

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
 Data File : VN073352.D
 Acq On : 06 Jul 2022 18:03
 Operator : JC\MD
 Sample : N3586-05 10X
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31487

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: VN073352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.240	902	910	920	rBV2	18608	49379	2.39%	0.158%
2	7.951	1020	1031	1036	rBV	221785	548293	26.57%	1.756%
3	8.016	1036	1042	1053	rVV	426384	994101	48.17%	3.184%
4	8.222	1070	1077	1087	rBV2	26615	63882	3.10%	0.205%
5	8.369	1092	1102	1116	rVV	230625	535710	25.96%	1.716%
6	8.757	1160	1168	1175	rBV5	15599	36627	1.77%	0.117%
7	8.898	1183	1192	1207	rBV	590390	1236726	59.93%	3.961%
8	9.386	1267	1275	1284	rBV3	9831	23856	1.16%	0.076%
9	10.380	1435	1444	1449	rBV	813075	1537856	74.52%	4.925%
10	10.439	1449	1454	1463	rVV	594806	1099718	53.29%	3.522%
11	10.557	1467	1474	1480	rVB3	21669	46678	2.26%	0.149%
12	11.286	1593	1598	1603	rVB5	15130	27242	1.32%	0.087%
13	11.392	1611	1616	1620	rBV5	13137	25892	1.25%	0.083%
14	11.469	1621	1629	1635	rBV4	43254	111897	5.42%	0.358%
15	11.569	1641	1646	1650	rVB	38077	62729	3.04%	0.201%
16	11.680	1658	1665	1673	rBV	893870	1569091	76.03%	5.025%
17	11.898	1693	1702	1710	rBV4	226550	436358	21.14%	1.397%
18	12.116	1735	1739	1744	rVB6	16951	26336	1.28%	0.084%
19	12.192	1745	1752	1754	rBV4	62870	116695	5.65%	0.374%
20	12.310	1767	1772	1776	rVB	82333	117359	5.69%	0.376%
21	12.422	1781	1791	1798	rBV8	72206	234233	11.35%	0.750%
22	12.522	1802	1808	1809	rBV5	25718	45004	2.18%	0.144%
23	12.569	1812	1816	1817	rBV4	29927	39535	1.92%	0.127%
24	12.598	1817	1821	1823	rBV2	58098	66975	3.25%	0.214%
25	12.622	1823	1825	1828	rVB2	65904	68893	3.34%	0.221%
26	12.669	1828	1833	1838	rBV	718868	1168987	56.65%	3.744%
27	12.839	1858	1862	1869	rVB4	46585	102227	4.95%	0.327%
28	12.921	1870	1876	1880	rBV3	136427	262076	12.70%	0.839%
29	12.986	1880	1887	1894	rVV	836246	1424482	69.03%	4.562%
30	13.045	1894	1897	1902	rVB2	71549	102413	4.96%	0.328%
31	13.098	1903	1906	1908	rBV4	24305	30251	1.47%	0.097%
32	13.157	1909	1916	1919	rBV4	58804	166237	8.06%	0.532%
33	13.221	1923	1927	1934	rVB2	180305	276261	13.39%	0.885%
34	13.304	1935	1941	1946	rVV	256518	459475	22.26%	1.472%
35	13.404	1955	1958	1960	rBV2	38994	47099	2.28%	0.151%
36	13.504	1968	1975	1979	rBV6	201499	431642	20.92%	1.382%

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37	13.545	1979	1982	1985	rVV2	153452	215250	10.43%	0.689%
38	13.610	1985	1993	2002	rVV2	1109581	2063665	100.00%	6.609%
39	13.686	2002	2006	2011	rVB2	144171	201431	9.76%	0.645%
40	13.804	2023	2026	2030	rBV2	137586	192110	9.31%	0.615%
41	13.851	2030	2034	2037	rBV3	82183	118537	5.74%	0.380%
42	13.933	2042	2048	2053	rBV	1123201	1654485	80.17%	5.299%
43	13.974	2053	2055	2058	rVV3	51311	56197	2.72%	0.180%
44	14.074	2068	2072	2073	rBV	59785	84073	4.07%	0.269%
45	14.098	2073	2076	2081	rVV3	142311	232974	11.29%	0.746%
46	14.151	2082	2085	2090	rVB	161198	212665	10.31%	0.681%
47	14.263	2098	2104	2109	rBV2	243066	415189	20.12%	1.330%
48	14.321	2110	2114	2120	rBV6	85864	209572	10.16%	0.671%
49	14.445	2121	2135	2139	rBV8	428586	1131152	54.81%	3.623%
50	14.557	2150	2154	2158	rBV3	190101	278414	13.49%	0.892%
51	14.604	2158	2162	2167	rVB5	208913	339766	16.46%	1.088%
52	14.663	2168	2172	2175	rVV6	112715	180847	8.76%	0.579%
53	14.698	2176	2178	2182	rVV	126522	164234	7.96%	0.526%
54	14.745	2182	2186	2187	rVV	160062	190060	9.21%	0.609%
55	14.786	2188	2193	2199	rVV3	638478	1114103	53.99%	3.568%
56	14.863	2199	2206	2211	rVV4	455007	1139089	55.20%	3.648%
57	14.910	2211	2214	2221	rVB4	255636	494785	23.98%	1.585%
58	15.021	2228	2233	2239	rVB2	203221	397863	19.28%	1.274%
59	15.127	2246	2251	2255	rBV4	170951	274623	13.31%	0.880%
60	15.239	2265	2270	2277	rVB3	165465	378545	18.34%	1.212%
61	15.398	2292	2297	2301	rBV3	171252	353800	17.14%	1.133%
62	15.486	2309	2312	2316	rVB	123033	176889	8.57%	0.567%
63	15.539	2317	2321	2332	rVV7	222966	647022	31.35%	2.072%
64	15.627	2332	2336	2346	rVB3	402276	802272	38.88%	2.569%
65	15.727	2346	2353	2361	rBV3	181129	511284	24.78%	1.637%
66	15.939	2385	2389	2396	rVB2	383164	708772	34.35%	2.270%
67	16.110	2412	2418	2432	rVB5	146893	522037	25.30%	1.672%
68	16.257	2435	2443	2448	rBV5	282136	667031	32.32%	2.136%
69	16.462	2472	2478	2484	rBV2	263422	546282	26.47%	1.750%
70	16.527	2484	2489	2494	rVV5	145284	314999	15.26%	1.009%
71	16.592	2496	2500	2510	rVB3	192234	399713	19.37%	1.280%
72	16.745	2519	2526	2531	rBV3	77759	242533	11.75%	0.777%

