.717	2502	2510	2513	rBV3	33496	79109	1.67%	0.389%
42	16.782	2513	2521	2522	rBV	1216911	1905320	40.20%	9.359%

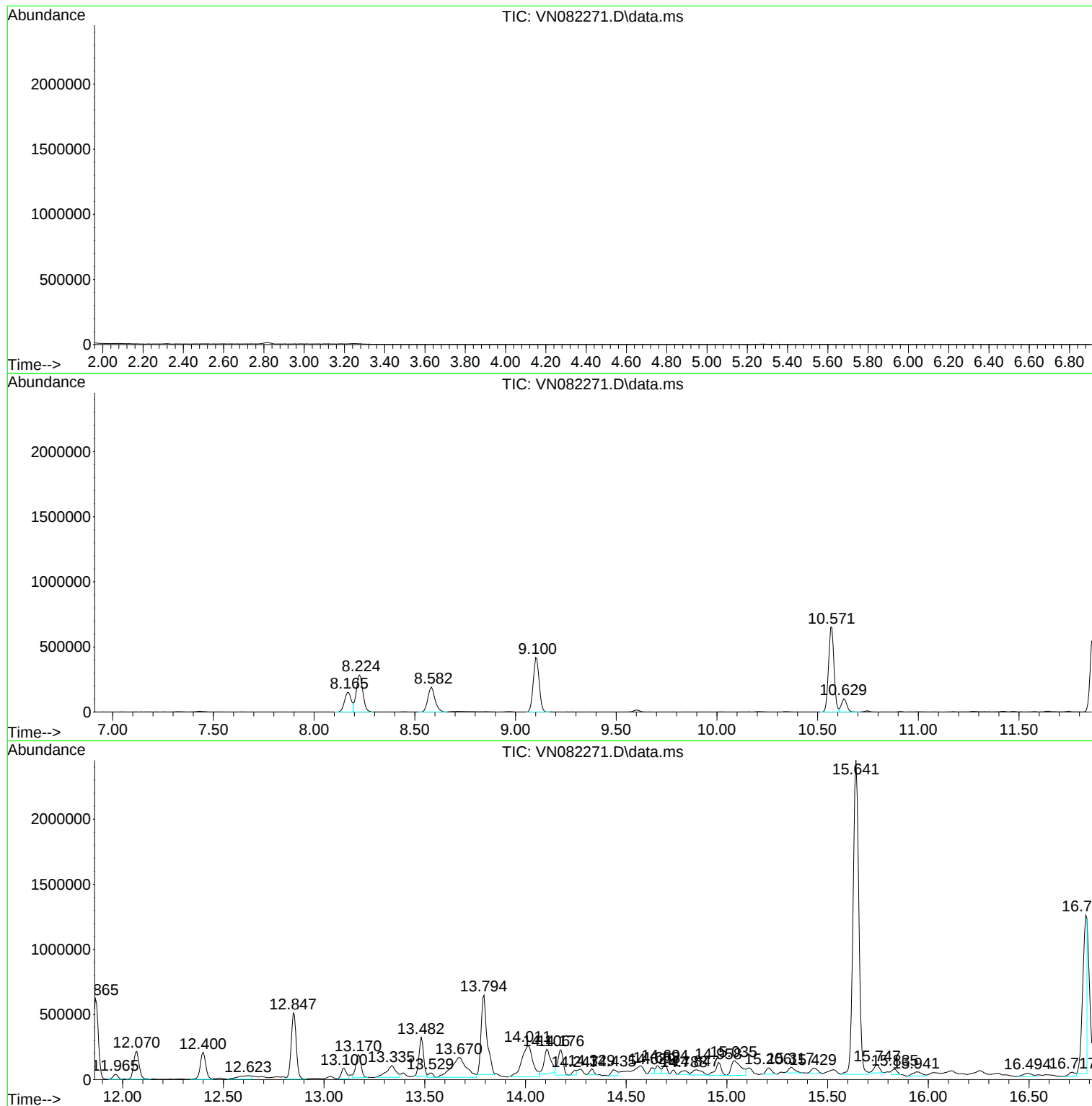
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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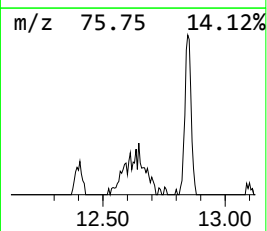
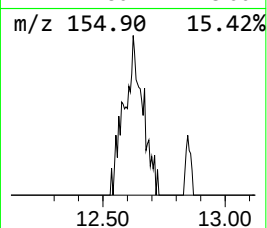
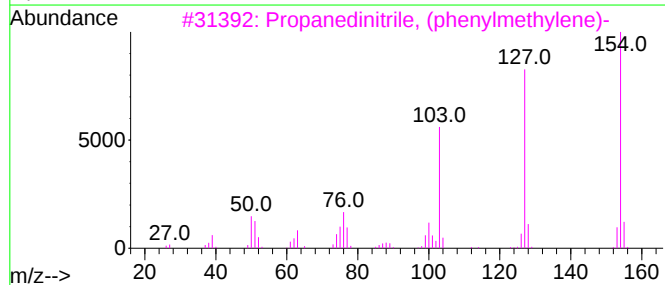
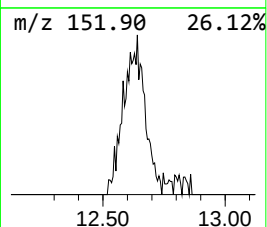
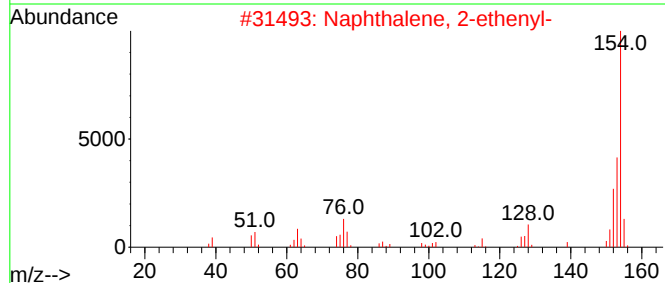
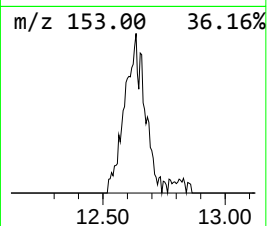
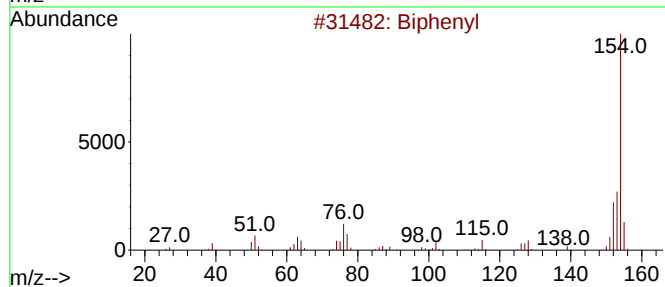
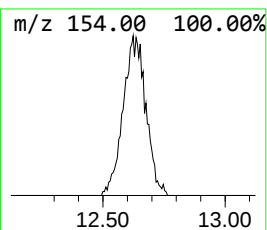
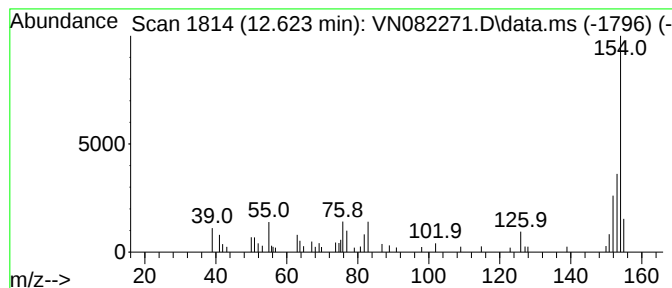
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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	5.46 ug/l	120994	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	76
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	68
3			Propanedinitrile, (phenylmethyle...	154	C10H6N2	002700-22-3	47
4			5,6-Difluoro-1H-indazole	154	C7H4F2N2	944898-96-8	38
5			2-Quinolinecarbonitrile	154	C10H6N2	001436-43-7	38



