

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073133.D
 Acq On : 26 Jun 2022 02:30
 Operator : JC\MD
 Sample : N3494-11
 Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SP-EXC-1-5

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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN073133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	552	566	584	rBV2	20072	93881	3.47%	0.240%
2	7.292	909	919	930	rBV	16968	50377	1.86%	0.129%
3	7.945	1020	1030	1035	rBV	216911	543428	20.11%	1.388%
4	8.004	1035	1040	1050	rVB	433630	985831	36.49%	2.519%
5	8.363	1091	1101	1112	rBV	230628	546871	20.24%	1.397%
6	8.586	1129	1139	1146	rBV2	20536	52600	1.95%	0.134%
7	8.898	1183	1192	1204	rBV	590233	1265659	46.85%	3.234%
8	9.657	1315	1321	1328	rBV5	13851	30766	1.14%	0.079%
9	10.133	1395	1402	1407	rBV5	12458	27744	1.03%	0.071%
10	10.374	1432	1443	1451	rBV	833622	1594641	59.02%	4.074%
11	10.674	1487	1494	1496	rBV4	22893	41887	1.55%	0.107%
12	10.716	1497	1501	1508	rVB2	47863	82392	3.05%	0.211%
13	10.816	1512	1518	1522	rBV6	19448	47792	1.77%	0.122%
14	10.898	1528	1532	1537	rVB3	19675	29684	1.10%	0.076%
15	10.986	1539	1547	1555	rBV2	63590	123734	4.58%	0.316%
16	11.092	1558	1565	1573	rBV2	55413	134101	4.96%	0.343%
17	11.163	1573	1577	1581	rBV2	29547	54765	2.03%	0.140%
18	11.280	1591	1597	1603	rBV2	166504	301589	11.16%	0.771%
19	11.339	1603	1607	1610	rVB3	30191	40086	1.48%	0.102%
20	11.392	1610	1616	1620	rBV4	64904	115243	4.27%	0.294%
21	11.486	1627	1632	1639	rVB2	132442	237716	8.80%	0.607%
22	11.557	1641	1644	1649	rBV4	25775	47710	1.77%	0.122%
23	11.680	1658	1665	1676	rBV2	922501	2109593	78.09%	5.390%
24	11.816	1684	1688	1692	rBV2	58406	85342	3.16%	0.218%
25	11.874	1692	1698	1702	rBV5	104353	216158	8.00%	0.552%
26	11.921	1702	1706	1710	rBV	111835	199030	7.37%	0.509%
27	12.027	1720	1724	1731	rBV5	61733	114736	4.25%	0.293%
28	12.186	1744	1751	1757	rBV3	326303	764558	28.30%	1.953%
29	12.239	1758	1760	1763	rVV2	76872	102115	3.78%	0.261%
30	12.304	1764	1771	1776	rVB2	301152	553035	20.47%	1.413%
31	12.392	1776	1786	1787	rBV4	322267	624102	23.10%	1.595%
32	12.416	1788	1790	1797	rVB4	372094	610022	22.58%	1.559%
33	12.557	1811	1814	1827	rVB7	203661	595748	22.05%	1.522%
34	12.668	1827	1833	1839	rBV	995982	1650077	61.08%	4.216%
35	12.757	1840	1848	1852	rBV6	175941	427511	15.82%	1.092%
36	12.833	1856	1861	1868	rVB2	495637	937727	34.71%	2.396%

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37	12.915	1868	1875	1880	rBV6	286338	700824	25.94%	1.791%
38	12.992	1881	1888	1893	rBV6	398612	1072057	39.68%	2.739%
39	13.133	1908	1912	1916	rBV3	282807	381391	14.12%	0.974%
40	13.186	1916	1921	1923	rBV3	171975	291898	10.80%	0.746%
41	13.221	1923	1927	1940	rVB4	601058	1199947	44.42%	3.066%
42	13.315	1940	1943	1945	rBV2	109783	133109	4.93%	0.340%
43	13.351	1945	1949	1953	rVV	243406	347290	12.85%	0.887%
44	13.398	1954	1957	1961	rVV	181979	242443	8.97%	0.619%
45	13.504	1967	1975	1978	rBV6	382577	892221	33.03%	2.280%
46	13.539	1978	1981	1986	rVV4	269722	452224	16.74%	1.155%
47	13.610	1988	1993	2002	rVB	1098516	2043749	75.65%	5.222%
48	13.751	2013	2017	2022	rBV5	259203	435443	16.12%	1.113%
49	13.933	2042	2048	2053	rBV3	951557	1711537	63.35%	4.373%
50	14.039	2063	2066	2069	rBV5	228308	324092	12.00%	0.828%
51	14.251	2099	2102	2107	rVB5	233034	346901	12.84%	0.886%
52	14.321	2110	2114	2120	rVB6	409281	701022	25.95%	1.791%
53	14.380	2120	2124	2126	rBV4	191598	286790	10.62%	0.733%
54	14.439	2130	2134	2140	rVV4	791599	1352589	50.07%	3.456%
55	14.604	2157	2162	2167	rBV5	736246	1260483	46.66%	3.221%
56	14.721	2179	2182	2185	rVB2	195661	215318	7.97%	0.550%
57	14.798	2192	2195	2199	rBV5	227022	342512	12.68%	0.875%
58	14.857	2201	2205	2208	rVV3	420754	714222	26.44%	1.825%
59	14.904	2209	2213	2221	rVB3	1122521	2162010	80.03%	5.524%
60	15.186	2259	2261	2264	rBV3	190558	207911	7.70%	0.531%
61	15.398	2292	2297	2305	rBV2	1384943	2701645	100.00%	6.903%
62	15.809	2363	2367	2373	rVB5	726459	1357198	50.24%	3.468%
63	16.380	2459	2464	2472	rVB	926841	1823211	67.49%	4.658%

