LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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: VN086318.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.212	1058	1064	1076	rVB3	330225	866782	2.52%	0.618%
2	8.577	1117	1126	1137	rBV2	156041	417031	1.21%	0.297%
3	8.753	1139	1156	1166	rBV2	121211	447983	1.30%	0.319%
4	9.094	1205	1214	1222	rBV	406104	846498	2.46%	0.603%
5	9.588	1285	1298	1304	rBV2	178443	465105	1.35%	0.331%
6	10.559	1456	1463	1469	rBV	651804	1252300	3.64%	0.892%
7	10.624	1469	1474	1482	rVB	1024739	1861550	5.40%	1.326%
8	10.741	1487	1494	1501	rVB	282466	525996	1.53%	0.375%
9	11.641	1639	1647	1658	rVB3	239859	528716	1.53%	0.377%
10	11.865	1677	1685	1693	rBV	505466	917091	2.66%	0.653%
11	11.959	1693	1701	1710	rBV	4701787	7833726	22.74%	5.581%
12	12.065	1710	1719	1730	rBV	18207298	34449899	100.00%	24.544%
13	12.394	1763	1775	1784	rBV	5810418	10036899	29.13%	7.151%
14	12.606	1794	1811	1821	rBV8	163507	795558	2.31%	0.567%
15	12.765	1830	1838	1840	rBV3	215258	415140	1.21%	0.296%
16	12.794	1840	1843	1847	rVB	274366	359020	1.04%	0.256%
17	12.847	1847	1852	1855	rBV	369566	622438	1.81%	0.443%
18	13.029	1877	1883	1888	rBV	371168	602477	1.75%	0.429%
19	13.094	1888	1894	1898	rBV	1278935	2227604	6.47%	1.587%
20	13.159	1898	1905	1912	rVB3	2105013	4471475	12.98%	3.186%
21	13.335	1925	1935	1941	rBV2	484016	1265403	3.67%	0.902%
22	13.388	1941	1944	1952	rVB2	335586	535723	1.56%	0.382%
23	13.482	1953	1960	1965	rBV	2175694	3553725	10.32%	2.532%
24	13.670	1986	1992	1996	rBV4	413567	823243	2.39%	0.587%
25	13.712	1996	1999	2002	rVV	341703	429955	1.25%	0.306%
26	13.782	2007	2011	2014	rVV2	928505	1446060	4.20%	1.030%
27	13.818	2014	2017	2020	rVV	614482	946506	2.75%	0.674%
28	13.853	2020	2023	2030	rVB	690878	1035042	3.00%	0.737%
29	13.947	2030	2039	2040	rBV6	316438	552796	1.60%	0.394%
30	13.982	2040	2045	2049	rVV2	815615	1597609	4.64%	1.138%
31	14.018	2049	2051	2060	rVB3	746178	1352156	3.92%	0.963%
32	14.100	2060	2065	2071	rBV	4548337	6701870	19.45%	4.775%
33	14.265	2086	2093	2098	rVB3	599152	1448105	4.20%	1.032%
34	14.323	2098	2103	2108	rBV	901919	1412112	4.10%	1.006%
35	14.435	2117	2122	2128	rBV3	584307	1075074	3.12%	0.766%
36	14.494	2128	2132	2138	rBV7	183874	377100	1.09%	0.269%

LSC Area Percent Report

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Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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	14.576	2141	2146	2150	rVV3	850031	1725564	5.01%	1.229%
38	14.623	2150	2154	2157	rVV2	1435235	2462202	7.15%	1.754%
39	14.659	2157	2160	2163	rVV2	1230668	1877067	5.45%	1.337%
40	14.688	2163	2165	2168	rVV	781242	968430	2.81%	0.690%
41	14.729	2168	2172	2176	rVV	1116568	1673676	4.86%	1.192%
42	14.765	2176	2178	2187	rVB4	420287	895494	2.60%	0.638%
43	14.841	2187	2191	2193	rBV2	220330	355062	1.03%	0.253%
44	14.870	2193	2196	2200	rVB	371746	513606	1.49%	0.366%
45	14.953	2200	2210	2217	rBV2	5229593	9358742	27.17%	6.668%
46	15.047	2218	2226	2241	rVB6	1399185	5934827	17.23%	4.228%
47	15.212	2249	2254	2259	rVB	450712	934667	2.71%	0.666%
48	15.312	2267	2271	2277	rVV4	540978	987685	2.87%	0.704%
49	15.423	2283	2290	2299	rBV7	525779	1911084	5.55%	1.362%
50	15.506	2300	2304	2312	rVB3	641683	1631544	4.74%	1.162%
51	15.582	2312	2317	2322	rBV2	747216	1469569	4.27%	1.047%
52	15.635	2322	2326	2331	rVB	483324	833160	2.42%	0.594%
53	15.741	2340	2344	2349	rBV2	365882	608039	1.76%	0.433%
54	15.823	2353	2358	2369	rVB	2604961	5041181	14.63%	3.592%
55	15.941	2369	2378	2385	rBV5	577228	1707286	4.96%	1.216%
56	16.117	2403	2408	2411	rBV5	157032	356793	1.04%	0.254%
57	16.159	2411	2415	2426	rVB2	542625	1148071	3.33%	0.818%
58	16.335	2438	2445	2451	rVB6	216582	614512	1.78%	0.438%
59	16.494	2461	2472	2476	rBV8	374097	1177318	3.42%	0.839%
60	16.706	2503	2508	2513	rVB2	224277	434400	1.26%	0.309%
61	16.776	2513	2520	2522	rBV	689109	1244840	3.61%	0.887%

