

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
 Data File : VN073347.D
 Acq On : 06 Jul 2022 16:00
 Operator : JC\MD
 Sample : N3564-31
 Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-16-2-3

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073347.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.775	481	491	502	rBV2	24293	77363	2.06%	0.165%
2	7.281	909	917	930	rBV3	27544	86192	2.29%	0.184%
3	7.945	1018	1030	1035	rBV2	203937	509758	13.55%	1.090%
4	8.004	1035	1040	1049	rVV	388988	918456	24.41%	1.963%
5	8.080	1049	1053	1066	rVB4	23017	59557	1.58%	0.127%
6	8.210	1066	1075	1080	rBV3	17263	41941	1.11%	0.090%
7	8.363	1092	1101	1111	rBV	218077	499040	13.27%	1.067%
8	8.486	1116	1122	1125	rVV3	26194	57851	1.54%	0.124%
9	8.539	1126	1131	1139	rVV5	36792	115222	3.06%	0.246%
10	8.622	1139	1145	1158	rVB4	35756	85632	2.28%	0.183%
11	8.898	1183	1192	1203	rBV	543426	1169164	31.08%	2.499%
12	9.386	1259	1275	1281	rBV	427697	1021058	27.14%	2.183%
13	9.563	1301	1305	1311	rVB2	37216	71276	1.89%	0.152%
14	9.657	1317	1321	1329	rVB3	43662	88232	2.35%	0.189%
15	9.804	1340	1346	1353	rBV2	73544	147959	3.93%	0.316%
16	9.951	1365	1371	1375	rBV2	65166	123190	3.27%	0.263%
17	10.004	1377	1380	1386	rVB5	25495	46855	1.25%	0.100%
18	10.139	1396	1403	1407	rBV3	57461	136381	3.63%	0.292%
19	10.374	1436	1443	1460	rVB2	1042224	2366115	62.89%	5.058%
20	10.498	1460	1464	1466	rVV3	36385	50113	1.33%	0.107%
21	10.551	1466	1473	1483	rVB6	105467	299965	7.97%	0.641%
22	10.716	1496	1501	1509	rVB	176562	321601	8.55%	0.687%
23	10.810	1510	1517	1524	rVV4	143366	334025	8.88%	0.714%
24	10.904	1528	1533	1538	rVB2	50559	92504	2.46%	0.198%
25	10.986	1543	1547	1554	rVB	162805	272588	7.25%	0.583%
26	11.086	1561	1564	1571	rVB	62737	111443	2.96%	0.238%
27	11.157	1573	1576	1579	rVV4	48407	64470	1.71%	0.138%
28	11.192	1580	1582	1583	rVV2	47217	43807	1.16%	0.094%
29	11.227	1584	1588	1593	rVV	267641	437559	11.63%	0.935%
30	11.280	1593	1597	1603	rVV	268589	456841	12.14%	0.977%
31	11.333	1603	1606	1610	rVB3	69786	95481	2.54%	0.204%
32	11.392	1611	1616	1621	rBV3	150275	245761	6.53%	0.525%
33	11.486	1628	1632	1636	rBV2	122319	178556	4.75%	0.382%
34	11.563	1642	1645	1649	rBV	82218	121717	3.24%	0.260%
35	11.710	1660	1670	1678	rBV2	1398715	3762063	100.00%	8.042%
36	11.816	1685	1688	1691	rBV2	68601	91103	2.42%	0.195%

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37	11.874	1693	1698	1702	rBV5	93384	189646	5.04%	0.405%
38	11.927	1703	1707	1711	rBV	168889	307471	8.17%	0.657%
39	12.027	1721	1724	1729	rBV5	54424	87440	2.32%	0.187%
40	12.186	1745	1751	1758	rBV5	321265	809348	21.51%	1.730%
41	12.310	1768	1772	1776	rVB	326460	470063	12.49%	1.005%
42	12.392	1776	1786	1787	rBV4	340323	681043	18.10%	1.456%
43	12.421	1788	1791	1798	rVB2	406551	831950	22.11%	1.778%
44	12.674	1828	1834	1841	rBV	867250	1648254	43.81%	3.523%
45	12.833	1856	1861	1868	rBV3	609024	1045179	27.78%	2.234%
46	12.998	1882	1889	1894	rBV6	490952	1286888	34.21%	2.751%
47	13.139	1909	1913	1917	rVB3	324025	480927	12.78%	1.028%
48	13.221	1924	1927	1934	rVB	608309	922945	24.53%	1.973%
49	13.310	1939	1942	1946	rVB3	158297	217786	5.79%	0.466%
50	13.351	1946	1949	1953	rBV	180397	201817	5.36%	0.431%
51	13.504	1968	1975	1979	rBV4	654163	1541538	40.98%	3.295%
52	13.545	1979	1982	1988	rVV5	455008	755420	20.08%	1.615%
53	13.615	1989	1994	2003	rVB2	1049246	2323004	61.75%	4.966%
54	13.757	2014	2018	2024	rBV4	312586	606259	16.12%	1.296%
55	13.933	2042	2048	2053	rBV3	1380787	2583838	68.68%	5.523%
56	14.151	2082	2085	2090	rVB	456763	660129	17.55%	1.411%
57	14.262	2100	2104	2109	rVB4	491257	854911	22.72%	1.827%
58	14.327	2111	2115	2121	rVB7	338511	653808	17.38%	1.398%
59	14.380	2121	2124	2126	rBV3	212638	299378	7.96%	0.640%
60	14.445	2130	2135	2139	rBV3	1017550	1705015	45.32%	3.645%
61	14.556	2151	2154	2158	rBV	325021	394816	10.49%	0.844%
62	14.609	2158	2163	2168	rBV4	811750	1447574	38.48%	3.094%
63	14.856	2200	2205	2210	rBV3	843507	1865308	49.58%	3.987%
64	14.909	2211	2214	2221	rVB5	723213	1388132	36.90%	2.967%
65	15.127	2248	2251	2255	rVB4	514609	648364	17.23%	1.386%
66	15.398	2293	2297	2306	rBV8	585732	1205039	32.03%	2.576%
67	15.809	2364	2367	2374	rVB5	566869	972838	25.86%	2.080%
68	16.251	2438	2442	2447	rVB6	440168	786773	20.91%	1.682%
69	16.727	2518	2523	2533	rVB4	862835	2307907	61.35%	4.933%