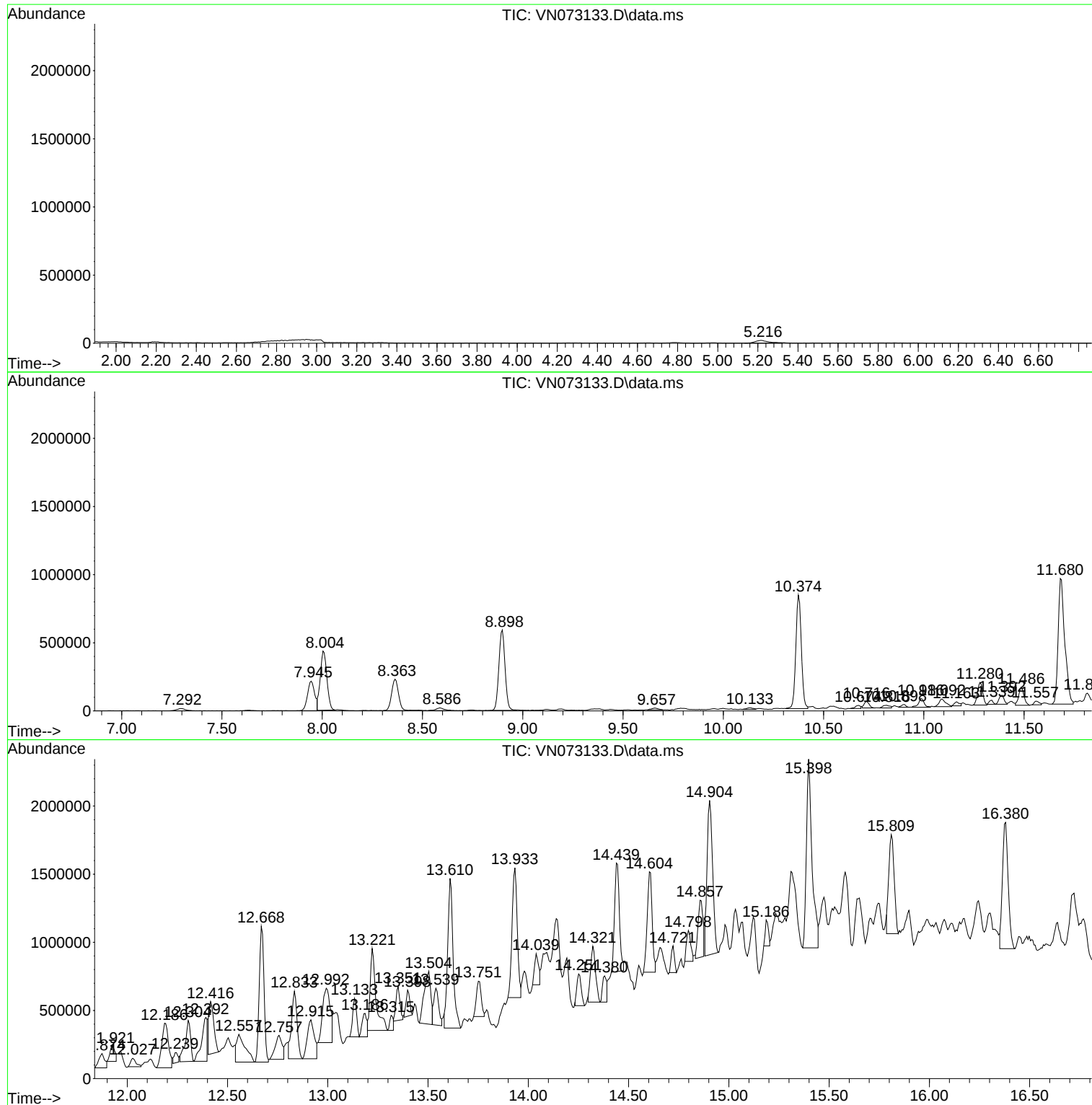
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ClientSampleId :
SP-EXC-1-5

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



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SP-EXC-1-5

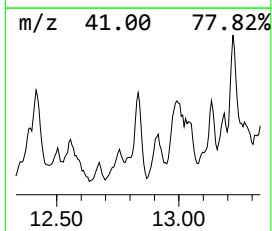
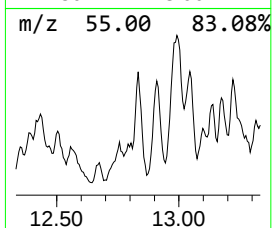
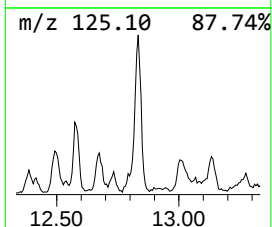
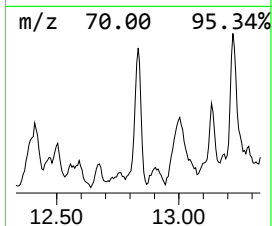
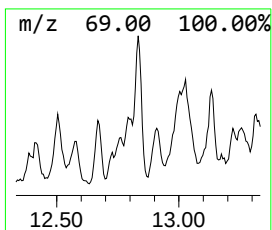
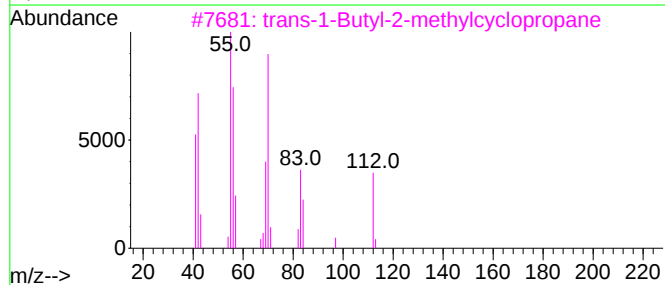
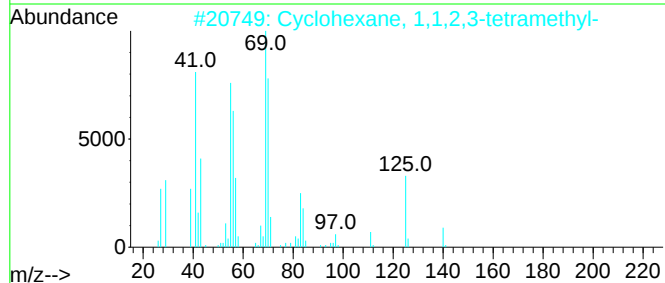
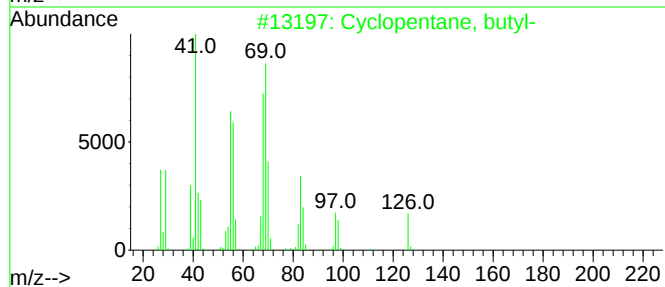
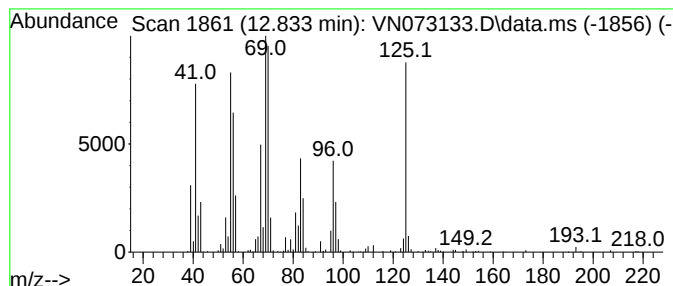
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.833	22.94 ug/l	937727	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, butyl-	126	C9H18	002040-95-1	55
2			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	47
3			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	46
4			cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	42
5			Cyclopropane, octyl-	154	C11H22	001472-09-9	38



