

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
 Data File : VN074566.D
 Acq On : 17 Sep 2022 19:19
 Operator : JC\MD
 Sample : N4663-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SVE-03

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\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	59	rBV	196913	367569	7.18%	0.920%
2	2.693	132	137	141	rBV4	45936	95436	1.86%	0.239%
3	7.622	966	975	990	rBV3	120527	297409	5.81%	0.745%
4	7.780	993	1002	1012	rVB2	86073	211979	4.14%	0.531%
5	7.957	1021	1032	1036	rBV2	227170	563893	11.01%	1.412%
6	8.016	1036	1042	1055	rVB	382173	864559	16.88%	2.165%
7	8.369	1094	1102	1115	rBV	268008	613585	11.98%	1.536%
8	8.904	1182	1193	1207	rBV2	602531	1224506	23.91%	3.066%
9	9.398	1263	1277	1286	rBV3	57123	144774	2.83%	0.362%
10	10.380	1436	1444	1459	rBV	962466	1764529	34.46%	4.418%
11	10.545	1467	1472	1482	rVB7	24033	58523	1.14%	0.147%
12	10.721	1495	1502	1509	rVB3	40300	77331	1.51%	0.194%
13	11.286	1594	1598	1603	rVB4	32084	55654	1.09%	0.139%
14	11.686	1659	1666	1674	rBV	957194	1645247	32.13%	4.119%
15	11.780	1677	1682	1687	rVV2	36263	57485	1.12%	0.144%
16	11.927	1701	1707	1720	rVB7	40013	110361	2.16%	0.276%
17	12.204	1745	1754	1758	rBV7	28131	69583	1.36%	0.174%
18	12.398	1775	1787	1792	rBV7	44750	123067	2.40%	0.308%
19	12.521	1803	1808	1814	rVB	157736	257500	5.03%	0.645%
20	12.674	1827	1834	1841	rBV	809284	1300211	25.39%	3.256%
21	12.751	1841	1847	1853	rBV5	33276	63330	1.24%	0.159%
22	12.862	1859	1866	1872	rVB	172079	313700	6.13%	0.785%
23	12.998	1882	1889	1895	rVB9	26898	59168	1.16%	0.148%
24	13.239	1923	1930	1931	rBV5	38495	62557	1.22%	0.157%
25	13.262	1931	1934	1941	rVB3	54147	86529	1.69%	0.217%
26	13.439	1957	1964	1970	rBV4	164997	344596	6.73%	0.863%
27	13.615	1987	1994	2003	rVB	1008166	1625674	31.75%	4.070%
28	13.709	2003	2010	2016	rBV	137457	239932	4.69%	0.601%
29	13.780	2016	2022	2025	rBV	333019	547583	10.69%	1.371%
30	13.815	2025	2028	2033	rVB	452627	693230	13.54%	1.736%
31	13.945	2045	2050	2056	rVB	368978	568163	11.10%	1.423%
32	14.157	2080	2086	2092	rBV	1099321	1684101	32.89%	4.217%
33	14.221	2092	2097	2100	rVV	314373	527515	10.30%	1.321%
34	14.268	2100	2105	2111	rVV2	1110295	1924801	37.59%	4.819%
35	14.333	2111	2116	2122	rVV5	78002	161151	3.15%	0.403%
36	14.409	2122	2129	2132	rVV	179905	312449	6.10%	0.782%

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37	14.480	2132	2141	2150	rVB	1085361	1919258	37.48%	4.806%
38	14.562	2150	2155	2158	rBV	117310	171931	3.36%	0.430%
39	14.604	2158	2162	2163	rVV3	65339	93016	1.82%	0.233%
40	14.633	2163	2167	2172	rVV	153283	256492	5.01%	0.642%
41	14.704	2172	2179	2183	rVV4	167301	408211	7.97%	1.022%
42	14.751	2183	2187	2192	rVV3	235840	422546	8.25%	1.058%
43	14.798	2192	2195	2199	rVV4	111086	168396	3.29%	0.422%
44	14.856	2199	2205	2213	rVV2	2397553	5120371	100.00%	12.821%
45	14.927	2213	2217	2223	rVV4	172633	362203	7.07%	0.907%
46	14.974	2223	2225	2230	rVB2	48662	73035	1.43%	0.183%
47	15.133	2235	2252	2255	rBV4	416069	1131098	22.09%	2.832%
48	15.174	2255	2259	2264	rVV2	281128	522307	10.20%	1.308%
49	15.245	2264	2271	2278	rVB2	593329	1350932	26.38%	3.383%
50	15.345	2284	2288	2291	rVB	64797	88590	1.73%	0.222%
51	15.392	2291	2296	2302	rVB3	171016	342234	6.68%	0.857%
52	15.492	2306	2313	2318	rBV	313937	621523	12.14%	1.556%
53	15.733	2347	2354	2361	rBV3	133168	286707	5.60%	0.718%
54	15.809	2361	2367	2373	rVV5	129369	252539	4.93%	0.632%
55	15.903	2377	2383	2386	rVV2	249176	518459	10.13%	1.298%
56	15.945	2386	2390	2399	rVB	442251	834366	16.30%	2.089%
57	16.033	2400	2405	2408	rBV4	107028	197271	3.85%	0.494%
58	16.092	2408	2415	2423	rVB	1398816	2899898	56.63%	7.261%
59	16.268	2436	2445	2454	rBV2	582067	1332173	26.02%	3.336%
60	16.462	2469	2478	2485	rBV3	120164	304314	5.94%	0.762%
61	16.533	2485	2490	2494	rBV5	83304	185885	3.63%	0.465%
62	16.739	2517	2525	2533	rBV3	371423	956869	18.69%	2.396%

