

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
 Data File : VN075824.D
 Acq On : 15 Dec 2022 17:47
 Operator : JC\MD
 Sample : N6074-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 221214029-02-VOA

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	38	43	53	rVB	84821	132868	1.95%	0.425%
2	4.442	395	406	425	rBV2	55188	184096	2.71%	0.589%
3	5.530	575	591	610	rBV	1444153	4962540	72.96%	15.887%
4	7.441	901	916	931	rBV	2523629	6801830	100.00%	21.775%
5	7.559	932	936	950	rVB3	43057	129688	1.91%	0.415%
6	7.841	972	984	1003	rBV	1078655	2798420	41.14%	8.959%
7	8.171	1031	1040	1044	rBV	234143	540731	7.95%	1.731%
8	8.230	1044	1050	1062	rVB	474315	1081000	15.89%	3.461%
9	8.583	1095	1110	1119	rBV2	252616	718677	10.57%	2.301%
10	8.659	1120	1123	1132	rVB2	51553	103357	1.52%	0.331%
11	9.106	1189	1199	1210	rBV	614534	1265019	18.60%	4.050%
12	10.441	1417	1426	1435	rBV4	31448	82882	1.22%	0.265%
13	10.571	1439	1448	1454	rVV	947617	1750486	25.74%	5.604%
14	10.635	1454	1459	1473	rVB2	165976	428317	6.30%	1.371%
15	11.171	1541	1550	1560	rBV	145556	277754	4.08%	0.889%
16	11.776	1646	1653	1658	rVV4	31719	81538	1.20%	0.261%
17	11.871	1658	1669	1677	rVV	809051	1555688	22.87%	4.980%
