LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032425\
Data File : VN086076.D
Acq On : 24 Mar 2025 16:49
Operator : JC\MD
Sample : Q1606-09
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

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\82N031825W.M
Title : SW846 8260

Signal : TIC: VN086076.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.889	138	159	162	rBV6	23469	127938	5.89%	0.587%
2	8.159	1044	1055	1060	rBV	136612	335806	15.47%	1.541%
3	8.218	1060	1065	1076	rVB	233686	508252	23.41%	2.332%
4	8.571	1116	1125	1135	rBV2	139688	316860	14.59%	1.454%
5	8.782	1159	1161	1178	rVB3	7443	22717	1.05%	0.104%
6	9.094	1206	1214	1225	rBV	332245	676558	31.16%	3.104%
7	10.565	1454	1464	1472	rBV	502296	917211	42.24%	4.209%
8	11.865	1676	1685	1698	rBV	441961	794561	36.59%	3.646%
9	12.476	1783	1789	1795	rVB2	20011	33003	1.52%	0.151%
10	12.588	1795	1808	1819	rBV4	18286	75748	3.49%	0.348%
11	12.729	1825	1832	1835	rBV6	12296	25148	1.16%	0.115%
12	12.764	1835	1838	1845	rVB4	18807	31945	1.47%	0.147%
13	12.847	1845	1852	1860	rBV	354918	612027	28.19%	2.808%
14	13.017	1877	1881	1887	rVB5	21996	41771	1.92%	0.192%
15	13.088	1887	1893	1898	rBV6	16842	38842	1.79%	0.178%
16	13.170	1899	1907	1912	rVV5	41450	106985	4.93%	0.491%
17	13.223	1913	1916	1921	rVB3	24725	39126	1.80%	0.180%
18	13.311	1921	1931	1934	rBV4	35380	68581	3.16%	0.315%
19	13.359	1934	1939	1940	rVV2	38045	49647	2.29%	0.228%
20	13.394	1941	1945	1950	rVV	115920	190412	8.77%	0.874%
21	13.453	1951	1955	1960	rVB2	39350	64972	2.99%	0.298%
22	13.517	1960	1966	1971	rBV3	58111	107507	4.95%	0.493%
23	13.576	1971	1976	1980	rBV2	50973	79117	3.64%	0.363%
24	13.682	1986	1994	1997	rBV4	94808	203861	9.39%	0.935%
25	13.711	1997	1999	2004	rVV	79696	116812	5.38%	0.536%
26	13.788	2007	2012	2021	rVB	461444	801683	36.92%	3.679%
27	13.935	2030	2037	2042	rBV8	61346	136547	6.29%	0.627%
28	14.117	2062	2068	2072	rBV5	188321	404554	18.63%	1.856%
29	14.153	2072	2074	2079	rVV3	126785	180824	8.33%	0.830%
30	14.211	2080	2084	2088	rVV3	136196	231224	10.65%	1.061%
31	14.258	2088	2092	2096	rVV2	160589	308545	14.21%	1.416%
32	14.317	2099	2102	2106	rVV4	162639	312870	14.41%	1.436%
33	14.364	2107	2110	2116	rVB	202933	308431	14.21%	1.415%
34	14.423	2116	2120	2126	rBV8	108538	213487	9.83%	0.980%
35	14.494	2128	2132	2138	rBV6	127160	240300	11.07%	1.103%
36	14.576	2139	2146	2148	rBV5	92964	185323	8.54%	0.850%

LSC Area Percent Report

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Operator : JC\MD
Sample : Q1606-09
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

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\82N031825W.M
Title : SW846 8260

37	14.623	2149	2154	2163	rVB4	388849	702601	32.36%	3.224%
38	14.729	2168	2172	2175	rBV5	94457	154248	7.10%	0.708%
39	14.794	2175	2183	2187	rBV6	254104	484946	22.33%	2.225%
40	14.976	2210	2214	2218	rBV5	99963	176359	8.12%	0.809%
41	15.035	2219	2224	2227	rVV3	367069	662070	30.49%	3.038%
42	15.076	2227	2231	2241	rVB2	757182	1683115	77.52%	7.723%
43	15.223	2253	2256	2259	rVB3	116426	132727	6.11%	0.609%
44	15.264	2260	2263	2267	rBV3	143388	220129	10.14%	1.010%
45	15.311	2267	2271	2277	rVB4	296065	527893	24.31%	2.422%
46	15.435	2287	2292	2298	rBV7	296444	654305	30.13%	3.002%
47	15.588	2313	2318	2327	rVB	1188462	2171268	100.00%	9.963%
48	15.682	2327	2334	2338	rBV7	223702	629852	29.01%	2.890%
49	15.788	2349	2352	2358	rVB6	224399	399119	18.38%	1.831%
50	15.941	2370	2378	2386	rBV4	393303	1416492	65.24%	6.500%
51	16.017	2387	2391	2400	rVB4	342575	815150	37.54%	3.740%
52	16.541	2476	2480	2485	rVB4	304768	557709	25.69%	2.559%
53	16.611	2486	2492	2500	rBV	757861	1496379	68.92%	6.866%

