

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
 Data File : VN074268.D
 Acq On : 02 Sep 2022 02:30
 Operator : JC\MD
 Sample : N4354-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-25

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\82N083022W.M
 Title : SW846 8260

Signal : TIC: VN074268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	51	63	79	rBV	419625	1984347	25.65%	2.142%
2	2.710	136	140	145	rVB2	54900	89583	1.16%	0.097%
3	3.087	199	204	217	rVB4	65421	164127	2.12%	0.177%
4	3.940	340	349	361	rVB4	29919	81339	1.05%	0.088%
5	4.881	500	509	522	rVB2	28795	89710	1.16%	0.097%
6	5.275	568	576	591	rBV3	39265	135041	1.75%	0.146%
7	5.534	605	620	635	rBV	683577	2419820	31.28%	2.611%
8	7.069	871	881	889	rBV3	34548	99868	1.29%	0.108%
9	7.951	1021	1031	1036	rBV	180062	435688	5.63%	0.470%
10	8.016	1036	1042	1055	rVB2	327866	754248	9.75%	0.814%
11	8.392	1093	1106	1123	rBV	2201237	5442519	70.35%	5.874%
12	8.904	1185	1193	1205	rBV	490299	997794	12.90%	1.077%
13	10.380	1436	1444	1449	rBV	738070	1365904	17.66%	1.474%
14	10.445	1449	1455	1469	rVV	3602772	6711808	86.75%	7.243%
15	10.580	1469	1478	1485	rVB2	157701	283375	3.66%	0.306%
16	10.657	1485	1491	1497	rBV	166608	292045	3.77%	0.315%
17	11.686	1657	1666	1675	rBV	733827	1327115	17.15%	1.432%
18	11.786	1675	1683	1692	rVV	4281113	7233627	93.50%	7.807%
19	11.898	1692	1702	1714	rVB	3753013	7182455	92.84%	7.751%
20	12.222	1749	1757	1768	rVB	4635117	7736515	100.00%	8.349%
21	12.516	1801	1807	1814	rBV	208391	338169	4.37%	0.365%
22	12.669	1825	1833	1844	rBV	640165	1098722	14.20%	1.186%
23	12.857	1860	1865	1871	rBV	454277	706866	9.14%	0.763%
24	12.921	1871	1876	1879	rVV	538576	901911	11.66%	0.973%
25	12.957	1879	1882	1885	rVV	573644	832594	10.76%	0.899%
26	12.998	1885	1889	1896	rVB	602003	928075	12.00%	1.002%
27	13.157	1909	1916	1925	rVB	1385468	2249794	29.08%	2.428%
28	13.304	1932	1941	1954	rBV	4474297	7164306	92.60%	7.732%
29	13.498	1968	1974	1979	rBV3	58304	108743	1.41%	0.117%
30	13.616	1987	1994	1995	rBV	865731	1335922	17.27%	1.442%
31	13.645	1995	1999	2007	rVB	1711936	2860959	36.98%	3.088%
32	13.816	2015	2028	2044	rBV	3474841	6444967	83.31%	6.955%
33	13.939	2044	2049	2053	rBV3	49443	79566	1.03%	0.086%
34	13.998	2053	2059	2066	rVV2	313931	592599	7.66%	0.640%
35	14.068	2066	2071	2074	rVV	309062	517546	6.69%	0.559%
36	14.098	2074	2076	2081	rVV	240714	315704	4.08%	0.341%

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37	14.157	2081	2086	2091	rVV	599861	930063	12.02%	1.004%
38	14.216	2091	2096	2100	rVV2	173214	304413	3.93%	0.329%
39	14.263	2100	2104	2112	rVB2	694878	1166034	15.07%	1.258%
40	14.398	2120	2127	2133	rBV	159482	256567	3.32%	0.277%
41	14.474	2133	2140	2144	rBV	459801	779298	10.07%	0.841%
42	14.516	2144	2147	2152	rVB	547629	781190	10.10%	0.843%
43	14.745	2181	2186	2191	rVV	693855	1124106	14.53%	1.213%
44	14.868	2198	2207	2213	rVV2	1566571	3029133	39.15%	3.269%
45	14.933	2213	2218	2225	rVV3	139618	261719	3.38%	0.282%
46	15.015	2226	2232	2240	rVV	362594	650745	8.41%	0.702%
47	15.127	2240	2251	2255	rVV4	210450	546437	7.06%	0.590%
48	15.163	2255	2257	2263	rVV3	126210	214141	2.77%	0.231%
49	15.239	2263	2270	2278	rVB4	214349	518986	6.71%	0.560%
50	15.433	2290	2303	2311	rBV	4032139	7347710	94.97%	7.930%
51	15.533	2314	2320	2327	rVV	382228	787465	10.18%	0.850%
52	15.598	2327	2331	2340	rVB2	76084	144156	1.86%	0.156%
53	15.733	2346	2354	2360	rBV2	118784	236911	3.06%	0.256%
54	15.904	2373	2383	2388	rBV3	89636	255270	3.30%	0.275%
55	16.110	2412	2418	2424	rVB3	56536	122863	1.59%	0.133%
56	16.257	2433	2443	2450	rBV7	42403	109623	1.42%	0.118%
57	16.462	2466	2478	2483	rBV2	62472	147541	1.91%	0.159%
58	16.527	2483	2489	2504	rVB4	94721	267310	3.46%	0.288%
59	16.733	2516	2524	2533	rBV	602297	1376233	17.79%	1.485%