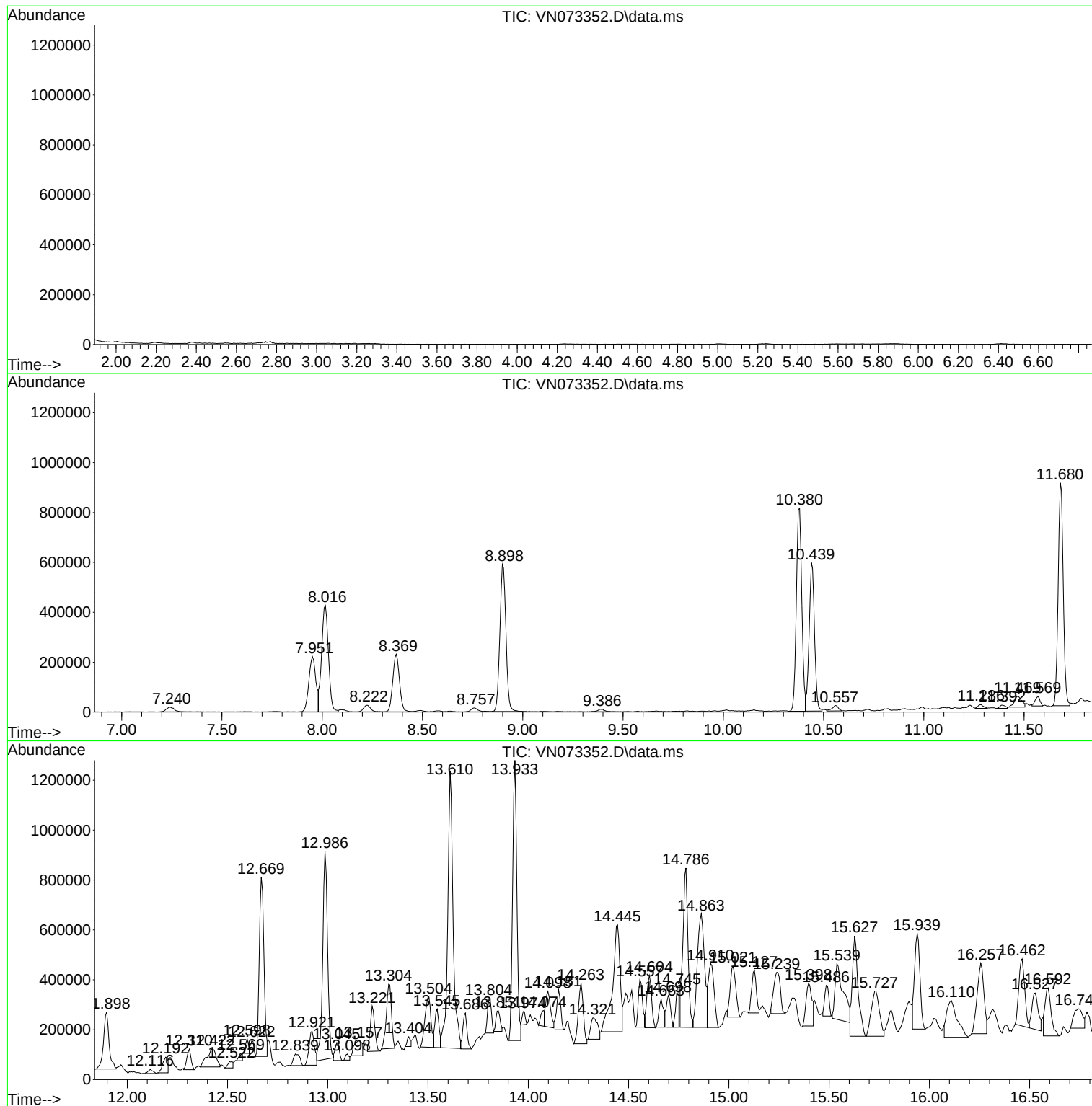
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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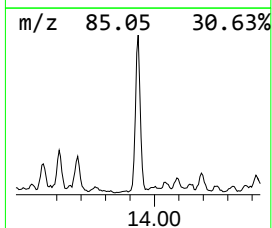
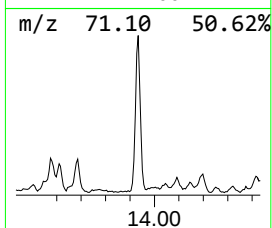
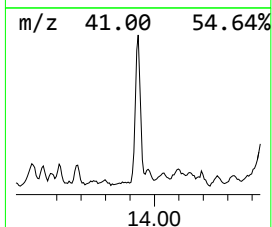
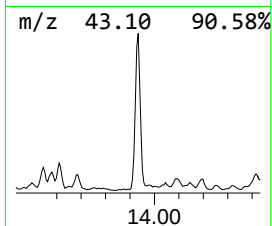
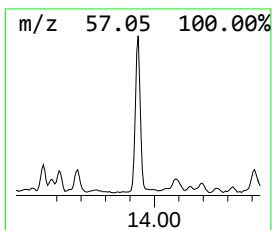
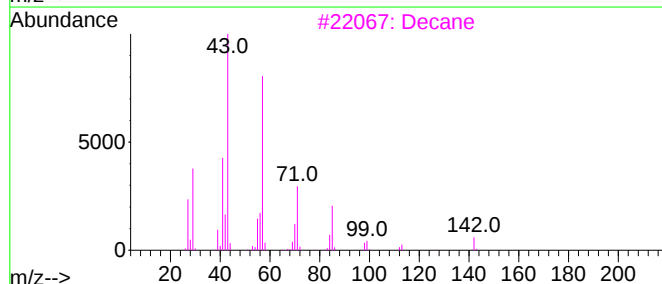
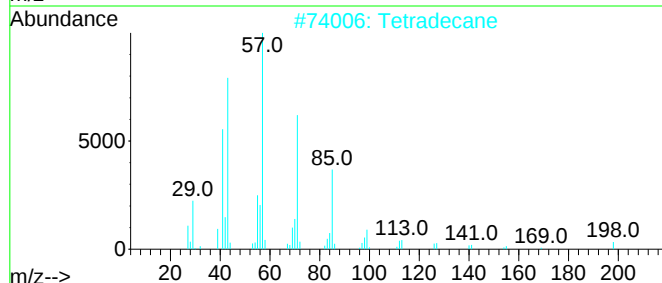
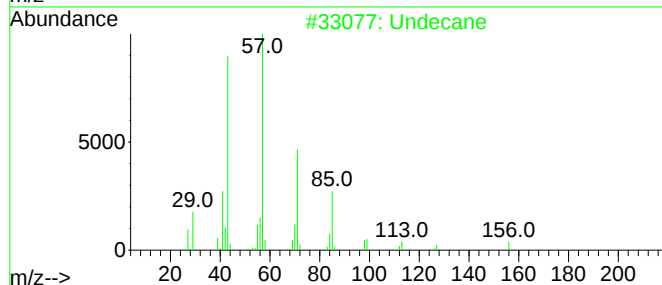
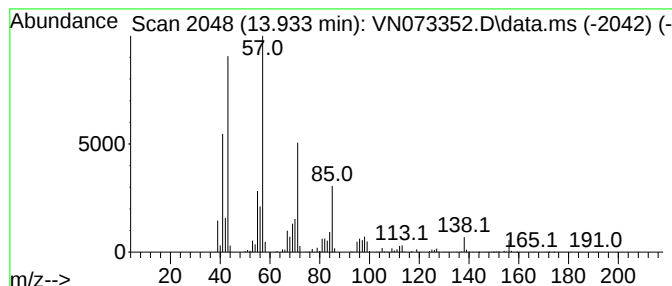
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	40.09 ug/l	1654490	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	90
2	Tetradecane			198	C14H30	000629-59-4	80
3	Decane			142	C10H22	000124-18-5	72
4	Hexadecane			226	C16H34	000544-76-3	59
5	Decane, 2,3,5-trimethyl-			184	C13H28	062238-11-3	59