Sum of corrected areas: 140360586

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Acq On : 17 Apr 2025 13:41
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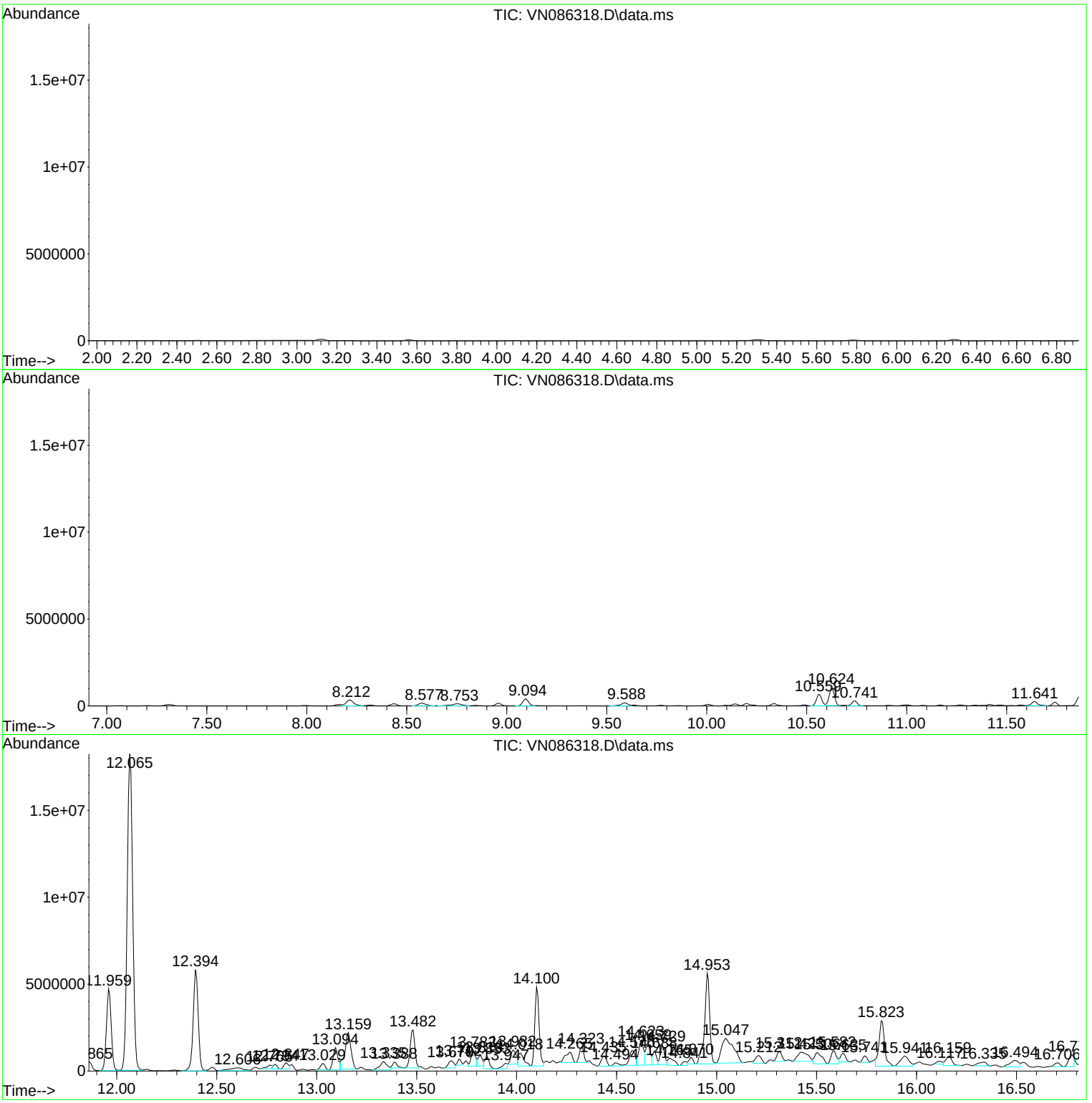
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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Instrument :
MSVOA_N
ClientSampleId :
288

