LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086310.D
Acq On : 16 Apr 2025 20:28
Operator : JC\MD
Sample : Q1791-12 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

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\82N041525W.M
Title : SW846 8260

Signal : TIC: VN086310.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.806	140	145	151	rVB	9017	22085	1.53%	0.125%
2	4.430	408	421	430	rBV2	21274	66227	4.60%	0.374%
3	7.477	930	939	950	rBV	15258	39743	2.76%	0.224%
4	8.165	1045	1056	1060	rBV	118916	286835	19.91%	1.620%
5	8.218	1060	1065	1077	rVB	246502	555536	38.56%	3.137%
6	8.577	1115	1126	1134	rBV	157659	354640	24.61%	2.003%
7	8.959	1185	1191	1199	rVB	7903	16114	1.12%	0.091%
8	9.100	1206	1215	1227	rBV	390544	801138	55.60%	4.524%
9	9.530	1280	1288	1294	rBV	17655	36275	2.52%	0.205%
10	10.441	1437	1443	1450	rBV2	16269	31328	2.17%	0.177%
11	10.565	1455	1464	1472	rVV	623519	1147174	79.62%	6.478%
12	10.653	1472	1479	1489	rVB3	11008	25556	1.77%	0.144%
13	11.194	1562	1571	1578	rBV2	13477	25662	1.78%	0.145%
14	11.865	1676	1685	1692	rBV	525575	958098	66.50%	5.410%
15	11.959	1692	1701	1706	rVB3	18622	44854	3.11%	0.253%
16	12.088	1714	1723	1729	rBV2	14003	29406	2.04%	0.166%
17	12.376	1765	1772	1781	rBV	23142	44466	3.09%	0.251%
18	12.476	1781	1789	1793	rBV3	10882	27230	1.89%	0.154%
19	12.747	1829	1835	1838	rBV4	12275	24455	1.70%	0.138%
20	12.847	1841	1852	1859	rVV2	400674	906527	62.92%	5.119%
21	12.923	1859	1865	1869	rVV3	20269	45308	3.14%	0.256%
22	12.988	1869	1876	1886	rVB3	80603	192191	13.34%	1.085%
23	13.112	1892	1897	1901	rBV2	14680	22471	1.56%	0.127%
24	13.194	1901	1911	1916	rBV	65437	168791	11.72%	0.953%
25	13.359	1935	1939	1941	rBV3	17780	23927	1.66%	0.135%
26	13.418	1941	1949	1956	rVB	369429	682303	47.36%	3.853%
27	13.482	1956	1960	1963	rBV3	30295	52131	3.62%	0.294%
28	13.535	1963	1969	1977	rBV	761574	1440803	100.00%	8.136%
29	13.641	1977	1987	1993	rVB	508634	1026682	71.26%	5.797%
30	13.706	1993	1998	2001	rBV2	50320	76114	5.28%	0.430%
31	13.753	2001	2006	2008	rBV2	100664	167481	11.62%	0.946%
32	13.788	2008	2012	2016	rBV	468163	712305	49.44%	4.022%
33	13.835	2016	2020	2024	rBV	710449	1343799	93.27%	7.588%
34	13.935	2031	2037	2041	rBV	770049	1407470	97.69%	7.948%
35	13.976	2041	2044	2046	rBV	200360	285317	19.80%	1.611%
36	14.135	2064	2071	2074	rBV3	110167	219615	15.24%	1.240%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
V1207

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\82N041525W.M
Title : SW846 8260

37	14.176	2074	2078	2089	rVB2	146699	354188	24.58%	2.000%
38	14.270	2090	2094	2095	rBV3	16767	22338	1.55%	0.126%
39	14.306	2095	2100	2102	rBV	58701	96176	6.68%	0.543%
40	14.341	2102	2106	2118	rVB2	128590	251332	17.44%	1.419%
41	14.441	2118	2123	2127	rBV	89226	139731	9.70%	0.789%
42	14.494	2127	2132	2144	rVB6	104373	304318	21.12%	1.718%
43	14.653	2148	2159	2163	rBV6	33571	91906	6.38%	0.519%
44	14.735	2167	2173	2182	rBV2	234841	464588	32.25%	2.623%
45	14.812	2184	2186	2189	rVV4	17589	20416	1.42%	0.115%
46	14.847	2189	2192	2195	rVV2	30097	49483	3.43%	0.279%
47	14.912	2199	2203	2206	rVB2	27671	33405	2.32%	0.189%
48	15.070	2225	2230	2234	rBV2	103892	177959	12.35%	1.005%
49	15.106	2234	2236	2242	rVB2	43671	62301	4.32%	0.352%
50	15.212	2242	2254	2256	rBV3	135433	377668	26.21%	2.133%
51	15.247	2257	2260	2262	rVV3	40824	55160	3.83%	0.311%
52	15.317	2268	2272	2280	rVB2	131413	324360	22.51%	1.832%
53	15.400	2280	2286	2291	rBV2	157572	312461	21.69%	1.764%
54	15.553	2300	2312	2325	rVV5	116451	550576	38.21%	3.109%
55	15.659	2325	2330	2338	rVB3	39525	74344	5.16%	0.420%
56	15.823	2354	2358	2369	rVB	112901	206243	14.31%	1.165%
57	15.941	2370	2378	2384	rVV9	18885	67525	4.69%	0.381%
58	16.017	2387	2391	2401	rVB5	28083	68145	4.73%	0.385%
59	16.300	2436	2439	2444	rBV4	14720	23900	1.66%	0.135%
60	16.400	2452	2456	2460	rBV3	18562	28923	2.01%	0.163%
61	16.453	2460	2465	2469	rBV2	22276	40993	2.85%	0.231%
62	16.535	2476	2479	2485	rVB2	39852	68884	4.78%	0.389%
63	16.606	2485	2491	2503	rVB2	62318	132121	9.17%	0.746%