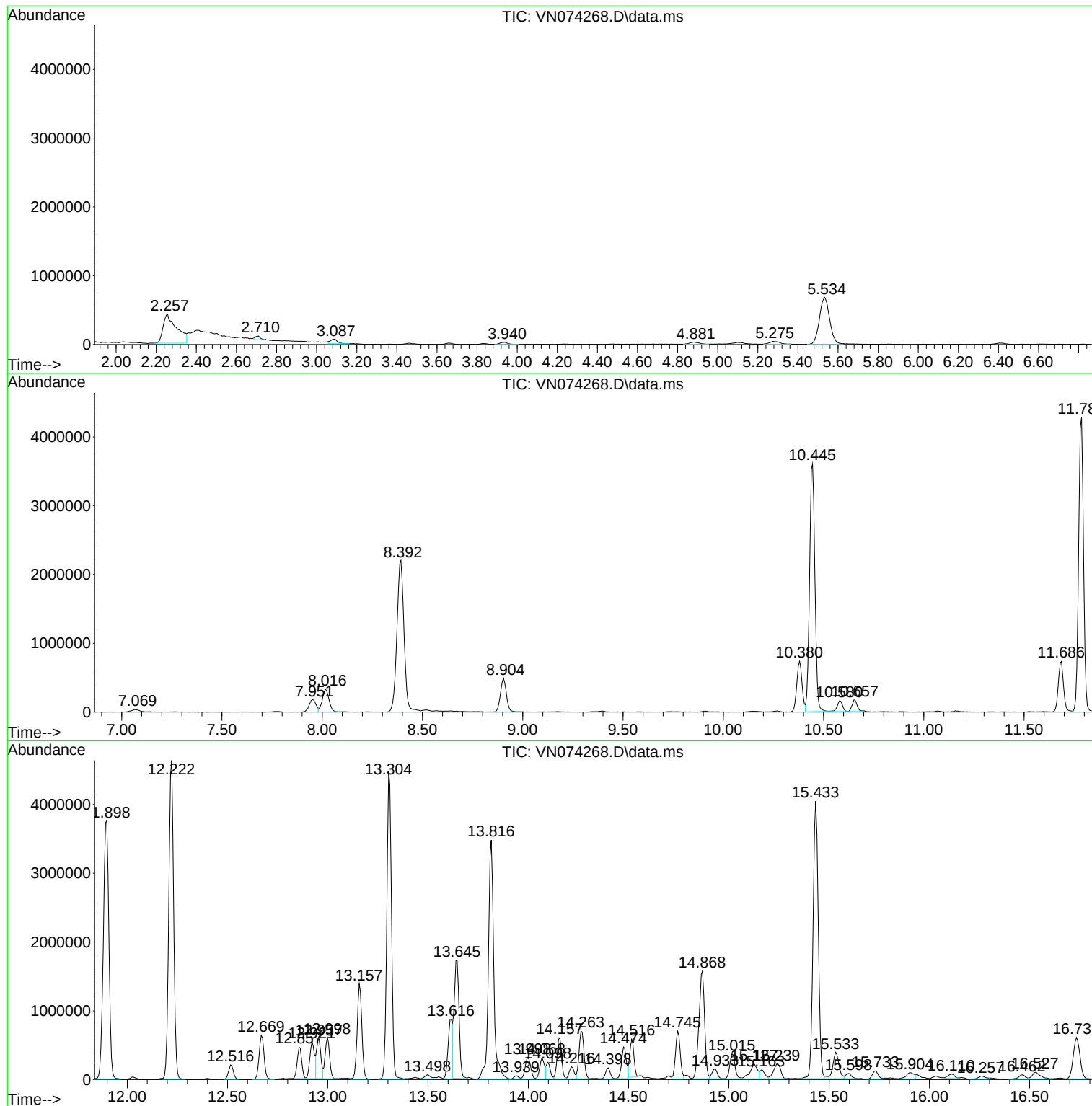
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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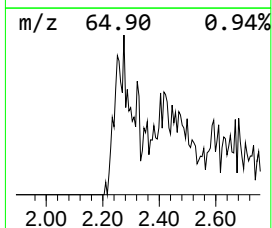
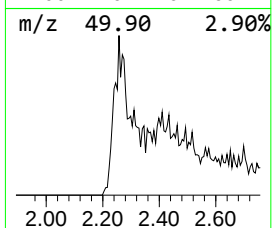
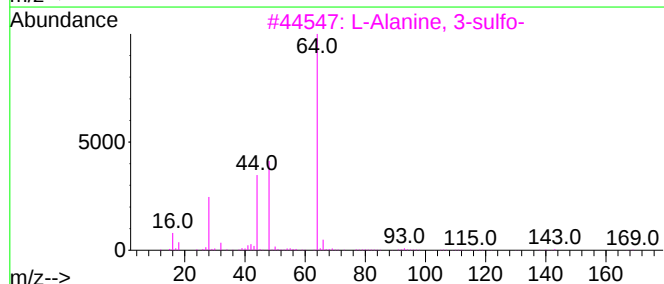
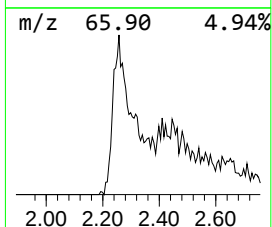
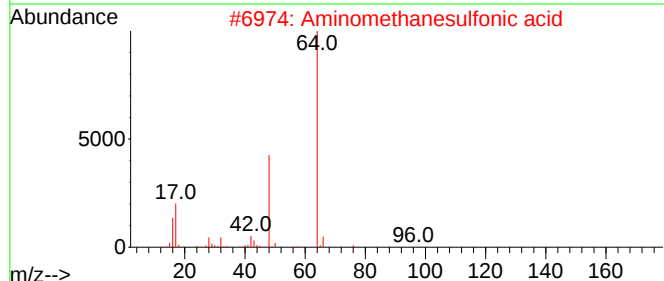
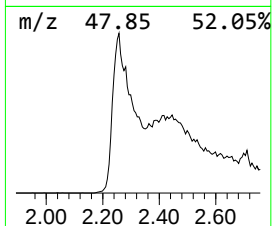
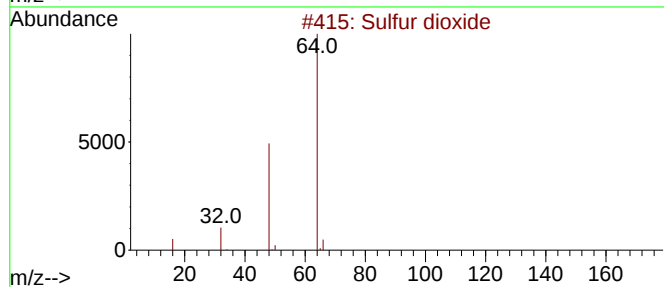
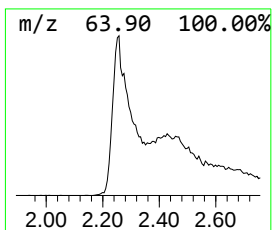
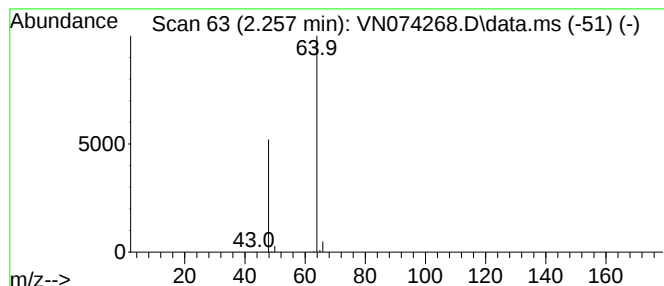
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	131.54 ug/l	1984350	