LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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: VN073116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	238	245	252	rVB3	12450	31229	1.03%	0.111%
2	4.769	478	490	506	rBV	102002	331364	10.92%	1.176%
3	5.210	551	565	575	rBV2	10826	41022	1.35%	0.146%
4	5.987	688	697	706	rVB5	13008	35130	1.16%	0.125%
5	7.292	908	919	927	rBV	28069	76663	2.53%	0.272%
6	7.945	1017	1030	1035	rBV	231381	579864	19.10%	2.057%
7	8.004	1035	1040	1052	rVB	451411	1040628	34.28%	3.692%
8	8.363	1091	1101	1113	rBV2	259459	639751	21.08%	2.270%
9	8.745	1158	1166	1173	rBV4	22094	50988	1.68%	0.181%
10	8.898	1181	1192	1201	rBV	612286	1299636	42.82%	4.611%
11	9.386	1264	1275	1281	rBV7	25154	77369	2.55%	0.275%
12	10.328	1431	1435	1436	rBV4	42300	47535	1.57%	0.169%
13	10.375	1437	1443	1450	rVV	868501	1633964	53.83%	5.797%
14	10.439	1450	1454	1459	rVB	57458	93697	3.09%	0.332%
15	10.675	1490	1494	1497	rBV4	19724	34344	1.13%	0.122%
16	10.716	1497	1501	1507	rVB3	44558	82720	2.73%	0.293%
17	11.275	1592	1596	1602	rBV2	57036	99964	3.29%	0.355%
18	11.333	1604	1606	1609	rVB3	30918	33879	1.12%	0.120%
19	11.486	1627	1632	1639	rVB	110722	190806	6.29%	0.677%
20	11.680	1659	1665	1676	rBV	941623	1832539	60.37%	6.502%
21	11.780	1679	1682	1685	rBV	48759	68993	2.27%	0.245%
22	11.810	1685	1687	1692	rVB4	47895	65003	2.14%	0.231%
23	11.886	1693	1700	1706	rBV5	250548	700760	23.09%	2.486%
24	12.027	1720	1724	1731	rVB4	90844	142190	4.68%	0.504%
25	12.186	1744	1751	1758	rBV3	272989	743696	24.50%	2.639%
26	12.392	1781	1786	1796	rVB4	314722	889444	29.30%	3.156%
27	12.504	1800	1805	1810	rVB5	163191	352430	11.61%	1.250%
28	12.669	1827	1833	1839	rBV	1817943	3035377	100.00%	10.769%
29	12.757	1841	1848	1852	rBV8	172692	402540	13.26%	1.428%
30	12.833	1857	1861	1868	rVB4	388230	768295	25.31%	2.726%
31	12.916	1869	1875	1882	rBV7	300039	776093	25.57%	2.754%
32	12.998	1883	1889	1892	rBV6	354580	790456	26.04%	2.804%
33	13.133	1909	1912	1917	rVB4	351303	533352	17.57%	1.892%
34	13.227	1924	1928	1929	rBV	219479	297143	9.79%	1.054%
35	13.316	1939	1943	1946	rBV4	201292	316917	10.44%	1.124%
36	13.351	1946	1949	1952	rVV3	146376	199049	6.56%	0.706%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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

37	13.492	1967	1973	1978	rBV4	325940	757351	24.95%	2.687%
38	13.610	1988	1993	2002	rVB	1210076	2411472	79.45%	8.556%
39	13.933	2043	2048	2054	rVB3	855441	1512084	49.82%	5.365%
40	14.321	2111	2114	2120	rVB8	315347	531492	17.51%	1.886%
41	14.439	2130	2134	2138	rBV3	541802	921510	30.36%	3.269%
42	14.604	2158	2162	2167	rBV2	621110	926549	30.53%	3.287%
43	15.198	2258	2263	2264	rBV5	271851	442393	14.57%	1.570%
44	15.639	2334	2338	2352	rVB7	448201	1238091	40.79%	4.393%
45	15.810	2364	2367	2376	rVB4	552445	1109607	36.56%	3.937%

