

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
 Data File : VN073979.D
 Acq On : 17 Aug 2022 16:22
 Operator : JC\MD
 Sample : N4136-03
 Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-5

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\82N081522W.M
 Title : SW846 8260

Signal : TIC: VN073979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.693	127	137	138	rBV8	16207	36180	1.10%	0.092%
2	4.775	479	491	505	rBV	40837	140254	4.25%	0.358%
3	4.969	513	524	534	rBV4	13242	45386	1.38%	0.116%
4	5.216	550	566	578	rBV	23802	101563	3.08%	0.259%
5	7.287	907	918	933	rBV2	36963	113994	3.46%	0.291%
6	7.945	1018	1030	1035	rBV	373611	906318	27.48%	2.310%
7	8.010	1035	1041	1063	rVB	709988	1634099	49.55%	4.165%
8	8.363	1090	1101	1112	rBV	337207	780966	23.68%	1.991%
9	8.686	1150	1156	1173	rVB3	20569	74012	2.24%	0.189%
10	8.898	1183	1192	1208	rVB	937850	1948218	59.07%	4.966%
11	10.380	1430	1444	1451	rBV	1302664	2454050	74.41%	6.255%
12	10.439	1451	1454	1461	rVB	42762	71373	2.16%	0.182%
13	11.133	1561	1572	1581	rBV2	45326	89477	2.71%	0.228%
14	11.686	1657	1666	1675	rBV	1502310	2615390	79.30%	6.667%
15	11.786	1677	1683	1692	rVV2	32923	79570	2.41%	0.203%
16	11.892	1692	1701	1711	rVV4	52420	135788	4.12%	0.346%
17	12.198	1744	1753	1755	rBV4	26809	56432	1.71%	0.144%
18	12.304	1765	1771	1776	rVB4	20637	42496	1.29%	0.108%
19	12.404	1781	1788	1789	rBV5	25999	45910	1.39%	0.117%
20	12.674	1827	1834	1844	rVB	1961074	3202995	97.12%	8.165%
21	12.845	1857	1863	1869	rVB5	40412	96509	2.93%	0.246%
22	12.922	1869	1876	1880	rBV2	70751	137338	4.16%	0.350%
23	12.992	1880	1888	1894	rVV3	223047	451508	13.69%	1.151%
24	13.051	1894	1898	1902	rVB6	33002	54544	1.65%	0.139%
25	13.098	1902	1906	1909	rBV2	35438	52669	1.60%	0.134%
26	13.227	1924	1928	1934	rVB2	93677	151914	4.61%	0.387%
27	13.310	1935	1942	1947	rBV	159915	278837	8.45%	0.711%
28	13.439	1961	1964	1968	rVB3	36399	45628	1.38%	0.116%
29	13.504	1968	1975	1979	rBV4	129799	258957	7.85%	0.660%
30	13.545	1979	1982	1986	rVV5	67133	101041	3.06%	0.258%
31	13.616	1986	1994	2003	rVB	1963903	3297992	100.00%	8.407%
32	13.686	2003	2006	2012	rBV3	58803	87013	2.64%	0.222%
33	13.810	2023	2027	2030	rBV2	120168	158604	4.81%	0.404%
34	13.851	2030	2034	2043	rVB3	171454	353222	10.71%	0.900%
35	13.933	2043	2048	2053	rBV	577338	907917	27.53%	2.314%
36	14.010	2058	2061	2065	rVV	66344	109665	3.33%	0.280%

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37	14.074	2068	2072	2073	rVV	67490	86869	2.63%	0.221%
38	14.098	2074	2076	2079	rVV2	121339	171104	5.19%	0.436%
39	14.151	2079	2085	2091	rVB3	327420	643968	19.53%	1.642%
40	14.263	2098	2104	2109	rBV2	318899	562980	17.07%	1.435%
41	14.321	2109	2114	2116	rBV2	79325	134516	4.08%	0.343%
42	14.398	2121	2127	2130	rBV6	110449	244516	7.41%	0.623%
43	14.445	2130	2135	2139	rVV3	268813	426000	12.92%	1.086%
44	14.516	2145	2147	2151	rVB	148150	172293	5.22%	0.439%
45	14.563	2151	2155	2158	rBV	261425	347442	10.53%	0.886%
46	14.604	2158	2162	2169	rVB5	264906	413837	12.55%	1.055%
47	14.668	2169	2173	2174	rBV3	111720	141331	4.29%	0.360%
48	14.704	2175	2179	2183	rVB	167391	260908	7.91%	0.665%
49	14.786	2183	2193	2199	rBV5	451601	1011094	30.66%	2.577%
50	14.857	2199	2205	2212	rBV3	464050	1263594	38.31%	3.221%
51	14.921	2212	2216	2221	rVB3	236242	414991	12.58%	1.058%
52	15.021	2229	2233	2239	rVB3	171430	308587	9.36%	0.787%
53	15.133	2247	2252	2256	rBV3	292589	524460	15.90%	1.337%
54	15.245	2265	2271	2277	rVB3	314482	717949	21.77%	1.830%
55	15.404	2293	2298	2301	rBV6	151162	322731	9.79%	0.823%
56	15.492	2308	2313	2317	rBV	262981	451702	13.70%	1.151%
57	15.545	2317	2322	2325	rBV4	266417	452836	13.73%	1.154%
58	15.633	2333	2337	2346	rVB4	291909	654786	19.85%	1.669%
59	15.733	2346	2354	2361	rBV4	241023	700601	21.24%	1.786%
60	15.810	2363	2367	2372	rVV4	102855	176911	5.36%	0.451%
61	15.898	2375	2382	2385	rVV3	204284	524140	15.89%	1.336%
62	15.945	2385	2390	2396	rVB	519051	1004204	30.45%	2.560%
63	16.033	2401	2405	2411	rVV7	189355	490012	14.86%	1.249%
64	16.115	2411	2419	2431	rVB6	274631	1081492	32.79%	2.757%
65	16.262	2436	2444	2450	rBV3	480265	1113150	33.75%	2.837%
66	16.462	2470	2478	2485	rBV3	687853	1618423	49.07%	4.125%
67	16.533	2485	2490	2503	rVB6	315880	969210	29.39%	2.471%
68	16.745	2518	2526	2531	rBV8	236689	705828	21.40%	1.799%

