

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
 Data File : VN076946.D
 Acq On : 11 Mar 2023 00:04
 Operator : JC\MD
 Sample : 01854-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 33952

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\82N031023W.M
 Title : SW846 8260

Signal : TIC: VN076946.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.096	20	27	36	rBV2	35556	65316	1.90%	0.238%
2	2.307	54	63	66	rBV	39803	82087	2.39%	0.299%
3	2.496	89	95	98	rBV	67574	118004	3.44%	0.429%
4	2.525	98	100	111	rVB2	57168	92225	2.69%	0.336%
5	2.825	148	151	162	rVB7	13086	36975	1.08%	0.135%
6	3.254	217	224	237	rVB3	25216	74361	2.17%	0.271%
7	3.807	308	318	327	rBV2	28817	82894	2.41%	0.302%
8	4.448	416	427	437	rBV2	14784	49168	1.43%	0.179%
9	5.813	648	659	673	rBV4	18894	66159	1.93%	0.241%
10	6.695	793	809	826	rBV3	58023	203040	5.91%	0.739%
11	7.242	893	902	910	rBV5	21929	60660	1.77%	0.221%
12	7.342	910	919	928	rVB5	10520	34606	1.01%	0.126%
13	8.178	1051	1061	1065	rBV	263782	650195	18.94%	2.366%
14	8.231	1065	1070	1088	rVB	540341	1232203	35.89%	4.485%
15	8.601	1121	1133	1145	rBV3	379110	1322701	38.53%	4.814%
16	9.107	1211	1219	1233	rBV	716045	1486082	43.29%	5.409%
17	10.572	1460	1468	1473	rBV	1044010	1961975	57.15%	7.141%
18	10.636	1473	1479	1503	rVB	1801875	3433225	100.00%	12.496%
19	11.871	1677	1689	1699	rBV	939983	1685614	49.10%	6.135%
20	11.966	1699	1705	1713	rVB	116994	203981	5.94%	0.742%
21	12.071	1715	1723	1734	rBV	983861	1930055	56.22%	7.025%
22	12.401	1772	1779	1786	rBV	825506	1405082	40.93%	5.114%
23	12.854	1846	1856	1864	rBV	751892	1325199	38.60%	4.823%
24	13.048	1882	1889	1891	rBV	20392	39345	1.15%	0.143%
25	13.101	1891	1898	1901	rBV	298801	521350	15.19%	1.898%
26	13.177	1907	1911	1918	rVB	216260	355072	10.34%	1.292%
27	13.342	1924	1939	1947	rBV	241731	459924	13.40%	1.674%
28	13.483	1957	1963	1970	rBV	479624	779200	22.70%	2.836%
29	13.677	1992	1996	2003	rBV5	33480	65969	1.92%	0.240%
30	13.795	2009	2016	2026	rBV2	928444	2185462	63.66%	7.954%
31	13.877	2026	2030	2038	rVV	141373	236273	6.88%	0.860%
32	13.960	2038	2044	2045	rVV3	41380	65463	1.91%	0.238%
33	13.995	2045	2050	2066	rVB4	191032	591643	17.23%	2.153%
34	14.183	2076	2082	2088	rVB3	48546	81087	2.36%	0.295%
35	14.248	2088	2093	2096	rBV2	64984	116667	3.40%	0.425%
36	14.277	2096	2098	2103	rVV2	59978	71795	2.09%	0.261%

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Integration Parameters: RTEINT.P

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	14.336	2103	2108	2113	rVB	128453	205945	6.00%	0.750%
38	14.401	2113	2119	2122	rBV2	23067	39825	1.16%	0.145%
39	14.448	2122	2127	2134	rVB2	85229	144022	4.19%	0.524%
40	14.577	2143	2149	2153	rBV3	51171	94078	2.74%	0.342%
41	14.660	2157	2163	2166	rVV	93412	150787	4.39%	0.549%
42	14.695	2166	2169	2174	rVB	138351	196728	5.73%	0.716%
43	14.777	2179	2183	2187	rVB3	23252	36252	1.06%	0.132%
44	14.877	2192	2200	2204	rBV8	19240	38658	1.13%	0.141%
45	14.930	2204	2209	2214	rVV2	85911	159678	4.65%	0.581%
46	14.965	2214	2215	2221	rVB2	29475	36737	1.07%	0.134%
47	15.054	2221	2230	2237	rBV3	223508	555748	16.19%	2.023%
48	15.118	2237	2241	2249	rVB5	38678	84725	2.47%	0.308%
49	15.212	2252	2257	2264	rVV	107891	198248	5.77%	0.722%
50	15.324	2265	2276	2289	rVV5	88157	340134	9.91%	1.238%
51	15.442	2289	2296	2306	rVB3	83119	232152	6.76%	0.845%
52	15.642	2324	2330	2336	rVB	67524	123158	3.59%	0.448%
53	15.707	2336	2341	2345	rBV3	40193	69074	2.01%	0.251%
54	15.754	2345	2349	2352	rBV4	24083	39692	1.16%	0.144%
55	15.948	2375	2382	2392	rBV3	62791	157070	4.57%	0.572%
56	16.130	2403	2413	2414	rBV4	55157	101998	2.97%	0.371%
57	16.171	2415	2420	2430	rVV2	153130	352843	10.28%	1.284%
58	16.259	2430	2435	2441	rVV5	30604	68479	1.99%	0.249%
59	16.348	2441	2450	2464	rVB5	64104	233602	6.80%	0.850%
60	16.501	2464	2476	2488	rBV5	121341	388217	11.31%	1.413%
61	16.718	2500	2513	2519	rBV5	82054	256407	7.47%	0.933%