18	11.965	1677	1685	1692	rVB3	56954	153380	2.25%	0.491%
19	12.071	1692	1703	1713	rBV2	147540	341794	5.03%	1.094%
20	12.400	1751	1759	1765	rBV	132774	233644	3.44%	0.748%
21	12.853	1828	1836	1845	rVB	644488	1164551	17.12%	3.728%
22	13.188	1886	1893	1900	rVB6	27905	79186	1.16%	0.254%
23	13.482	1931	1943	1950	rBV	62074	129602	1.91%	0.415%
24	13.606	1957	1964	1972	rBV3	116042	245601	3.61%	0.786%
25	13.688	1972	1978	1981	rVV3	40865	81214	1.19%	0.260%
26	13.735	1981	1986	1989	rVV	90846	153574	2.26%	0.492%
27	13.794	1989	1996	2003	rVV	806783	1517002	22.30%	4.856%
28	13.870	2003	2009	2019	rVB3	142335	346938	5.10%	1.111%
29	13.994	2025	2030	2045	rVB2	50827	125263	1.84%	0.401%
30	14.253	2066	2074	2077	rBV5	120754	228005	3.35%	0.730%
31	14.306	2077	2083	2092	rVB	510052	872852	12.83%	2.794%
32	14.453	2100	2108	2116	rVB8	48731	125703	1.85%	0.402%
33	14.676	2140	2146	2153	rVB	783588	1293904	19.02%	4.142%
34	15.029	2200	2206	2213	rBV5	40402	91914	1.35%	0.294%
35	15.100	2213	2218	2225	rVV2	39529	74633	1.10%	0.239%
36	15.276	2241	2248	2257	rBV7	94164	271694	3.99%	0.870%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

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\82N121422W.M
