LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

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\82N030722W.M
Title : SW846 8260

Signal : TIC: VN071325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.281	379	390	402	rBV	869113	2571592	10.28%	1.694%
2	4.569	423	439	458	rBV	395650	1328913	5.31%	0.876%
3	4.851	476	487	503	rVB2	112082	364687	1.46%	0.240%
4	7.328	894	908	924	rBV2	97552	309182	1.24%	0.204%
5	8.016	1014	1025	1031	rBV	561085	1393142	5.57%	0.918%
6	8.080	1031	1036	1053	rVB	1101542	2514735	10.06%	1.657%
7	8.433	1084	1096	1109	rBV	662022	1610122	6.44%	1.061%
8	8.963	1177	1186	1209	rVB	1603206	3348817	13.39%	2.206%
9	9.151	1210	1218	1239	rBV	791359	1847627	7.39%	1.217%
10	10.327	1411	1418	1426	rBV	362178	658165	2.63%	0.434%
11	10.439	1426	1437	1444	rBV	2571768	4701881	18.80%	3.098%
12	10.945	1515	1523	1539	rBV	1437635	2701448	10.80%	1.780%
13	11.127	1549	1554	1559	rVB	232328	369066	1.48%	0.243%
14	11.457	1604	1610	1617	rBV	255960	462552	1.85%	0.305%
15	11.739	1648	1658	1668	rBV	2346734	4345606	17.38%	2.863%
16	11.945	1685	1693	1705	rVB	783113	1386257	5.54%	0.913%
17	12.727	1819	1826	1835	rVB	1988992	3414751	13.65%	2.250%
18	12.815	1835	1841	1848	rBV	586656	1138659	4.55%	0.750%
19	12.927	1855	1860	1871	rVB	457254	721136	2.88%	0.475%
20	13.057	1877	1882	1893	rVB	163766	310671	1.24%	0.205%
21	13.304	1918	1924	1935	rBV6	118107	337859	1.35%	0.223%
22	13.586	1967	1972	1979	rVB5	165100	288836	1.15%	0.190%
23	13.668	1979	1986	1993	rBV	2087423	3758164	15.03%	2.476%
24	13.739	1993	1998	1999	rVV	841224	1319304	5.28%	0.869%
25	13.762	1999	2002	2010	rVV	2150005	3701847	14.80%	2.439%
26	13.833	2010	2014	2023	rVB3	186388	387530	1.55%	0.255%
27	13.986	2035	2040	2044	rBV	392872	633209	2.53%	0.417%
28	14.027	2044	2047	2055	rVV3	261683	425860	1.70%	0.281%
29	14.133	2059	2065	2073	rVV2	987412	1756139	7.02%	1.157%
30	14.339	2092	2100	2106	rBV2	759931	2211109	8.84%	1.457%
31	14.415	2106	2113	2121	rVV	10426834	16670178	66.66%	10.983%
32	14.521	2126	2131	2135	rBV	1113701	1699305	6.79%	1.120%
33	14.586	2139	2142	2144	rBV2	360786	433586	1.73%	0.286%
34	14.627	2144	2149	2151	rBV	4007605	6136827	24.54%	4.043%
35	14.662	2151	2155	2161	rBV2	9563555	25009534	100.00%	16.477%
36	14.780	2170	2175	2182	rVV	5666997	8653983	34.60%	5.702%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

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\82N030722W.M
Title : SW846 8260

37	14.833	2182	2184	2190	rVB2	525540	708318	2.83%	0.467%
38	14.992	2201	2211	2219	rBV3	3267812	7236456	28.93%	4.768%
39	15.098	2219	2229	2231	rVV3	1294591	3284661	13.13%	2.164%
40	15.133	2232	2235	2237	rVV2	1939671	3109859	12.43%	2.049%
41	15.162	2238	2240	2243	rVV2	2363591	3634362	14.53%	2.394%
42	15.203	2244	2247	2255	rVV3	2084991	5075585	20.29%	3.344%
43	15.286	2255	2261	2265	rVV	2169535	4788260	19.15%	3.155%
44	15.333	2266	2269	2274	rVV2	1580171	3102405	12.40%	2.044%
45	15.439	2274	2287	2295	rVV4	1750329	7526793	30.10%	4.959%
46	15.521	2296	2301	2318	rVB4	985553	3064000	12.25%	2.019%
47	15.880	2355	2362	2373	rBV	461728	978708	3.91%	0.645%
48	16.192	2412	2415	2422	rVB2	200220	352338	1.41%	0.232%