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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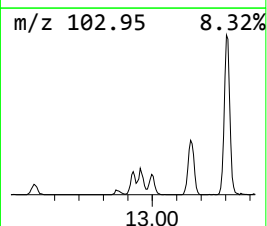
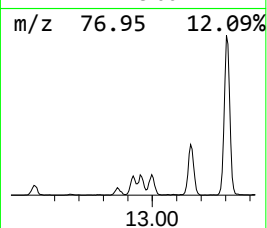
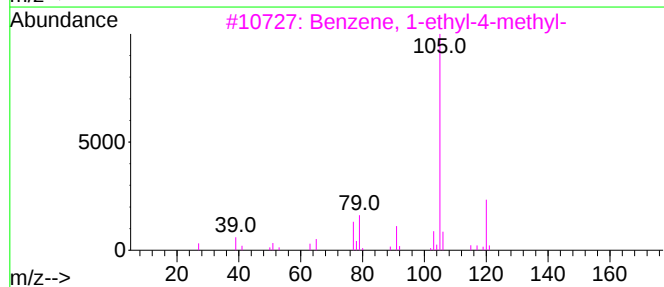
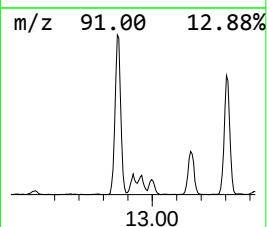
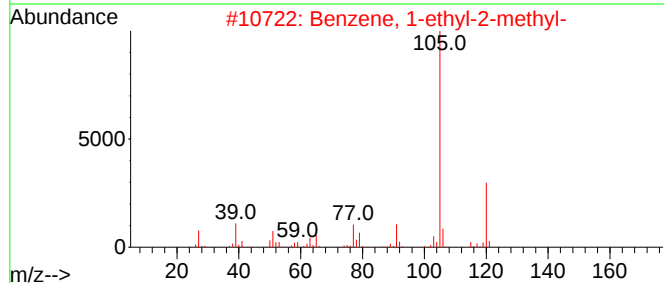
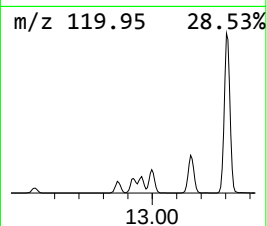
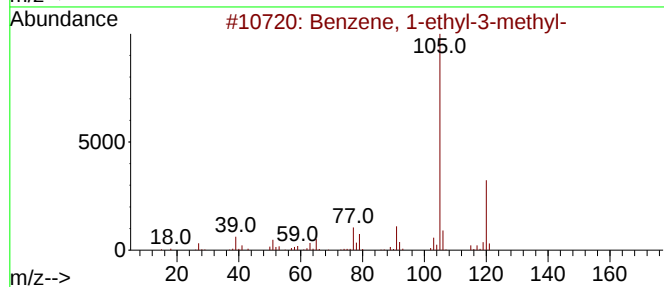
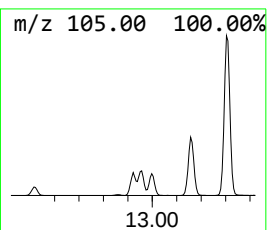
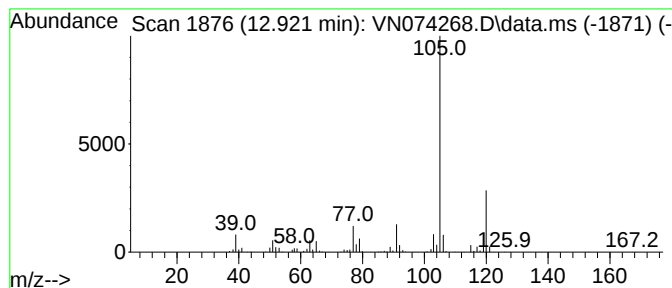
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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.
12.922	33.76 ug/l	901911	1,4-Dichlorobenzene-d4	13.610