Sum of corrected areas: 17709501

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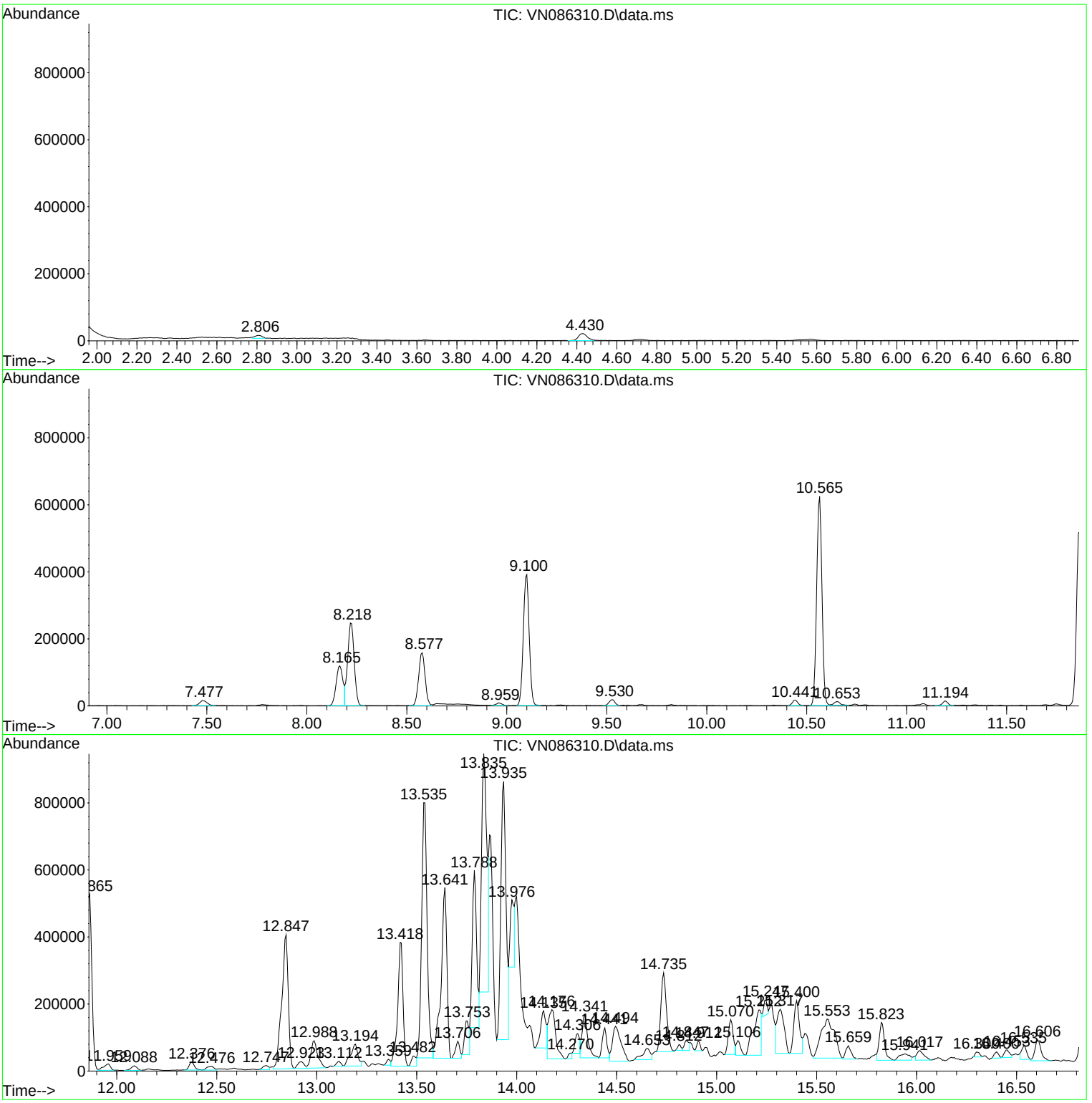
MSVOA_N
ClientSampleId :
V1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086310.D
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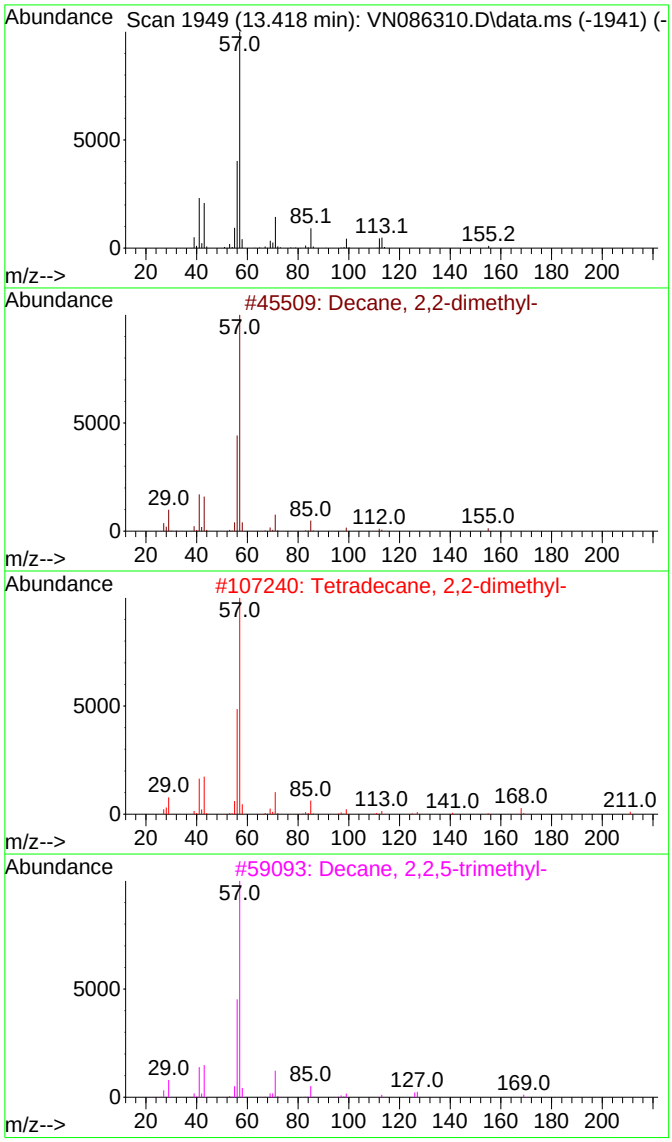
Quant Title : SW846 8260

