

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
 Data File : VN073763.D
 Acq On : 05 Aug 2022 15:30
 Operator : JC\MD
 Sample : N3887-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-12

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	77	87	94	rBV	53637	94712	1.02%	0.135%
2	3.087	195	204	217	rVB	220019	502883	5.39%	0.717%
3	4.993	516	528	537	rBV2	39371	146741	1.57%	0.209%
4	5.104	537	547	568	rVB3	70863	297860	3.19%	0.425%
5	5.534	606	620	633	rBV2	28325	94549	1.01%	0.135%
6	6.522	776	788	797	rBV2	49757	143599	1.54%	0.205%
7	7.069	869	881	888	rBV2	210073	628325	6.74%	0.896%
8	7.145	888	894	904	rVB	74980	202679	2.17%	0.289%
9	7.775	985	1001	1011	rBV	304319	775546	8.32%	1.106%
10	7.951	1018	1031	1036	rBV	274950	676957	7.26%	0.966%
11	8.022	1036	1043	1053	rVV2	753609	1836927	19.70%	2.621%
12	8.110	1053	1058	1069	rVB4	34470	96708	1.04%	0.138%
13	8.375	1095	1103	1114	rBV	271327	660882	7.09%	0.943%
14	8.522	1116	1128	1142	rVV6	93044	344489	3.70%	0.491%
15	8.639	1142	1148	1158	rVB2	44867	106646	1.14%	0.152%
16	8.904	1184	1193	1205	rBV	721941	1595694	17.12%	2.277%
17	9.180	1235	1240	1254	rVB	174611	352122	3.78%	0.502%
18	9.363	1259	1271	1272	rBV4	108592	213864	2.29%	0.305%
19	9.398	1272	1277	1286	rVB	210934	458831	4.92%	0.655%
20	9.745	1328	1336	1337	rBV2	67900	125843	1.35%	0.180%
21	9.822	1344	1349	1356	rVB3	84182	165548	1.78%	0.236%
22	9.910	1356	1364	1369	rBV	422226	824068	8.84%	1.176%
23	9.951	1369	1371	1383	rVB4	107448	206552	2.22%	0.295%