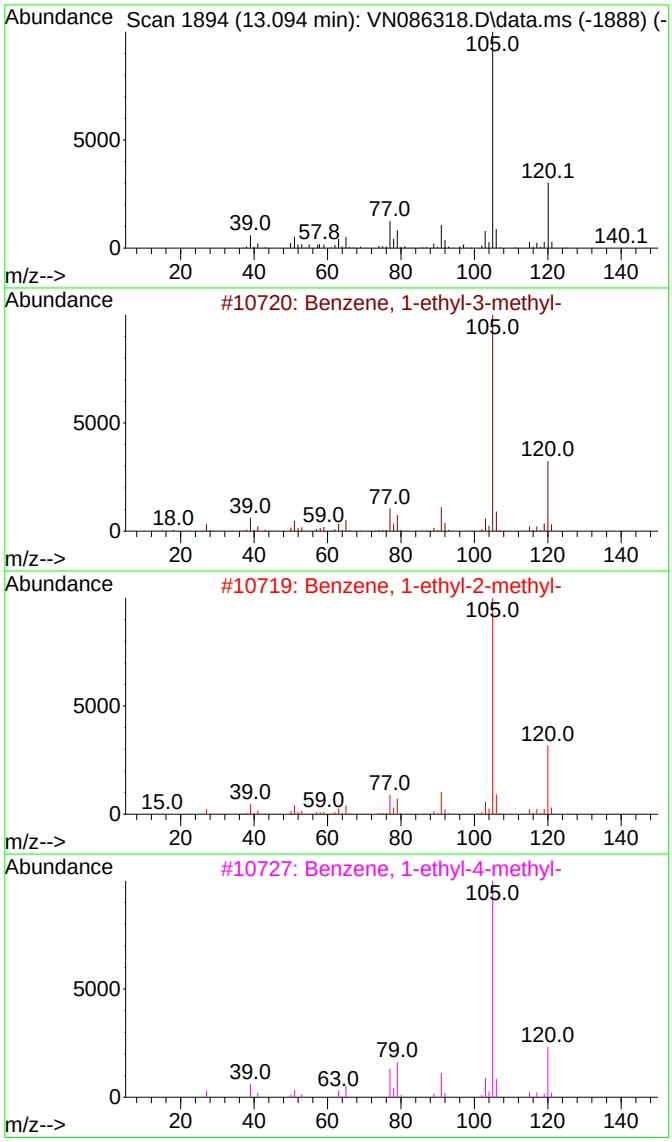
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

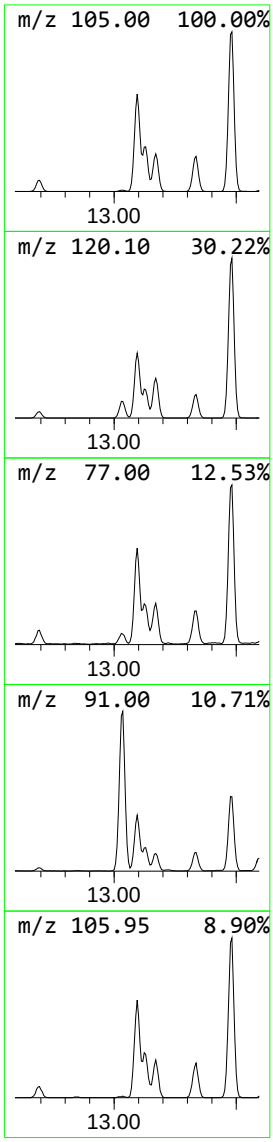
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	77.02 ug/l	2227600	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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

