

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
 Data File : VN071754.D
 Acq On : 01 Apr 2022 15:43
 Operator : JC\MD
 Sample : N2090-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-48

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\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071754.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	37	43	45	rBV3	29803	51481	1.48%	0.169%
2	3.828	303	313	327	rBV3	22208	56585	1.63%	0.186%
3	5.192	532	545	559	rVB3	22181	83041	2.39%	0.273%
4	5.357	562	573	593	rVV	61549	223638	6.43%	0.736%
5	5.610	605	616	637	rVB2	102006	371975	10.69%	1.224%
6	6.492	752	766	779	rBV3	40680	140960	4.05%	0.464%
7	7.145	862	877	885	rBV4	41022	133624	3.84%	0.440%
8	7.216	885	889	898	rVB4	17052	42561	1.22%	0.140%
9	7.845	986	996	1004	rVB2	30314	74449	2.14%	0.245%
10	8.022	1015	1026	1031	rBV	410401	1010113	29.03%	3.323%
11	8.080	1031	1036	1048	rVB	796877	1848792	53.14%	6.082%
12	8.433	1086	1096	1106	rBV	433236	992939	28.54%	3.267%
13	8.592	1116	1123	1128	rBV3	22088	54361	1.56%	0.179%
14	8.698	1136	1141	1150	rVB5	15505	45962	1.32%	0.151%
15	8.963	1176	1186	1201	rBV	1169183	2477405	71.21%	8.150%
16	9.245	1229	1234	1241	rVB3	19723	38410	1.10%	0.126%
17	9.451	1265	1269	1278	rVB5	28913	65372	1.88%	0.215%