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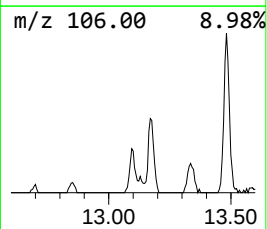
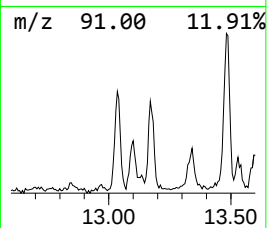
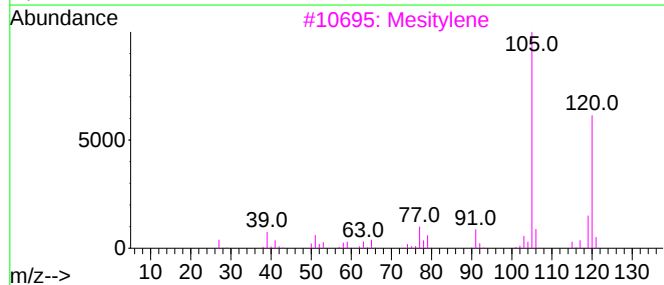
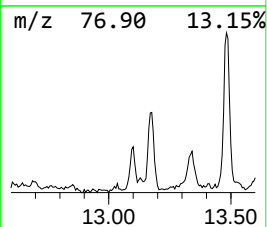
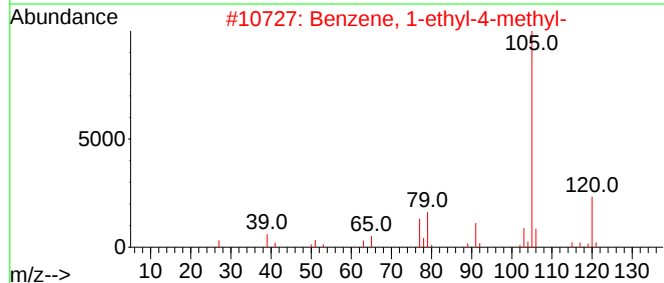
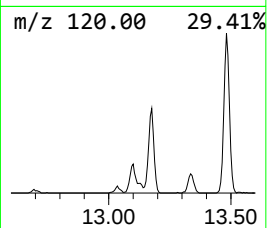
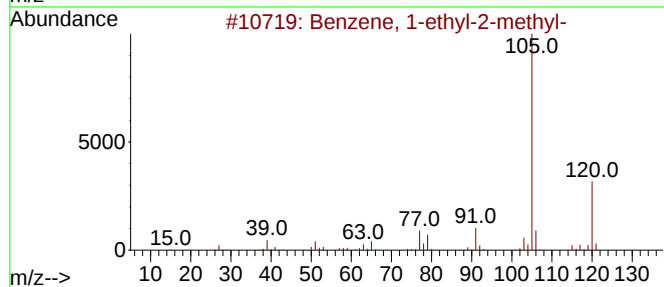
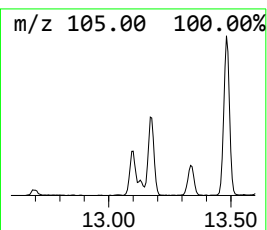
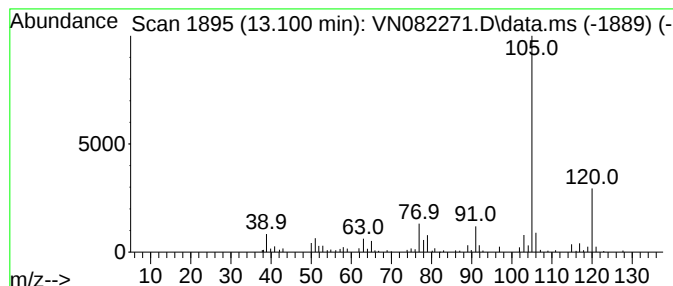
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	5.93 ug/l	148042	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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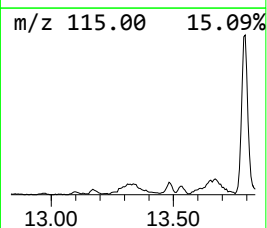
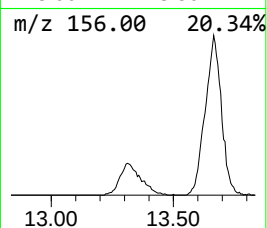
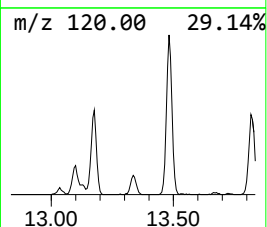
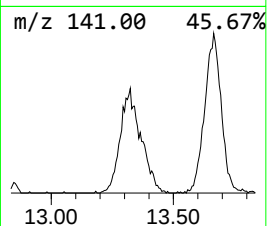
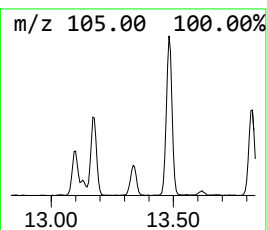
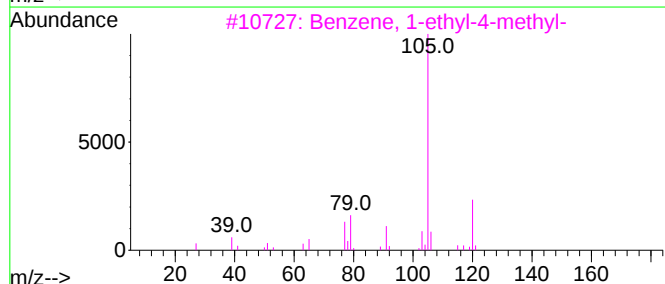
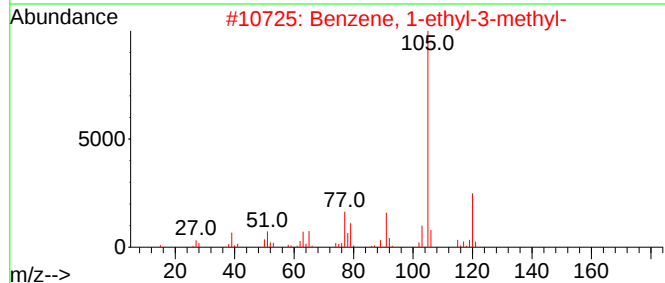
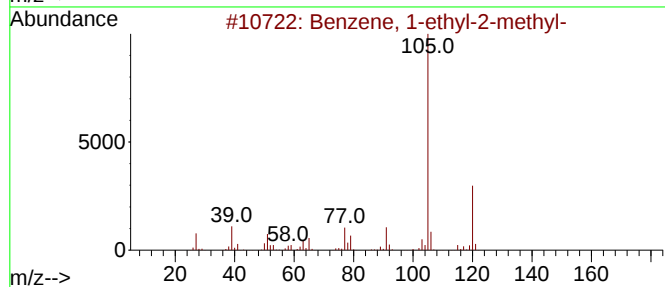
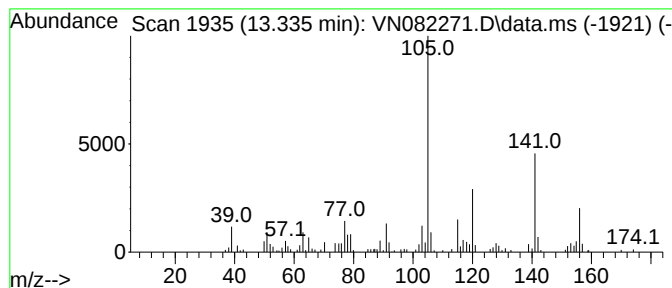
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Quant Title : SW846 8260

