

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073105.D
 Acq On : 25 Jun 2022 13:02
 Operator : JC\MD
 Sample : N3431-15
 Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-14B-2-4

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN073105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	503	517	526	rBV2	75685	311762	1.11%	0.050%
2	5.481	595	611	627	rBV2	200010	715027	2.55%	0.114%
3	6.775	820	831	845	rBV2	89160	305344	1.09%	0.048%
4	6.939	847	859	869	rBV	184606	587625	2.10%	0.093%
5	7.945	1019	1030	1034	rBV	216207	532024	1.90%	0.085%
6	8.004	1034	1040	1047	rVV2	526686	1280068	4.57%	0.203%
7	8.086	1047	1054	1066	rVB	971308	2459544	8.77%	0.391%
8	8.216	1066	1076	1080	rBV	250124	612689	2.19%	0.097%
9	8.275	1080	1086	1094	rVV	481403	1173016	4.18%	0.186%
10	8.363	1094	1101	1111	rVB2	236493	563989	2.01%	0.090%
11	8.486	1111	1122	1128	rBV2	1102597	2806095	10.01%	0.446%
12	8.557	1128	1134	1140	rVV	844548	1921326	6.85%	0.305%
13	8.628	1140	1146	1155	rVB	1133217	2582116	9.21%	0.410%
14	8.898	1184	1192	1203	rBV	619866	1368340	4.88%	0.217%
15	9.204	1237	1244	1254	rVB	220355	497618	1.78%	0.079%
16	9.386	1261	1275	1280	rBV2	3562664	10934299	39.00%	1.737%
17	9.439	1280	1284	1293	rVB	1234337	2352235	8.39%	0.374%
18	9.569	1300	1306	1311	rVB	291879	522326	1.86%	0.083%
19	9.657	1311	1321	1330	rVB2	2206031	4971803	17.74%	0.790%
20	9.804	1338	1346	1356	rBV2	2163018	4290070	15.30%	0.681%
21	9.951	1365	1371	1375	rBV	1191715	2184985	7.79%	0.347%
22	9.992	1375	1378	1384	rVB	766699	1278752	4.56%	0.203%
23	10.045	1384	1387	1393	rVB2	227519	392207	1.40%	0.062%
24	10.133	1394	1402	1406	rBV	1485012	3069671	10.95%	0.488%
25	10.180	1406	1410	1417	rVB	1232089	2219367	7.92%	0.353%
26	10.263	1418	1424	1427	rBV3	558664	1164362	4.15%	0.185%
27	10.369	1435	1442	1446	rBV2	5778052	11445673	40.83%	1.818%
28	10.410	1446	1449	1457	rVB	3120039	5207105	18.57%	0.827%
29	10.498	1458	1464	1466	rBV	1149457	1843774	6.58%	0.293%
30	10.545	1466	1472	1483	rVB4	2890739	8399062	29.96%	1.334%
31	10.674	1484	1494	1496	rBV2	1547042	3022614	10.78%	0.480%
32	10.716	1496	1501	1509	rVB	4920549	9104190	32.48%	1.446%
33	10.810	1509	1517	1522	rBV3	2625203	5941448	21.19%	0.944%
34	10.851	1522	1524	1528	rVB2	424203	525669	1.88%	0.083%
35	10.898	1528	1532	1537	rVB	1894193	3000116	10.70%	0.477%
36	10.986	1537	1547	1554	rBV	5278395	9660971	34.46%	1.534%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073105.D
 Acq On : 25 Jun 2022 13:02
 Operator : JC\MD
 Sample : N3431-15
 Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-14B-2-4

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\82N061722W.M
 Title : SW846 8260

37	11.092	1554	1565	1572	rBV	3157083	8199014	29.25%	1.302%
38	11.163	1572	1577	1580	rBV2	1636090	2767660	9.87%	0.440%
39	11.198	1580	1583	1584	rVV2	824515	1005863	3.59%	0.160%
40	11.227	1584	1588	1592	rVV	3562898	5422620	19.34%	0.861%
41	11.280	1592	1597	1603	rVB	10899353	19681915	70.21%	3.126%
42	11.333	1603	1606	1610	rVB2	1130661	1391915	4.97%	0.221%
43	11.386	1610	1615	1620	rBV3	3749251	6579250	23.47%	1.045%
44	11.433	1620	1623	1627	rVB2	1561545	2032989	7.25%	0.323%
45	11.486	1627	1632	1640	rVB	4704280	8437928	30.10%	1.340%
46	11.557	1640	1644	1649	rBV	1761542	2853429	10.18%	0.453%
47	11.604	1649	1652	1660	rVB5	762417	1506064	5.37%	0.239%
48	11.680	1660	1665	1668	rBV3	828090	1426049	5.09%	0.227%
49	11.721	1669	1672	1675	rVB2	618796	761527	2.72%	0.121%
50	11.774	1677	1681	1684	rBV	713435	1017659	3.63%	0.162%
51	11.816	1684	1688	1691	rBV	2594671	3834583	13.68%	0.609%
52	11.863	1691	1696	1701	rVB4	3259851	6535055	23.31%	1.038%
53	11.927	1701	1707	1711	rBV	6458096	12454685	44.43%	1.978%
54	11.969	1711	1714	1719	rVB2	5145440	8347209	29.78%	1.326%
55	12.027	1719	1724	1731	rBV3	1776359	4031721	14.38%	0.640%
56	12.116	1731	1739	1744	rVB4	2003420	4857990	17.33%	0.772%
57	12.192	1744	1752	1759	rBV3	9207446	21953842	78.31%	3.487%
58	12.310	1764	1772	1776	rVB	10279475	17573517	62.69%	2.791%
59	12.392	1776	1786	1788	rBV3	9236517	19403792	69.22%	3.082%
60	12.421	1788	1791	1802	rVB3	10297262	23401535	83.48%	3.717%
61	12.516	1803	1807	1810	rBV3	1930392	3782768	13.49%	0.601%
62	12.674	1828	1834	1839	rBV3	3878415	7027145	25.07%	1.116%
63	12.757	1840	1848	1852	rBV5	3485506	8539464	30.46%	1.356%
64	12.833	1856	1861	1868	rVB3	11309543	21874325	78.03%	3.474%
65	12.916	1868	1875	1880	rBV4	4473008	10593522	37.79%	1.683%
66	12.998	1880	1889	1894	rVV4	9439852	28033754	100.00%	4.453%
67	13.045	1894	1897	1903	rVB3	5386222	9213808	32.87%	1.463%
68	13.133	1908	1912	1916	rVV3	4756596	7331215	26.15%	1.164%
69	13.180	1916	1920	1923	rVV4	2329733	4036789	14.40%	0.641%
70	13.221	1923	1927	1935	rVB2	5924771	11132703	39.71%	1.768%
71	13.315	1940	1943	1945	rBV2	1511171	1820619	6.49%	0.289%
72	13.351	1946	1949	1954	rVB2	2374190	2916522	10.40%	0.463%
73	13.404	1954	1958	1961	rBV	2710128	4601764	16.42%	0.731%
74	13.504	1967	1975	1980	rBV4	9985240	23003400	82.06%	3.654%
75	13.757	2013	2018	2032	rVB4	5095205	14429855	51.47%	2.292%
76	13.933	2042	2048	2053	rBV3	12234842	22602152	80.62%	3.590%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073105.D
 Acq On : 25 Jun 2022 13:02
 Operator : JC\MD
 Sample : N3431-15
 Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-14B-2-4