Sum of corrected areas: 28185379

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
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Operator : JC\MD
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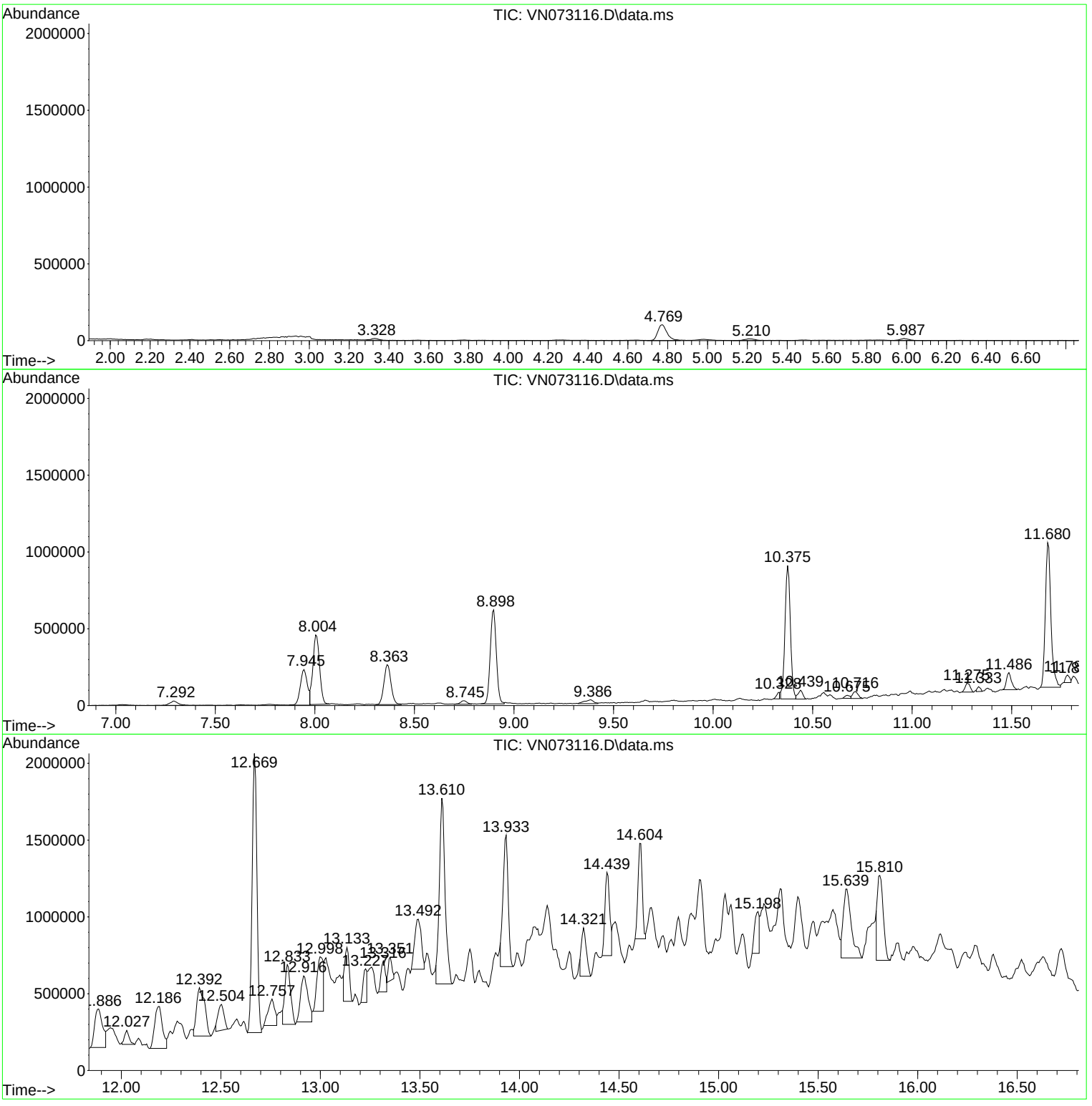
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

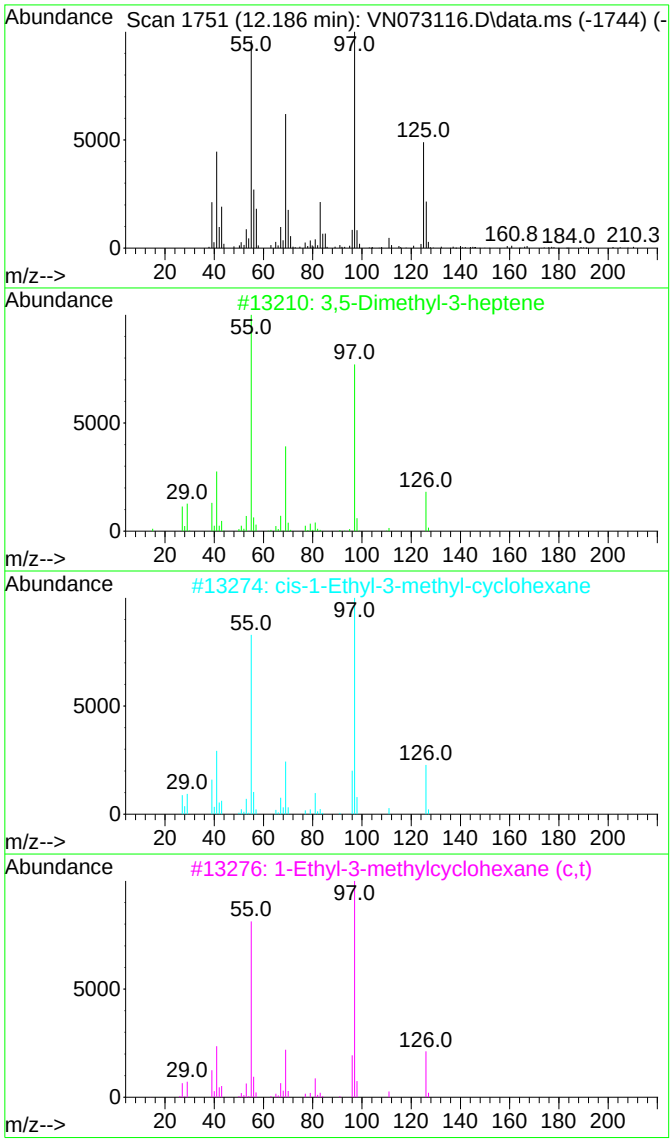
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

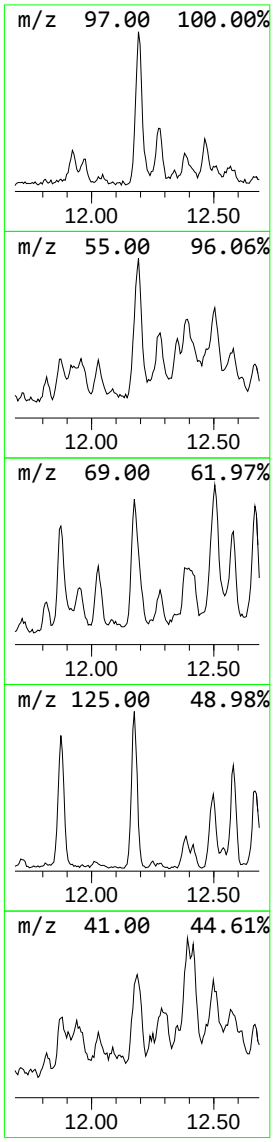
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3,5-Dimethyl-3-heptene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	20.29 ug/l	743696	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	53
2	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	52
3	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	52
4	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	50
5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