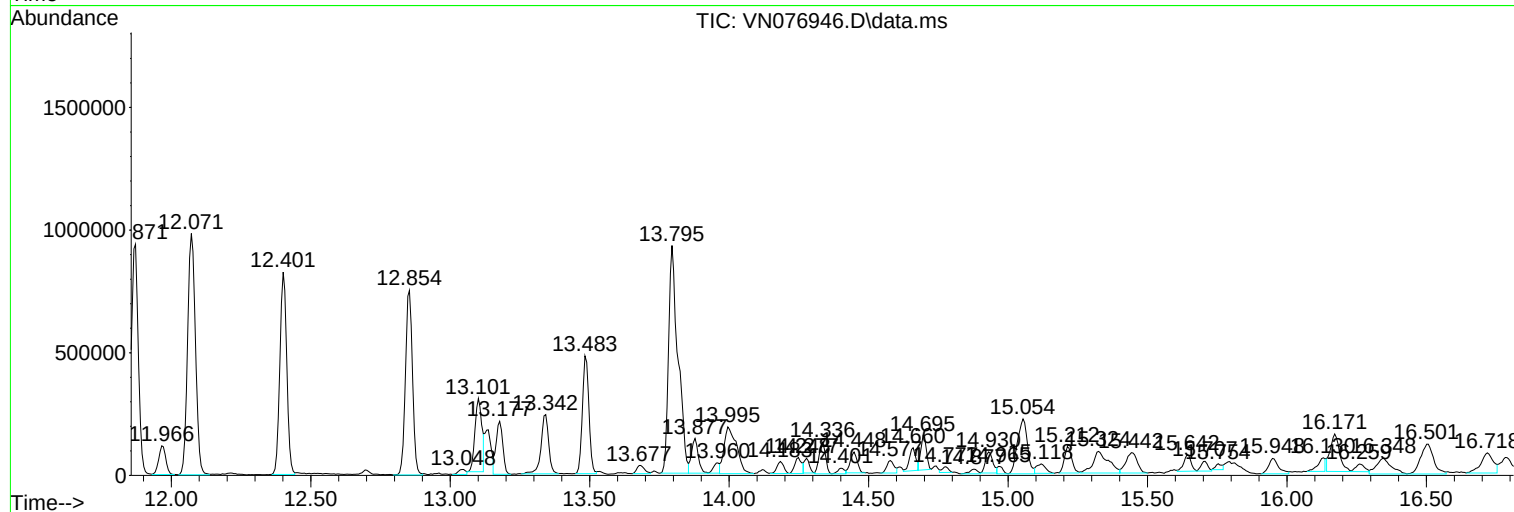
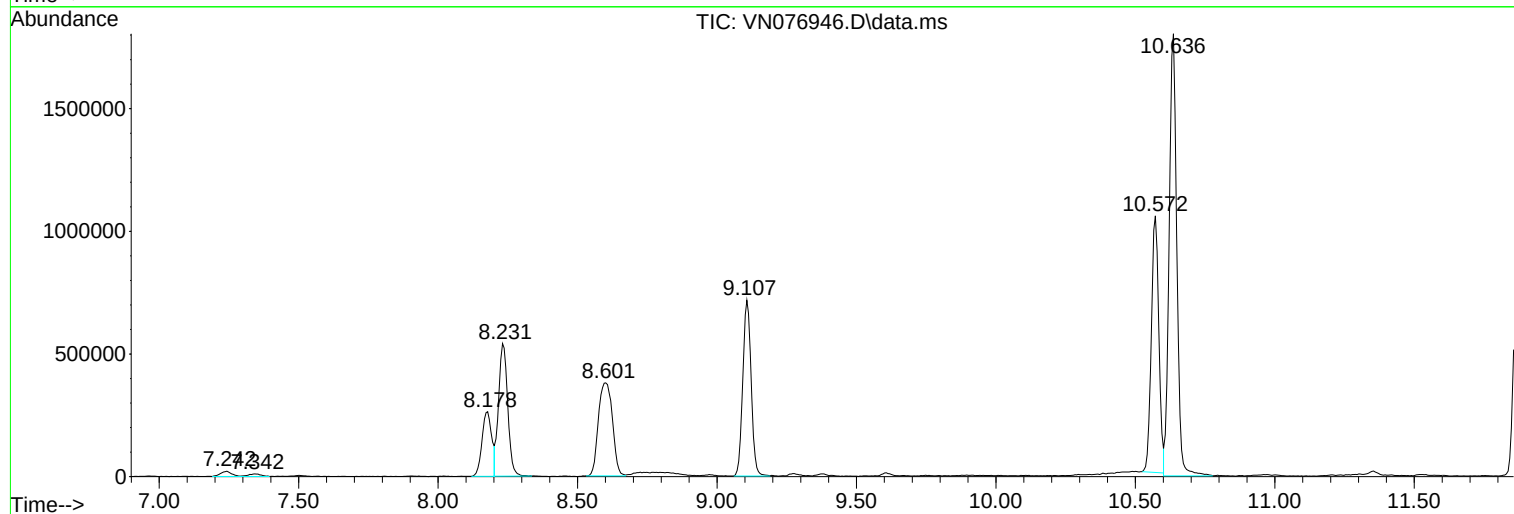
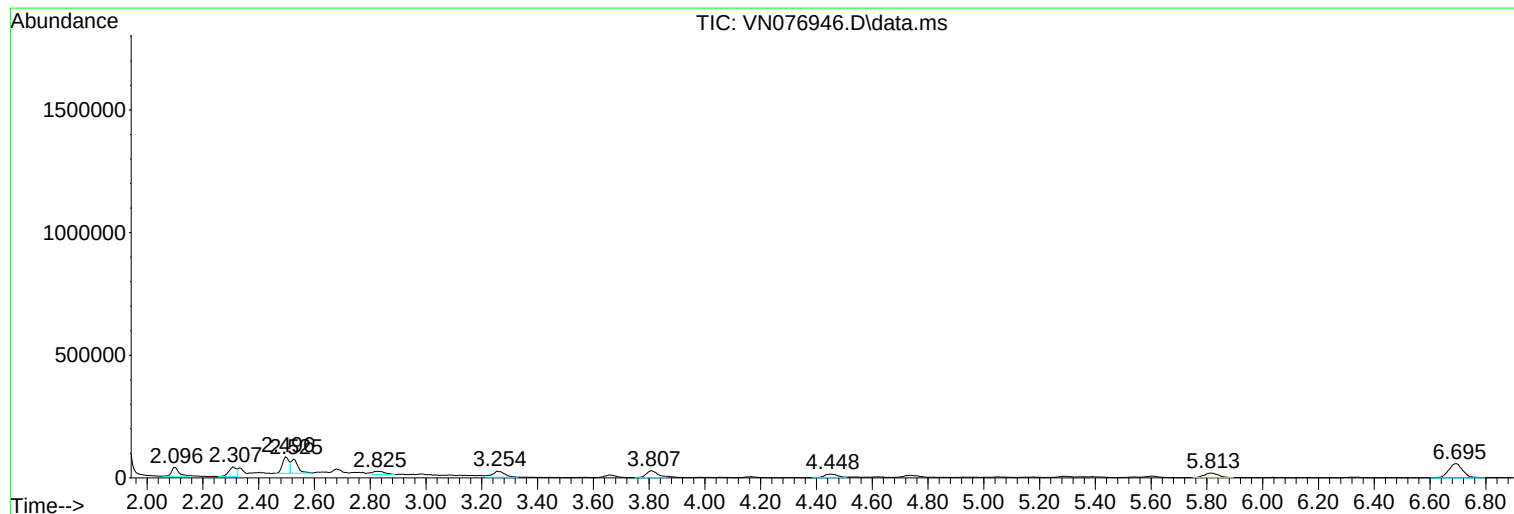
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031023W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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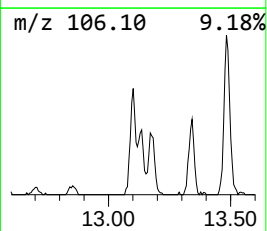
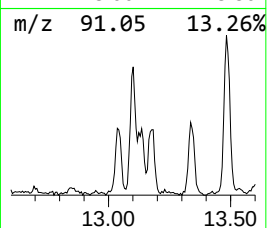
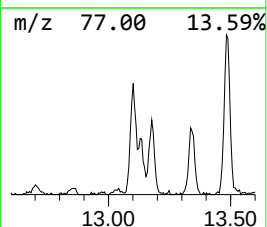
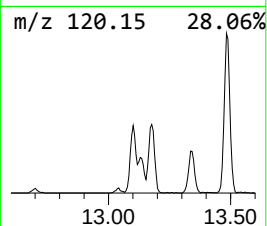
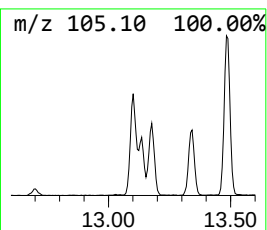
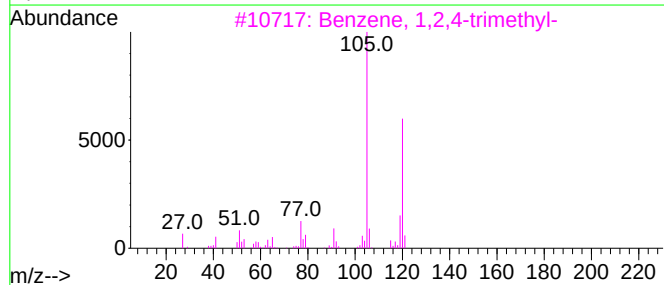
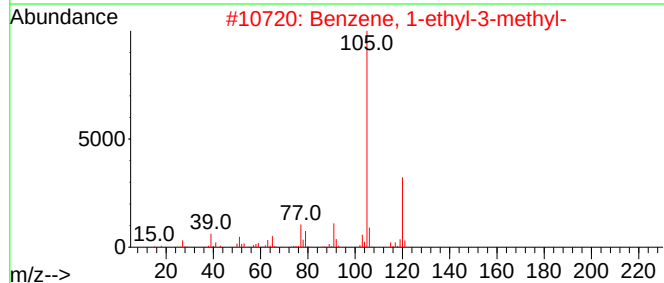
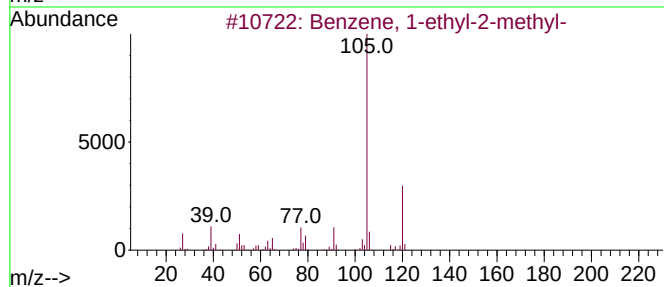
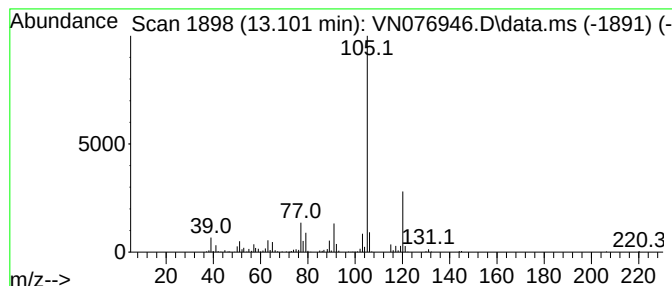
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.101	11.93 ug/l	521350	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5			Mesitylene	120	C9H12	000108-67-8	87