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\82N061722W.M
 Title : SW846 8260

77	13.980	2053	2056	2060	rVB2	3196671	4264883	15.21%	0.677%
78	14.039	2062	2066	2069	rBV4	2813380	4402906	15.71%	0.699%
79	14.151	2082	2085	2098	rVB	8338751	16009003	57.11%	2.543%
80	14.262	2098	2104	2110	rVB5	5081587	9982189	35.61%	1.586%
81	14.321	2110	2114	2120	rBV7	2925278	5449811	19.44%	0.866%
82	14.380	2121	2124	2127	rBV3	1315987	1947166	6.95%	0.309%
83	14.445	2129	2135	2139	rBV3	11139240	20537511	73.26%	3.262%
84	14.557	2150	2154	2157	rBV2	2653908	3937028	14.04%	0.625%
85	14.610	2158	2163	2169	rVV3	6770717	12788914	45.62%	2.031%
86	14.792	2191	2194	2198	rBV3	1892933	2818446	10.05%	0.448%
87	14.851	2199	2204	2210	rVV3	8551733	18263355	65.15%	2.901%
88	14.915	2211	2215	2221	rVB5	5331111	9298936	33.17%	1.477%
89	15.033	2232	2235	2238	rBV3	1541226	2343118	8.36%	0.372%
90	15.127	2247	2251	2255	rVB3	3866702	5927293	21.14%	0.941%
91	15.168	2255	2258	2260	rBV	1671694	2459078	8.77%	0.391%
92	15.239	2265	2270	2276	rVB4	4809048	9667688	34.49%	1.536%
93	15.398	2292	2297	2304	rVB5	3478744	6719888	23.97%	1.067%
94	15.809	2362	2367	2373	rBV6	2303651	4665130	16.64%	0.741%
95	16.251	2435	2442	2448	rBV5	3251951	8196208	29.24%	1.302%
96	16.721	2517	2522	2533	rBV6	1489484	4245275	15.14%	0.674%

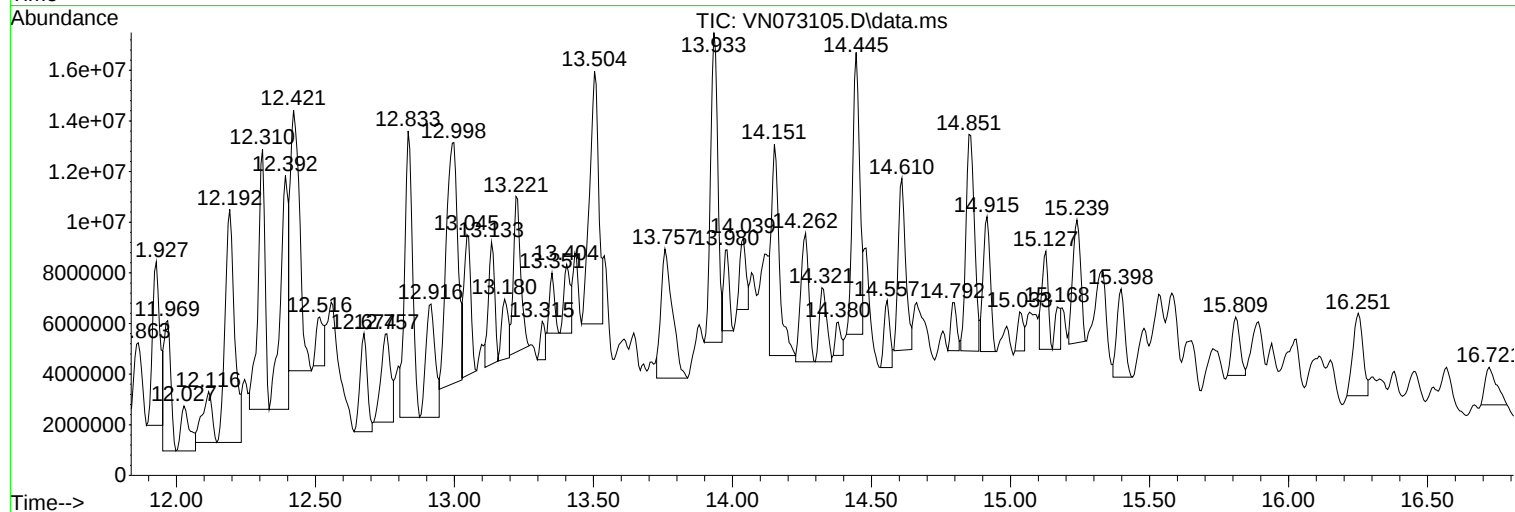
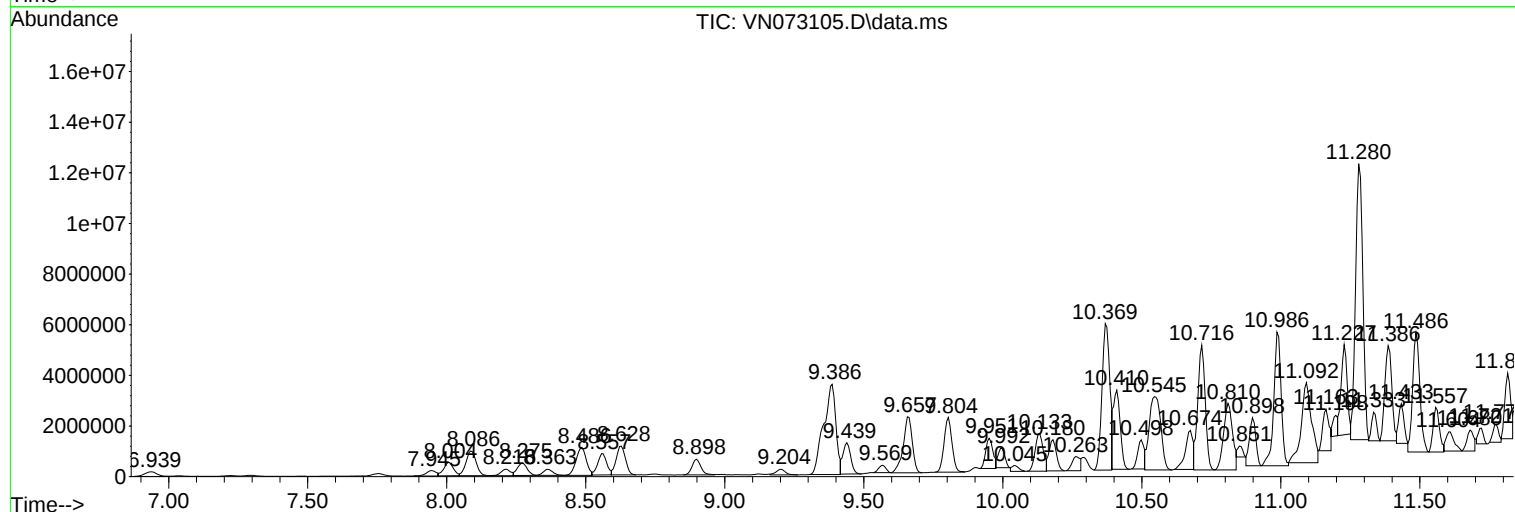
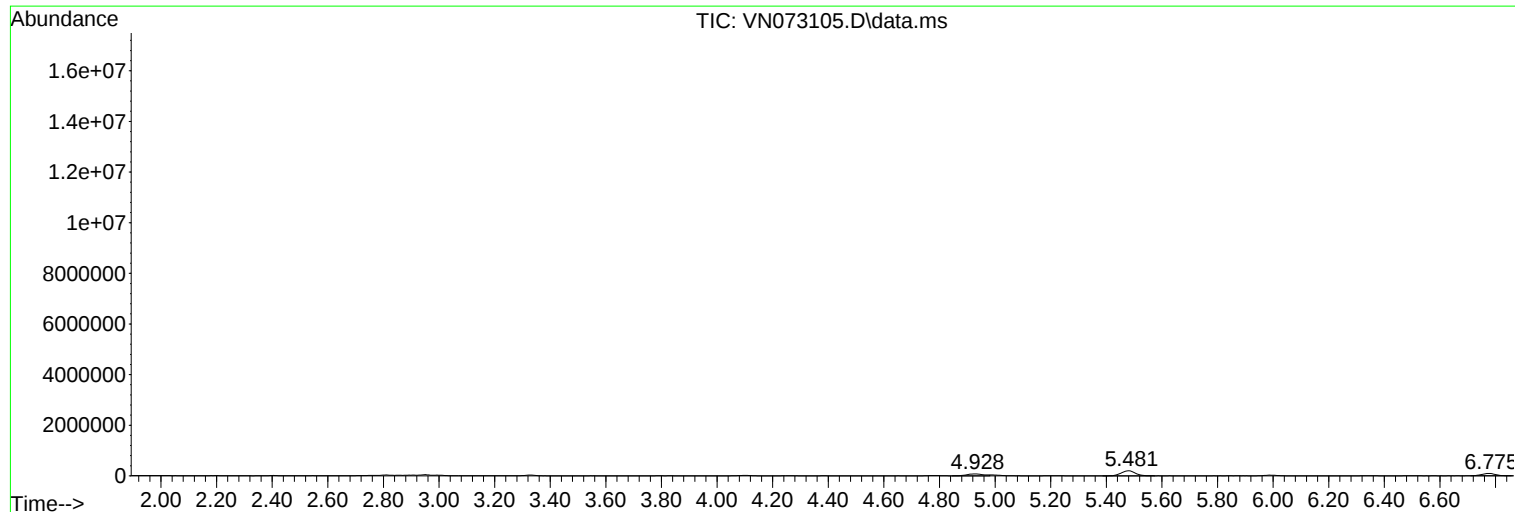
Sum of corrected areas: 629588724