Sum of corrected areas: 21793557

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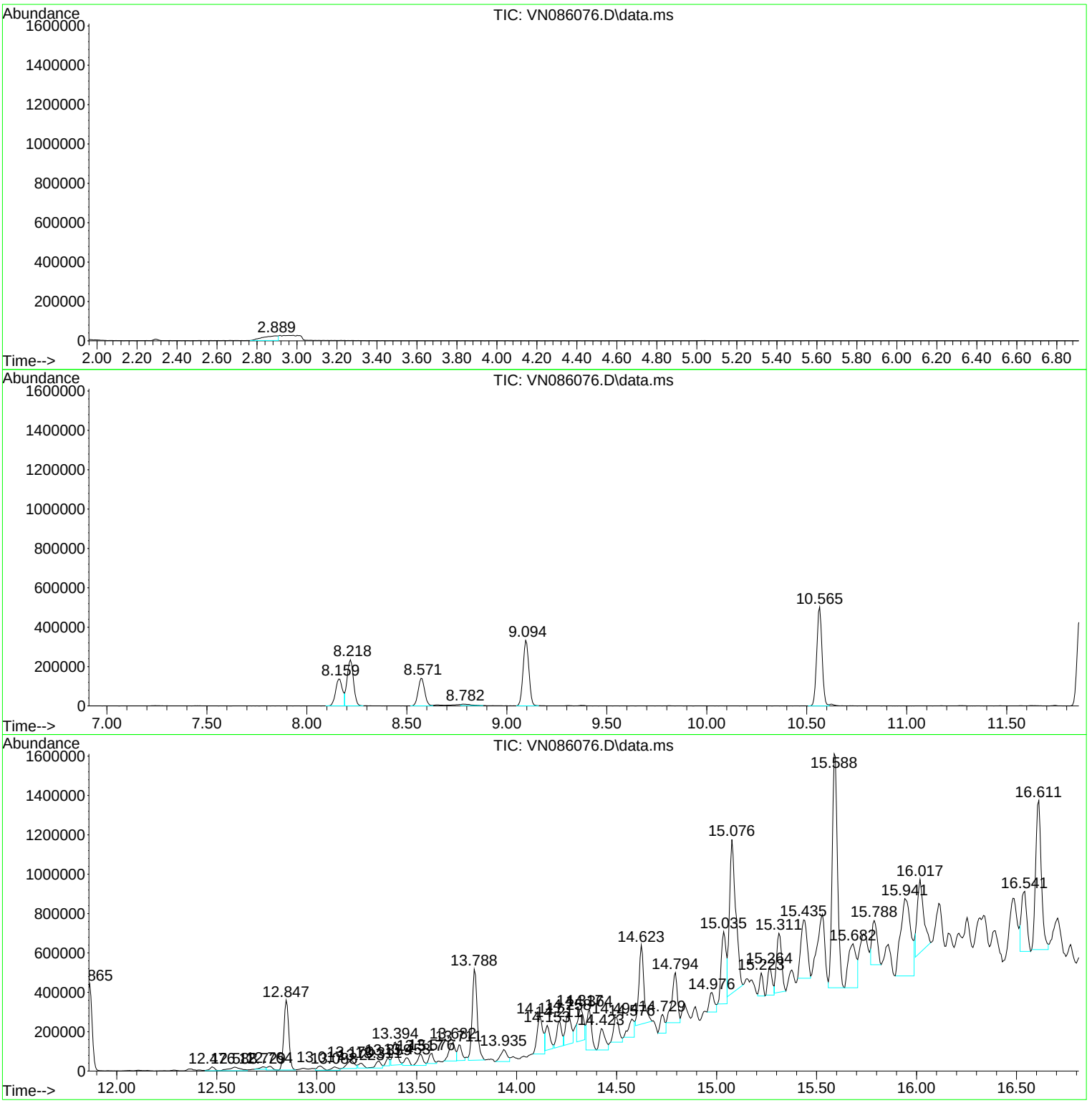
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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



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Data File : VN086076.D
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Operator : JC\MD
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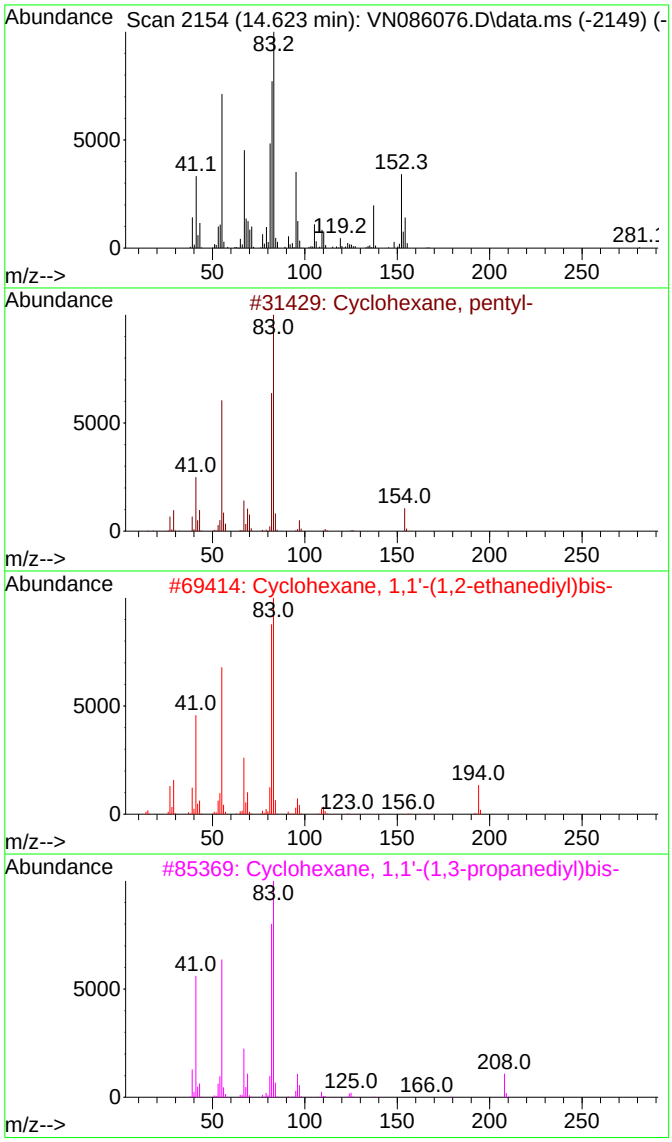
Quant Title : SW846 8260