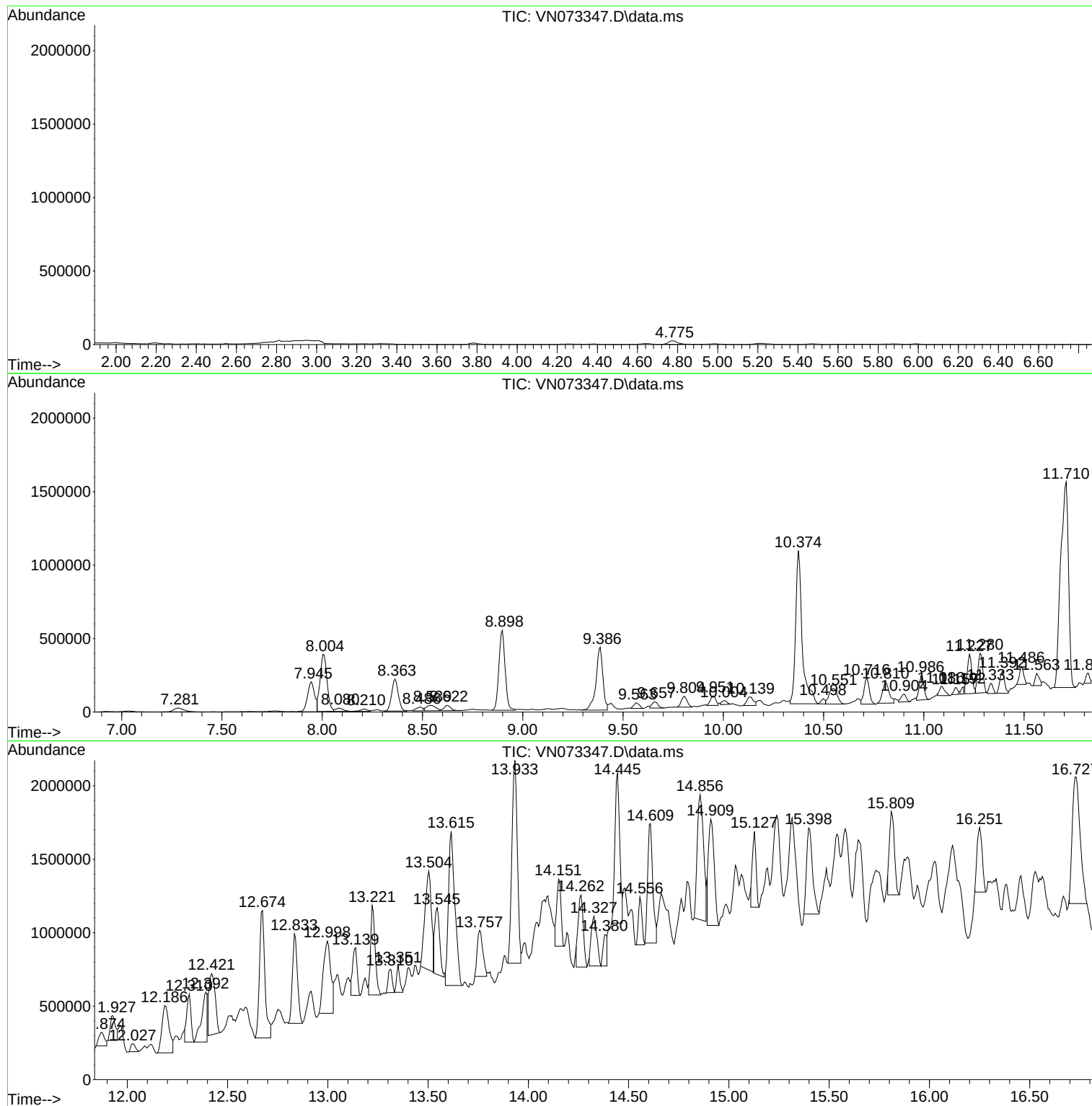
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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Instrument :
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WC-16-2-3

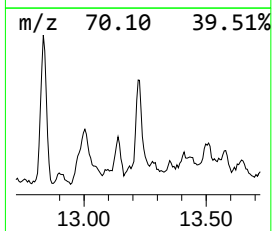
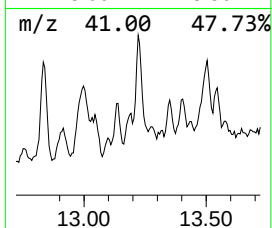
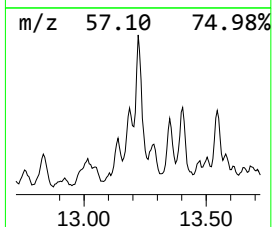
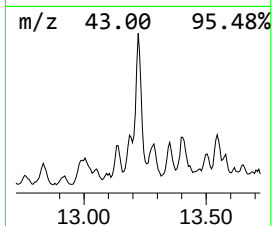
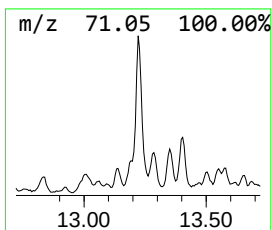
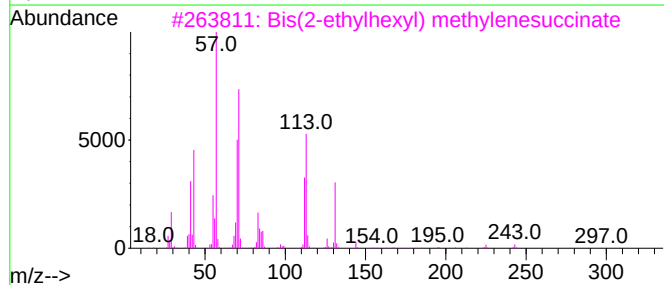
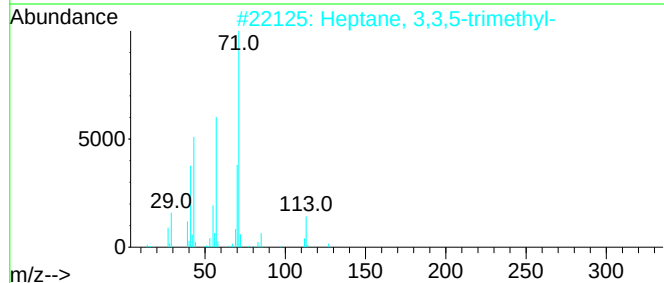
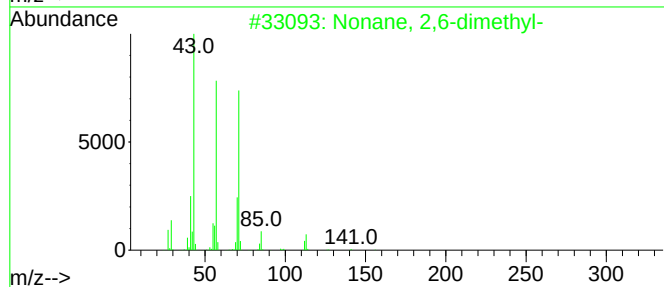
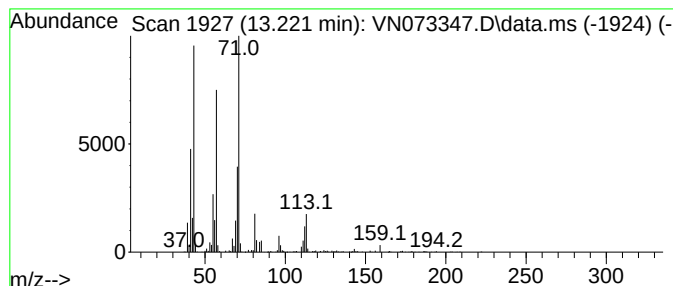
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Nonane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	19.87 ug/l	922945	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	72
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
3			Bis(2-ethylhexyl) methylenesucci...	354	C21H38O4	002287-83-4	53
4			4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	53
5			Carbonic acid, dipentyl ester	202	C11H22O3	002050-94-4	52



