

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030624\
 Data File : VN081333.D
 Acq On : 06 Mar 2024 17:51
 Operator : JC\MD
 Sample : P1683-01
 Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1132

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\82N030524W.M
 Title : SW846 8260

Signal : TIC: VN081333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.483	86	90	96	rBV5	14379	32333	1.92%	0.285%
2	2.818	136	147	149	rBV5	34771	100715	5.97%	0.887%
3	8.165	1047	1056	1060	rBV	232156	541990	32.13%	4.774%
4	8.224	1060	1066	1082	rVB	433432	986311	58.48%	8.688%
5	8.577	1116	1126	1133	rBV	266871	597144	35.40%	5.260%
6	8.659	1133	1140	1144	rBV3	21414	61320	3.64%	0.540%
7	9.100	1204	1215	1230	rBV	639862	1296762	76.88%	11.422%
8	9.383	1257	1263	1270	rBV5	8002	17449	1.03%	0.154%
9	10.565	1455	1464	1472	rBV	904145	1686658	100.00%	14.857%
10	11.871	1677	1686	1698	rBV	789849	1409943	83.59%	12.419%
11	12.071	1713	1720	1727	rBV3	27139	51753	3.07%	0.456%
12	12.853	1846	1853	1862	rVB	614795	1045367	61.98%	9.208%
13	13.165	1901	1906	1913	rBV4	20731	38786	2.30%	0.342%
14	13.706	1986	1998	2003	rBV4	19222	56720	3.36%	0.500%
15	13.794	2005	2013	2020	rBV	818758	1359104	80.58%	11.972%
16	13.923	2030	2035	2042	rBV10	10904	29400	1.74%	0.259%
17	14.106	2061	2066	2073	rBV3	156823	285059	16.90%	2.511%
18	14.223	2080	2086	2089	rBV6	22142	37924	2.25%	0.334%
19	14.441	2118	2123	2126	rBV7	28711	48468	2.87%	0.427%
20	14.506	2130	2134	2141	rVV9	37715	74217	4.40%	0.654%
21	14.576	2142	2146	2150	rBV7	39495	67869	4.02%	0.598%
22	14.629	2150	2155	2159	rBV3	105745	166855	9.89%	1.470%
23	14.735	2169	2173	2176	rBV5	46262	75732	4.49%	0.667%
24	14.770	2176	2179	2180	rVV2	39556	49096	2.91%	0.432%
25	14.794	2180	2183	2188	rVV4	70702	118395	7.02%	1.043%
26	14.847	2188	2192	2197	rVV5	62535	117184	6.95%	1.032%
27	14.959	2207	2211	2218	rBV	158275	260967	15.47%	2.299%
28	15.176	2246	2248	2251	rBV4	31112	42502	2.52%	0.374%
29	15.229	2253	2257	2260	rBV5	99048	168843	10.01%	1.487%
30	15.317	2268	2272	2278	rBV7	95445	175704	10.42%	1.548%
31	15.676	2328	2333	2338	rBV6	149163	352254	20.88%	3.103%