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SP-EXC-1-5

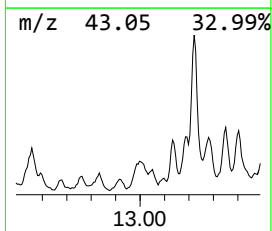
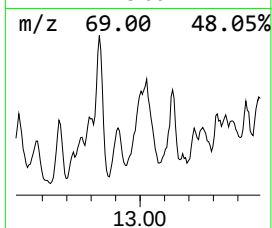
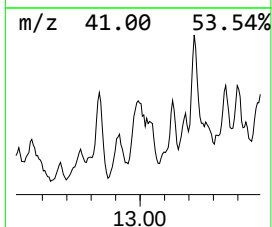
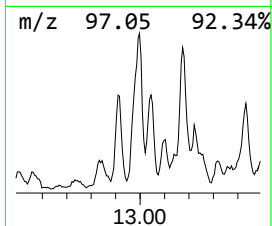
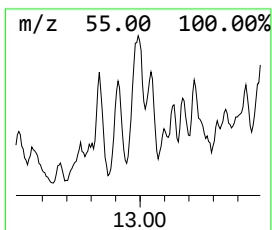
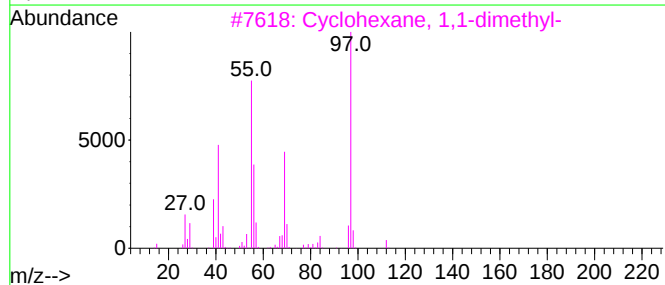
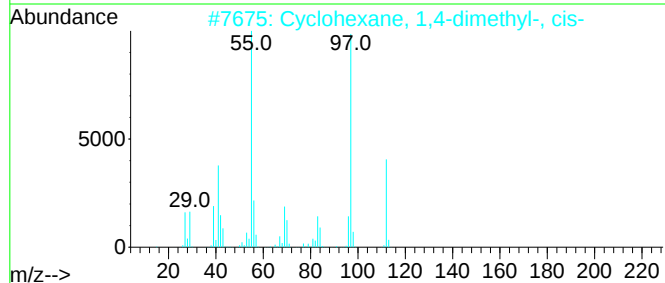
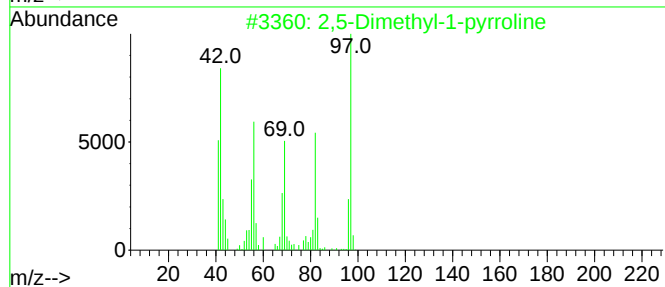
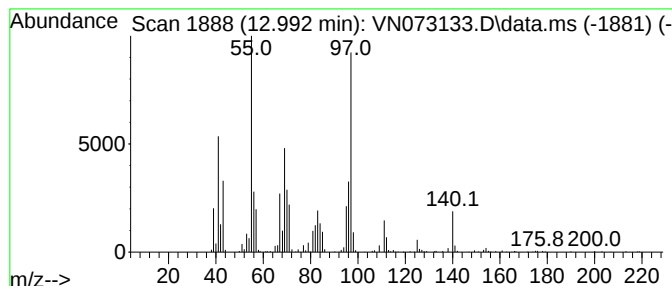
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.992 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	26.23 ug/l	1072060	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	49
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	49
3			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	43
4			1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	38
5			2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	1000283-20-9	38



