

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073112.D
 Acq On : 25 Jun 2022 15:54
 Operator : JC\MD
 Sample : N3454-02
 Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-16-1A-4-GR

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: VN073112.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.210	553	565	579	rBV3	20400	75861	1.28%	0.262%
2	7.292	910	919	929	rBV	65109	184066	3.10%	0.635%
3	7.945	1021	1030	1035	rBV	235984	593458	10.01%	2.048%
4	8.004	1035	1040	1050	rVB	449028	1054660	17.79%	3.639%
5	8.363	1093	1101	1111	rBV	248000	568612	9.59%	1.962%
6	8.898	1184	1192	1203	rBV	627841	1328472	22.41%	4.584%
7	10.374	1437	1443	1450	rVB	868506	1548045	26.11%	5.342%
8	11.680	1659	1665	1675	rVB	981323	1775756	29.95%	6.128%
9	11.880	1693	1699	1706	rBV4	249730	621609	10.48%	2.145%
10	12.174	1744	1749	1759	rBV3	198843	467608	7.89%	1.614%
11	12.498	1799	1804	1809	rBV4	250949	567978	9.58%	1.960%
12	12.668	1828	1833	1840	rBV	1042757	1800790	30.37%	6.214%
13	12.833	1857	1861	1866	rVB4	353248	572259	9.65%	1.975%
14	13.033	1884	1895	1898	rBV7	788359	2598913	43.83%	8.968%
15	13.257	1928	1933	1938	rBV6	331797	693421	11.70%	2.393%
16	13.315	1939	1943	1946	rBV5	304223	498056	8.40%	1.719%
17	13.492	1961	1973	1984	rBV4	1380096	5928910	100.00%	20.460%
18	13.609	1988	1993	2013	rVB3	1674518	4832571	81.51%	16.676%
19	14.445	2131	2135	2136	rBV3	226494	307458	5.19%	1.061%
20	14.604	2160	2162	2166	rVB2	258735	286815	4.84%	0.990%
21	15.215	2258	2266	2274	rBV4	475035	1708651	28.82%	5.896%
22	16.721	2518	2522	2530	rVB3	467775	964715	16.27%	3.329%