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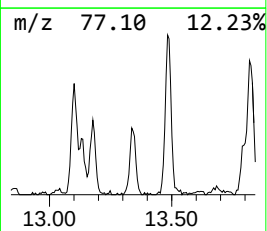
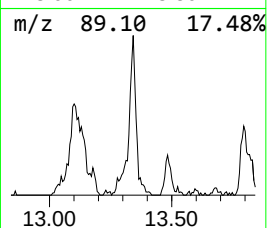
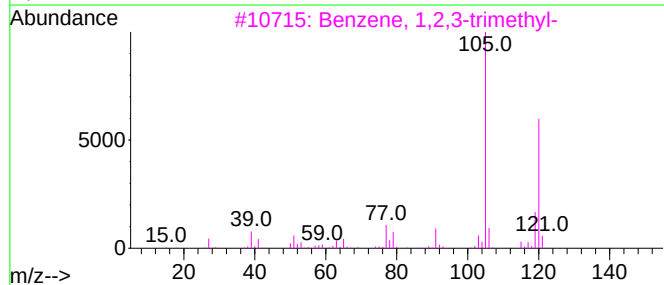
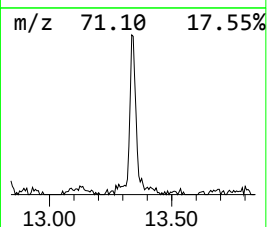
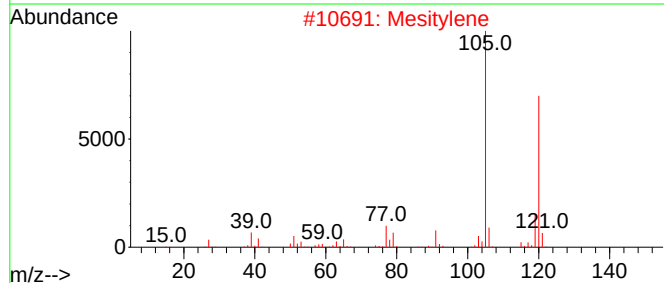
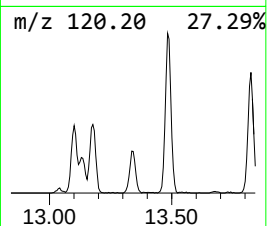
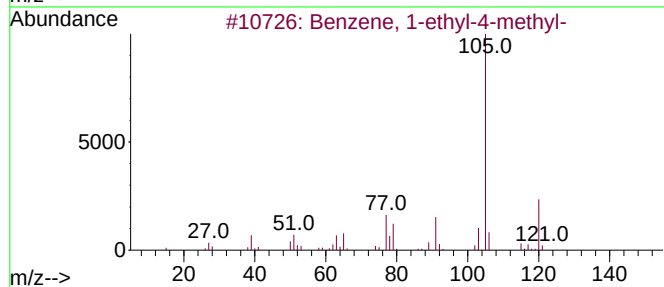
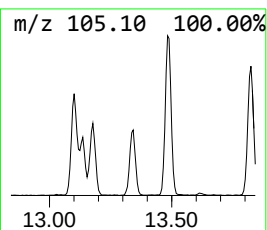
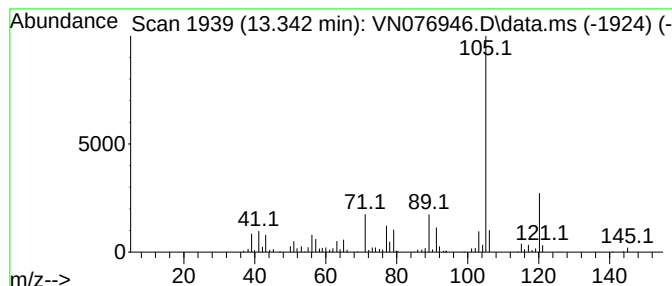
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031023W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.342	10.52 ug/l	459924	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2			Mesitylene	120	C9H12	000108-67-8	81
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	81
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	81
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	81