Sum of corrected areas: 151784024

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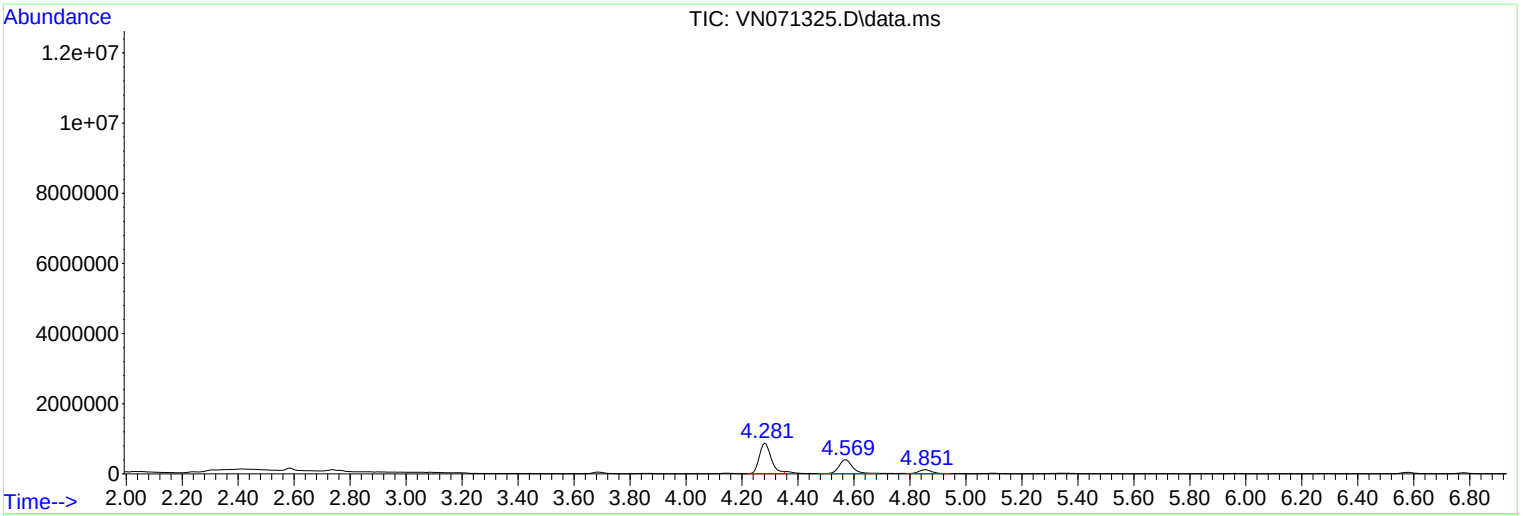
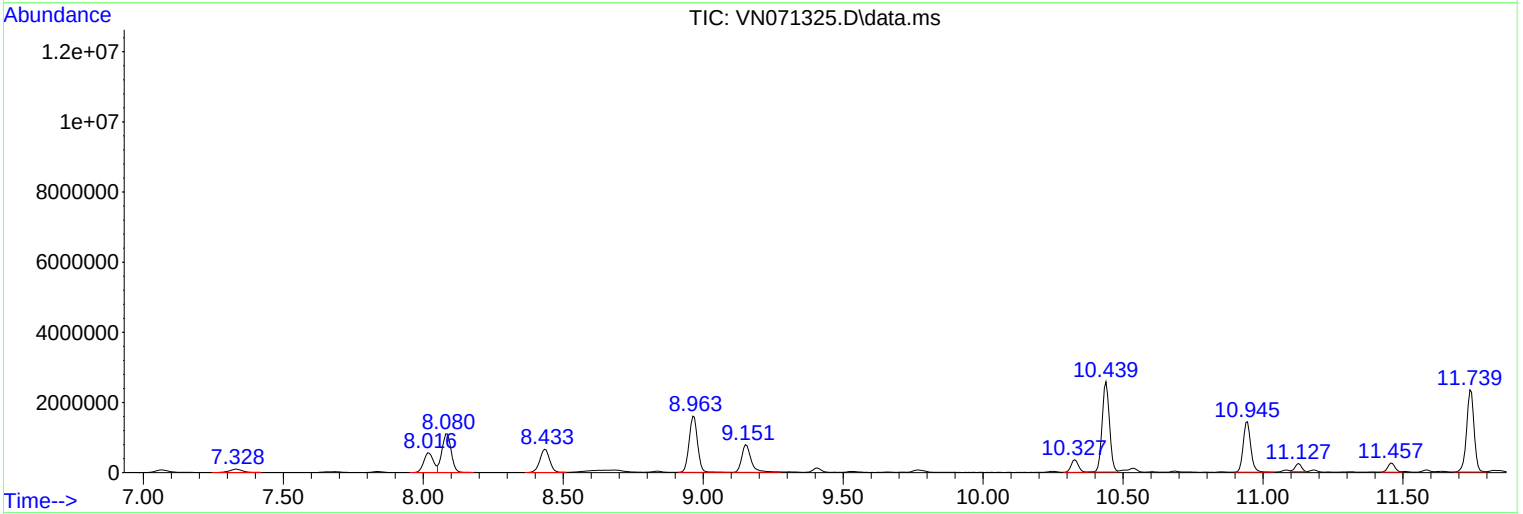
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

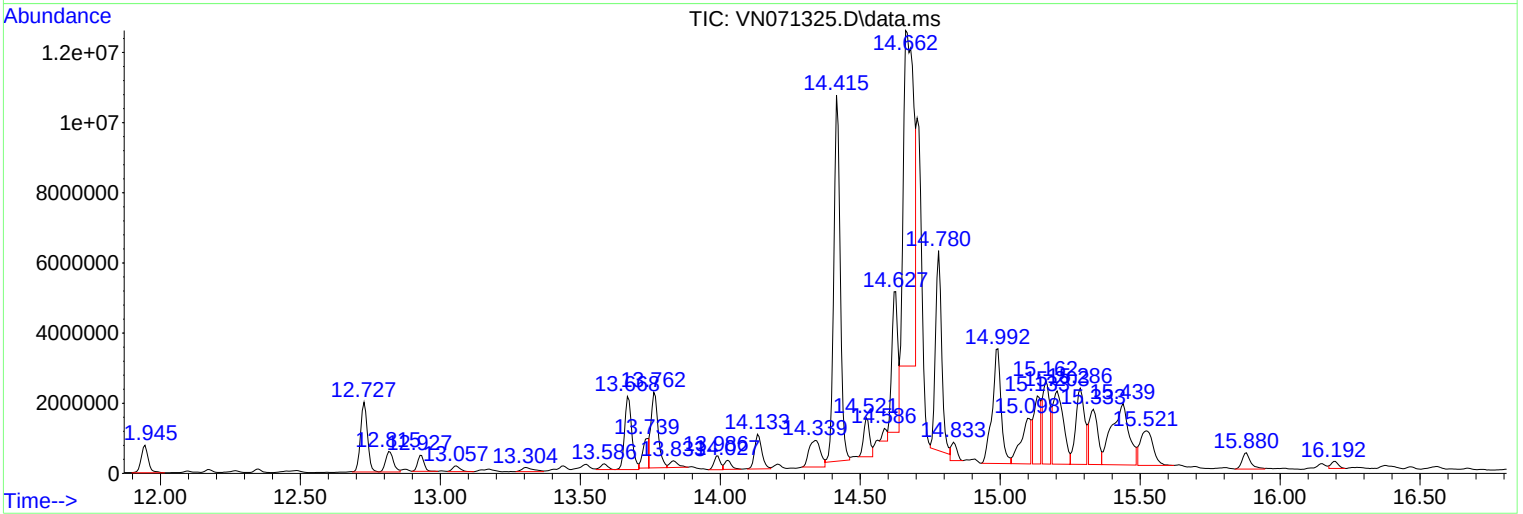
Instrument :
MSVOA_N
ClientSampleId :
2822-B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
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Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