Title : SW846 8260

37	15.364	2257	2263	2275	rVB5	243434	546834	8.04%	1.751%
38	15.641	2299	2310	2317	rVB	112847	264586	3.89%	0.847%

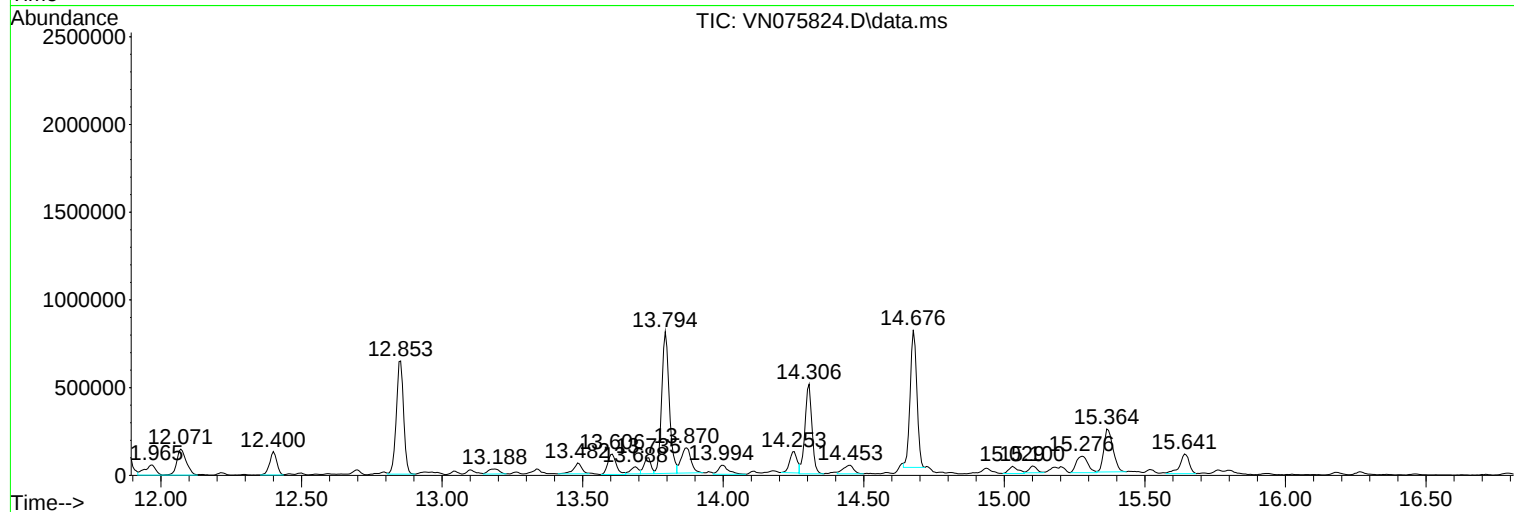
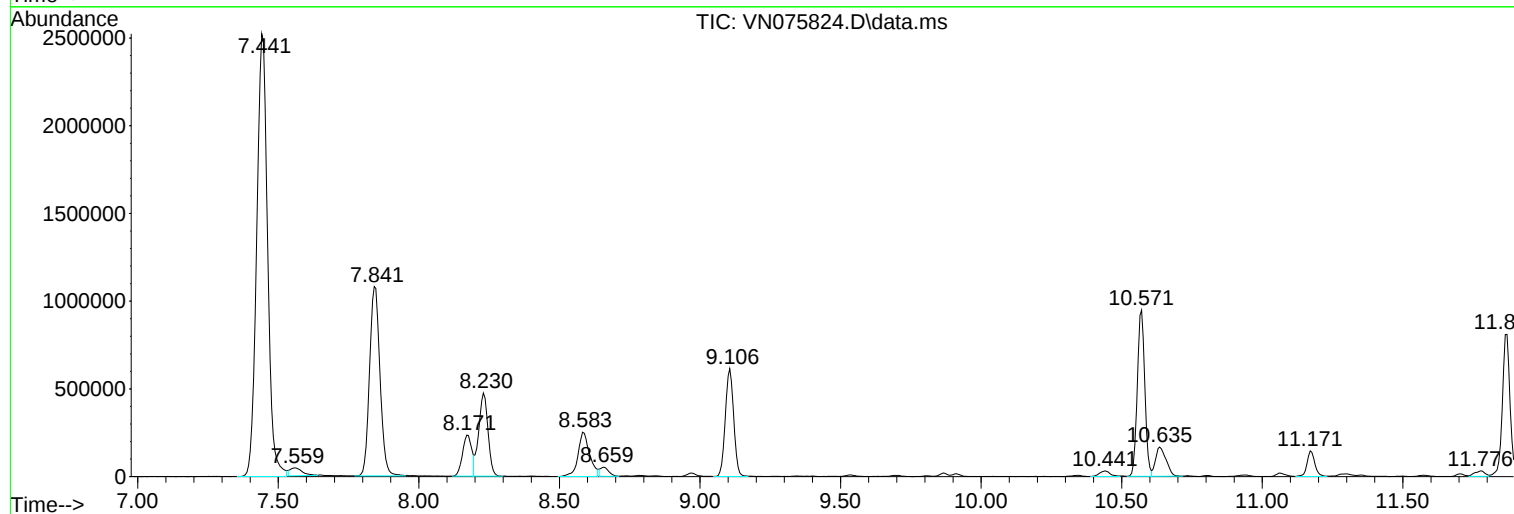
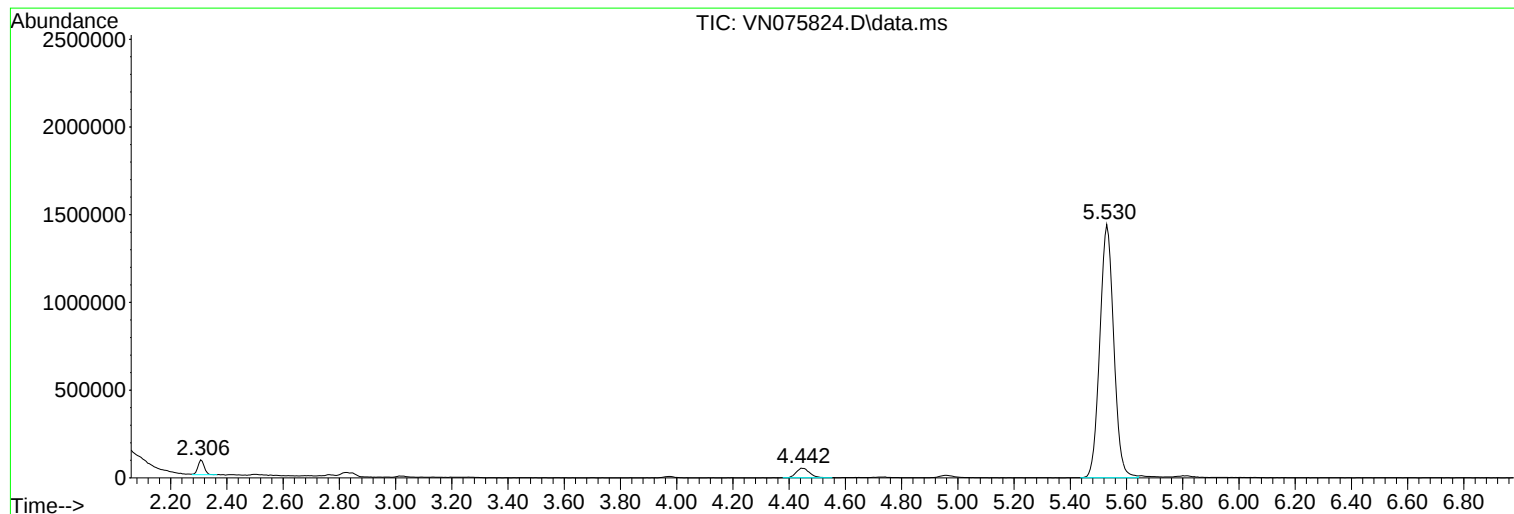
Sum of corrected areas: 31236765

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

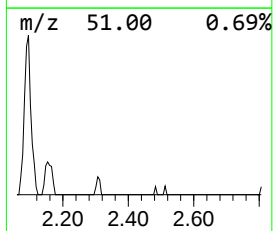
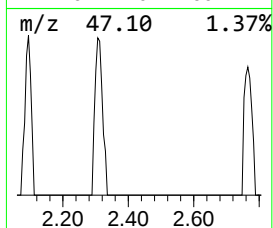
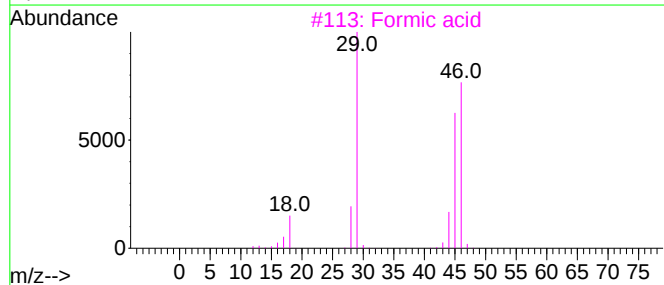
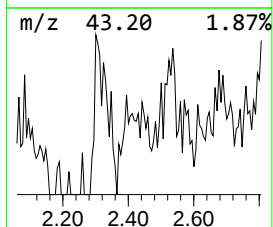
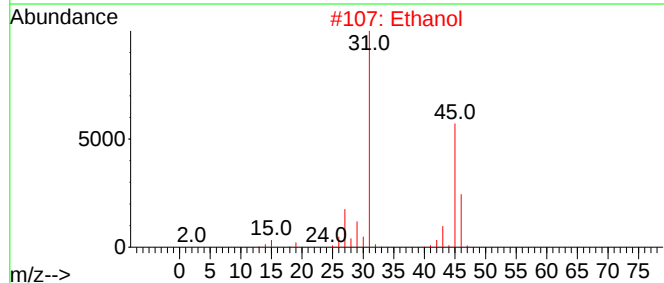
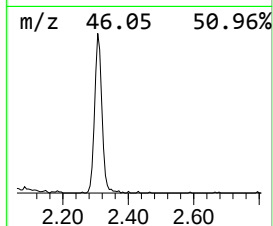
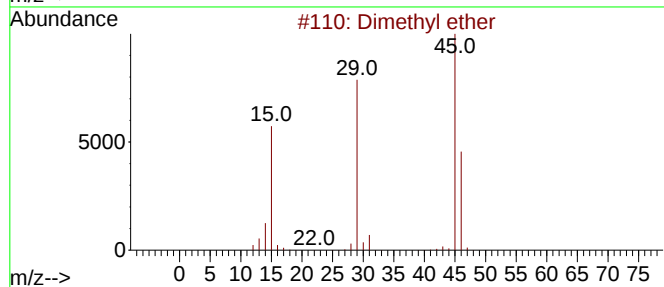
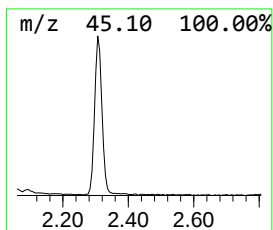
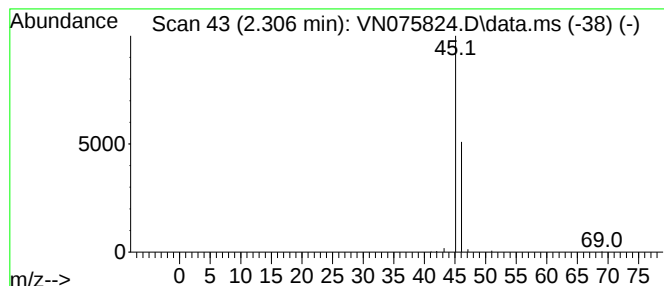
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	6.15 ug/l	132868	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	74
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Hydrazine, methyl-	46	CH6N2	000060-34-4	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

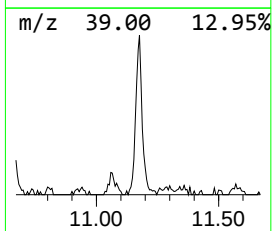
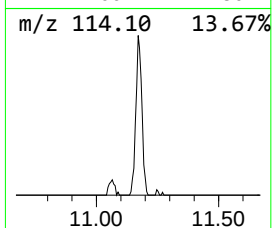
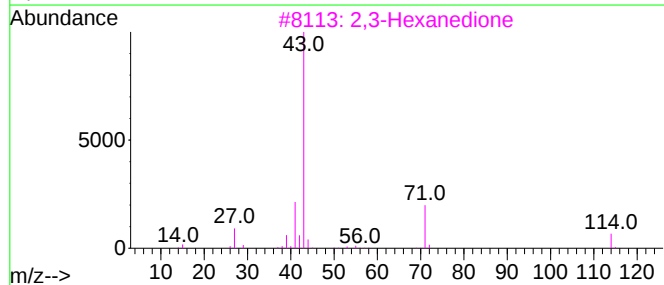
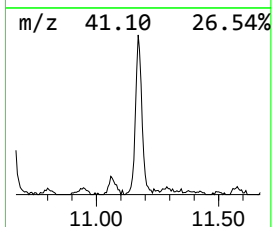
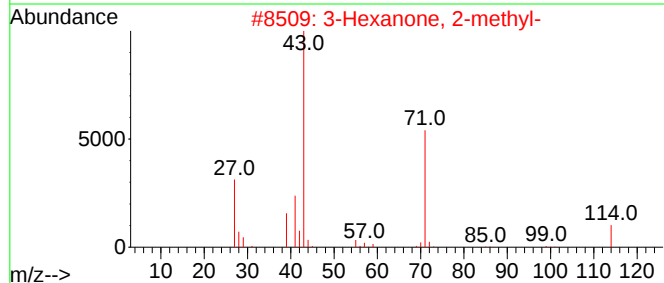