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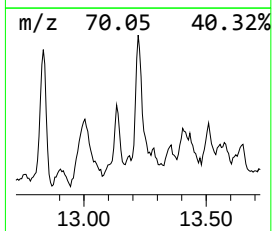
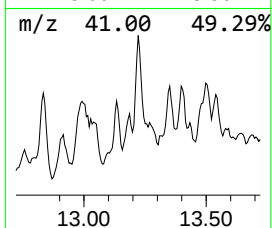
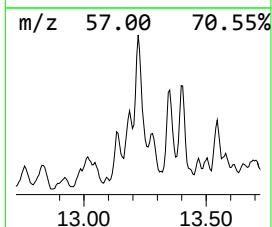
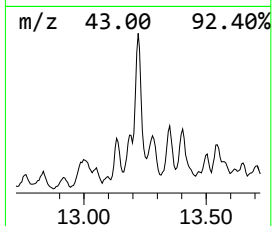
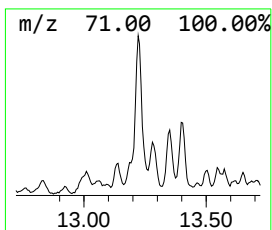
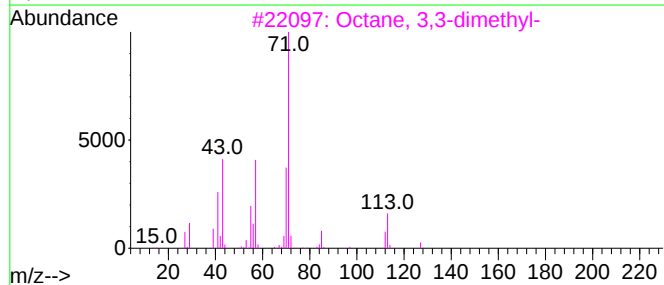
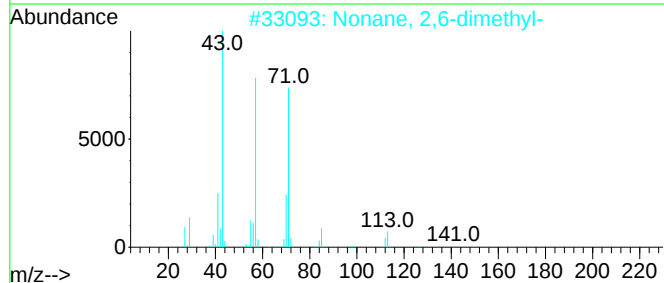
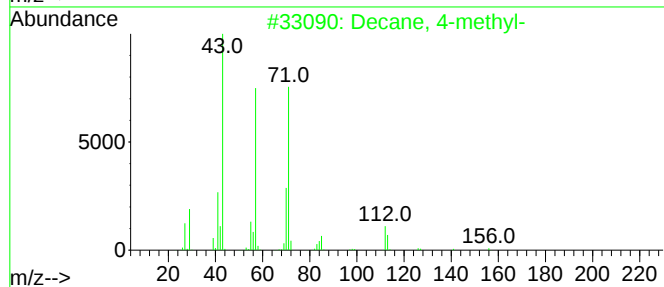
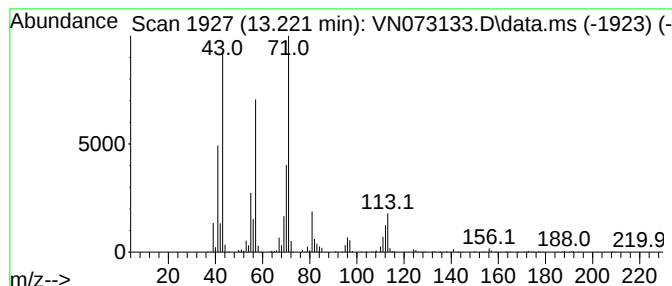
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 3 Decane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	29.36 ug/l	1199950	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	74
2			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	72
3			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
4			n-Amyl ether	158	C10H22O	000693-65-2	53
5			Methoxyacetic acid, 2-octyl ester	202	C11H22O3	1000282-69-6	50



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ClientSampleId :
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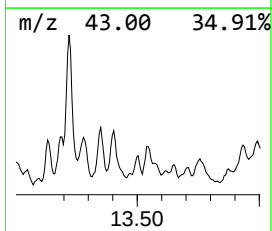
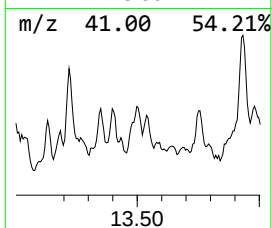
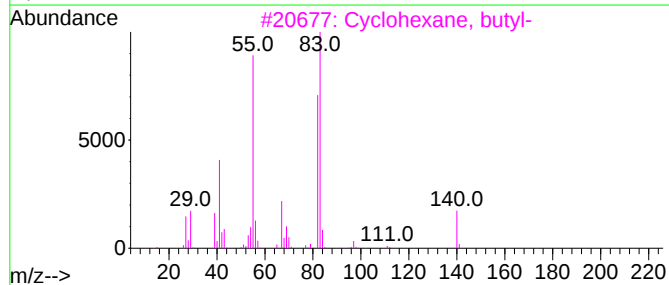
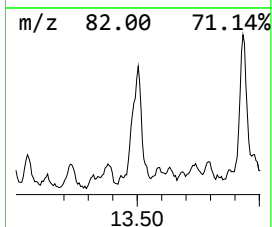
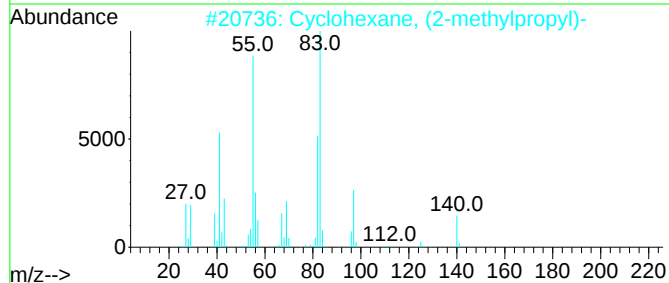
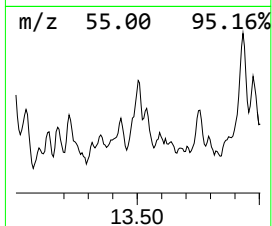
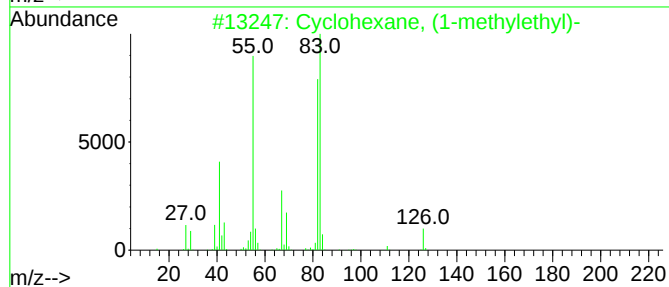
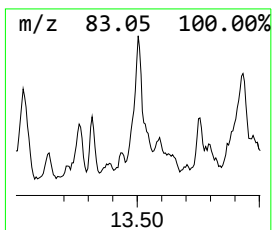
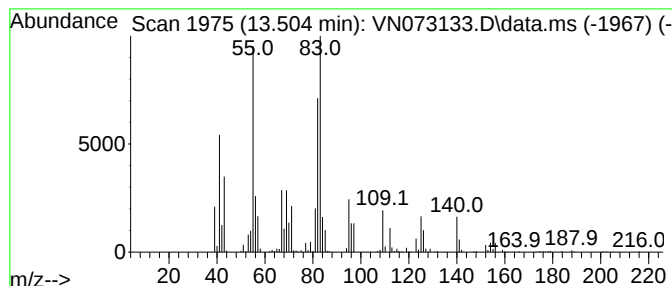
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, (1-methylethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	21.83 ug/l	892221	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	53
2			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	53
3			Cyclohexane, butyl-	140	C10H20	001678-93-9	49
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	49
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