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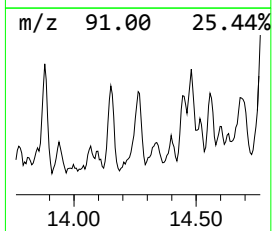
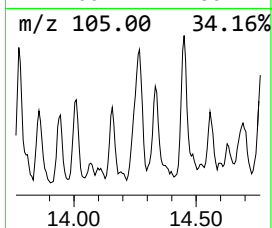
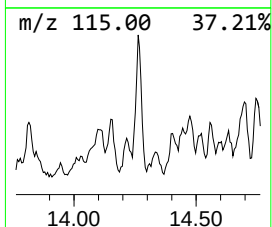
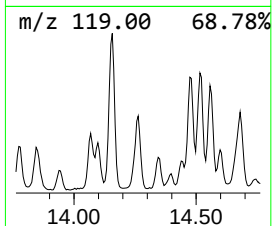
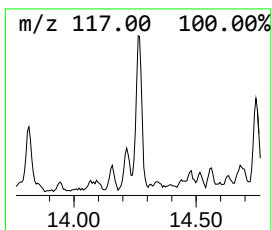
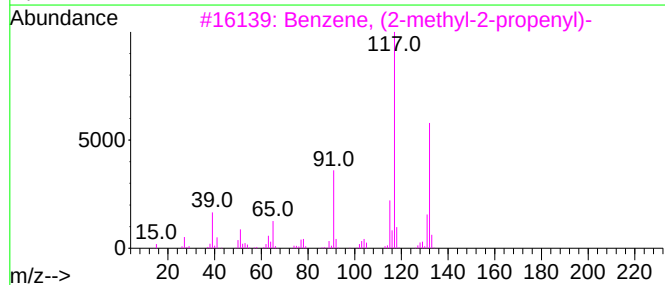
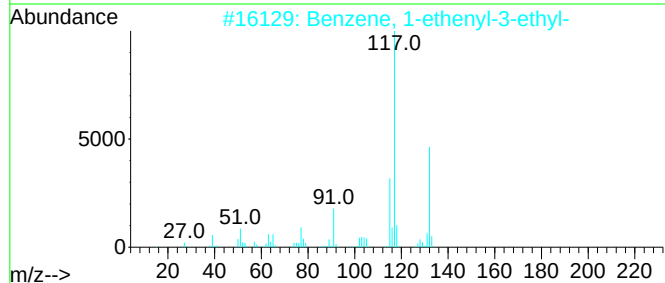
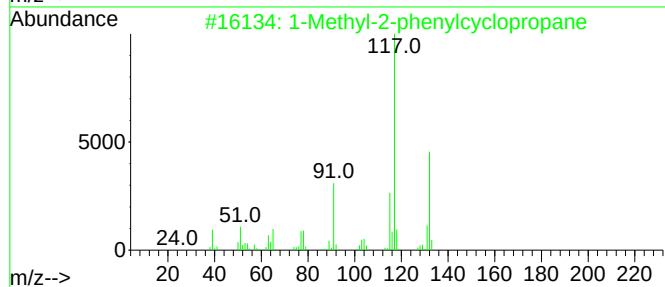
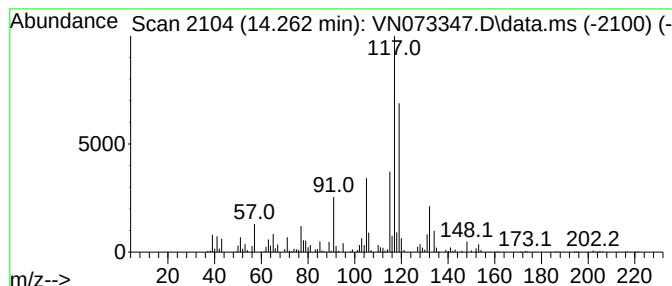
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Methyl-2-phenylcyclopropane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	18.40 ug/l	854911	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	60
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	53
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	53
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	49
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	49