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	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



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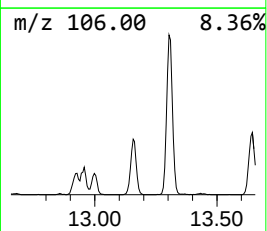
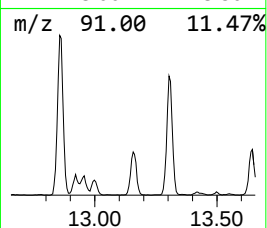
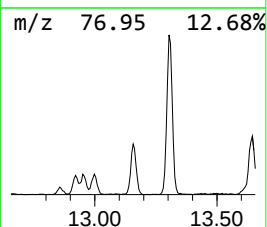
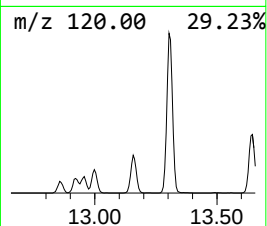
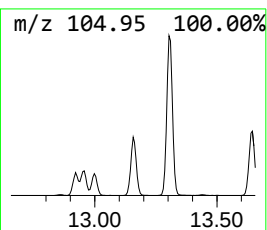
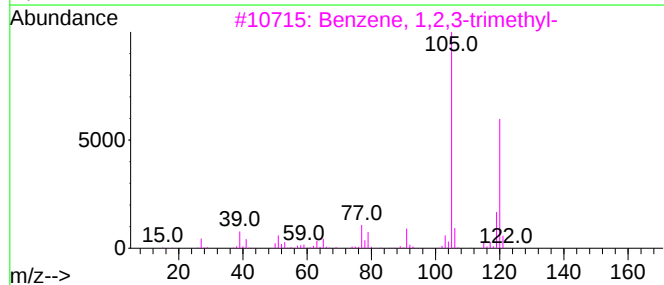
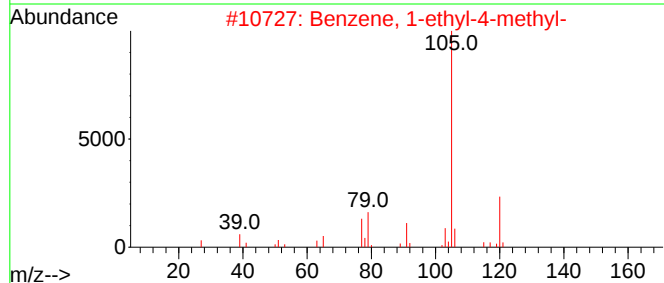
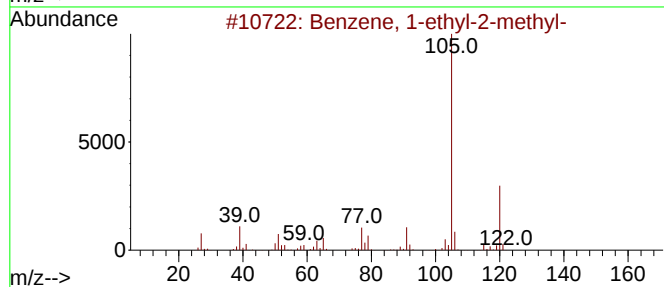
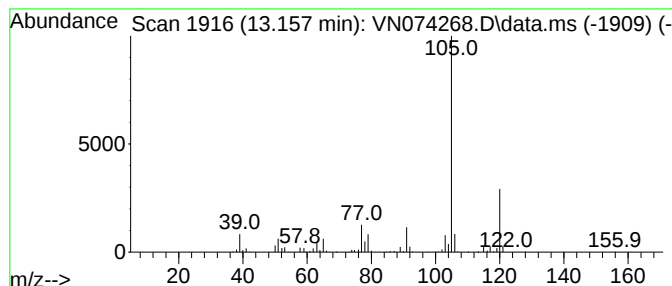
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	84.20 ug/l	2249790	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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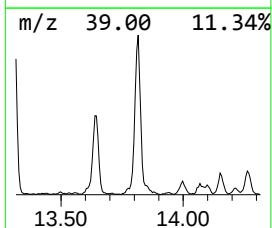
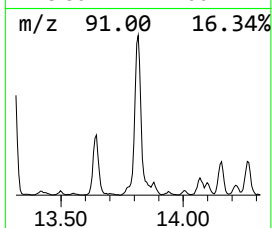
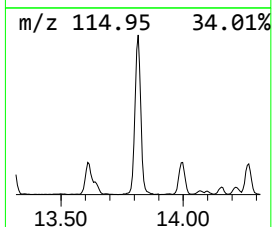
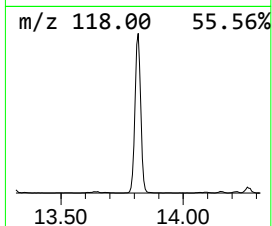
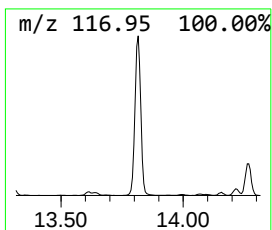
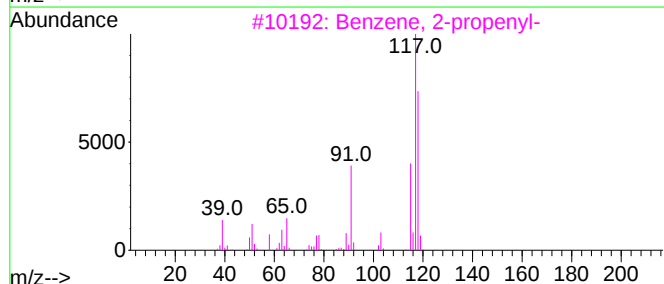
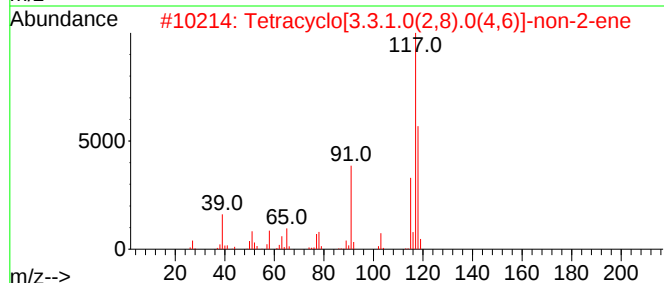
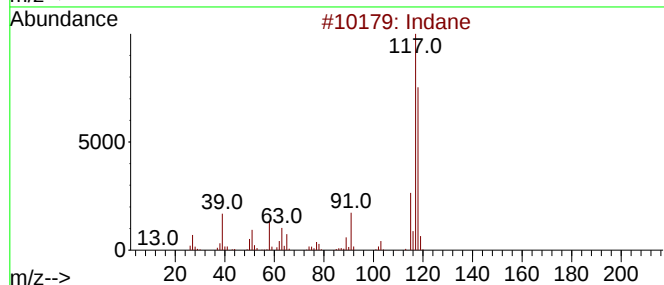
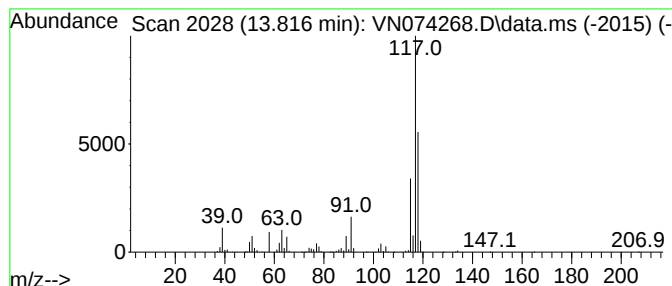
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	241.22 ug/l	6444970	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	96
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	83
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72