24	10.263	1416	1424	1437	rBV	338647	669205	7.18%	0.955%
25	10.380	1437	1444	1458	rVV	1044788	1949471	20.91%	2.781%
26	10.580	1466	1478	1484	rBV6	55353	146251	1.57%	0.209%
27	10.798	1507	1515	1524	rBV2	164823	338258	3.63%	0.483%
28	11.686	1658	1666	1672	rBV	1015398	1757807	18.86%	2.508%
29	12.674	1824	1834	1841	rBV	868051	1479302	15.87%	2.110%
30	13.163	1910	1917	1924	rBV	426267	695228	7.46%	0.992%
31	13.257	1924	1933	1944	rVV5	46258	112909	1.21%	0.161%
32	13.615	1986	1994	2006	rBV	1112486	2095999	22.48%	2.990%
33	13.710	2006	2010	2015	rVB	102719	159769	1.71%	0.228%
34	13.780	2015	2022	2023	rBV	853924	1135075	12.18%	1.619%
35	13.815	2023	2028	2043	rVB	5610627	9322694	100.00%	13.300%
36	13.945	2043	2050	2054	rBV	471985	751048	8.06%	1.071%

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37	13.998	2054	2059	2065	rVB2	235079	387199	4.15%	0.552%
38	14.068	2067	2071	2079	rBV2	70040	139298	1.49%	0.199%
39	14.157	2079	2086	2092	rBV	2005197	3040228	32.61%	4.337%
40	14.215	2092	2096	2099	rVV	345389	525816	5.64%	0.750%
41	14.268	2099	2105	2112	rVB2	3278369	5311024	56.97%	7.577%
42	14.404	2122	2128	2132	rBV	141248	229432	2.46%	0.327%
43	14.480	2132	2141	2150	rVB	2187968	3552065	38.10%	5.068%
44	14.562	2150	2155	2157	rBV	91167	132879	1.43%	0.190%
45	14.598	2157	2161	2165	rVV2	95509	134132	1.44%	0.191%
46	14.698	2171	2178	2182	rBV2	180647	363440	3.90%	0.519%
47	14.751	2182	2187	2192	rVV2	886886	1507021	16.17%	2.150%