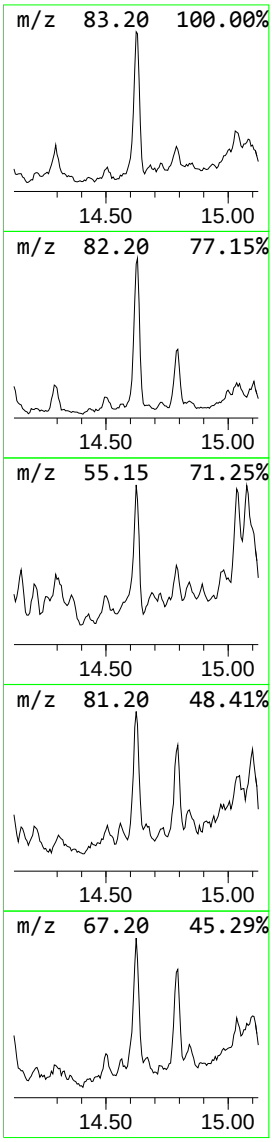
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, pentyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.623	43.82 ug/l	702601	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	53
2	Cyclohexane, 1,1'-(1,2-ethanediy...	194	C14H26	003321-50-4	47
3	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	47
4	(E)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	120603-00-1	43
5	(Z)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	067883-79-8	43





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Operator : JC\MD
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Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

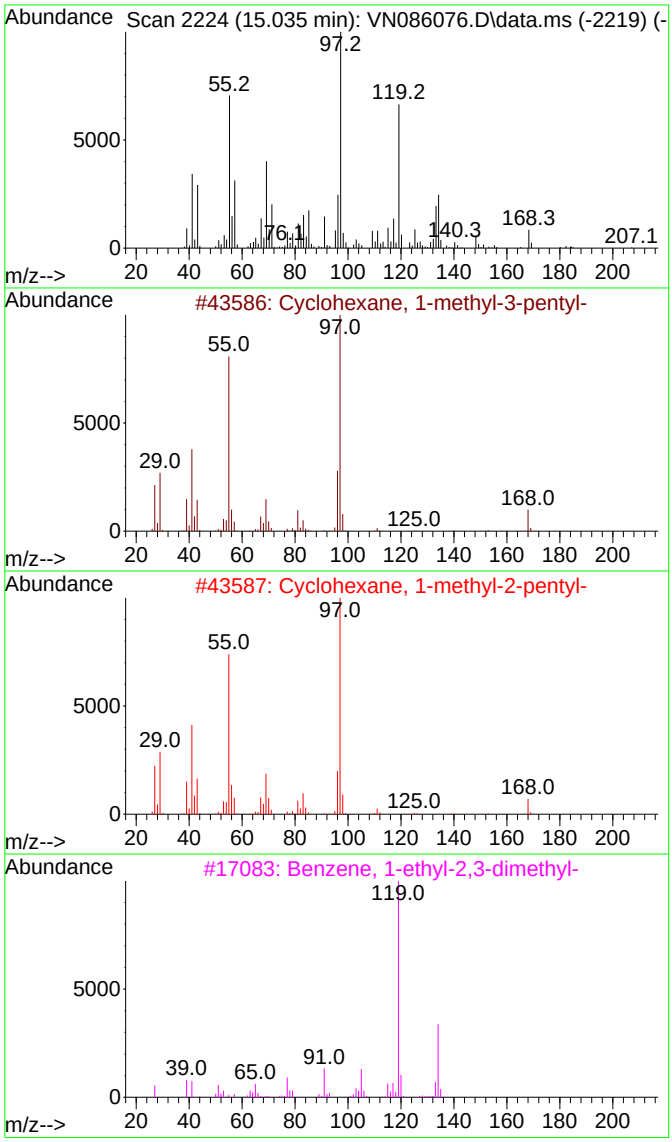
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

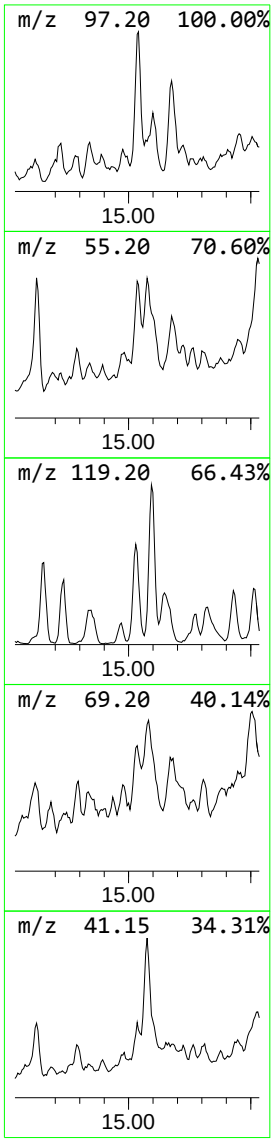
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown15.035 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.035	41.29 ug/l	662070	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	38
2	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	38
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	35
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	35
5	o-Cymene	134	C10H14	000527-84-4	35





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Operator : JC\MD
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

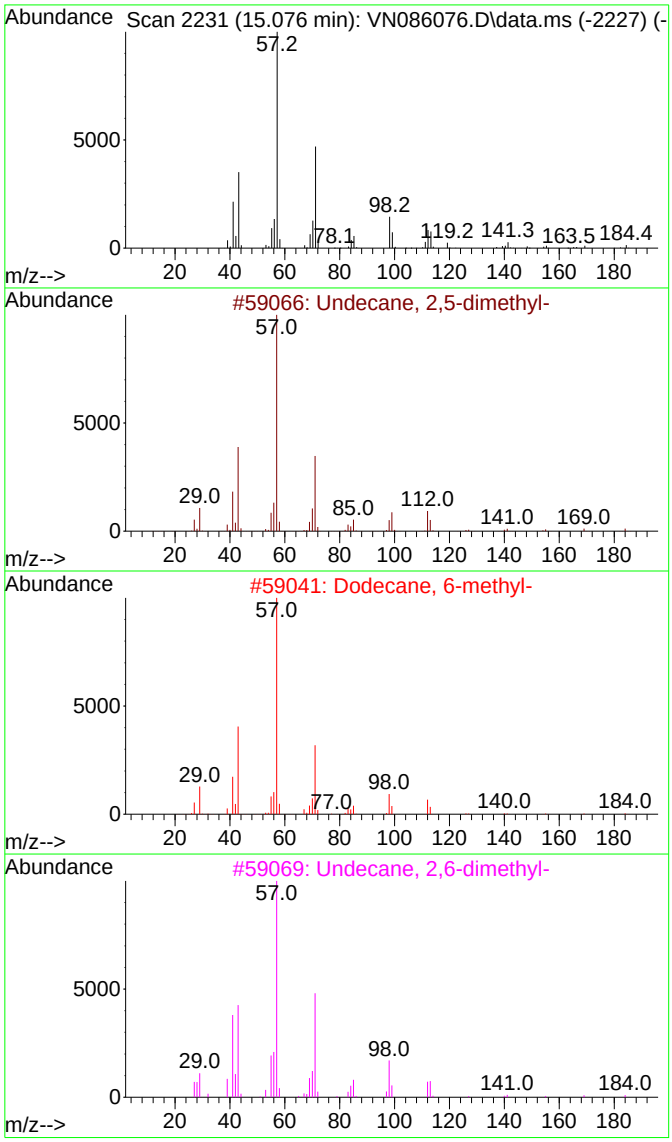
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