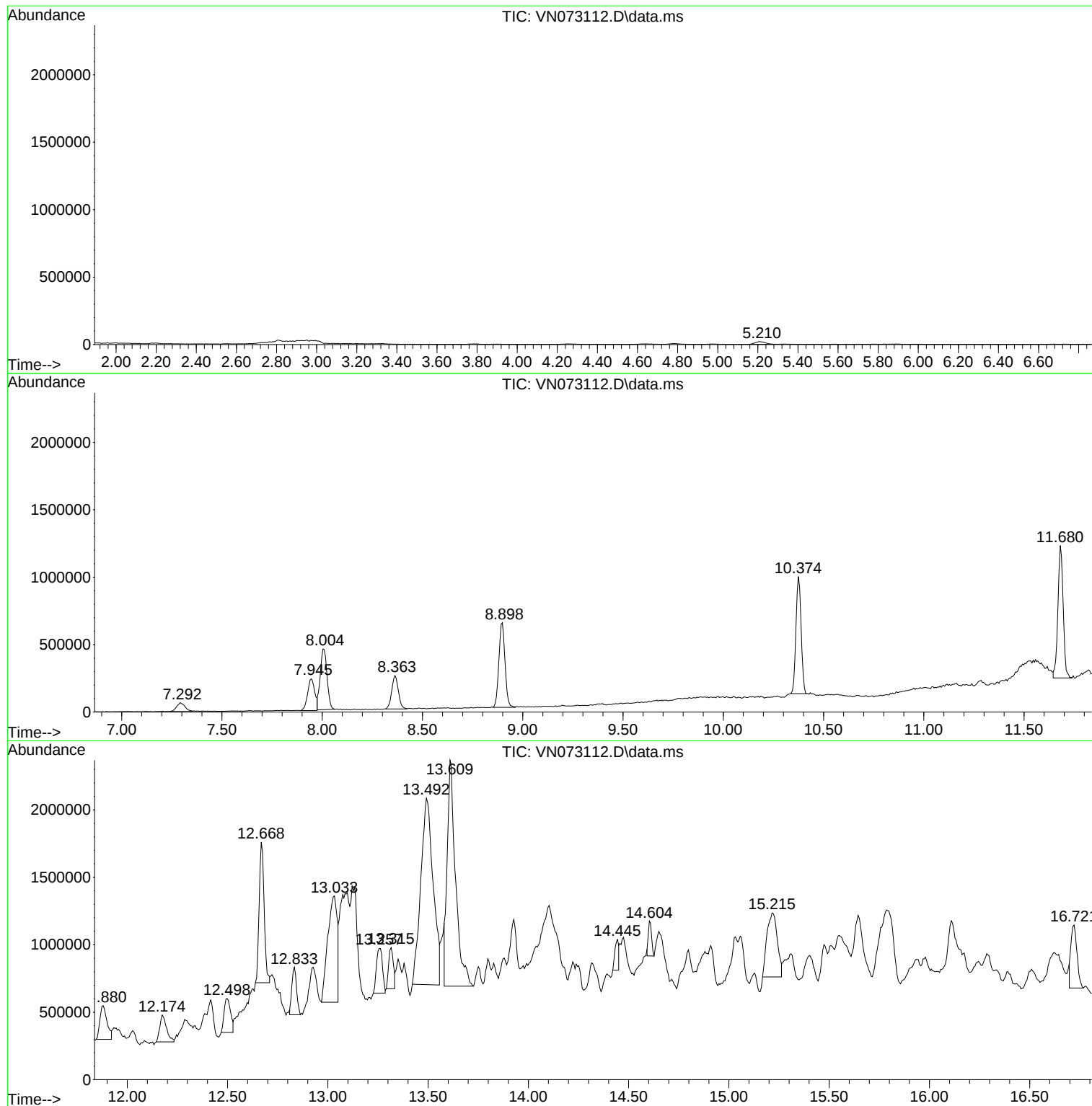
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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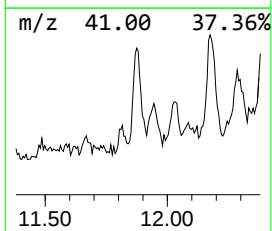
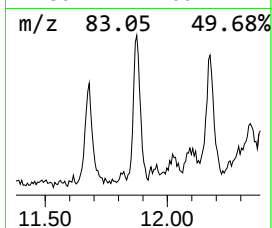
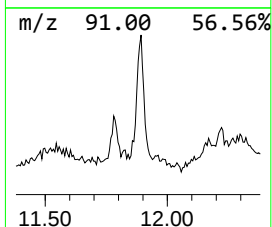
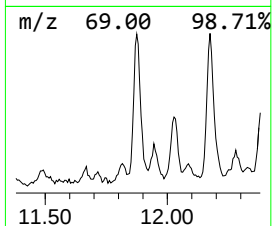
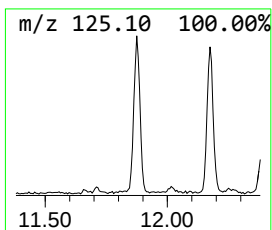
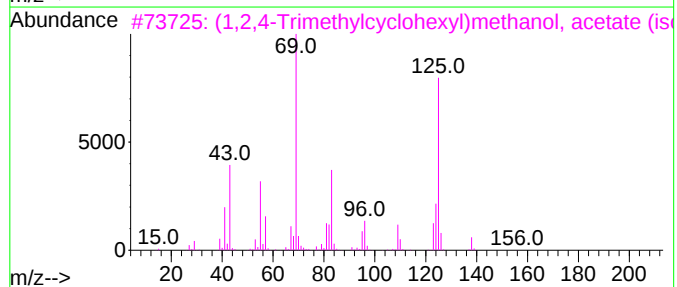
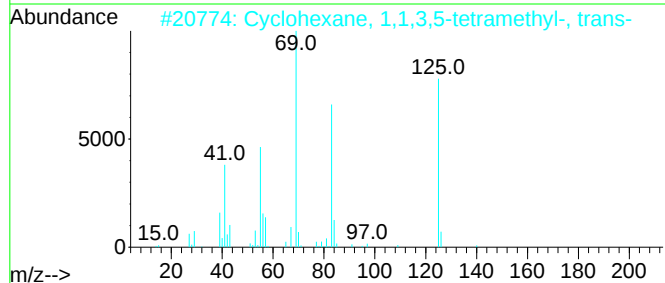
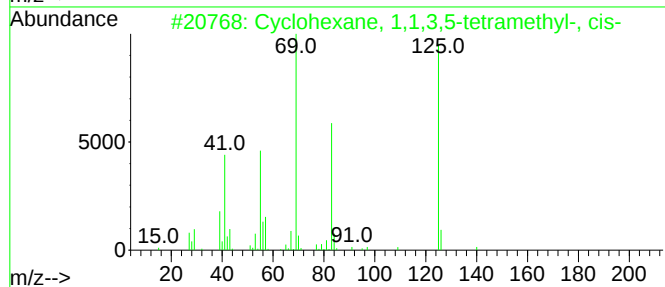
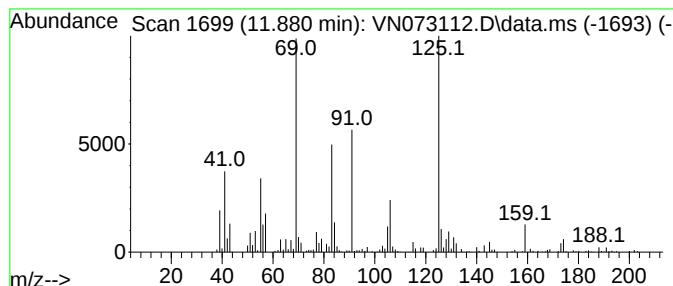
Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-4-GR

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, 1,1,3,5-tetram... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.880	17.50 ug/l	621609	Chlorobenzene-d5	11.680	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	81
2	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	58
3	(1,2,4-Trimethylcyclohexyl)metha...	198	C12H22O2	1010499-04-6	50
4	(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-03-8	50
5	Borinic acid, diethyl-, anhydride	154	C8H20B2O	007318-84-5	38