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

Peak Number 3 unknown13.335 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	11.73 ug/l	292731	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	42
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	42
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	42
4			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	38
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	38



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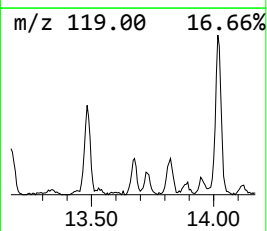
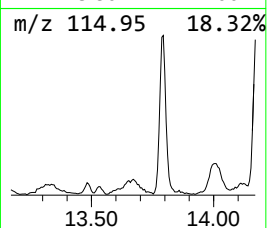
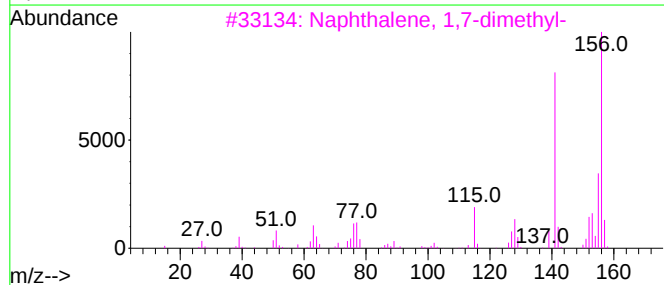
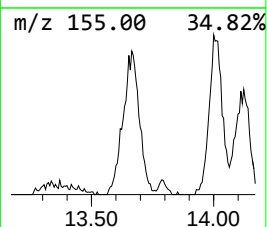
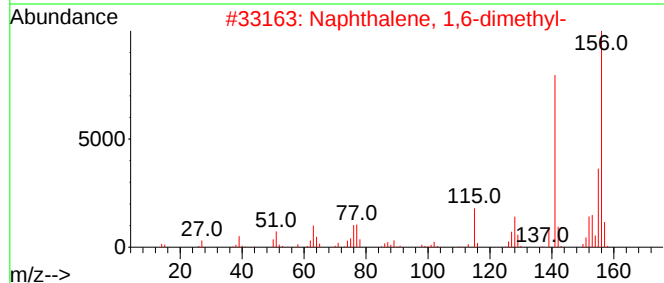
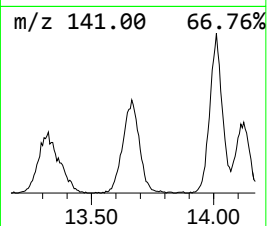
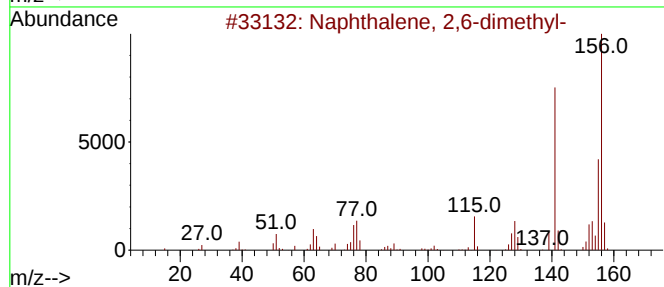
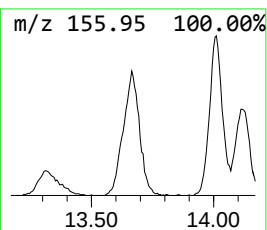
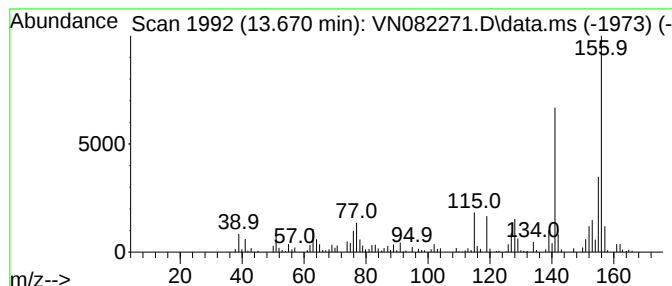
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	32.03 ug/l	799130	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, 1,6-dimethyl-	156	C12H12	000575-43-9	98