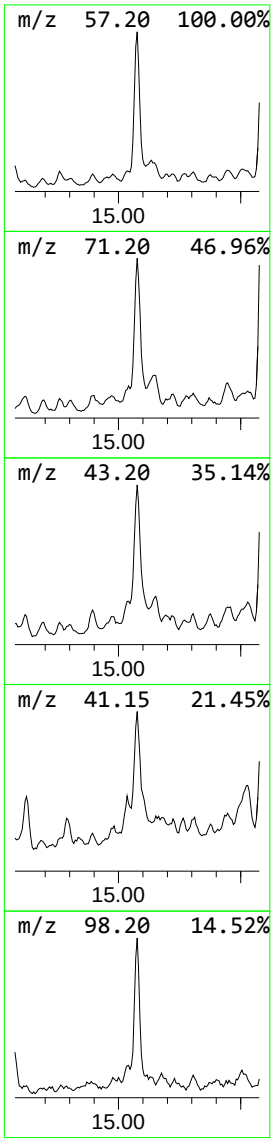
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Undecane, 2,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.076	104.97 ug/l	1683120	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	93
2	Dodecane, 6-methyl-	184	C13H28	006044-71-9	81
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	78
4	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	72
5	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	64





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Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

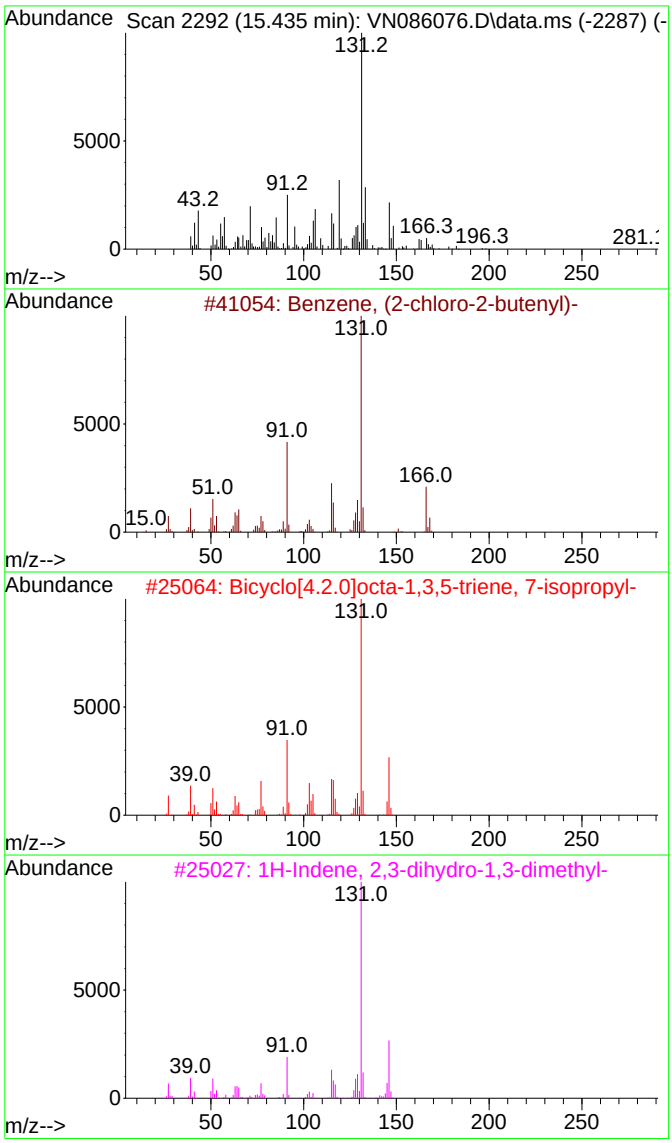
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

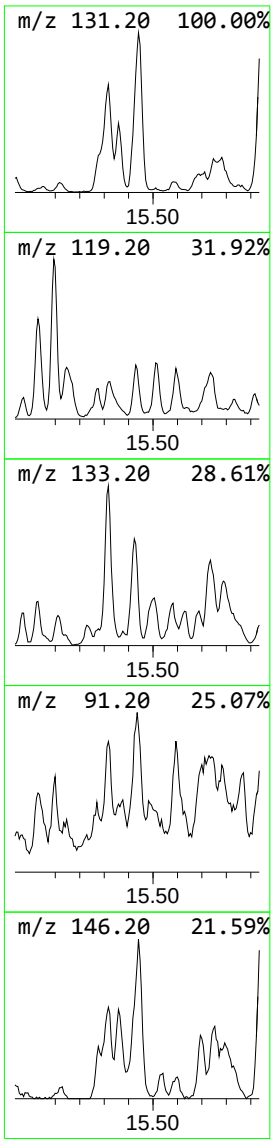
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (2-chloro-2-butenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.435	40.81 ug/l	654305	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	91
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	70
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
4	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	70