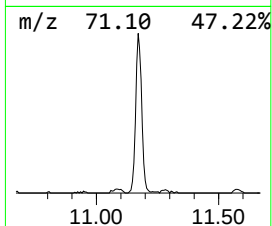
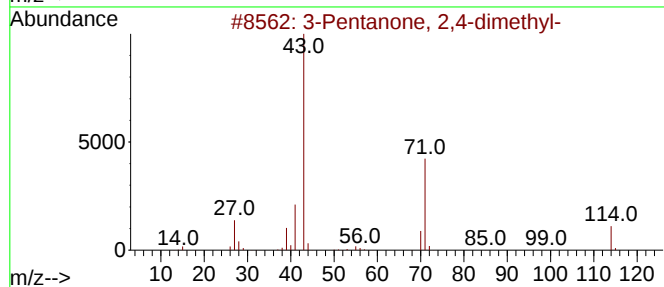
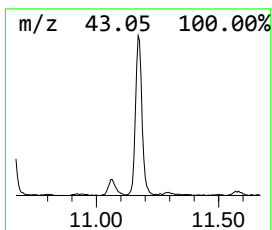
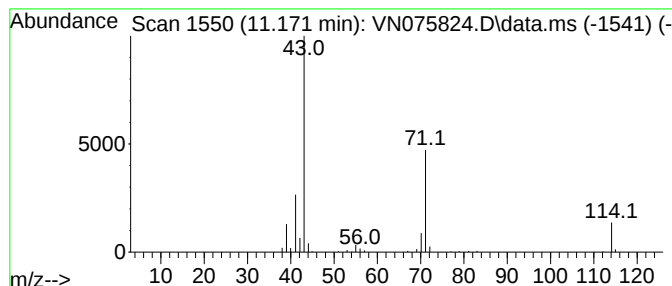
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	8.93 ug/l	277754	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	78
4			4-Heptanone	114	C7H14O	000123-19-3	59
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

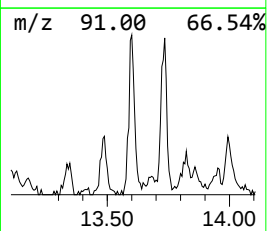
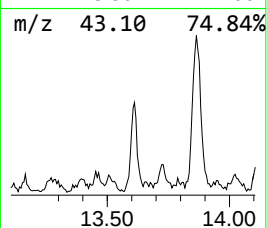
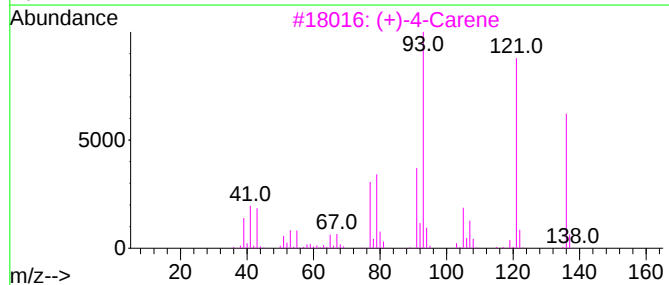
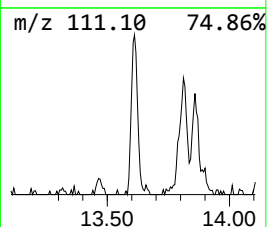
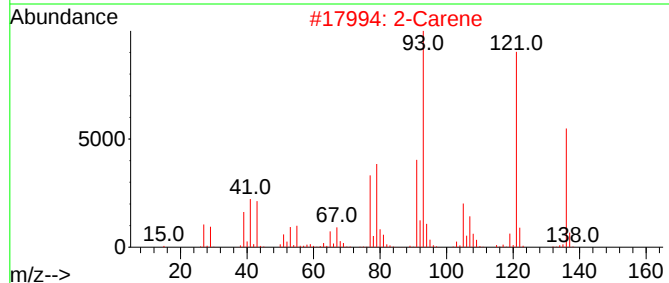
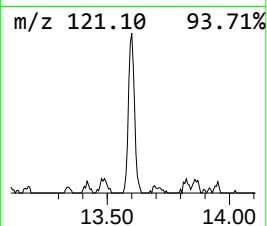
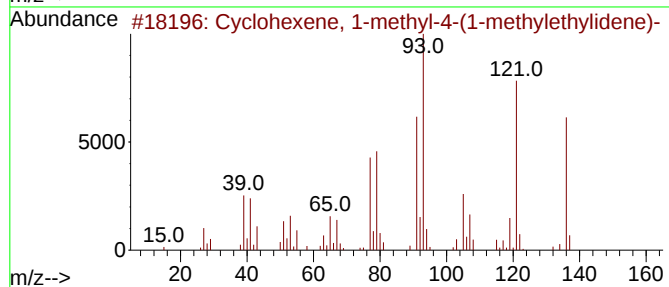
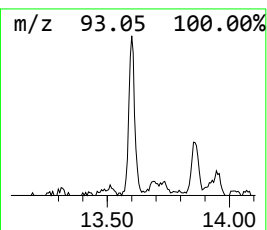
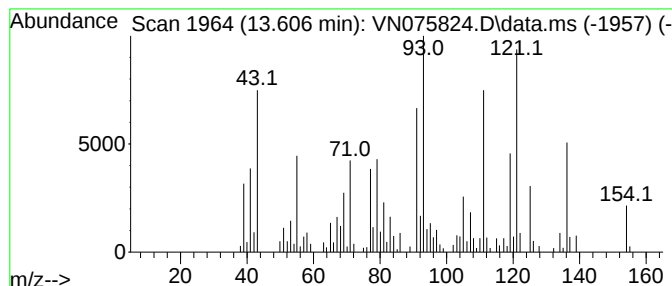
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.606	8.09 ug/l	245601	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	95
2			2-Carene	136	C10H16	000554-61-0	95
3			(+)-4-Carene	136	C10H16	029050-33-7	91
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	90
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

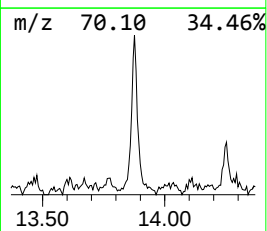
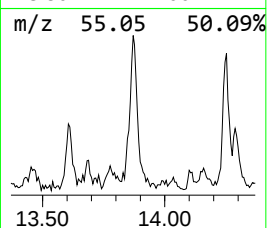