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

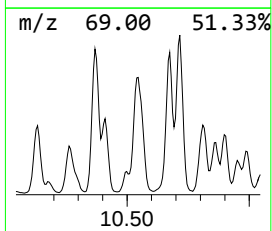
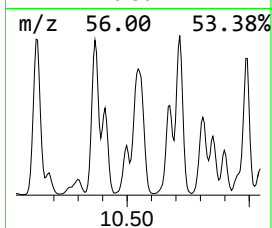
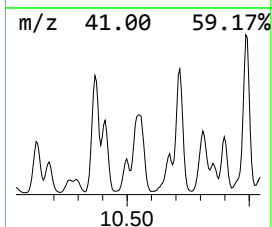
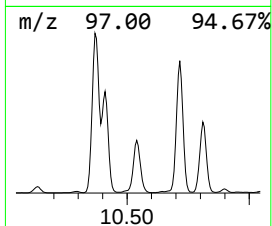
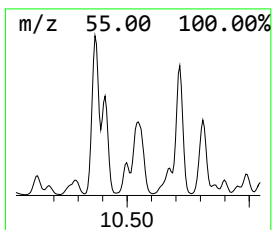
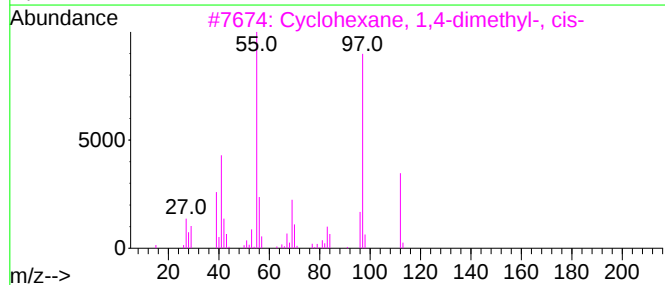
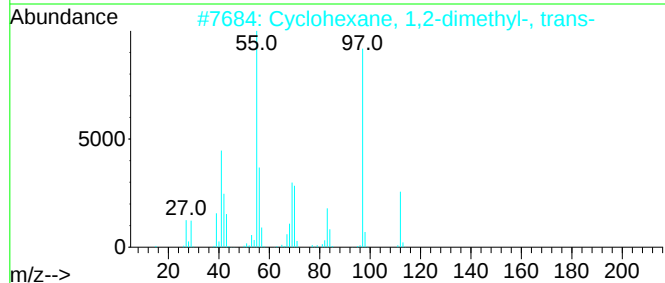
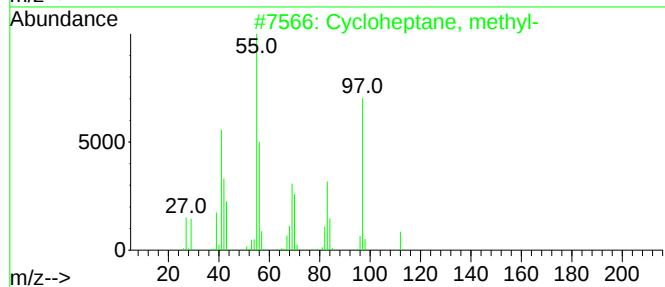
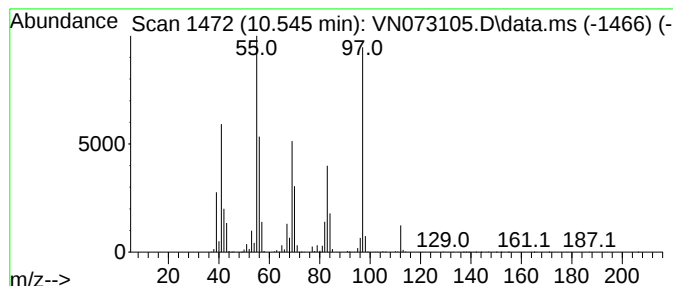
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Cycloheptane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	294.49 ug/l	8399060	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane, methyl-	112	C8H16	004126-78-7	93
2			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	76
3			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	52
4			4-Octene, (E)-	112	C8H16	014850-23-8	49
5			1H-Pyrazol-4-amine, 3-methyl-	97	C4H7N3	1010338-28-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