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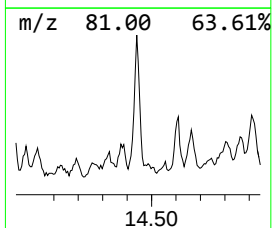
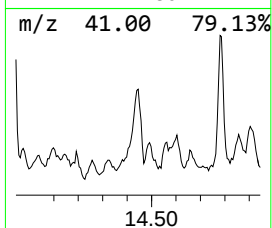
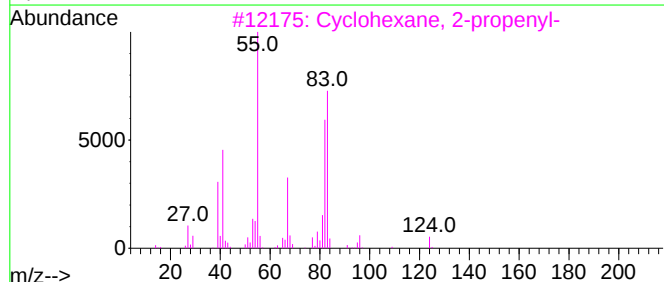
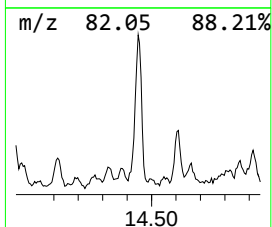
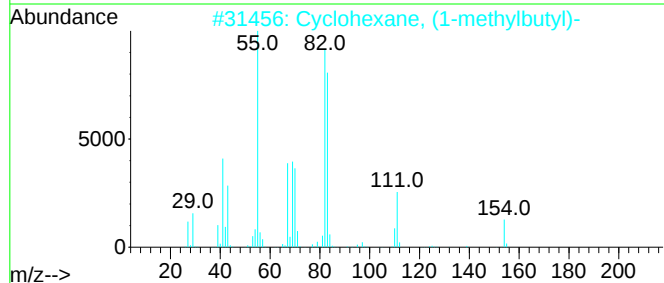
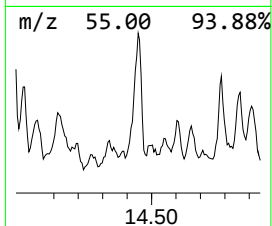
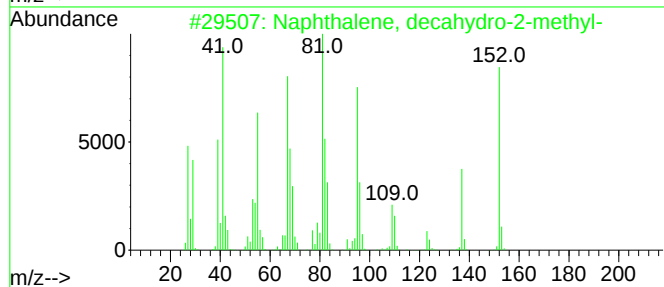
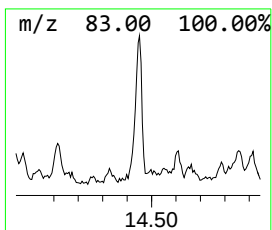
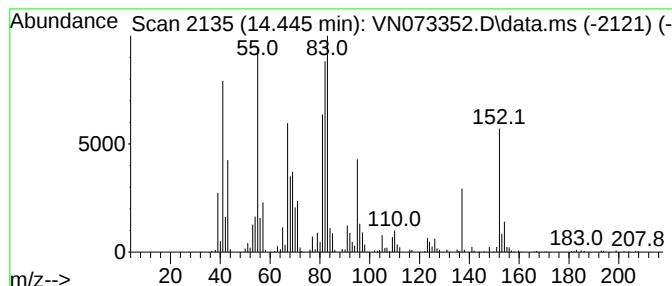
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, decahydro-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	27.41 ug/l	1131150	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	64
2			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	60
3			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	49
4			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	49
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	46