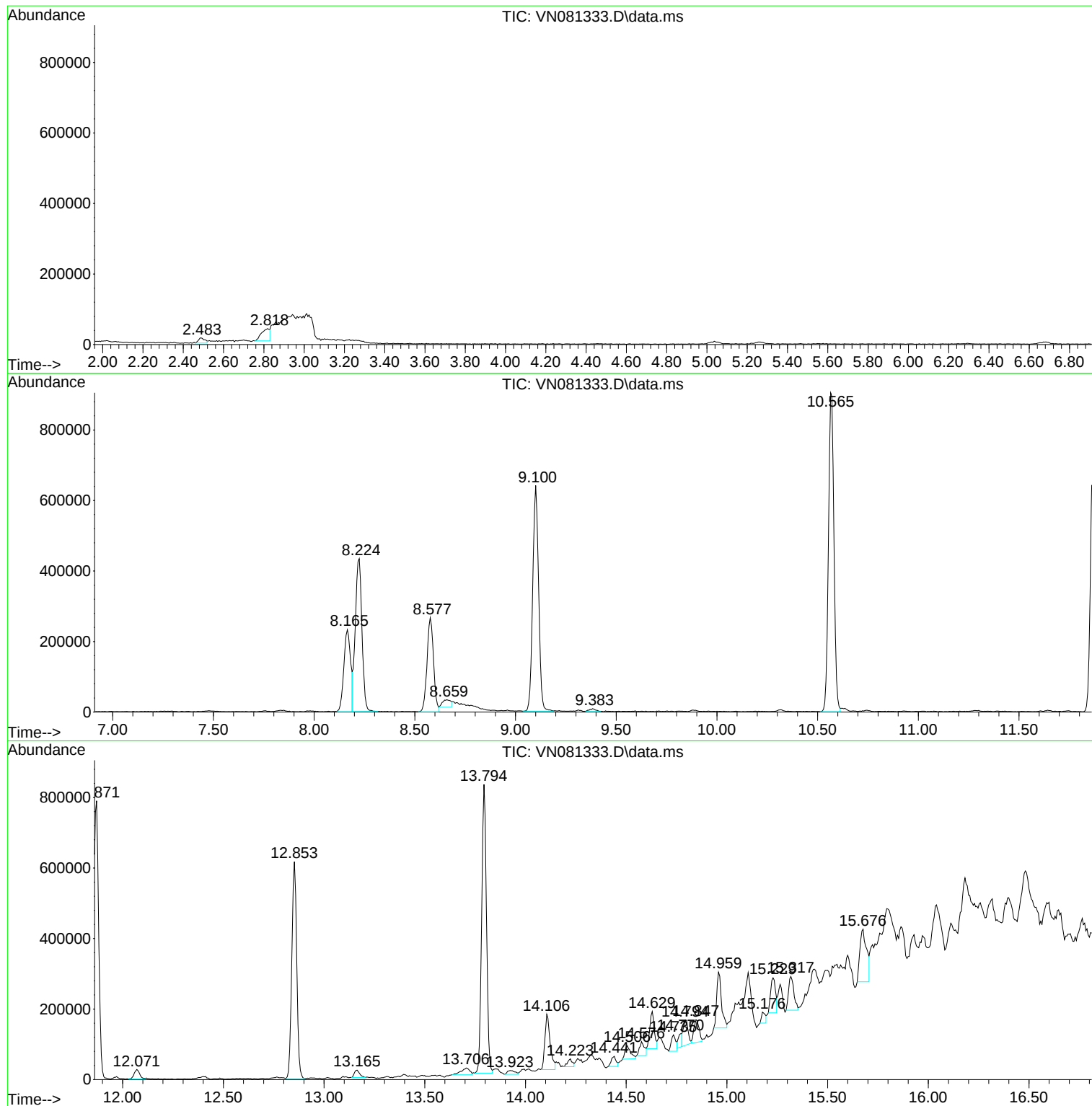
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



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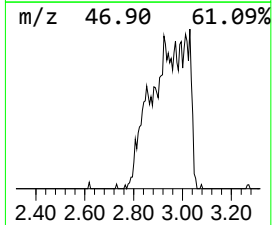
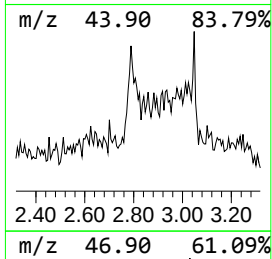
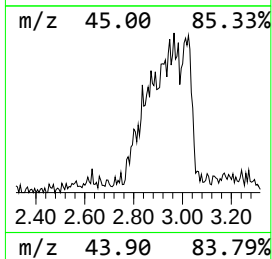
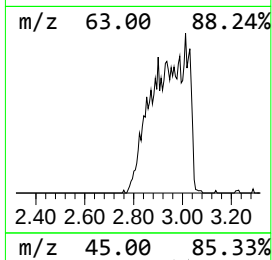
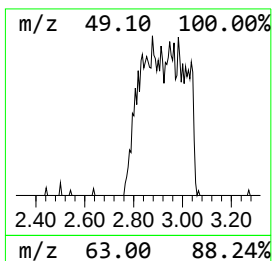
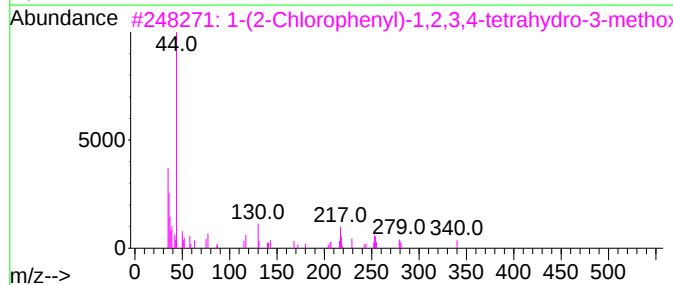
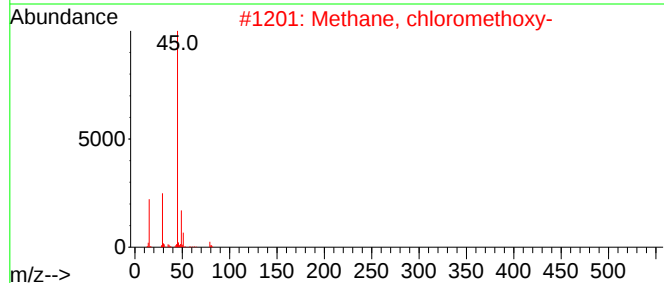
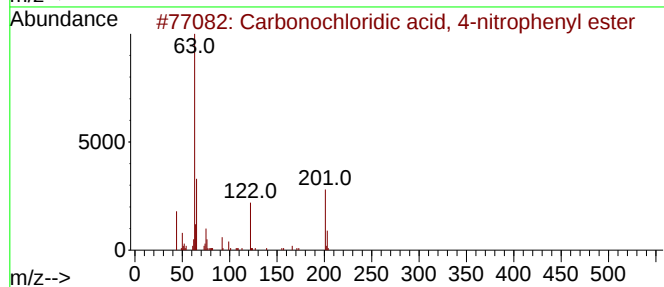
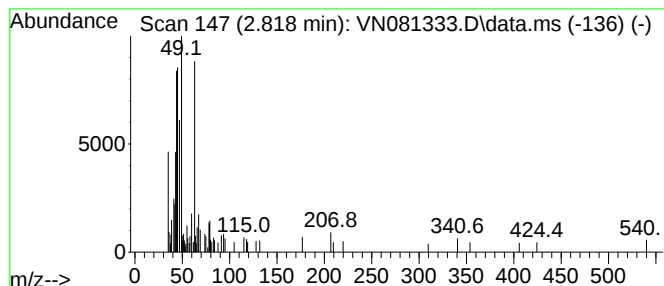
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.818 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.818	5.11 ug/l	100715	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonochloridic acid, 4-nitroph...	201	C7H4ClNO4	007693-46-1	10
2			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
3			1-(2-Chlorophenyl)-1,2,3,4-tetra...	340	C19H17ClN2O2	223690-84-4	9
4			Chloromethanesulfonyl chloride	148	CH2Cl2O2S	003518-65-8	9
5			4-Bromo-1,2-bis-(2-chloro-ethoxy...	312	C10H11BrCl2O2	1000317-37-9	9