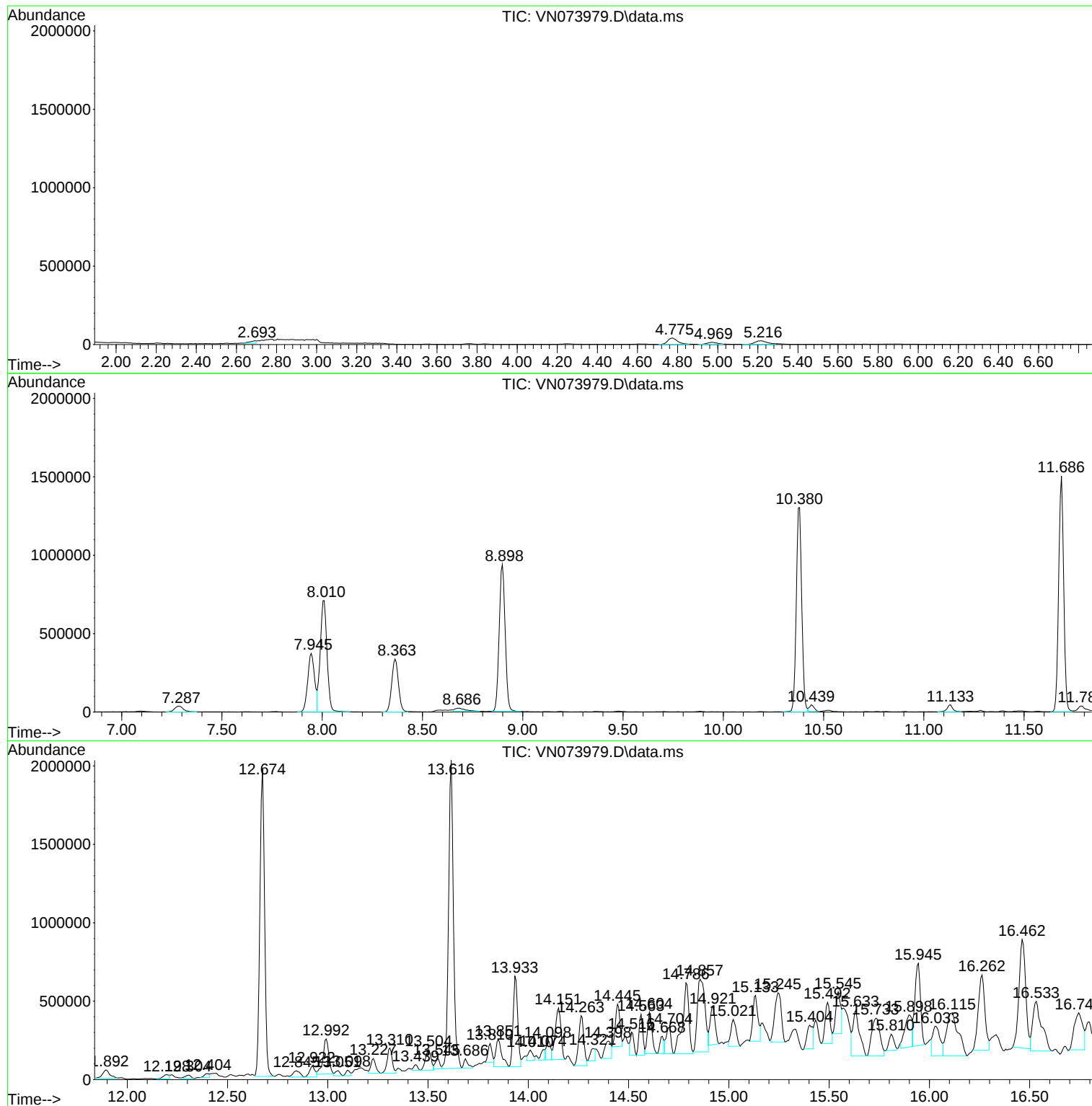
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ClientSampleId :
WC-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
WC-5

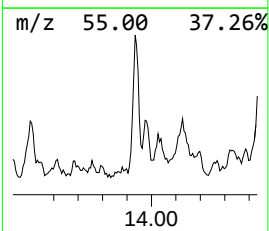
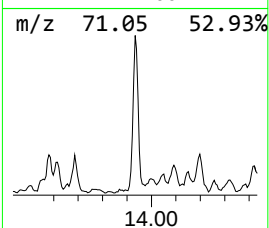
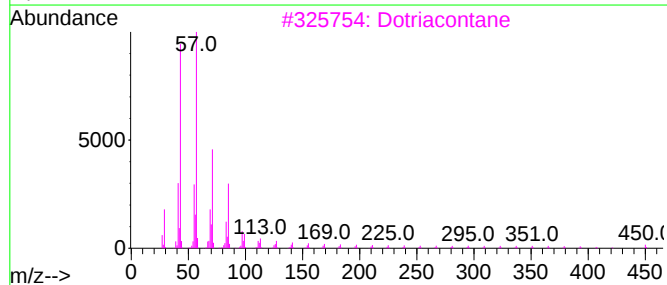
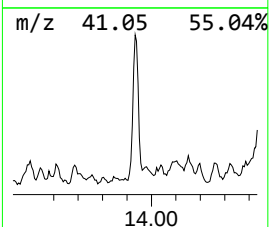
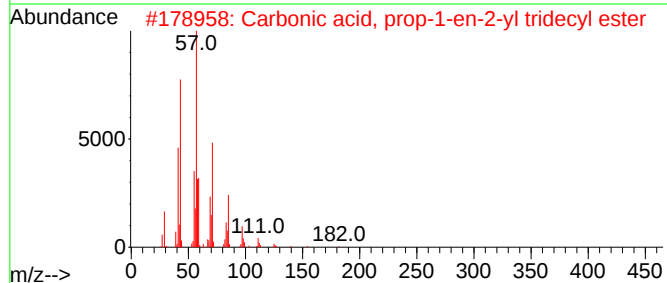
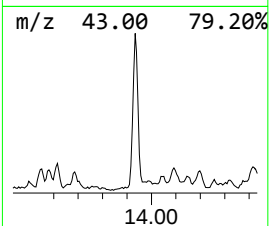
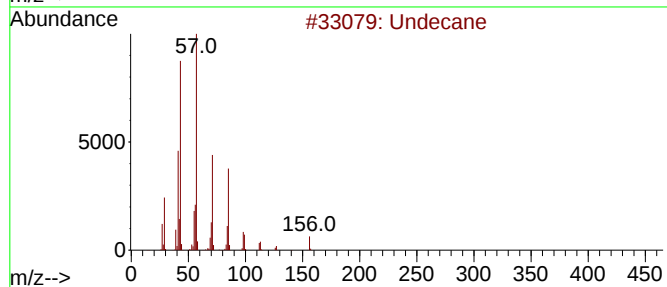
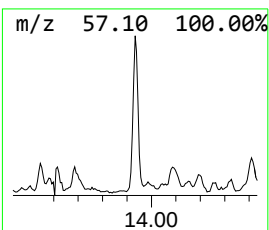
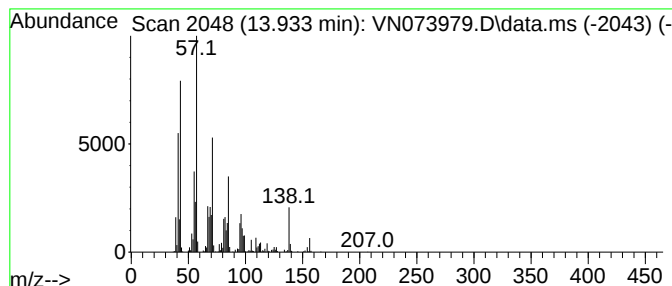
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	13.76 ug/l	907917	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	95
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	47
3			Dotriacontane	451	C32H66	000544-85-4	46
4			Tetradecane	198	C14H30	000629-59-4	46
5			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	43