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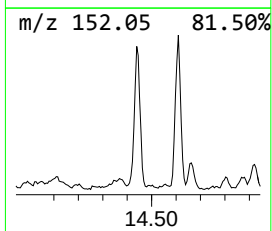
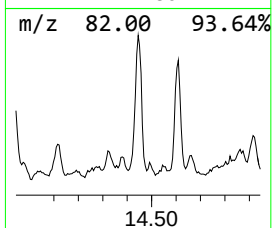
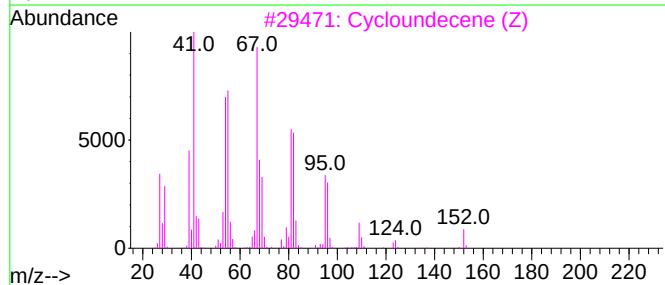
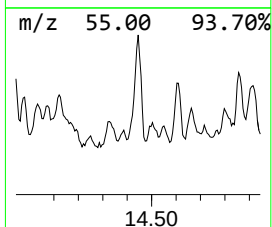
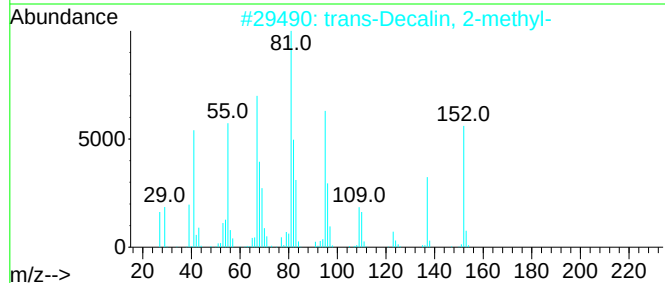
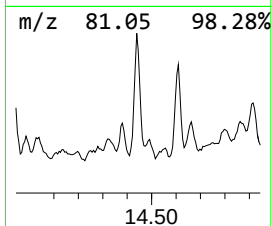
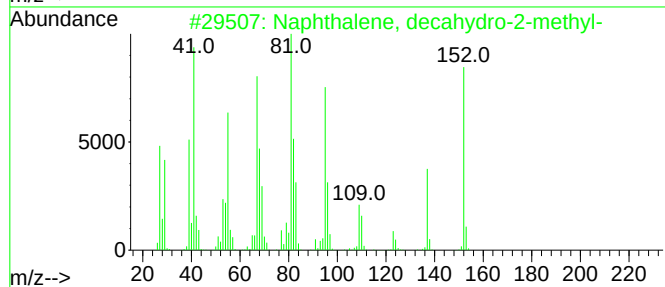
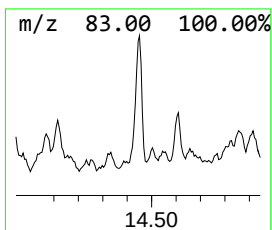
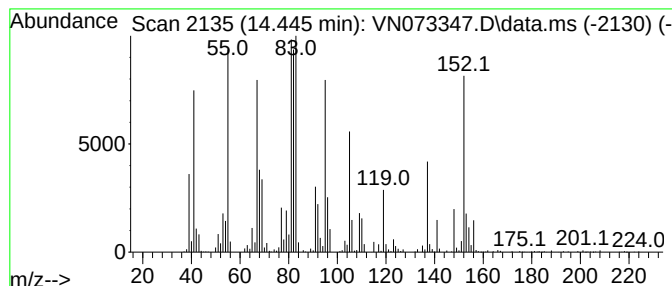
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Naphthalene, decahydro-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	36.70 ug/l	1705020	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	70
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	55
3			Cycloundecene (Z)	152	C11H20	013151-61-6	49
4			Pulegone	152	C10H16O	000089-82-7	46
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	46



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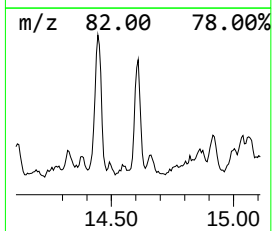
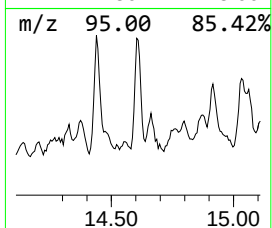
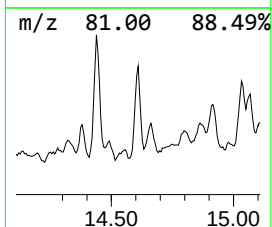
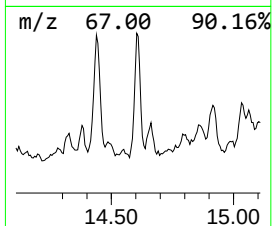
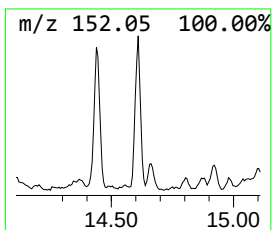
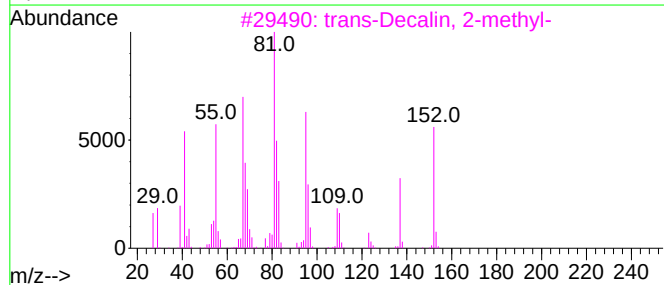
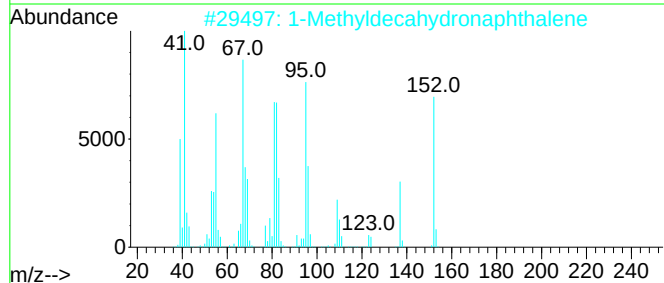
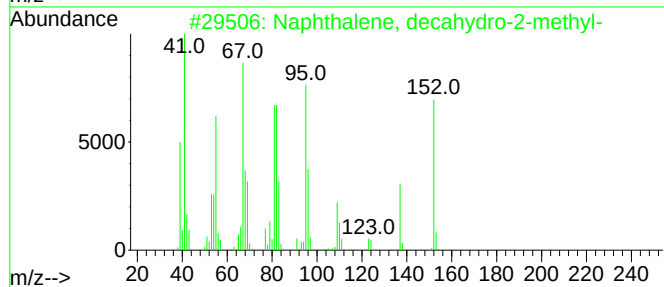
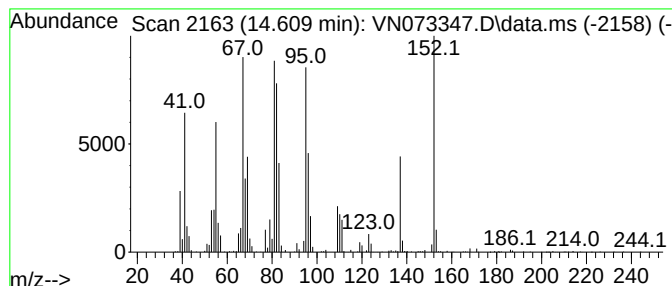
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.609	31.16 ug/l	1447570	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	96
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	90
4			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	70
5			cis-9-Tetradecen-1-ol	212	C14H28O	035153-15-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