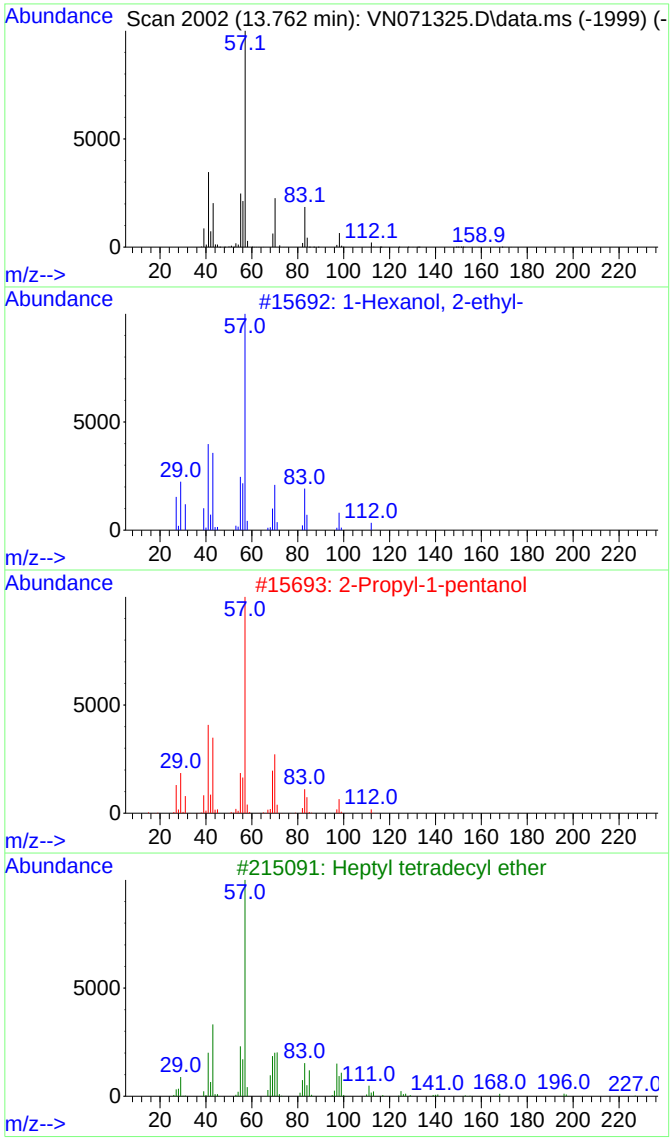
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

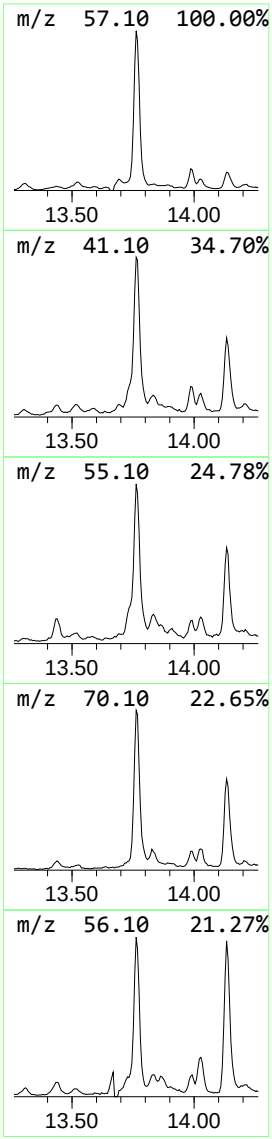
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.762	49.25 ug/l	3701850	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	40
3	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	39
4	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	38
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

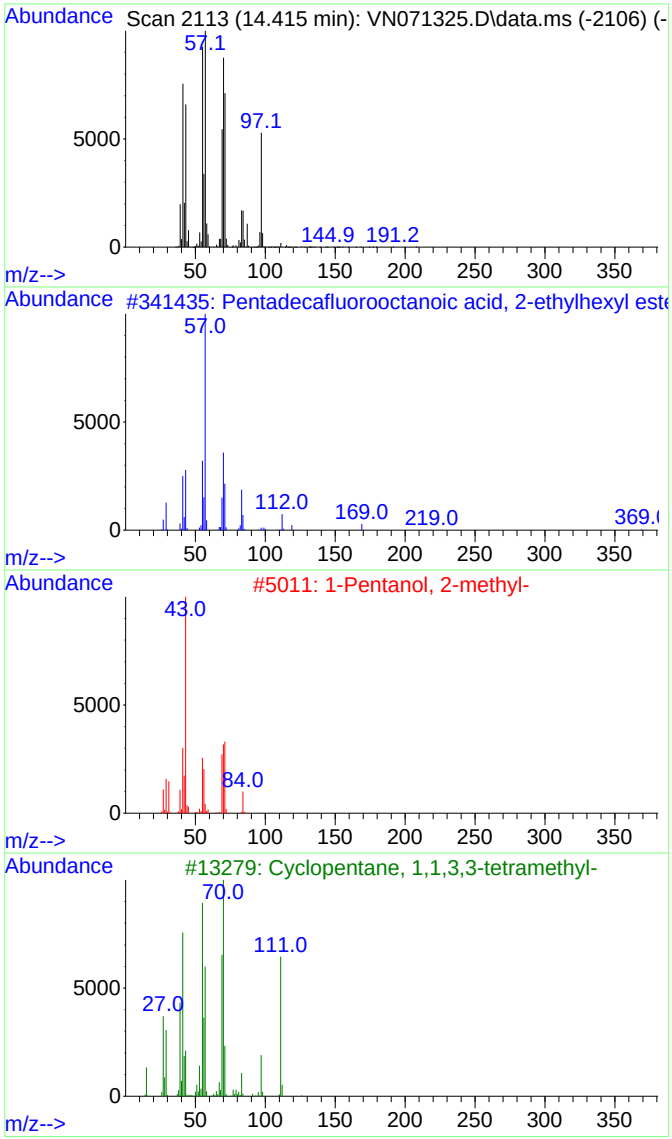
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

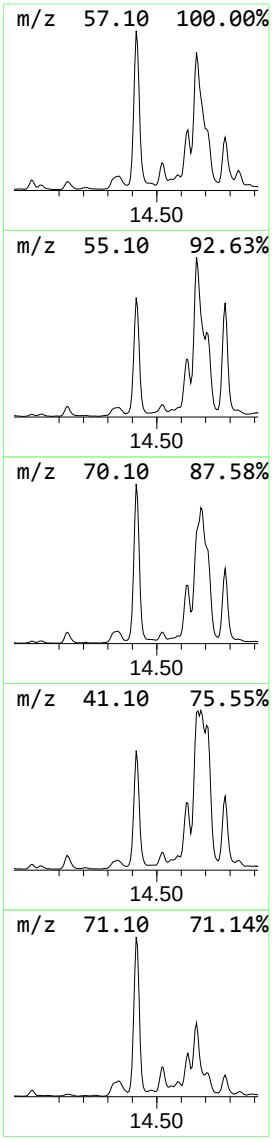
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.415	221.79 ug/l	16670200	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
2	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
3	Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	50
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	47
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