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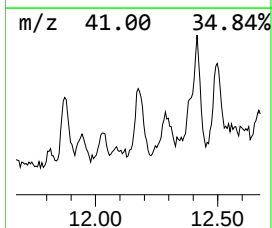
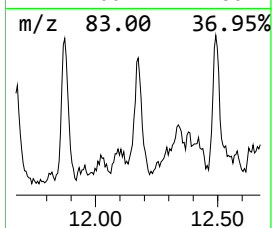
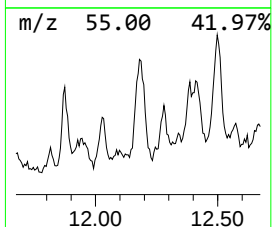
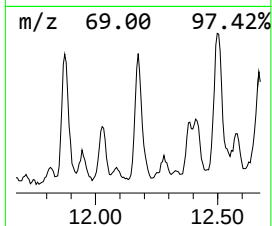
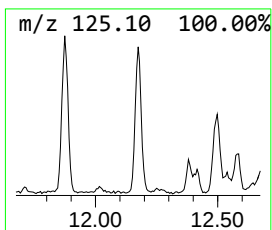
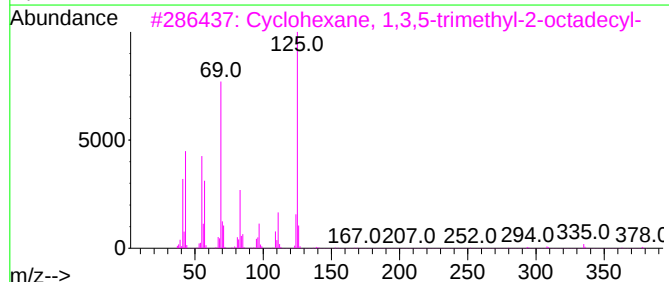
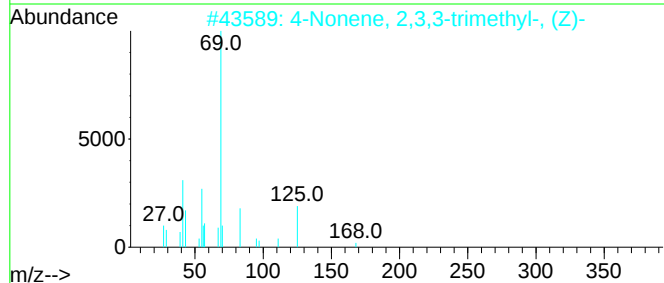
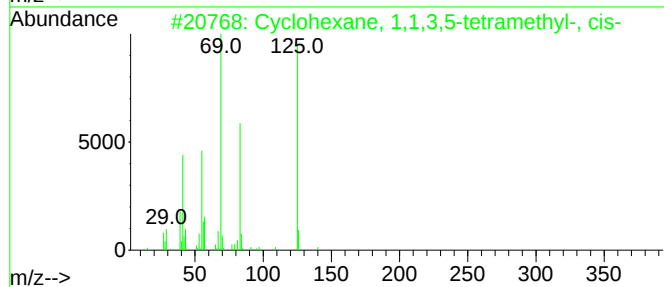
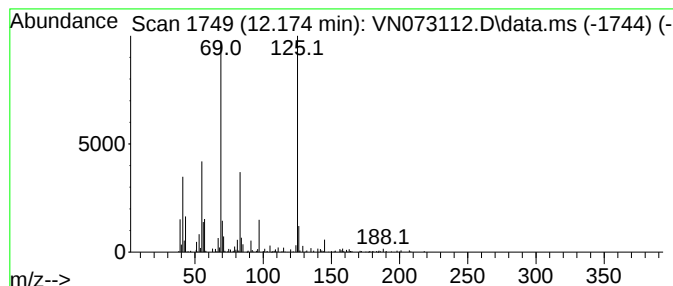
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 3 4-Nonene, 2,3,3-trimethyl-,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.174	13.17 ug/l	467608	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	87
2			4-Nonene, 2,3,3-trimethyl-, (Z)-	168	C12H24	063830-68-2	72
3			Cyclohexane, 1,3,5-trimethyl-2-o...	378	C27H54	055282-34-3	64
4			Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	64
5			Zinc, bis[2-(1,1-dimethylethyl)-...	314	C18H34Zn	074793-36-5	56