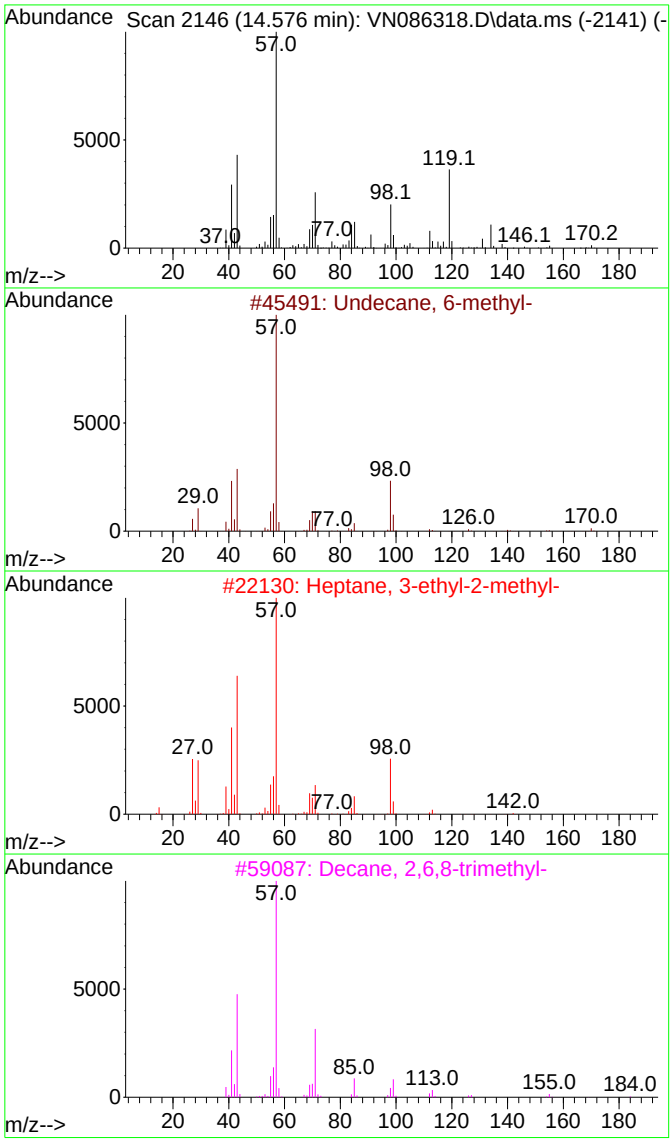
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

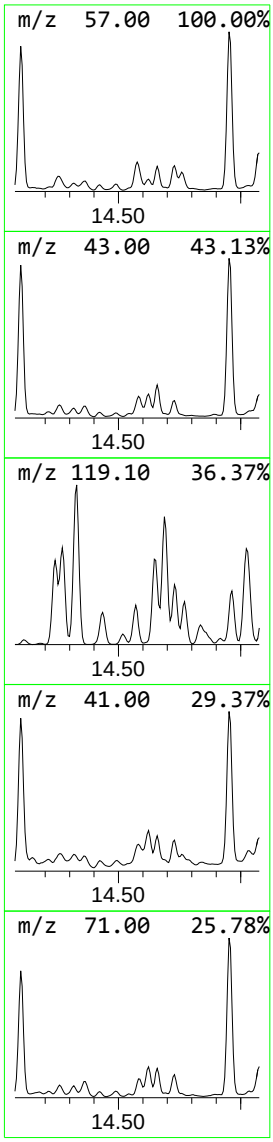
****

Peak Number 2 unknown14.576 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.576	59.66 ug/l	1725560	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-methyl-	170	C12H26	017302-33-9	38
2	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	38
3	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	35
4	1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	35
5	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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

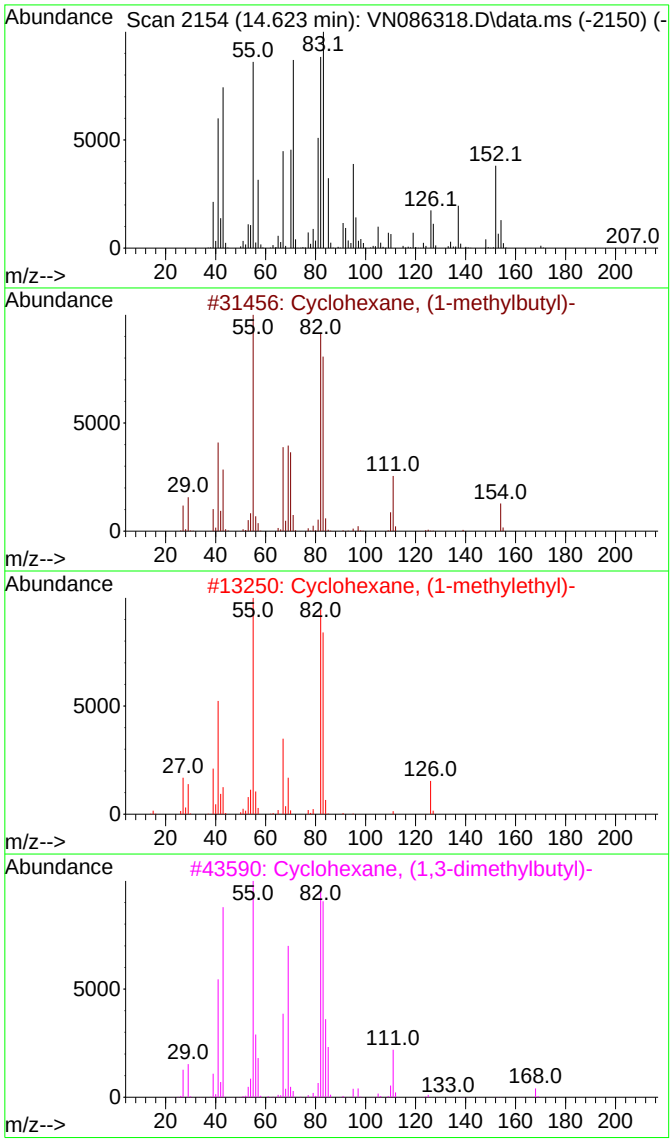
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