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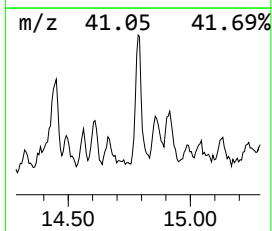
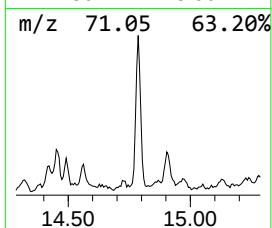
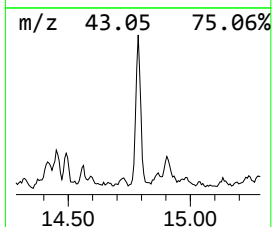
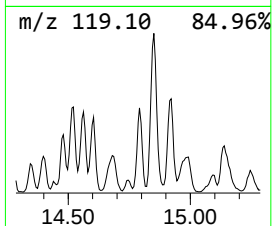
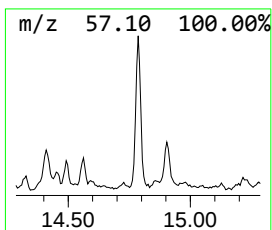
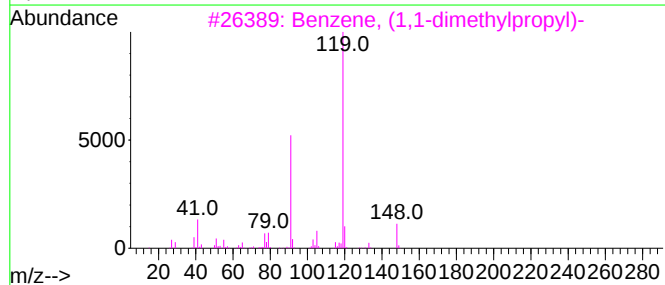
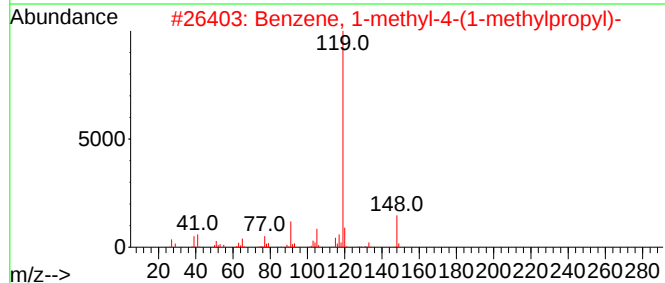
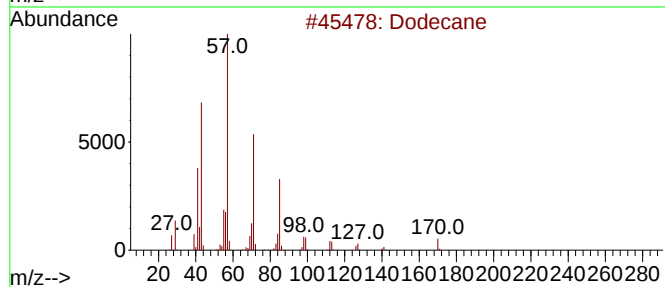
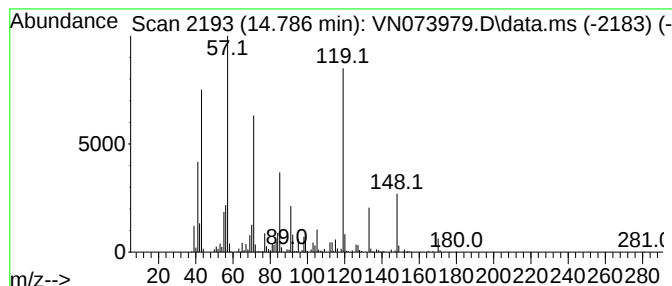
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	15.33 ug/l	1011090	1,4-Dichlorobenzene-d4	13.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane	170	C12H26	000112-40-3	89
2		Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	41
3		Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	38
4		Tridecane	184	C13H28	000629-50-5	38
5		Hexadecane	226	C16H34	000544-76-3	30