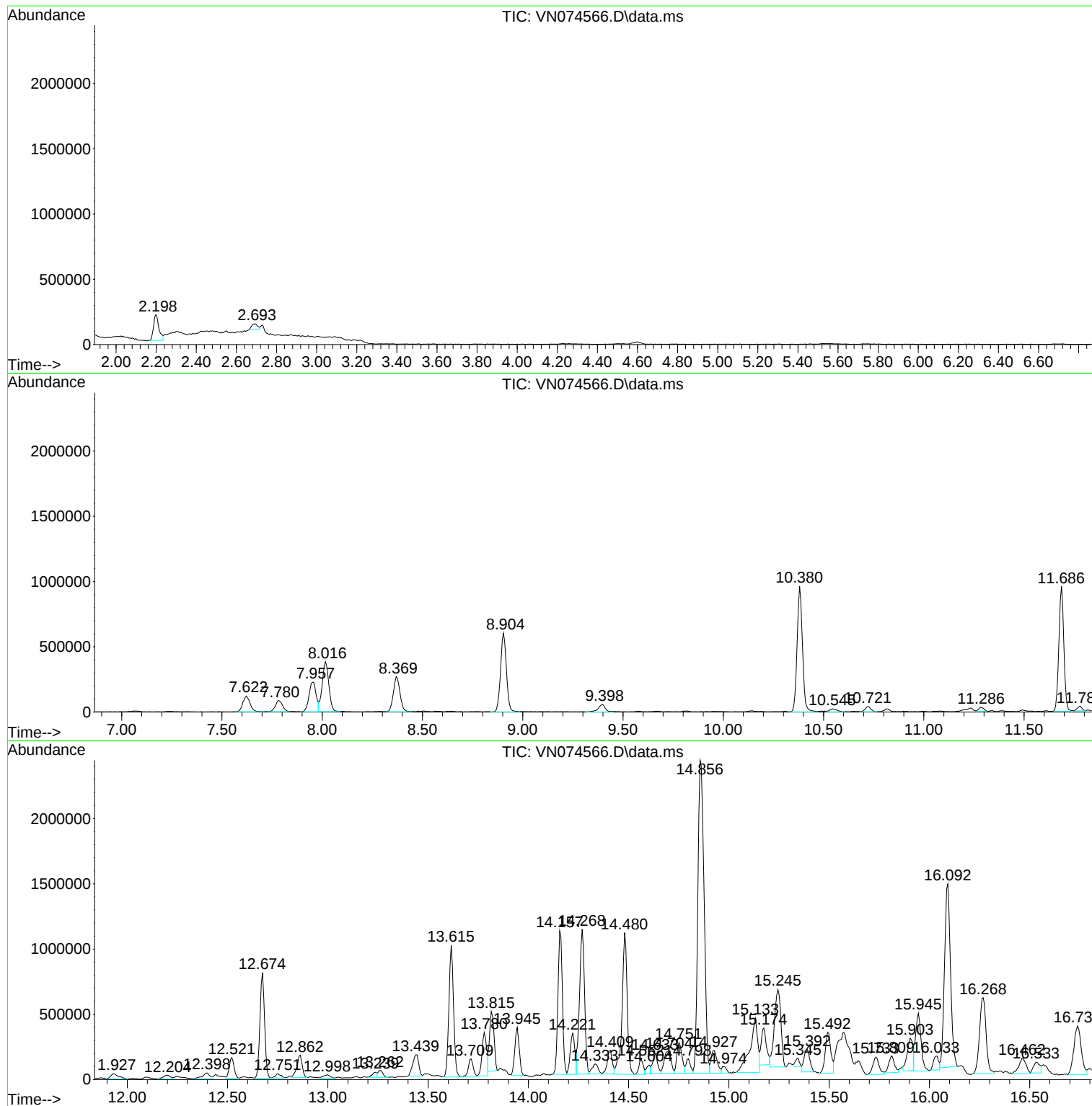
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Quant Title : SW846 8260

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



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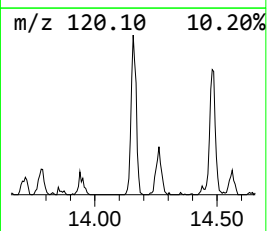
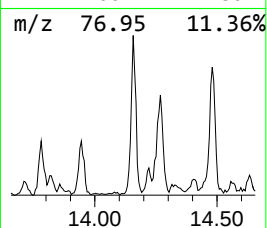
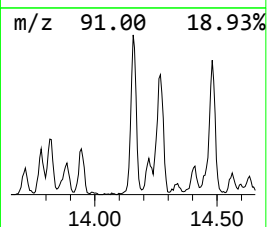
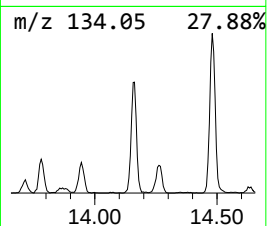
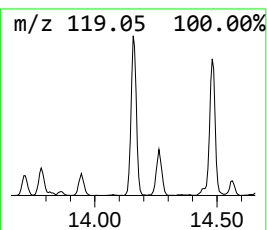
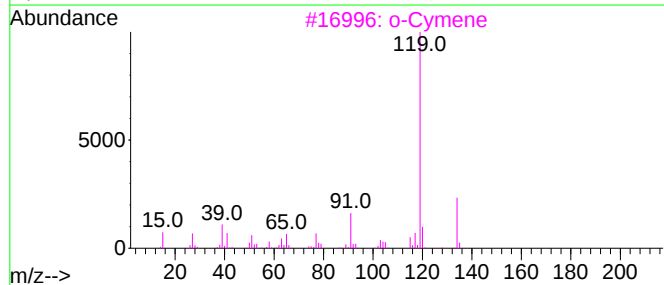
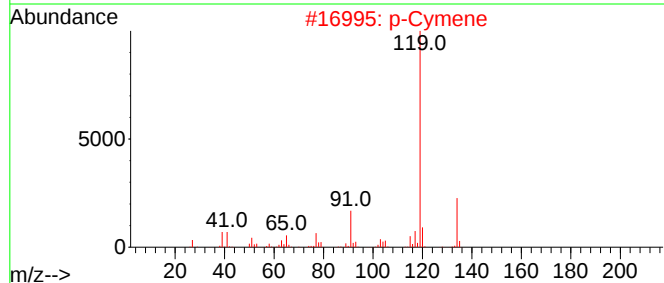
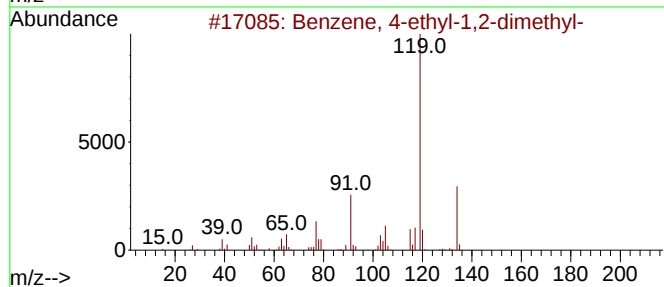
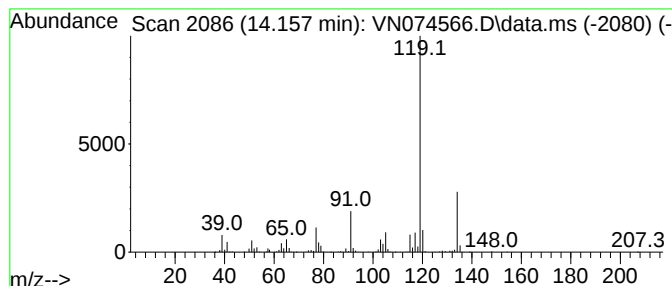
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.156	51.80 ug/l	1684100	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			p-Cymene	134	C10H14	000099-87-6	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