48	14.792	2192	2194	2199	rVV2	145426	197872	2.12%	0.282%
49	14.868	2199	2207	2213	rVV3	4418047	8699014	93.31%	12.411%
50	14.921	2213	2216	2223	rVV3	225361	499730	5.36%	0.713%
51	15.021	2227	2233	2242	rVV2	758317	1444760	15.50%	2.061%
52	15.127	2244	2251	2256	rVV2	1040069	2230180	23.92%	3.182%
53	15.168	2256	2258	2264	rVV	452731	746199	8.00%	1.065%
54	15.239	2264	2270	2279	rVB2	1048430	2399450	25.74%	3.423%
55	15.398	2291	2297	2306	rVB3	160798	394863	4.24%	0.563%
56	15.492	2307	2313	2317	rBV2	172260	334886	3.59%	0.478%
57	15.545	2317	2322	2324	rVV	232930	427383	4.58%	0.610%
58	15.592	2328	2330	2346	rVB	365795	742221	7.96%	1.059%
59	15.733	2346	2354	2360	rBV	503145	1017490	10.91%	1.452%
60	15.904	2375	2383	2395	rVV	426070	1196936	12.84%	1.708%
61	16.033	2400	2405	2411	rVV2	278181	616702	6.62%	0.880%
62	16.109	2411	2418	2433	rVB2	332536	1051982	11.28%	1.501%
63	16.262	2435	2444	2455	rBV3	301629	792015	8.50%	1.130%
64	16.462	2473	2478	2485	rVV3	138457	328085	3.52%	0.468%
65	16.727	2516	2523	2533	rBV8	148889	486269	5.22%	0.694%

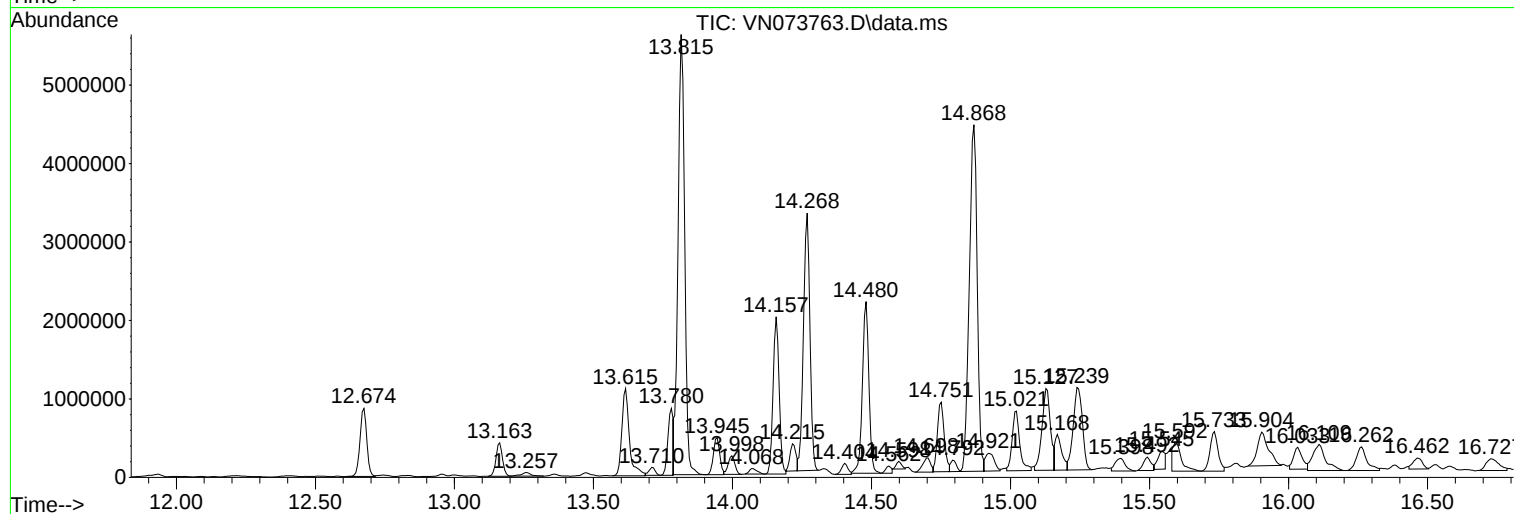
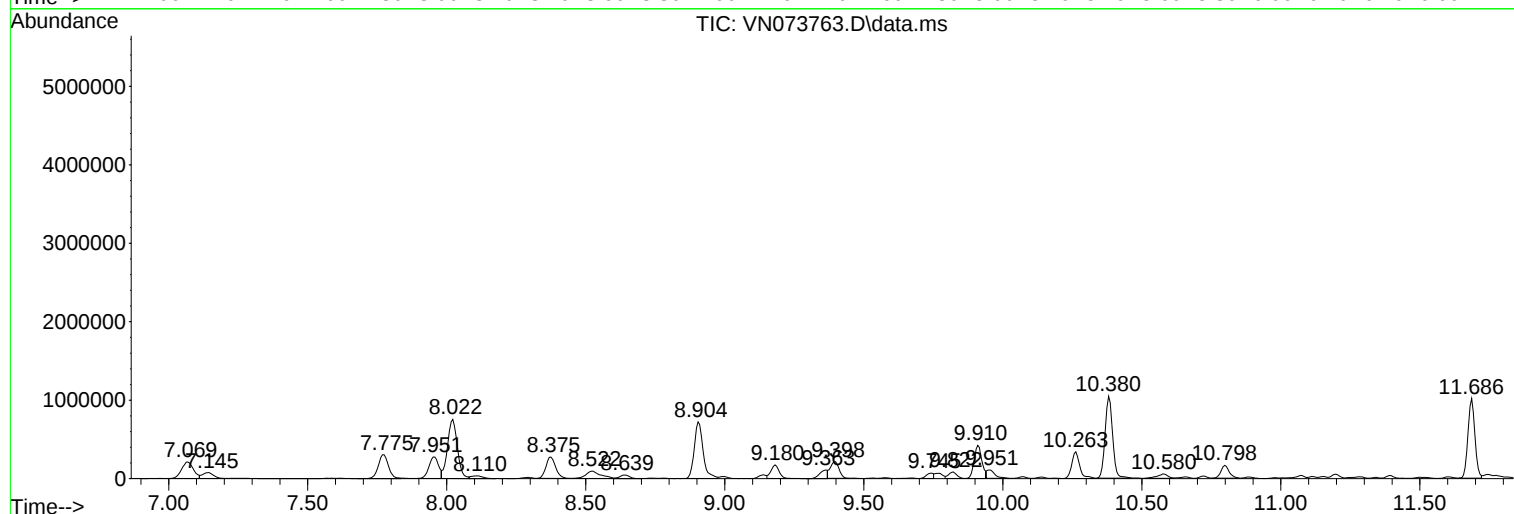
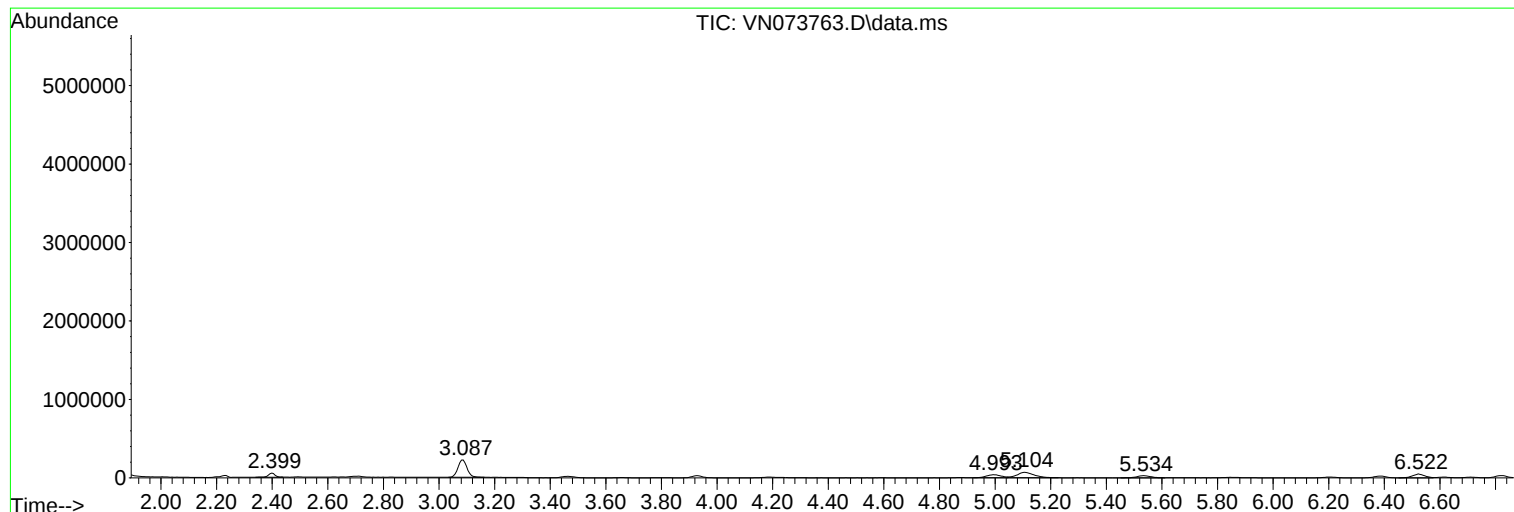
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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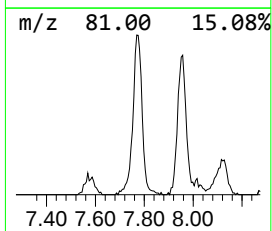
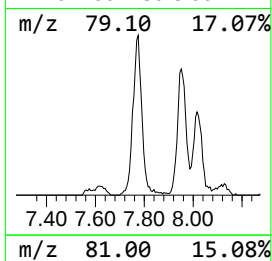
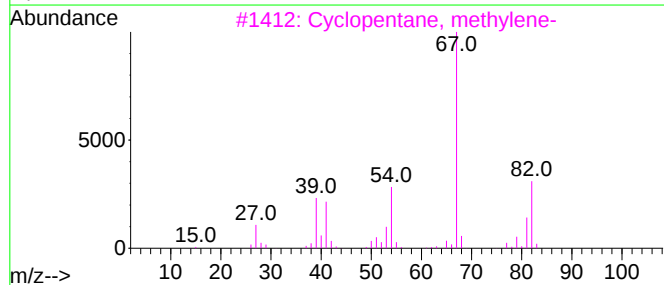
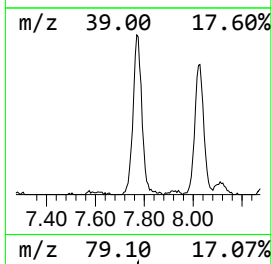
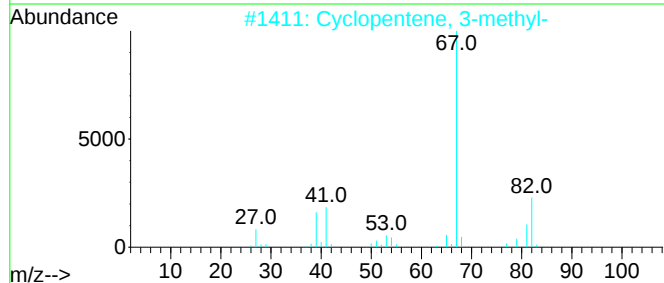