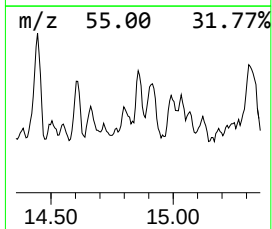
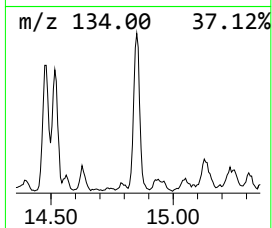
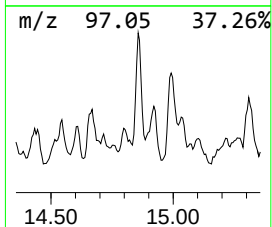
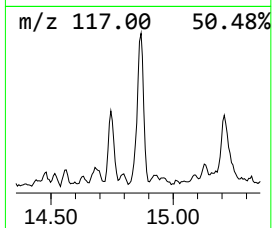
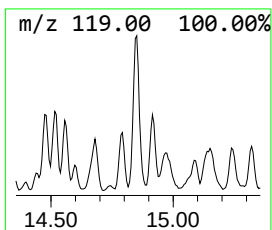
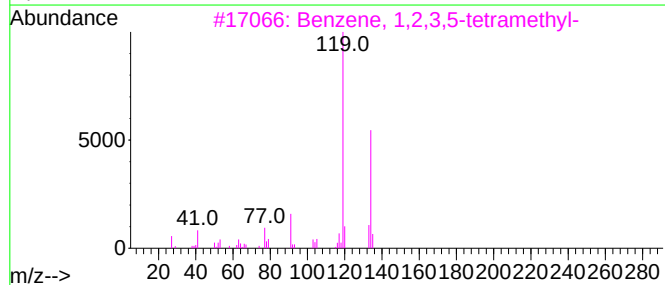
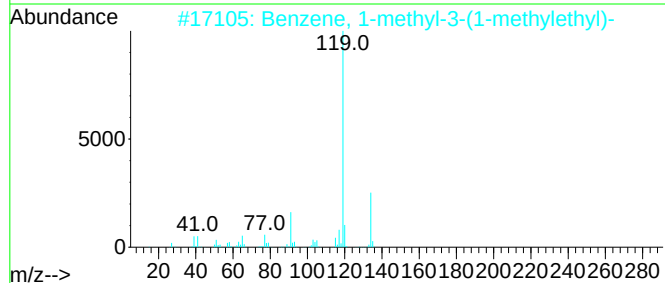
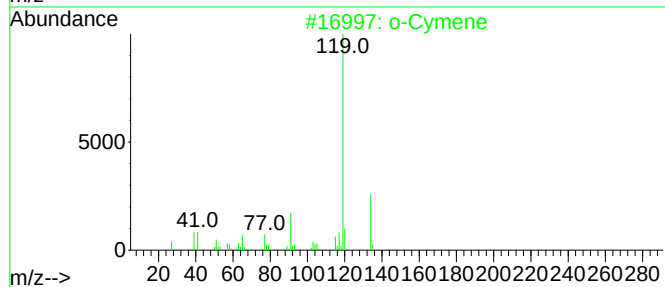
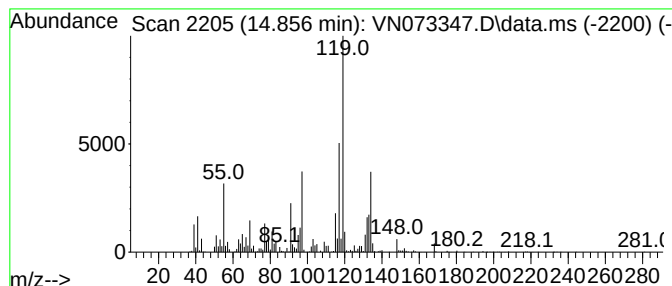
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Quant Title : SW846 8260

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

Peak Number 5 o-Cymene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	40.15 ug/l	1865310	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	55
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	55
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	55
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	55
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

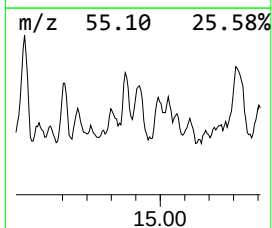
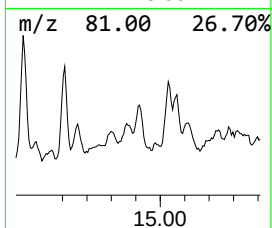
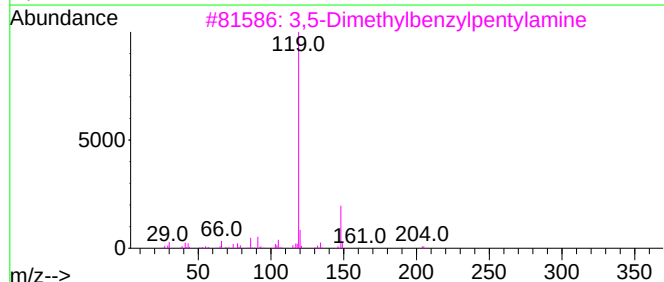
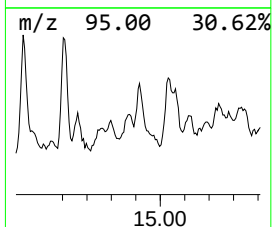
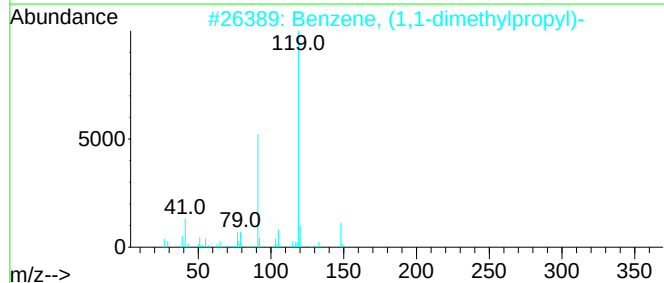
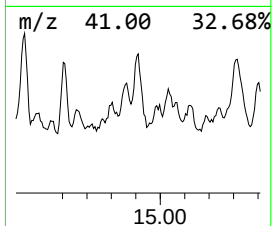
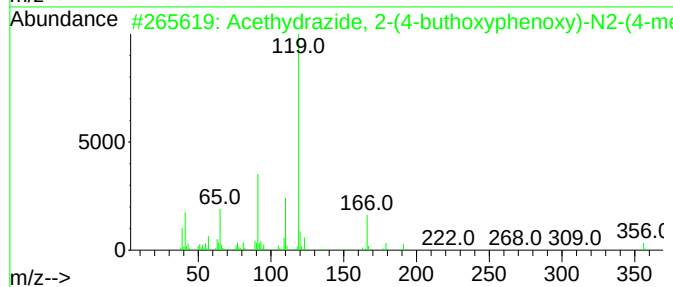
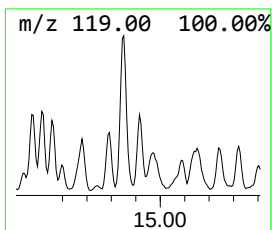
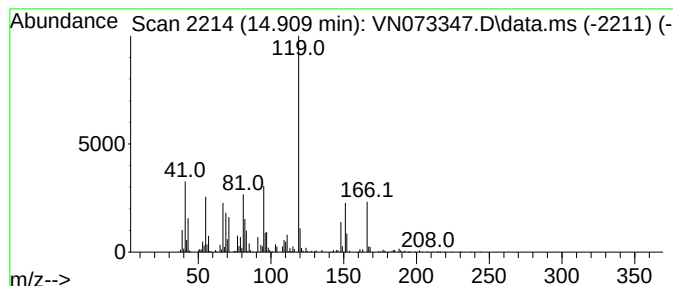
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.909 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.909	29.88 ug/l	1388130	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acethydrazide, 2-(4-butoxypheno...	356	C20H24N2O4	1000263-84-3	43
2			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	38
3			3,5-Dimethylbenzylpentylamine	205	C14H23N	1000491-60-8	38
4			Butyric acid, 2-phenyl-, dodec-2...	330	C22H34O2	1000406-86-7	37
5			Butyric acid, 2-phenyl-, undec-2...	316	C21H32O2	1000406-92-0	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