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-4-GR

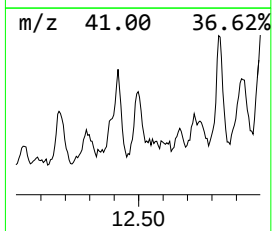
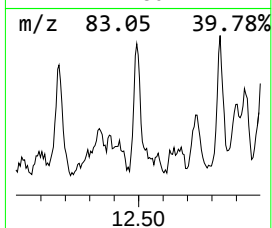
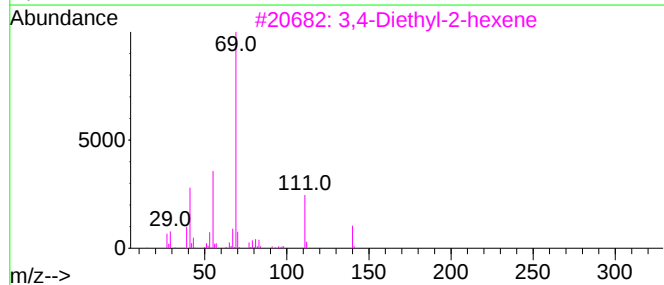
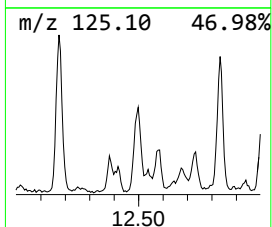
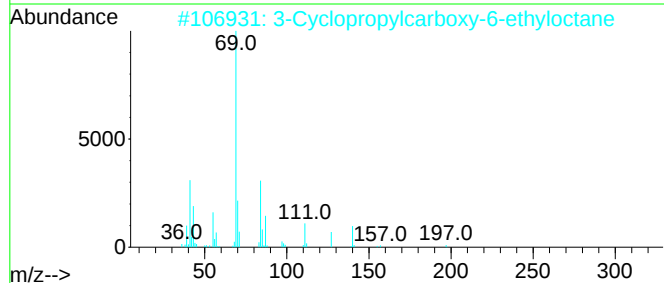
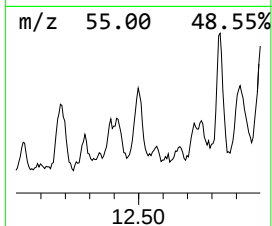
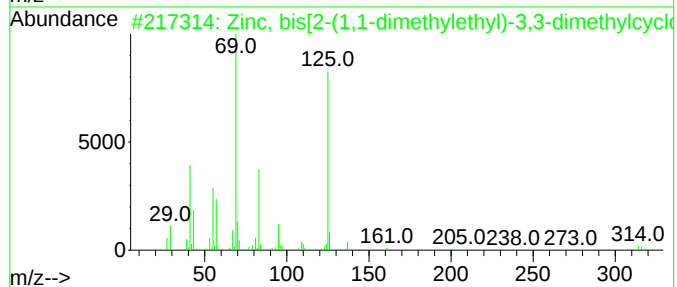
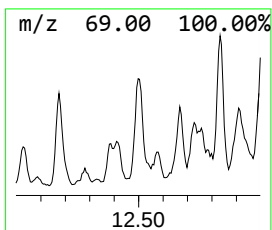
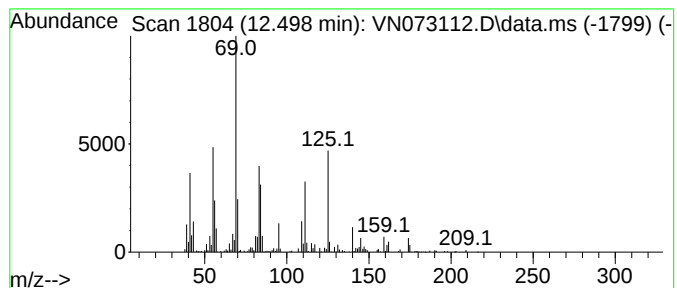
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 Zinc, bis[2-(1,1-dimethylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	15.99 ug/l	567978	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Zinc, bis[2-(1,1-dimethylethyl)-...	314	C18H34Zn	074793-36-5	50
2			3-Cyclopropylcarboxy-6-ethyloctane	226	C14H26O2	1000245-65-5	43
3			3,4-Diethyl-2-hexene	140	C10H20	1000113-54-8	41
4			4-Nonene, 2,3,3-trimethyl-, (Z)-	168	C12H24	063830-68-2	38
5			Heptane, 2-methyl-3-methylene-	126	C9H18	062187-11-5	38



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Operator : JC\MD
Sample : N3454-02
Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