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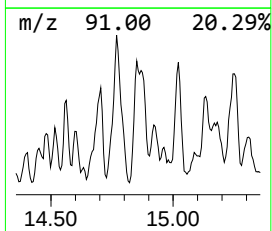
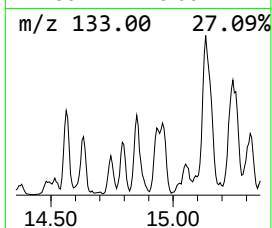
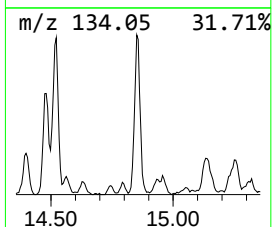
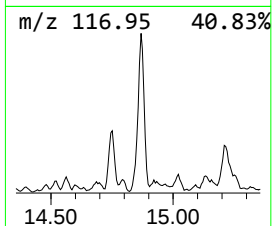
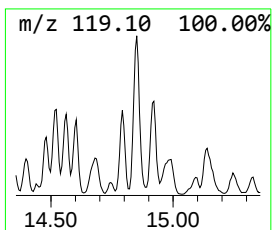
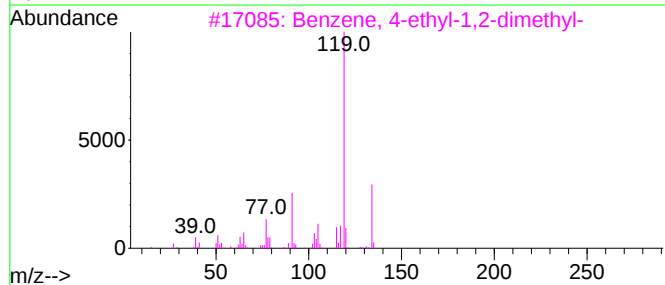
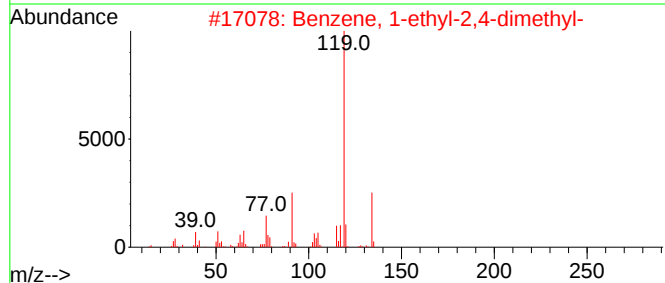
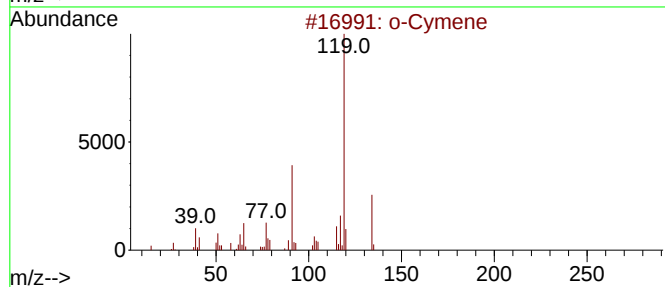
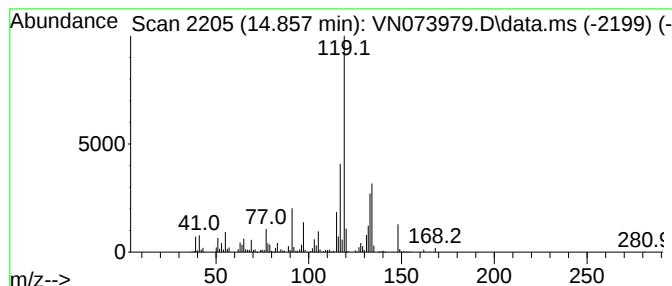
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 o-Cymene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	19.16 ug/l	1263590	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	55
2			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	55
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	55
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	55
5			p-Cymene	134	C10H14	000099-87-6	55



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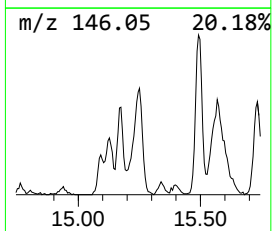
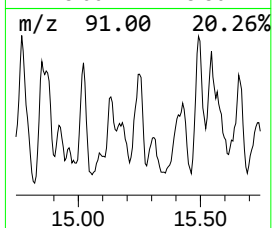
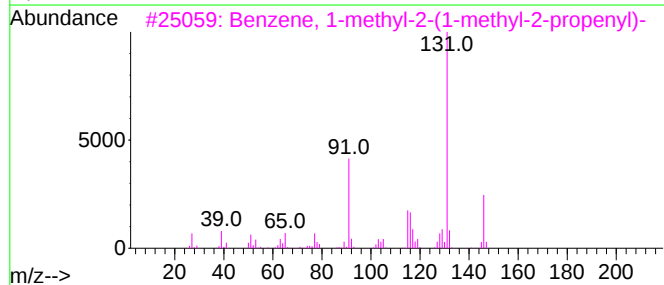
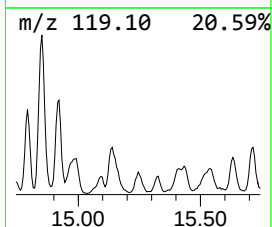
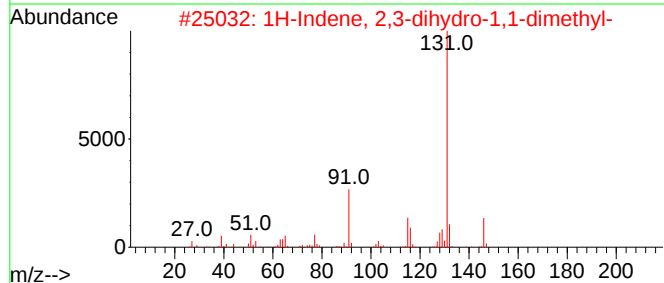
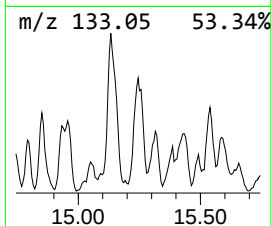
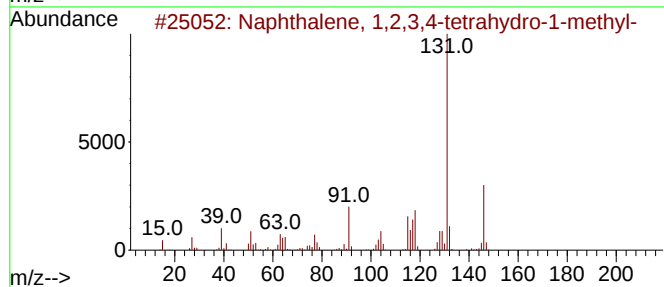
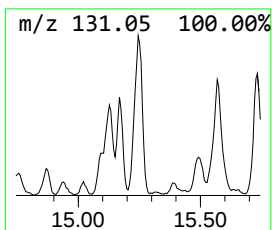
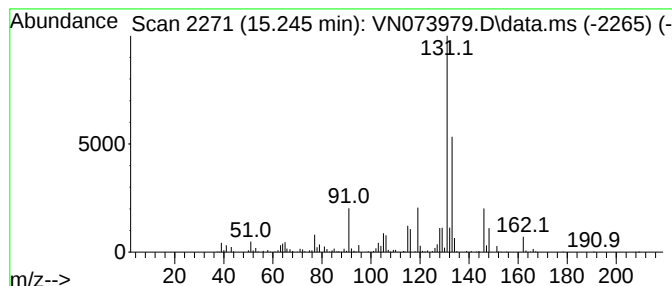
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Peak Number 4 Naphthalene, 1,2,3,4-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	10.88 ug/l	717949	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
2			1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	64
3			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	60
4			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	58
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