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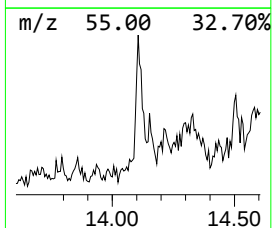
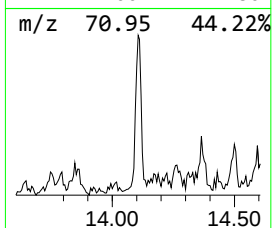
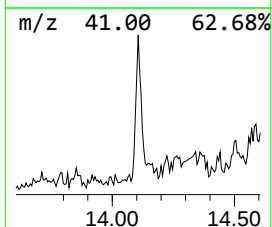
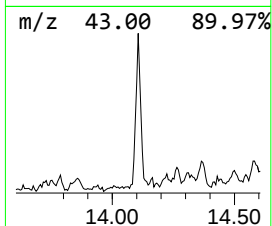
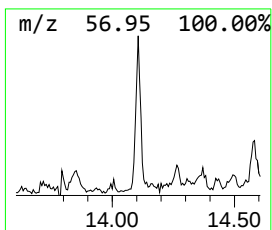
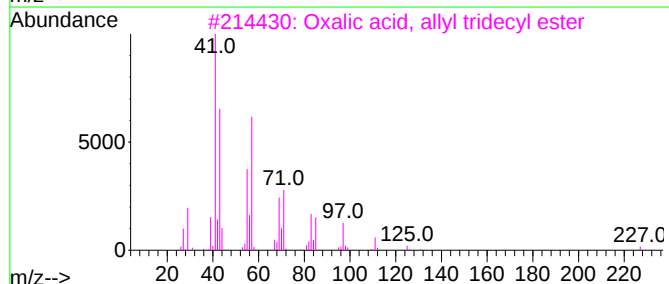
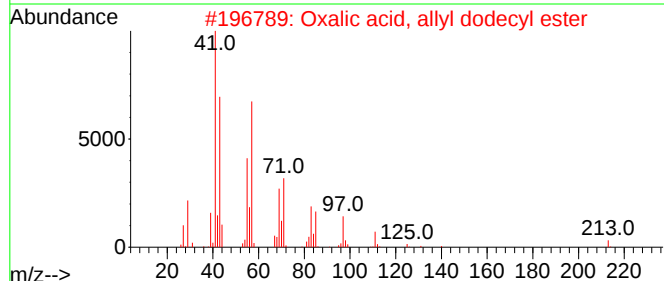
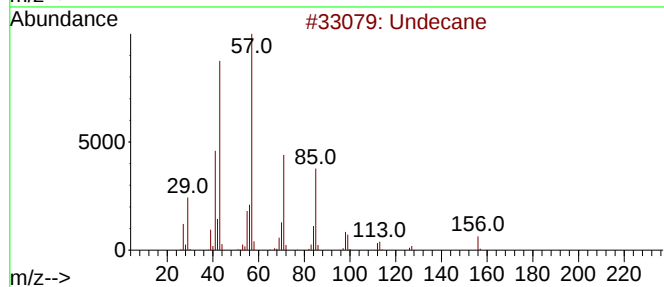
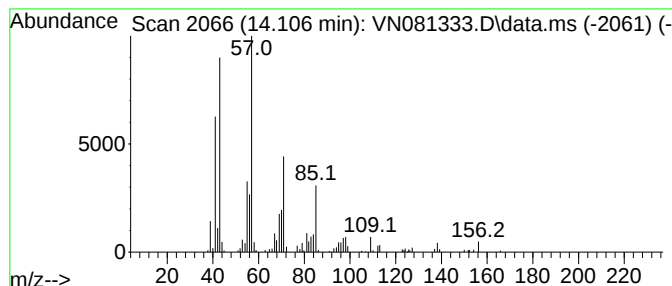
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	10.49 ug/l	285059	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	76
2	Oxalic acid, allyl dodecyl ester			298	C17H30O4	1000309-24-0	72
3	Oxalic acid, allyl tridecyl ester			312	C18H32O4	1000309-24-1	72
4	Oxalic acid, isobutyl nonyl ester			272	C15H28O4	1010309-37-4	58
5	Ether, heptyl hexyl			200	C13H28O	007289-40-9	49