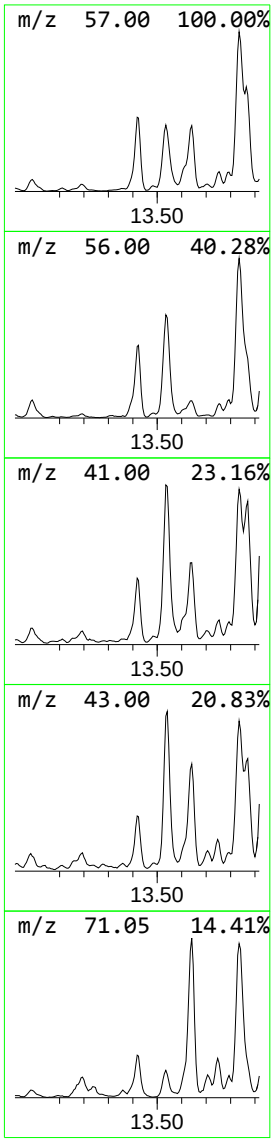
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Decane, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	47.89 ug/l	682303	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	78
2	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
3	Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	72
4	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
5	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

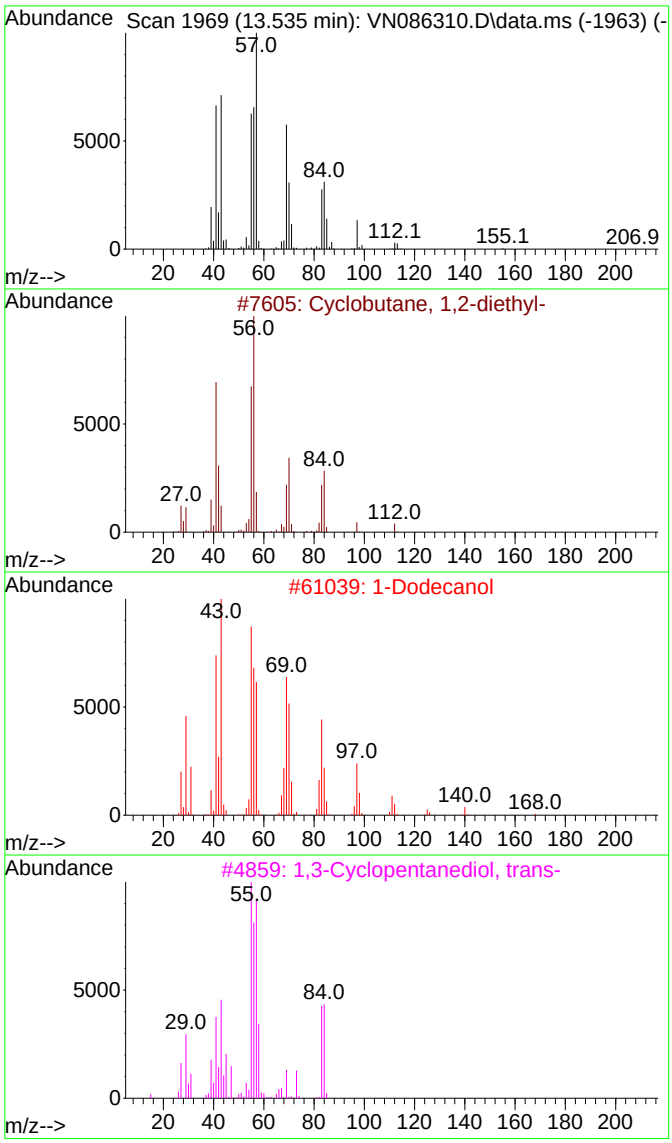
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

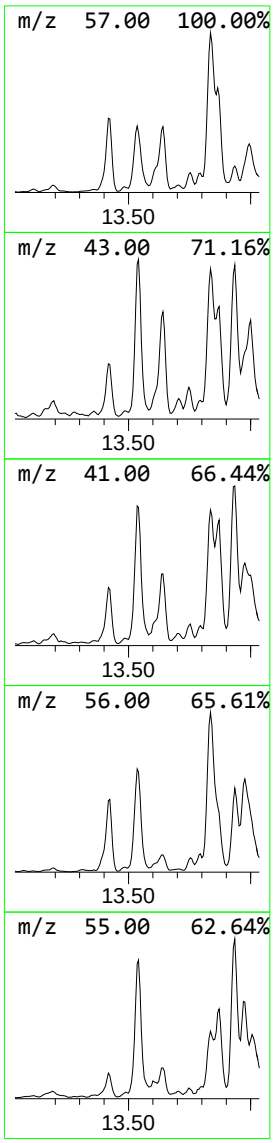
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclobutane, 1,2-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.535	101.14 ug/l	1440800	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	64
2	1-Dodecanol	186	C12H26O	000112-53-8	50
3	1,3-Cyclopentanediol, trans-	102	C5H10O2	016326-98-0	50
4	Cyclopentanone, 2,3-dimethyl-	112	C7H12O	1000151-06-7	47
5	Propanoic acid, octyl ester	186	C11H22O2	000142-60-9	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
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Operator : JC\MD
Sample : Q1791-12 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