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ALS Vial : 35 Sample Multiplier: 1

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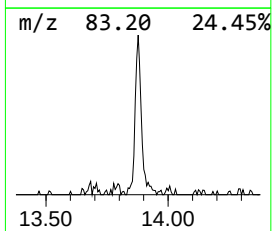
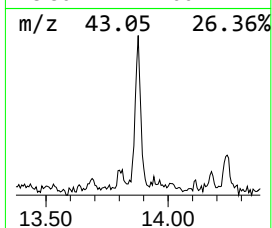
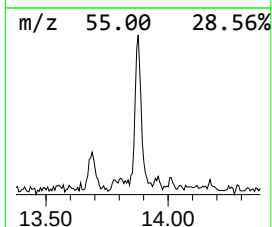
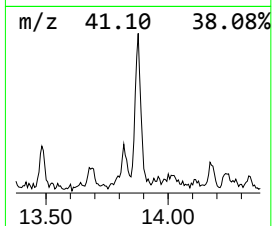
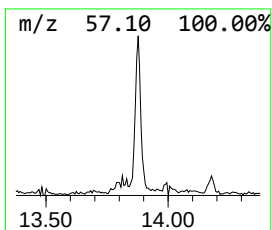
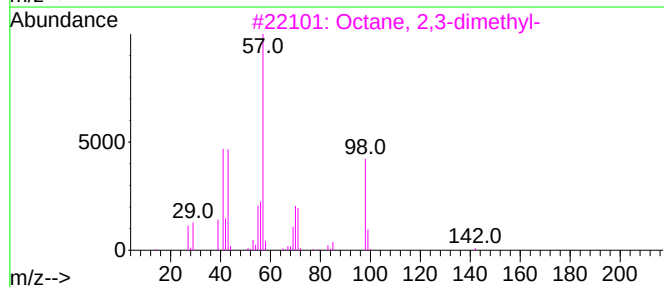
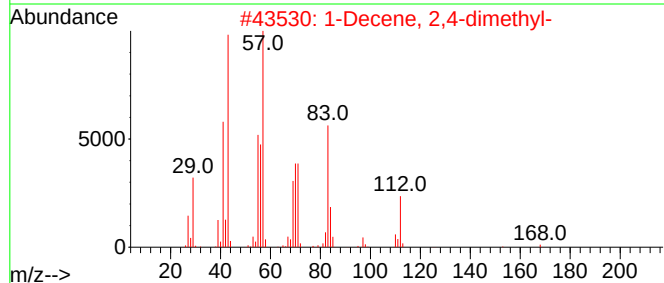
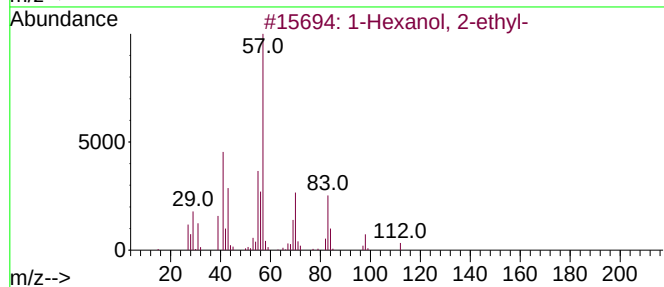
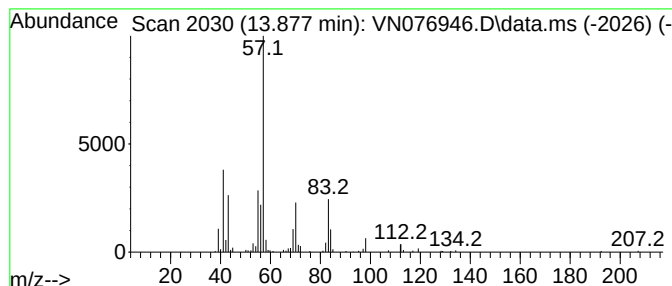
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Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.877	5.41 ug/l	236273	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
3			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
4			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	47
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47