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Instrument :
MSVOA_N
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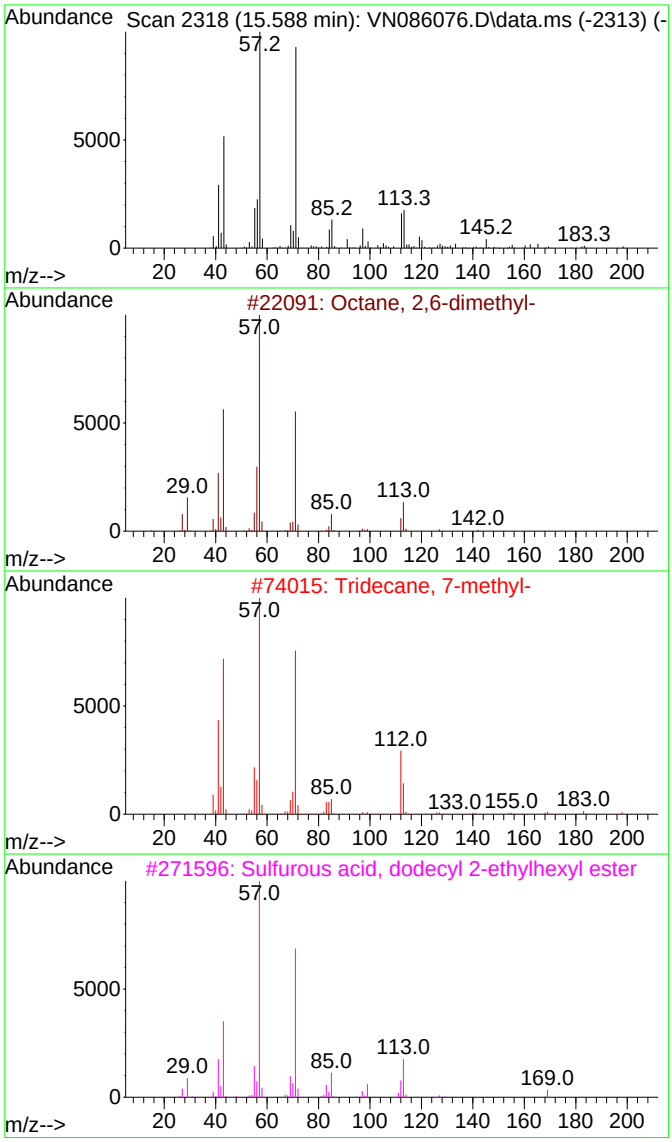
Quant Title : SW846 8260

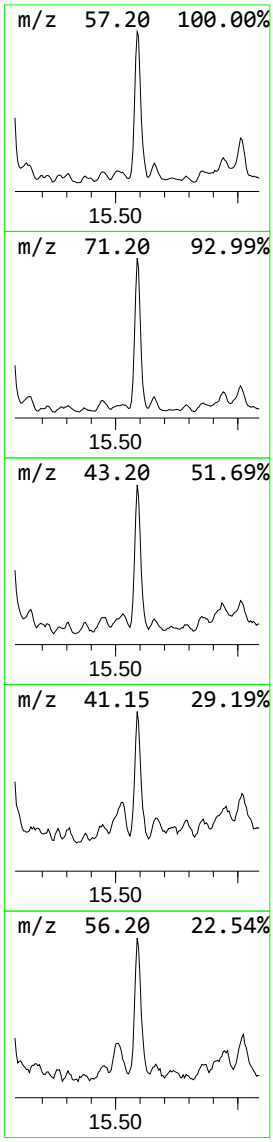
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.588	135.42 ug/l	2171270	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	80
2	Tridecane, 7-methyl-	198	C14H30	026730-14-3	68
3	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	59
4	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	59
5	2-Bromo-6-methylheptane	192	C8H17Br	004730-24-9	59





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

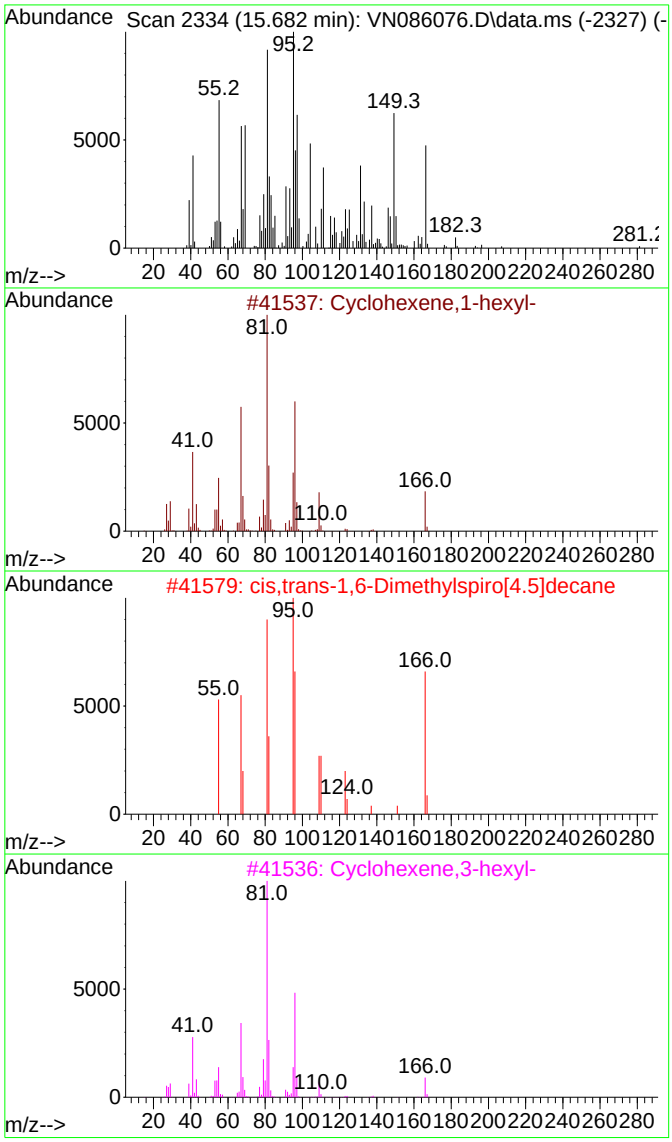
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