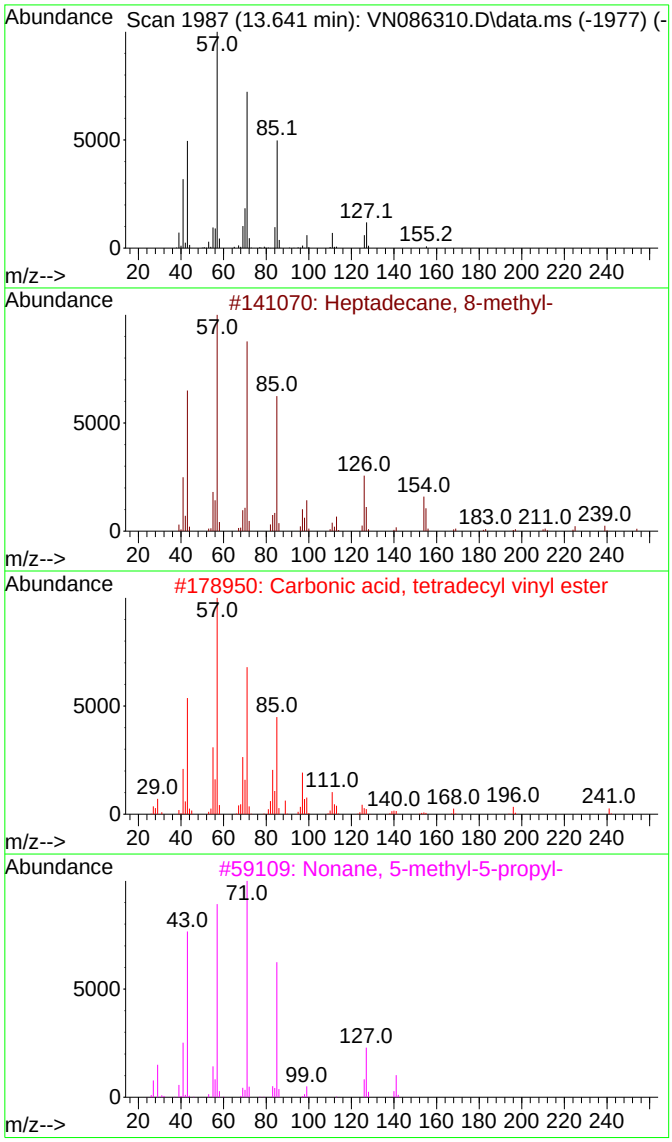
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

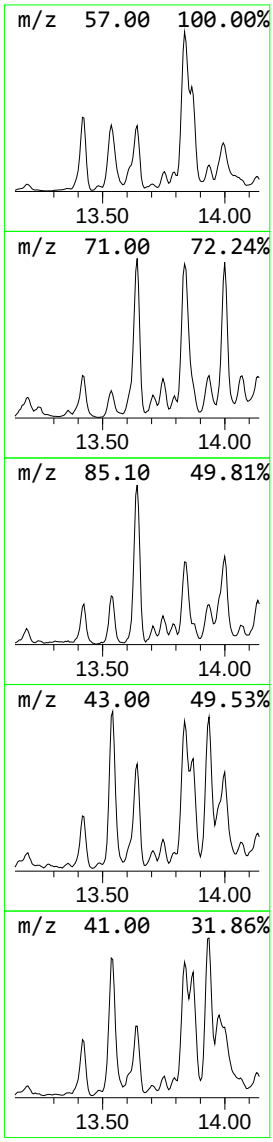
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecane, 8-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	72.07 ug/l	1026680	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	78
2	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	72
3	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	64
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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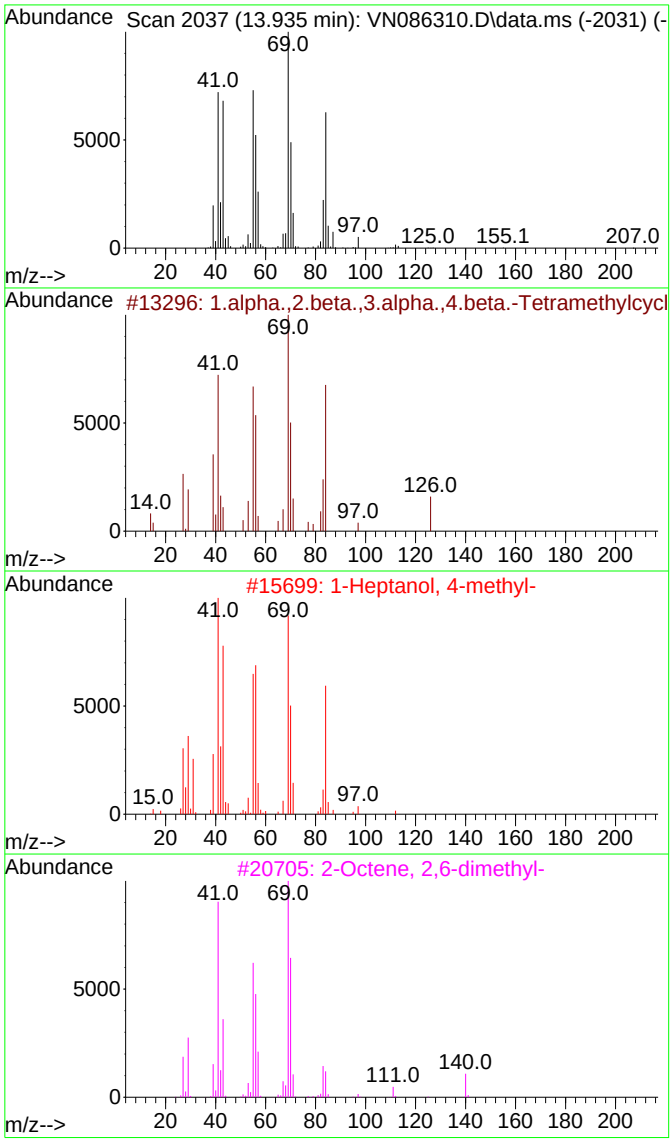
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

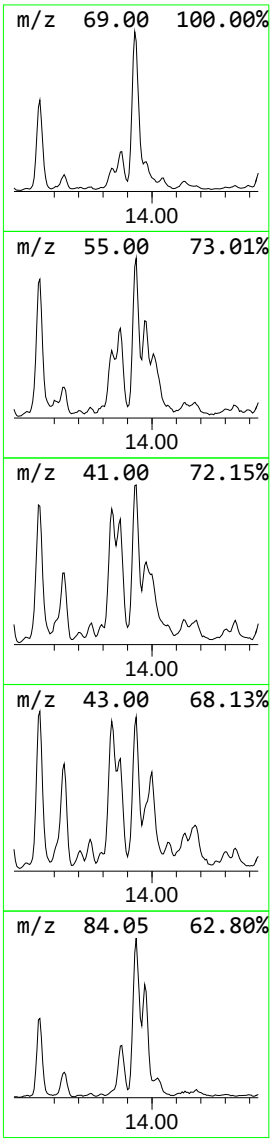
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1.alpha.,2.beta.,3.alpha.,4... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.935	98.80 ug/l	1407470	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1.alpha.,2.beta.,3.alpha.,4.beta...	126	C9H18	002532-67-4	83
2	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	78
3	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	59
4	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	59
5	Ornithine	132	C5H12N2O2	000070-26-8	50