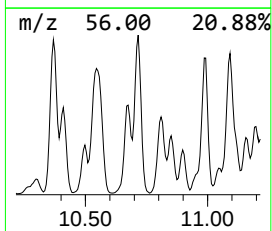
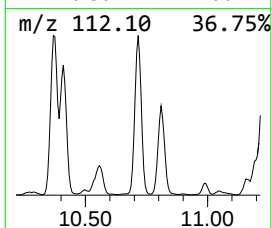
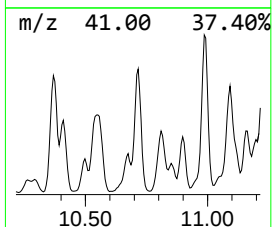
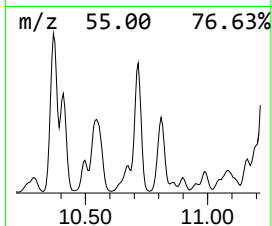
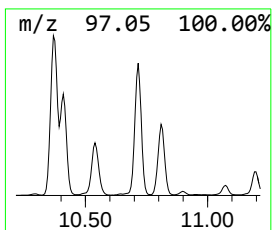
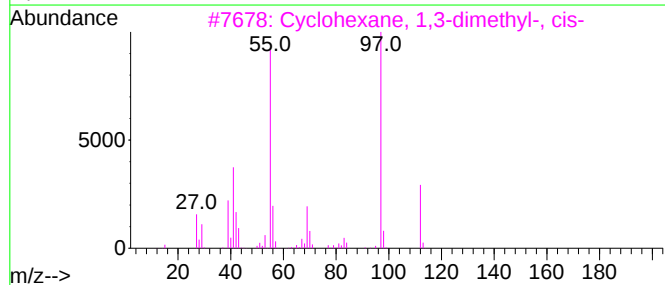
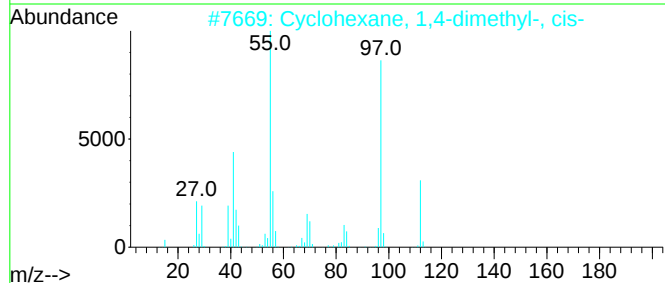
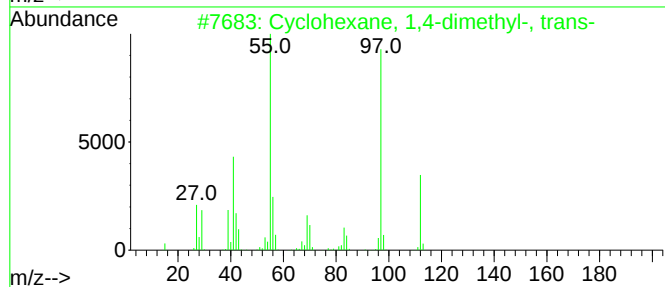
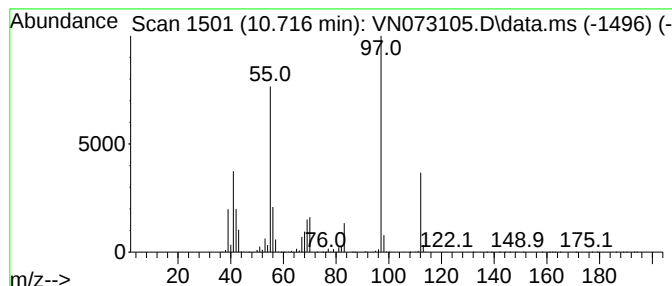
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.716	319.21 ug/l	9104190	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	90
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	87
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	83
4			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	80
5			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

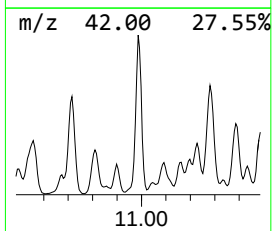
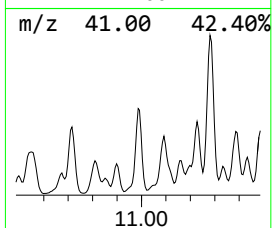
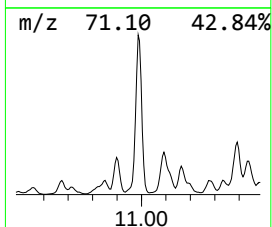
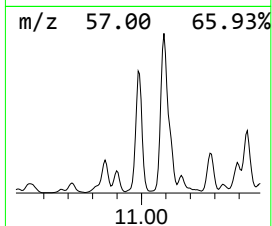
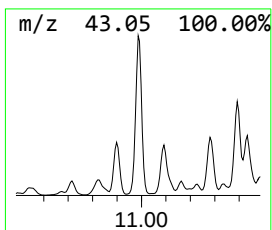
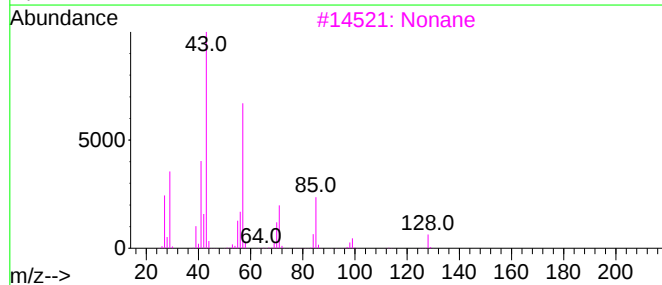
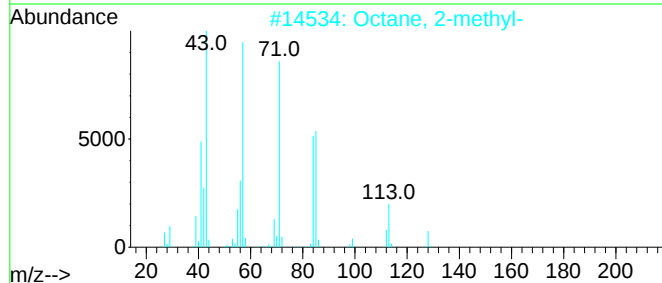
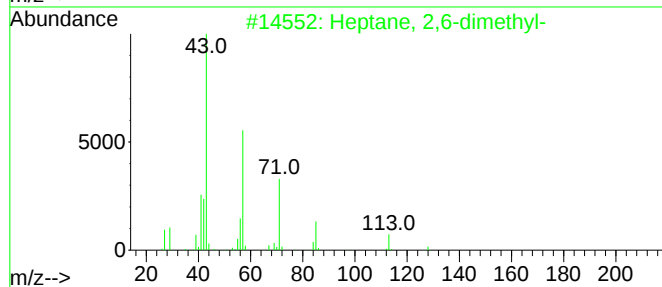
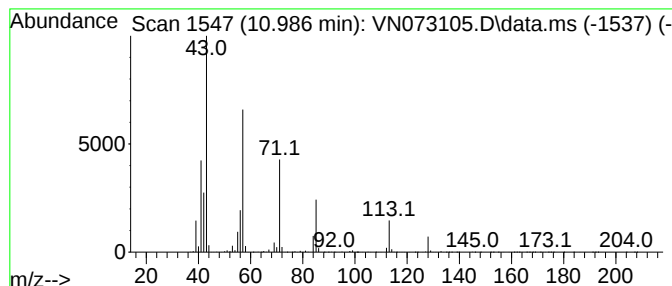
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.986	338.73 ug/l	9660970	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	91
2			Octane, 2-methyl-	128	C9H20	003221-61-2	91
3			Nonane	128	C9H20	000111-84-2	58
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