18	9.969	1350	1357	1362	rBV2	54905	104522	3.00%	0.344%
19	10.198	1389	1396	1410	rBV3	19054	48695	1.40%	0.160%
20	10.321	1410	1417	1422	rBV2	32911	62820	1.81%	0.207%
21	10.439	1429	1437	1457	rBV	1909337	3479252	100.00%	11.446%
22	10.639	1459	1471	1477	rBV	243477	429577	12.35%	1.413%
23	10.710	1477	1483	1490	rVB	255320	448086	12.88%	1.474%
24	10.857	1502	1508	1518	rVB2	23610	48497	1.39%	0.160%
25	11.739	1651	1658	1671	rBV	1785936	3163206	90.92%	10.407%
26	11.951	1687	1694	1703	rBV2	24775	53686	1.54%	0.177%
27	12.574	1793	1800	1807	rBV	361302	597173	17.16%	1.965%
28	12.727	1819	1826	1837	rBV	1349114	2326320	66.86%	7.653%
29	12.915	1851	1858	1867	rVB	397157	642785	18.47%	2.115%
30	13.215	1903	1909	1917	rVB	81653	137826	3.96%	0.453%
31	13.498	1948	1957	1963	rBV2	63559	139487	4.01%	0.459%
32	13.668	1979	1986	1997	rBV	1419029	2438088	70.08%	8.021%
33	13.768	1997	2003	2008	rVB	30937	48113	1.38%	0.158%
34	13.833	2008	2014	2016	rBV	168763	264544	7.60%	0.870%
35	13.874	2016	2021	2037	rVB	1698839	2883976	82.89%	9.488%
36	13.998	2037	2042	2048	rVB	80096	130030	3.74%	0.428%

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37	14.145	2059	2067	2072	rBV3	29812	56540	1.63%	0.186%
38	14.209	2072	2078	2084	rBV	348882	562674	16.17%	1.851%