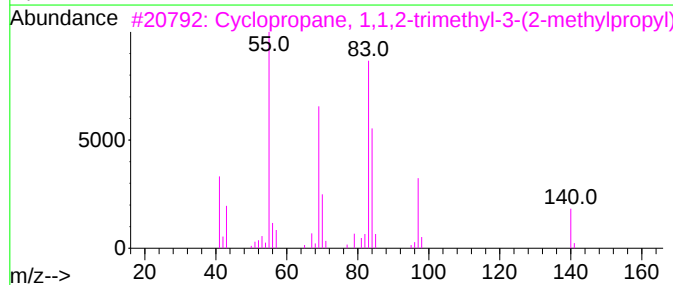
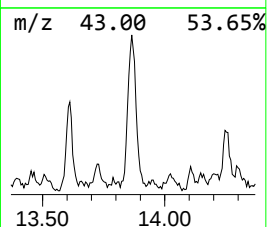
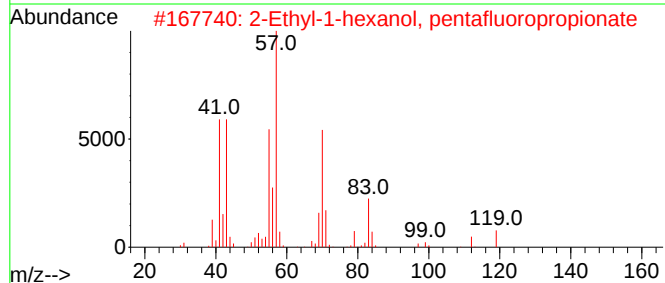
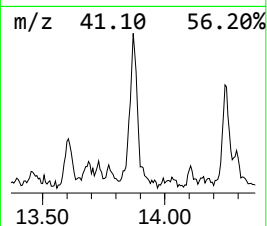
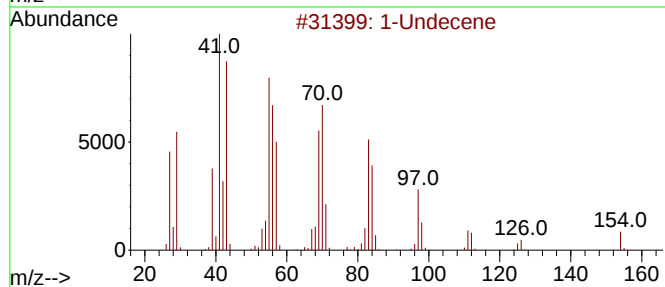
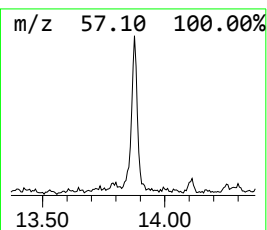
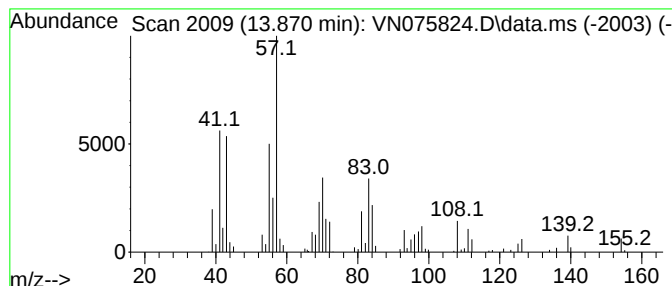
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.870 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	11.44 ug/l	346938	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Undecene	154	C11H22	000821-95-4	43
2			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	35
3			Cyclopropane, 1,1,2-trimethyl-3-...	140	C10H20	041977-43-9	30
4			2-Undecene, (Z)-	154	C11H22	000821-96-5	27
5			Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

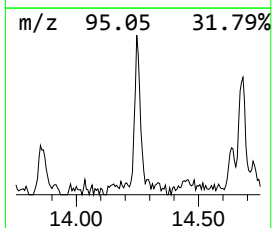
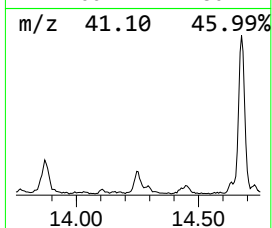
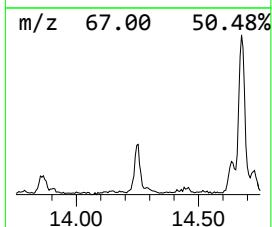
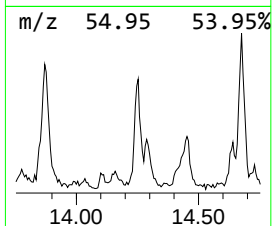
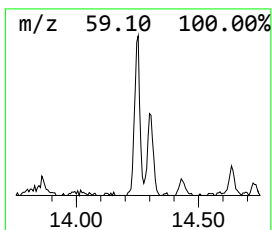
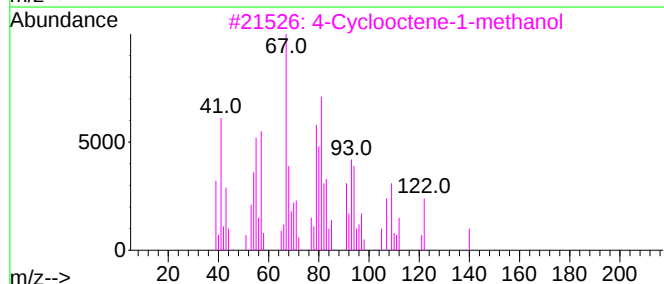
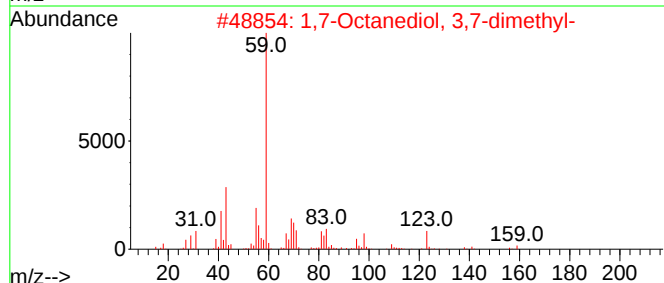
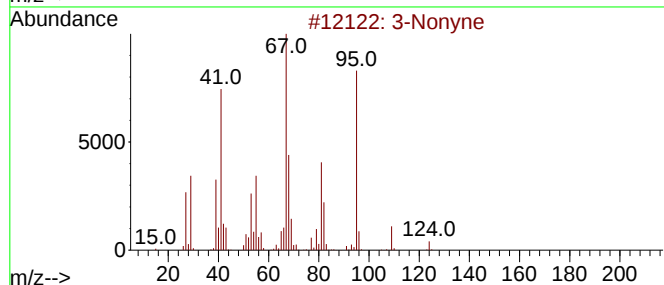
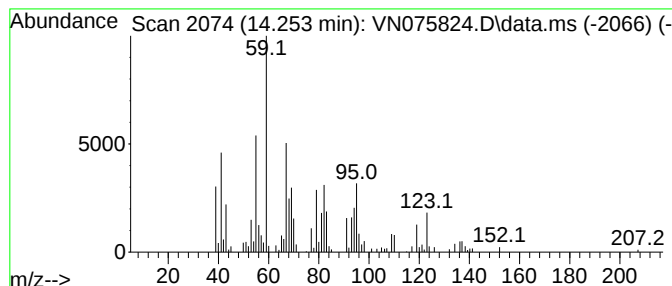