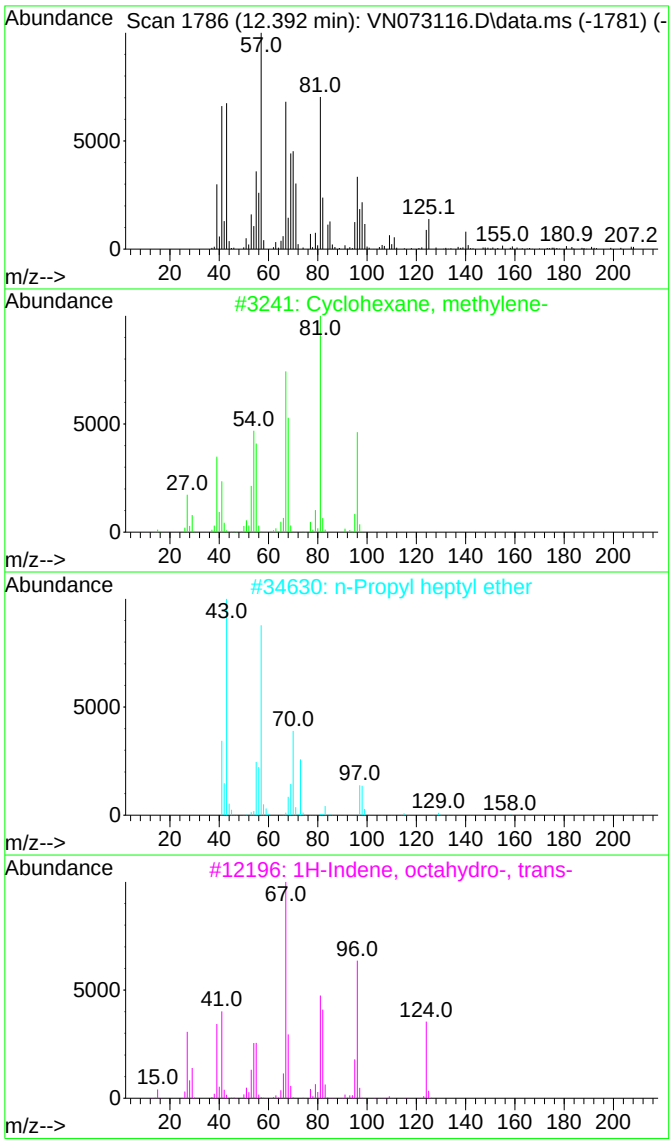
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

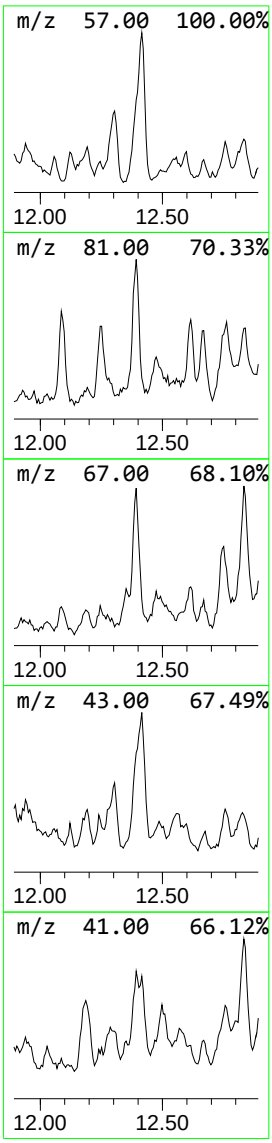
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown12.392 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	24.27 ug/l	889444	Chlorobenzene-d5	11.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, methylene-	96	C7H12	001192-37-6	38
2	n-Propyl heptyl ether	158	C10H22O	071112-89-5	30
3	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	30
4	Cycloheptene	96	C7H12	000628-92-2	25
5	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	18





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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

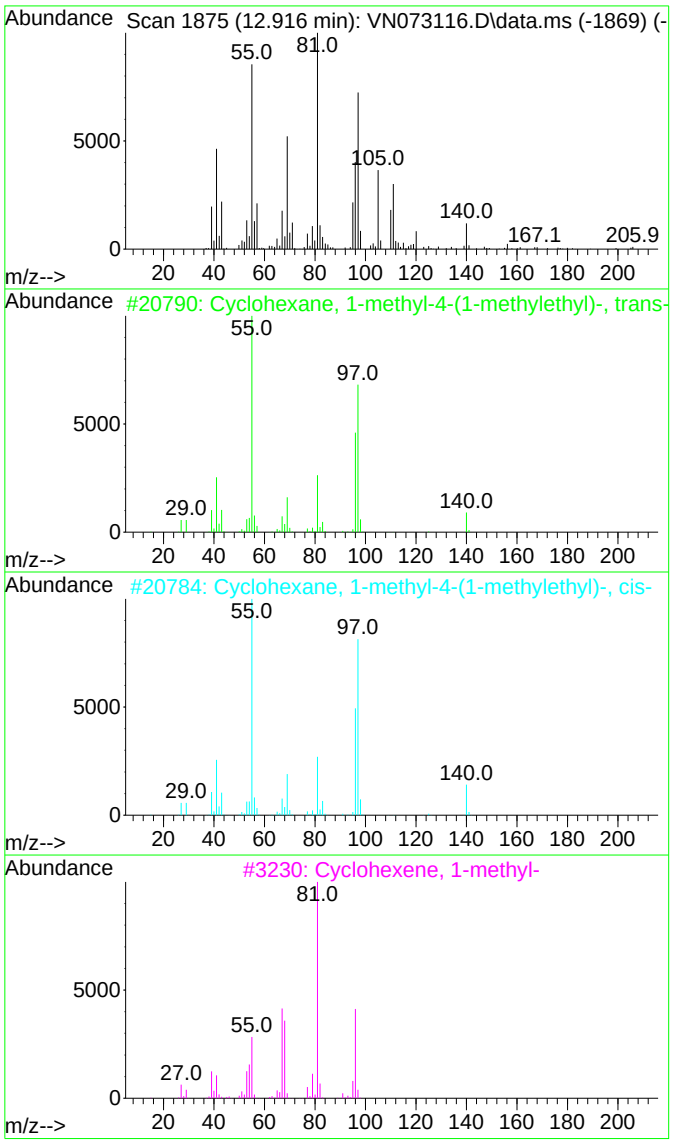
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