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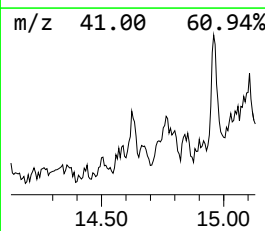
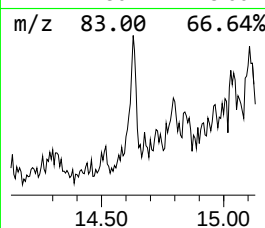
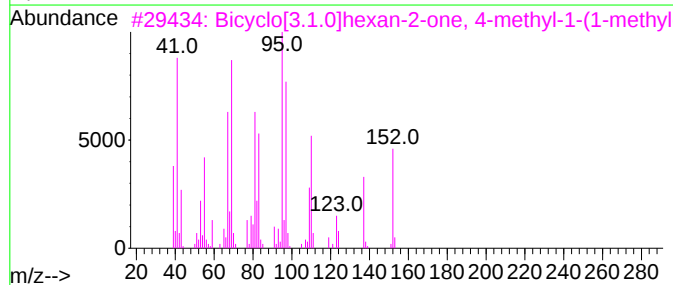
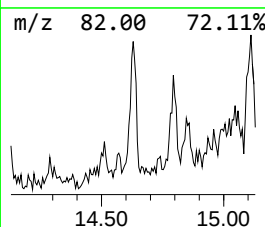
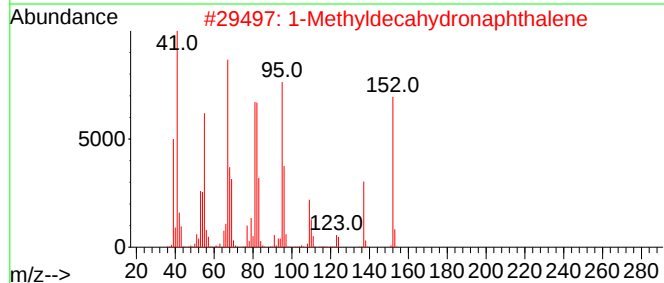
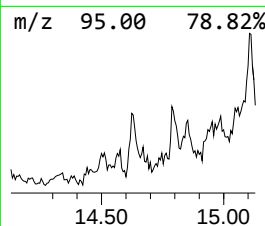
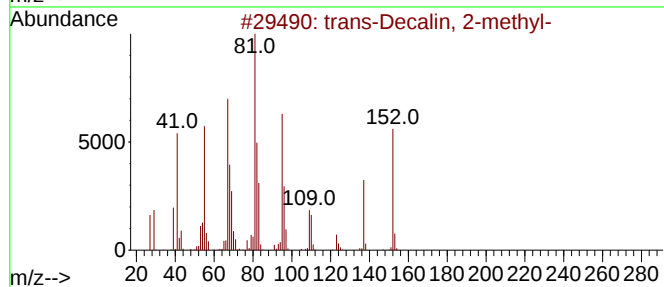
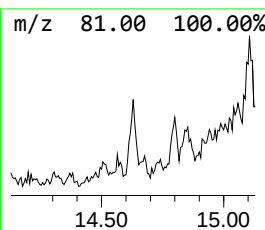
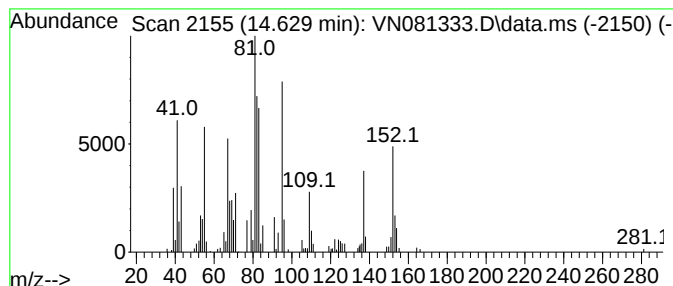
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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