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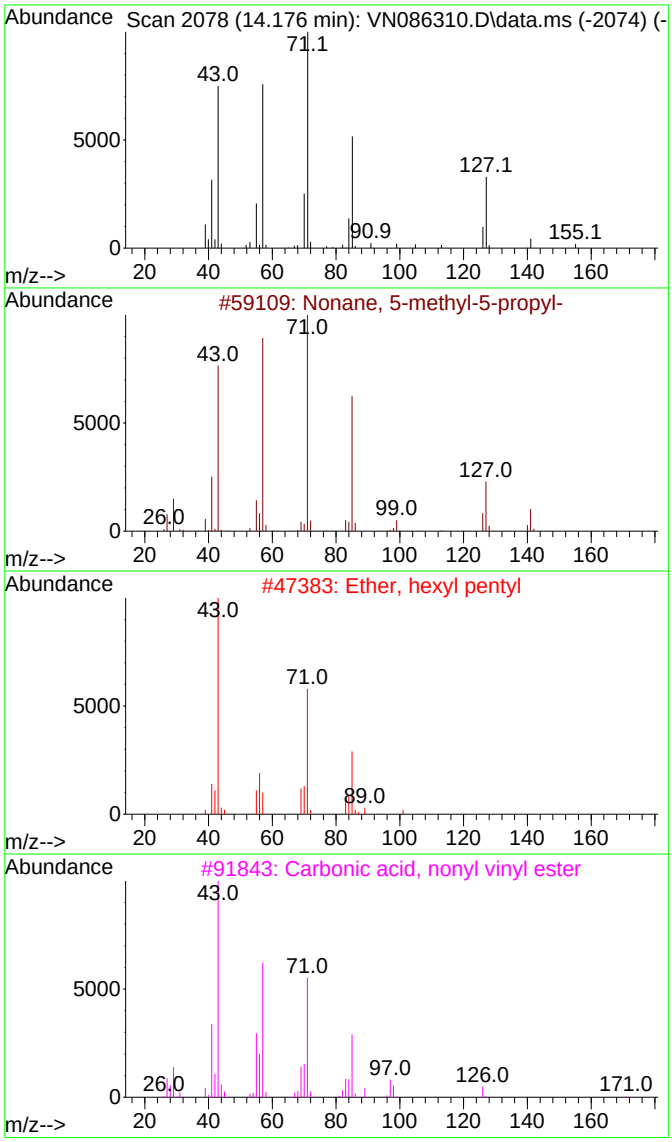
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

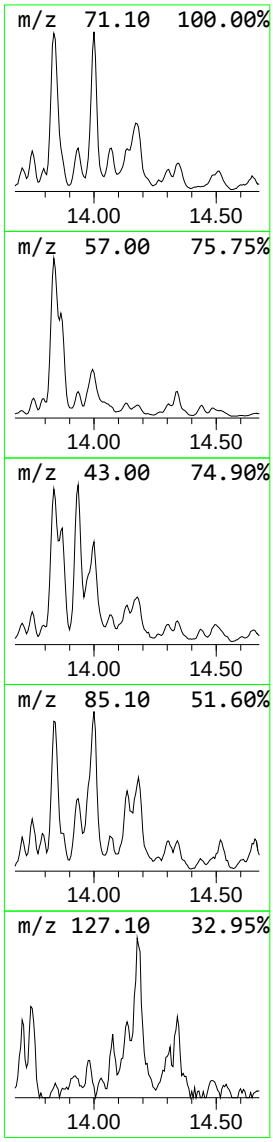
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Nonane, 5-methyl-5-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	24.86 ug/l	354188	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	72
2	Ether, hexyl pentyl	172	C11H24O	032357-83-8	64
3	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	56
4	4-Octanone	128	C8H16O	000589-63-9	53
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50





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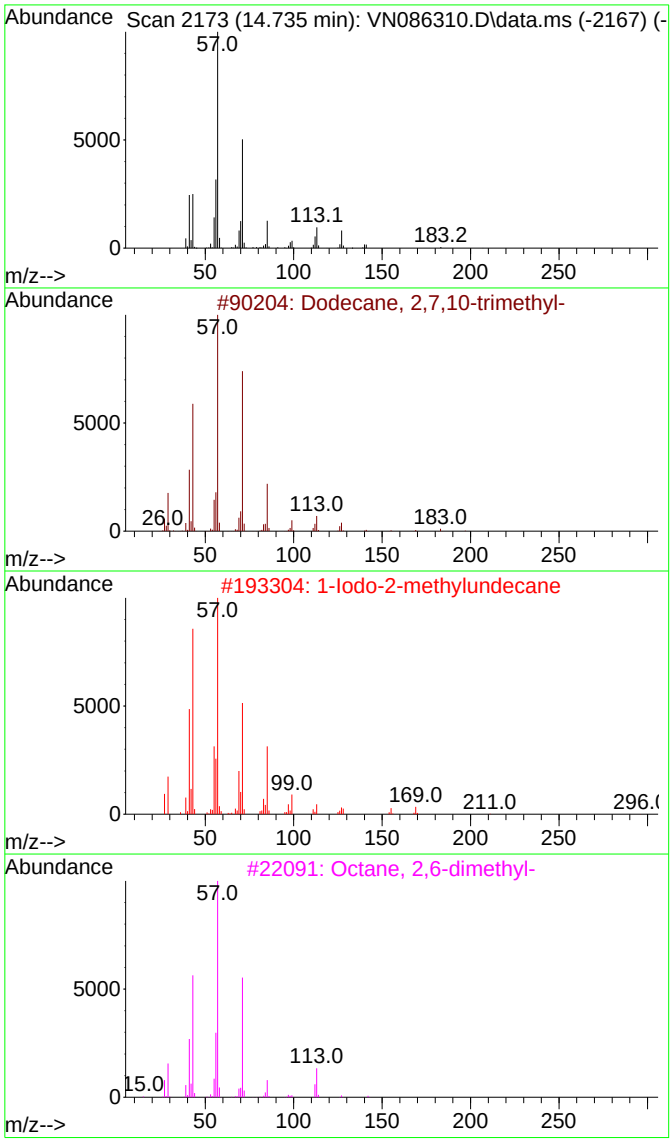
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