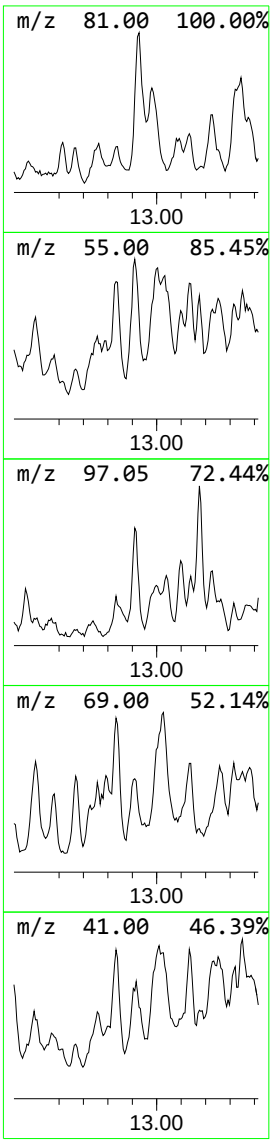
****

Peak Number 3 unknown12.916 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	16.09 ug/l	776093	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	46
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	46
3	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	43
4	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	38
5	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

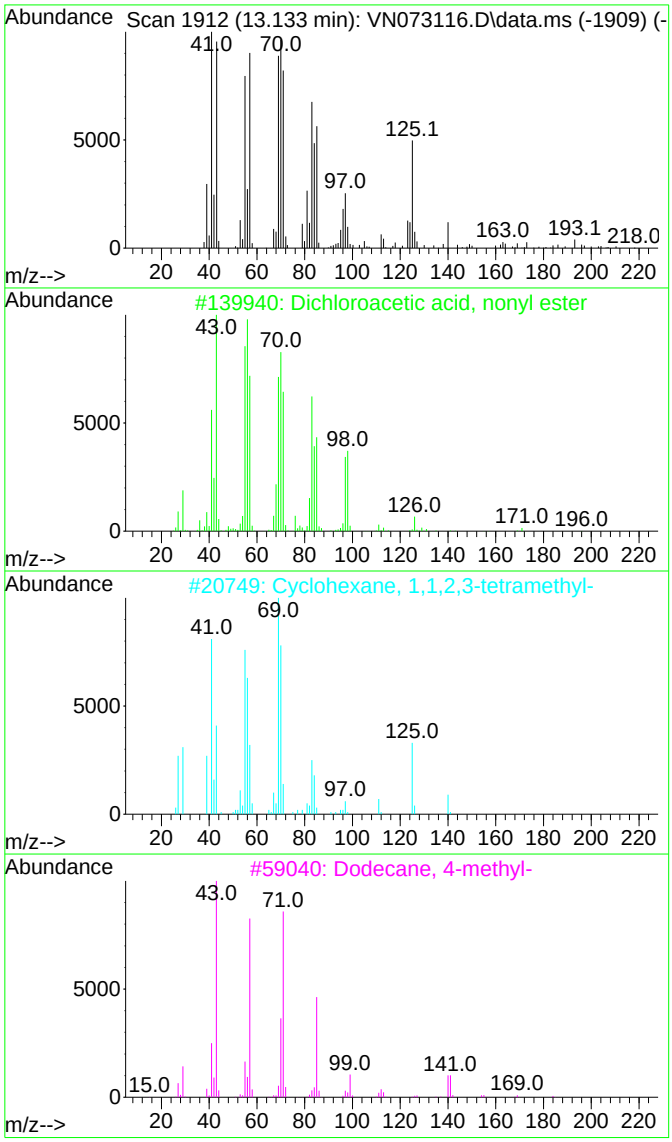
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

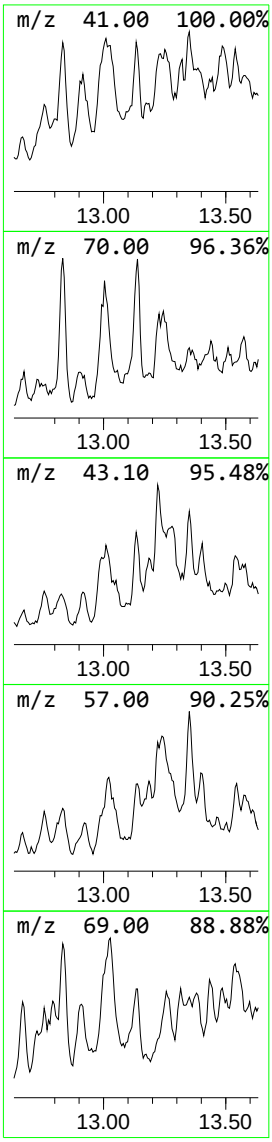
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Dichloroacetic acid, nonyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.133	11.06 ug/l	533352	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, nonyl ester	254	C11H20Cl2O2	083004-99-3	72
2	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	43
3	Dodecane, 4-methyl-	184	C13H28	006117-97-1	30
4	3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	25
5	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