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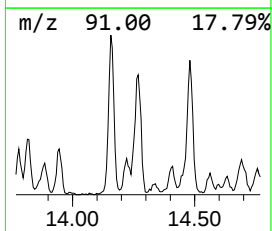
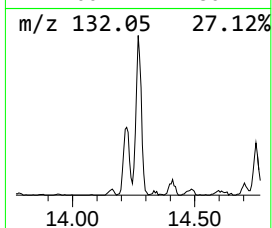
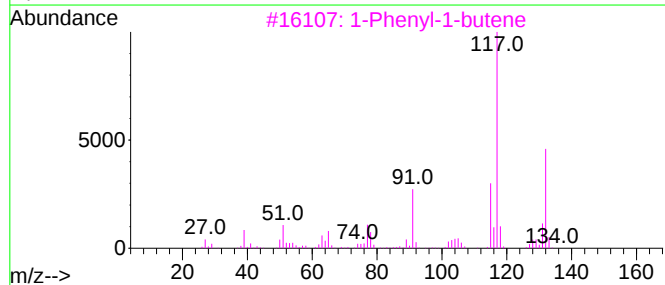
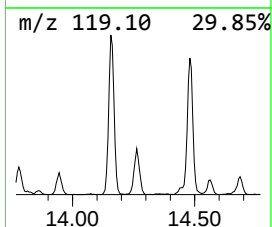
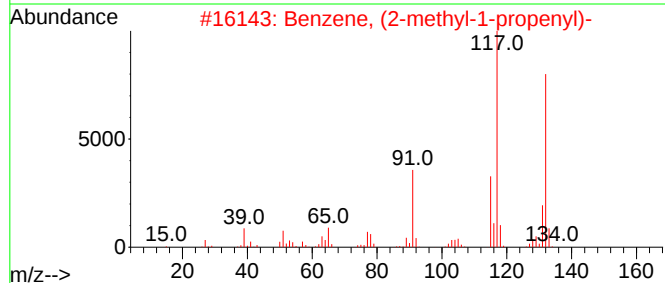
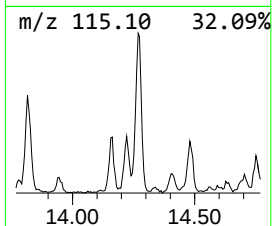
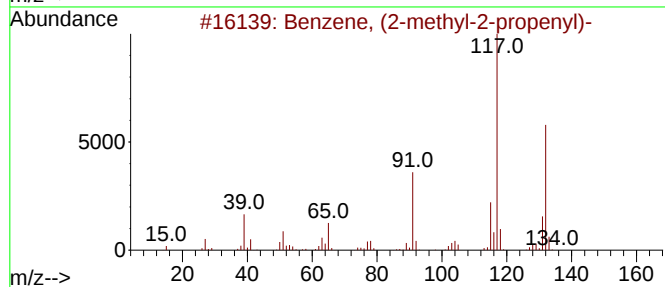
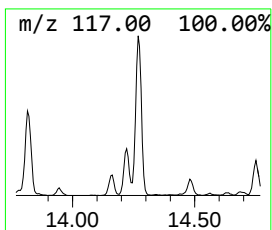
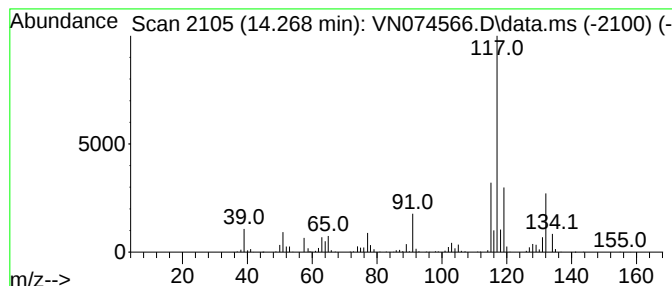
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, (2-methyl-2-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	59.20 ug/l	1924800	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	81
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74