39	14.274	2084	2089	2092	rVV	110993	173617	4.99%	0.571%
40	14.327	2092	2098	2105	rVV	574956	969074	27.85%	3.188%
41	14.462	2115	2121	2125	rBV	32372	48668	1.40%	0.160%
42	14.533	2125	2133	2143	rVB	396712	639692	18.39%	2.105%
43	14.756	2164	2171	2175	rBV4	31303	63856	1.84%	0.210%
44	14.804	2175	2179	2185	rVV2	98977	166008	4.77%	0.546%
45	14.927	2191	2200	2207	rBV3	633784	1312240	37.72%	4.317%
46	14.998	2207	2212	2217	rVB5	41409	77742	2.23%	0.256%
47	15.186	2237	2244	2249	rVV3	82899	179531	5.16%	0.591%
48	15.233	2249	2252	2256	rVV3	37989	66487	1.91%	0.219%
49	15.304	2256	2264	2272	rVB4	90861	237336	6.82%	0.781%
50	15.556	2302	2307	2312	rBV	47669	89369	2.57%	0.294%
51	15.639	2312	2321	2338	rVB4	66377	229193	6.59%	0.754%
52	15.798	2342	2348	2356	rBV2	38349	72747	2.09%	0.239%
53	15.980	2368	2379	2391	rBV3	30942	96556	2.78%	0.318%
54	16.103	2395	2400	2408	rBV	17818	40285	1.16%	0.133%
55	16.186	2408	2414	2421	rVB5	21052	48296	1.39%	0.159%
56	16.339	2432	2440	2449	rBV3	49482	107741	3.10%	0.354%

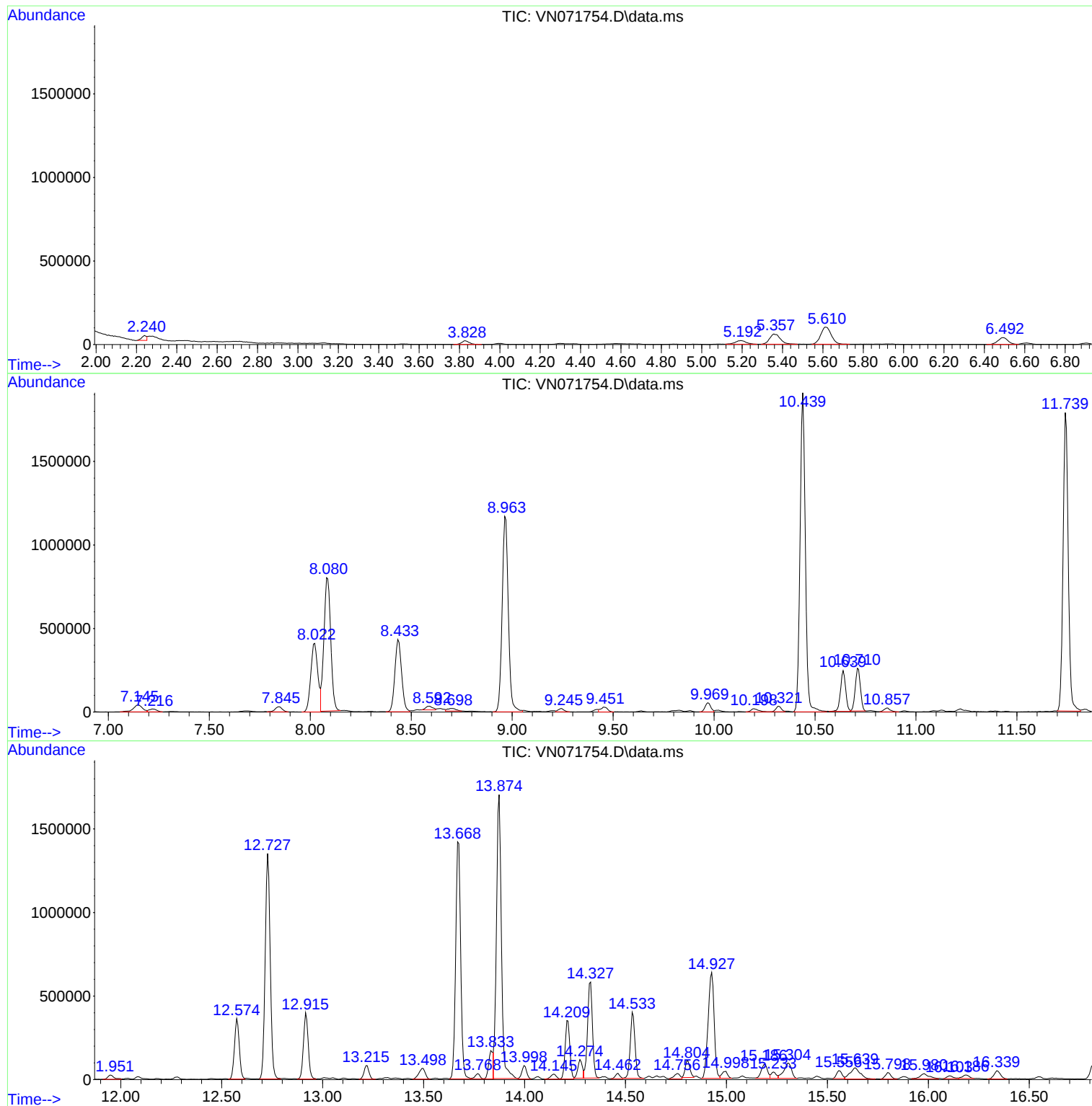
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Quant Title : SW846 8260

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



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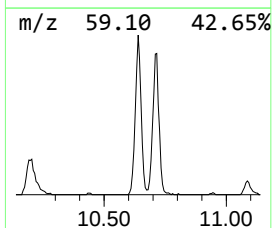