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



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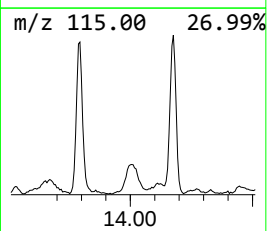
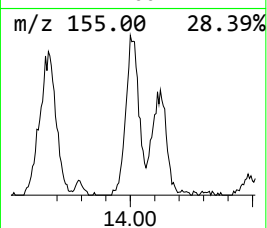
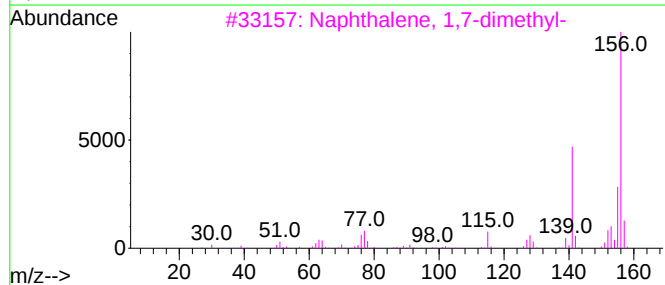
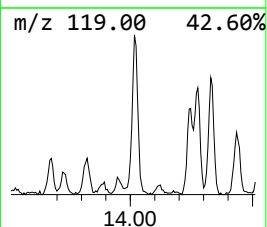
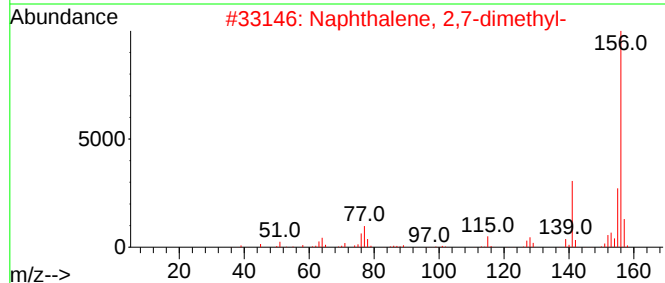
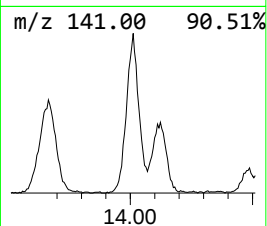
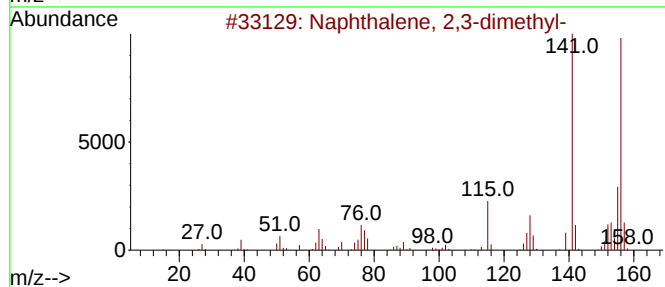
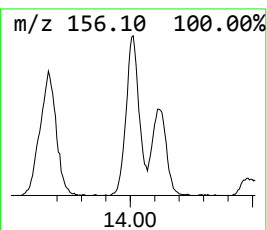
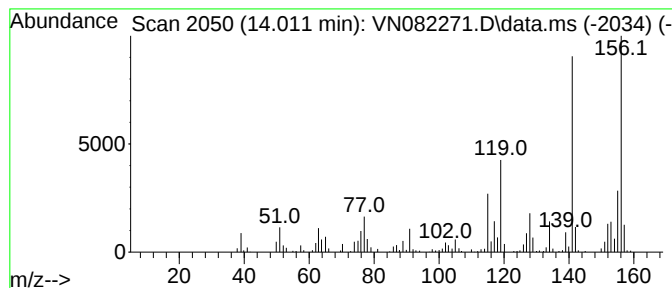
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Quant Title : SW846 8260

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	36.71 ug/l	915934	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, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
11

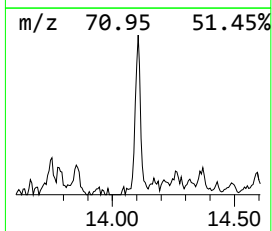
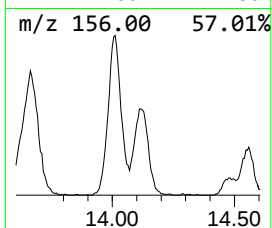
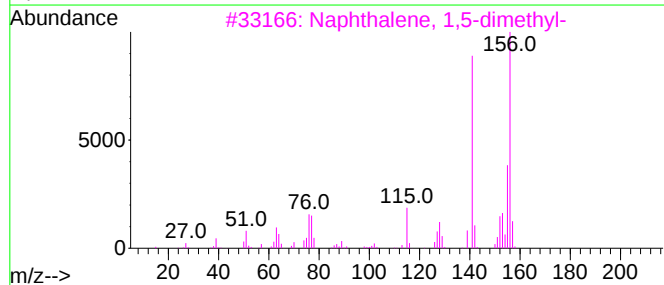
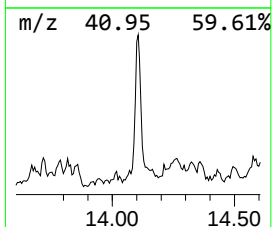
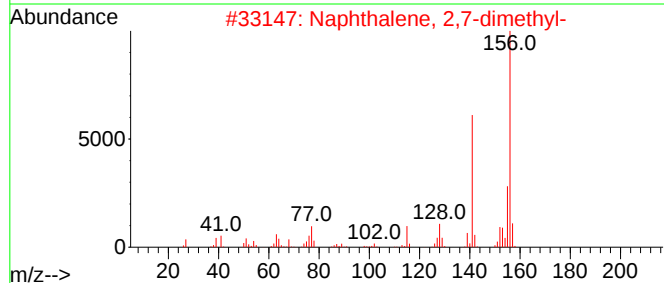
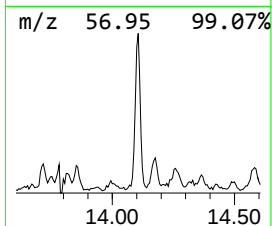
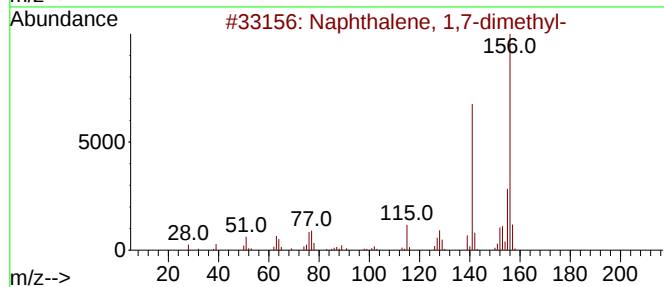