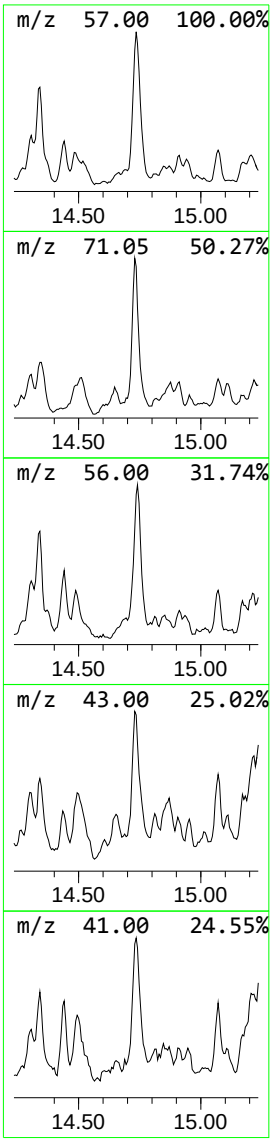
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dodecane, 2,7,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	32.61 ug/l	464588	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
4	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
5	Dodecane	170	C12H26	000112-40-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086310.D
Acq On : 16 Apr 2025 20:28
Operator : JC\MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

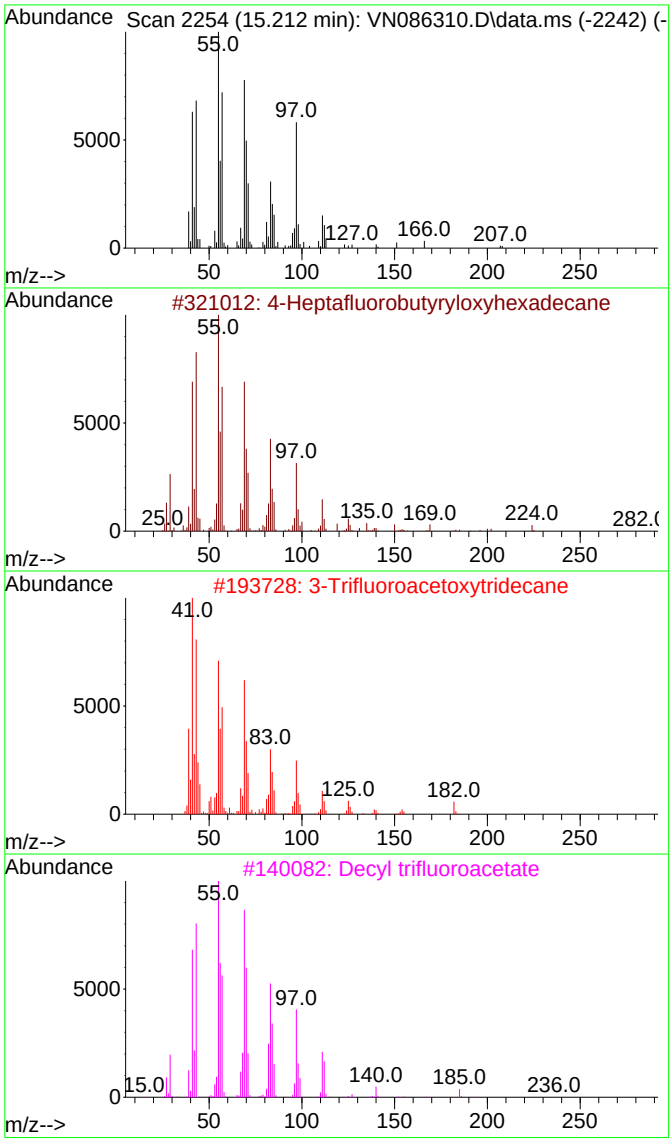
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

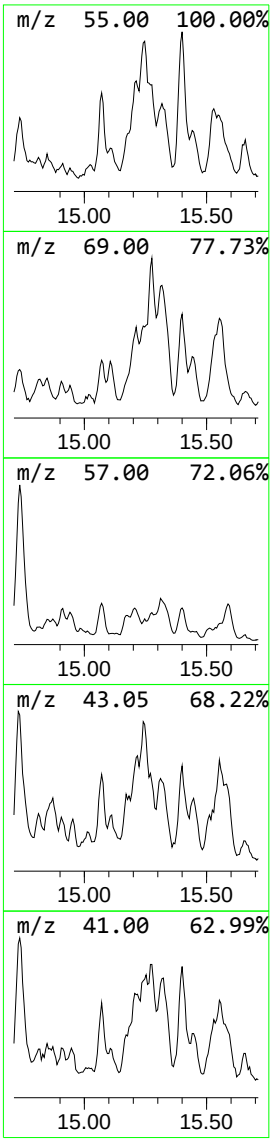
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptafluorobutyryloxyhexa... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	26.51 ug/l	377668	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1010282-97-2	86
2	3-Trifluoroacetoxytridecane	296	C15H27F3O2	1000245-47-2	86
3	Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	50
4	5-Undecene, 6-methyl-	168	C12H24	083687-45-0	50
5	Cyclopentane, ethyl-	98	C7H14	001640-89-7	49





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Data File : VN086310.D
Acq On : 16 Apr 2025 20:28
Operator : JC\MD
Sample : Q1791-12 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