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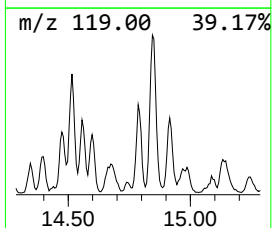
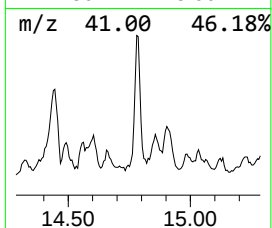
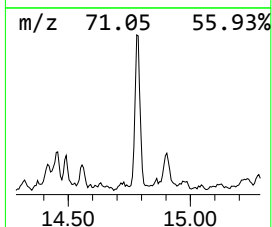
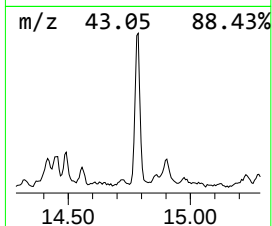
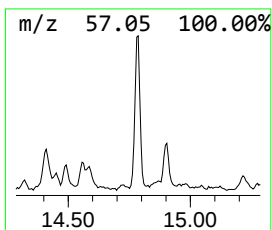
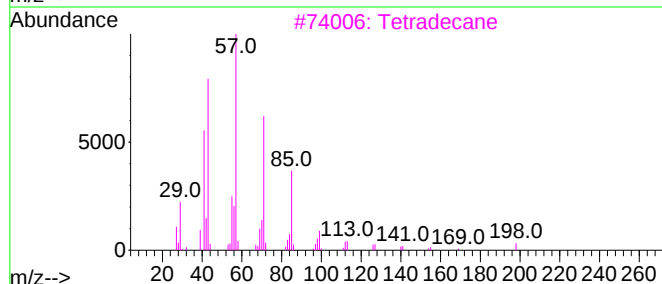
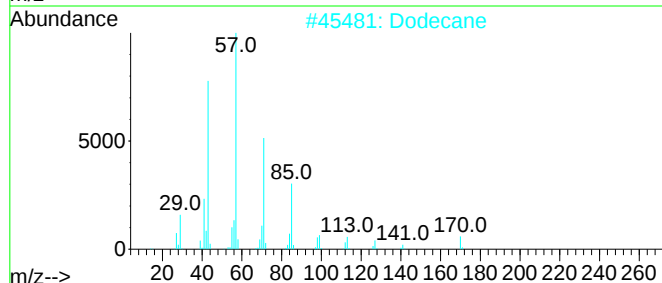
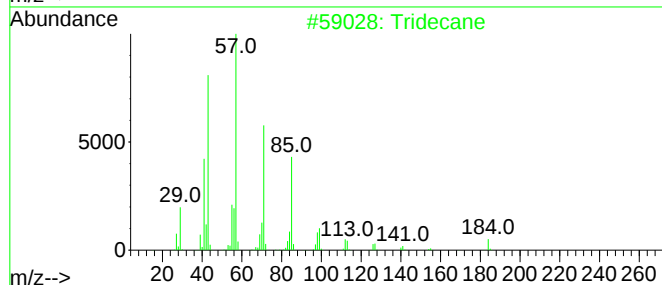
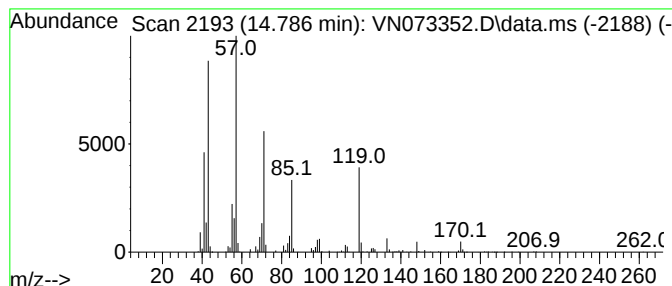
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Peak Number 3 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	26.99 ug/l	1114100	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	92
2			Dodecane	170	C12H26	000112-40-3	78
3			Tetradecane	198	C14H30	000629-59-4	49
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	49
5			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	47