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MW-25

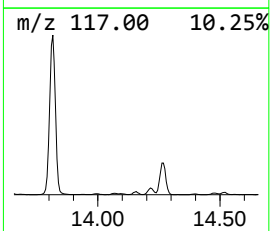
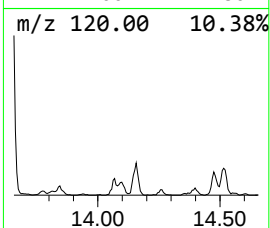
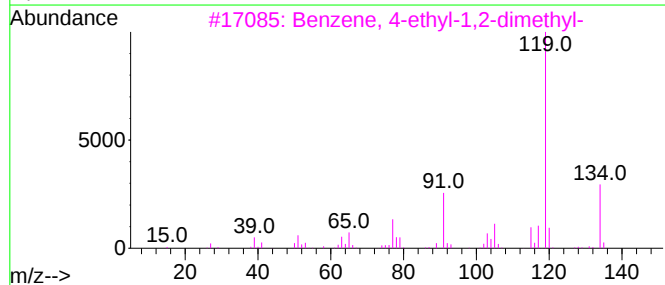
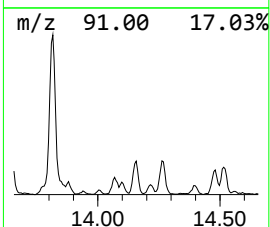
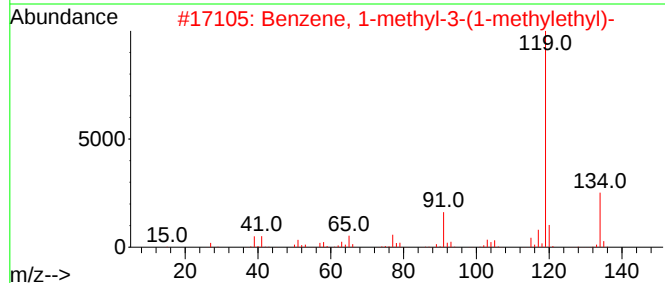
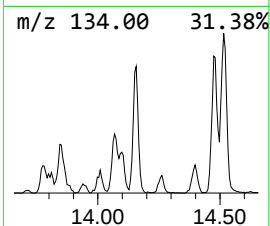
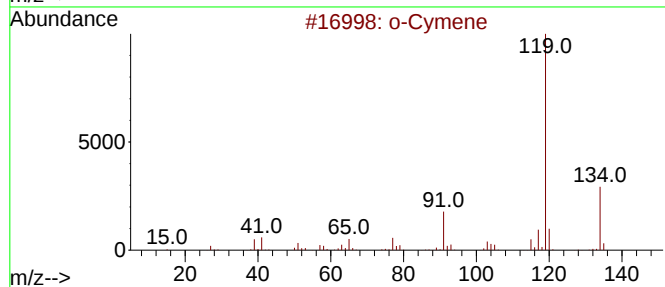
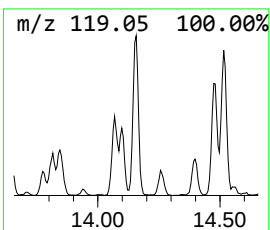
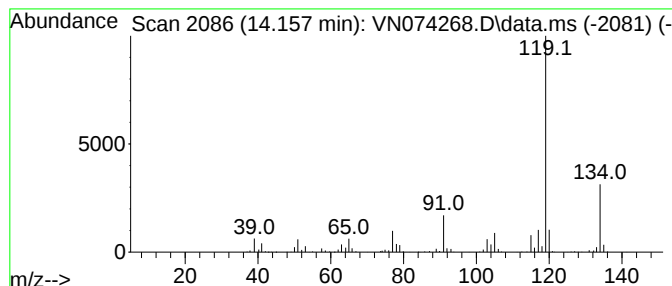
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	34.81 ug/l	930063	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

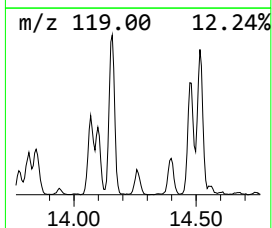
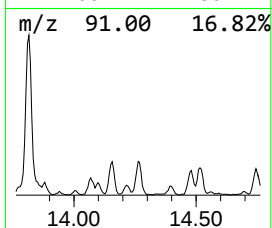
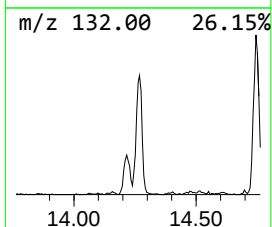
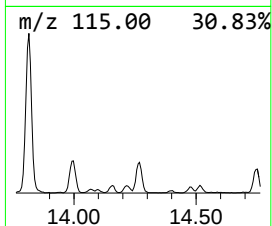
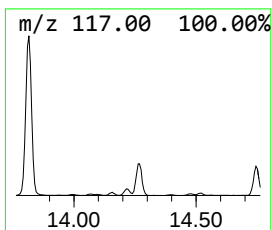
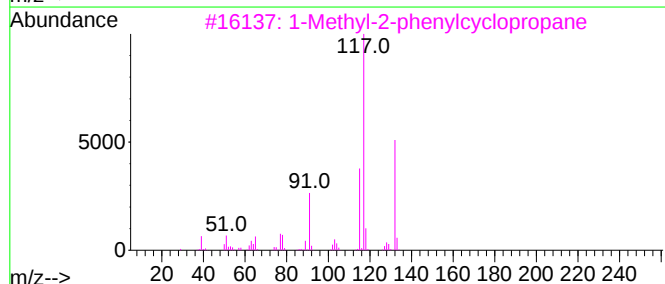
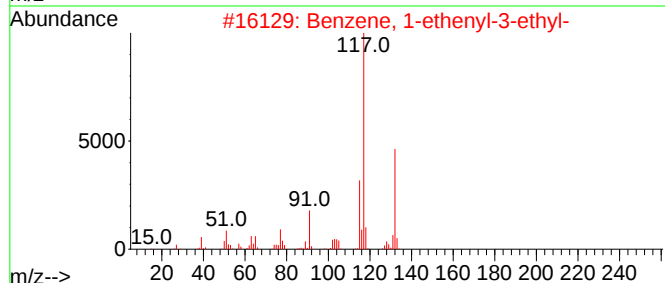
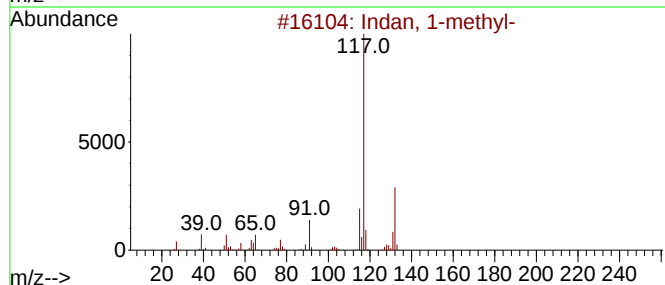
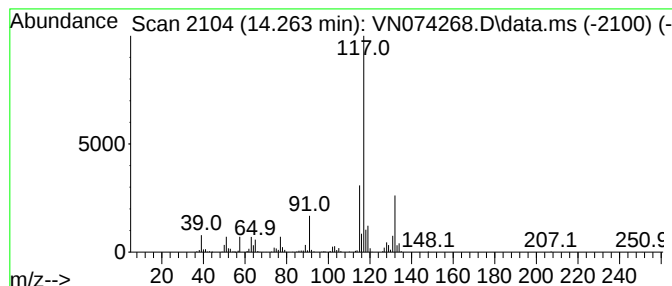
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	43.64 ug/l	1166030	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