Peak Number 3 trans-Decalin, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.629	6.14 ug/l	166855	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	86
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	52
3			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	52
4			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	52
5			Naphthalene, 2-ethyldecahydro-	166	C12H22	001618-23-1	50



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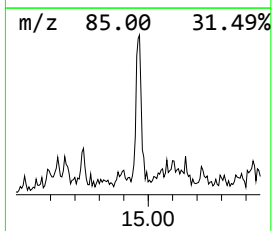
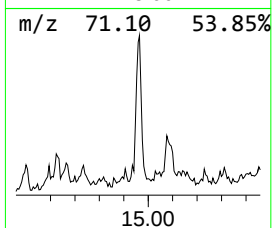
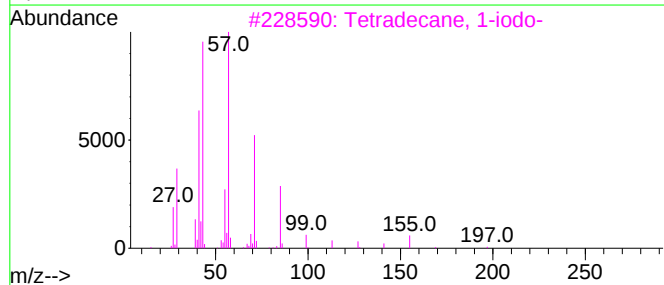
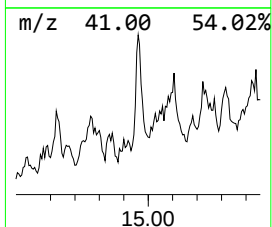
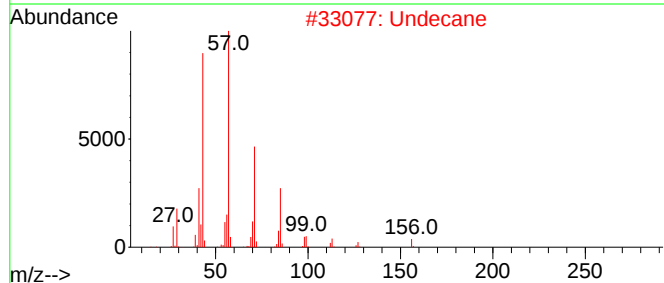
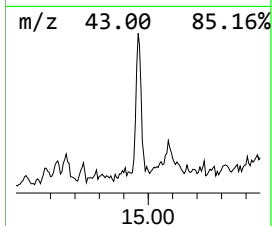
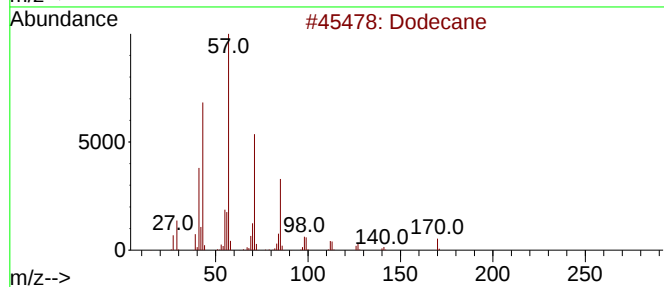
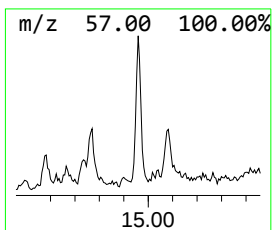
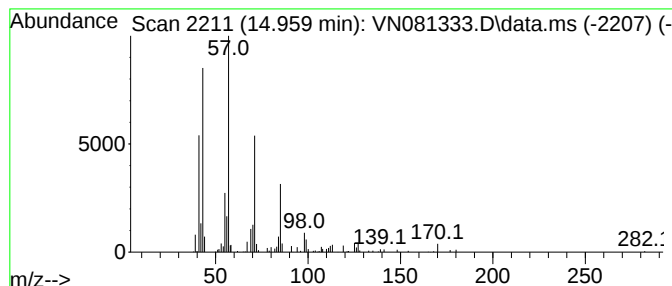
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	9.60 ug/l	260967	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	96
2			Undecane	156	C11H24	001120-21-4	80
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4			Tridecane	184	C13H28	000629-50-5	80
5			Hexadecane	226	C16H34	000544-76-3	80