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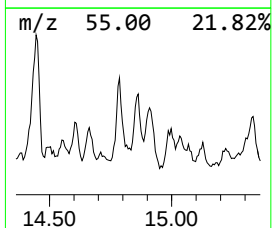
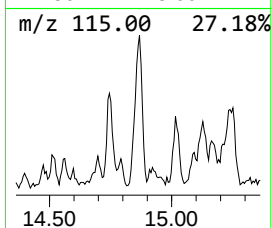
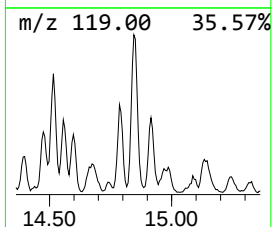
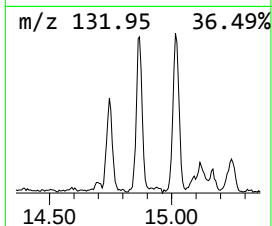
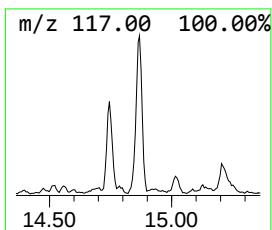
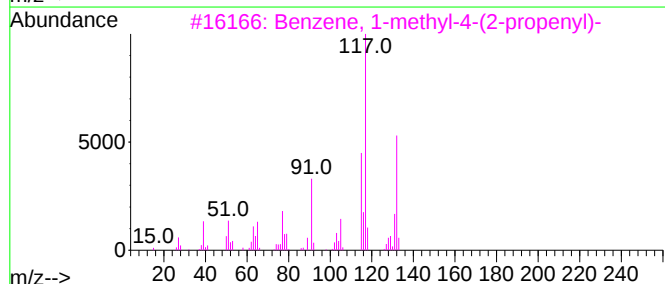
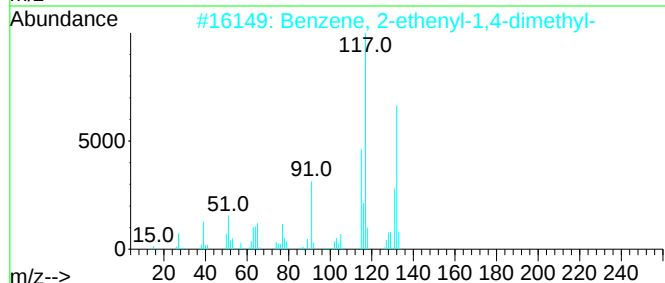
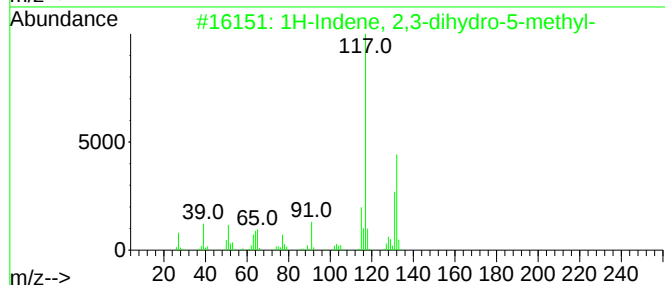
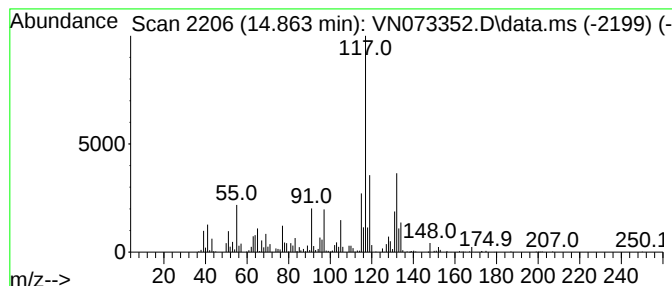
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.863	27.60 ug/l	1139090	1,4-Dichlorobenzene-d4			13.610
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-		132	C10H12	000874-35-1	91
2	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	91
3	Benzene, 1-methyl-4-(2-propenyl)-		132	C10H12	003333-13-9	89
4	Benzene, 1-methyl-2-(2-propenyl)-		132	C10H12	001587-04-8	70
5	Benzene, 2-ethenyl-1,3-dimethyl-		132	C10H12	002039-90-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31487

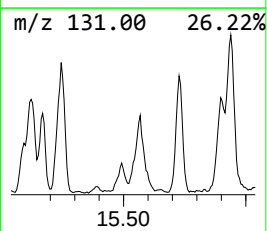
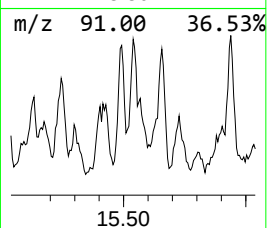
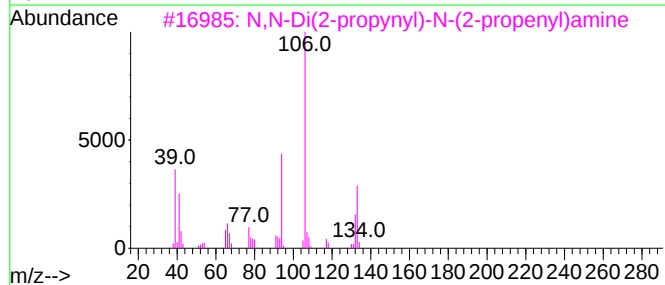
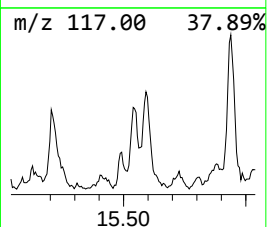
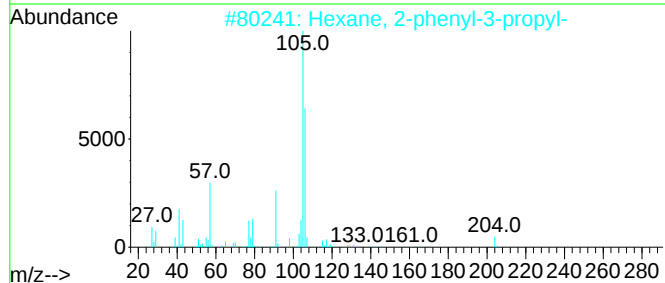
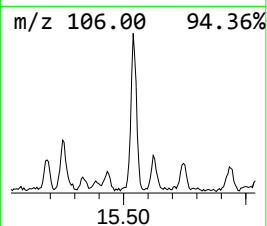
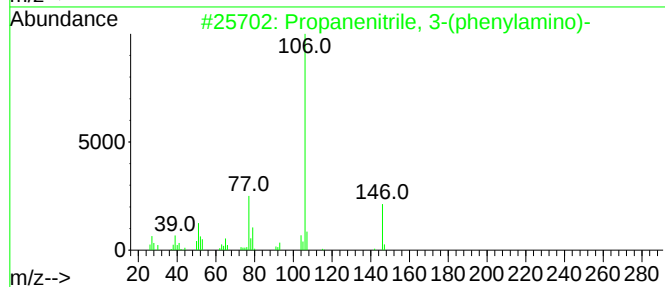
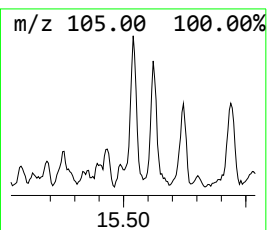
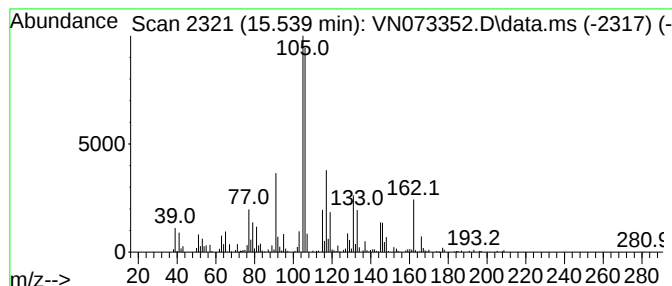
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Quant Title : SW846 8260