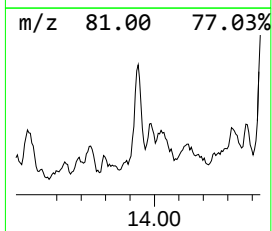
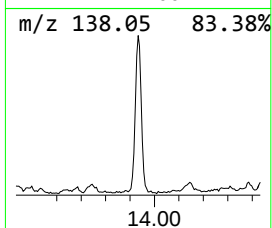
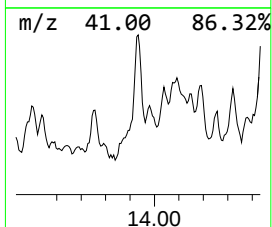
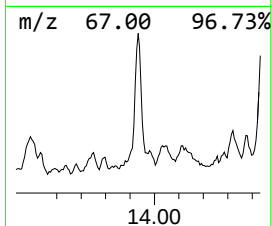
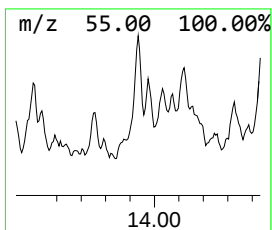
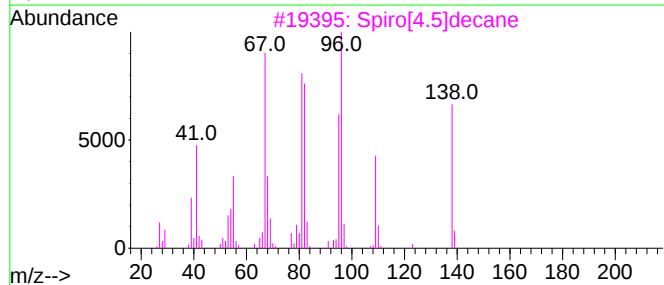
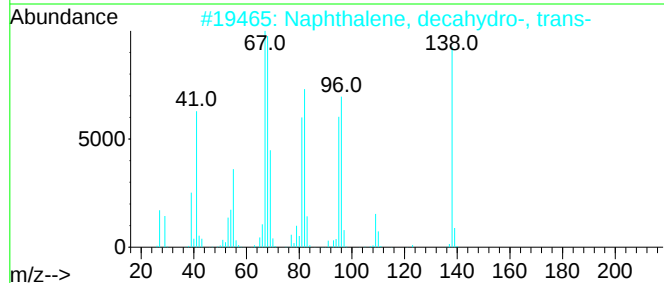
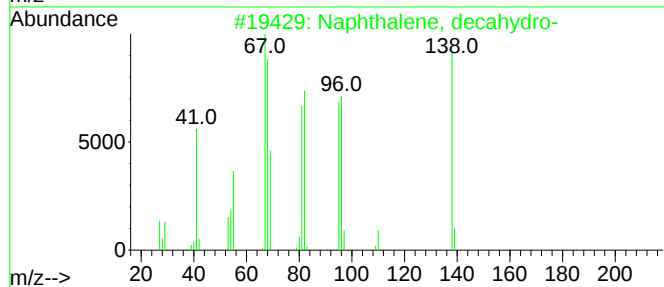
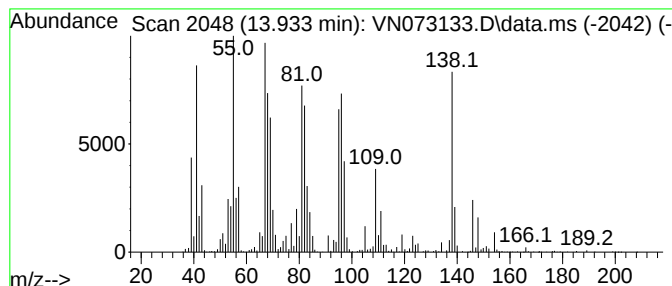
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, decahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	41.87 ug/l	1711540	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	94
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	90
3			Spiro[4.5]decane	138	C10H18	000176-63-6	89
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

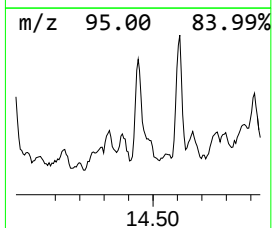
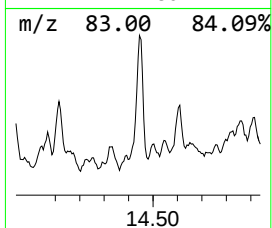
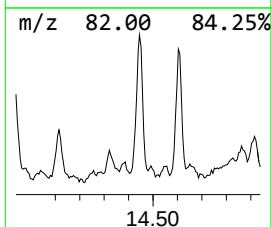
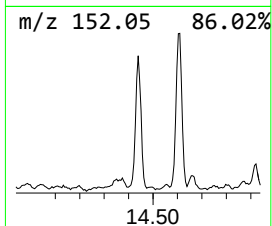
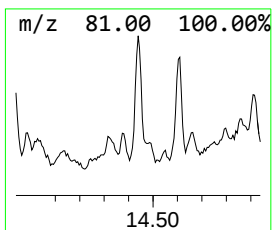
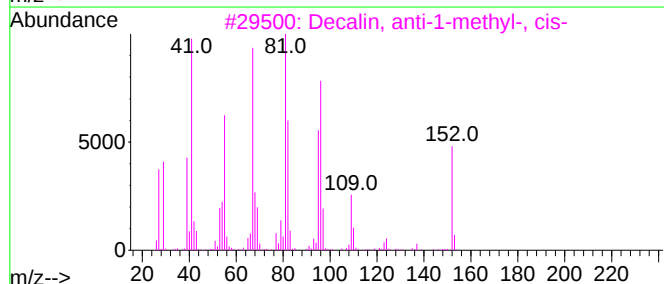
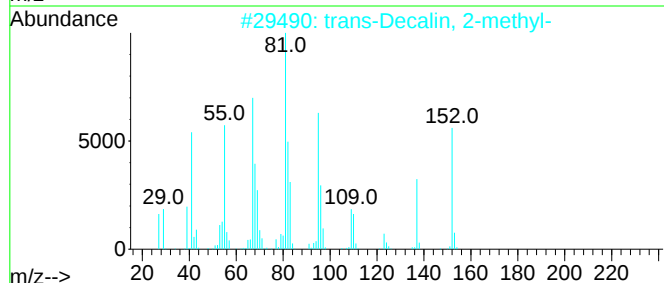
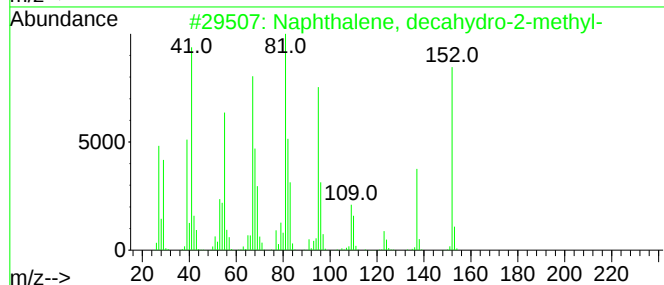
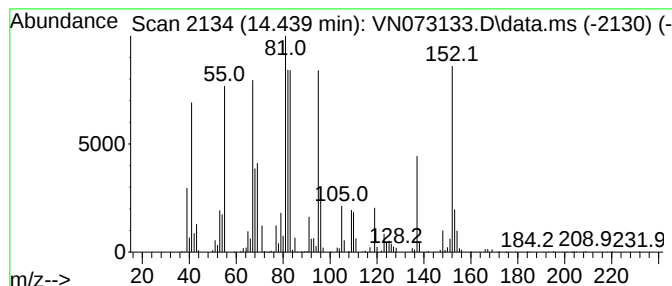
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	33.09 ug/l	1352590	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	96
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	76
3			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	64
4			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	52
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