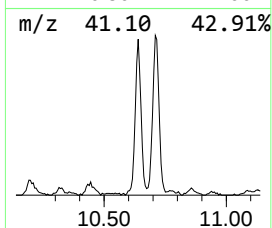
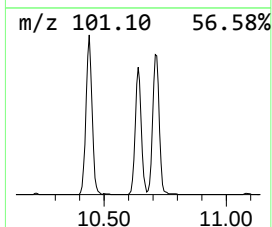
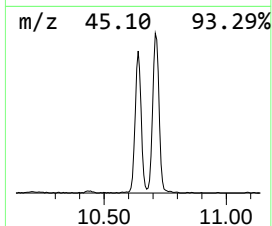
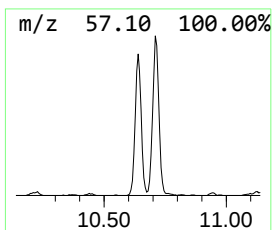
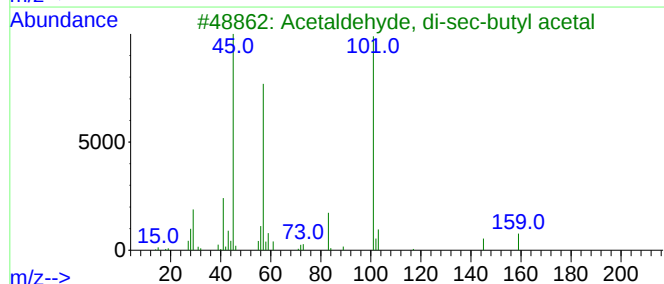
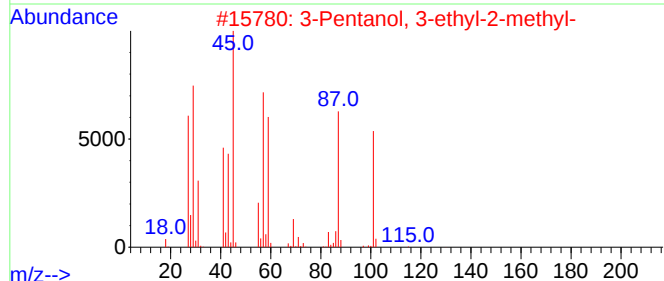
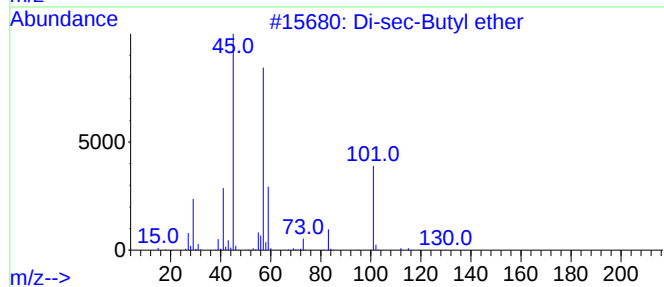
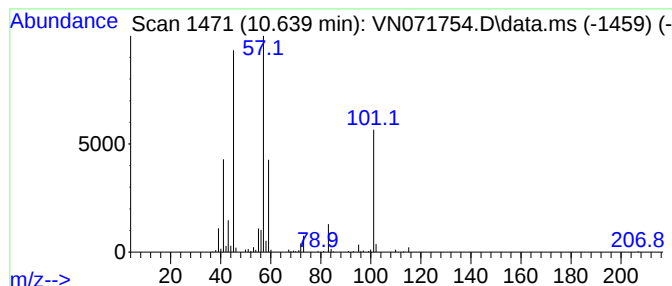
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Di-sec-Butyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	6.79 ug/l	429577	Chlorobenzene-d5	11.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
3			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	64
4			Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53
5			3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	50



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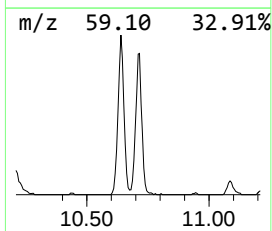
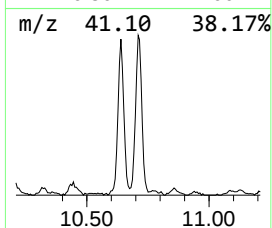
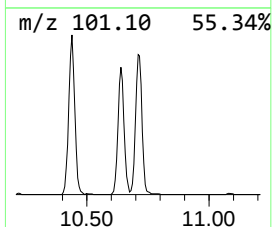
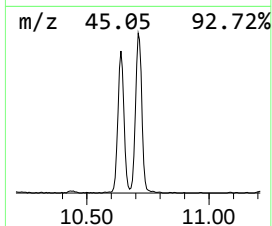
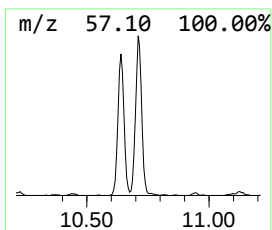
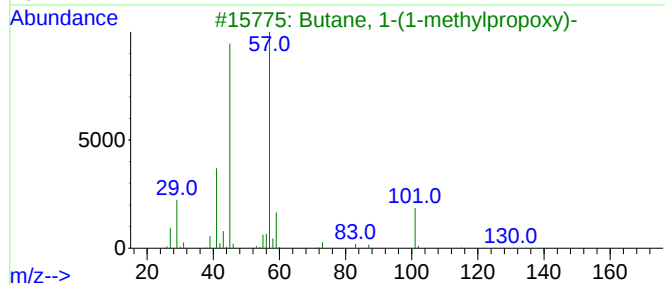
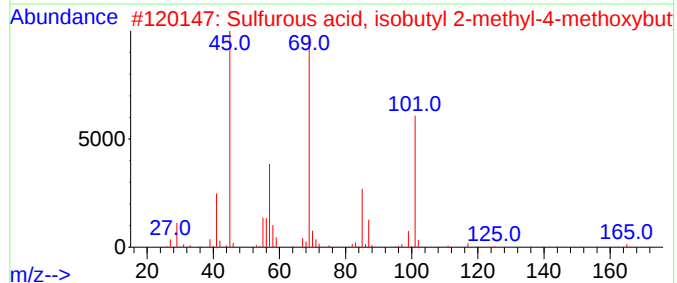
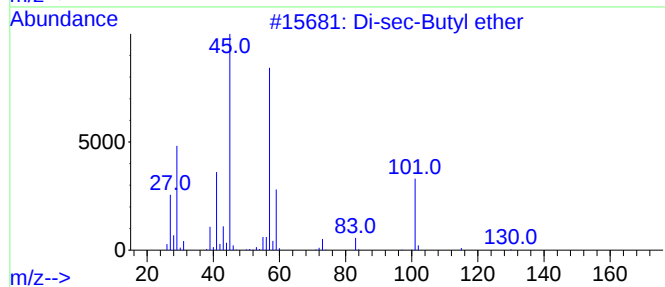
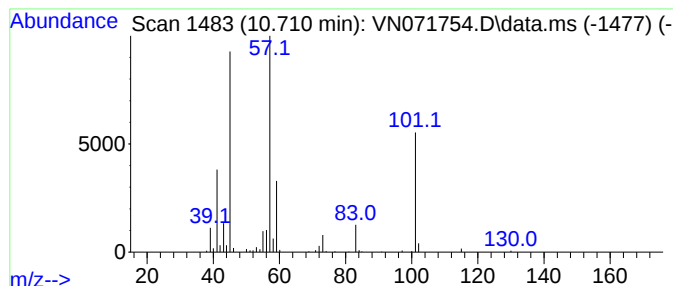
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfurous acid, isobutyl 2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	7.08 ug/l	448086	Chlorobenzene-d5	11.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	59