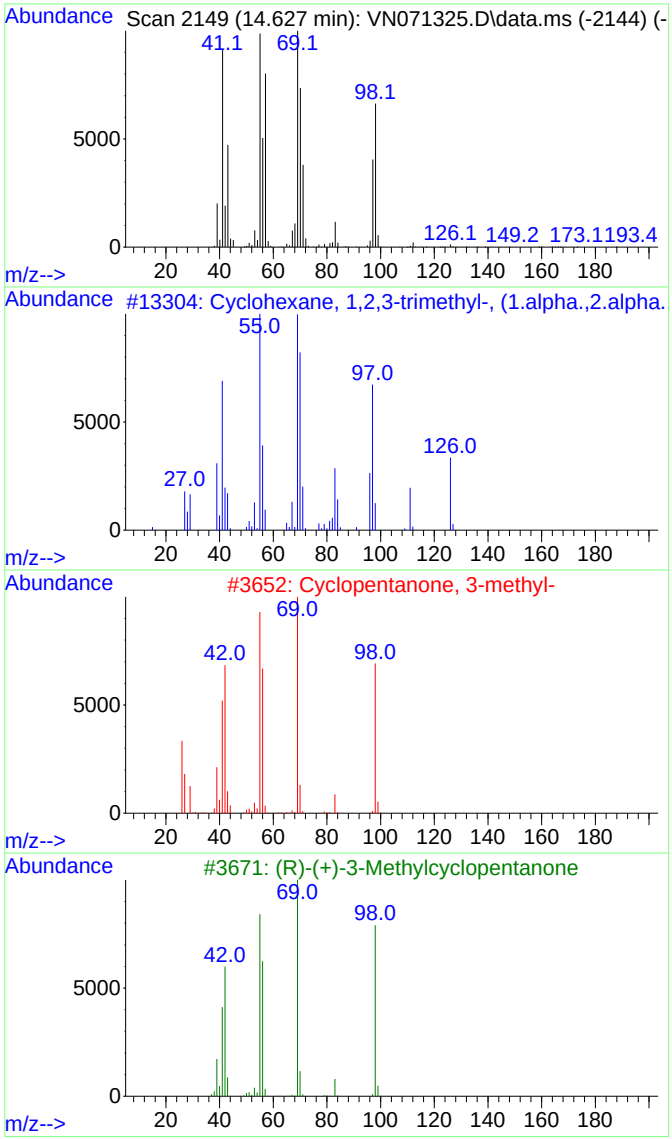
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

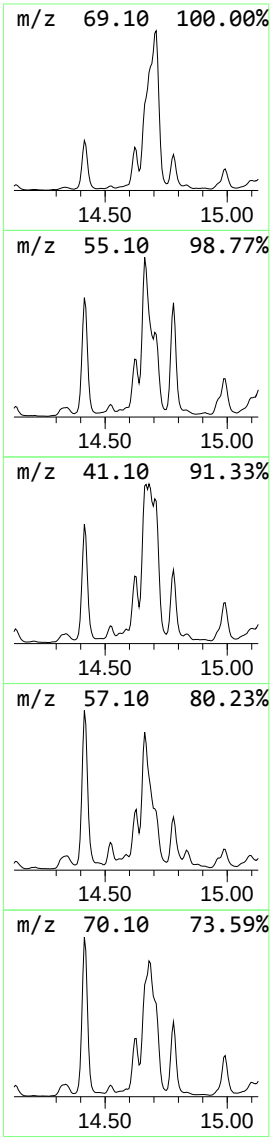
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,2,3-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.627	81.65 ug/l	6136830	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001839-88-9	64
2	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	46
3	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	46
4	Cyclopentanecarboxaldehyde	98	C6H10O	000872-53-7	38
5	2-Pentene, 3-ethyl-	98	C7H14	000816-79-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
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Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

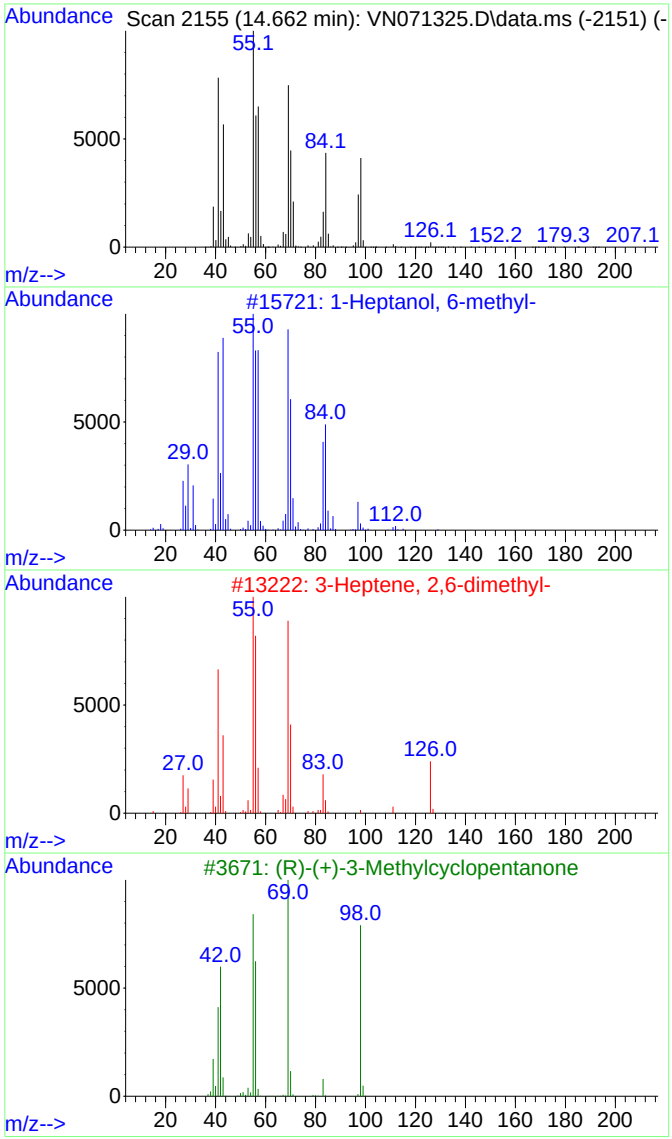
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