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ClientSampleId :
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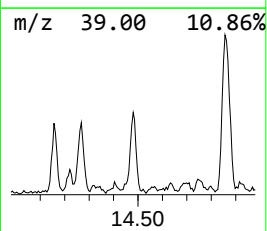
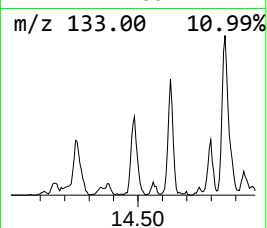
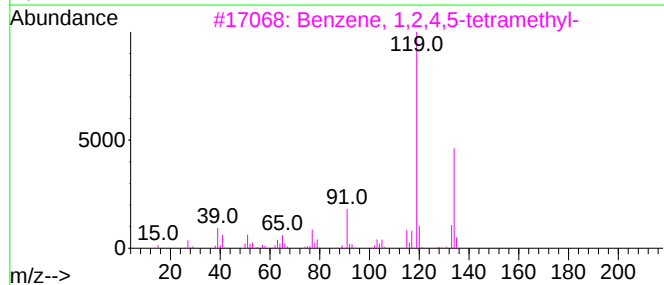
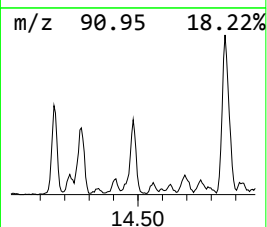
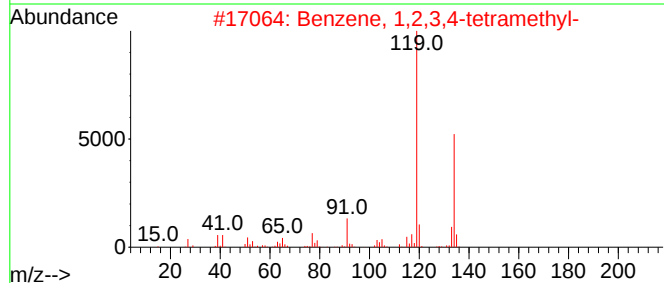
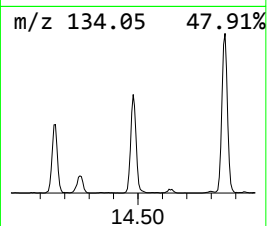
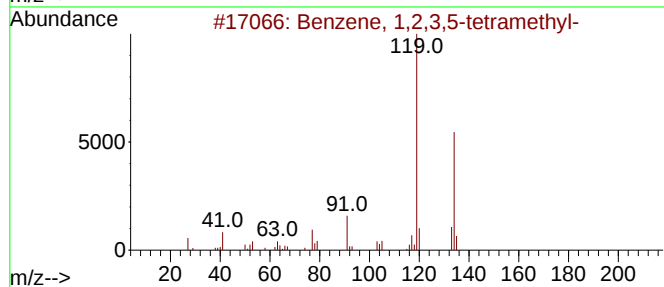
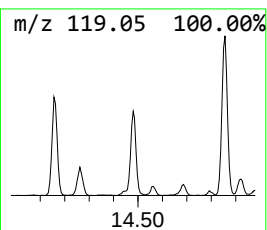
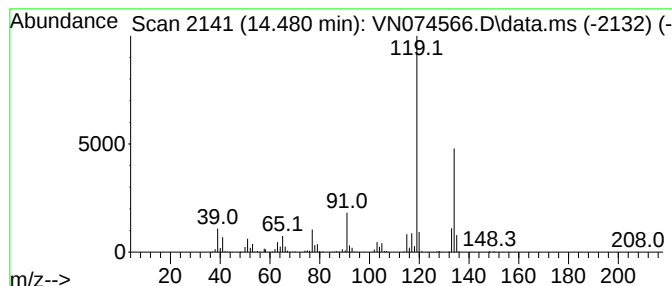
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	59.03 ug/l	1919260	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			p-Cymene	134	C10H14	000099-87-6	94
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94



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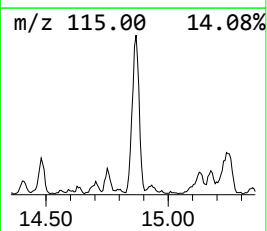
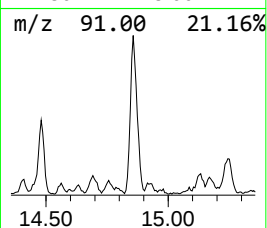
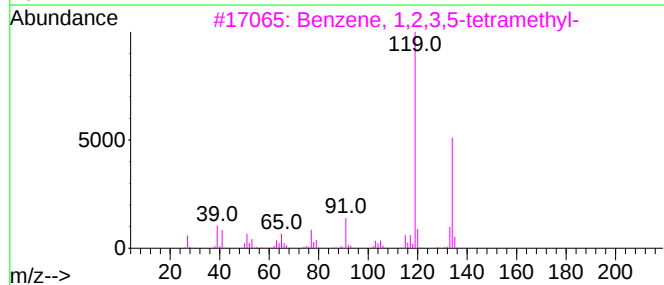
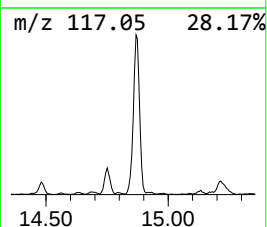
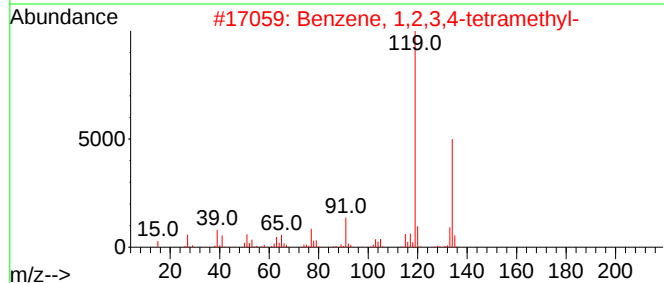
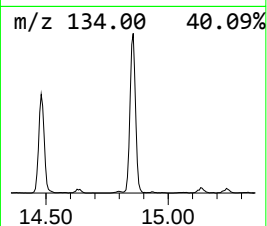
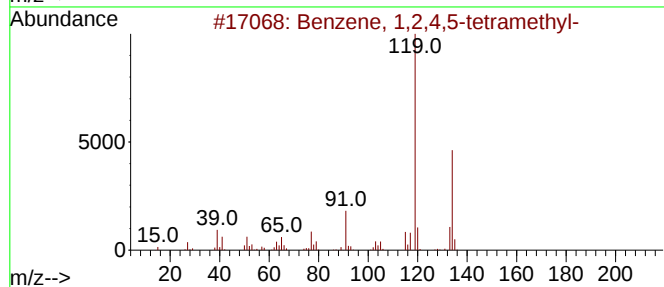
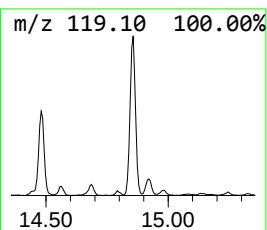
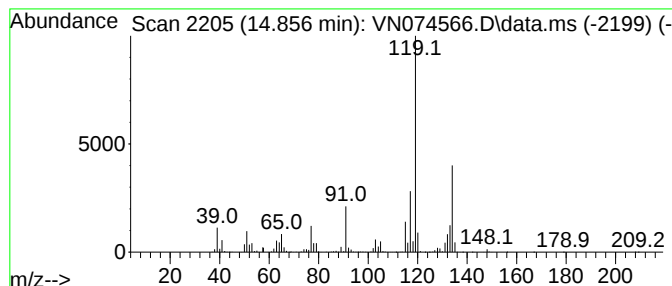
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	157.49 ug/l	5120370	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	87
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	87
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	83
5			o-Cymene	134	C10H14	000527-84-4	81



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Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