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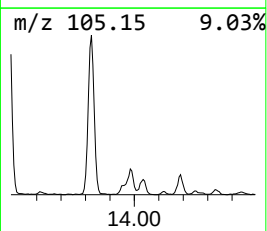
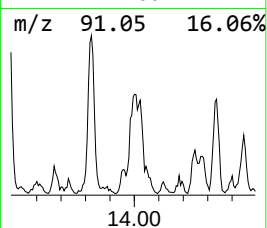
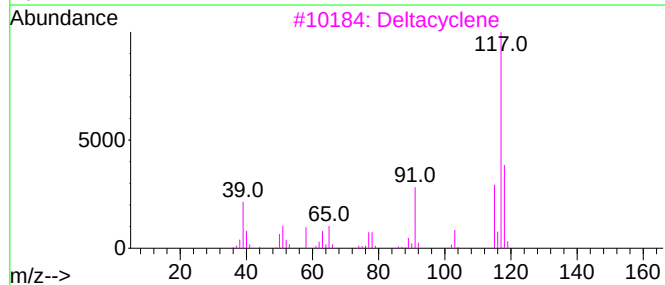
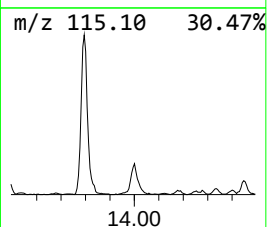
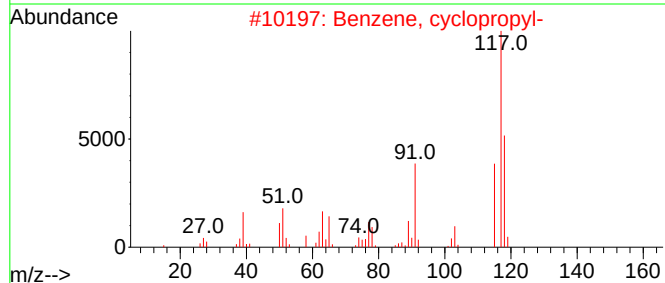
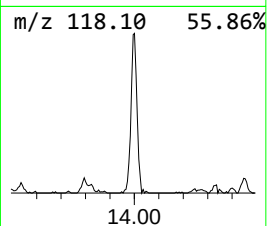
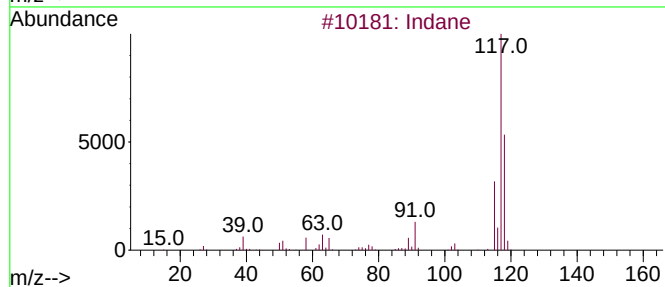
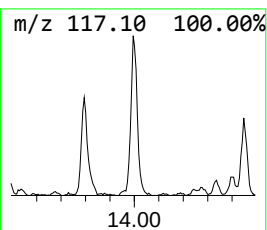
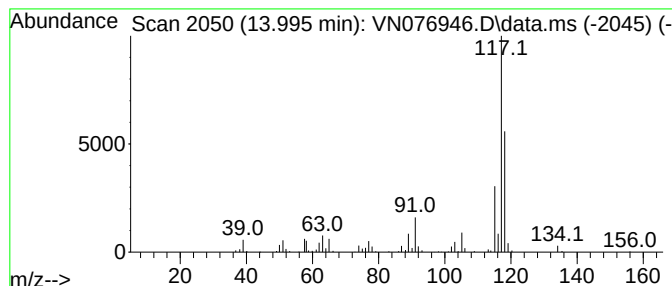
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031023W.M
Quant Title : SW846 8260

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.
13.995	13.54 ug/l	591643	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Deltacyclene	118	C9H10	007785-10-6	58
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
5			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50