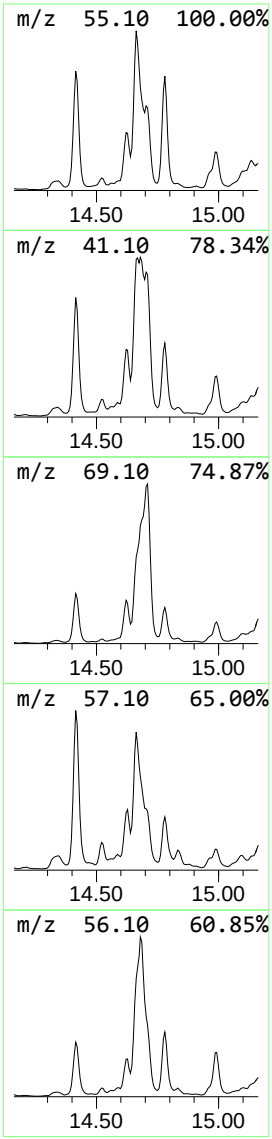
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heptanol, 6-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.662	332.74 ug/l	25009500	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	53
2	3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	49
3	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	47
4	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	43
5	2-Pentene, 2-methyl-	84	C6H12	000625-27-4	38





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

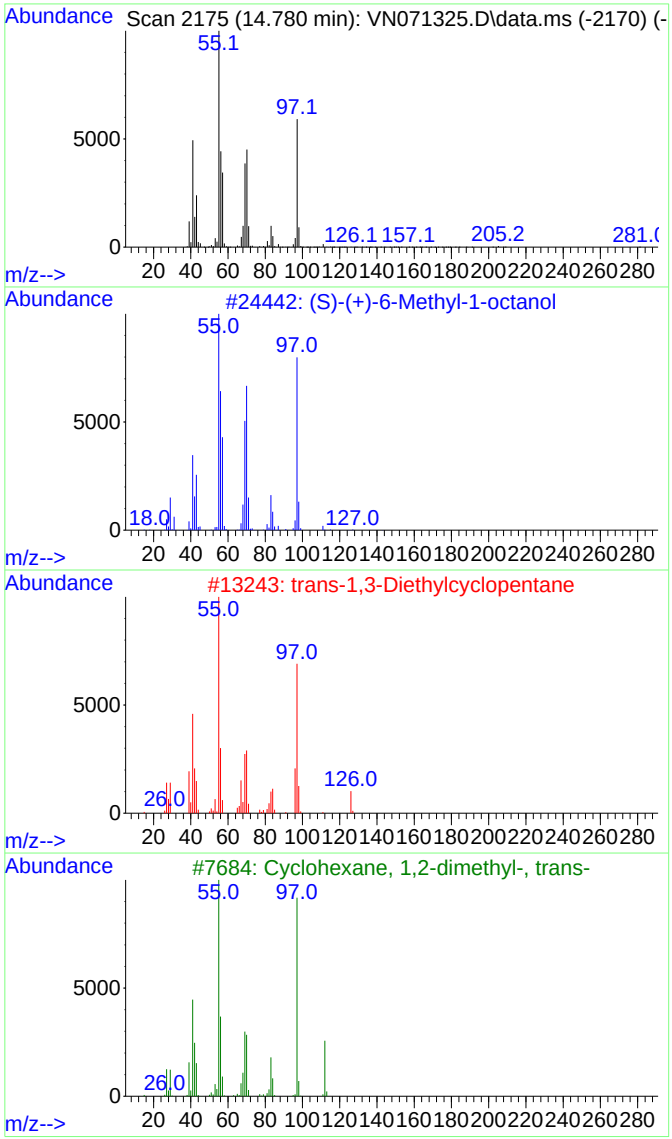
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

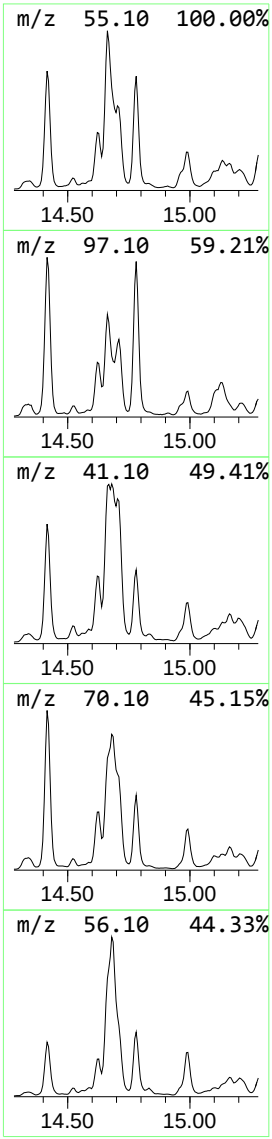
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (S)-(+)-6-Methyl-1-octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	115.14 ug/l	8653980	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2	trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	53
3	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50
4	trans-2,4-Dimethylthiane, S,S-di...	162	C7H14O2S	1000215-67-6	50
5	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