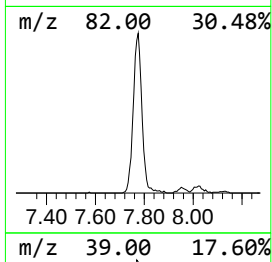
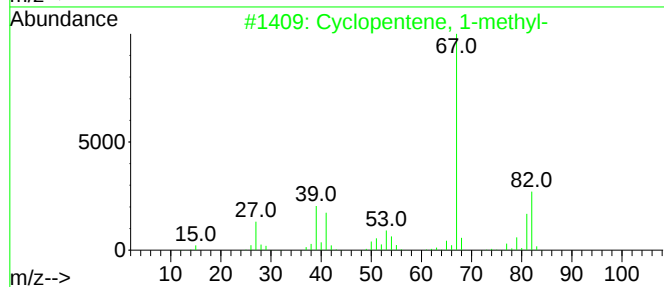
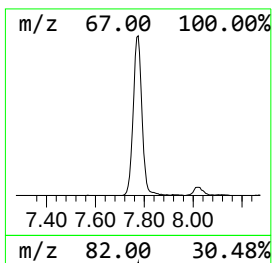
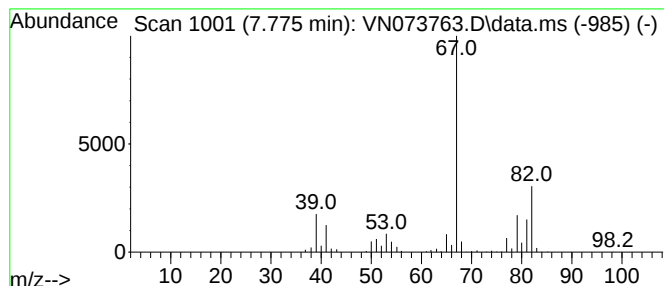
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentene, 1-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.775	21.11 ug/l	775546	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	87
2			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
3			Cyclopentane, methylene-	82	C6H10	001528-30-9	81
4			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	80
5			Cyclohexene	82	C6H10	000110-83-8	74



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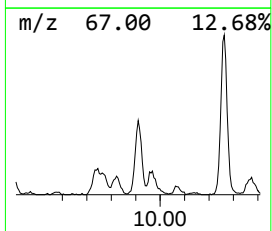
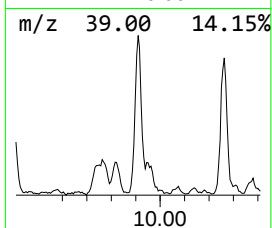
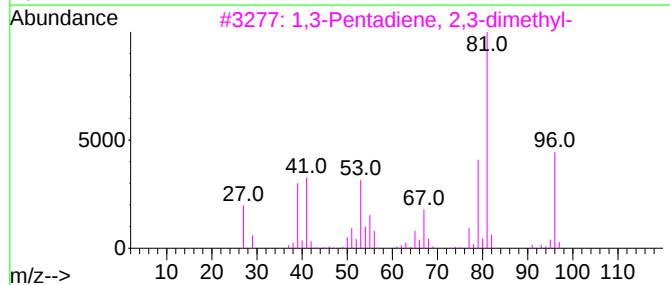
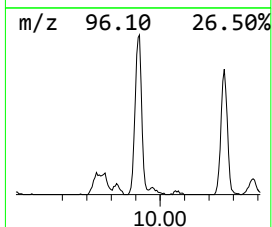
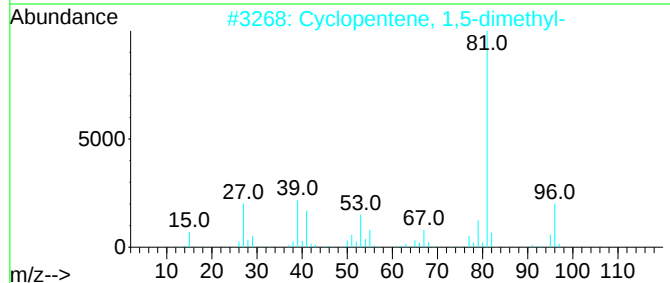
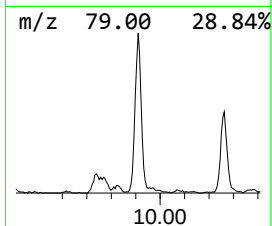
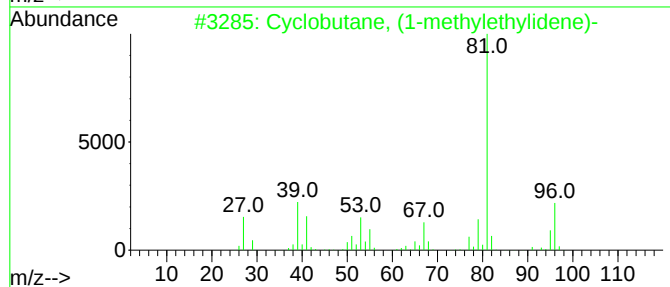
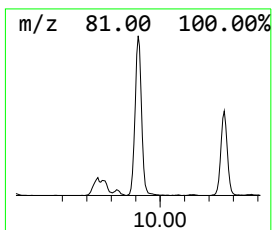
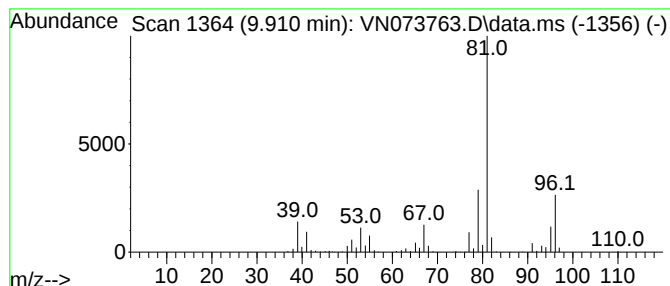
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclobutane, (1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.910	25.82 ug/l	824068	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2			Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	87
3			1,3-Pentadiene, 2,3-dimethyl-	96	C7H12	001113-56-0	80
4			3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5			Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	72



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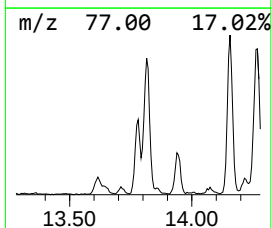