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ClientSampleId :
33952

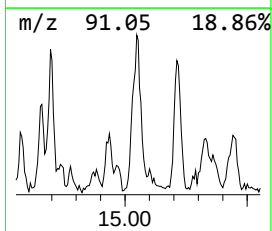
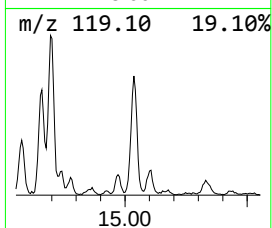
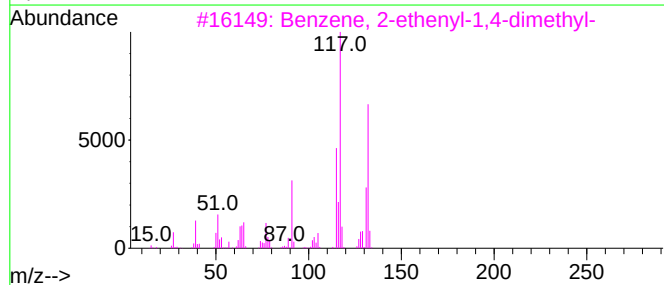
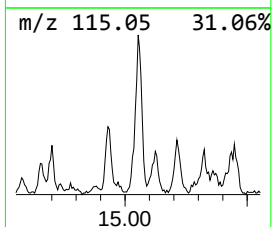
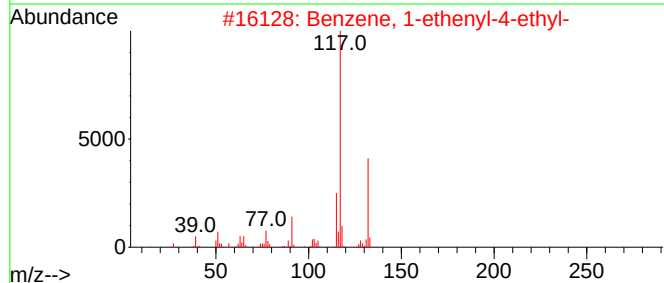
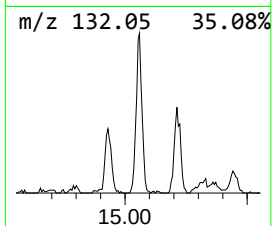
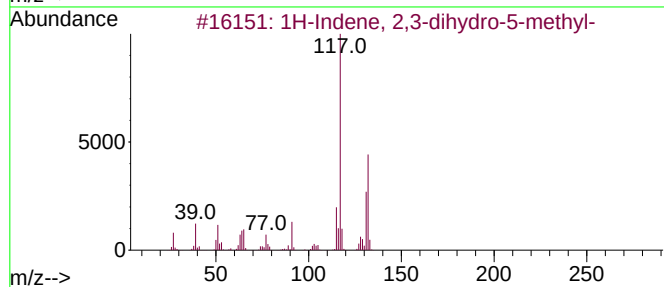
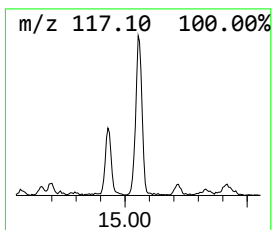
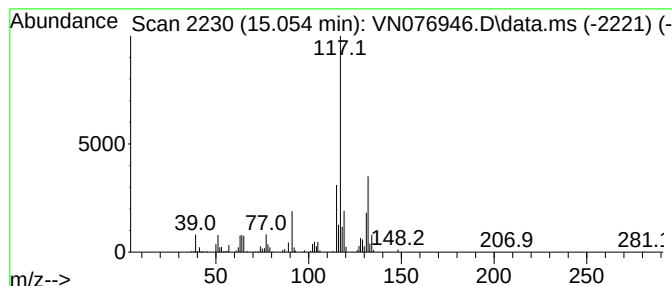
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.054	12.71 ug/l	555748	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	87
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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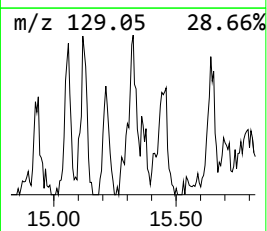
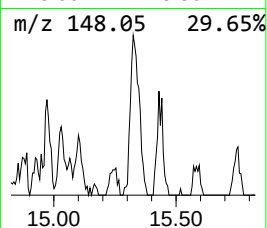
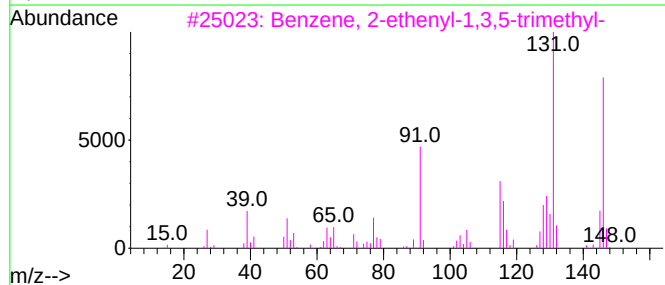
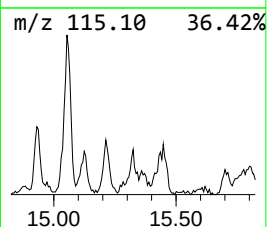
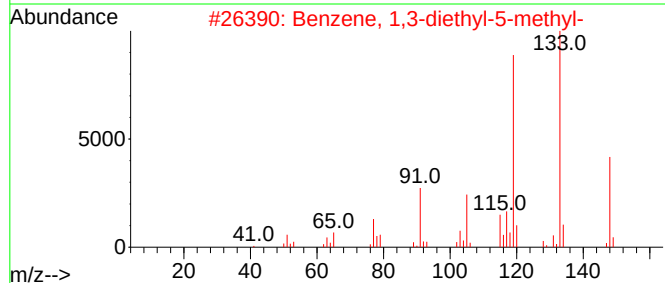
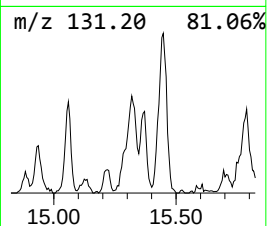
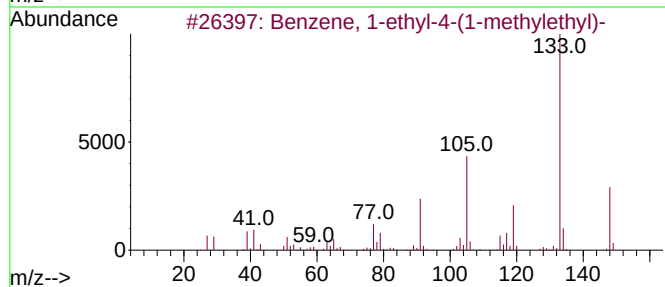
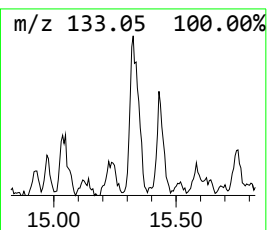
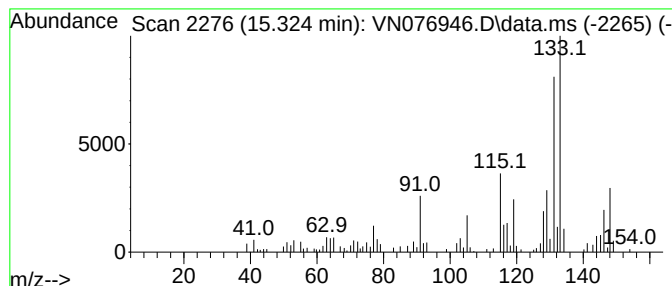
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.324	7.78 ug/l	340134	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	50
2			Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	46
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	46
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	46
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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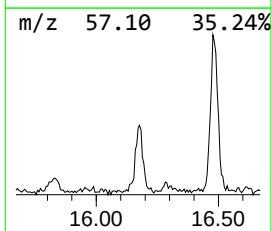
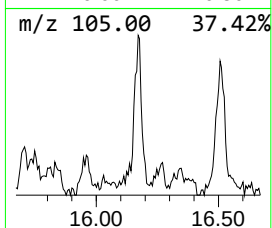
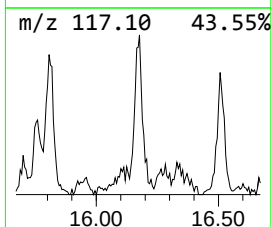
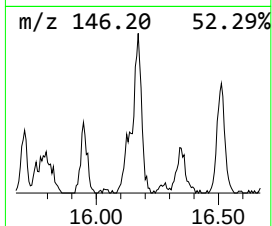
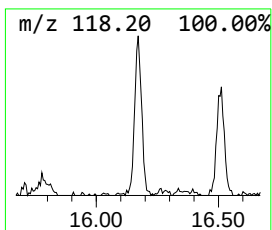
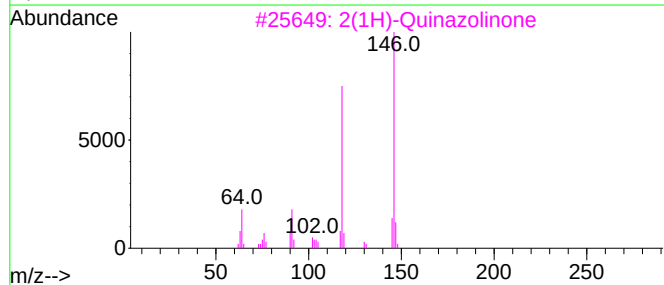
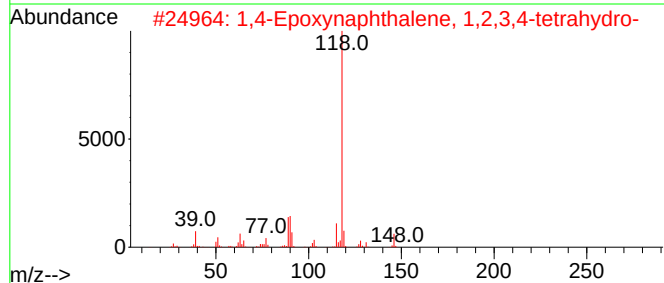
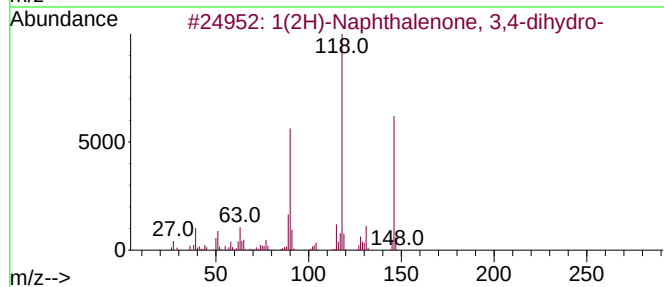
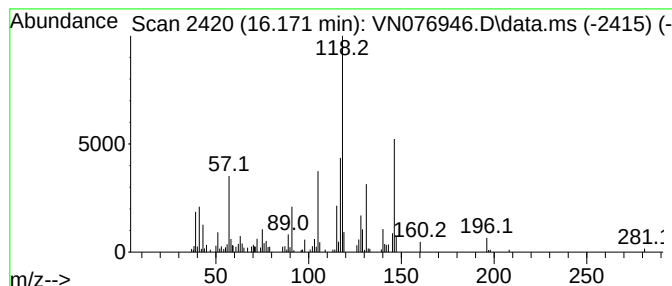
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Quant Title : SW846 8260