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			DL-Lactamide, butyl ether	145	C7H15N02	1000452-56-5	50
5			2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	39



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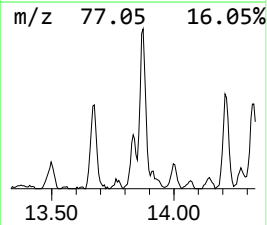
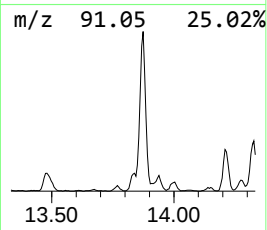
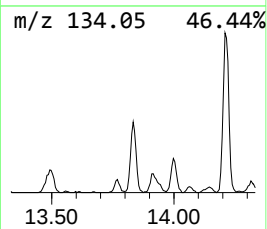
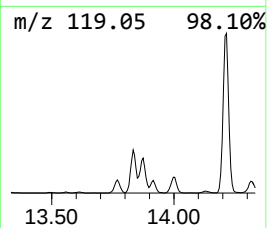
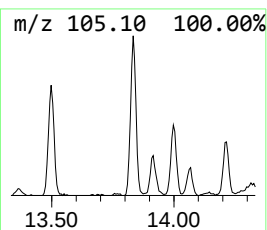
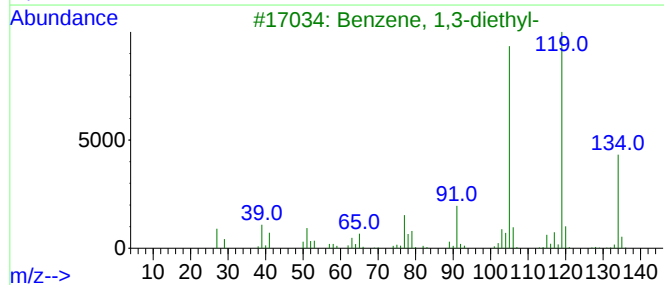
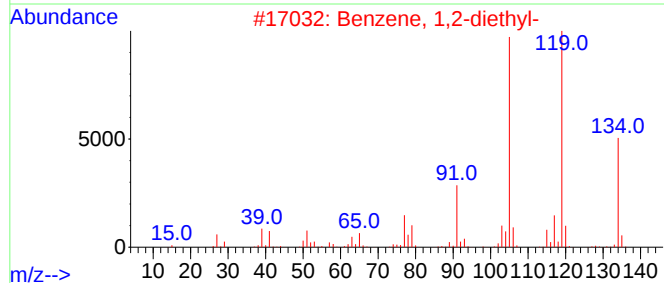
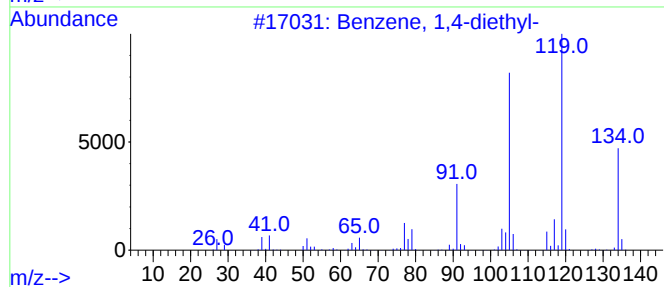
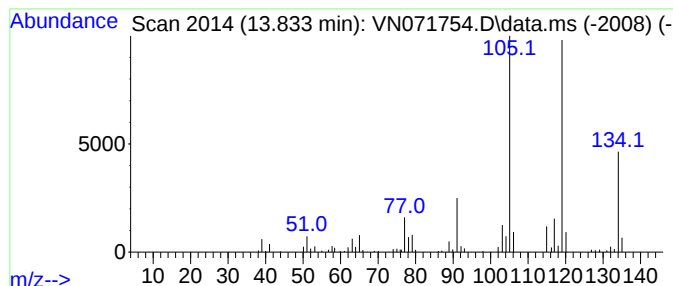
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,4-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	5.43 ug/l	264544	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5			2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	87



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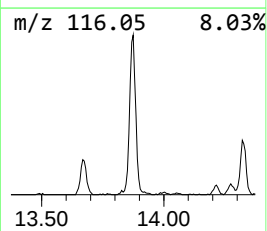
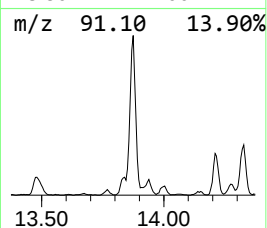
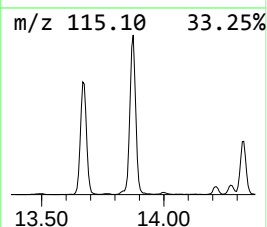
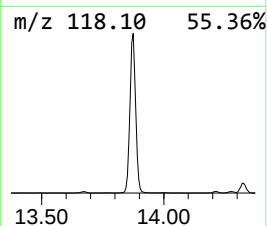
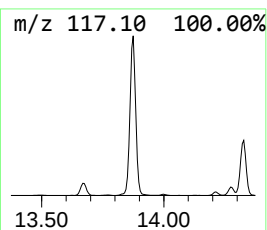
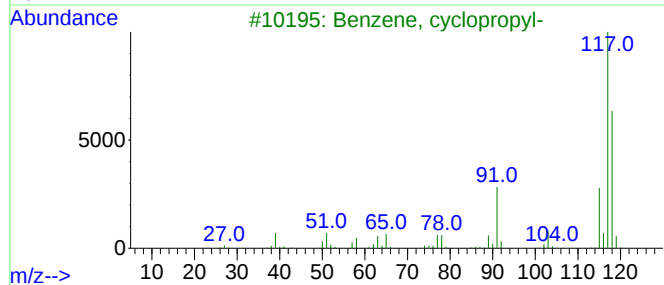