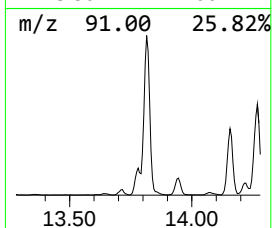
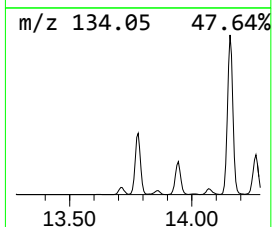
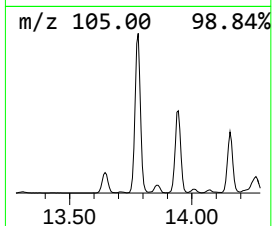
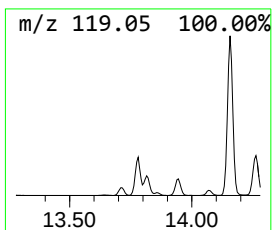
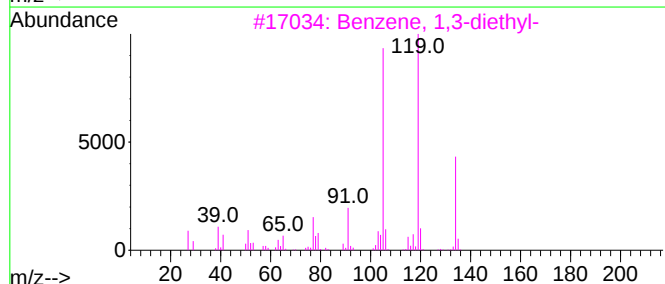
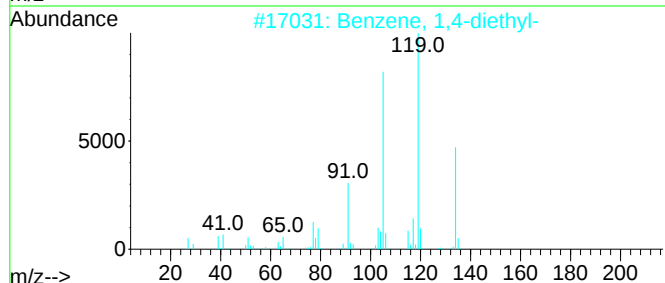
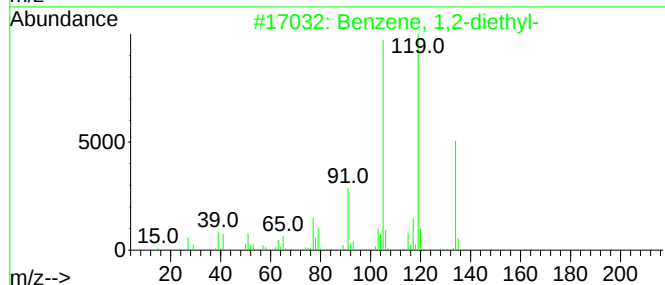
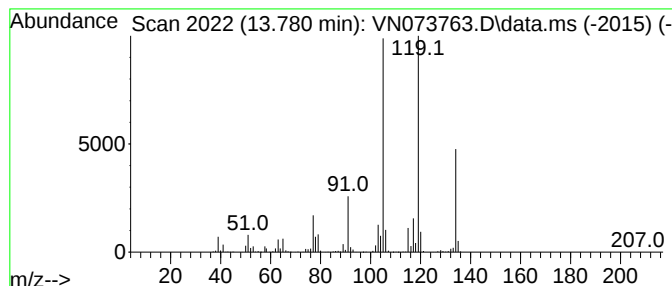
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1,2-diethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	27.08 ug/l	1135080	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	95
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			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	87



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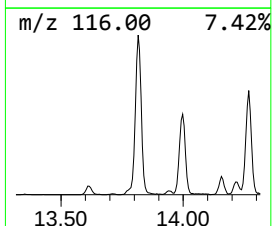
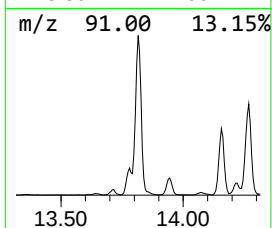
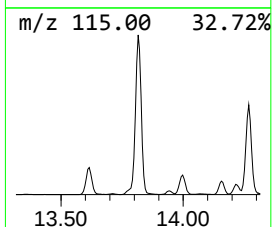
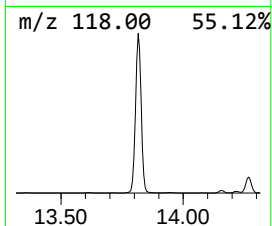
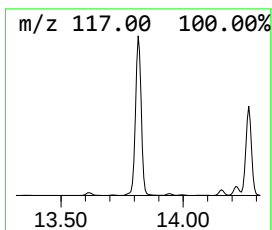
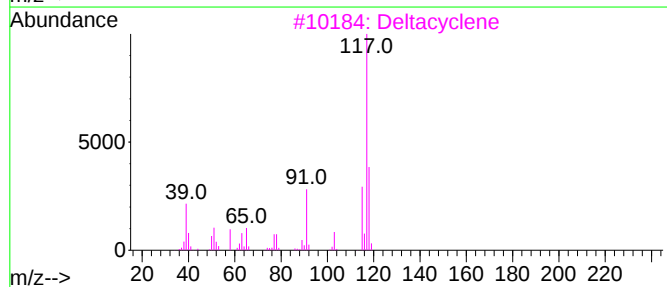
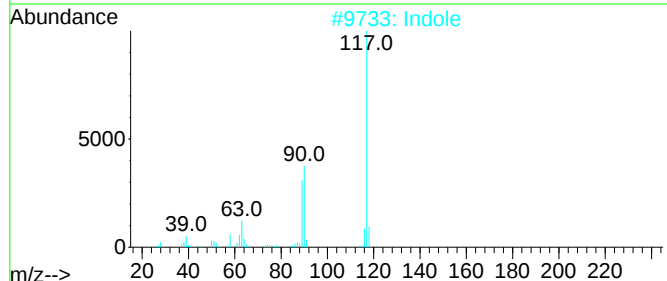
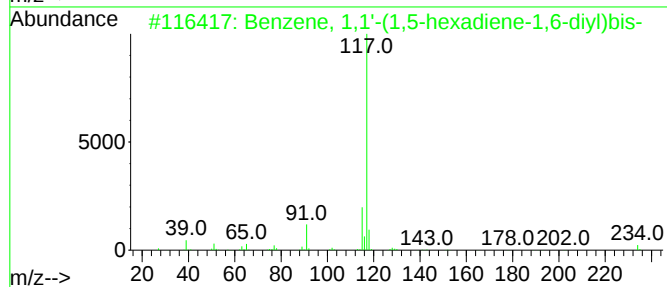
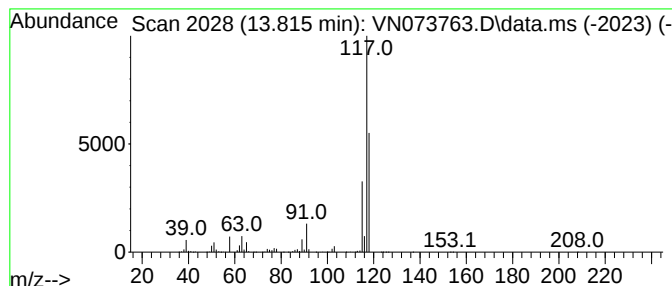
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Quant Title : SW846 8260

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Peak Number 4 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	222.39 ug/l	9322690	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2			Indole	117	C8H7N	000120-72-9	47
3			Deltacyclene	118	C9H10	007785-10-6	45