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

Peak Number 5 unknown15.539 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.539	15.68 ug/l	647022	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile, 3-(phenylamino)-	146	C9H10N2	001075-76-9	38
2			Hexane, 2-phenyl-3-propyl-	204	C15H24	1000161-01-5	35
3			N,N-Di(2-propynyl)-N-(2-propenyl)...	133	C9H11N	053146-05-7	35
4			2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	35
5			Benzaldehyde	106	C7H6O	000100-52-7	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31487

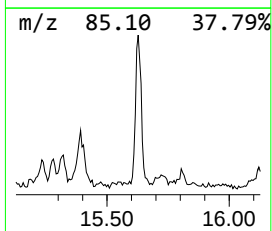
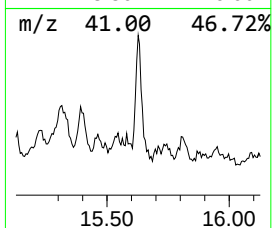
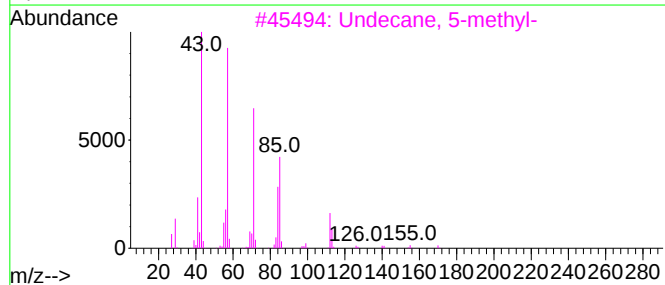
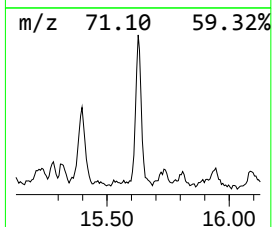
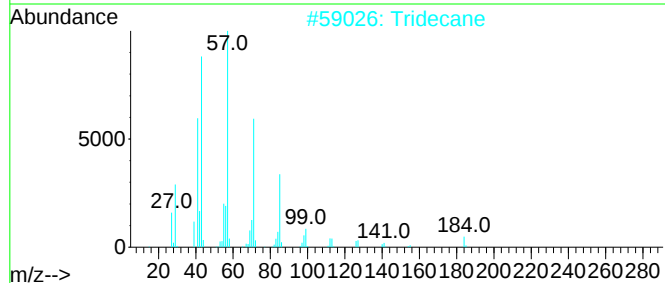
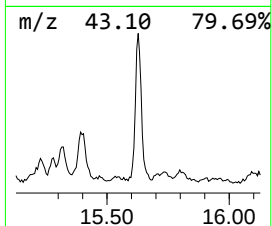
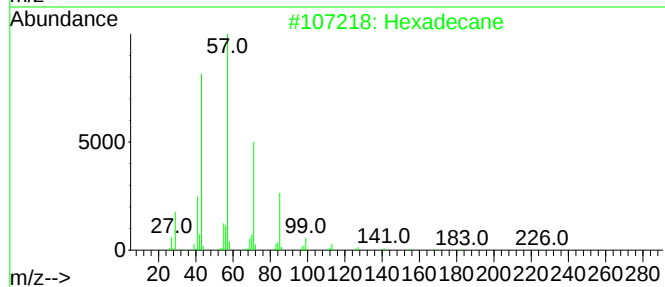
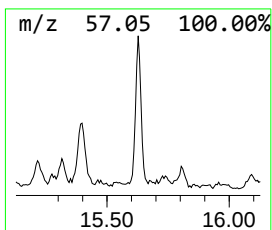
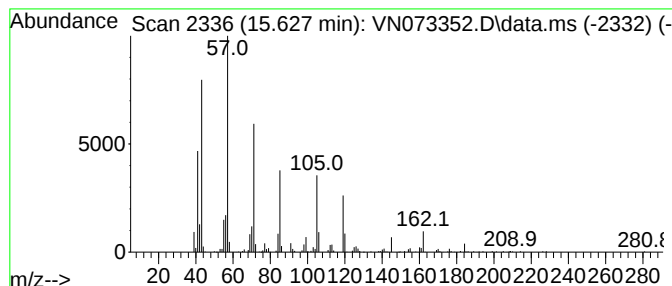
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Quant Title : SW846 8260

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

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.627	19.44 ug/l	802272	1,4-Dichlorobenzene-d4	13.610