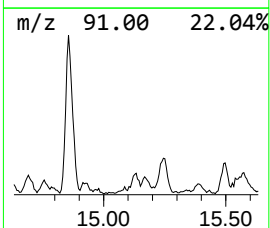
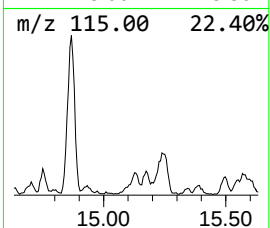
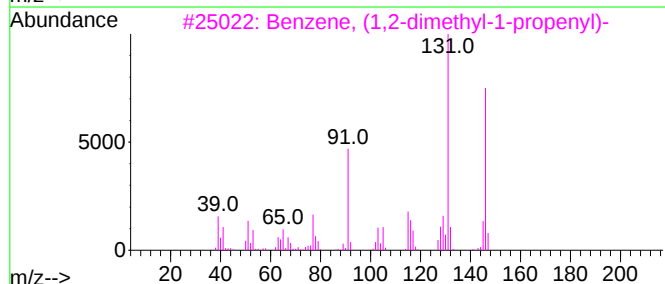
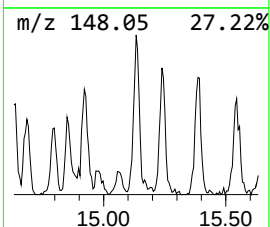
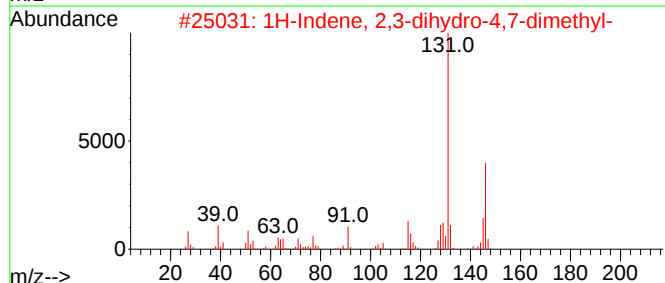
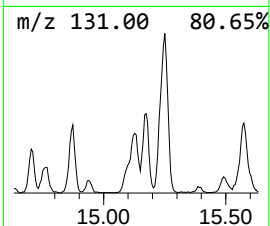
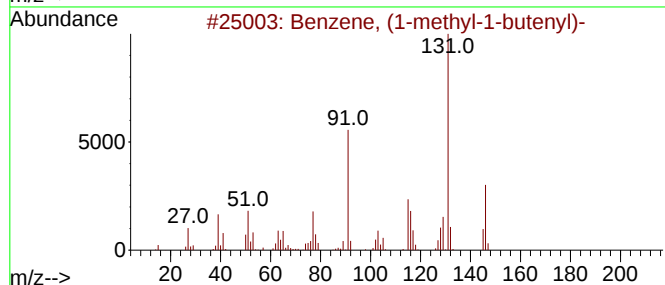
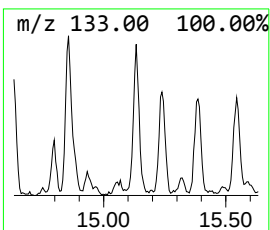
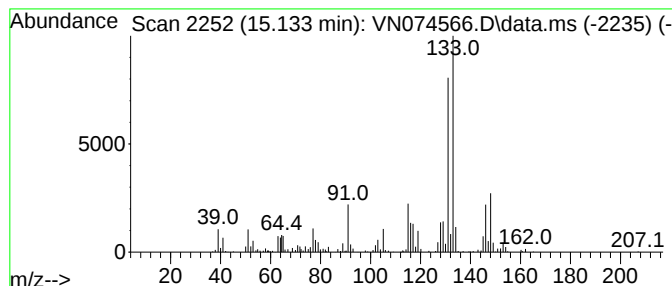
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (1-methyl-1-butenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	34.79 ug/l	1131100	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	90
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	86
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	64
4			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	50
5			1,3-Cyclopentadiene, 5-(trans-2-...	146	C11H14	079209-36-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

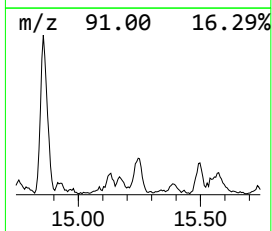
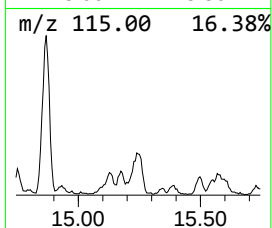
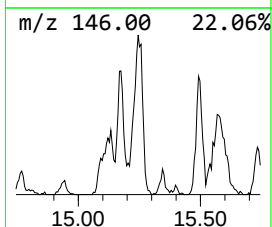
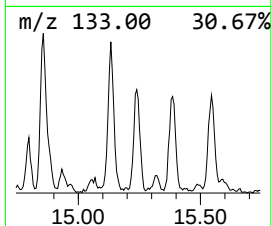
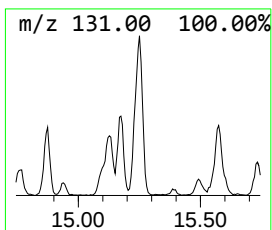
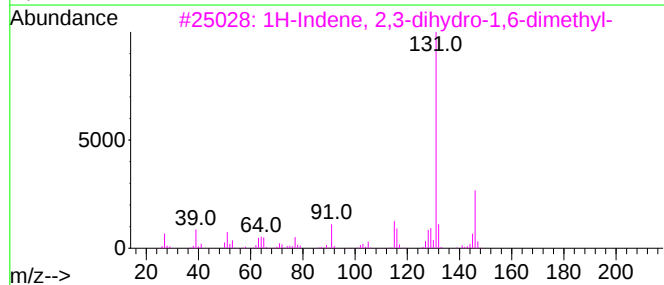
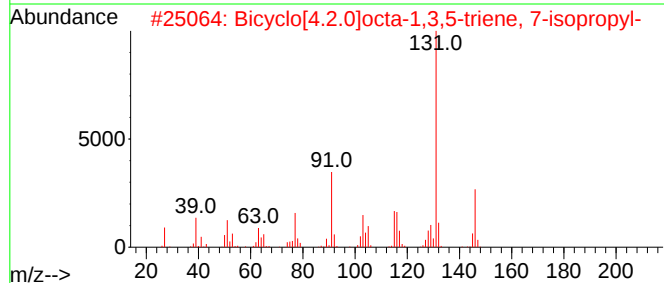
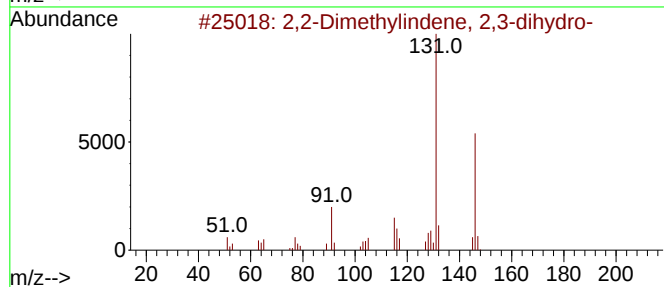
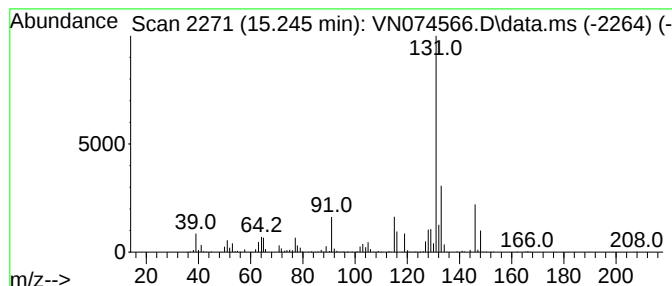
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Quant Title : SW846 8260