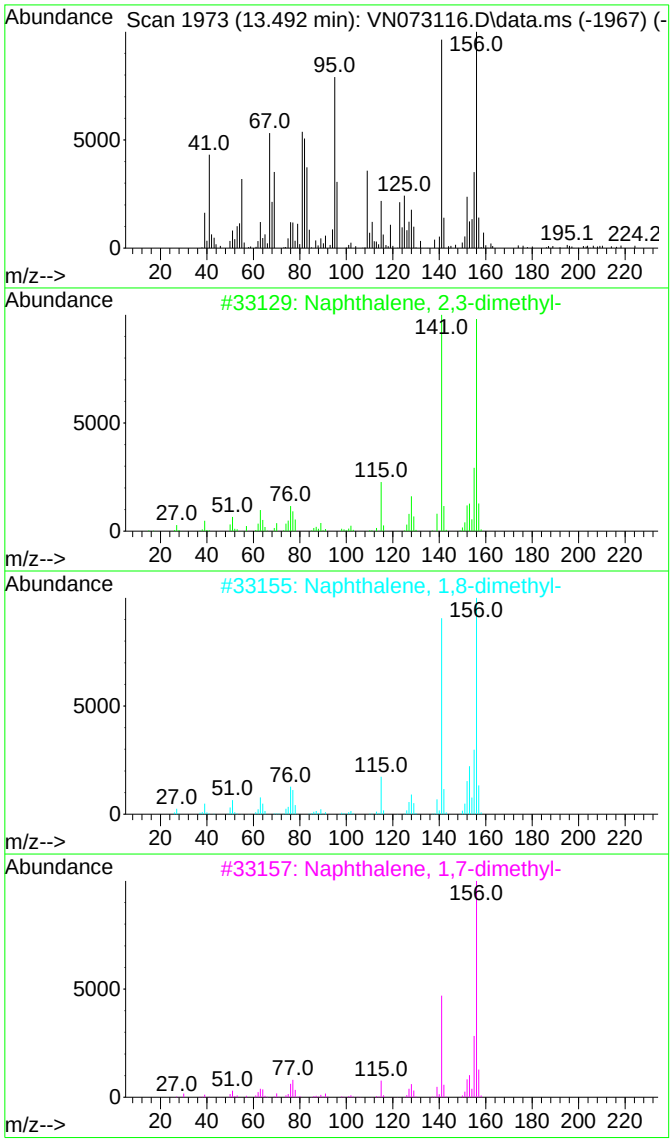
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

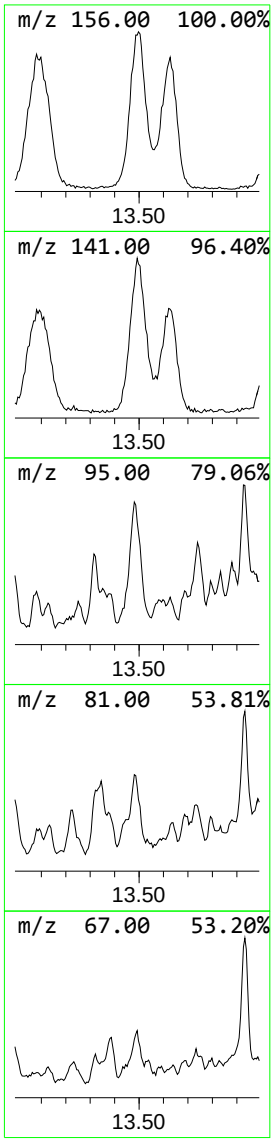
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	15.70 ug/l	757351	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
2	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	94
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	89
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	89
5	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	89





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

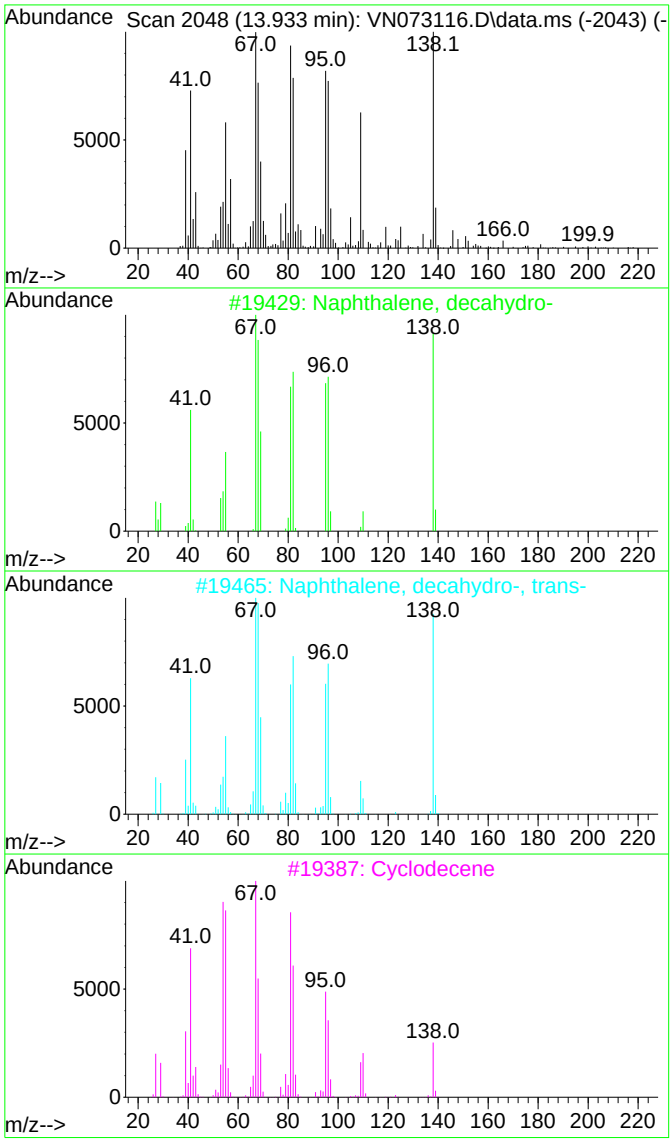
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