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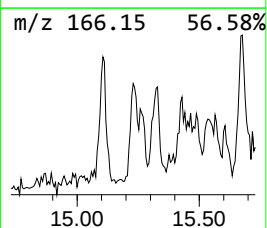
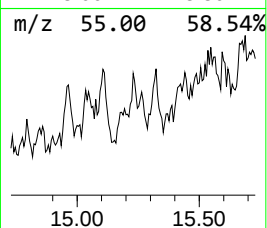
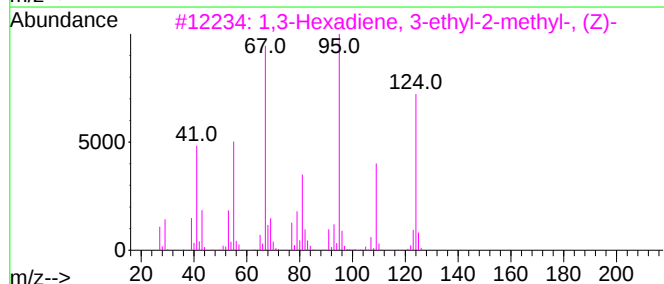
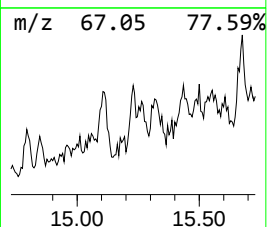
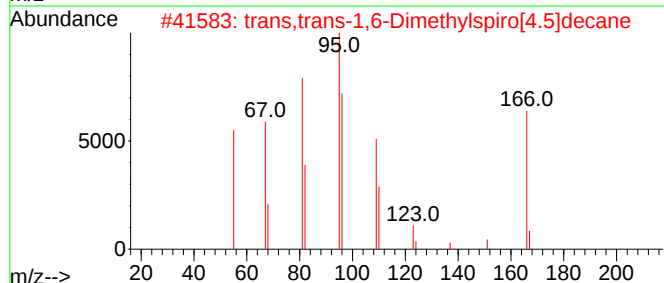
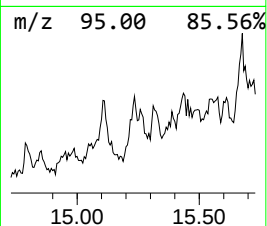
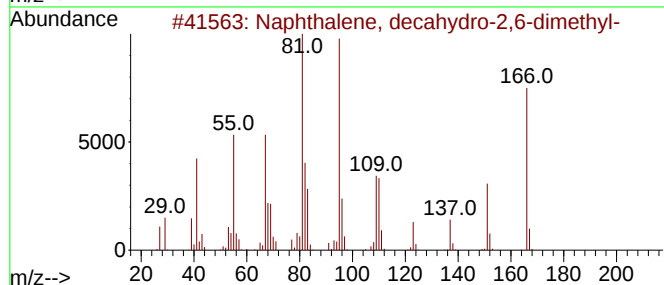
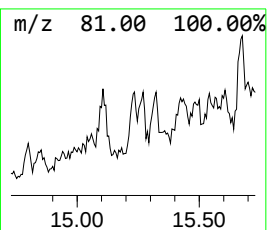
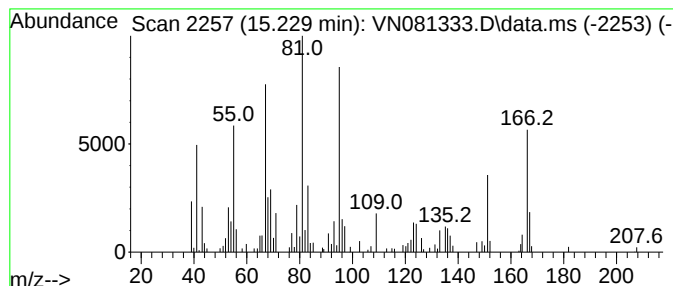
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.229	6.21 ug/l	168843	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	87
2			trans,trans-1,6-Dimethylspiro[4...	166	C12H22	1000111-72-1	58
3			1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	38
4			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	25
5			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	18