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

Peak Number 6 2,2-Dimethylindene, 2,3-dih... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	41.55 ug/l	1350930	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	81
3		1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	81
4		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81
5		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

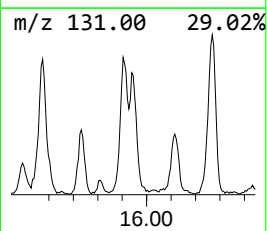
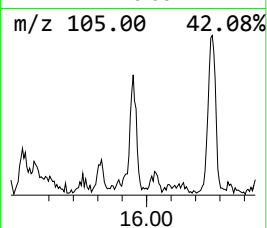
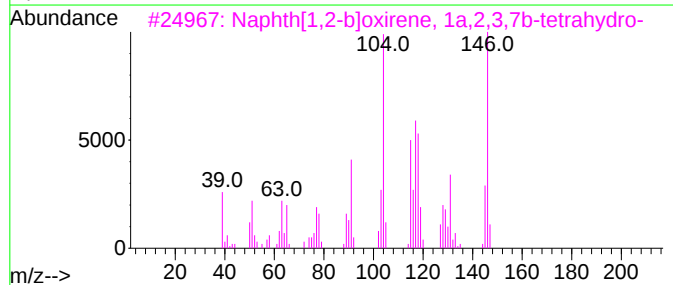
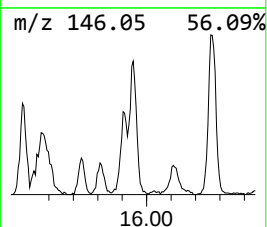
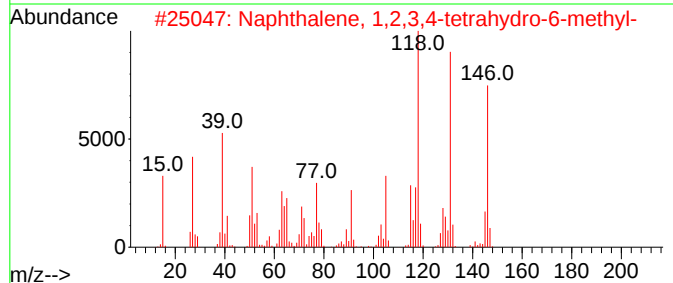
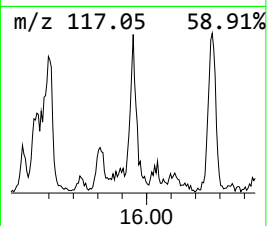
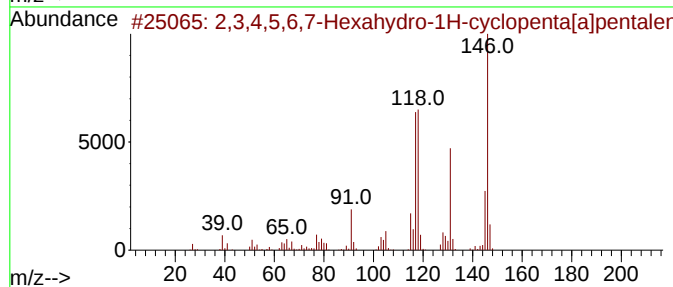
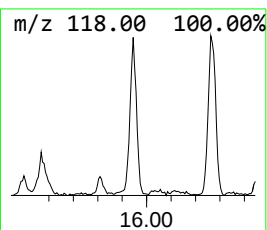
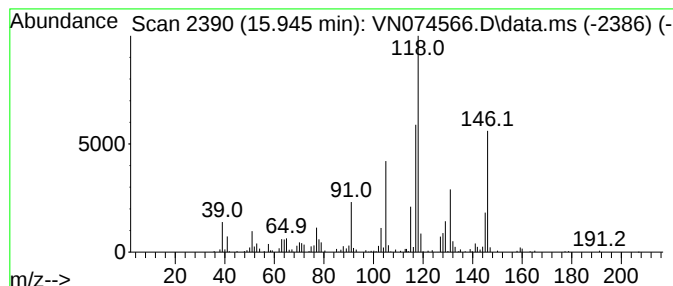
Instrument :
MSVOA_N
ClientSampleId :
SVE-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 7 2,3,4,5,6,7-Hexahydro-1H-cy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.945	25.66 ug/l	834366	1,4-Dichlorobenzene-d4		13.615	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,3,4,5,6,7-Hexahydro-1H-cyclope...		146	C11H14	1010189-31-0	74
2	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001680-51-9	72
3	Naphth[1,2-b]oxirene, 1a,2,3,7b-...		146	C10H10O	002461-34-9	46
4	Pyridine, 3-(3,4-dihydro-2H-pyrr...		146	C9H10N2	000532-12-7	43
5	1H-Tetrazole, 5-phenyl-		146	C7H6N4	018039-42-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