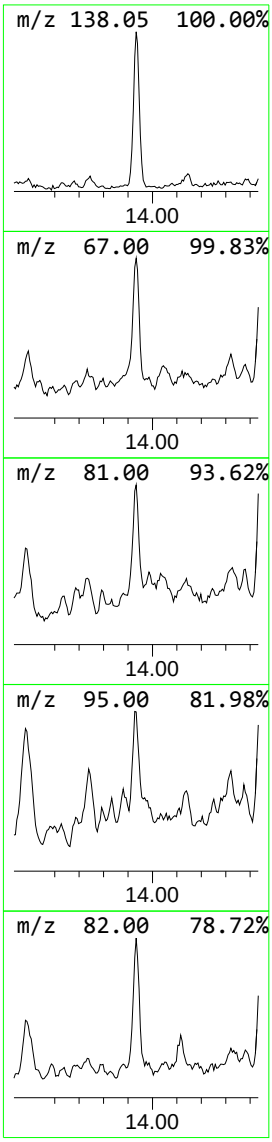
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, decahydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	31.35 ug/l	1512080	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	90
3	Cyclodecene	138	C10H18	003618-12-0	87
4	Spiro[4.5]decane	138	C10H18	000176-63-6	81
5	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	74





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Operator : JC\MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

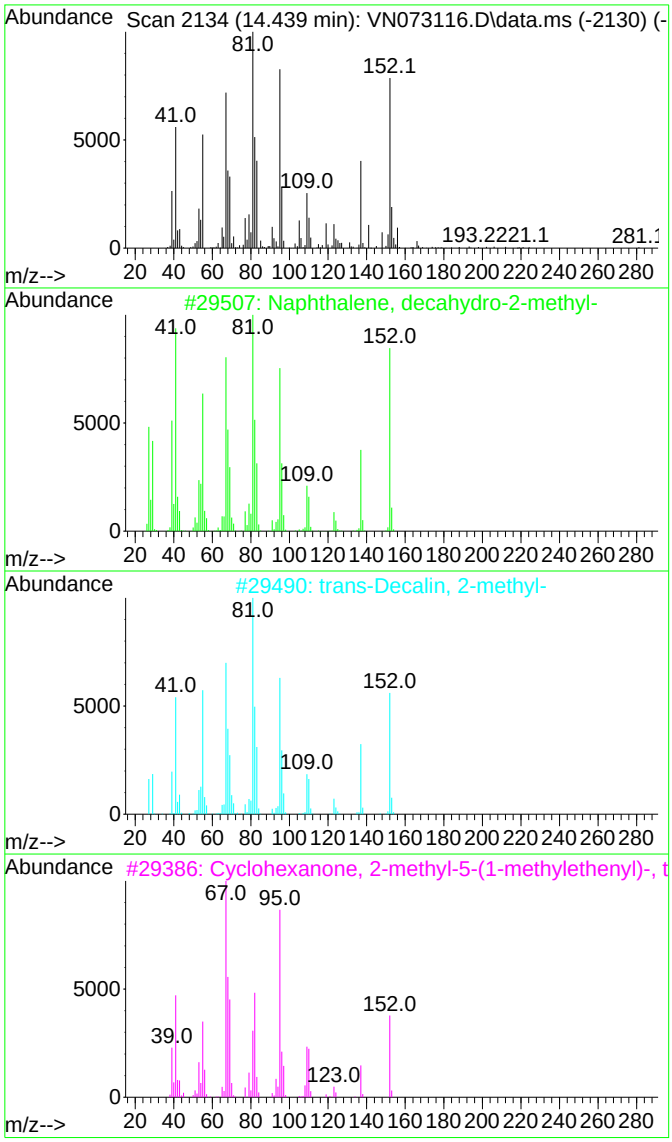
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

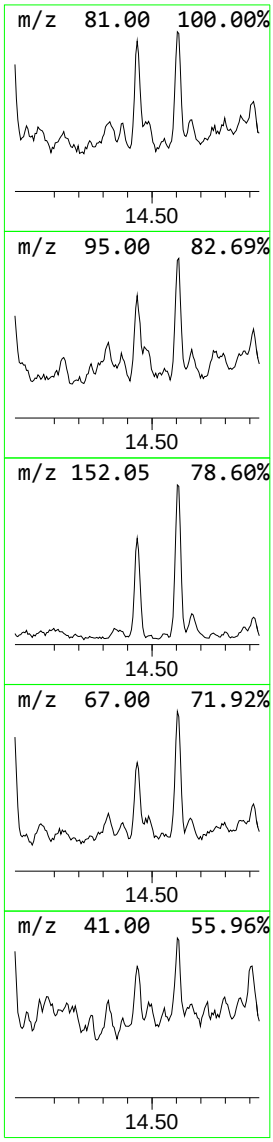
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, decahydro-2-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	19.11 ug/l	921510	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	94
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	87
3	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	60
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	53
5	1-Adamantanol	152	C10H16O	000768-95-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