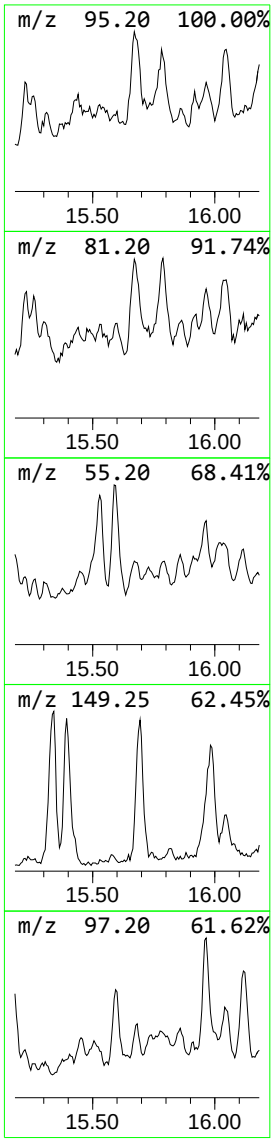
****

Peak Number 6 unknown15.682 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.682	39.28 ug/l	629852	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	42
2	cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	42
3	Cyclohexene,3-hexyl-	166	C12H22	015232-78-7	38
4	1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	35
5	Cyclohexane, ethenyl-	110	C8H14	000695-12-5	15





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ClientSampleId :
CHRT28607

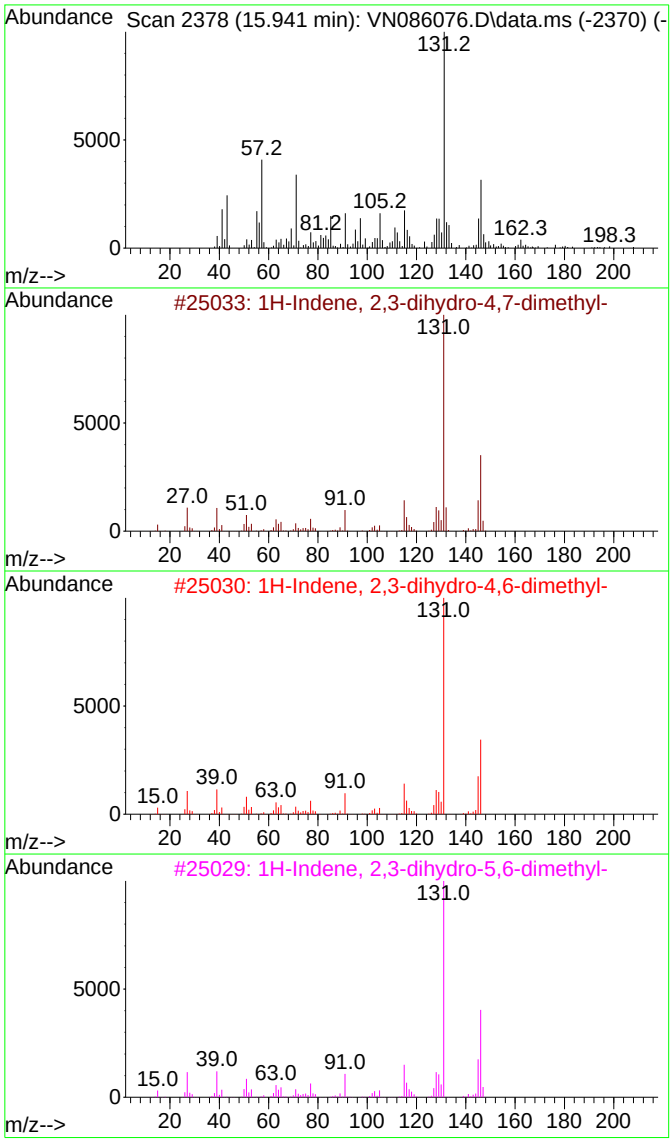
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

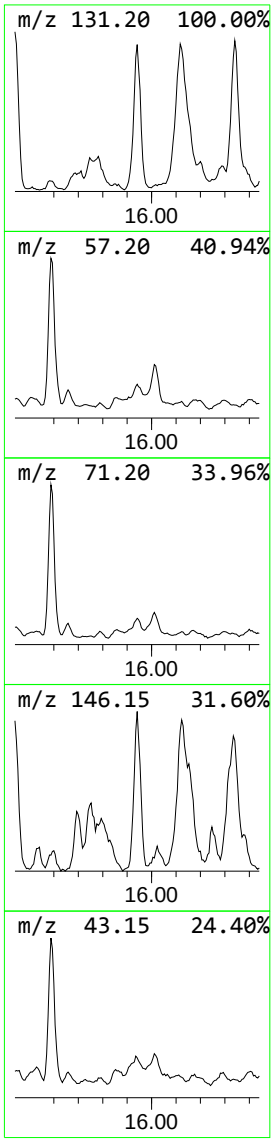
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	88.34 ug/l	1416490	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	96
2	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	93
3	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	93
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	89
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	76





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Operator : JC\MD
Sample : Q1606-09
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