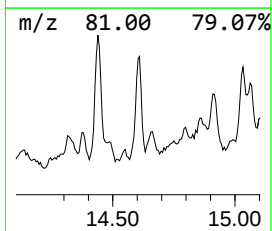
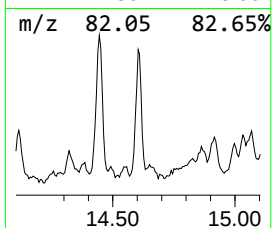
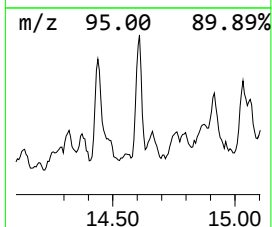
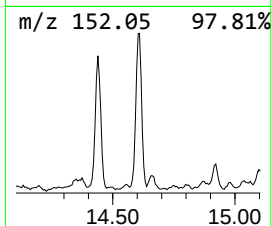
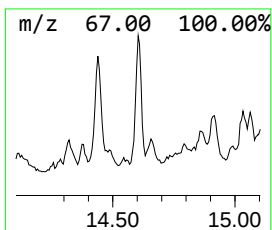
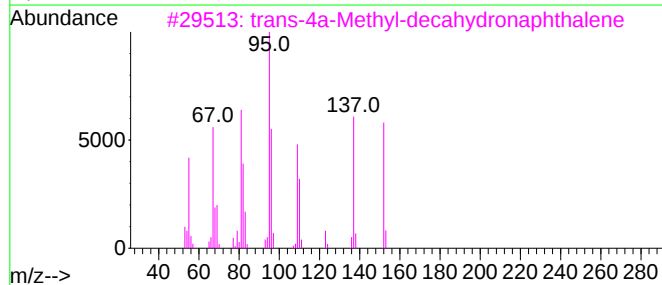
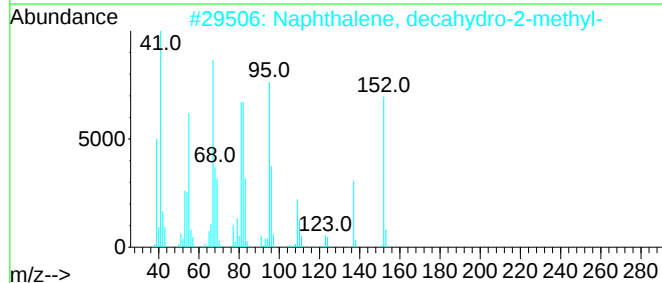
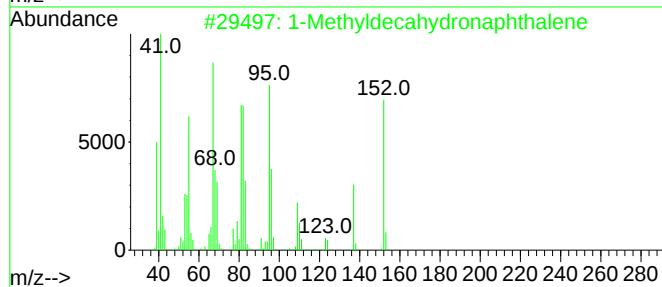
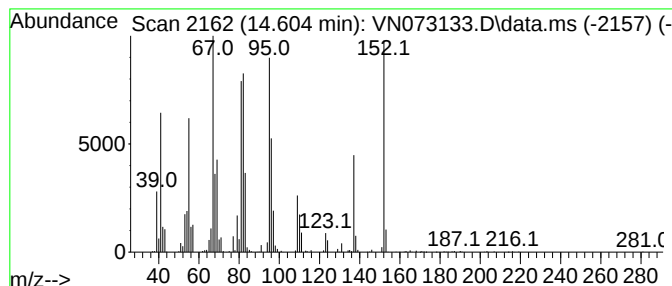
Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

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 1-Methyldecahydronaphthalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.604	30.84 ug/l	1260480	1,4-Dichlorobenzene-d4	13.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	97
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	97
3	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	89
4	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	87
5	8-Dodecen-1-ol, (Z)-	184	C12H24O	040642-40-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