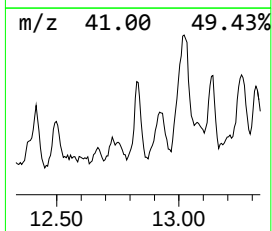
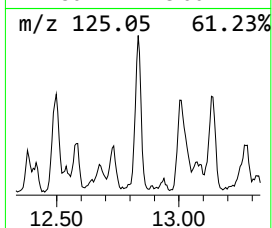
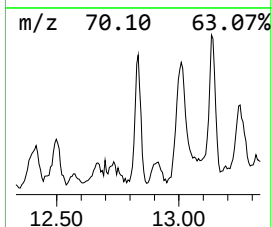
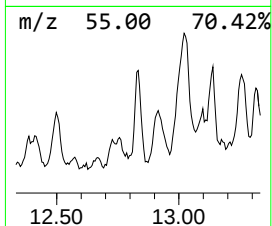
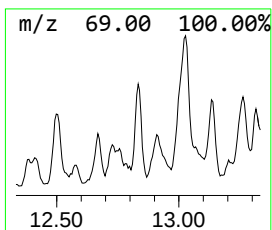
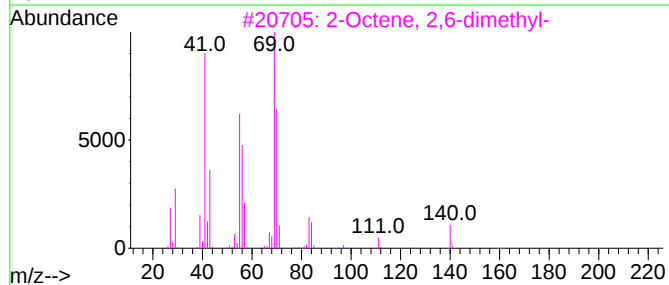
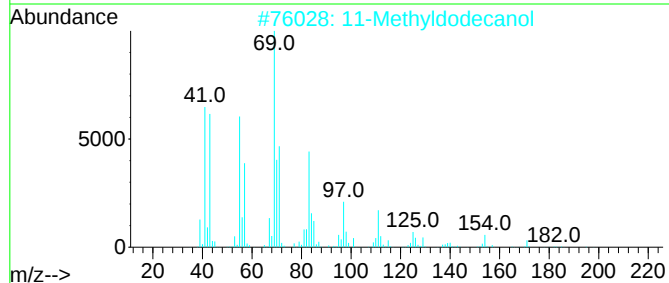
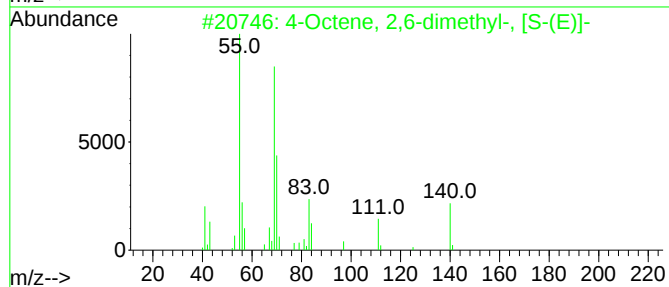
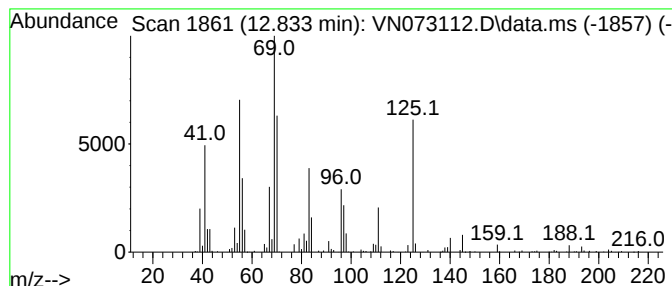
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Quant Title : SW846 8260

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

Peak Number 5 4-Octene, 2,6-dimethyl-, [S... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.833	5.92 ug/l	572259	1,4-Dichlorobenzene-d4			13.610
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Octene, 2,6-dimethyl-, [S-(E)]-		140	C10H20	062960-76-3	70
2	11-Methyldodecanol		200	C13H28O	085763-57-1	47
3	2-Octene, 2,6-dimethyl-		140	C10H20	004057-42-5	43
4	Cyclohexane, 1,2,4-trimethyl-		126	C9H18	002234-75-5	43
5	(1,2,4-Trimethylcyclohexyl)metha...		156	C10H20O	1000499-03-8	38



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Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

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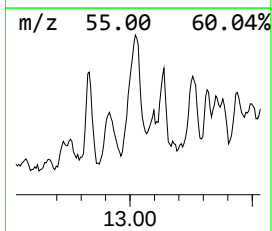
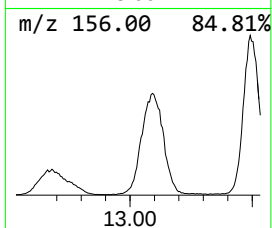
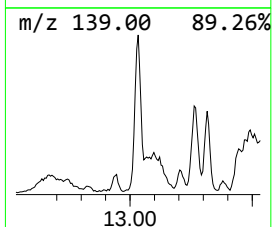
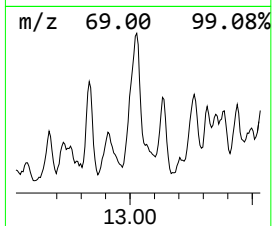
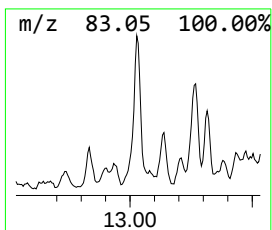
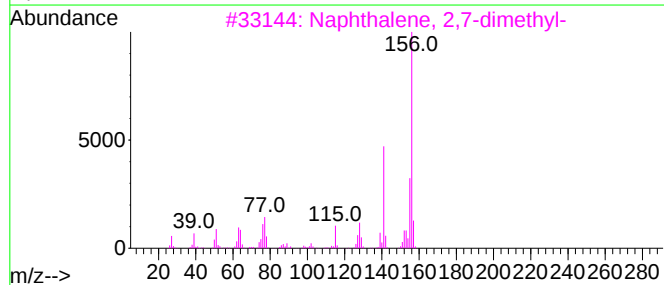
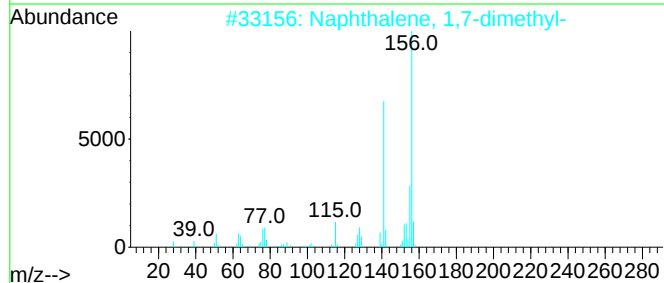
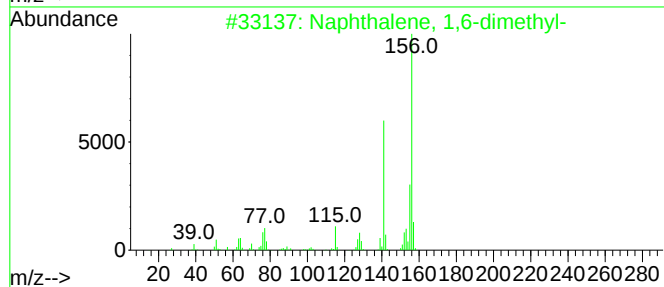
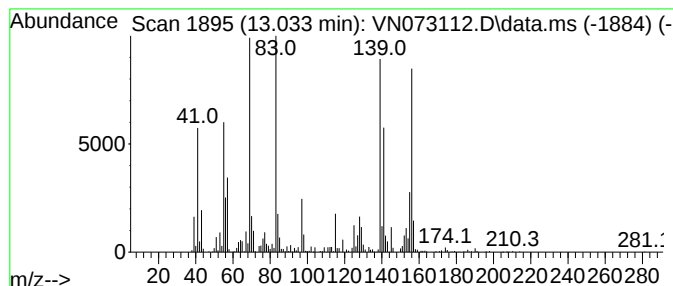
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.033	26.89 ug/l	2598910	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	74
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	74
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	74
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	70
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	51