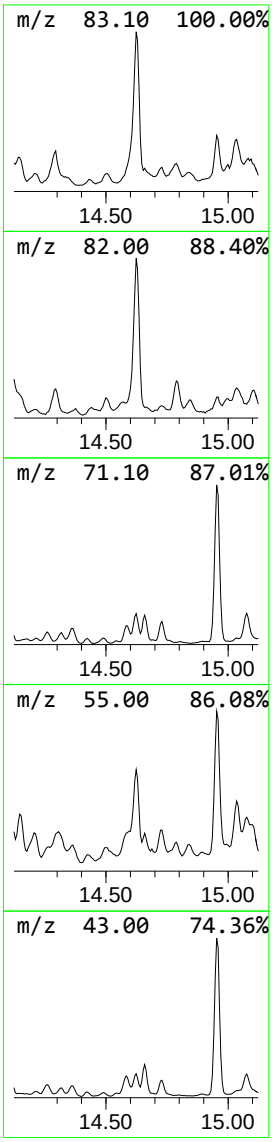
****

Peak Number 3 unknown14.623 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.623	85.13 ug/l	2462200	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	46
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	41
3	Cyclohexane, (1,3-dimethylbutyl)-	168	C12H24	061142-19-6	38
4	Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	35
5	1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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

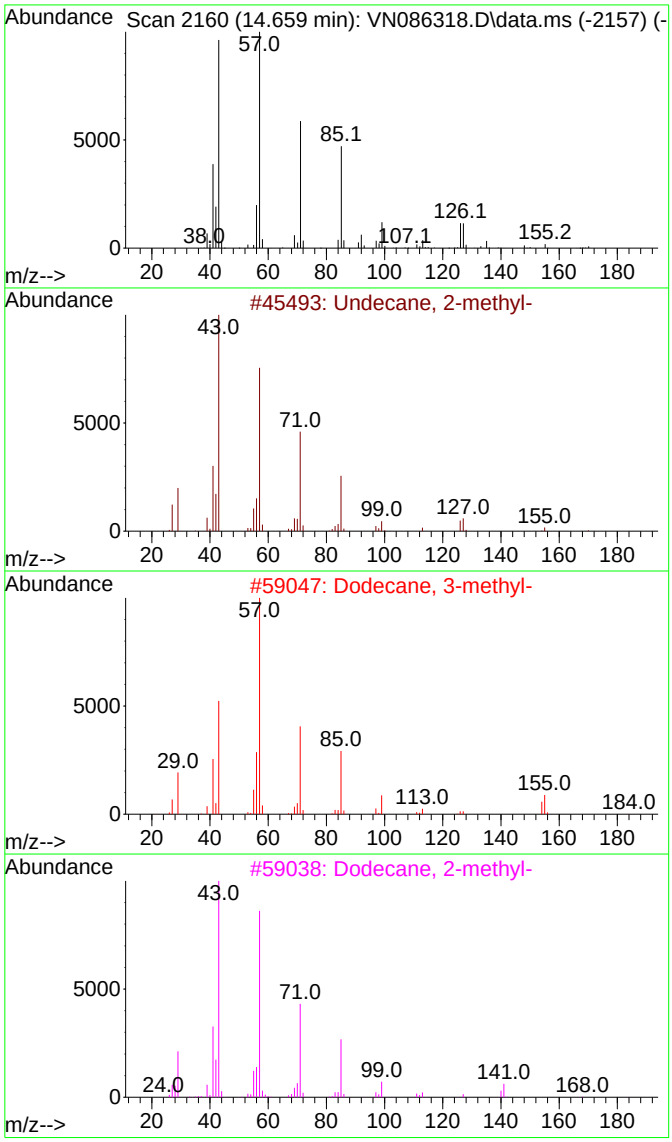
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

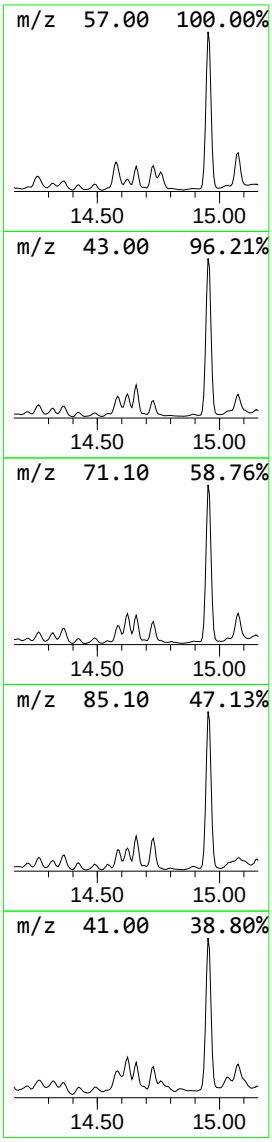
****

Peak Number 4 Undecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	64.90 ug/l	1877070	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2-methyl-	170	C12H26	007045-71-8	87
2	Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	59
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
5	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