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1132

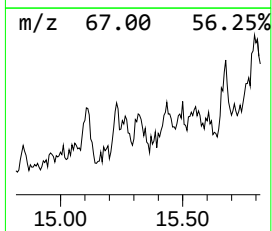
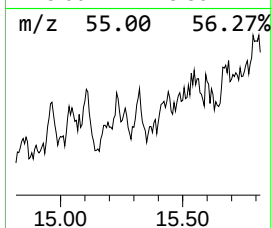
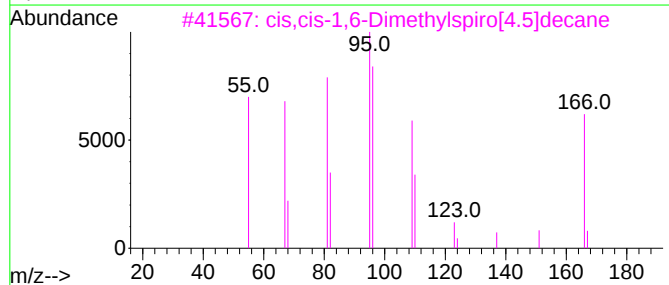
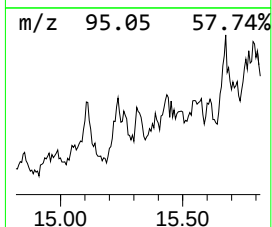
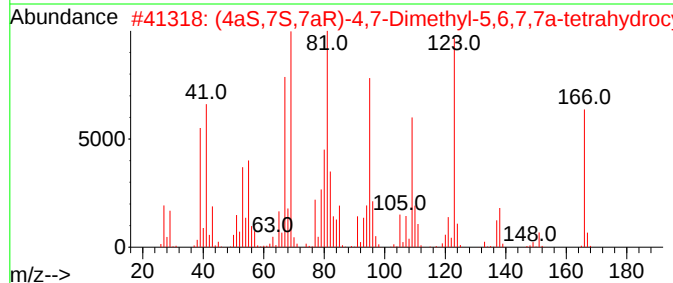
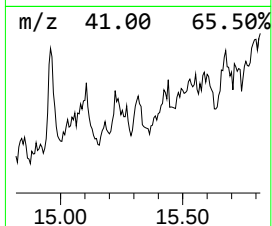
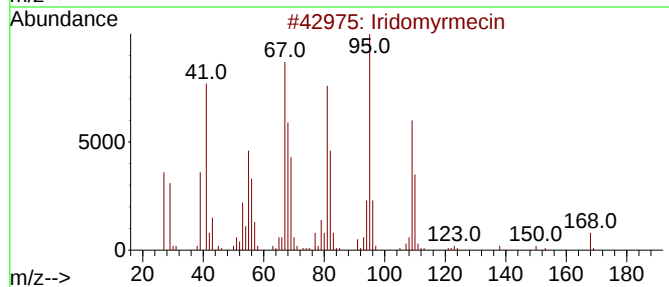
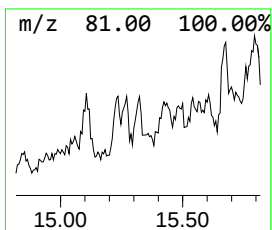
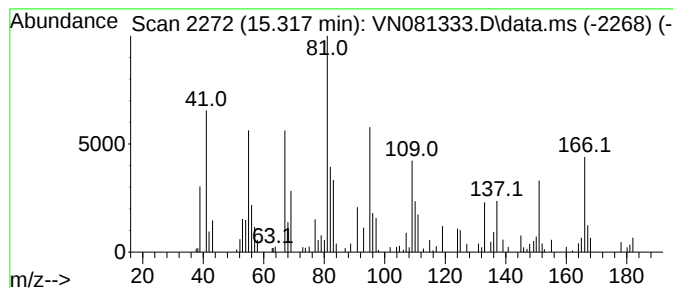
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Quant Title : SW846 8260

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

Peak Number 6 Iridomyrmecin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	6.46 ug/l	175704	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Iridomyrmecin	168	C10H16O2	000485-43-8	64
2			(4aS,7S,7aR)-4,7-Dimethyl-5,6,7,...	166	C10H14O2	021651-62-7	62
3			cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	53
4			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	43
5			3,5-Octadiene, 4,5-diethyl-	166	C12H22	067652-84-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030624\
Data File : VN081333.D
Acq On : 06 Mar 2024 17:51
Operator : JC\MD
Sample : P1683-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1132