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown14.253 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.253	7.51 ug/l	228005	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Nonyne	124	C9H16	020184-89-8	30
2			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	27
3			4-Cyclooctene-1-methanol	140	C9H16O	013366-81-9	27
4			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	25
5			3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-97-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

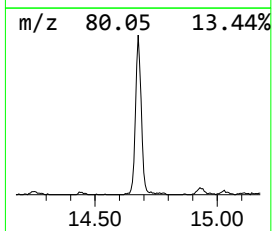
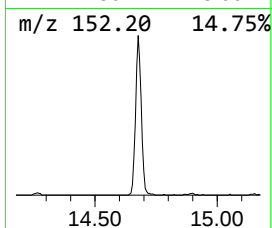
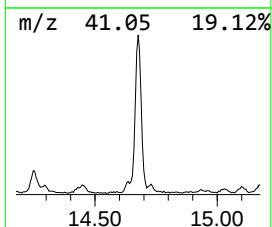
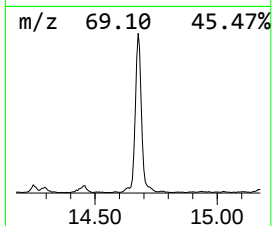
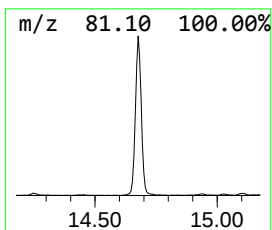
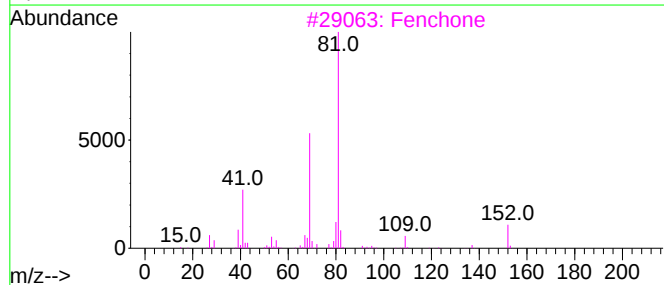
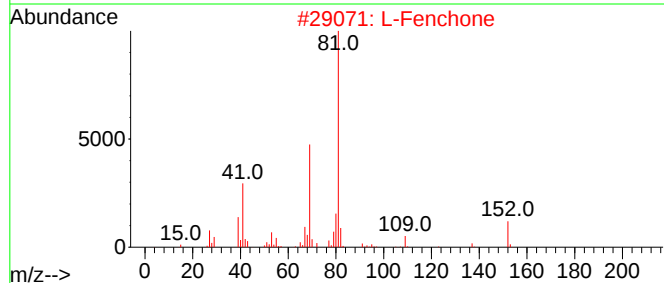
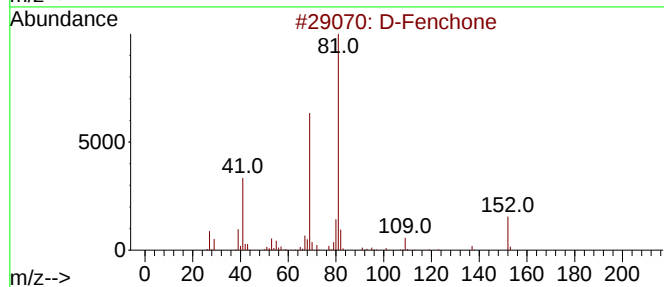
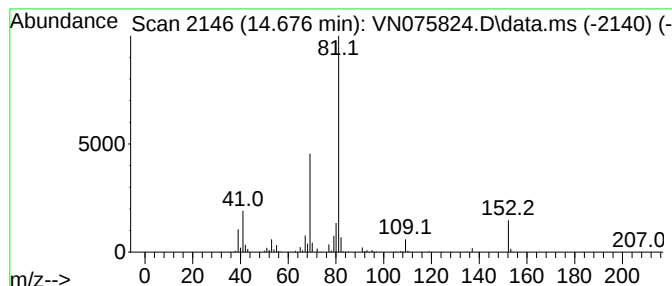
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 8 D-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	42.65 ug/l	1293900	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Fenchone	152	C10H16O	004695-62-9	94
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			Fenchone	152	C10H16O	001195-79-5	94
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	59