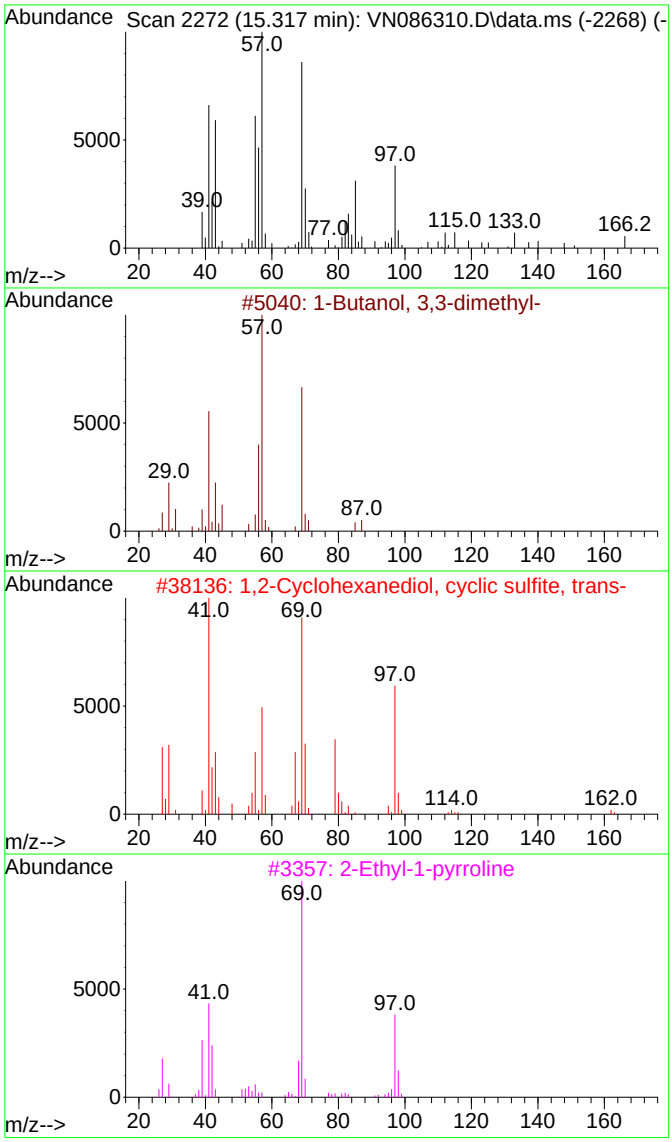
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

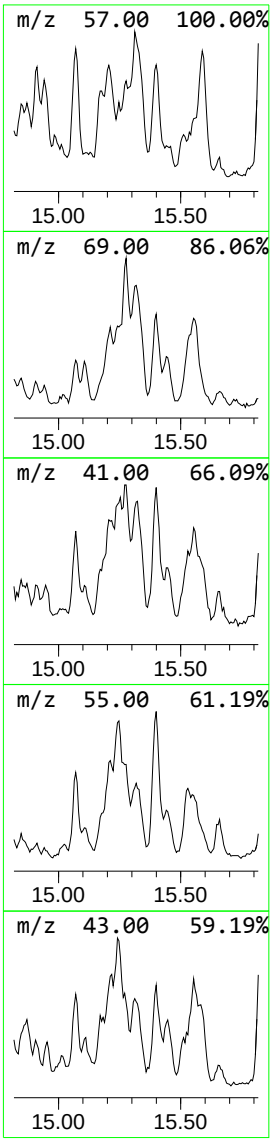
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown15.317 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	22.77 ug/l	324360	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	47
2	1,2-Cyclohexanediol, cyclic sulf...	162	C6H10O3S	019456-19-0	43
3	2-Ethyl-1-pyrroline	97	C6H11N	1000422-81-4	43
4	3-Octanol, acetate	172	C10H20O2	004864-61-3	38
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	27





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

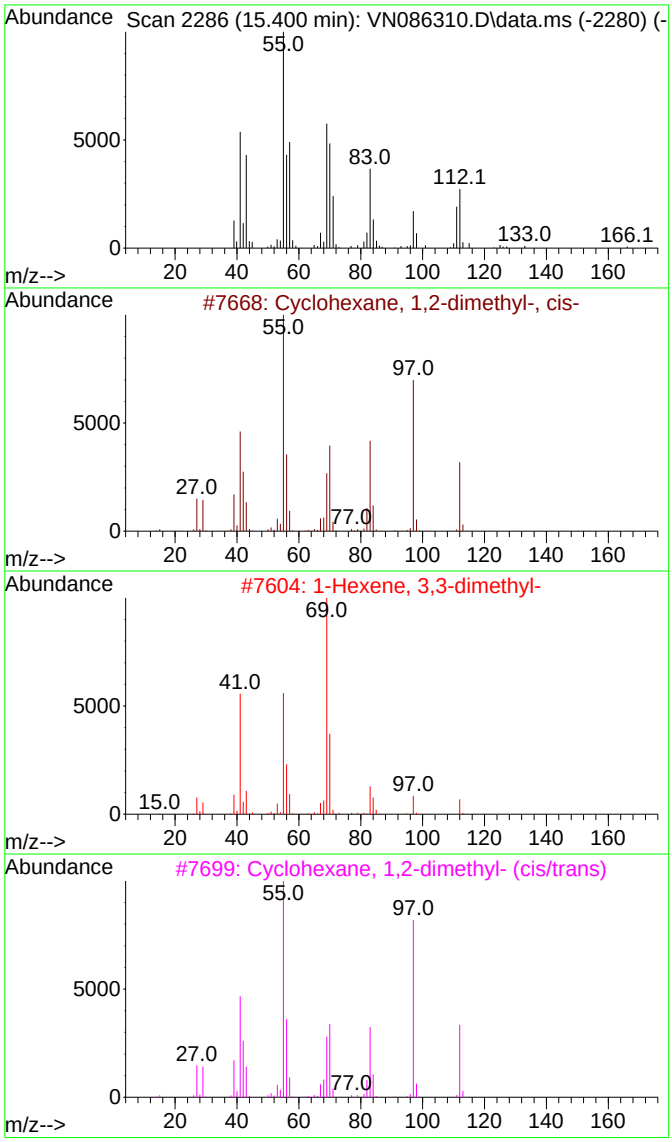
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