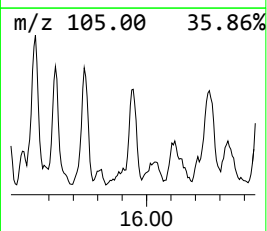
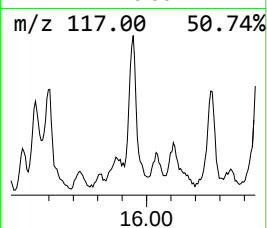
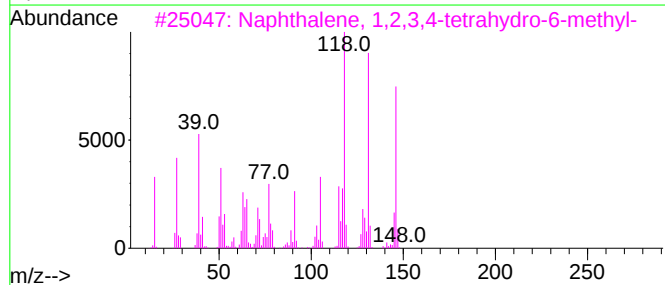
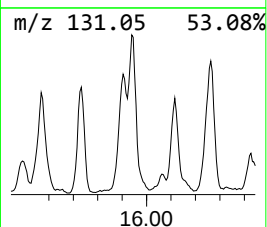
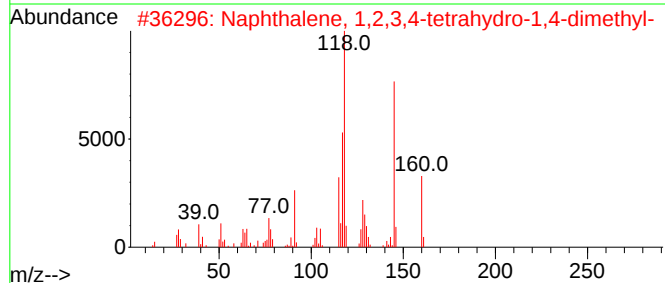
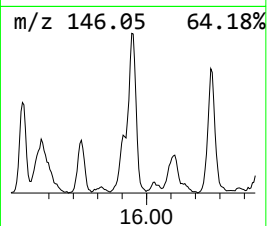
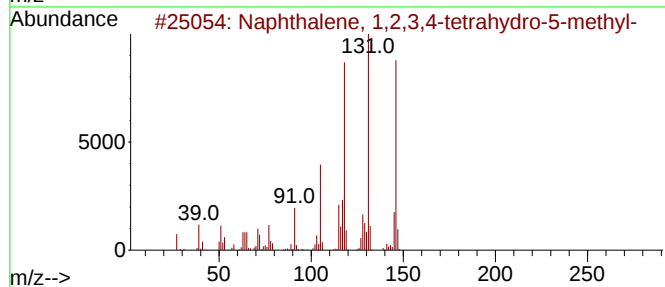
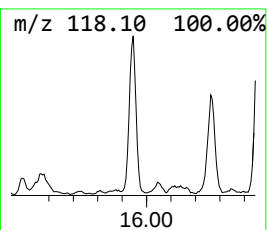
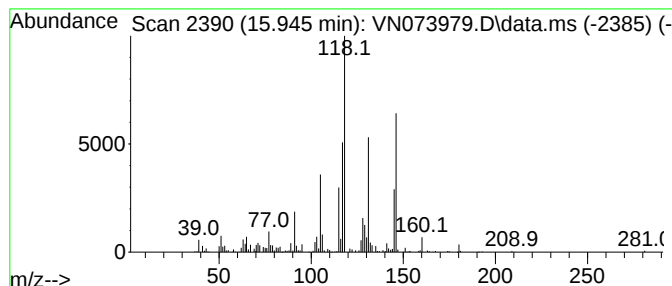
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	15.22 ug/l	1004200	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	68
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	58
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	53
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	50
5			1H-Indene-4-carboxaldehyde, 2,3-...	146	C10H10O	051932-70-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