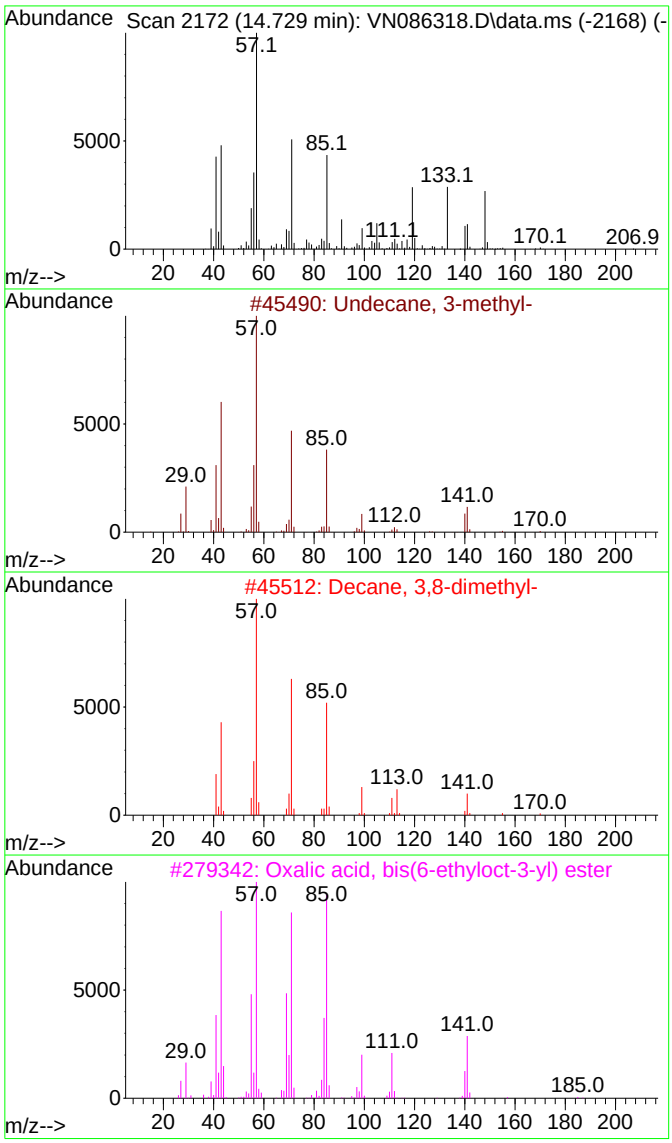
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

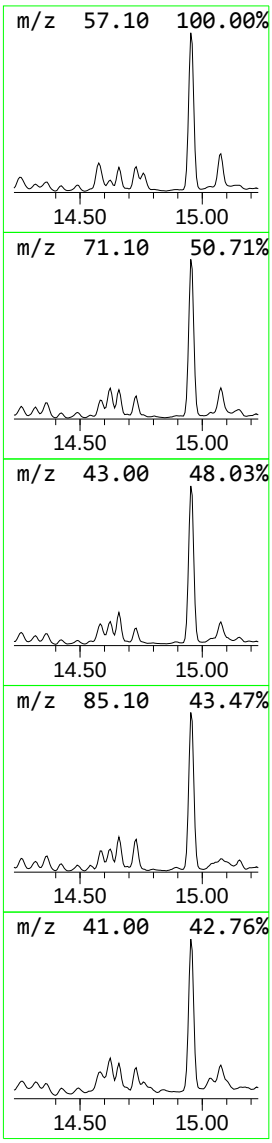
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Undecane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.729	57.87 ug/l	1673680	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3-methyl-	170	C12H26	001002-43-3	92
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	60
3	Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	49
4	Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	47
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

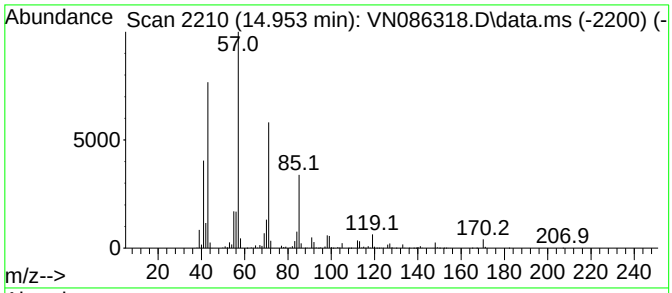
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