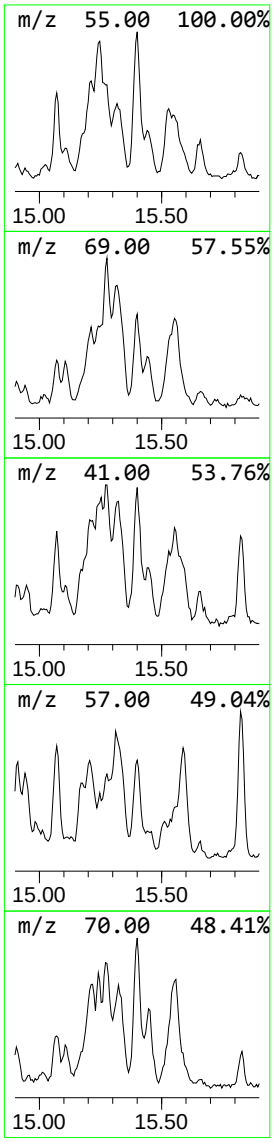
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.400	21.93 ug/l	312461	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	76
2	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	64
3	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	58
4	1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	53
5	1-Undecanol	172	C11H24O	000112-42-5	50





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Data File : VN086310.D
Acq On : 16 Apr 2025 20:28
Operator : JC\MD
Sample : Q1791-12 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

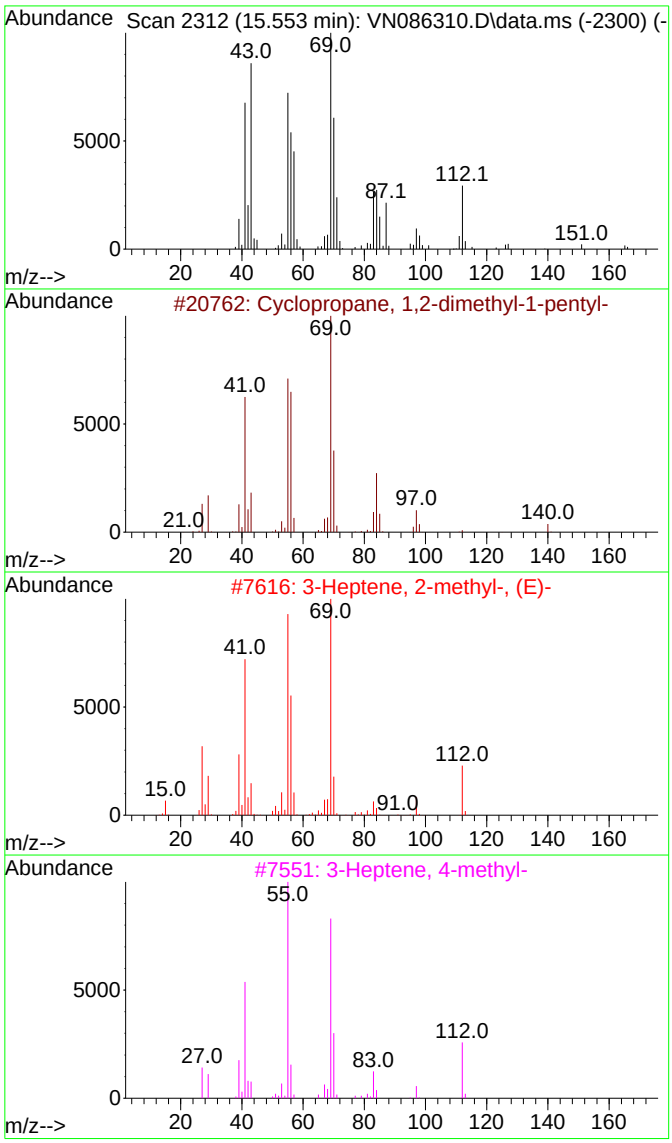
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

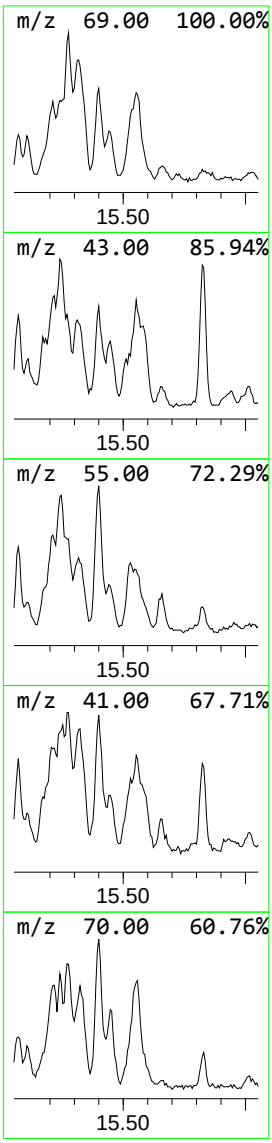
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.553	38.65 ug/l	550576	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	50
2	3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	49
3	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	46
4	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	45
5	3-Octene, (E)-	112	C8H16	014919-01-8	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086310.D
Acq On : 16 Apr 2025 20:28
Operator : JC\MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
V1207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
Decane, 2,2-dim...	13.418	47.9	ug/l	682303	4	13.788	712305	50.0
Cyclobutane, 1,...	13.535	101.1	ug/l	1440800	4	13.788	712305	50.0
Heptadecane, 8-...	13.641	72.1	ug/l	1026680	4	13.788	712305	50.0
1.alpha.,2.beta...	13.935	98.8	ug/l	1407470	4	13.788	712305	50.0
Nonane, 5-methy...	14.176	24.9	ug/l	354188	4	13.788	712305	50.0
Dodecane, 2,7,1...	14.735	32.6	ug/l	464588	4	13.788	712305	50.0
4-Heptafluorobu...	15.212	26.5	ug/l	377668	4	13.788	712305	50.0
unknown15.317	15.317	22.8	ug/l	324360	4	13.788	712305	50.0
Cyclohexane, 1,...	15.400	21.9	ug/l	312461	4	13.788	712305	50.0
Cyclopropane, 1...	15.553	38.6	ug/l	550576	4	13.788	712305	50.0