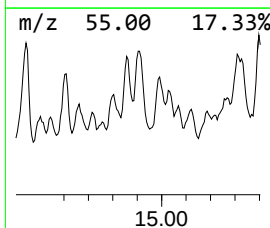
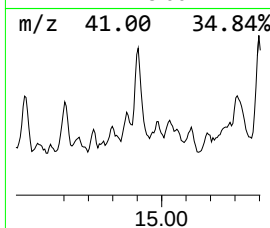
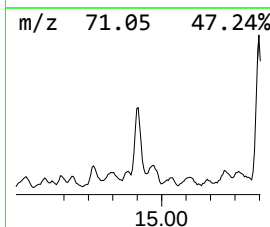
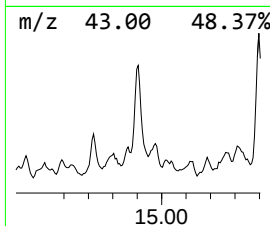
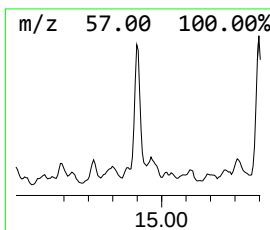
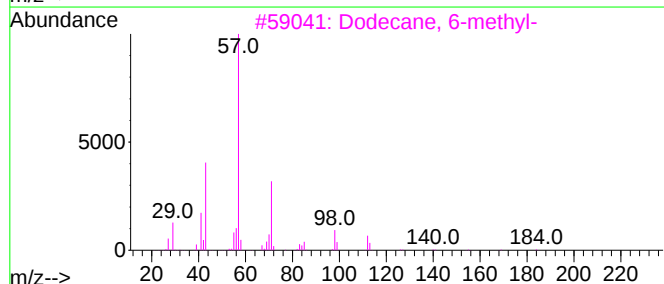
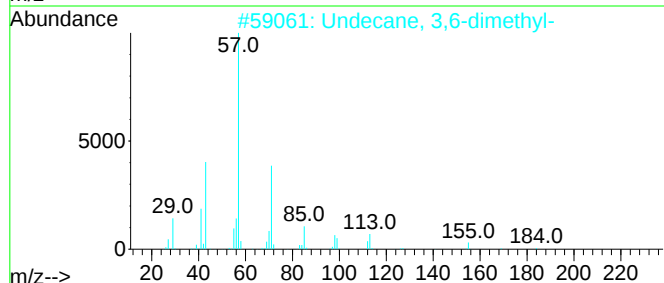
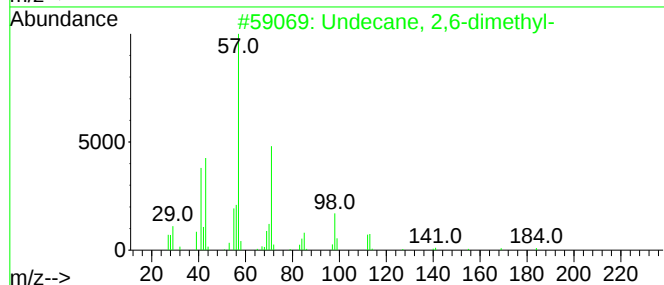
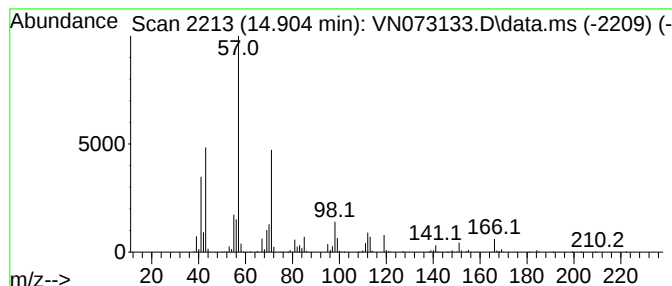
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	52.89 ug/l	2162010	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	90		
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	62		
3	Dodecane, 6-methyl-	184	C13H28	006044-71-9	60		
4	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	60		
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	47		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

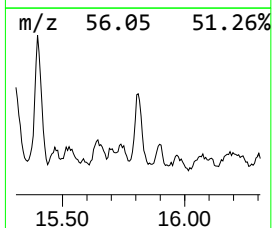
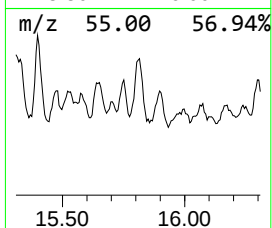
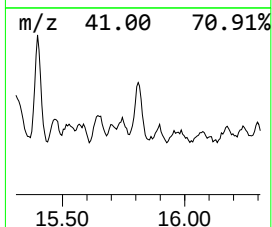
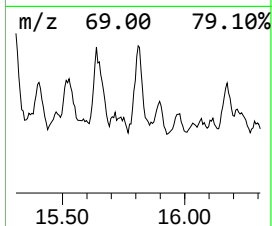
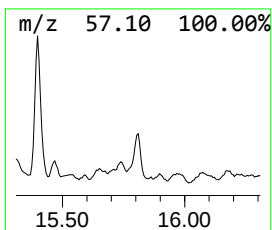
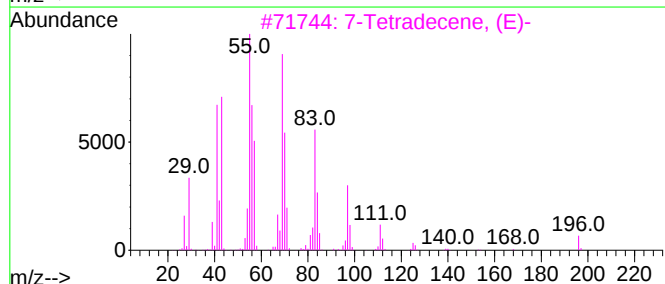
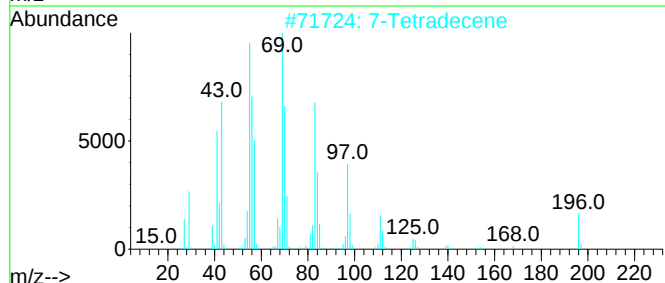
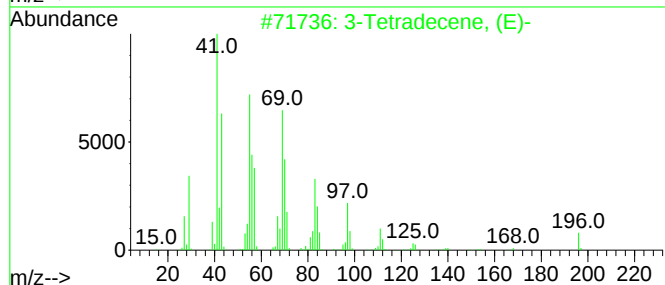
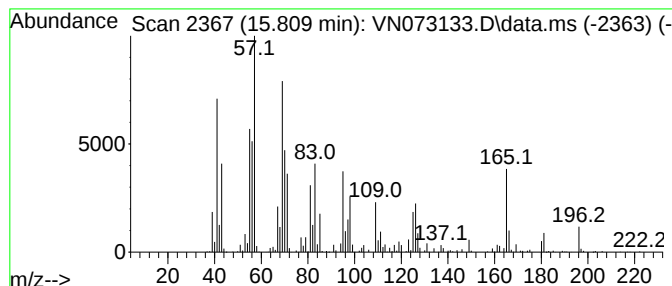
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Quant Title : SW846 8260