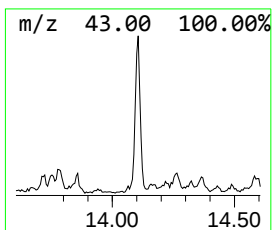
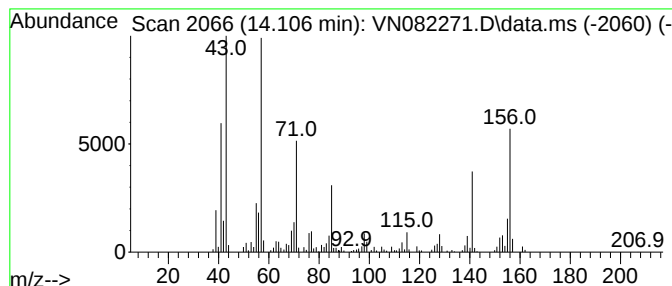
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	17.57 ug/l	438377	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	86
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	64
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	60
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	60
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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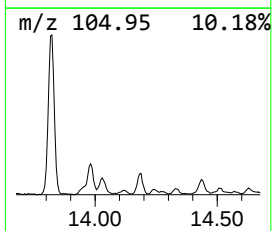
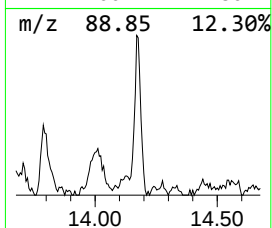
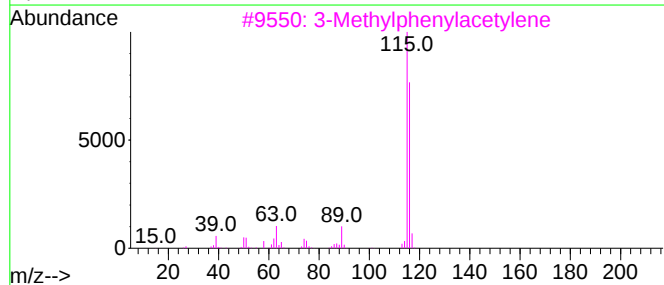
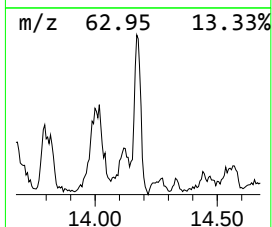
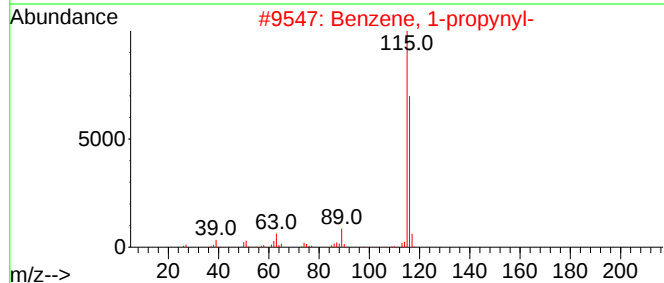
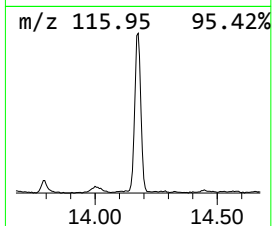
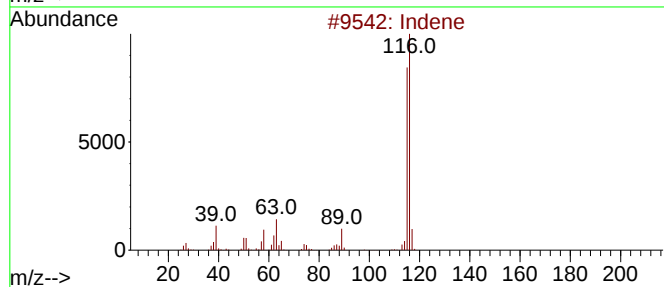
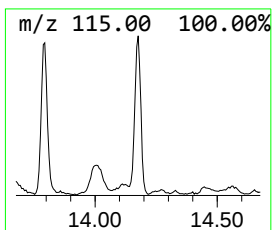
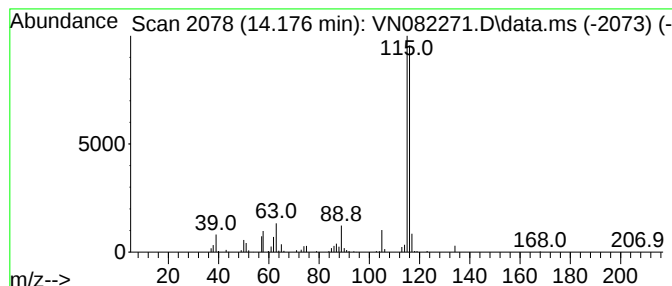
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	14.24 ug/l	355370	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	96
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	93