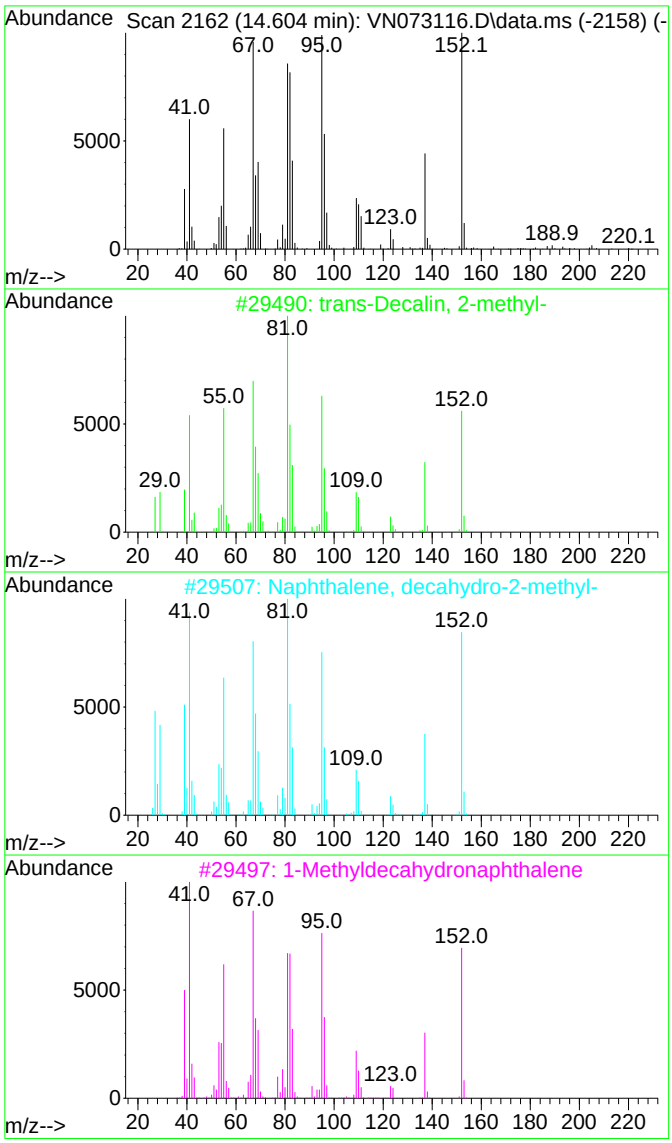
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

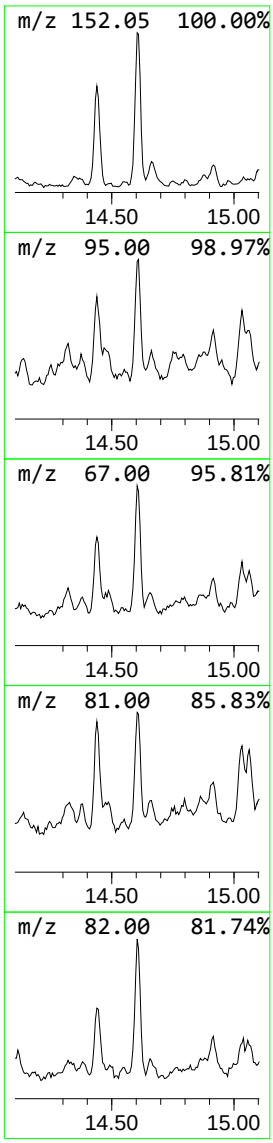
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 trans-Decalin, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.604	19.21 ug/l	926549	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
3	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	90
4	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	76
5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	58





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Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

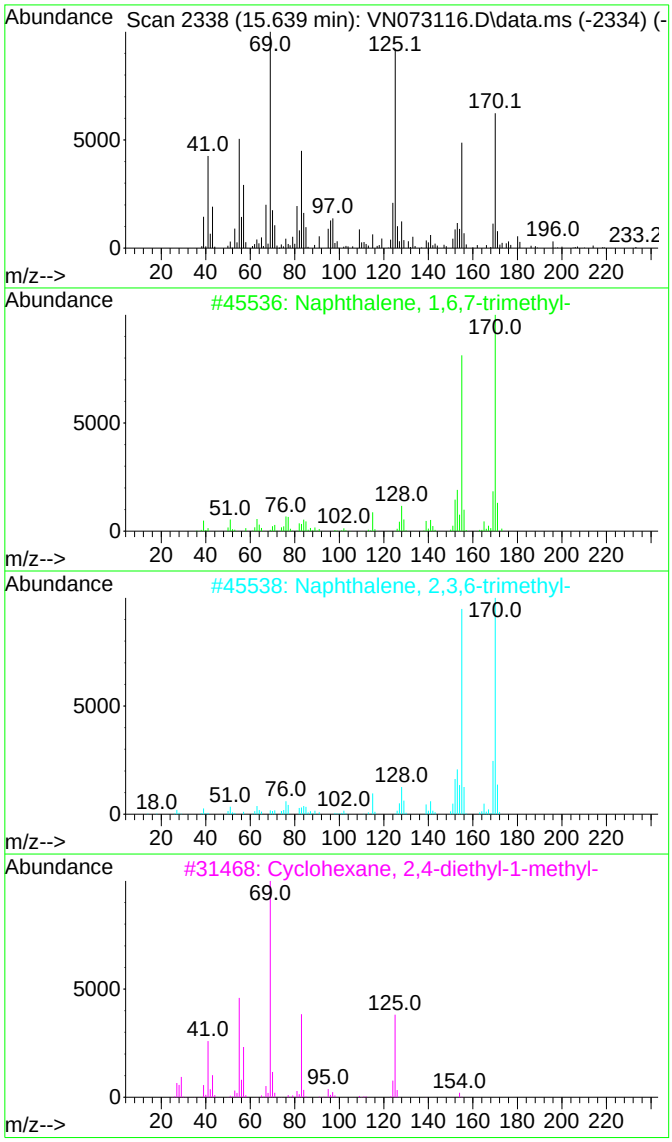
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