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

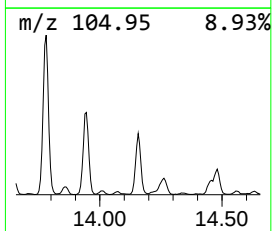
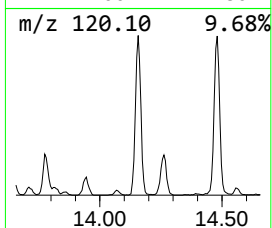
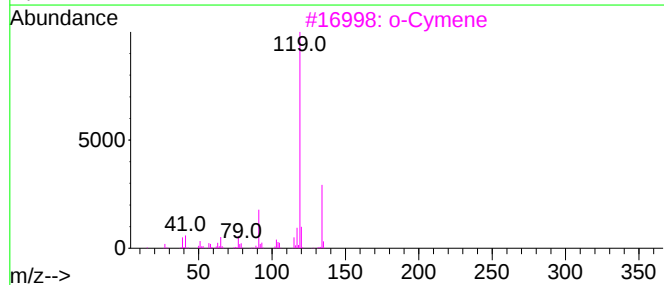
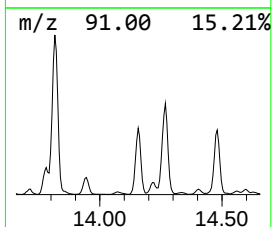
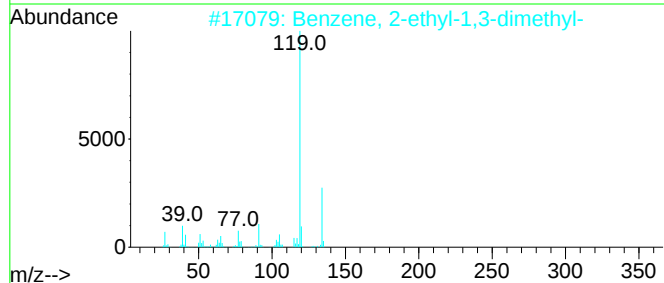
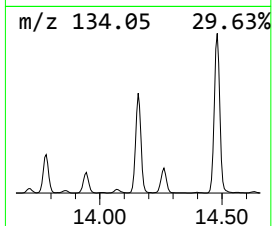
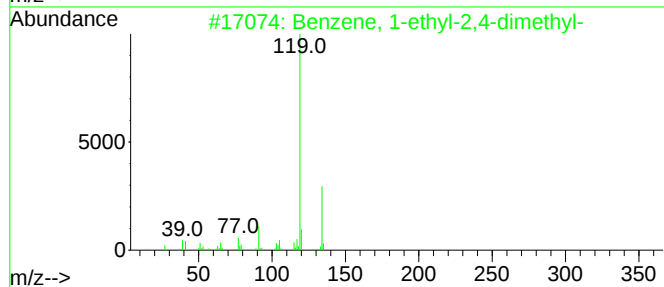
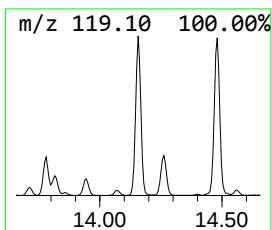
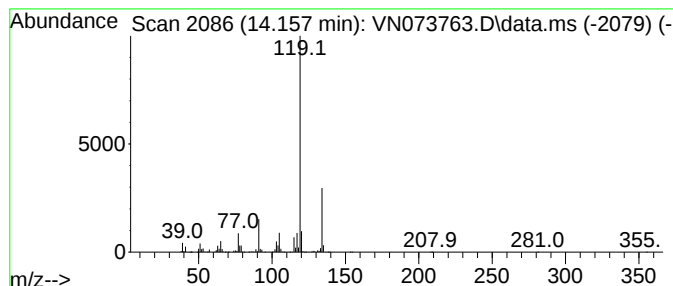
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	72.52 ug/l	3040230	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	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, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

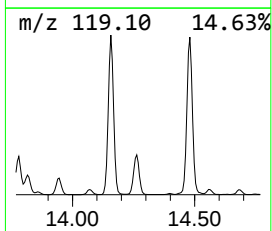
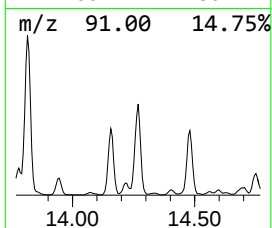
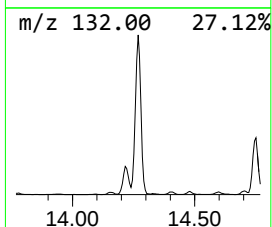
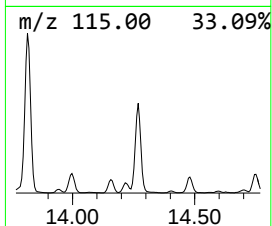
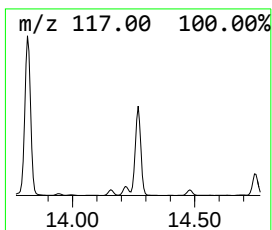
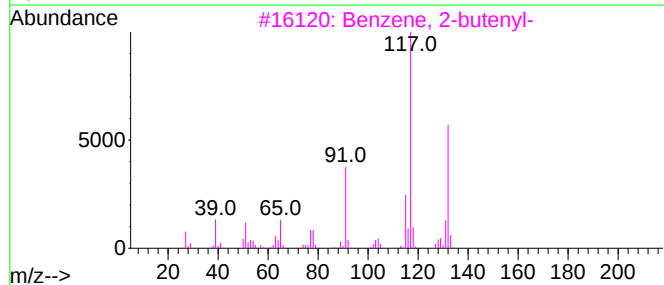
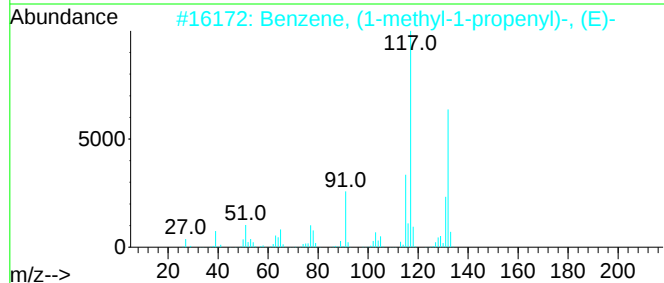
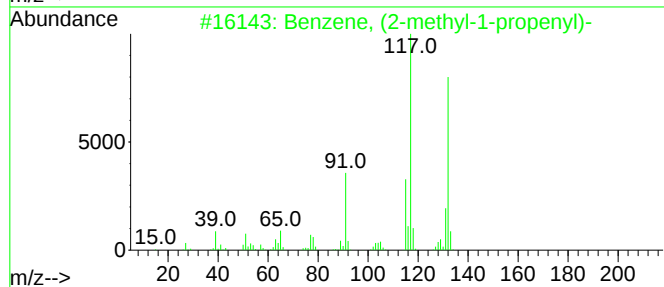
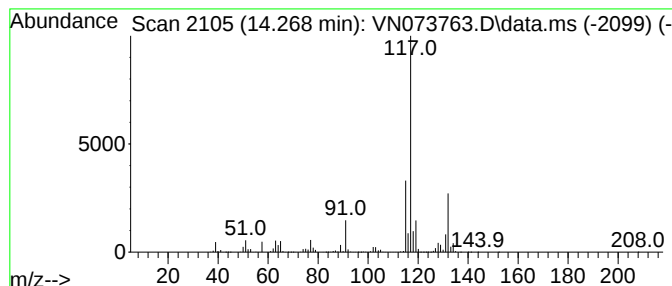
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, (2-methyl-1-propen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	126.69 ug/l	5311020	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	83
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

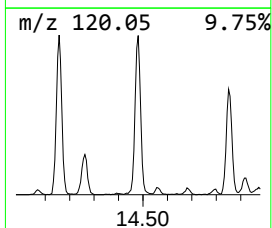
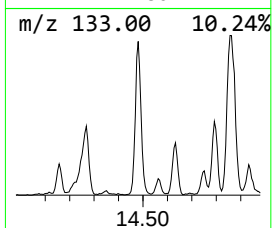
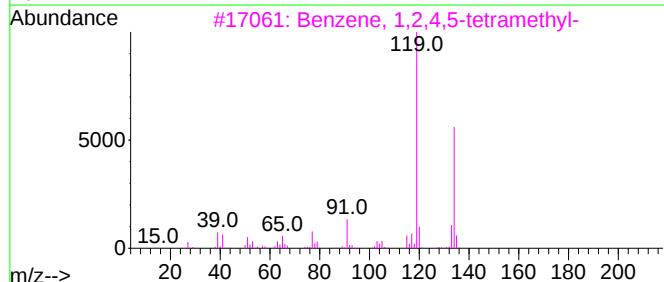
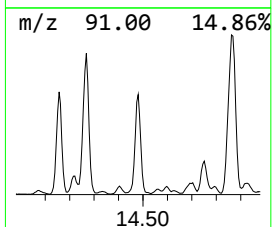
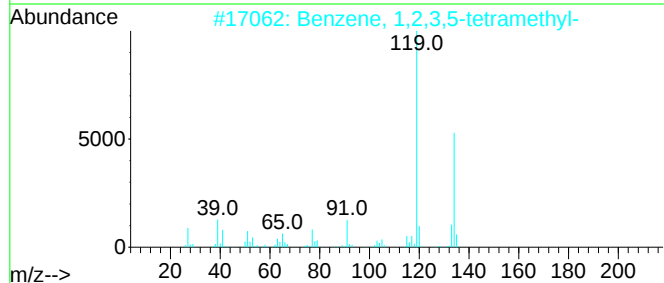