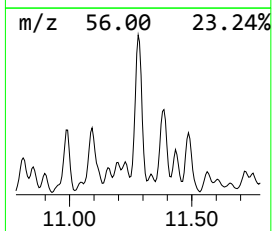
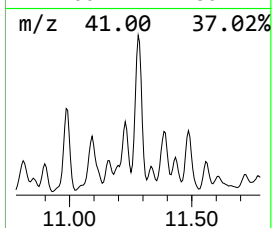
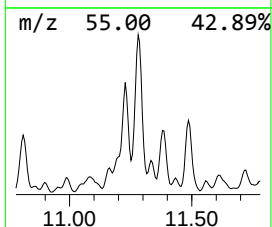
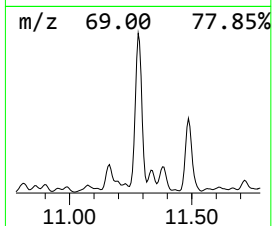
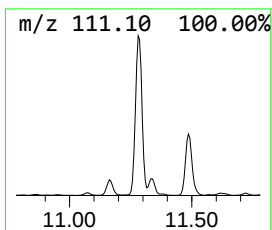
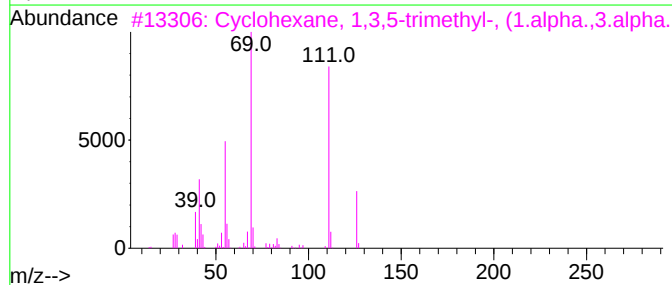
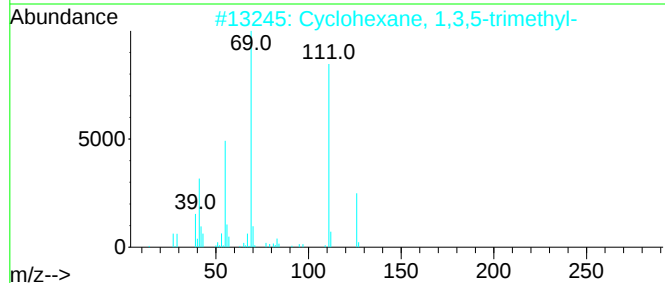
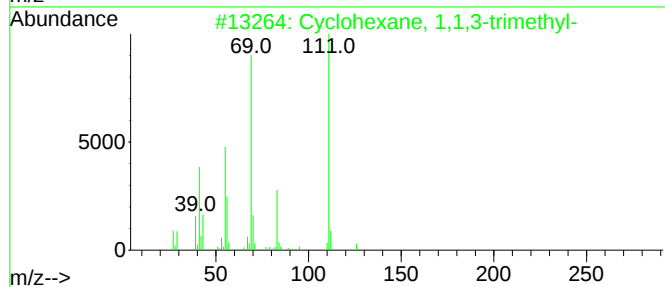
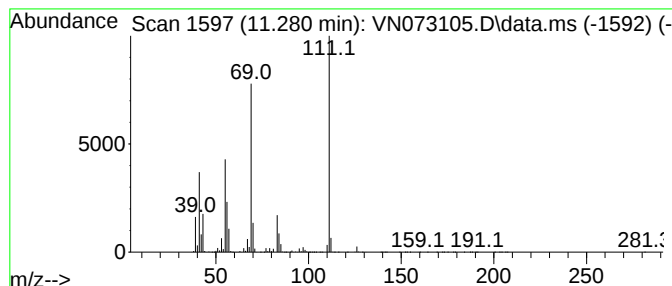
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.280	690.09 ug/l	19681900	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
2			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	72
4			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	72
5			6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

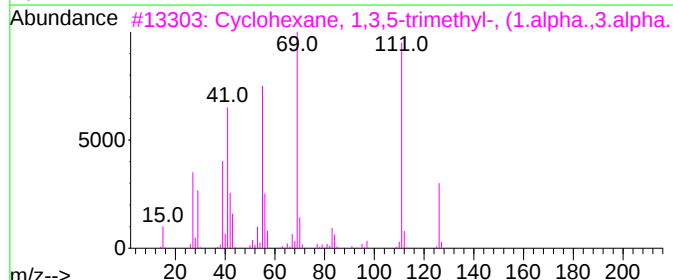
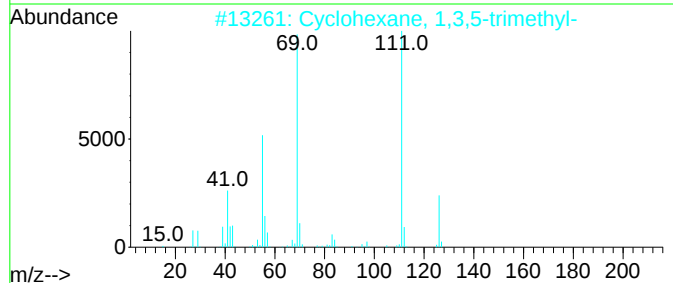
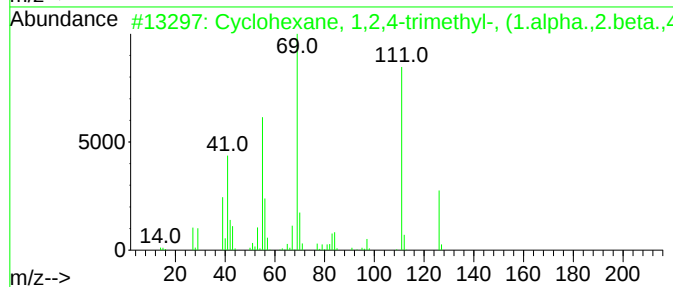
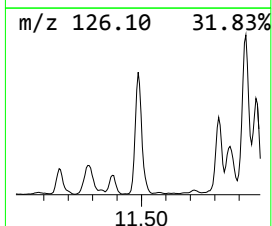
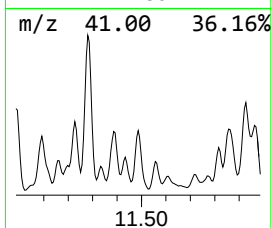
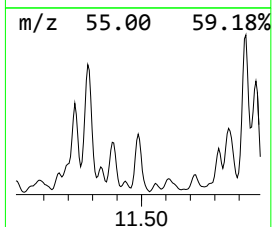
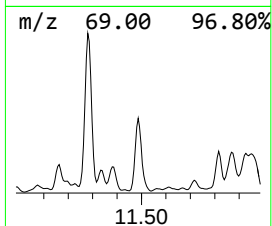
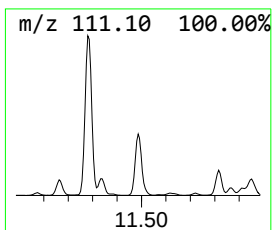
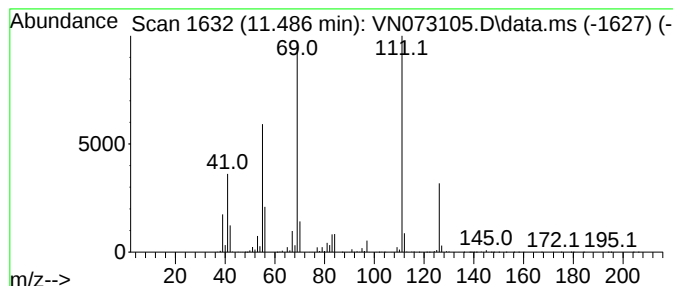
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,2,4-trimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.486	295.85 ug/l	8437930	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	95
2			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	93
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	93
4			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	90
5			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