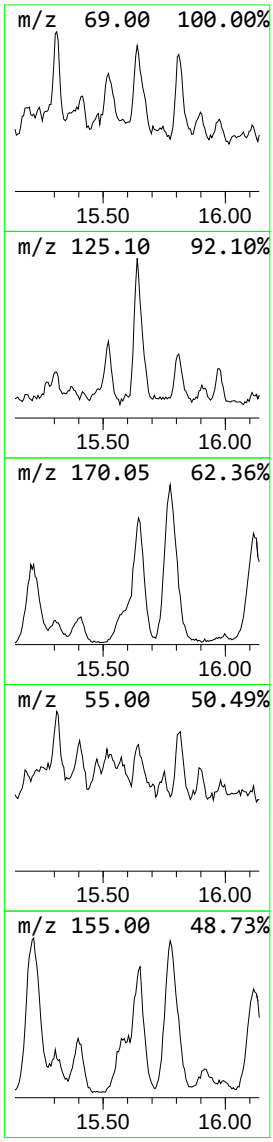
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,6,7-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	25.67 ug/l	1238090	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	92
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	78
3	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	64
4	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	52
5	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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

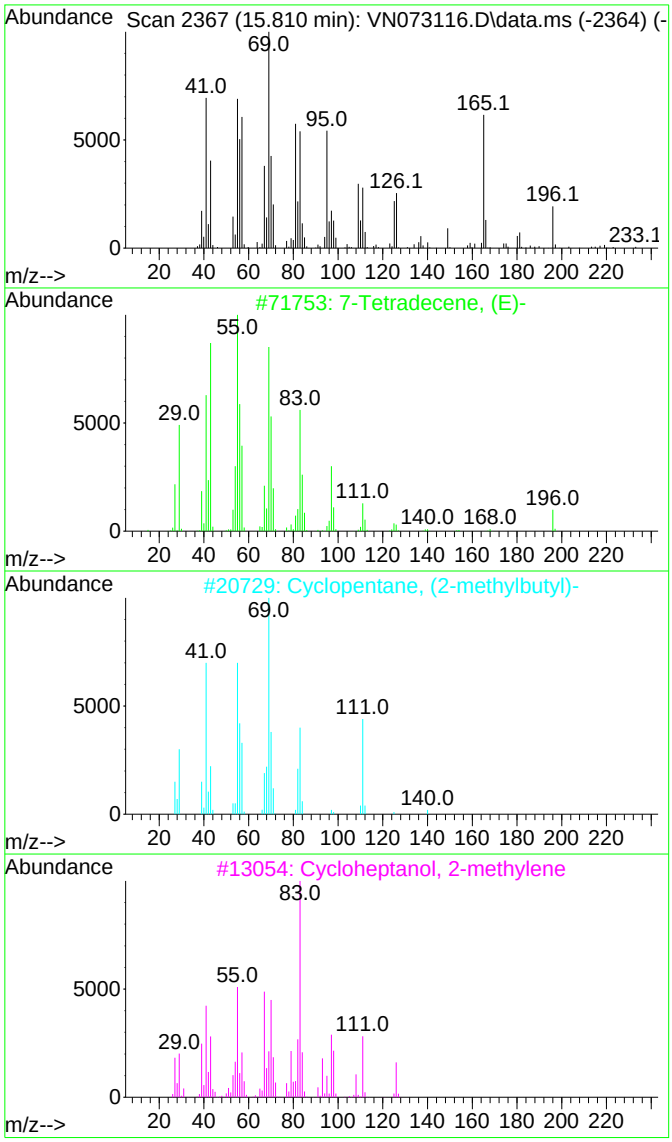
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

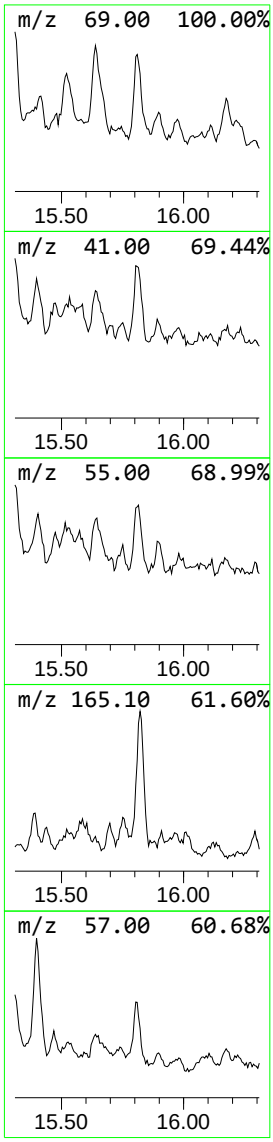
****

Peak Number 10 unknown15.810 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.810	23.01 ug/l	1109610	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tetradecene, (E)-	196	C14H28	041446-63-3	49
2	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	41
3	Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	38
4	Cyclopropane, 1,1-dimethyl-2-nonyl-	196	C14H28	041977-38-2	38
5	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
Data File : VN073116.D
Acq On : 25 Jun 2022 17:32
Operator : JC\MD
Sample : N3455-17
Misc : 3.90g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SP-EXC-2-3

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3,5-Dimethyl-3-...	12.186	20.3	ug/l	743696	3	11.680	1832540	50.0
unknown12.392	12.392	24.3	ug/l	889444	3	11.680	1832540	50.0
unknown12.916	12.916	16.1	ug/l	776093	4	13.610	2411470	50.0
Dichloroacetic ...	13.133	11.1	ug/l	533352	4	13.610	2411470	50.0
Naphthalene, 2,...	13.492	15.7	ug/l	757351	4	13.610	2411470	50.0
Naphthalene, de...	13.933	31.4	ug/l	1512080	4	13.610	2411470	50.0
Naphthalene, de...	14.439	19.1	ug/l	921510	4	13.610	2411470	50.0
trans-Decalin, ...	14.604	19.2	ug/l	926549	4	13.610	2411470	50.0
Naphthalene, 1,...	15.639	25.7	ug/l	1238090	4	13.610	2411470	50.0
unknown15.810	15.810	23.0	ug/l	1109610	4	13.610	2411470	50.0