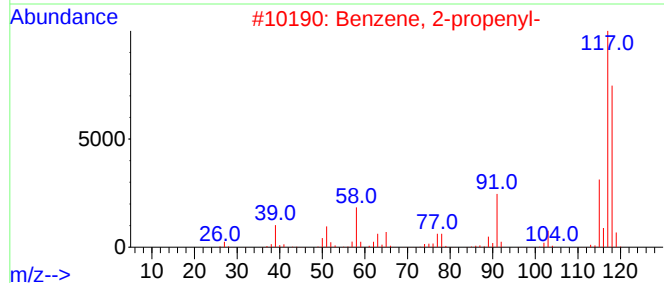
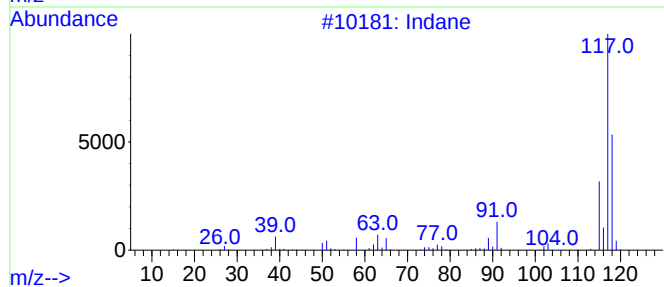
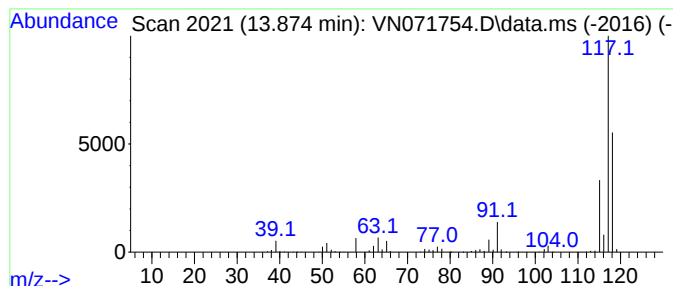
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	59.14 ug/l	2883980	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Delatacyclene	118	C9H10	007785-10-6	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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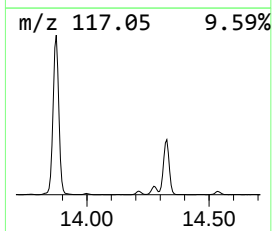
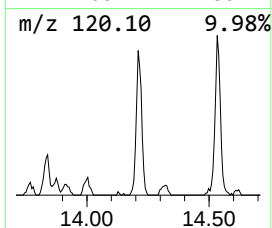
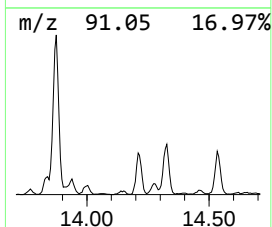
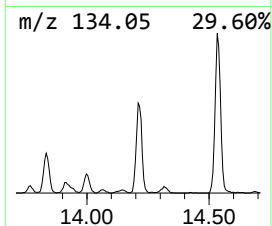
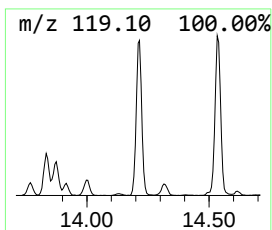
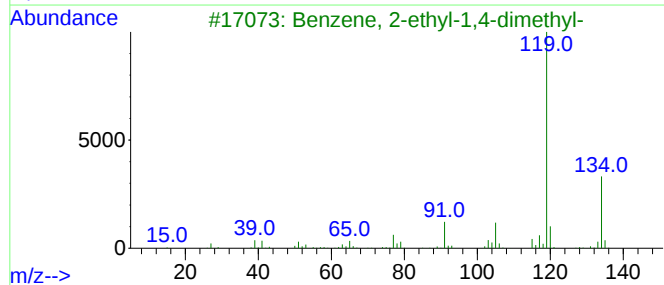
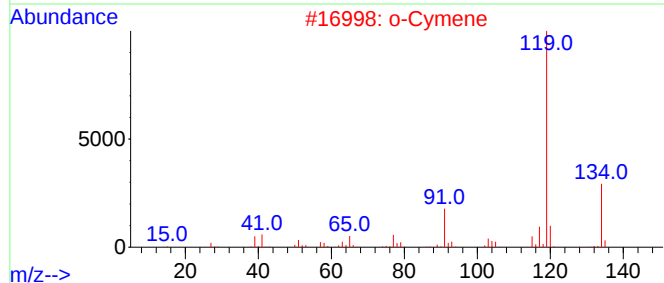
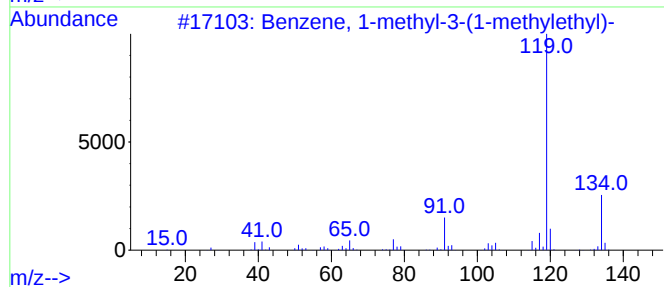
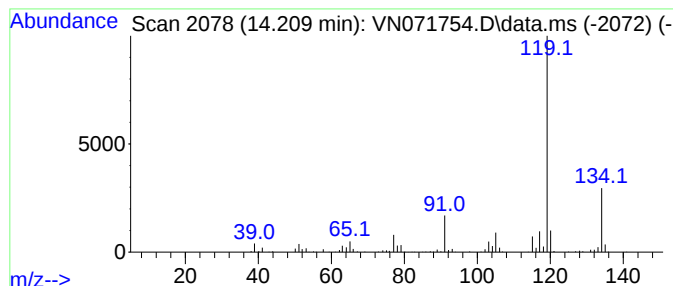
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methyl-3-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	11.54 ug/l	562674	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071754.D
Acq On : 01 Apr 2022 15:43
Operator : JC\MD
Sample : N2090-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

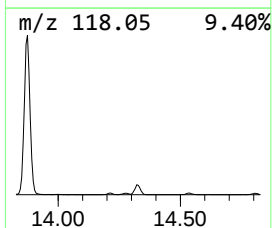
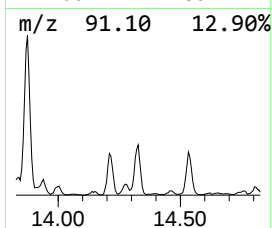
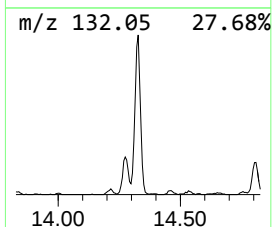
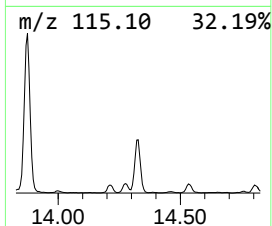
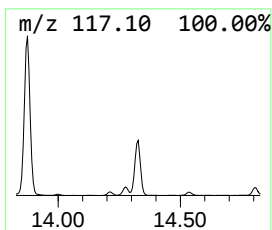