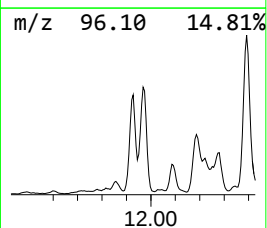
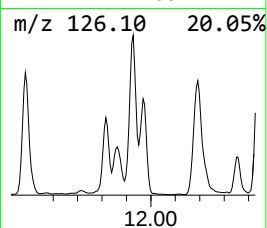
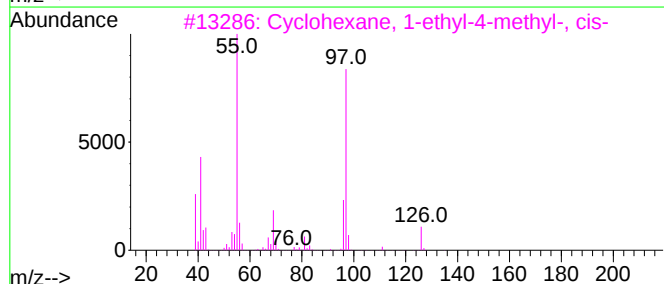
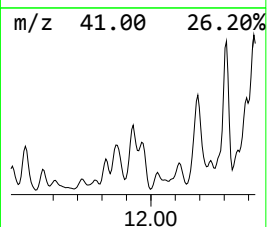
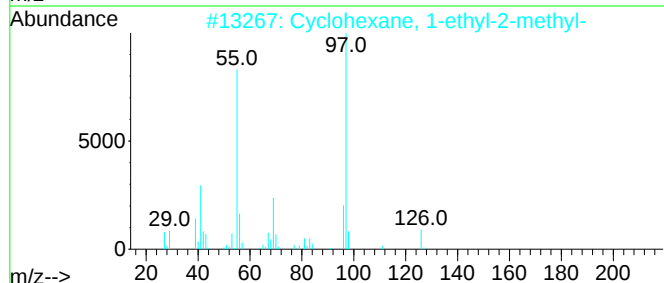
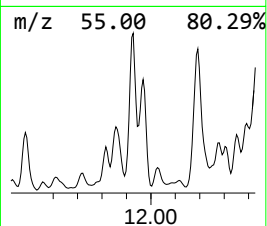
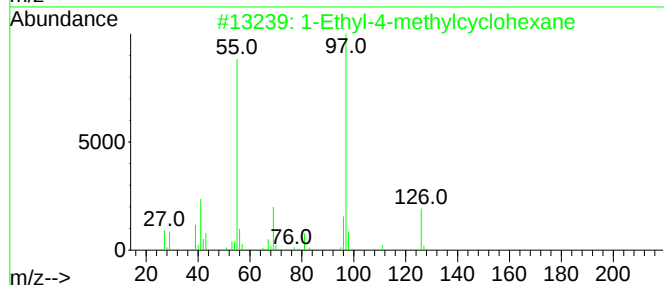
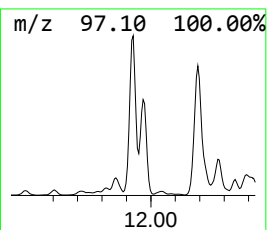
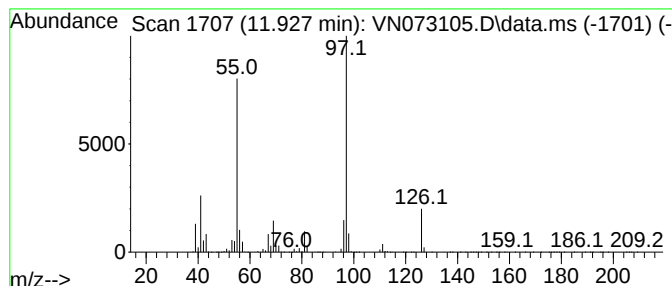
Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Ethyl-4-methylcyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.927	436.69 ug/l	12454700	Chlorobenzene-d5	11.680	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	94
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	83
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

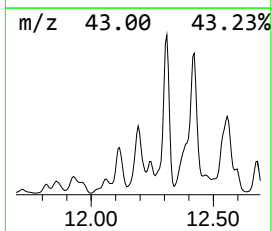
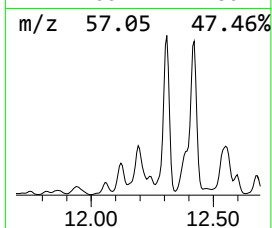
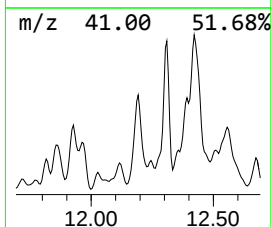
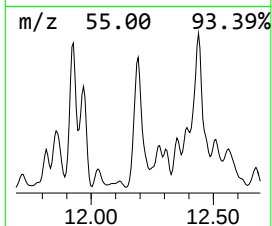
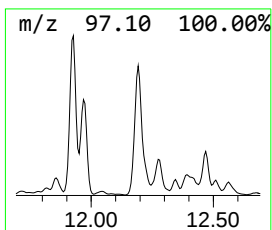
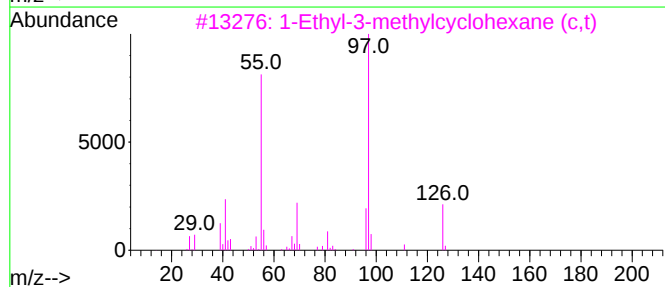
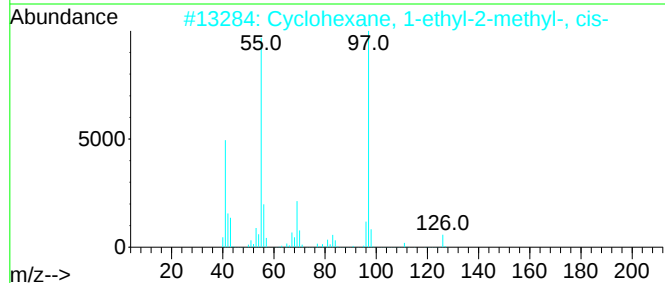
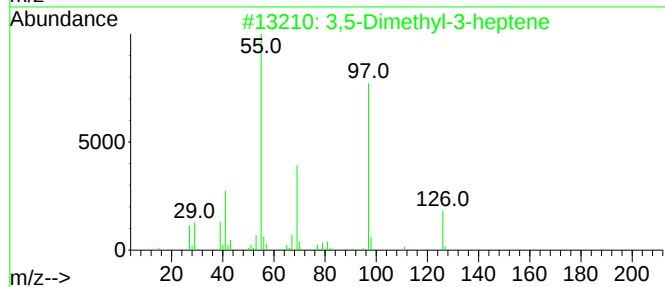
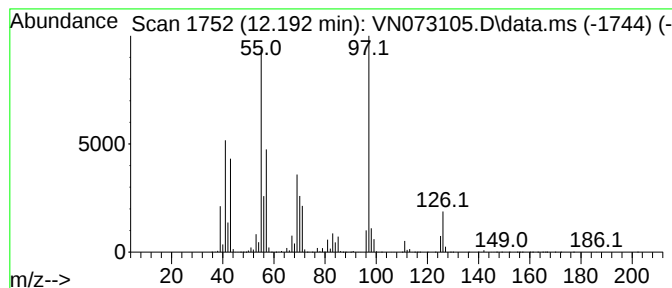
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 7 3,5-Dimethyl-3-heptene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.192	769.74 ug/l	21953800	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	58
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
3			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	52
4			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	52
5			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