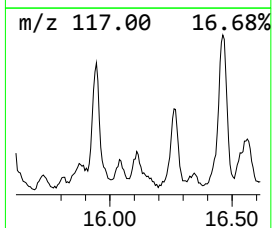
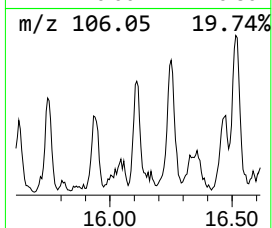
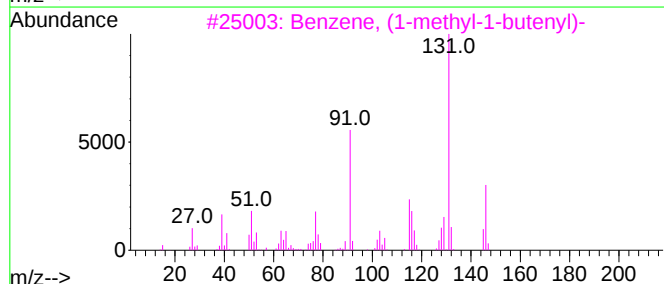
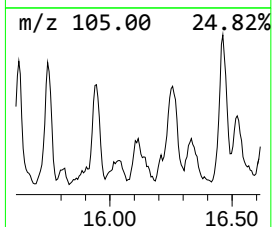
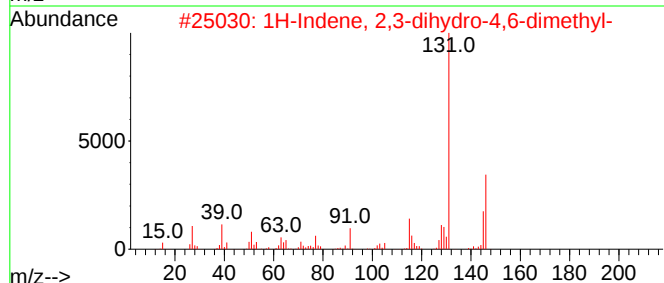
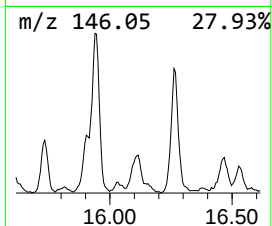
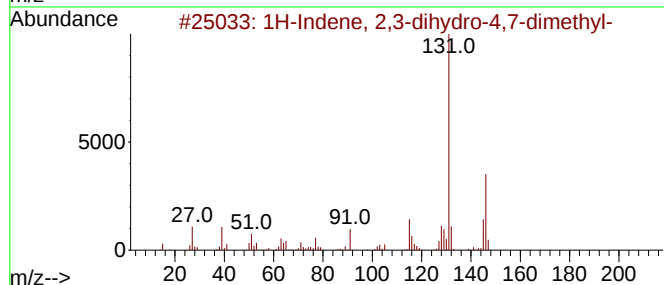
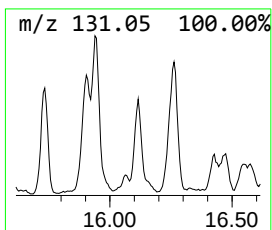
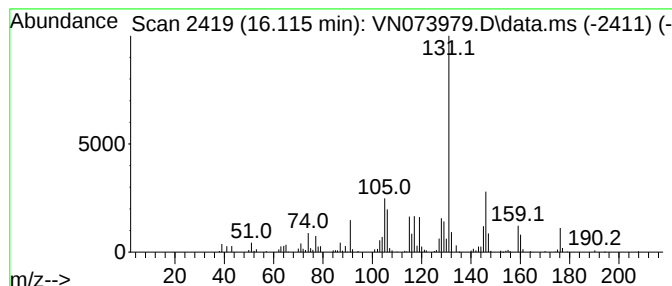
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.115	16.40 ug/l	1081490	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	93		
2	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	70		
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	70		
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70		
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

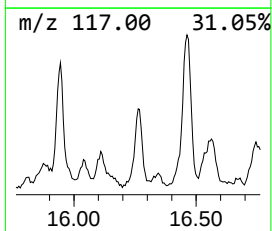
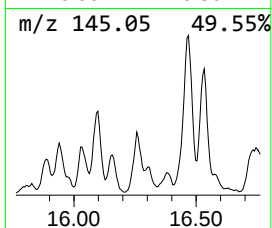
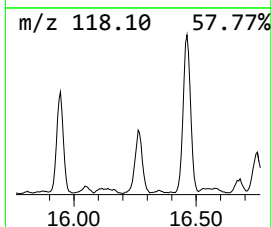
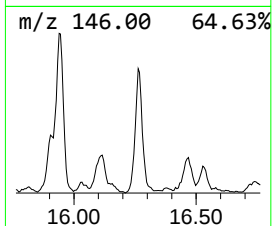
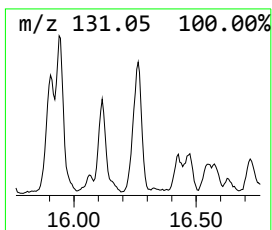
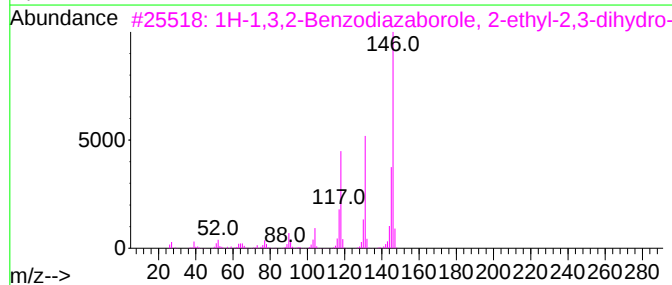
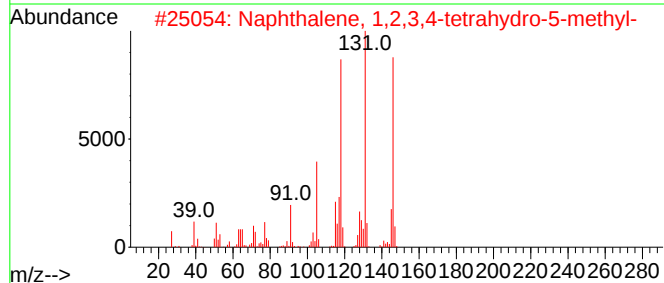
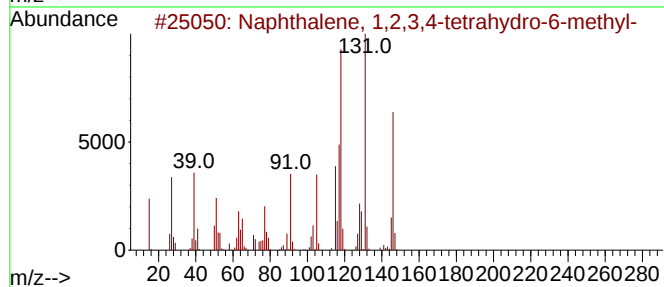
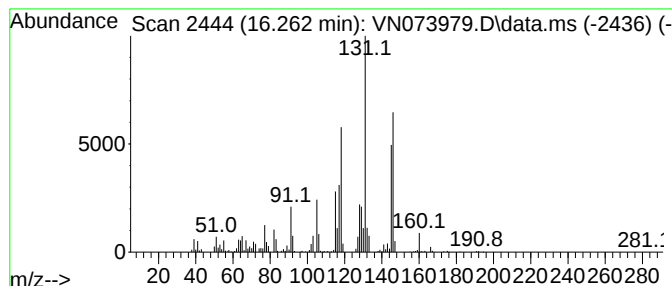
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	16.88 ug/l	1113150	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	89
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	74
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
4			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	52
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