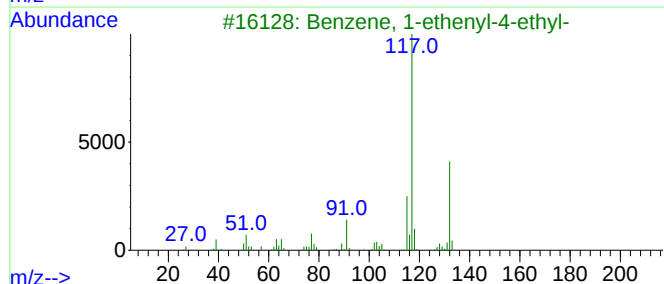
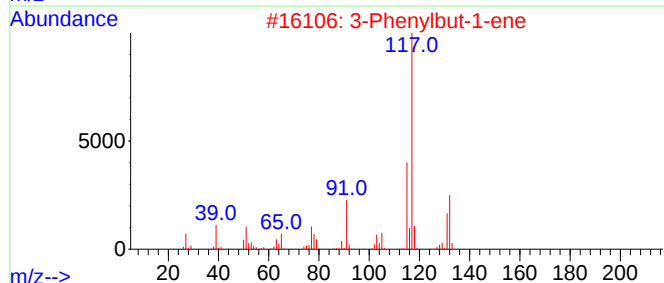
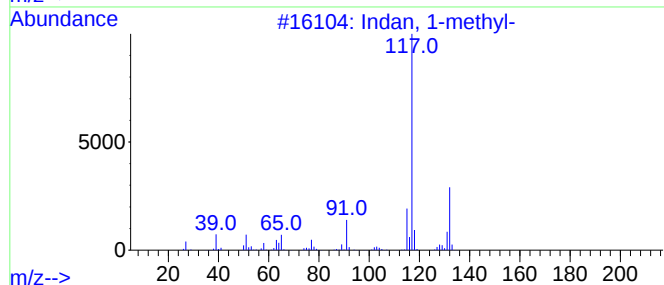
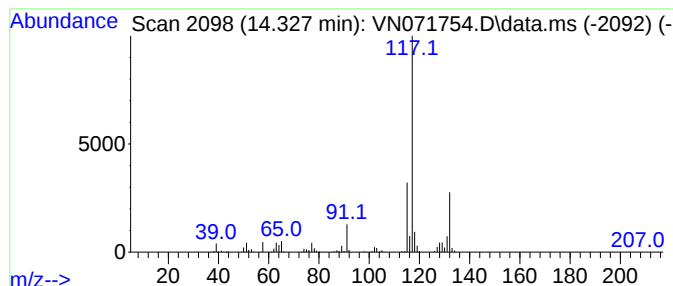
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	19.87 ug/l	969074	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	90
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	80
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	78
4			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	78
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071754.D
Acq On : 01 Apr 2022 15:43
Operator : JC\MD
Sample : N2090-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

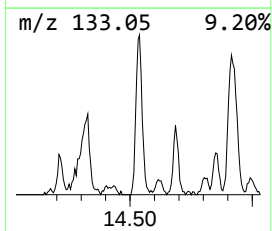
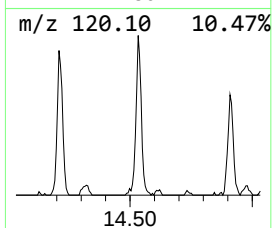
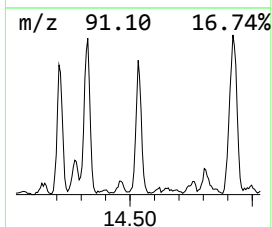
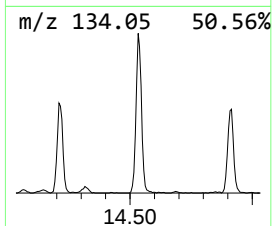
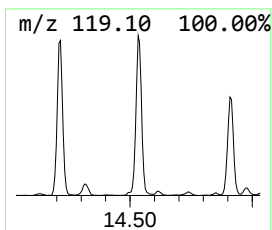
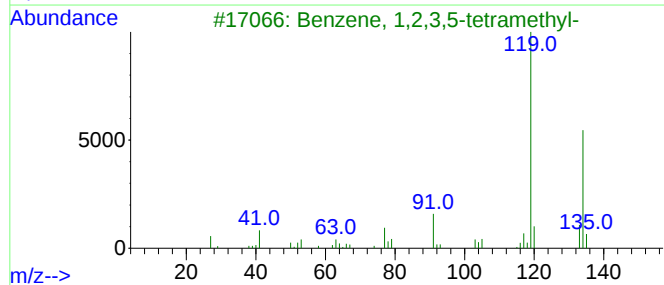
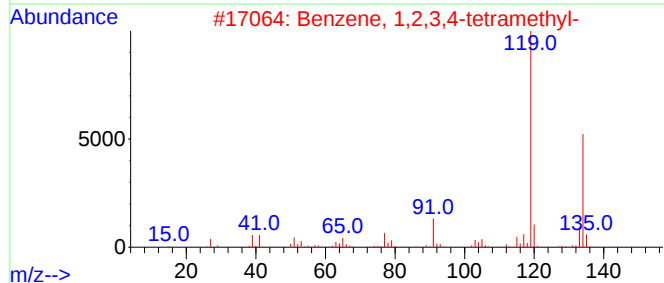
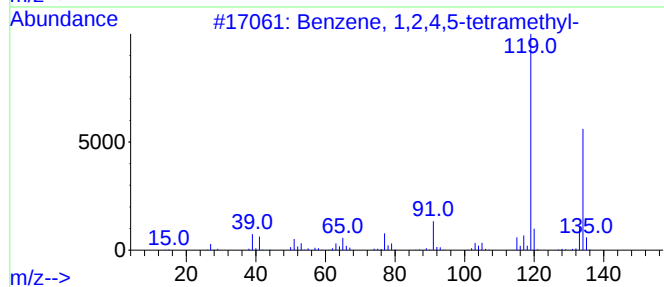
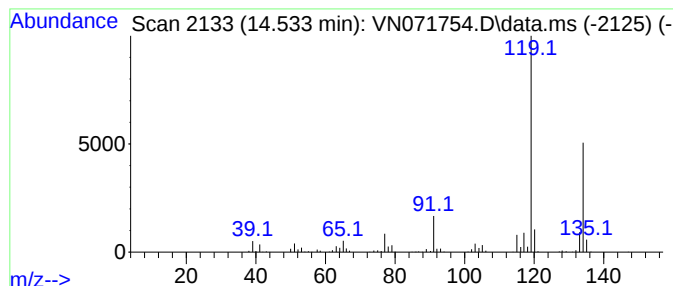
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	13.12 ug/l	639692	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071754.D
Acq On : 01 Apr 2022 15:43
Operator : JC\MD
Sample : N2090-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