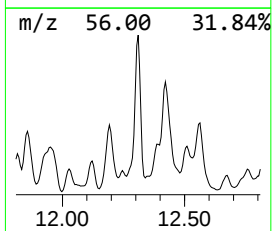
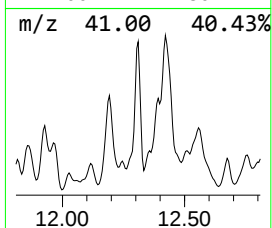
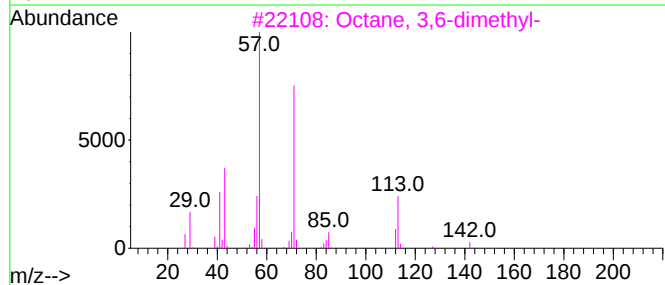
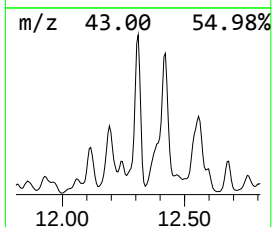
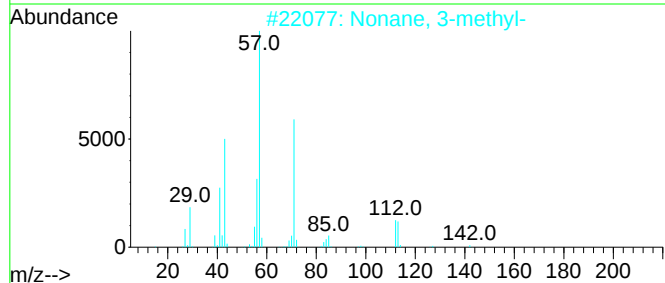
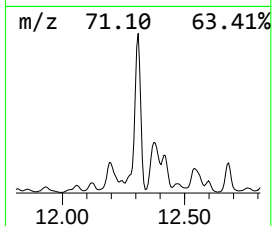
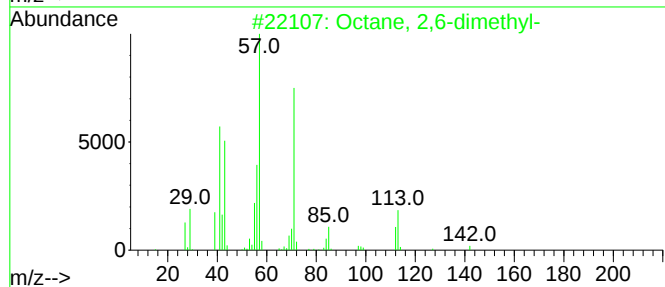
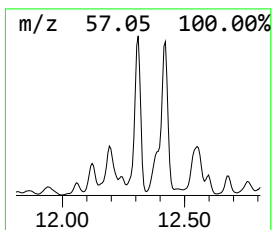
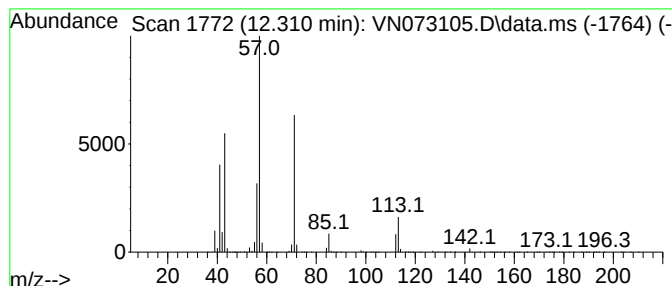
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 8 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.310	616.16 ug/l	17573500	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	90
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
4			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