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	93
4			2-Methylphenylacetylene	116	C9H8	000766-47-2	90
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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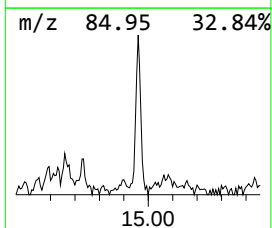
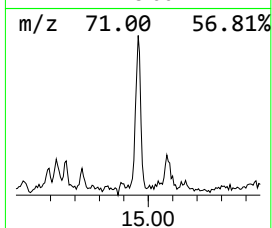
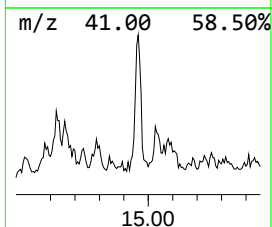
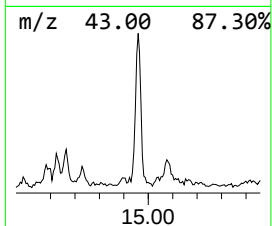
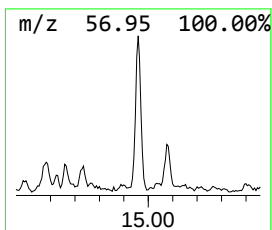
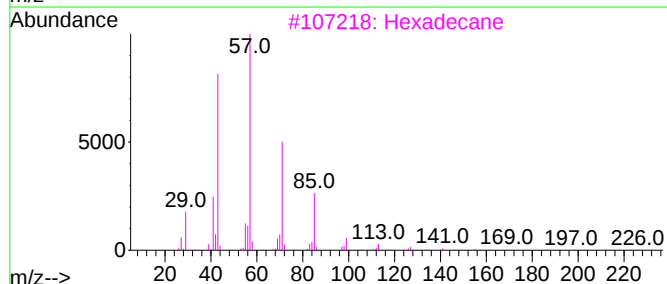
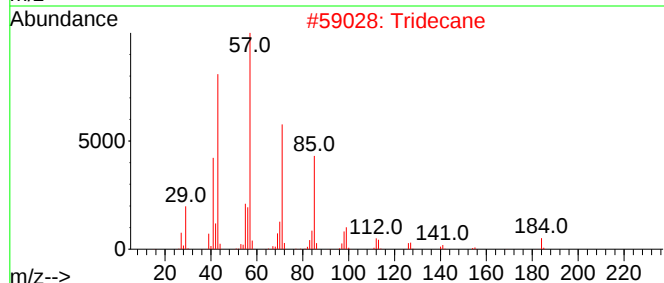
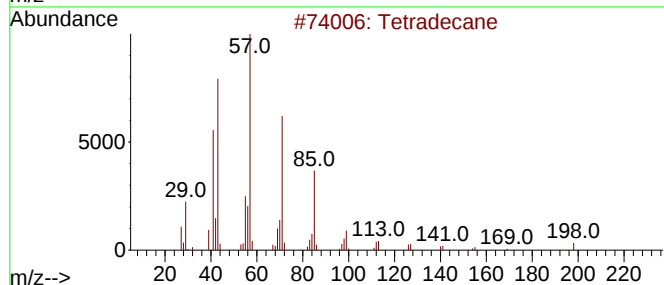
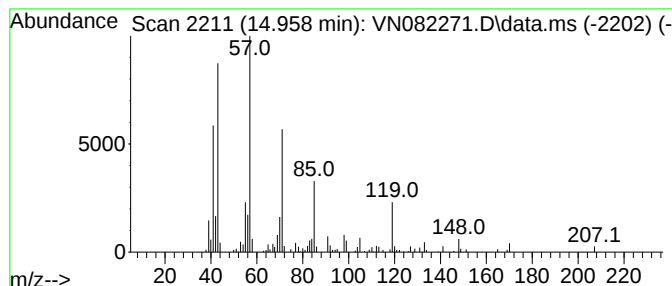
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Quant Title : SW846 8260

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

Peak Number 8 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	8.01 ug/l	199796	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	58
2			Tridecane	184	C13H28	000629-50-5	53
3			Hexadecane	226	C16H34	000544-76-3	53
4			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	50