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

Peak Number 9 3-Tetradecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.809	33.20 ug/l	1357200	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Tetradecene, (E)-	196	C14H28	041446-68-8	58
2			7-Tetradecene	196	C14H28	010374-74-0	52
3			7-Tetradecene, (E)-	196	C14H28	041446-63-3	50
4			Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	49
5			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

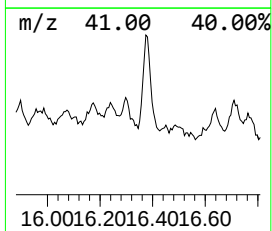
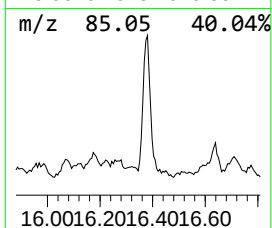
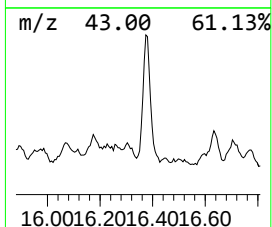
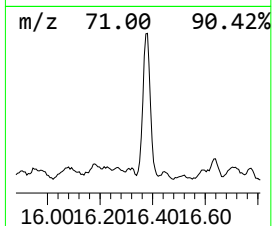
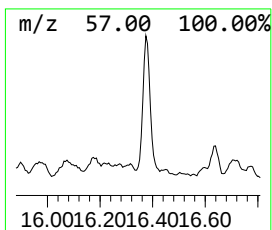
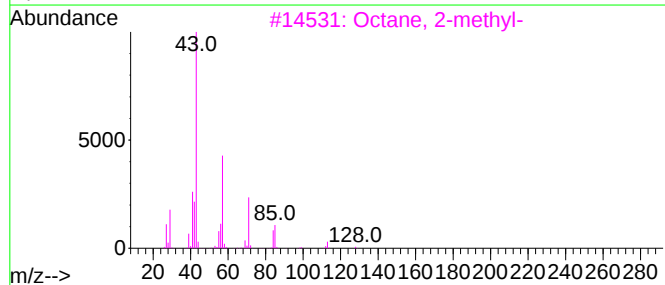
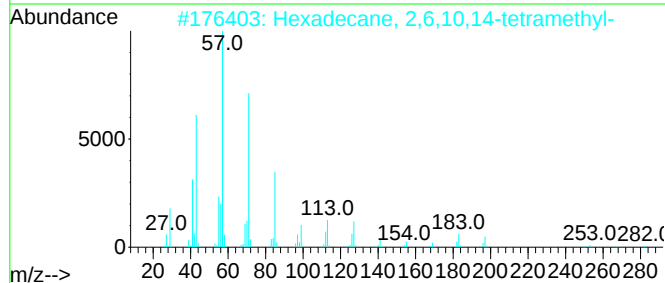
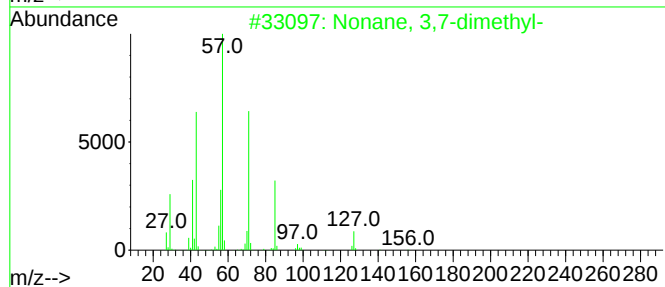
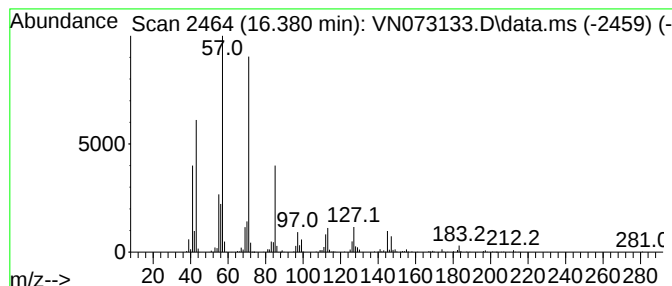
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Quant Title : SW846 8260

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

Peak Number 10 Nonane, 3,7-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.380	44.60 ug/l	1823210	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3			Octane, 2-methyl-	128	C9H20	003221-61-2	81
4			1-Undecene, 4-methyl-	168	C12H24	074630-39-0	72
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073133.D
Acq On : 26 Jun 2022 02:30
Operator : JC\MD
Sample : N3494-11
Misc : 1.28g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-1-5

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
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unknown12.992	12.992	26.2	ug/l	1072060	4	13.610	2043750	50.0
Decane, 4-methyl-	13.221	29.4	ug/l	1199950	4	13.610	2043750	50.0
Cyclohexane, (1...	13.504	21.8	ug/l	892221	4	13.610	2043750	50.0
Naphthalene, de...	13.933	41.9	ug/l	1711540	4	13.610	2043750	50.0
Naphthalene, de...	14.439	33.1	ug/l	1352590	4	13.610	2043750	50.0
1-Methyldecahyd...	14.604	30.8	ug/l	1260480	4	13.610	2043750	50.0
Undecane, 2,6-d...	14.904	52.9	ug/l	2162010	4	13.610	2043750	50.0
3-Tetradecene, ...	15.809	33.2	ug/l	1357200	4	13.610	2043750	50.0
Nonane, 3,7-dim...	16.380	44.6	ug/l	1823210	4	13.610	2043750	50.0