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Sample : N3454-02
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ALS Vial : 15 Sample Multiplier: 1

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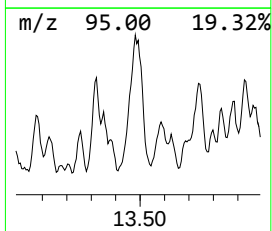
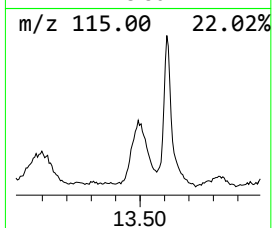
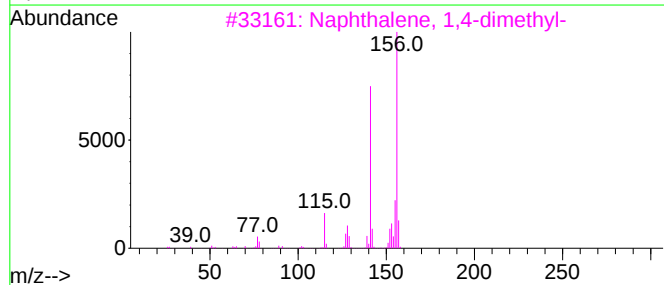
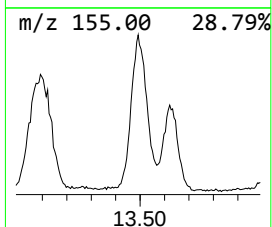
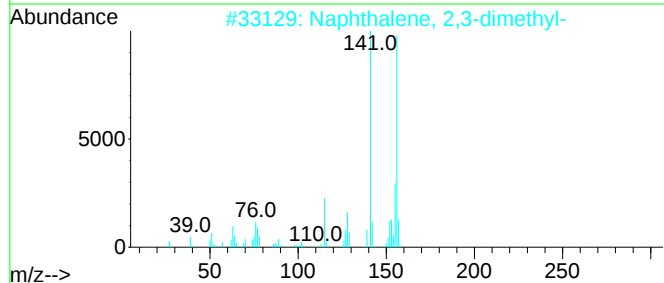
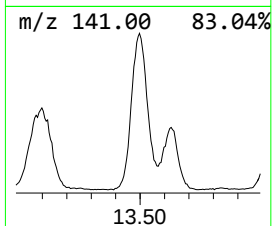
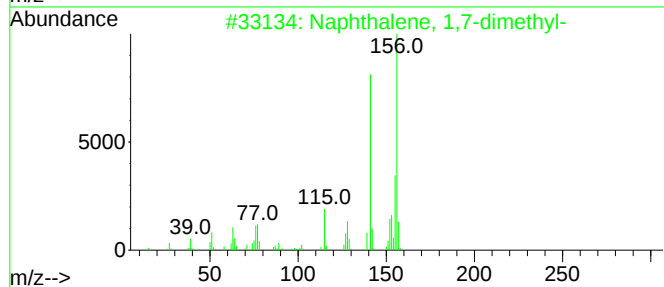
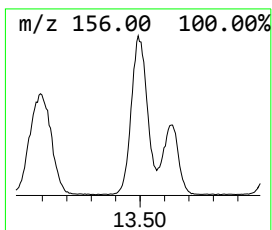
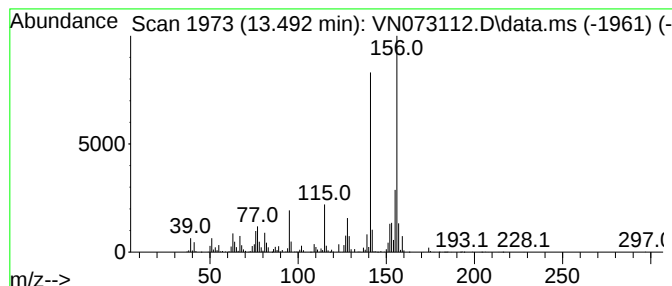
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,7-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	61.34 ug/l	5928910	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073112.D
Acq On : 25 Jun 2022 15:54
Operator : JC\MD
Sample : N3454-02
Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-4-GR