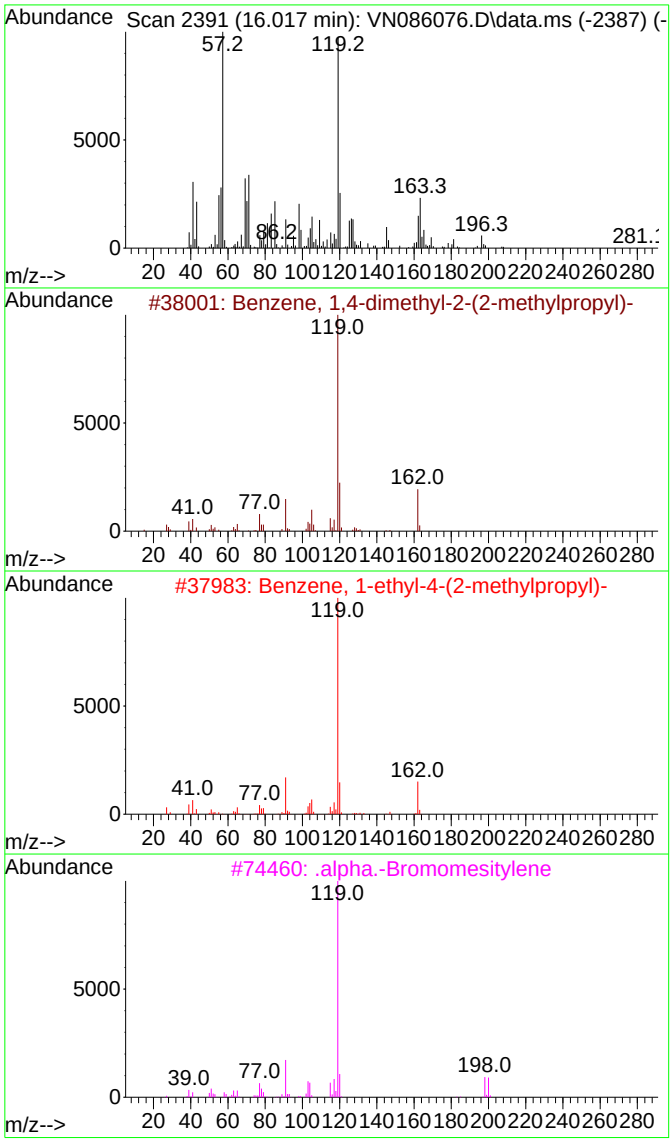
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

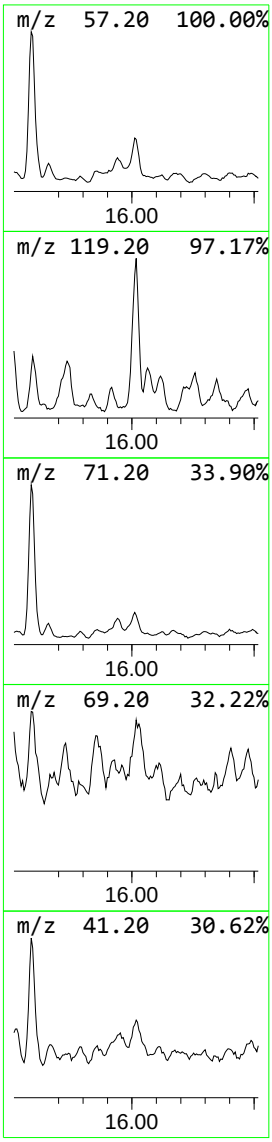
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,4-dimethyl-2-(2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.017	50.84 ug/l	815150	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-dimethyl-2-(2-methy...	162	C12H18	055669-88-0	55
2	Benzene, 1-ethyl-4-(2-methylprop...	162	C12H18	100319-40-2	43
3	.alpha.-Bromomesitylene	198	C9H11Br	027129-86-8	38
4	Succinic acid, monochloride pent...	204	C9H13ClO3	1000353-45-9	38
5	Benzene, (1,1-dimethylbutyl)-	162	C12H18	001985-57-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032425\
Data File : VN086076.D
Acq On : 24 Mar 2025 16:49
Operator : JC\MD
Sample : Q1606-09
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

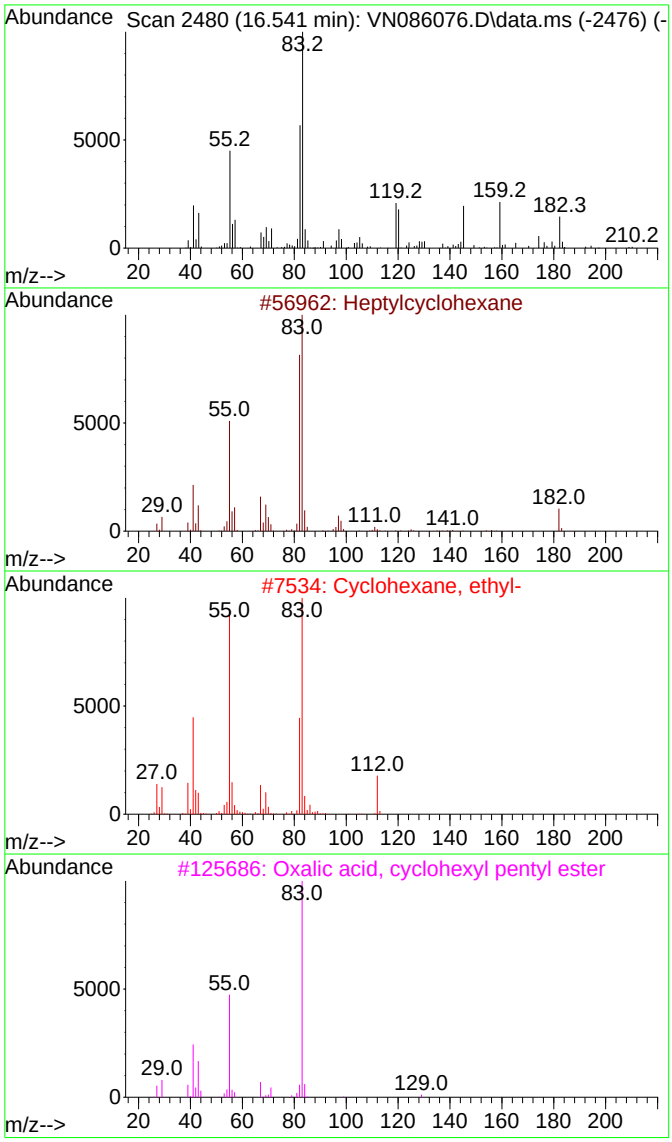
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