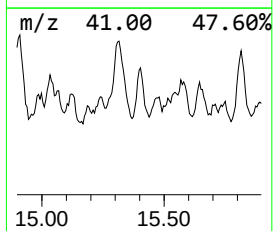
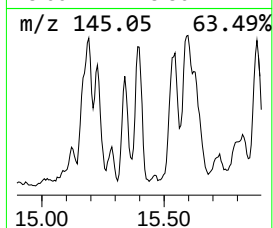
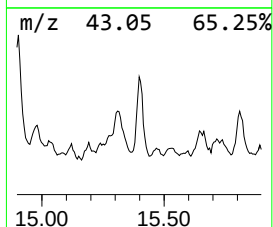
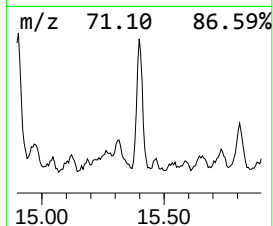
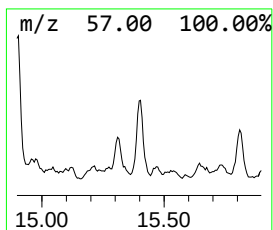
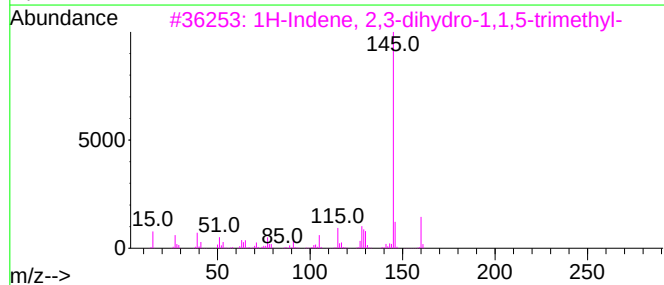
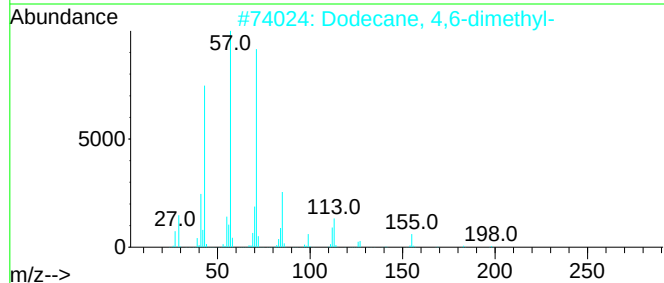
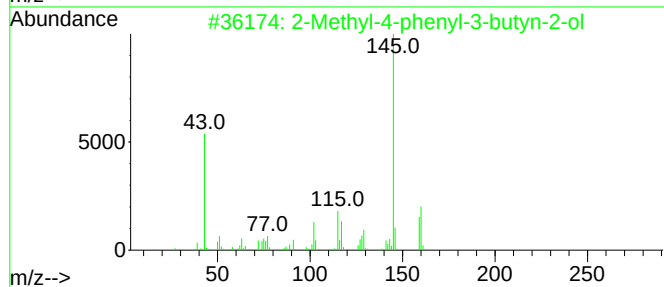
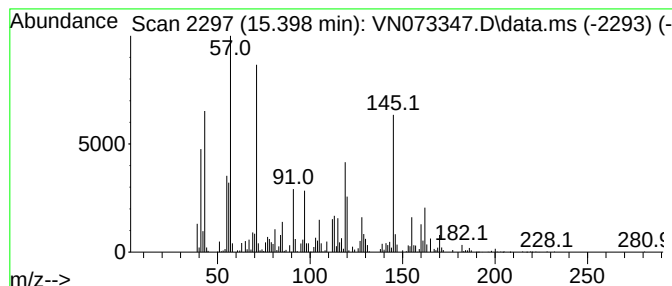
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	25.94 ug/l	1205040	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-phenyl-3-butyne-2-ol	160	C11H12O	001719-19-3	25		
2	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	25		
3	1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	160	C12H16	040650-41-7	25		
4	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	25		
5	1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	160	C12H16	016204-72-1	25		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