5			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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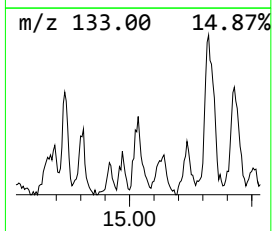
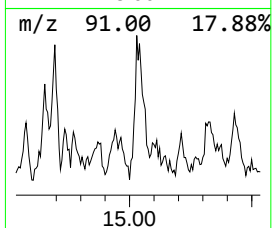
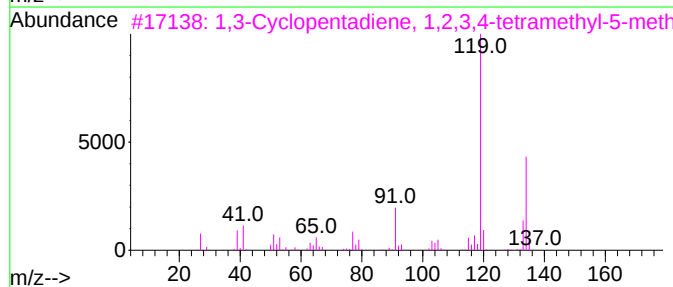
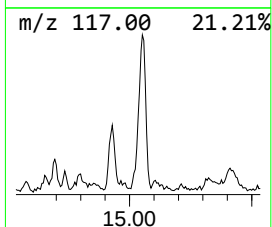
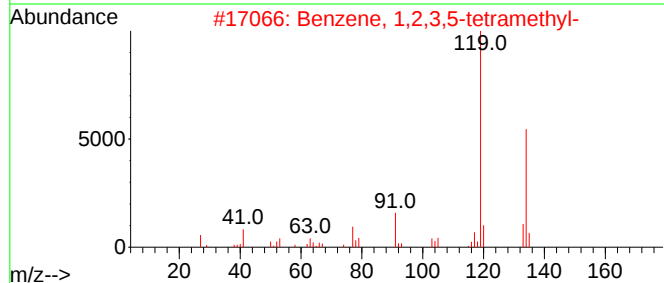
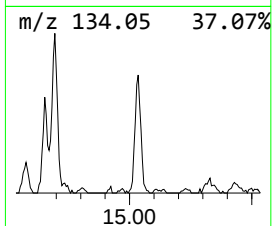
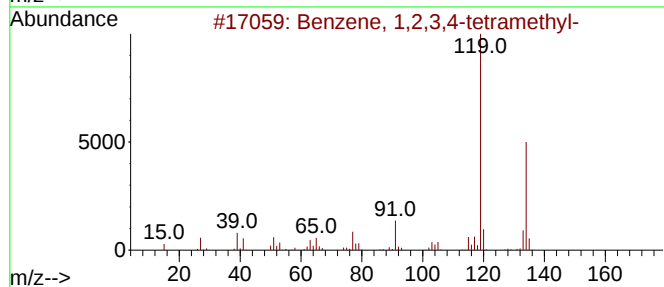
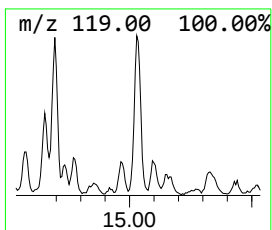
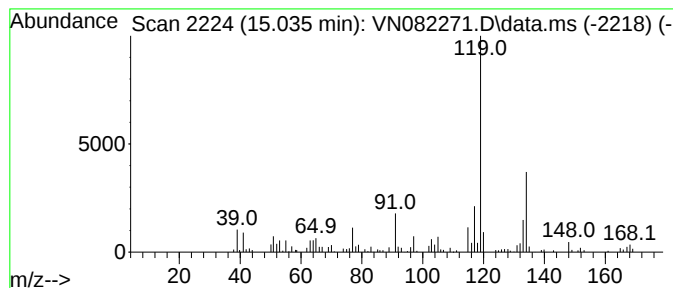
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	15.28 ug/l	381297	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
3			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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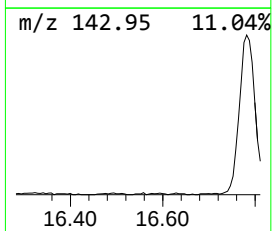
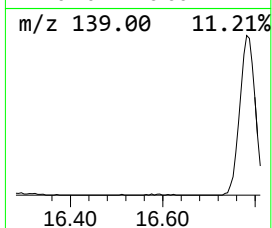
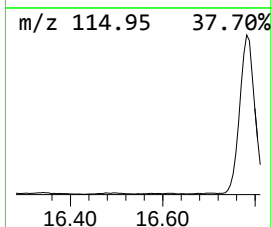
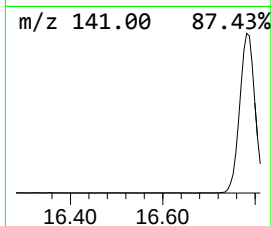
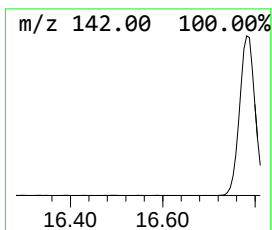
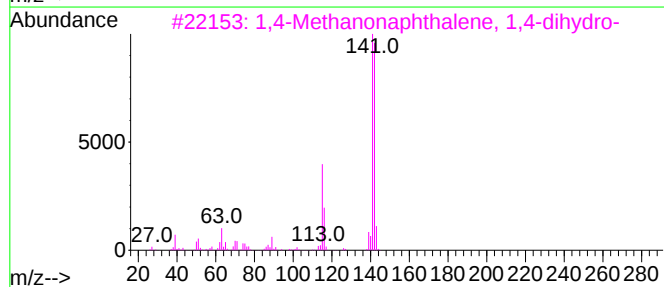
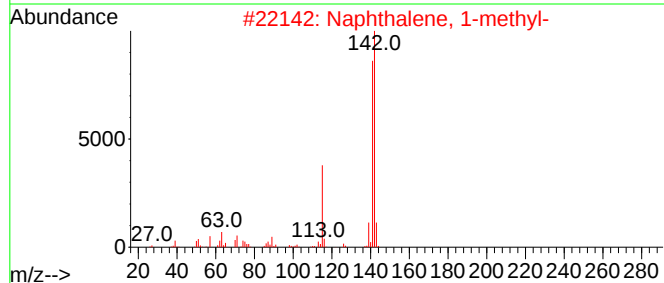
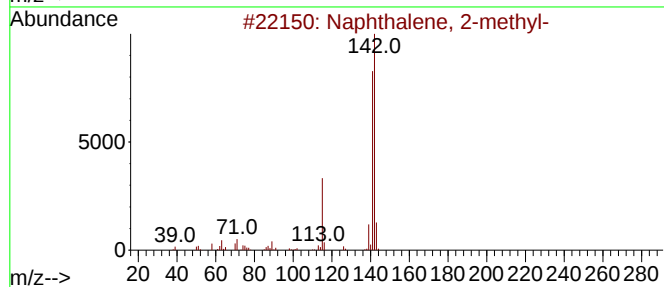