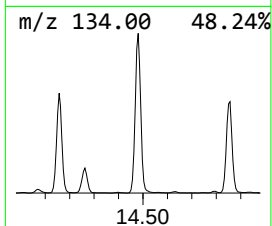
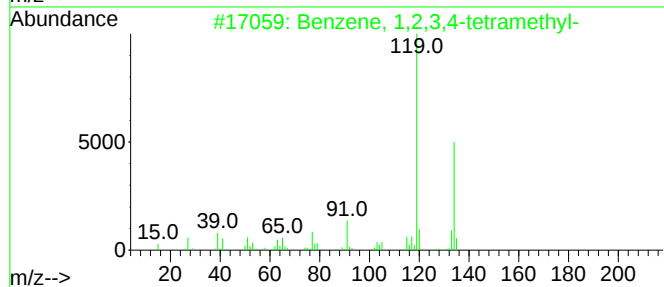
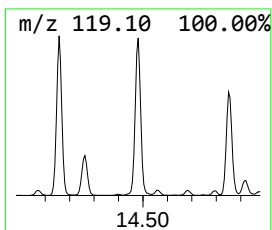
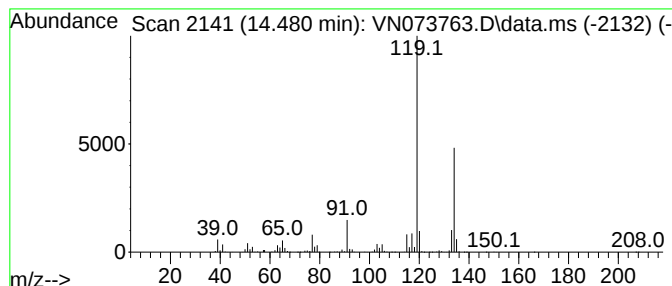
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	84.73 ug/l	3552070	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

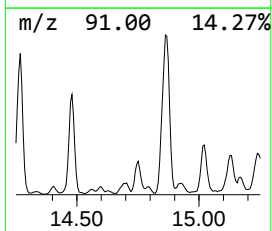
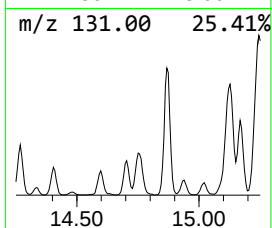
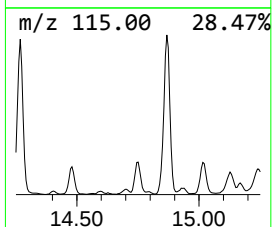
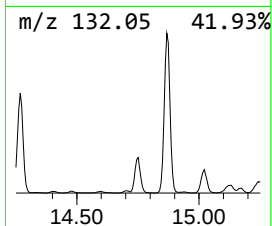
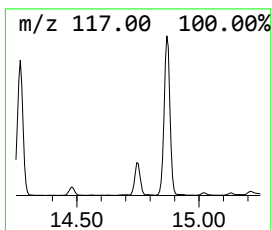
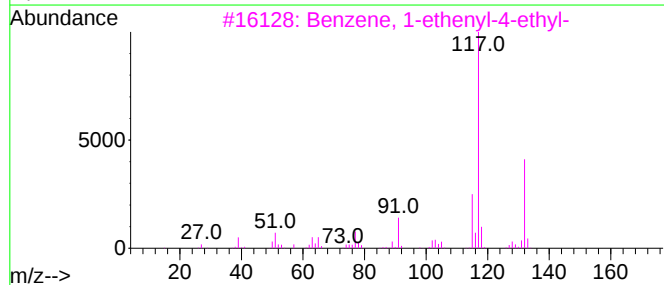
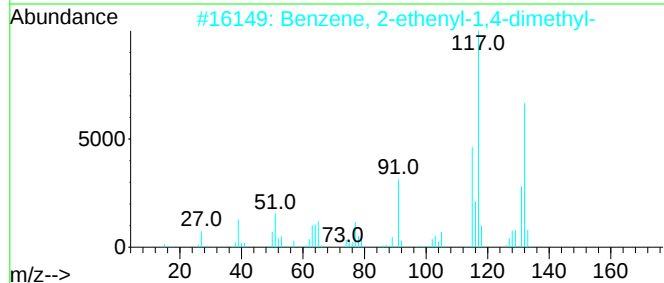
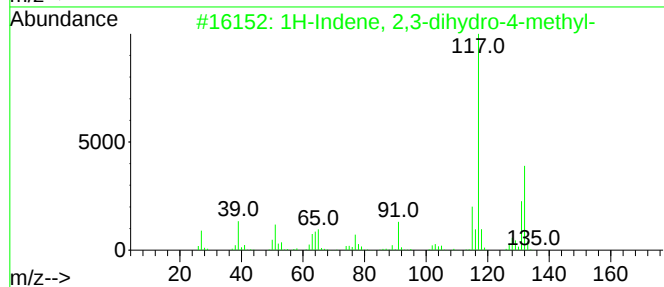
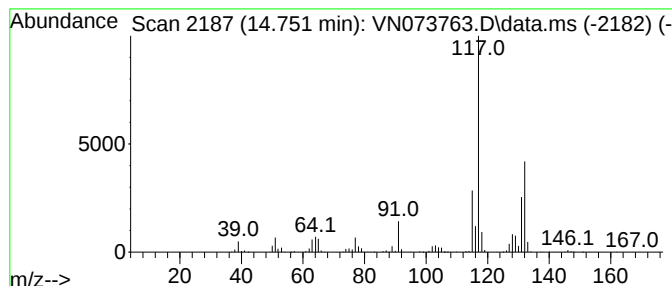
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	35.95 ug/l	1507020	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

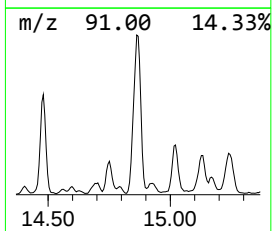
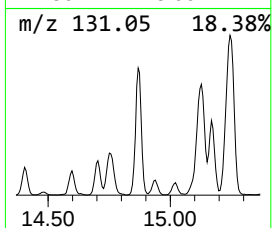
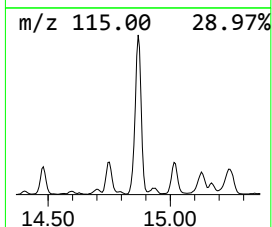
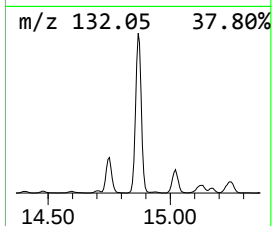
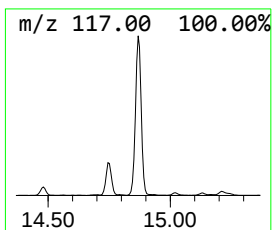
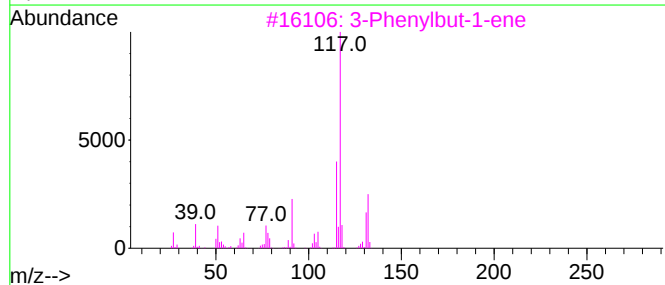
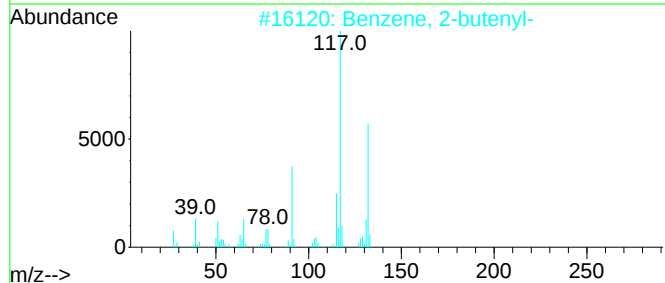
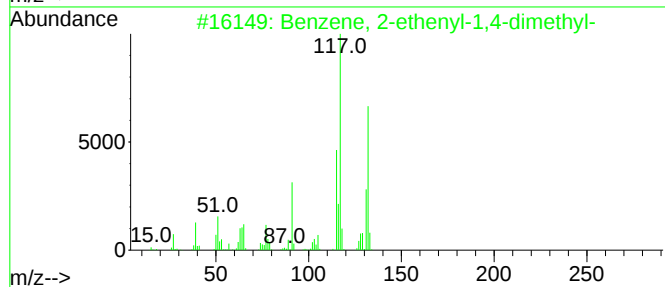
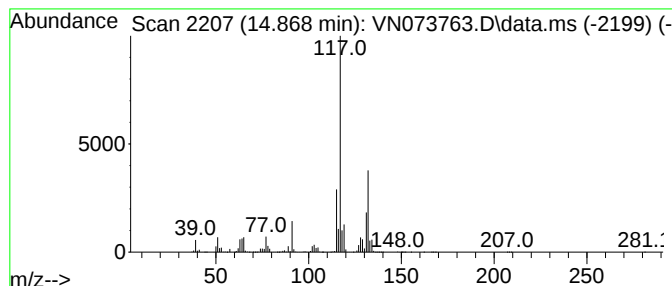
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	207.51 ug/l	8699010	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

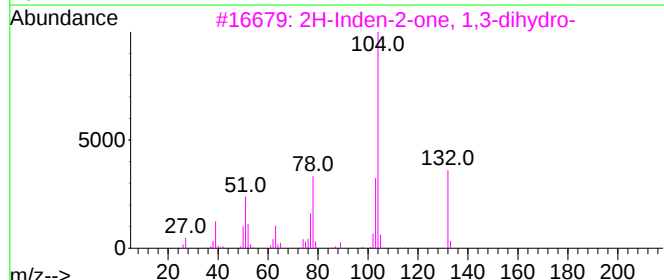
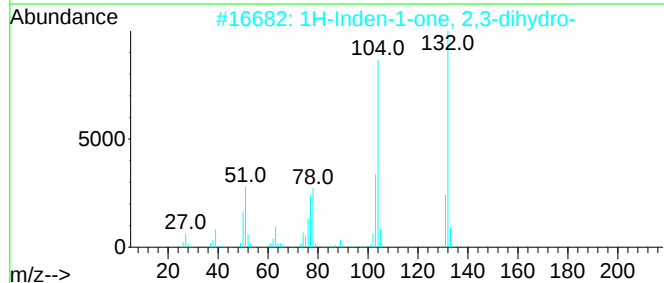
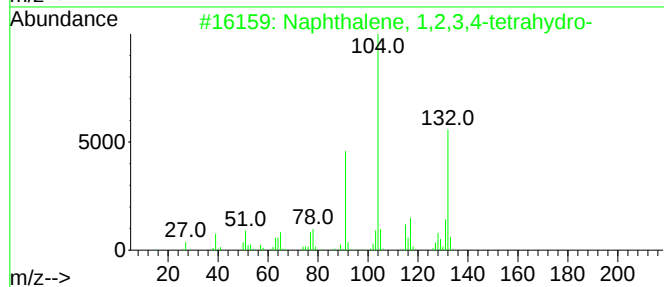
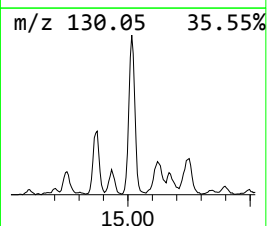