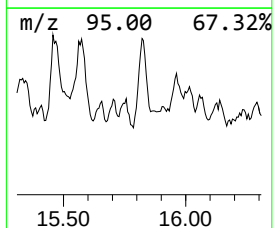
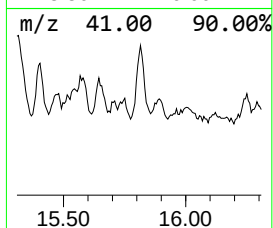
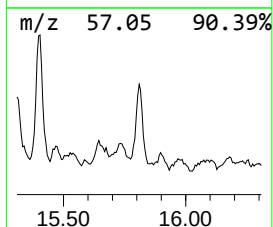
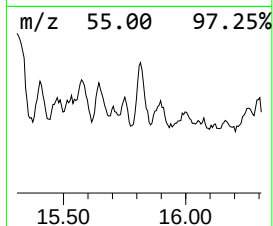
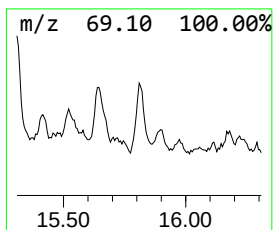
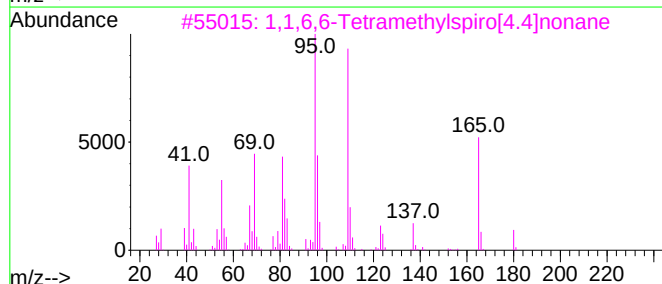
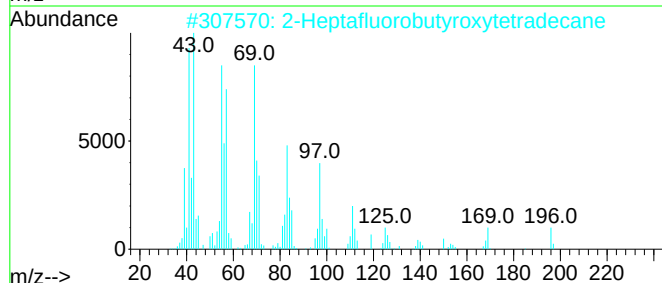
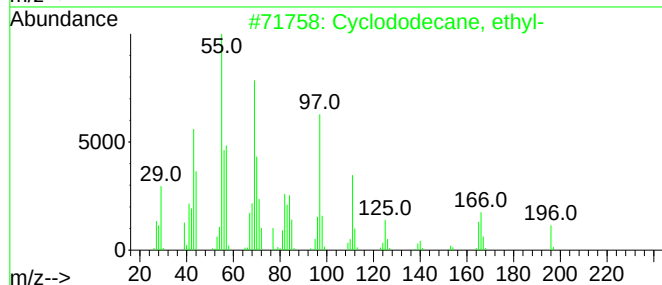
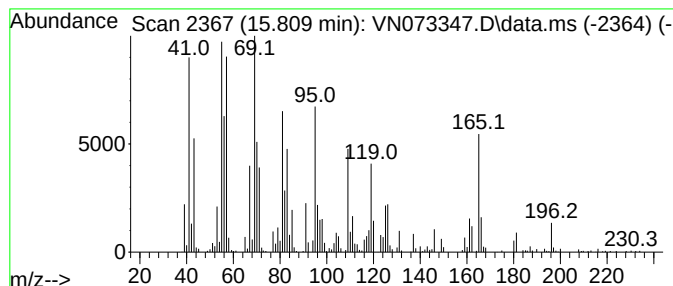
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.809 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.809	20.94 ug/l	972838	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane, ethyl-	196	C14H28	028981-49-9	42
2			2-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1010245-49-7	30
3			1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	25
4			7-Tetradecene, (Z)-	196	C14H28	041446-60-0	20
5			3-Tetradecene, (E)-	196	C14H28	041446-68-8	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

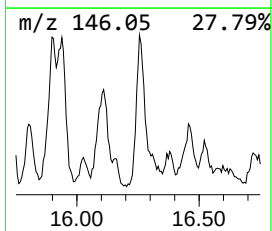
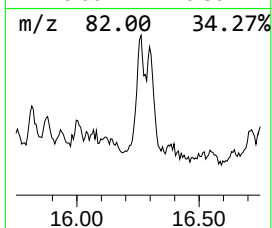
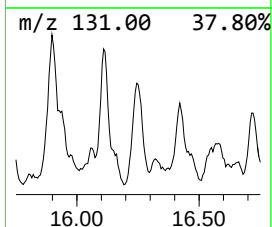
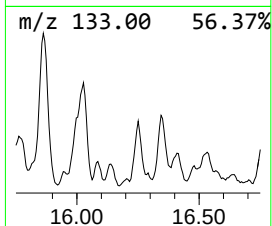
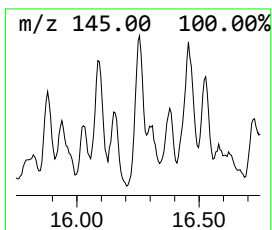
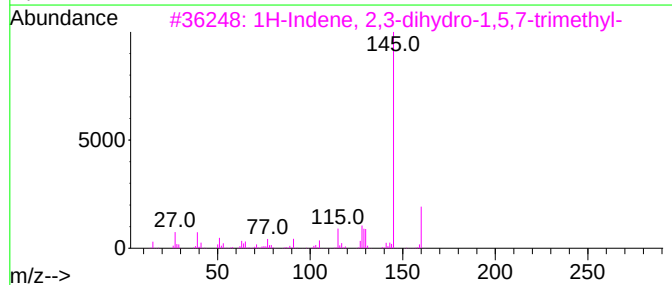
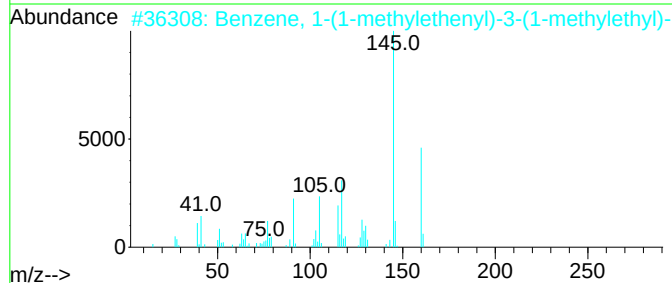
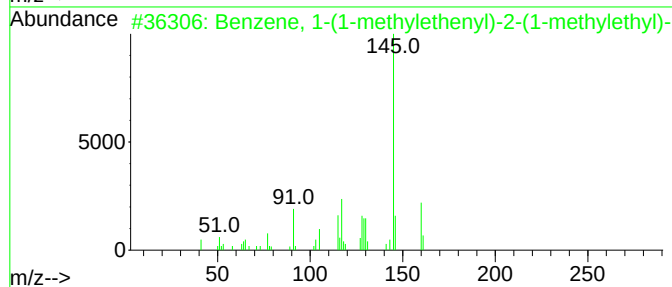
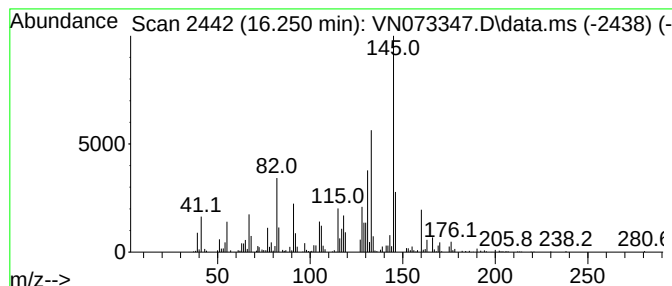
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-(1-methylethenyl)... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.250	16.93 ug/l	786773	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	64
2			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	62
3			1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	60
4			1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	60
5			1H-Indene, 2,3-dihydro-1,4,7-tri...	160	C12H16	054340-87-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