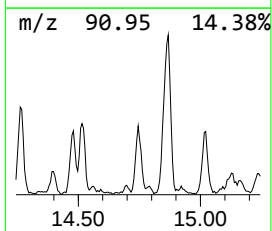
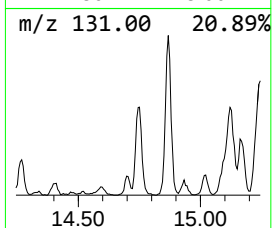
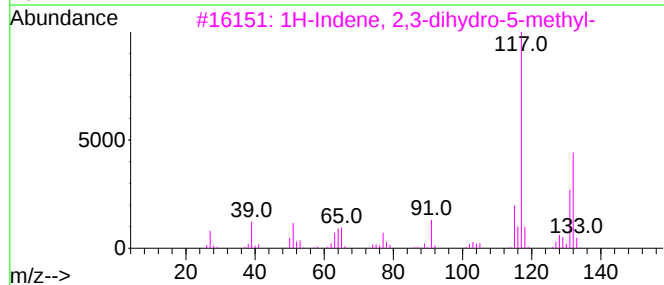
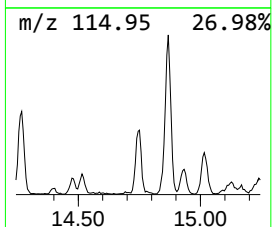
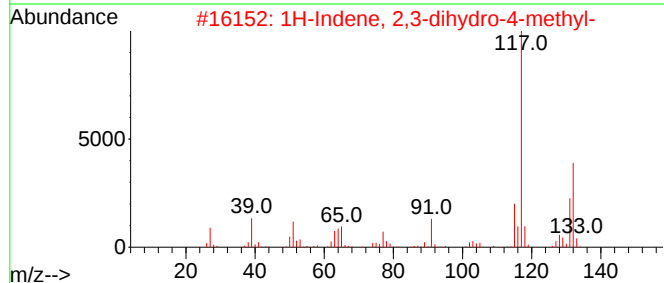
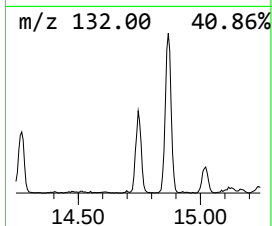
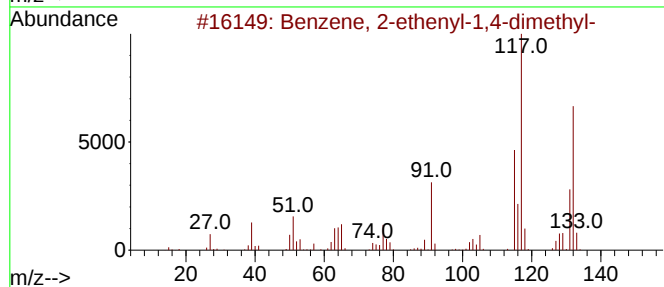
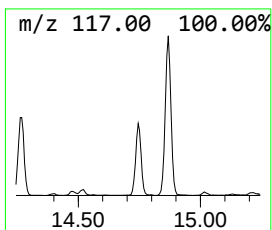
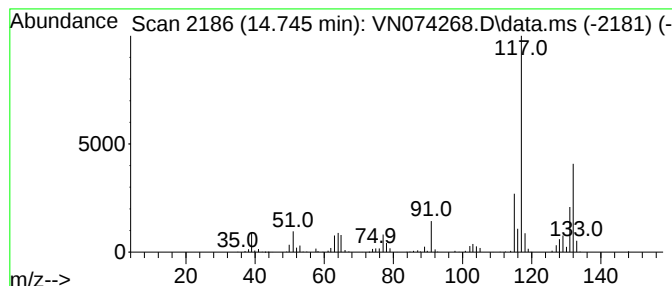
Instrument :
MSVOA_N
ClientSampleId :
MW-25

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.745	42.07 ug/l	1124110	1,4-Dichlorobenzene-d4			13.610
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-4-methyl-		132	C10H12	000824-22-6	96
3	1H-Indene, 2,3-dihydro-5-methyl-		132	C10H12	000874-35-1	96
4	Benzene, 1-ethenyl-4-ethyl-		132	C10H12	003454-07-7	94
5	3-Phenylbut-1-ene		132	C10H12	000934-10-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