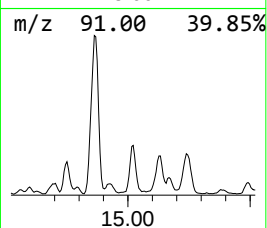
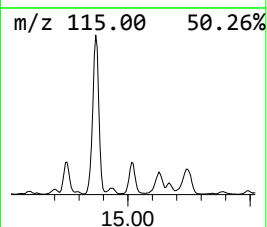
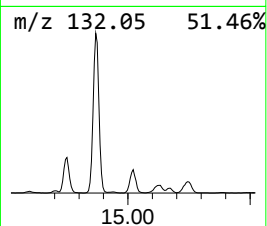
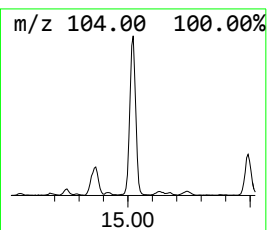
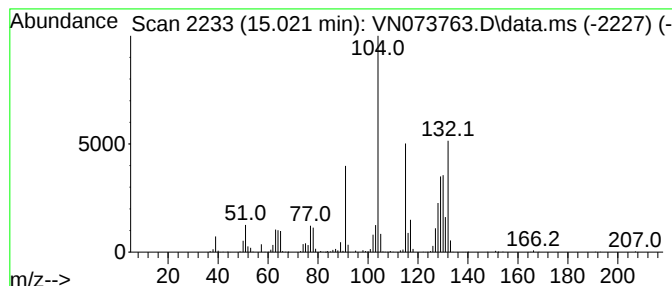
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	34.46 ug/l	1444760	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	92
2			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	45
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	38
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	35
5			2-Phenylethylamine, N,N-di(trifl...	313	C12H9F6NO2	1000463-67-7	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080522\
Data File : VN073763.D
Acq On : 05 Aug 2022 15:30
Operator : JC\MD
Sample : N3887-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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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Cyclobutane, (1...	9.910	25.8	ug/l	824068	2	8.904	1595690	50.0
Benzene, 1,2-di...	13.780	27.1	ug/l	1135080	4	13.616	2096000	50.0
Benzene, 1,1'-(...	13.816	222.4	ug/l	9322690	4	13.616	2096000	50.0
Benzene, 1-ethy...	14.157	72.5	ug/l	3040230	4	13.616	2096000	50.0
Benzene, (2-met...	14.268	126.7	ug/l	5311020	4	13.616	2096000	50.0
Benzene, 1,2,3,...	14.480	84.7	ug/l	3552070	4	13.616	2096000	50.0
1H-Indene, 2,3-...	14.751	36.0	ug/l	1507020	4	13.616	2096000	50.0
Benzene, 2-ethe...	14.868	207.5	ug/l	8699010	4	13.616	2096000	50.0
Naphthalene, 1,...	15.021	34.5	ug/l	1444760	4	13.616	2096000	50.0