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

Peak Number 7 1(2H)-Naphthalenone, 3,4-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.171	8.07 ug/l	352843	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	52
2			1,4-Epoxy naphthalene, 1,2,3,4-tetrahydro-	146	C10H10O	035185-96-7	47
3			2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	46
4			Butanoic acid, 3-phenylpropyl ester	206	C13H18O2	007402-29-1	43
5			2-Hydroxy-1,8-naphthyridine	146	C8H6N2O	015936-09-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
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ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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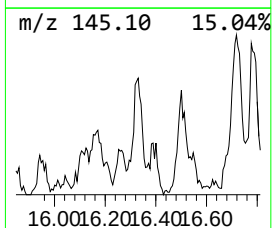
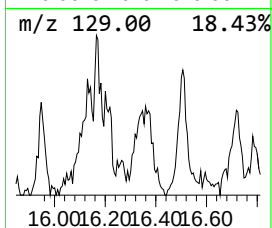
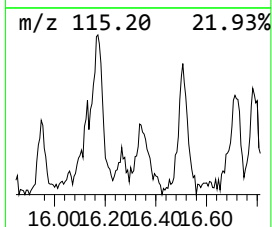
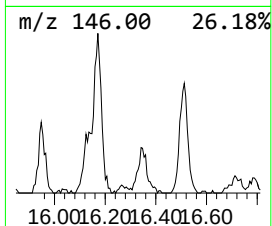
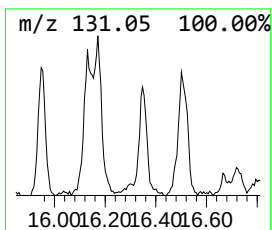
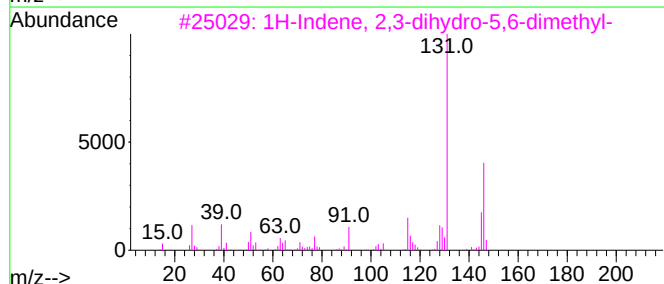
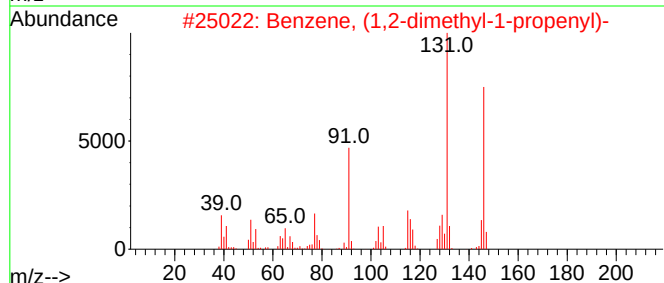
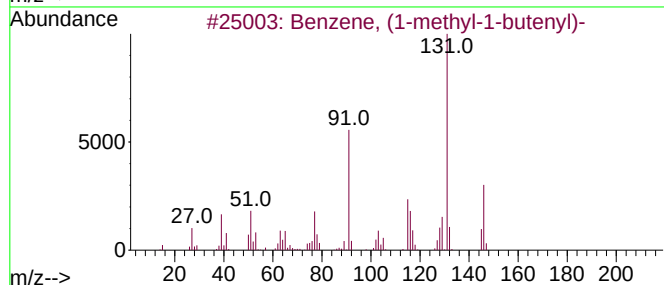
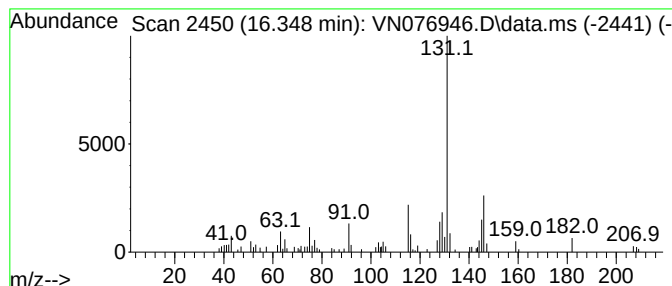
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (1-methyl-1-butenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.348	5.34 ug/l	233602	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	90
2			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	87
3			1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	87
4			1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	87
5			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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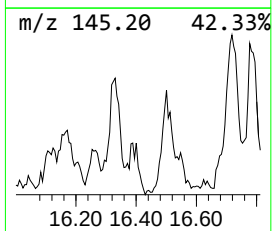
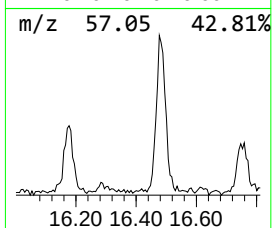
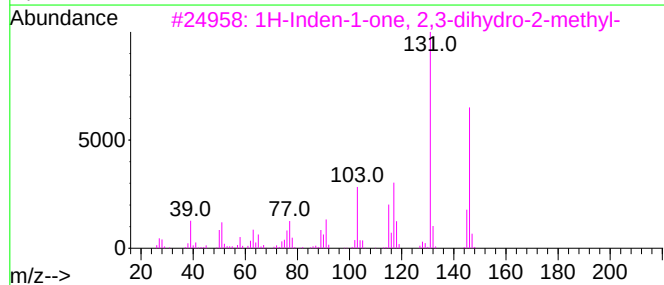
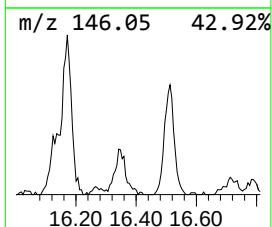
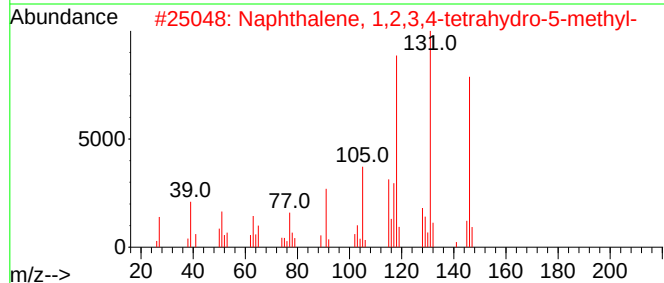
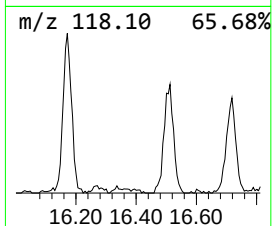
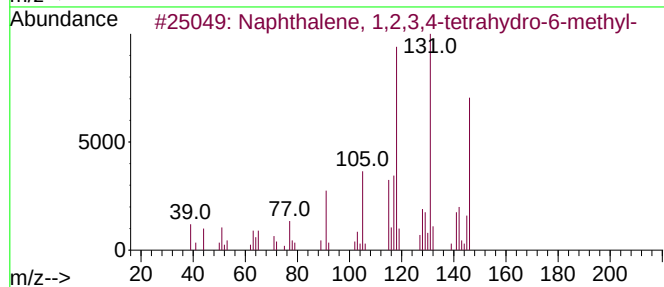
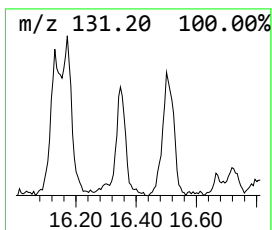