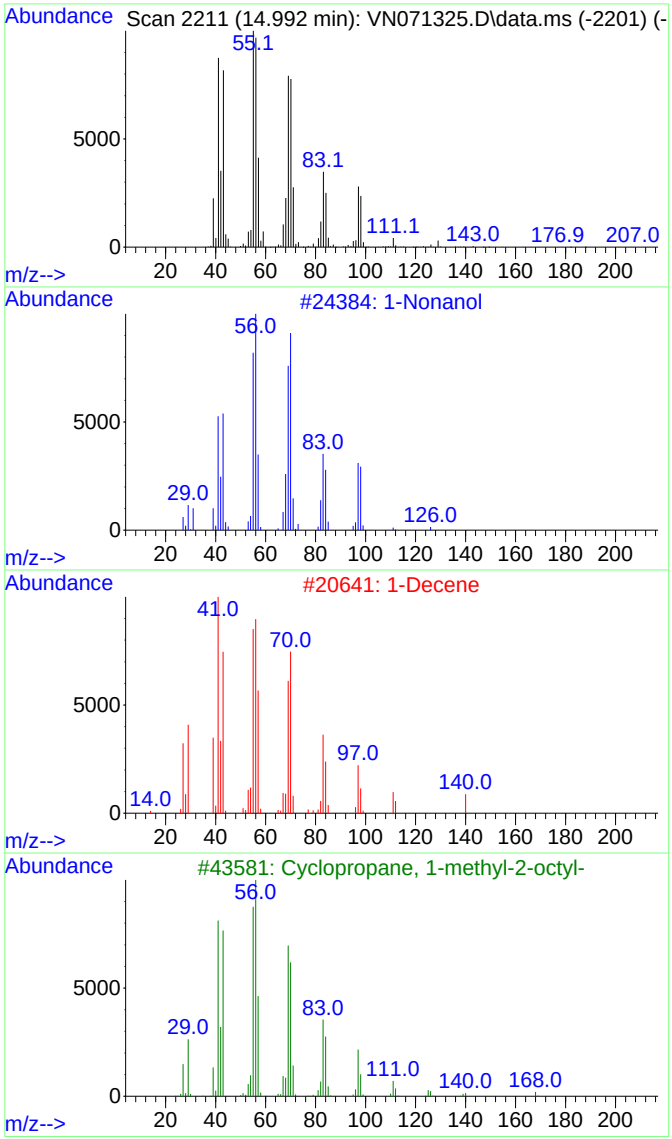
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

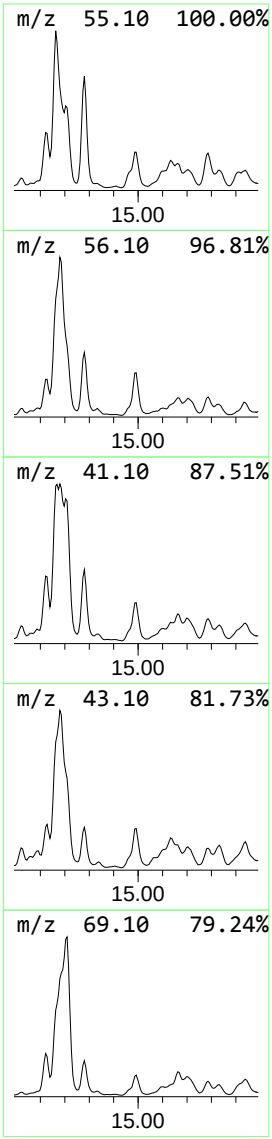
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Nonanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	96.28 ug/l	7236460	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	90
2	1-Decene	140	C10H20	000872-05-9	80
3	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	78
4	1-Octanol	130	C8H18O	000111-87-5	59
5	Cycloheptane	98	C7H14	000291-64-5	52





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Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

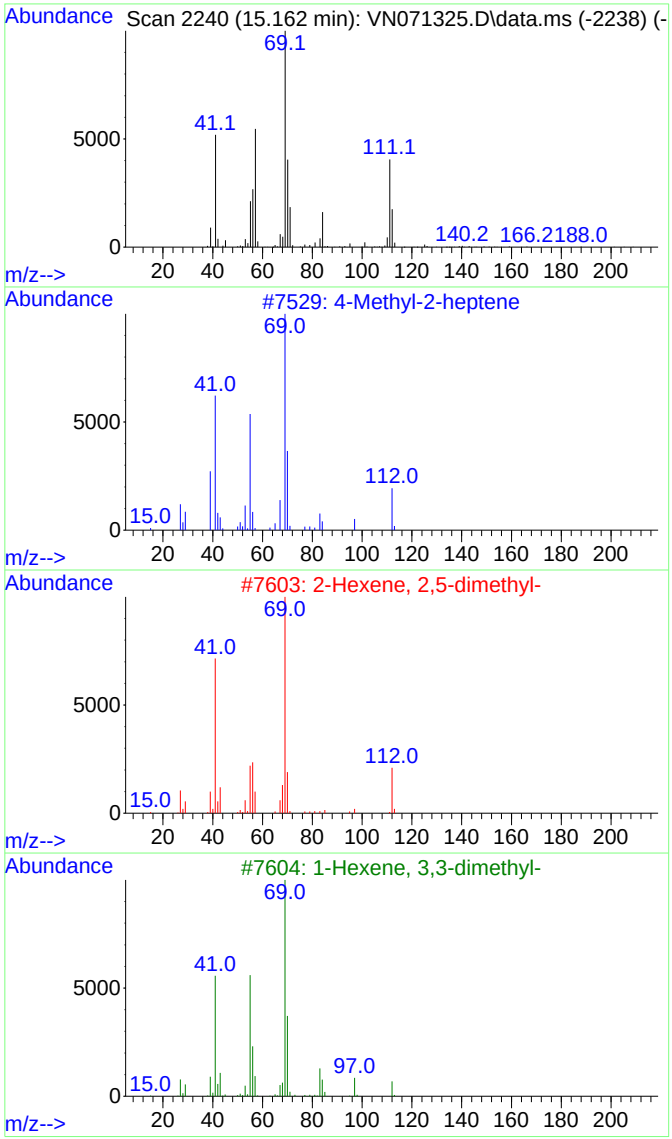
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