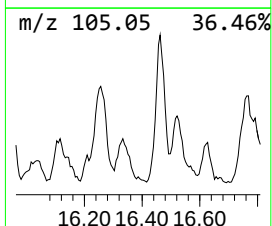
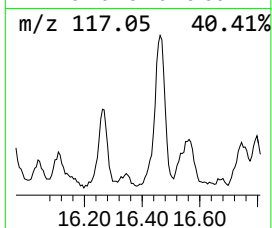
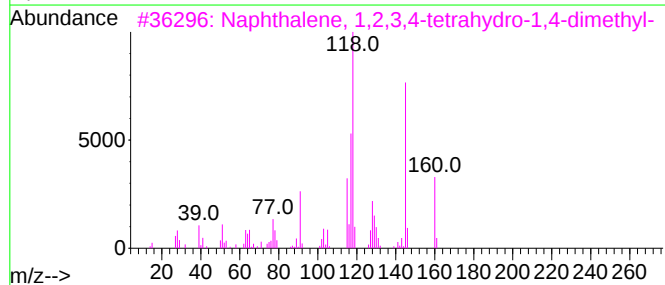
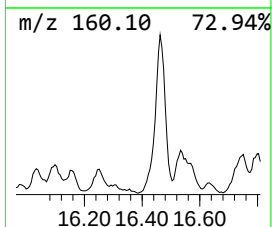
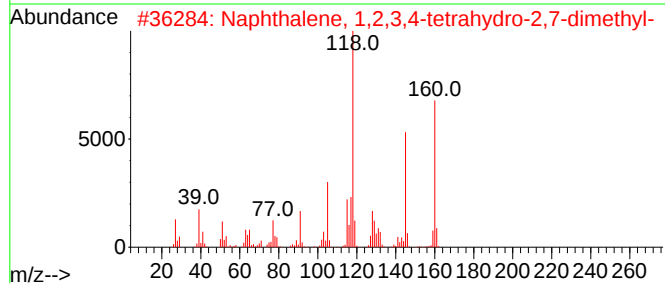
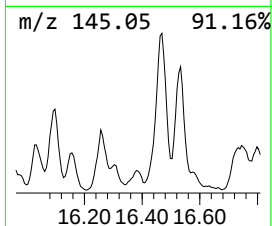
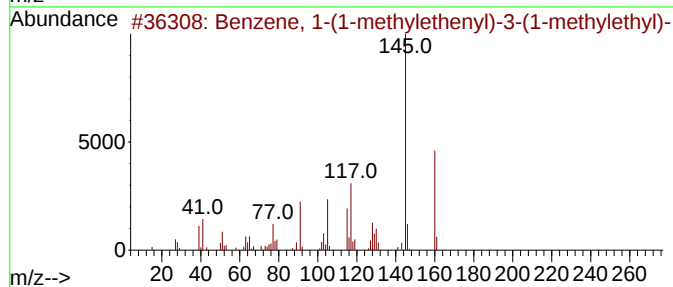
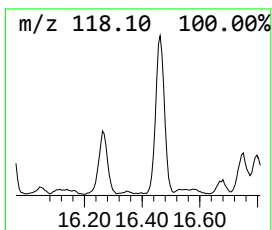
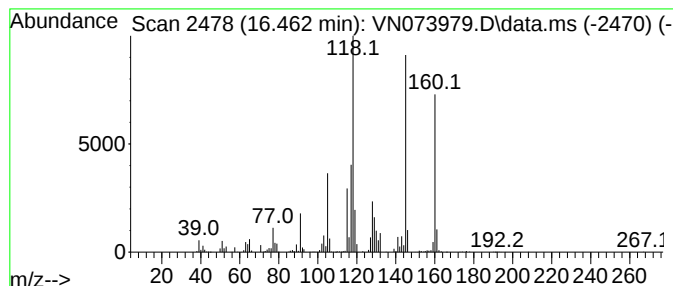
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-(1-methylethenyl)... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	24.54 ug/l	1618420	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	74
4			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

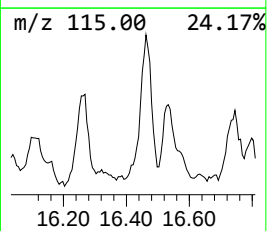
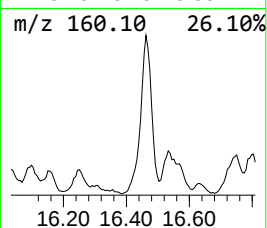
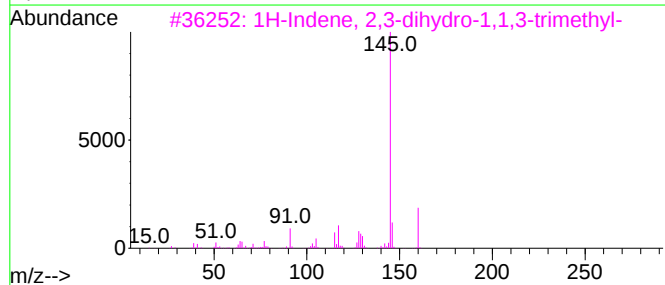
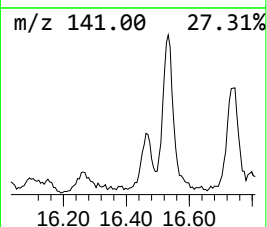
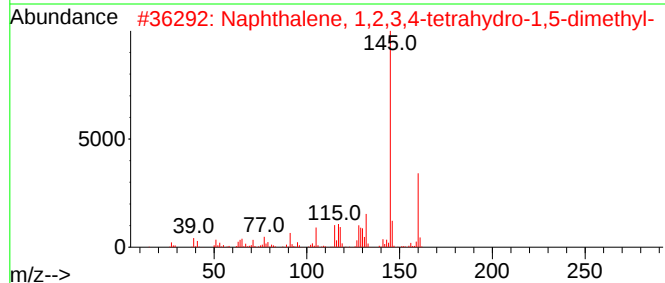
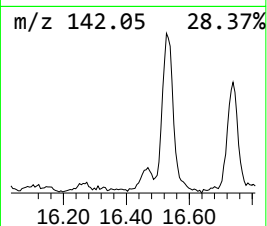
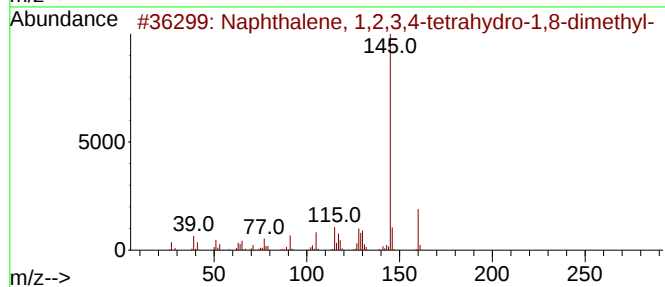
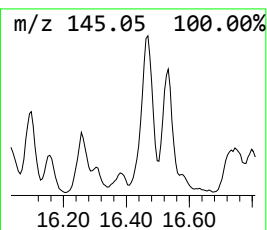
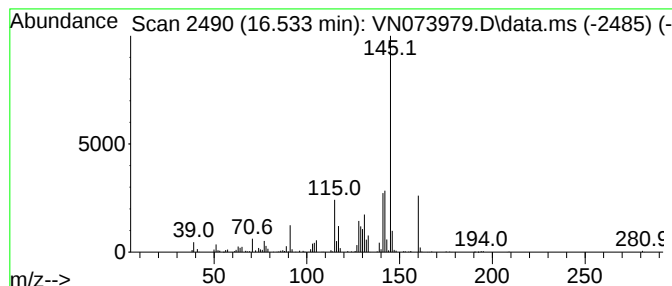
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Quant Title : SW846 8260