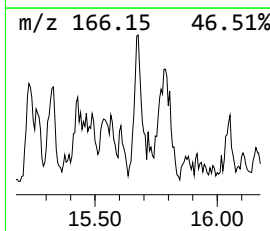
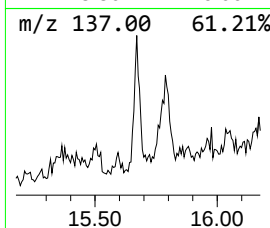
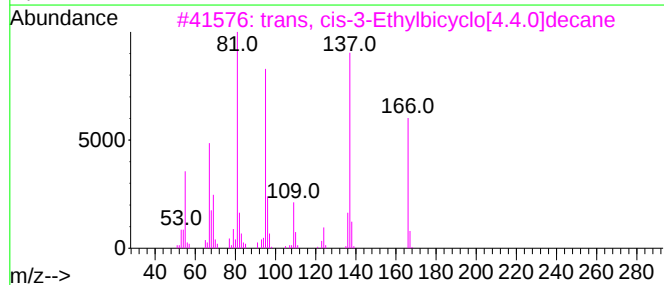
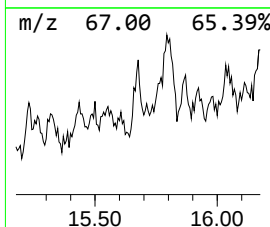
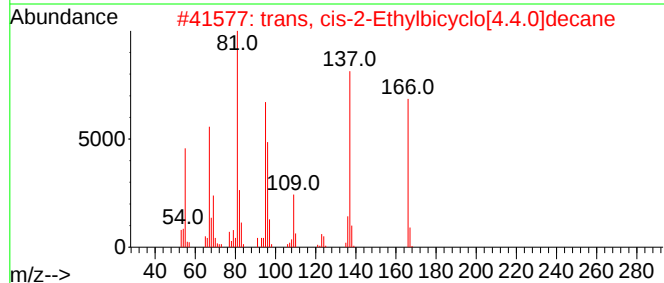
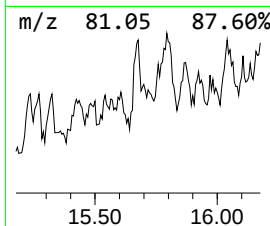
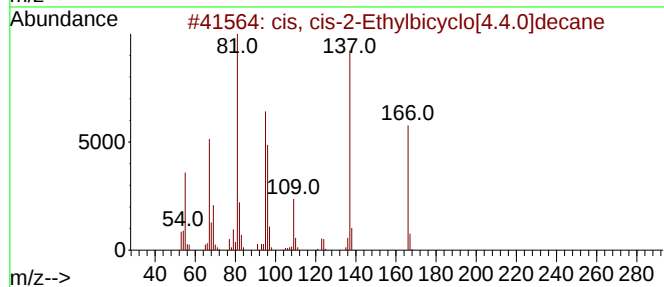
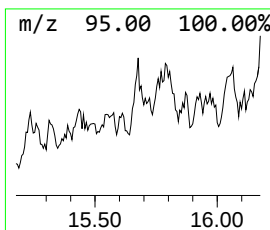
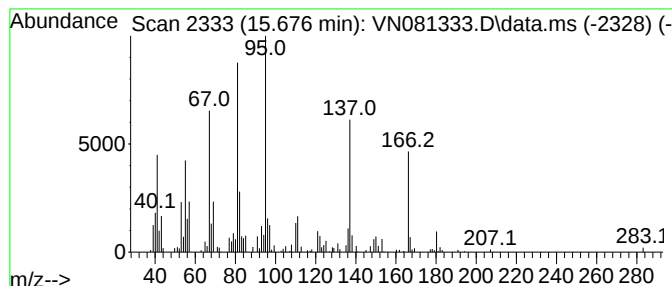
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Quant Title : SW846 8260

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

Peak Number 7 cis, cis-2-Ethylbicyclo[4.4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.676	12.96 ug/l	352254	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	68
2			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	68
3			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	62
4			4a(2H)-Naphthalenecarboxylic aci...	182	C11H18O2	007112-20-1	52
5			Naphthalene, 2-butyldcahydro-	194	C14H26	006305-52-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030624\
Data File : VN081333.D
Acq On : 06 Mar 2024 17:51
Operator : JC\MD
Sample : P1683-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.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
unknown2.818	2.818	5.1	ug/l	100715	1	8.224	986311	50.0
Undecane	14.106	10.5	ug/l	285059	4	13.794	1359100	50.0
trans-Decalin, ...	14.629	6.1	ug/l	166855	4	13.794	1359100	50.0
Dodecane	14.959	9.6	ug/l	260967	4	13.794	1359100	50.0
Naphthalene, de...	15.229	6.2	ug/l	168843	4	13.794	1359100	50.0
Iridomyrmecin	15.317	6.5	ug/l	175704	4	13.794	1359100	50.0
cis, cis-2-Ethy...	15.676	13.0	ug/l	352254	4	13.794	1359100	50.0