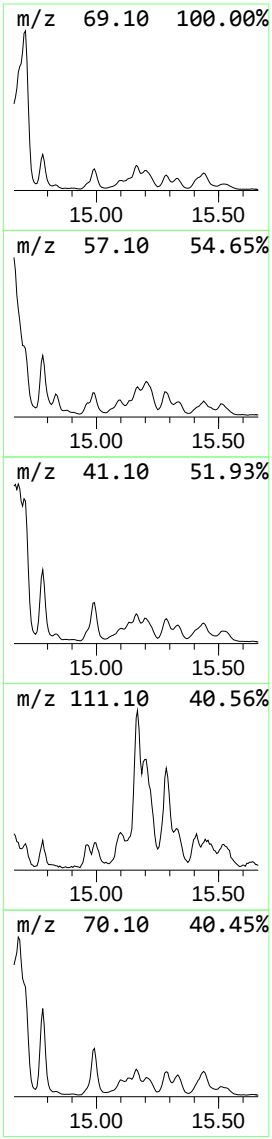
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown15.162 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.162	48.35 ug/l	3634360	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-2-heptene	112	C8H16	003404-56-6	49
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	43
3	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	40
4	Trichloroacetic acid, 6-ethyl-3-...	302	C12H21Cl3O2	1010282-57-4	39
5	2-Methyl-1,8-octanediol	160	C9H20O2	1000433-27-9	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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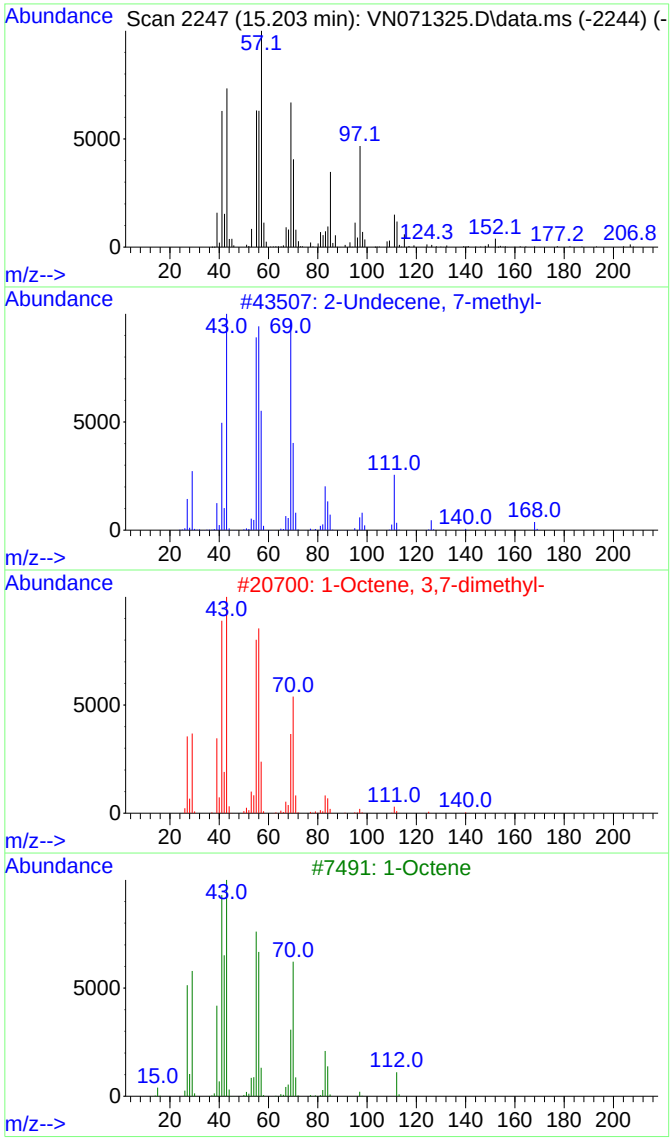
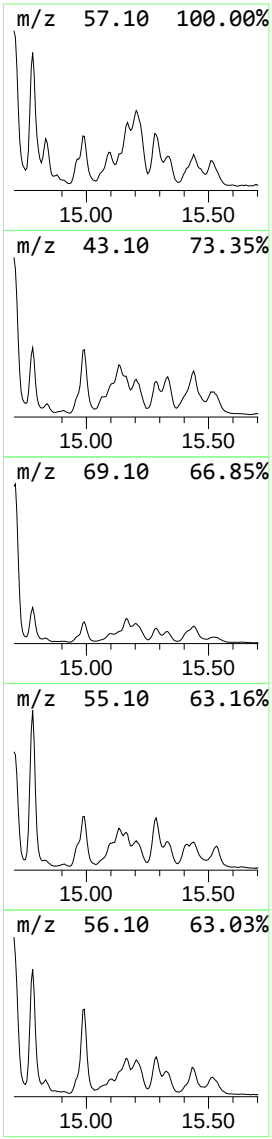
Peak Number 8 unknown15.204 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	67.53 ug/l	5075590	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecene, 7-methyl-	168	C12H24	1000061-83-0	46
2	1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	46
3	1-Octene	112	C8H16	000111-66-0	43
4	Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	30
5	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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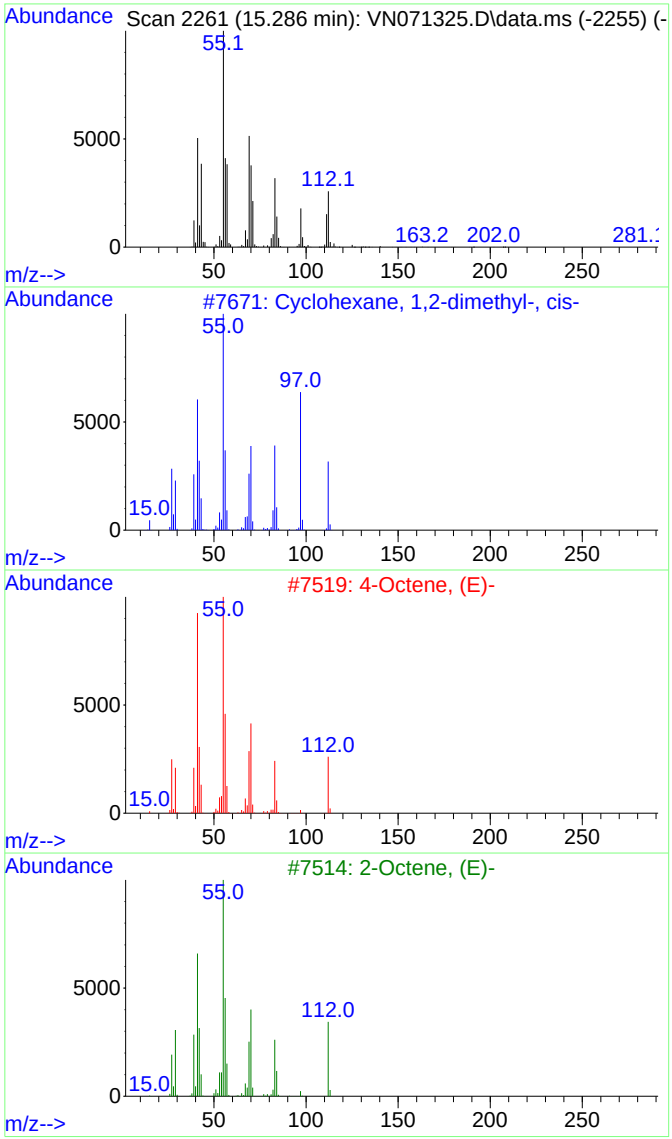
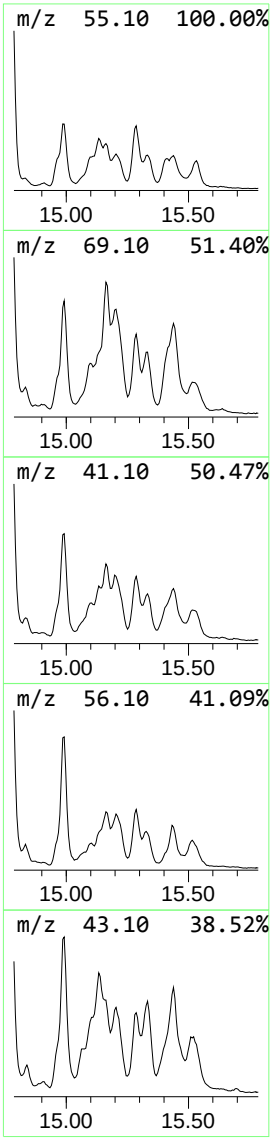
Peak Number 9 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	63.70 ug/l	4788260	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	76
2	4-Octene, (E)-	112	C8H16	014850-23-8	64
3	2-Octene, (E)-	112	C8H16	013389-42-9	59