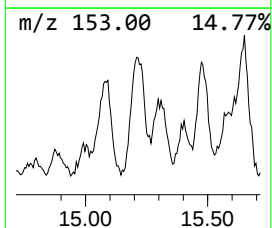
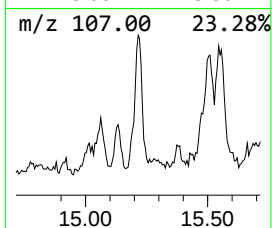
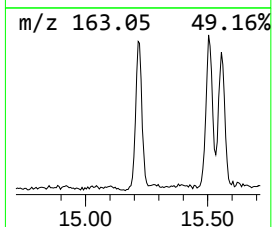
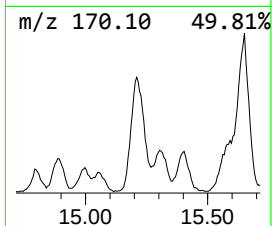
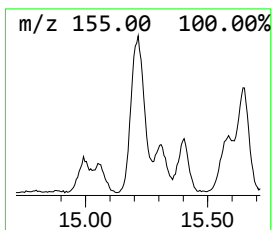
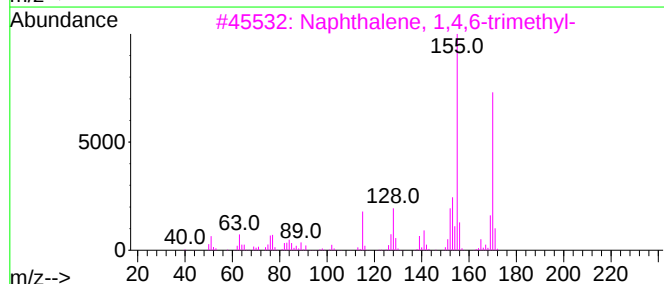
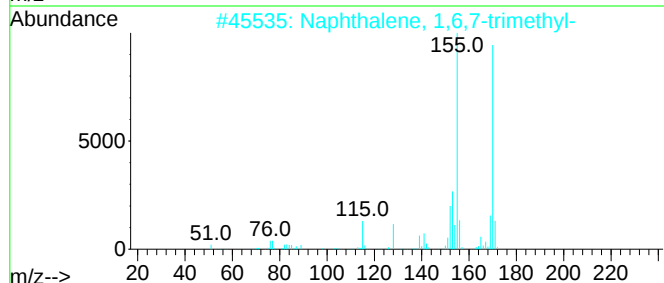
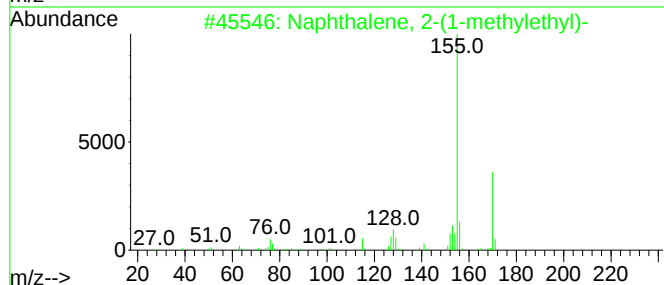
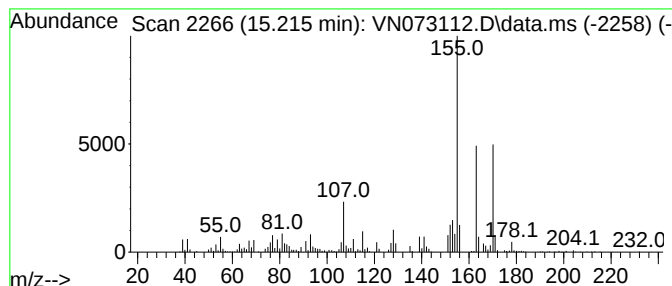
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2-(1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.215	17.68 ug/l	1708650	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-(1-methylethyl)-	170	C13H14	002027-17-0	70
2			Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	70
3			Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	70
4			Naphthalene, 1-(1-methylethyl)-	170	C13H14	006158-45-8	55
5			Naphthalene, 2-methyl-1-propyl-	184	C14H16	054774-89-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073112.D
Acq On : 25 Jun 2022 15:54
Operator : JC\MD
Sample : N3454-02
Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-4-GR