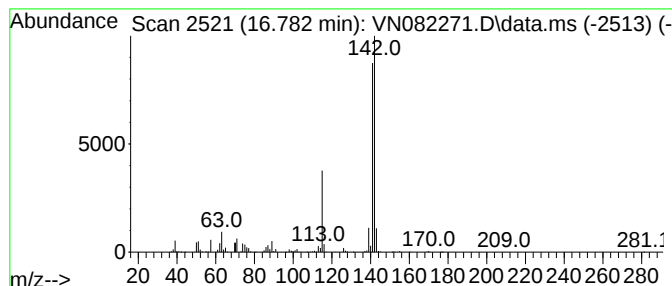
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Quant Title : SW846 8260

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	76.37 ug/l	1905320	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	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052124\
Data File : VN082271.D
Acq On : 22 May 2024 04:21
Operator : JC\MD
Sample : P2494-11 40X
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 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...	13.100	5.9	ug/l	148042	4	13.794	1247440	50.0
unknown13.335	13.335	11.7	ug/l	292731	4	13.794	1247440	50.0
Naphthalene, 2,...	13.670	32.0	ug/l	799130	4	13.794	1247440	50.0
Naphthalene, 2,...	14.012	36.7	ug/l	915934	4	13.794	1247440	50.0
Naphthalene, 1,...	14.106	17.6	ug/l	438377	4	13.794	1247440	50.0
Indene	14.176	14.2	ug/l	355370	4	13.794	1247440	50.0
Tetradecane	14.959	8.0	ug/l	199796	4	13.794	1247440	50.0
Benzene, 1,2,3,...	15.035	15.3	ug/l	381297	4	13.794	1247440	50.0
Naphthalene, 2-...	16.782	76.4	ug/l	1905320	4	13.794	1247440	50.0