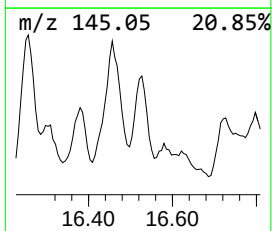
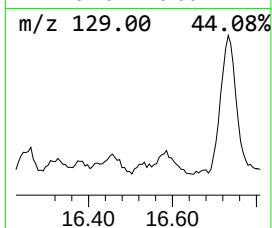
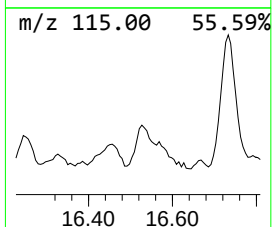
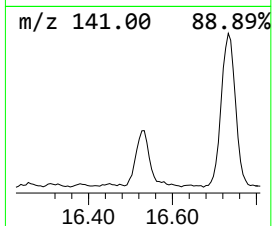
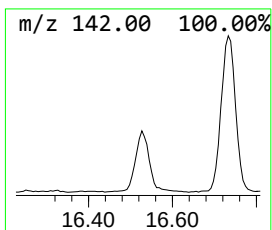
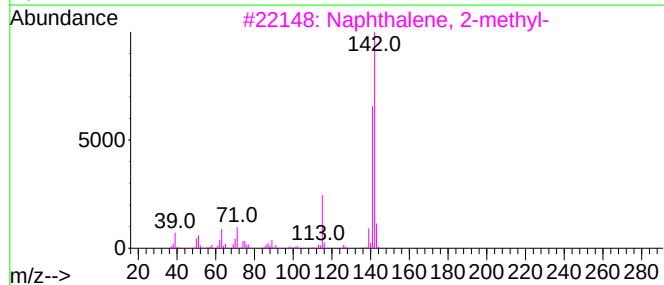
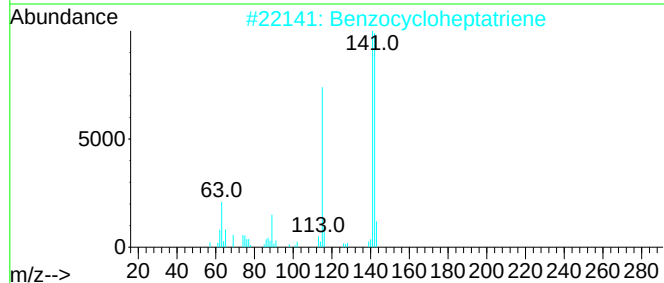
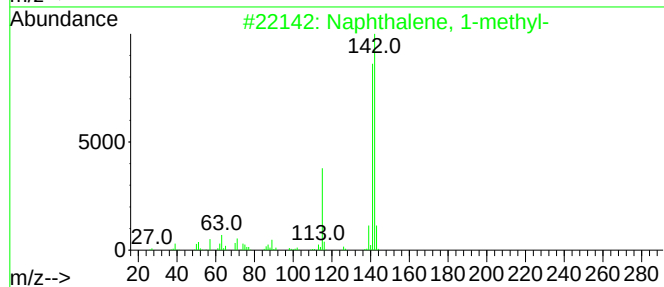
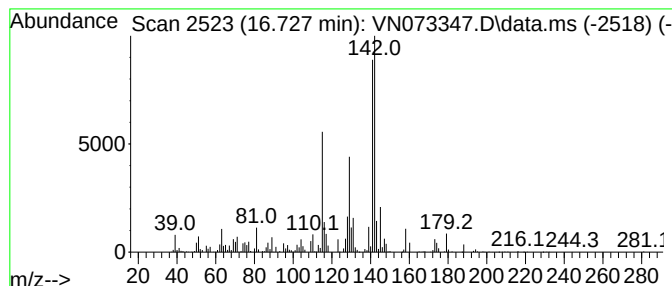
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Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	49.68 ug/l	2307910	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	93
2			Benzocycloheptatriene	142	C11H10	000264-09-5	70
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	64
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	64
5			Benzeneacetonitrile, 4-cyano-	142	C9H6N2	000876-31-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073347.D
Acq On : 06 Jul 2022 16:00
Operator : JC\MD
Sample : N3564-31
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-2-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.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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1-Methyl-2-phen...	14.262	18.4	ug/l	854911	4	13.615	2323000	50.0
Naphthalene, de...	14.445	36.7	ug/l	1705020	4	13.615	2323000	50.0
1-Methyldecahyd...	14.609	31.2	ug/l	1447570	4	13.615	2323000	50.0
o-Cymene	14.857	40.1	ug/l	1865310	4	13.615	2323000	50.0
unknown14.909	14.909	29.9	ug/l	1388130	4	13.615	2323000	50.0
unknown15.398	15.398	25.9	ug/l	1205040	4	13.615	2323000	50.0
unknown15.809	15.809	20.9	ug/l	972838	4	13.615	2323000	50.0
Benzene, 1-(1-m...	16.250	16.9	ug/l	786773	4	13.615	2323000	50.0
Benzocyclohepta...	16.727	49.7	ug/l	2307910	4	13.615	2323000	50.0