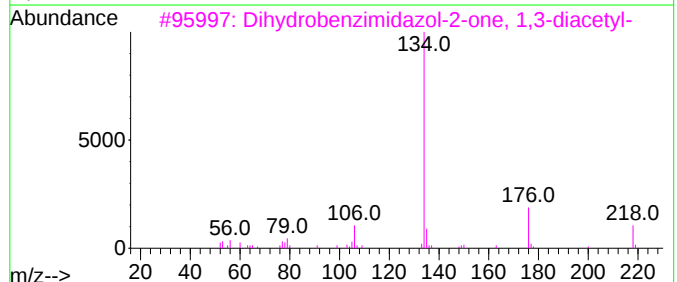
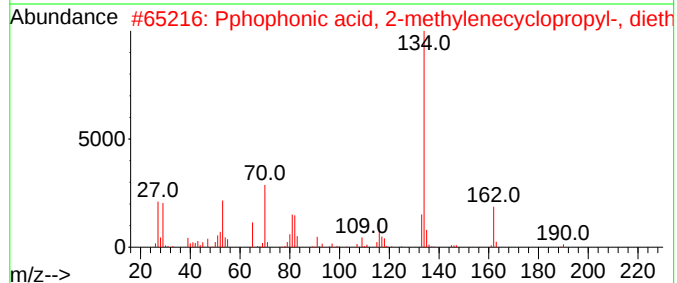
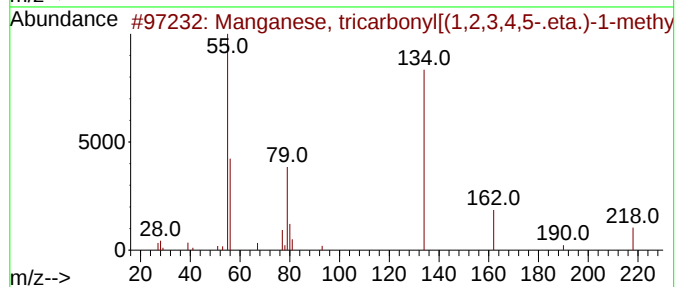
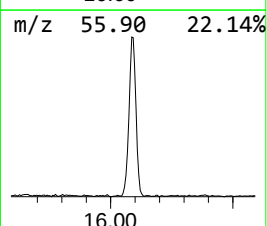
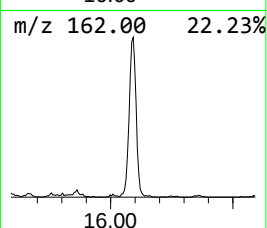
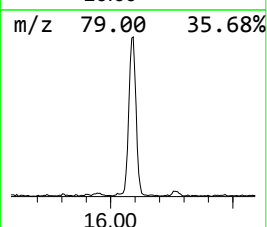
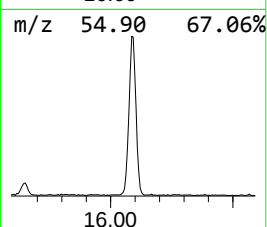
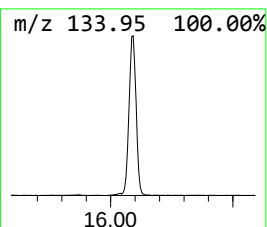
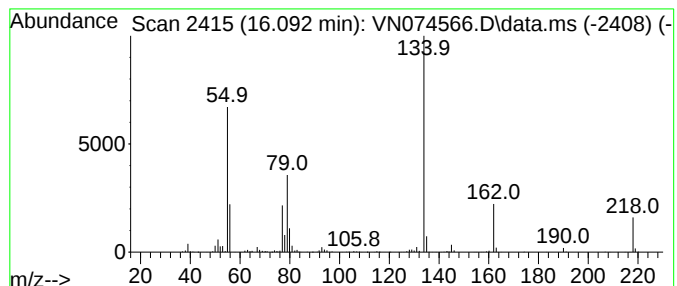
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Quant Title : SW846 8260

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

Peak Number 8 Manganese, tricarbonyl[(1,2... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	89.19 ug/l	2899900	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Manganese, tricarbonyl[(1,2,3,4,...	218	C9H7MnO3	012108-13-3	50
2			Pphophonic acid, 2-methylenecycl...	190	C8H15O3P	1000157-98-6	43
3			Dihydrobenzimidazol-2-one, 1,3-d...	218	C11H10N2O3	002735-73-1	32
4			3-Amino-4-hydroxybenzonitrile	134	C7H6N2O	014543-43-2	28
5			Pyrazolo[5,1-c]-as-triazine-3-ca...	206	C9H10N4O2	006726-54-1	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

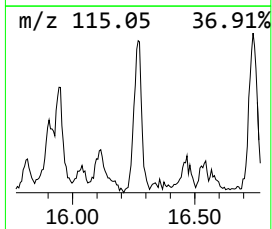
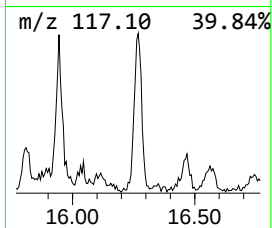
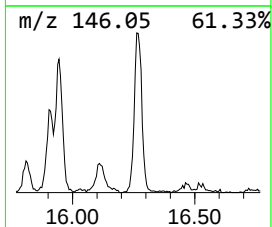
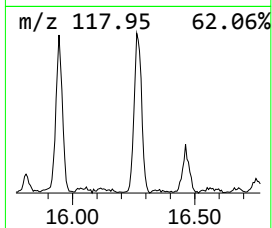
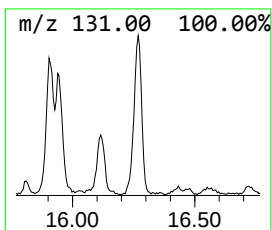
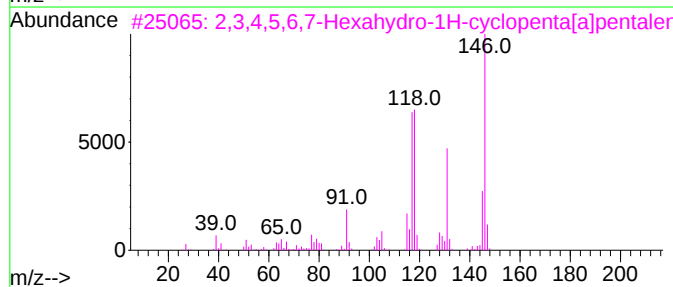
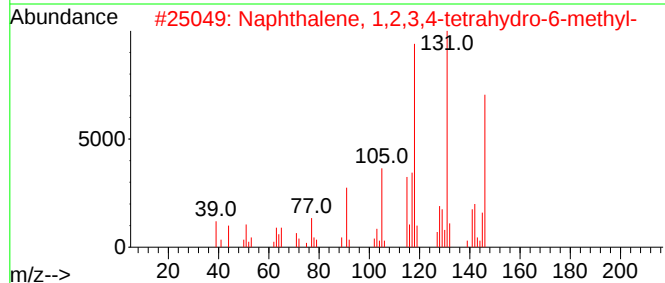
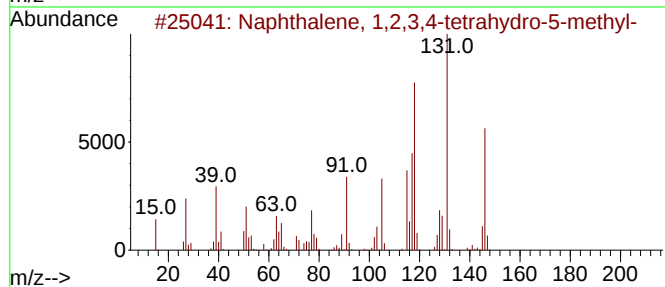
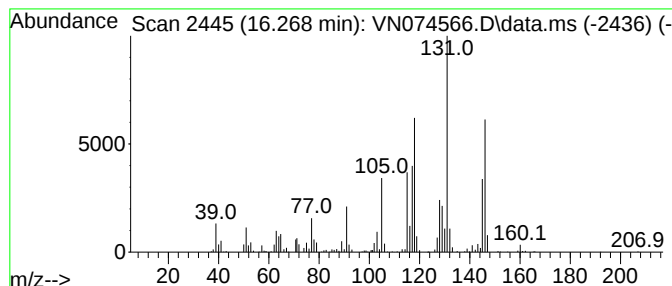
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.268	40.97 ug/l	1332170	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	87
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	76
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