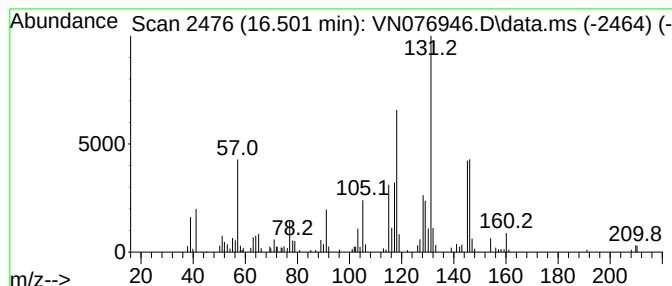
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.501	8.88 ug/l	388217	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
3			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	60
4			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	60
5			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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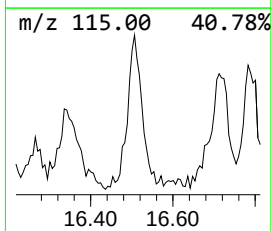
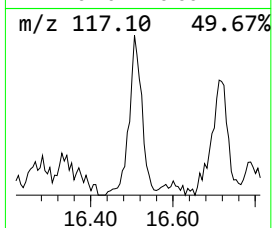
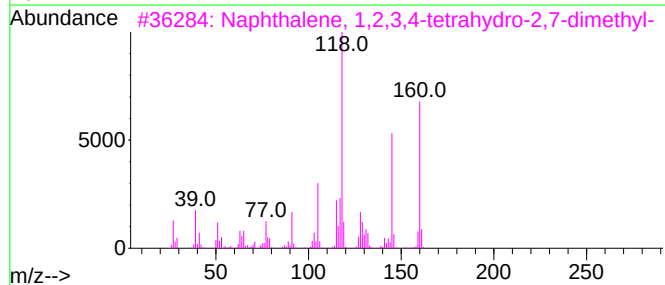
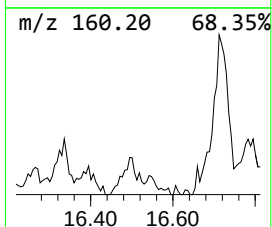
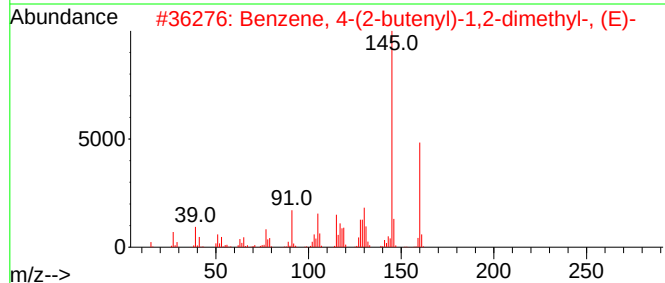
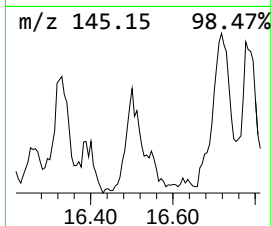
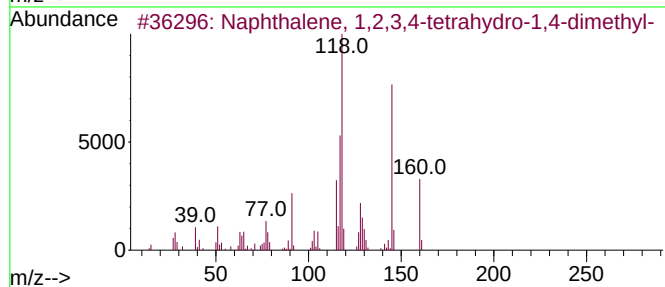
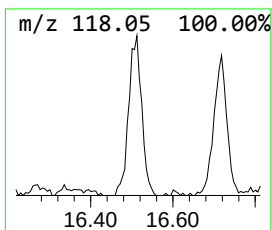
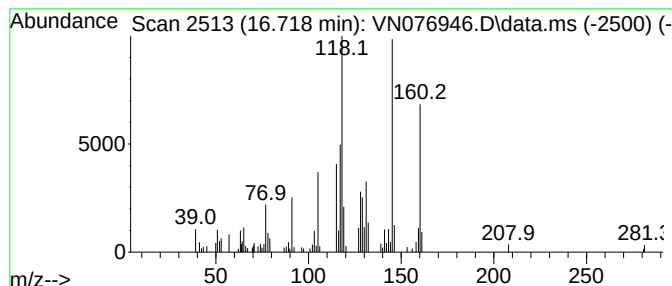
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.718	5.87 ug/l	256407	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	96
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	78
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
4			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	53
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031023\
Data File : VN076946.D
Acq On : 11 Mar 2023 00:04
Operator : JC\MD
Sample : 01854-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031023W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1-ethy...	13.342	10.5	ug/l	459924	4	13.795	2185460	50.0
1-Hexanol, 2-et...	13.877	5.4	ug/l	236273	4	13.795	2185460	50.0
Indane	13.995	13.5	ug/l	591643	4	13.795	2185460	50.0
1H-Indene, 2,3-...	15.054	12.7	ug/l	555748	4	13.795	2185460	50.0
Benzene, 1-ethy...	15.324	7.8	ug/l	340134	4	13.795	2185460	50.0
1(2H)-Naphthale...	16.171	8.1	ug/l	352843	4	13.795	2185460	50.0
Benzene, (1-met...	16.348	5.3	ug/l	233602	4	13.795	2185460	50.0
Naphthalene, 1,...	16.501	8.9	ug/l	388217	4	13.795	2185460	50.0
Naphthalene, 1,...	16.718	5.9	ug/l	256407	4	13.795	2185460	50.0