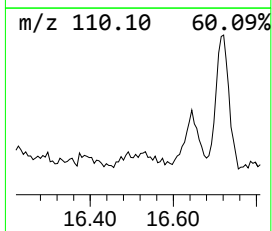
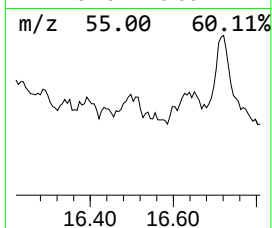
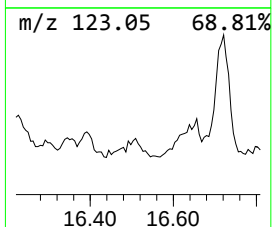
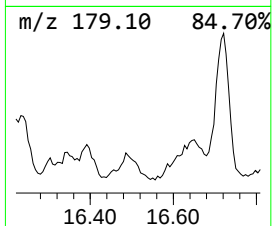
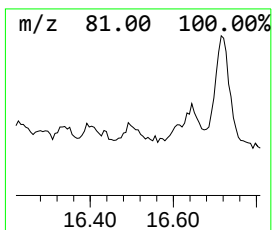
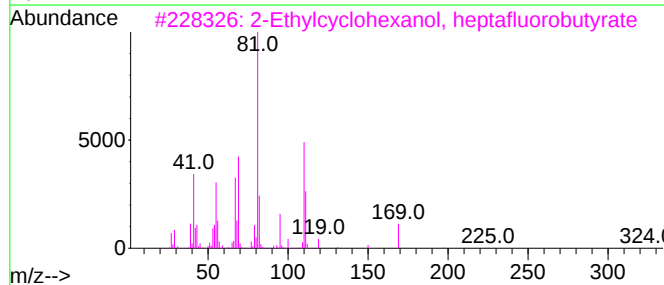
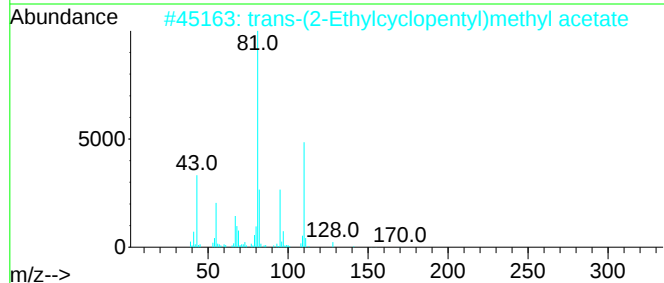
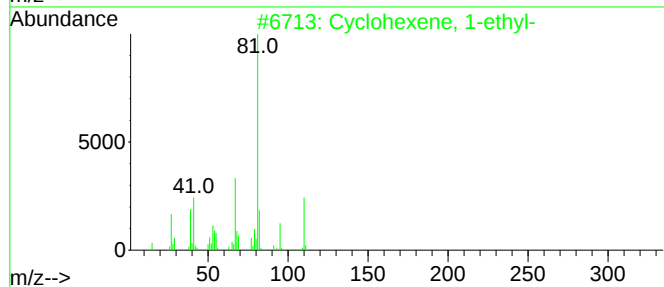
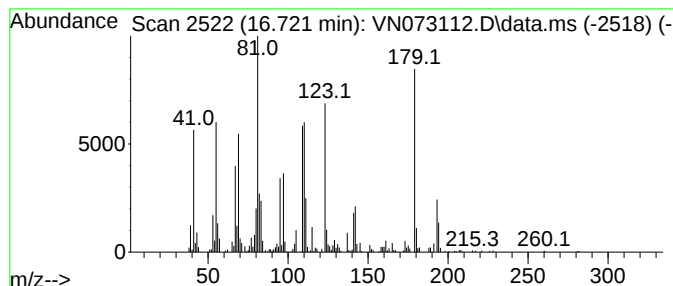
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.721 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.721	9.98 ug/l	964715	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	25
2			trans-(2-Ethylcyclopentyl)methyl...	170	C10H18O2	1000099-13-9	22
3			2-Ethylcyclohexanol, heptafluoro...	324	C12H15F7O2	959079-92-6	22
4			4,11-Dimethyl-8-(propan-2-yl)-5,...	268	C16H28O3	1010493-61-7	22
5			2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073112.D
Acq On : 25 Jun 2022 15:54
Operator : JC\MD
Sample : N3454-02
Misc : 3.95g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-16-1A-4-GR

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
Cyclohexane, 1,...	11.880	17.5	ug/l	621609	3	11.680	1775760	50.0
4-Nonene, 2,3,3...	12.174	13.2	ug/l	467608	3	11.680	1775760	50.0
Zinc, bis[2-(1,...	12.498	16.0	ug/l	567978	3	11.680	1775760	50.0
4-Octene, 2,6-d...	12.833	5.9	ug/l	572259	4	13.610	4832570	50.0
Naphthalene, 1,...	13.033	26.9	ug/l	2598910	4	13.610	4832570	50.0
Naphthalene, 1,...	13.492	61.3	ug/l	5928910	4	13.610	4832570	50.0
Naphthalene, 2-...	15.215	17.7	ug/l	1708650	4	13.610	4832570	50.0
unknown16.721	16.721	10.0	ug/l	964715	4	13.610	4832570	50.0