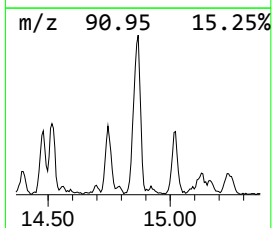
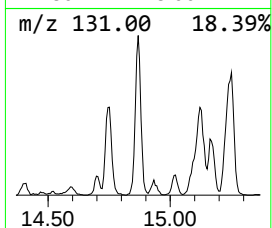
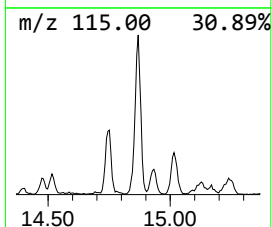
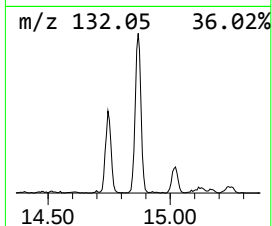
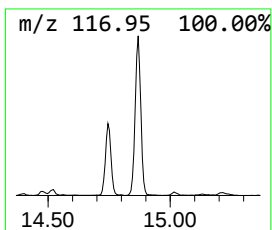
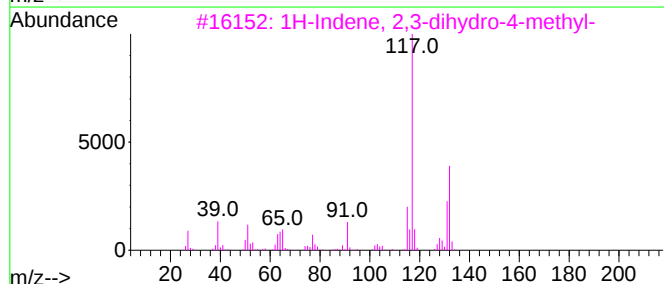
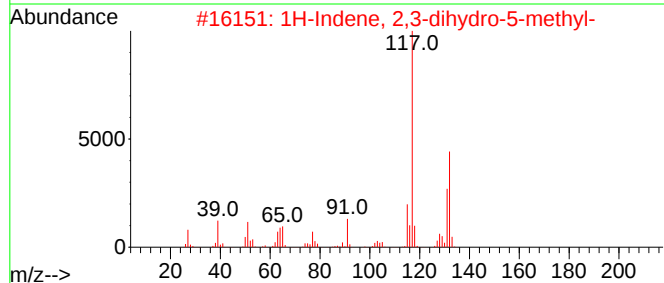
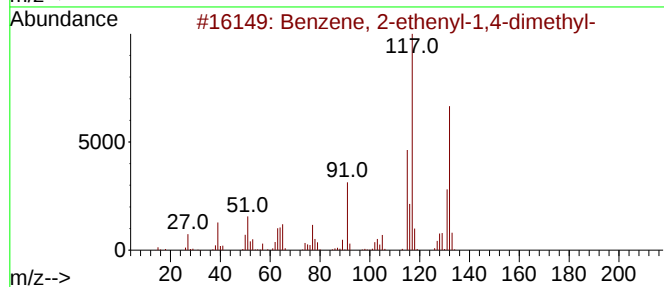
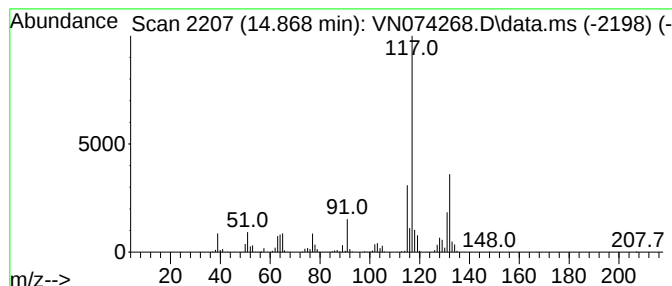
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	113.37 ug/l	3029130	1,4-Dichlorobenzene-d4	13.610

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

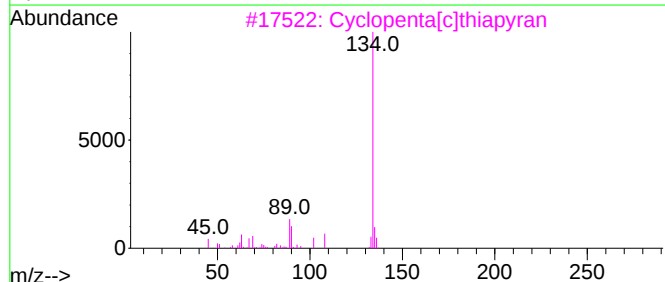
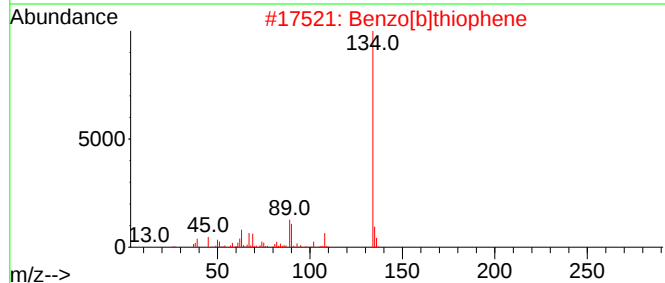
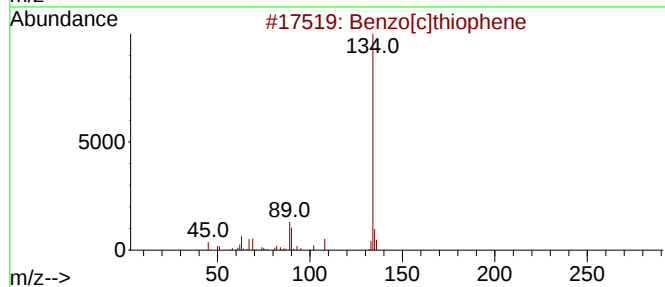
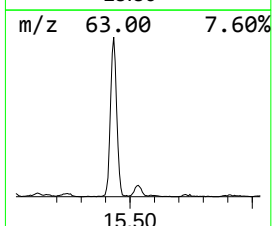
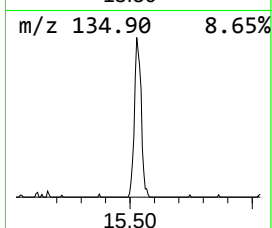
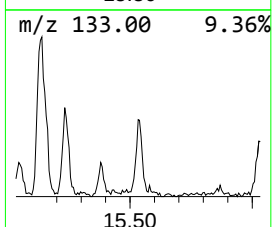
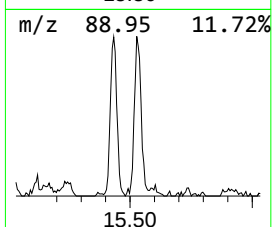
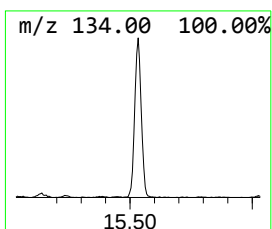
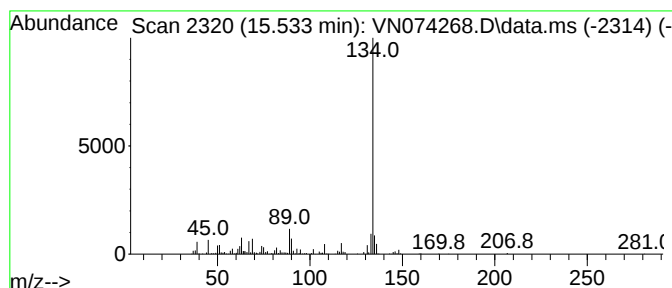
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Quant Title : SW846 8260