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

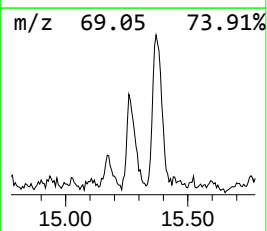
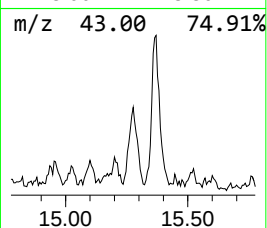
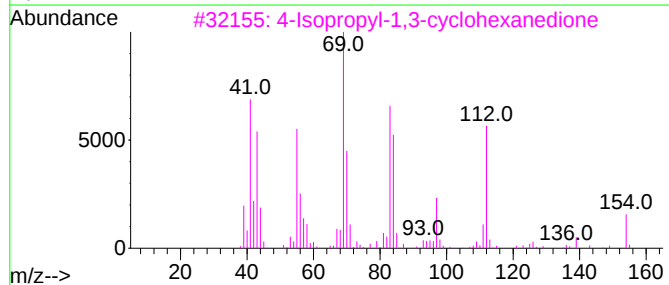
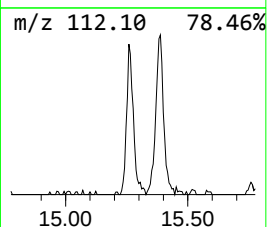
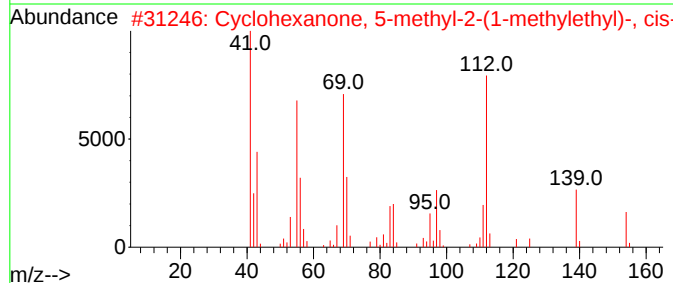
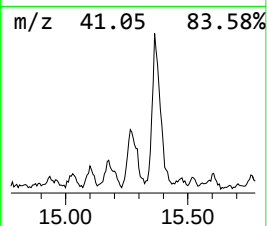
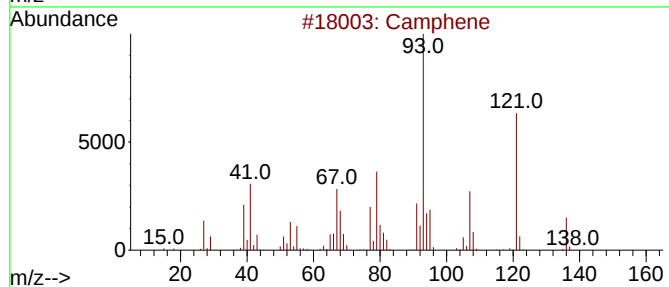
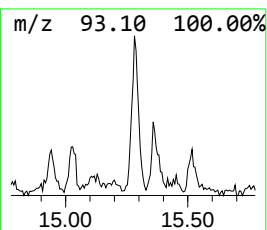
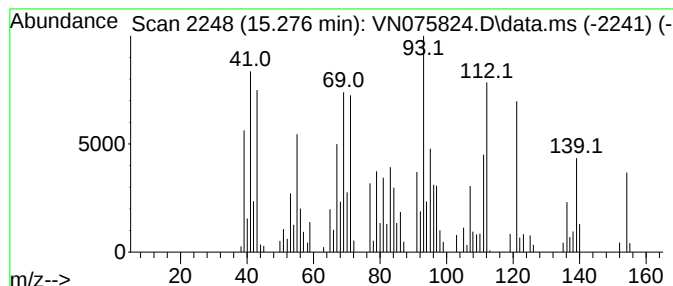
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 9 Camphene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.276	8.95 ug/l	271694	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	62
2			Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	42
3			4-Isopropyl-1,3-cyclohexanedione	154	C9H14O2	062831-62-3	41
4			L-Menthone	154	C10H18O	014073-97-3	38
5			Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

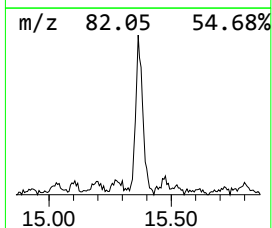
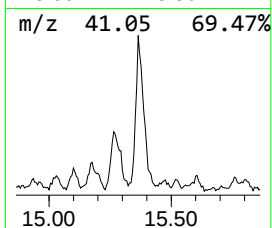
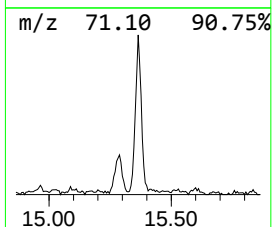
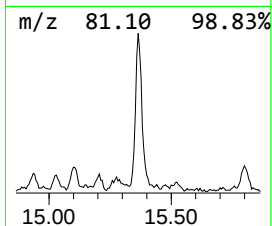
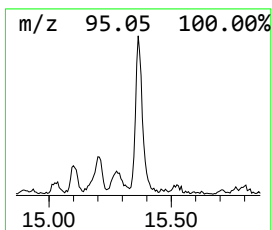
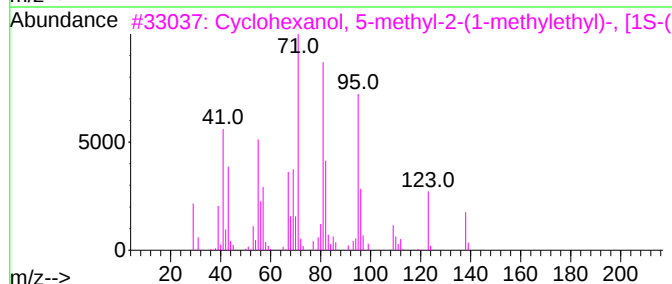
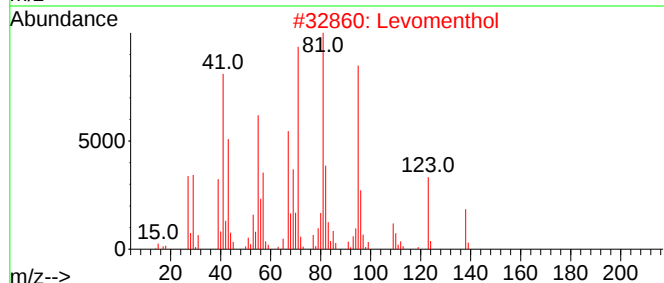
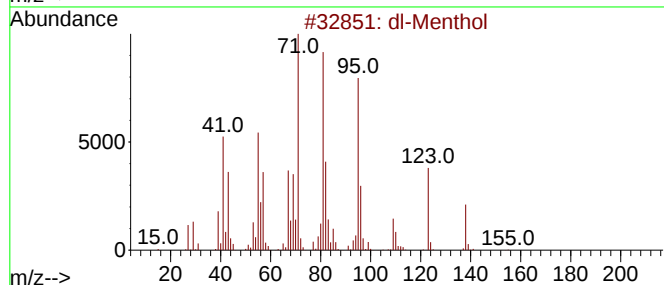
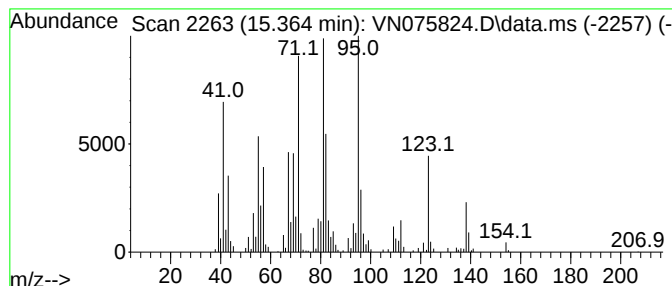
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 10 dl-Menthol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.365	18.02 ug/l	546834	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			dl-Menthol	156	C10H20O	000089-78-1	91
2			Levomenthol	156	C10H20O	002216-51-5	80
3			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	72
4			Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	72
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075824.D
Acq On : 15 Dec 2022 17:47
Operator : JC\MD
Sample : N6074-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
221214029-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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
Dimethyl ether	2.306	6.2	ug/l	132868	1	8.230	1081000	50.0
3-Pentanone, 2,...	11.171	8.9	ug/l	277754	3	11.871	1555690	50.0
Cyclohexene, 1-...	13.606	8.1	ug/l	245601	4	13.794	1517000	50.0
unknown13.870	13.870	11.4	ug/l	346938	4	13.794	1517000	50.0
unknown14.253	14.253	7.5	ug/l	228005	4	13.794	1517000	50.0
D-Fenchone	14.676	42.6	ug/l	1293900	4	13.794	1517000	50.0
Camphene	15.276	8.9	ug/l	271694	4	13.794	1517000	50.0
dl-Menthol	15.365	18.0	ug/l	546834	4	13.794	1517000	50.0