4	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	52
5	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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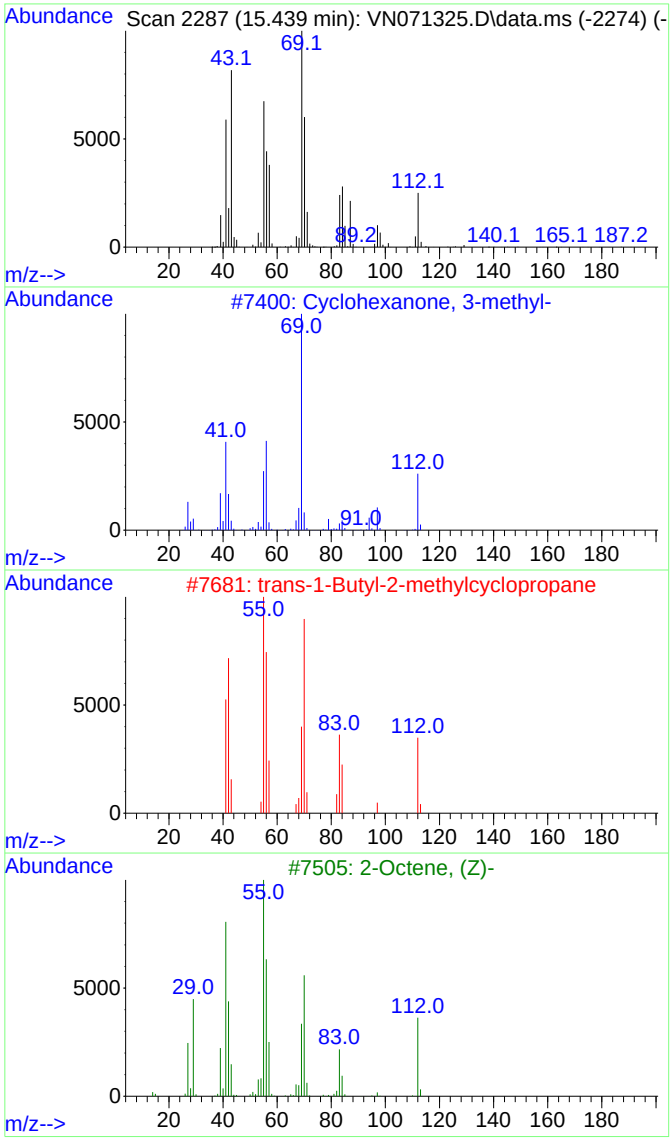
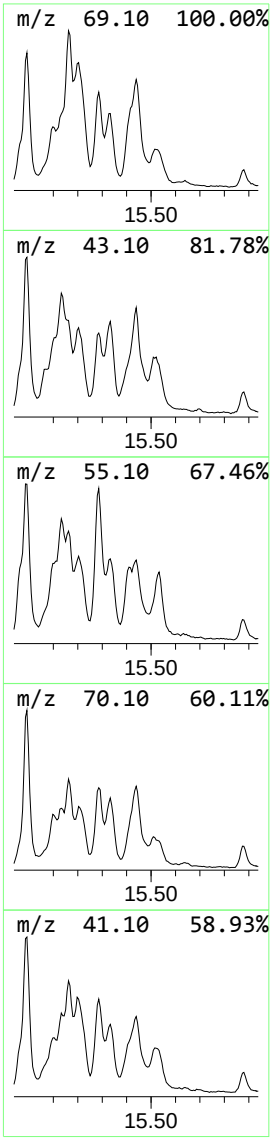
Peak Number 10 unknown15.439 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	100.14 ug/l	7526790	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-methyl-	112	C7H12O	000591-24-2	49
2	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	45
3	2-Octene, (Z)-	112	C8H16	007642-04-8	43
4	3-Octene, (E)-	112	C8H16	014919-01-8	43
5	3-Octene, (Z)-	112	C8H16	014850-22-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031622\
Data File : VN071325.D
Acq On : 16 Mar 2022 17:12
Operator : JC\MD
Sample : N1886-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2822-B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	13.762	49.3	ug/l	3701850	4	13.668	3758160	50.0
Pentadecafluoro...	14.415	221.8	ug/l	16670200	4	13.668	3758160	50.0
Cyclohexane, 1,...	14.627	81.7	ug/l	6136830	4	13.668	3758160	50.0
1-Heptanol, 6-m...	14.662	332.7	ug/l	25009500	4	13.668	3758160	50.0
(S)-(+)-6-Methy...	14.780	115.1	ug/l	8653980	4	13.668	3758160	50.0
1-Nonanol	14.992	96.3	ug/l	7236460	4	13.668	3758160	50.0
unknown15.162	15.162	48.4	ug/l	3634360	4	13.668	3758160	50.0
unknown15.204	15.204	67.5	ug/l	5075590	4	13.668	3758160	50.0
Cyclohexane, 1,...	15.286	63.7	ug/l	4788260	4	13.668	3758160	50.0
unknown15.439	15.439	100.1	ug/l	7526790	4	13.668	3758160	50.0