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	89
2		Tridecane	184	C13H28	000629-50-5	87
3		Undecane, 5-methyl-	170	C12H26	001632-70-8	55
4		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	55
5		Dodecane	170	C12H26	000112-40-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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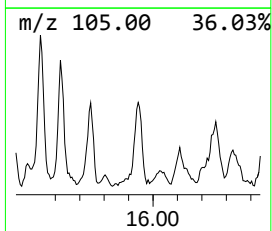
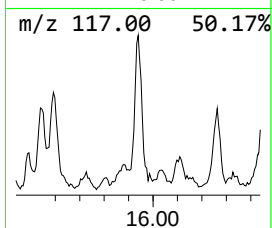
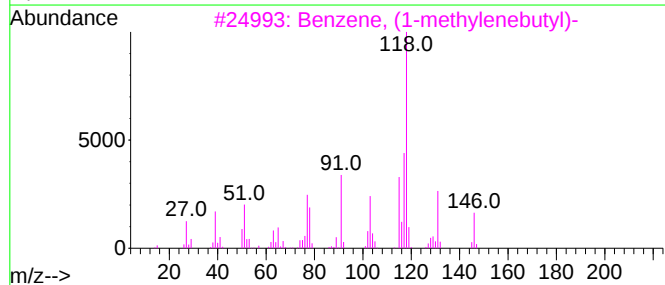
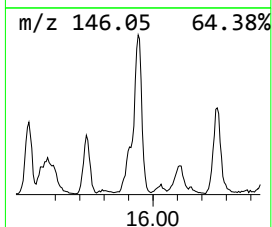
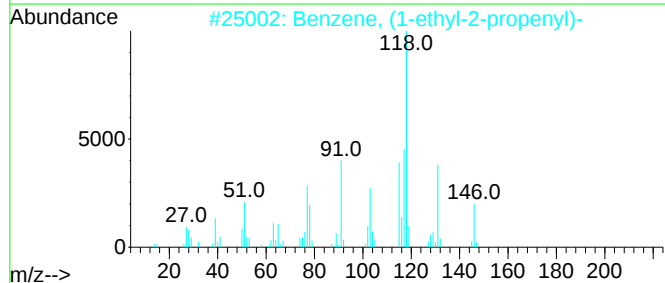
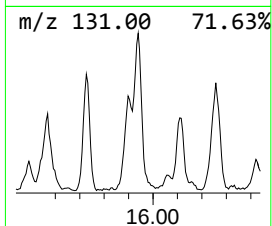
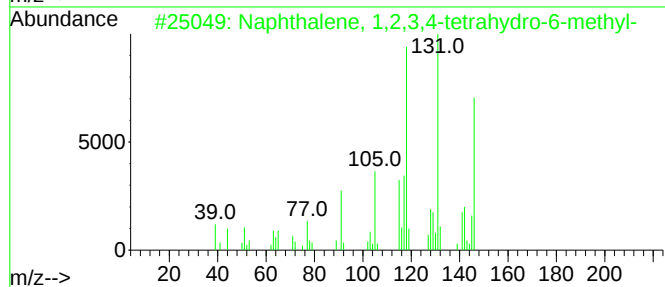
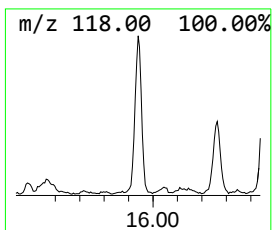
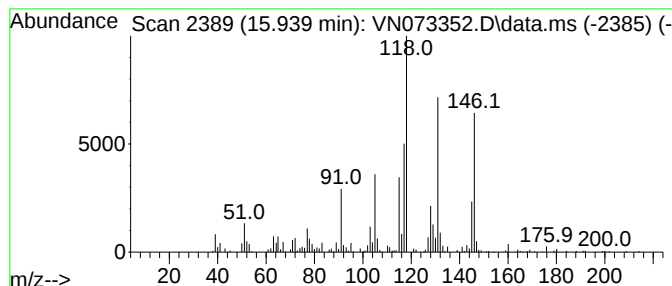
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	17.17 ug/l	708772	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	74
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	68
4			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	58
5			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31487