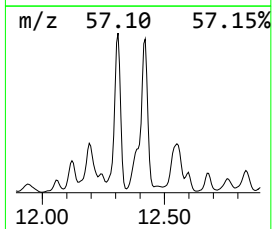
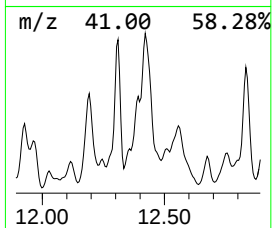
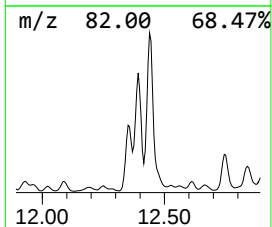
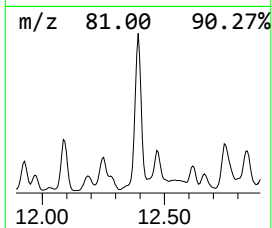
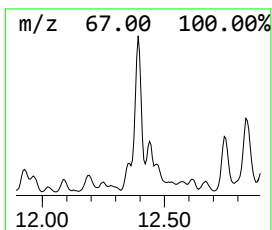
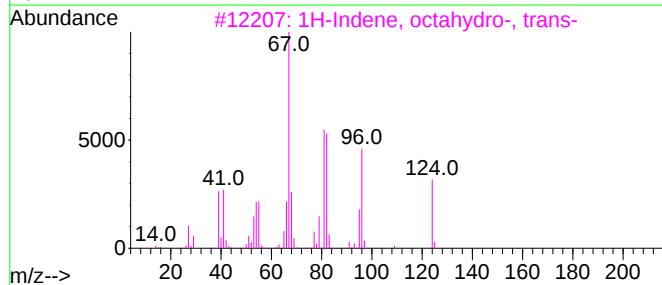
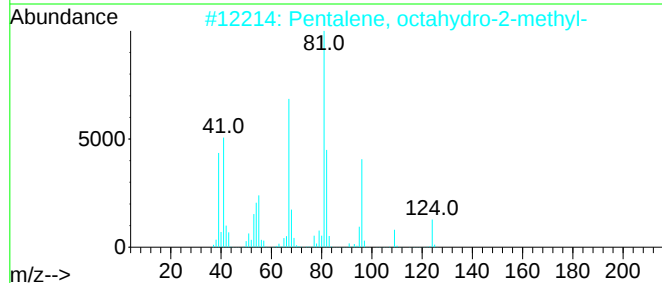
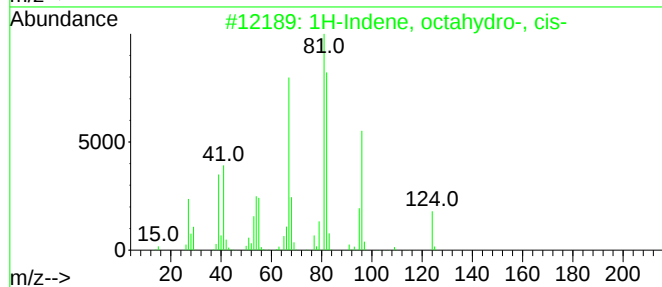
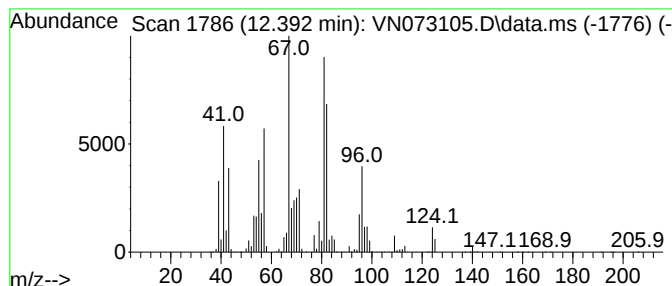
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, octahydro-, cis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	680.33 ug/l	19403800	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	70
2			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	60
3			1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
4			Bicyclo[2.2.1]heptane, 2-ethyl-	124	C9H16	002146-41-0	43
5			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

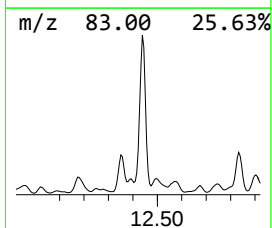
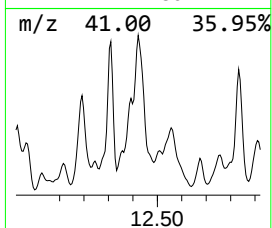
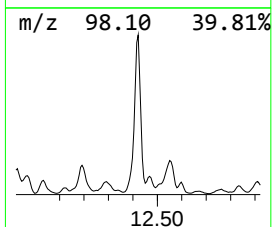
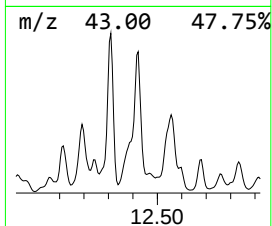
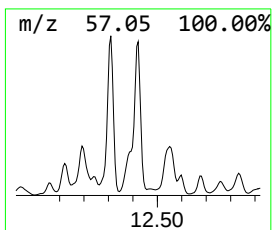
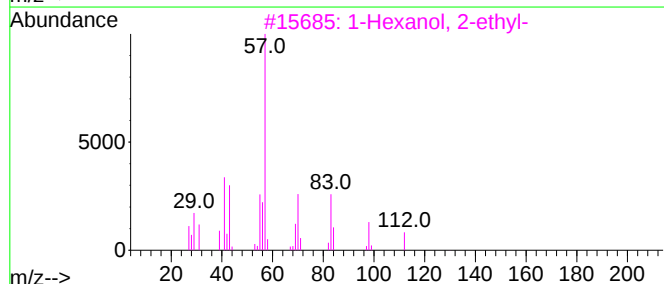
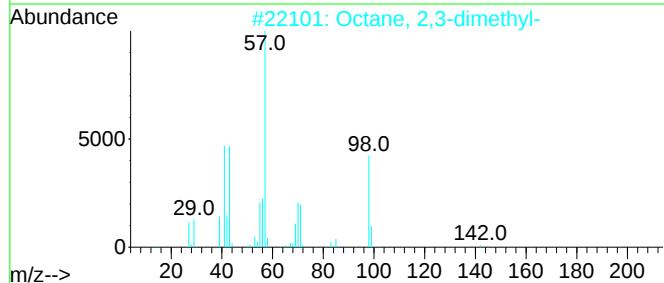
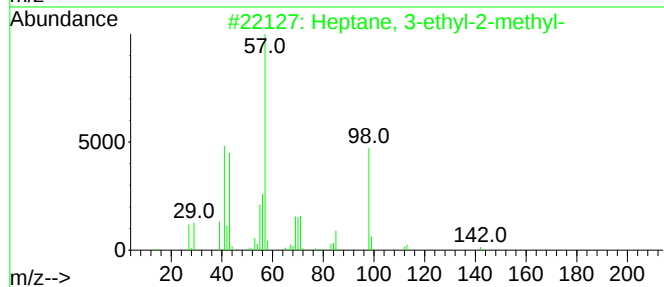
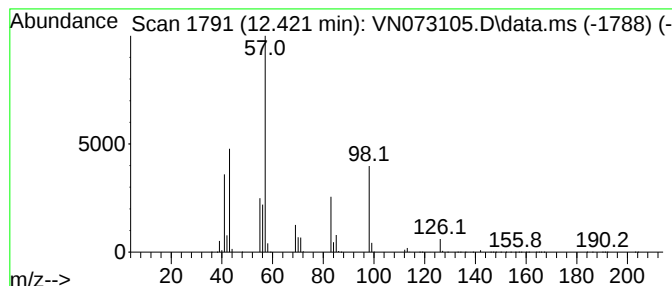
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 10 Heptane, 3-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	820.50 ug/l	23401500	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	62
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	58
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4			4-Octylcyclohexanone	210	C14H26O	1000428-94-1	45
5			2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073105.D
Acq On : 25 Jun 2022 13:02
Operator : JC\MD
Sample : N3431-15
Misc : 5.63g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-14B-2-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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
Cycloheptane, m...	10.545	294.5	ug/l	8399060	3	11.680	1426050	50.0
Cyclohexane, 1,...	10.716	319.2	ug/l	9104190	3	11.680	1426050	50.0
Heptane, 2,6-di...	10.986	338.7	ug/l	9660970	3	11.680	1426050	50.0
Cyclohexane, 1,...	11.280	690.1	ug/l	19681900	3	11.680	1426050	50.0
Cyclohexane, 1,...	11.486	295.9	ug/l	8437930	3	11.680	1426050	50.0
1-Ethyl-4-methy...	11.927	436.7	ug/l	12454700	3	11.680	1426050	50.0
3,5-Dimethyl-3-...	12.192	769.7	ug/l	21953800	3	11.680	1426050	50.0
Octane, 2,6-dim...	12.310	616.2	ug/l	17573500	3	11.680	1426050	50.0
1H-Indene, octa...	12.392	680.3	ug/l	19403800	3	11.680	1426050	50.0
Heptane, 3-ethy...	12.421	820.5	ug/l	23401500	3	11.680	1426050	50.0