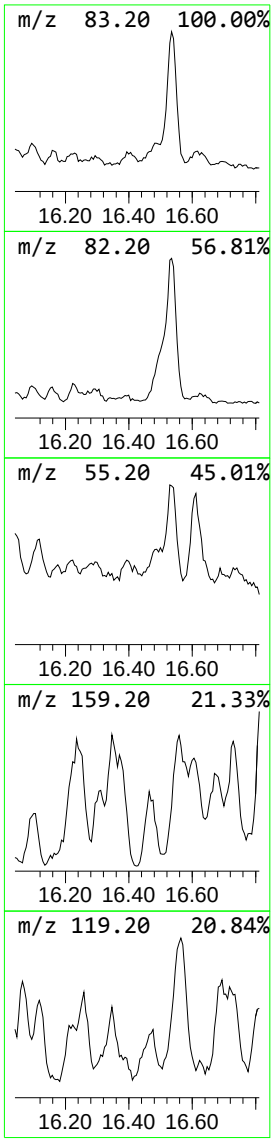
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Heptylcyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.541	34.78 ug/l	557709	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptylcyclohexane	182	C13H26	005617-41-4	60
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	43
3	Oxalic acid, cyclohexyl pentyl e...	242	C13H22O4	1000309-30-6	27
4	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	27
5	2,6-Octadiene, 2,4-dimethyl-	138	C10H18	063843-03-8	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032425\
Data File : VN086076.D
Acq On : 24 Mar 2025 16:49
Operator : JC\MD
Sample : Q1606-09
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

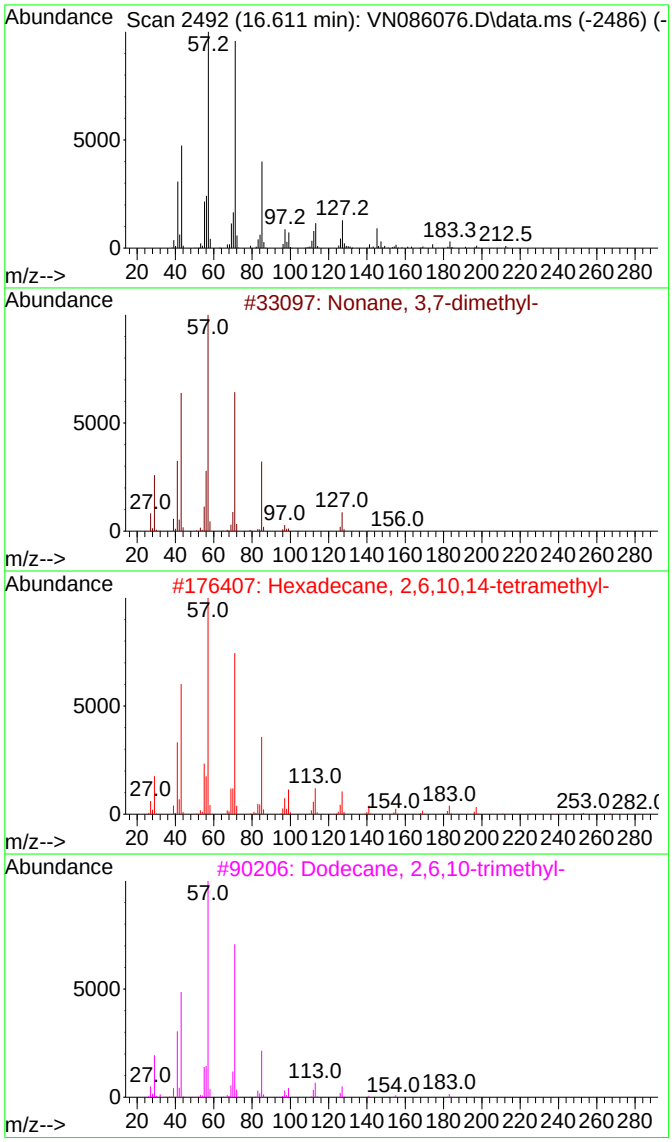
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

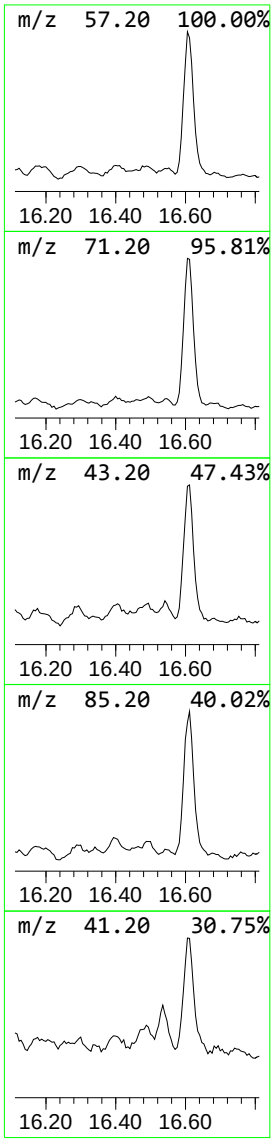
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Nonane, 3,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.611	93.33 ug/l	1496380	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032425\
Data File : VN086076.D
Acq On : 24 Mar 2025 16:49
Operator : JC\MD
Sample : Q1606-09
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHRT28607

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.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
Cyclohexane, pe...	14.623	43.8	ug/l	702601	4	13.788	801683	50.0
unknown15.035	15.035	41.3	ug/l	662070	4	13.788	801683	50.0
Undecane, 2,5-d...	15.076	105.0	ug/l	1683120	4	13.788	801683	50.0
Benzene, (2-chl...	15.435	40.8	ug/l	654305	4	13.788	801683	50.0
Octane, 2,6-dim...	15.588	135.4	ug/l	2171270	4	13.788	801683	50.0
unknown15.682	15.682	39.3	ug/l	629852	4	13.788	801683	50.0
1H-Indene, 2,3-...	15.941	88.3	ug/l	1416490	4	13.788	801683	50.0
Benzene, 1,4-di...	16.017	50.8	ug/l	815150	4	13.788	801683	50.0
Heptylcyclohexane	16.541	34.8	ug/l	557709	4	13.788	801683	50.0
Nonane, 3,7-dim...	16.611	93.3	ug/l	1496380	4	13.788	801683	50.0