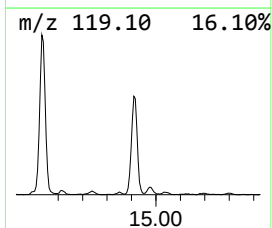
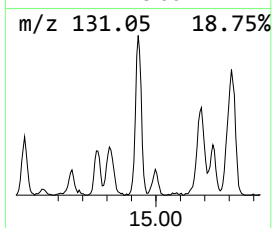
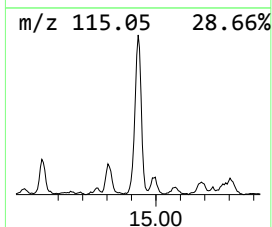
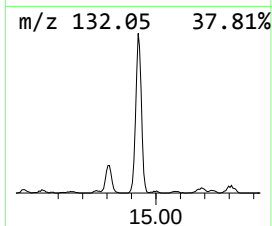
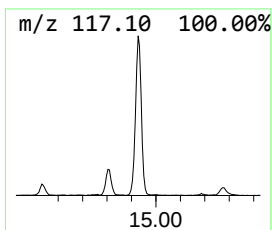
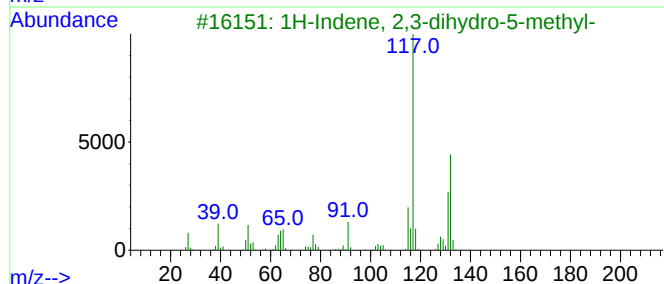
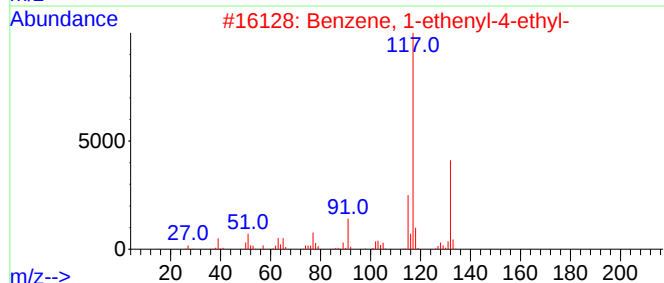
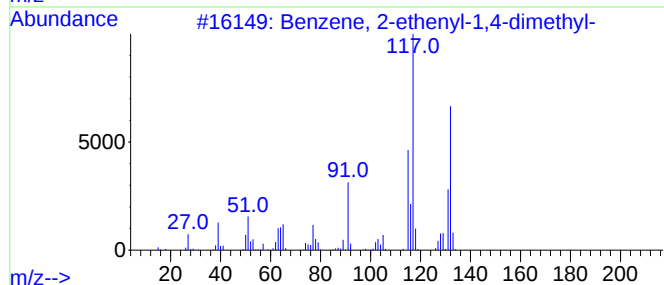
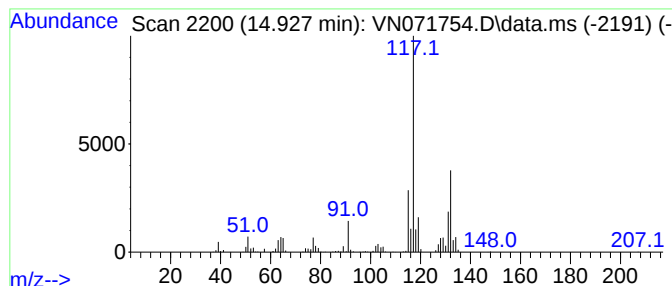
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	26.91 ug/l	1312240	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
Data File : VN071754.D
Acq On : 01 Apr 2022 15:43
Operator : JC\MD
Sample : N2090-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-48

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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
Di-sec-Butyl ether	10.639	6.8	ug/l	429577	3	11.739	3163210	50.0
Sulfurous acid,...	10.710	7.1	ug/l	448086	3	11.739	3163210	50.0
Benzene, 1,4-di...	13.833	5.4	ug/l	264544	4	13.674	2438090	50.0
Indane	13.874	59.1	ug/l	2883980	4	13.674	2438090	50.0
Benzene, 1-meth...	14.210	11.5	ug/l	562674	4	13.674	2438090	50.0
Indan, 1-methyl-	14.327	19.9	ug/l	969074	4	13.674	2438090	50.0
Benzene, 1,2,4,...	14.533	13.1	ug/l	639692	4	13.674	2438090	50.0
Benzene, 2-ethe...	14.927	26.9	ug/l	1312240	4	13.674	2438090	50.0