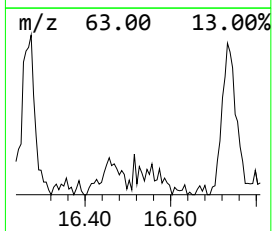
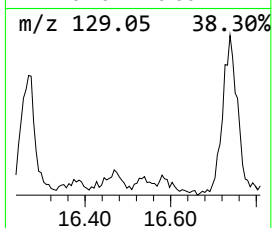
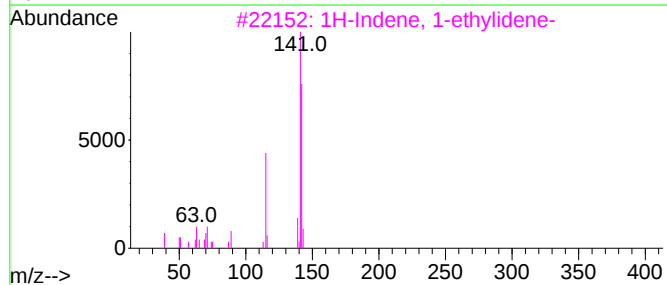
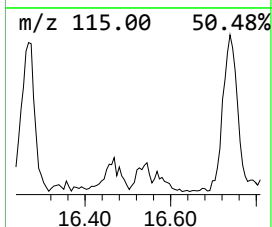
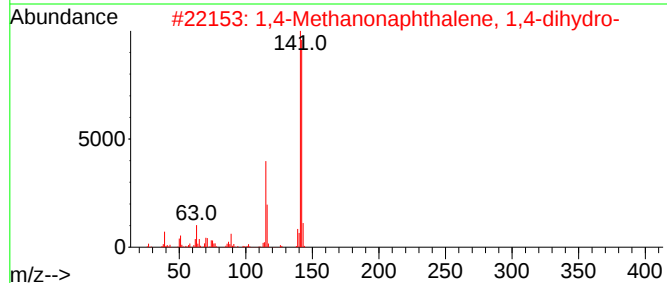
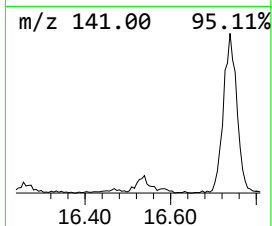
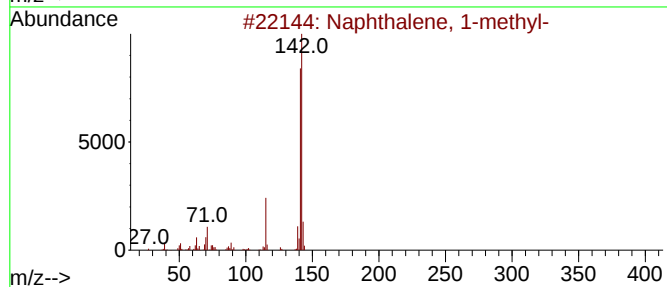
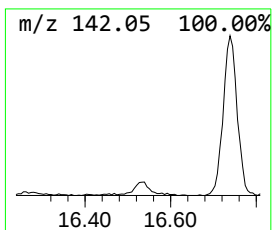
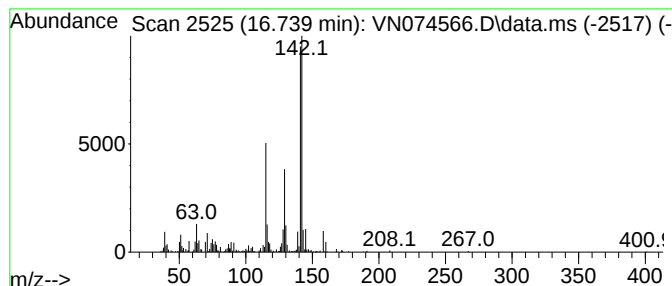
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	29.43 ug/l	956869	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	86
2		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	70
3		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	70
4		Benzocycloheptatriene	142	C11H10	000264-09-5	68
5		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091722\
Data File : VN074566.D
Acq On : 17 Sep 2022 19:19
Operator : JC\MD
Sample : N4663-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SVE-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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, (2-met...	14.268	59.2	ug/l	1924800	4	13.615	1625670	50.0
Benzene, 1,2,3,...	14.480	59.0	ug/l	1919260	4	13.615	1625670	50.0
Benzene, 1,2,4,...	14.857	157.5	ug/l	5120370	4	13.615	1625670	50.0
Benzene, (1-met...	15.133	34.8	ug/l	1131100	4	13.615	1625670	50.0
2,2-Dimethylind...	15.245	41.5	ug/l	1350930	4	13.615	1625670	50.0
2,3,4,5,6,7-Hex...	15.945	25.7	ug/l	834366	4	13.615	1625670	50.0
Manganese, tric...	16.092	89.2	ug/l	2899900	4	13.615	1625670	50.0
Naphthalene, 1,...	16.268	41.0	ug/l	1332170	4	13.615	1625670	50.0
Naphthalene, 1-...	16.739	29.4	ug/l	956869	4	13.615	1625670	50.0