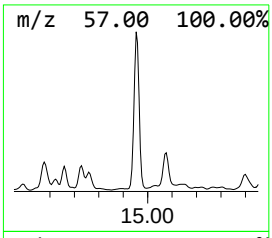
****

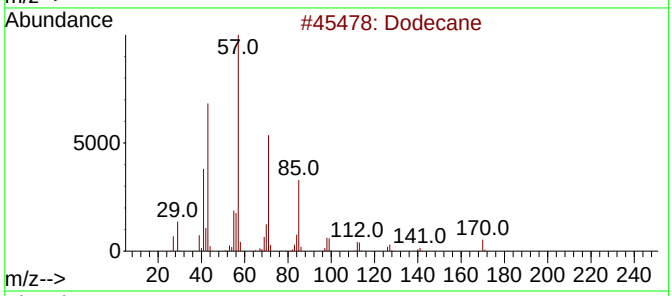
Peak Number 6 Dodecane Concentration Rank 1

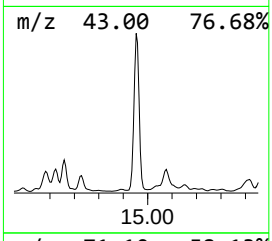
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.953	323.60 ug/l	9358740	1,4-Dichlorobenzene-d4	13.788

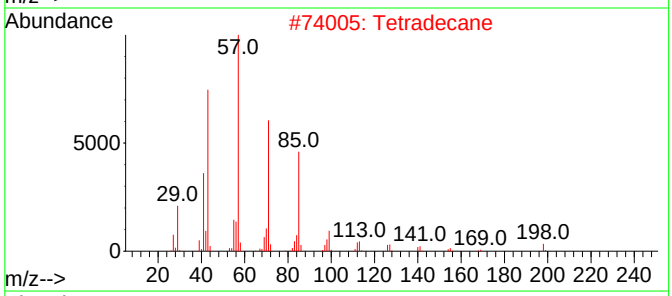
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	94
2	Tetradecane	198	C14H30	000629-59-4	86
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tridecane	184	C13H28	000629-50-5	78

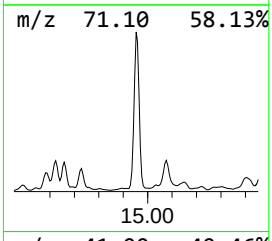


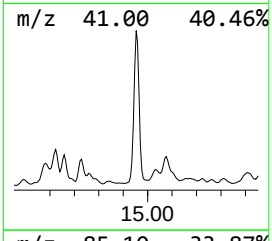


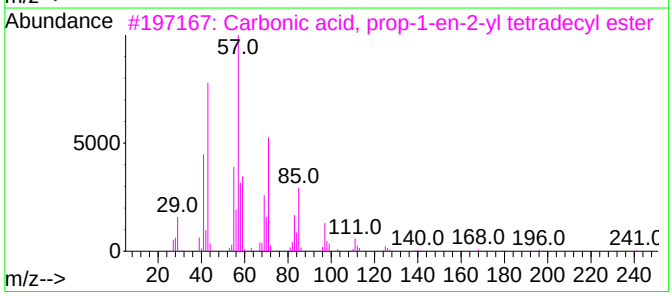


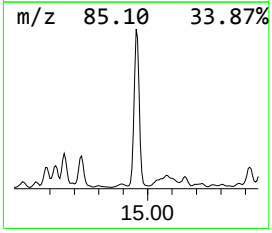












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

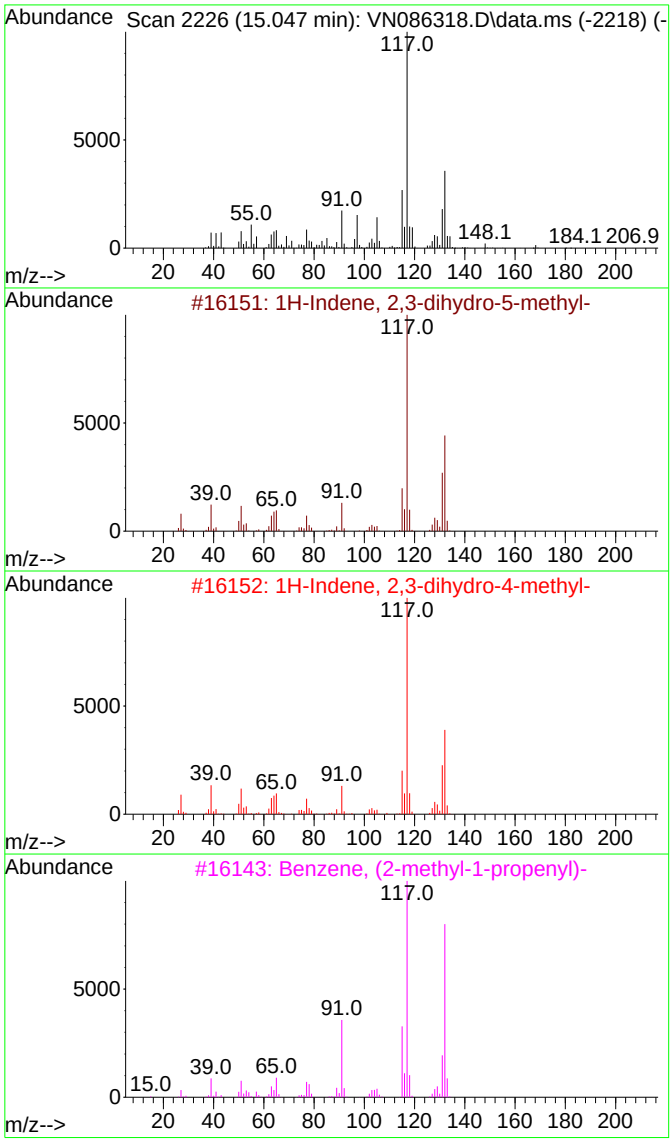
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