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

Peak Number 9 Benzo[c]thiophene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.533	29.47 ug/l	787465	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	87
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	87
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	87
4			3-(2'-Methyl benzenaminomethyl),...	324	C18H16N2O2S	312926-67-3	56
5			[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

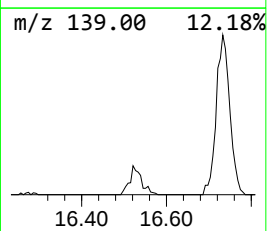
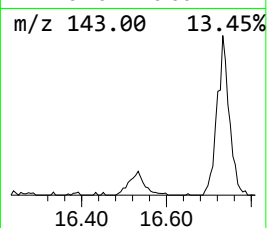
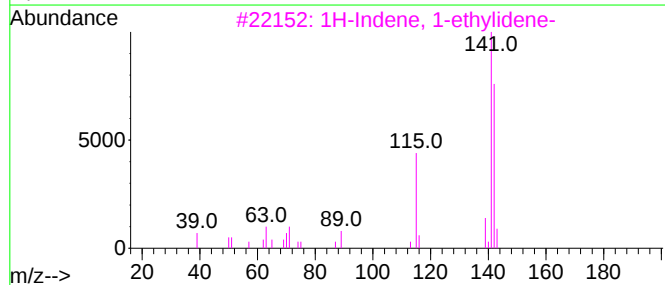
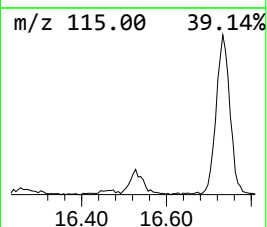
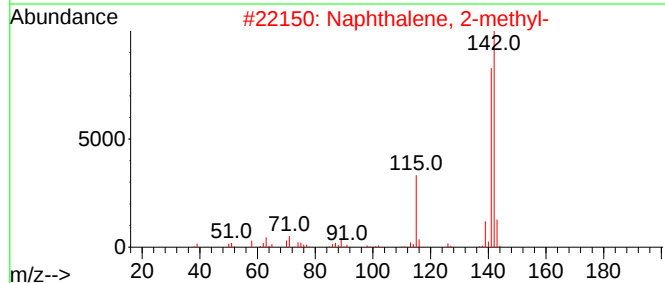
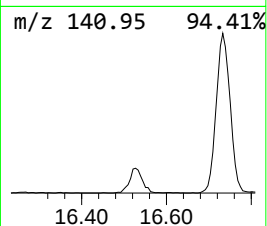
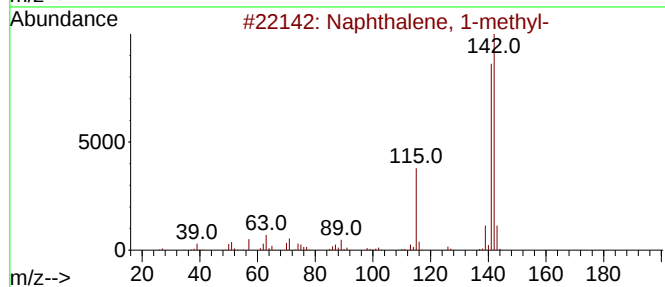
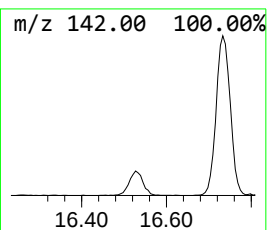
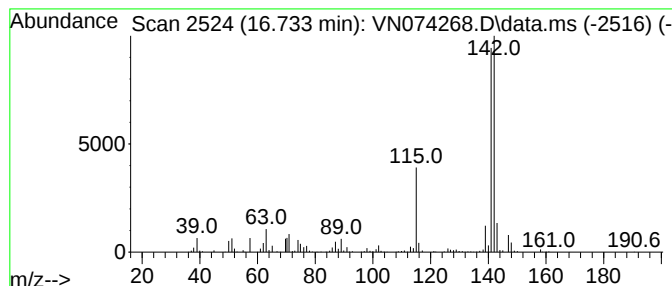
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 1-ethylidene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.733	51.51 ug/l	1376230	1,4-Dichlorobenzene-d4	13.610

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
3		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	94
4		Benzocycloheptatriene	142	C11H10	000264-09-5	93
5		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074268.D
Acq On : 02 Sep 2022 02:30
Operator : JC\MD
Sample : N4354-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-25

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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...	12.922	33.8	ug/l	901911	4	13.610	1335920	50.0
Benzene, 1-ethy...	13.157	84.2	ug/l	2249790	4	13.610	1335920	50.0
Indane	13.816	241.2	ug/l	6444970	4	13.610	1335920	50.0
o-Cymene	14.157	34.8	ug/l	930063	4	13.610	1335920	50.0
Indan, 1-methyl-	14.263	43.6	ug/l	1166030	4	13.610	1335920	50.0
Benzene, 2-ethe...	14.745	42.1	ug/l	1124110	4	13.610	1335920	50.0
1H-Indene, 2,3-...	14.868	113.4	ug/l	3029130	4	13.610	1335920	50.0
Benzo[c]thiophene	15.533	29.5	ug/l	787465	4	13.610	1335920	50.0
1H-Indene, 1-et...	16.733	51.5	ug/l	1376230	4	13.610	1335920	50.0