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.
16.533	14.69 ug/l	969210	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	68
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	64
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	62
4			Benzene, (2,2-dimethyl-1-methyle...	160	C12H16	005676-29-9	58
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

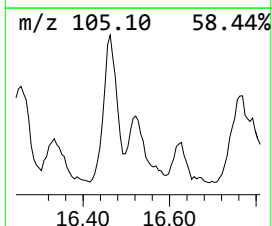
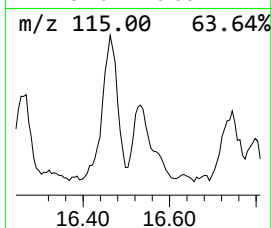
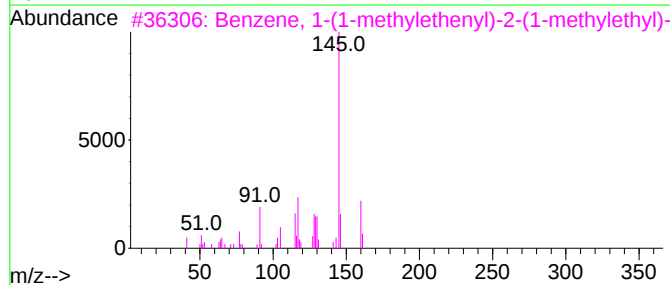
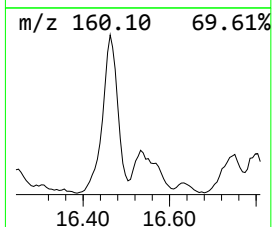
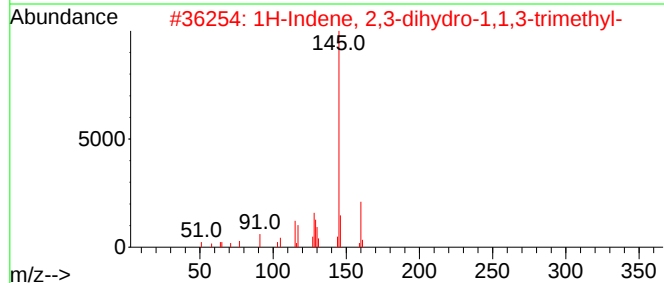
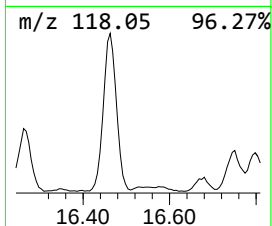
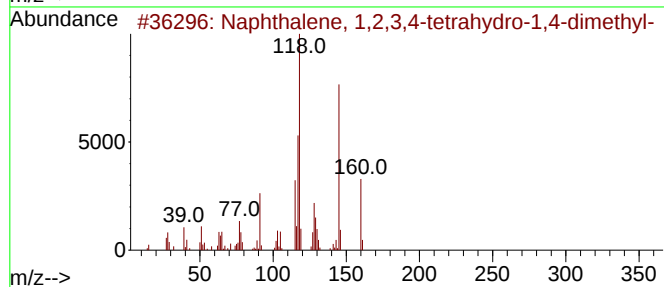
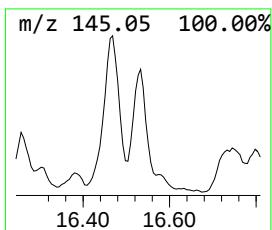
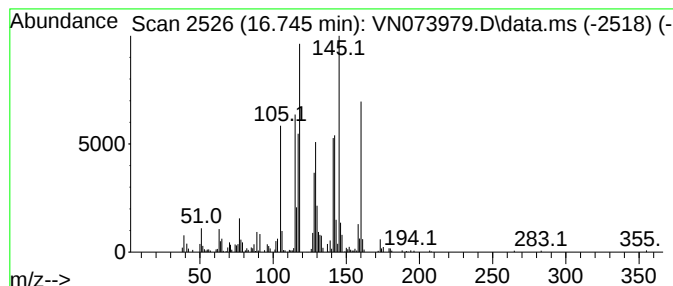
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	10.70 ug/l	705828	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	58
2			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	50
3			Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	43
4			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	42
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081722\
Data File : VN073979.D
Acq On : 17 Aug 2022 16:22
Operator : JC\MD
Sample : N4136-03
Misc : 7.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.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
Undecane	13.933	13.8	ug/l	907917	4	13.616	3297990	50.0
Dodecane	14.786	15.3	ug/l	1011090	4	13.616	3297990	50.0
o-Cymene	14.857	19.2	ug/l	1263590	4	13.616	3297990	50.0
Naphthalene, 1,...	15.245	10.9	ug/l	717949	4	13.616	3297990	50.0
Naphthalene, 1,...	15.945	15.2	ug/l	1004200	4	13.616	3297990	50.0
1H-Indene, 2,3-...	16.115	16.4	ug/l	1081490	4	13.616	3297990	50.0
Naphthalene, 1,...	16.262	16.9	ug/l	1113150	4	13.616	3297990	50.0
Benzene, 1-(1-m...	16.462	24.5	ug/l	1618420	4	13.616	3297990	50.0
Naphthalene, 1,...	16.533	14.7	ug/l	969210	4	13.616	3297990	50.0
Naphthalene, 1,...	16.745	10.7	ug/l	705828	4	13.616	3297990	50.0