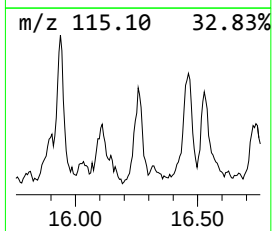
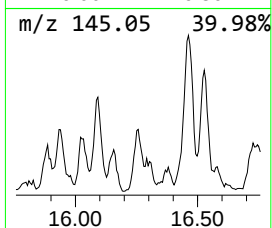
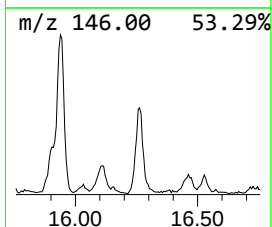
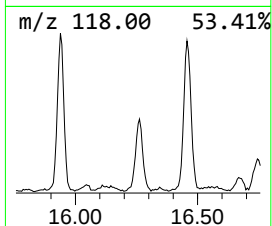
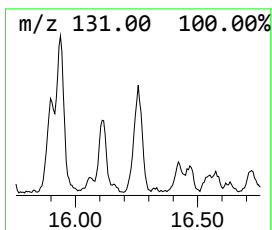
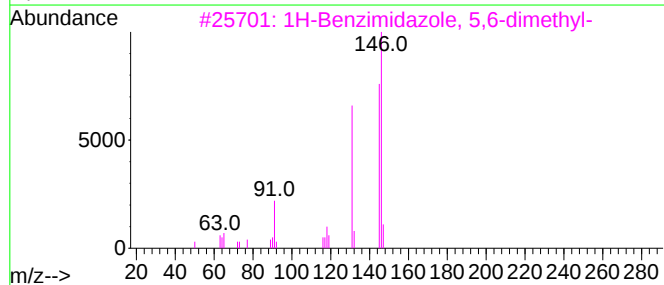
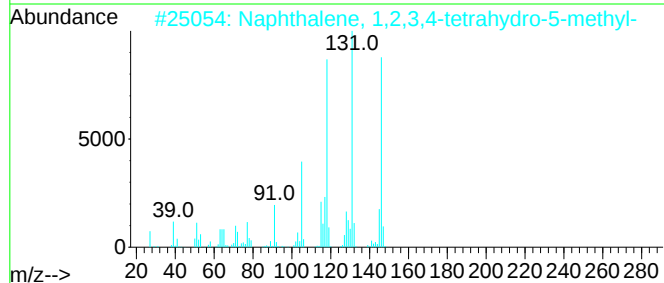
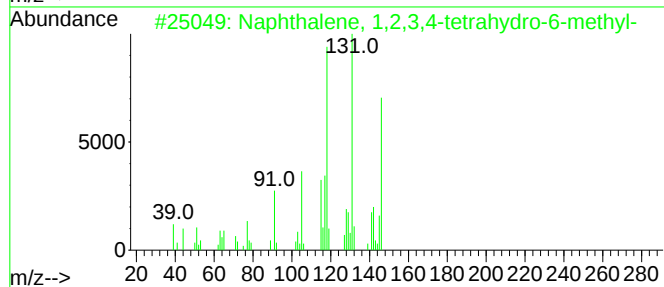
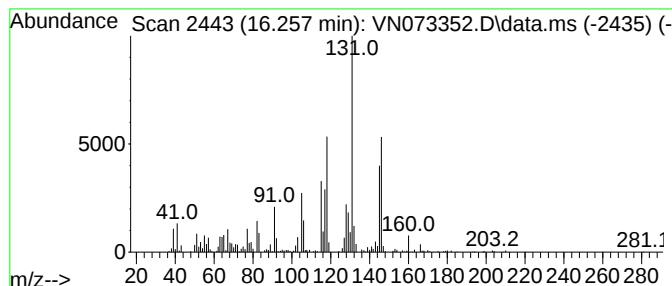
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	16.16 ug/l	667031	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	86
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	83
3			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	58
4			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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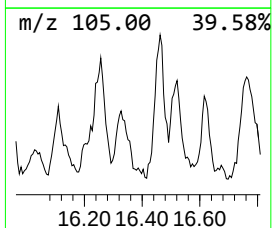
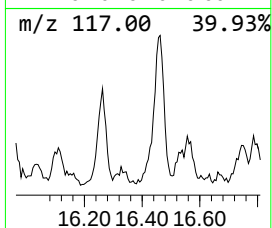
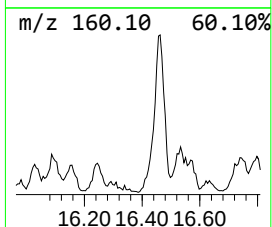
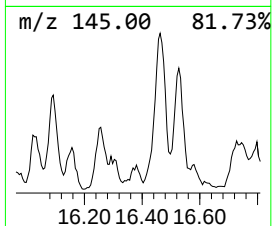
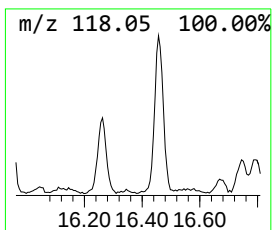
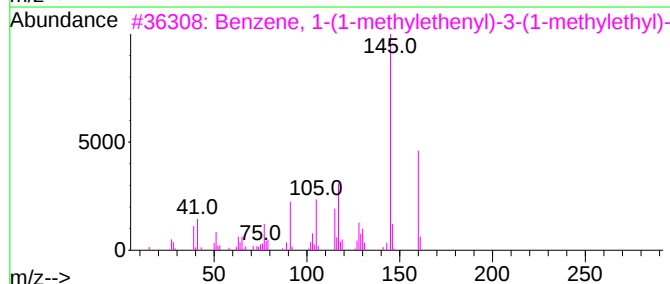
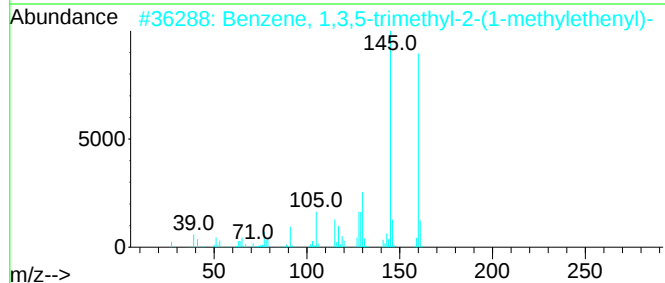
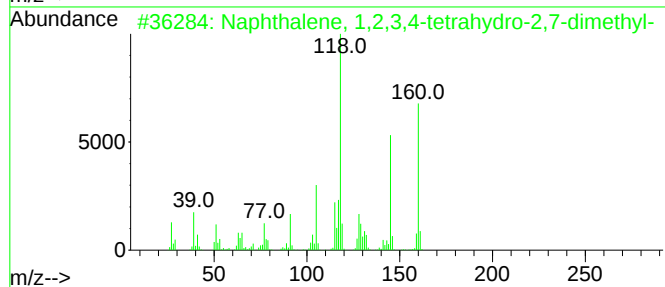
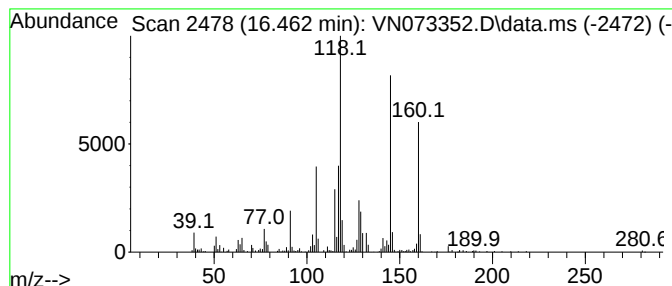
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	13.24 ug/l	546282	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	93
2			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
3			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	70
4			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	60
5			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070622\
Data File : VN073352.D
Acq On : 06 Jul 2022 18:03
Operator : JC\MD
Sample : N3586-05 10X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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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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Naphthalene, de...	14.445	27.4	ug/l	1131150	4	13.610	2063670	50.0
Tridecane	14.786	27.0	ug/l	1114100	4	13.610	2063670	50.0
1H-Indene, 2,3-...	14.863	27.6	ug/l	1139090	4	13.610	2063670	50.0
unknown15.539	15.539	15.7	ug/l	647022	4	13.610	2063670	50.0
Hexadecane	15.627	19.4	ug/l	802272	4	13.610	2063670	50.0
Naphthalene, 1,...	15.939	17.2	ug/l	708772	4	13.610	2063670	50.0
Naphthalene, 1,...	16.257	16.2	ug/l	667031	4	13.610	2063670	50.0
Naphthalene, 1,...	16.462	13.2	ug/l	546282	4	13.610	2063670	50.0