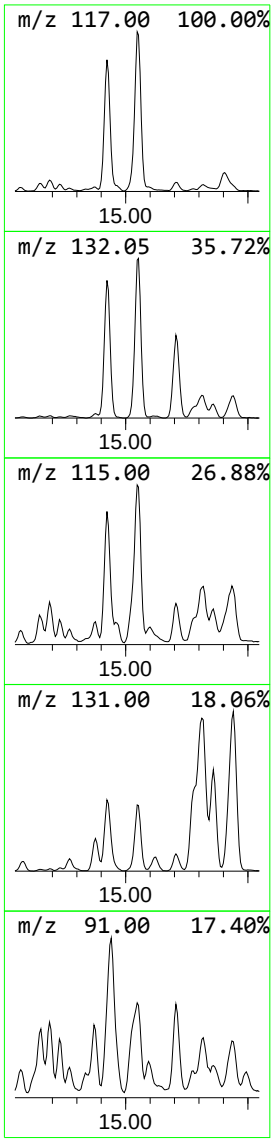
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	205.21 ug/l	5934830	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5	Indan, 1-methyl-	132	C10H12	000767-58-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

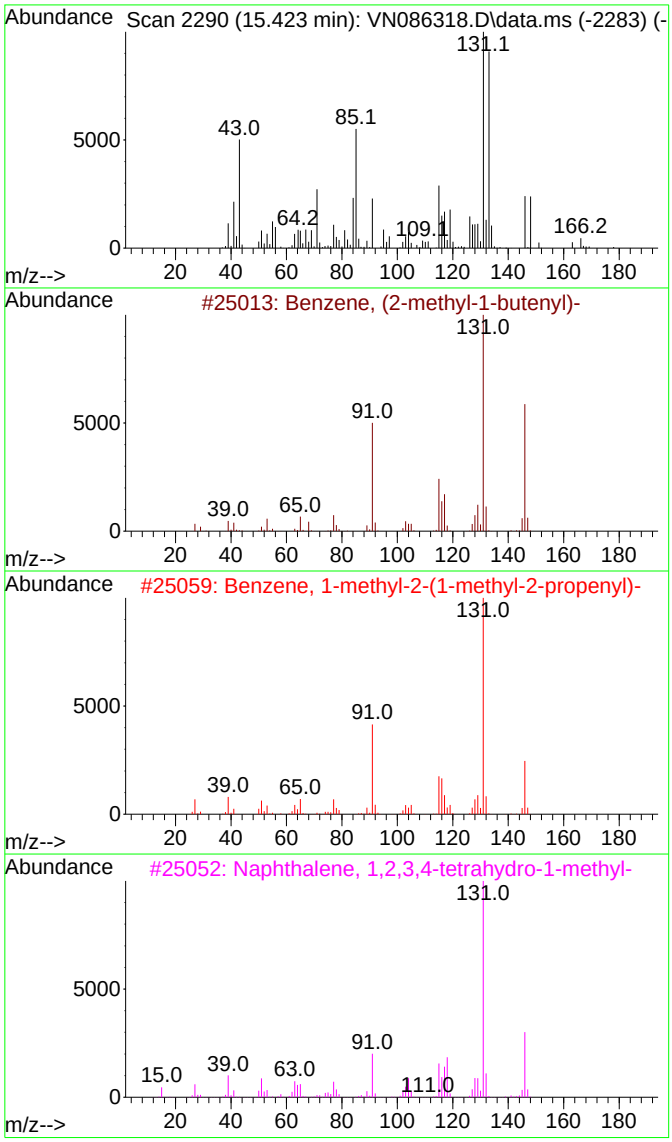
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

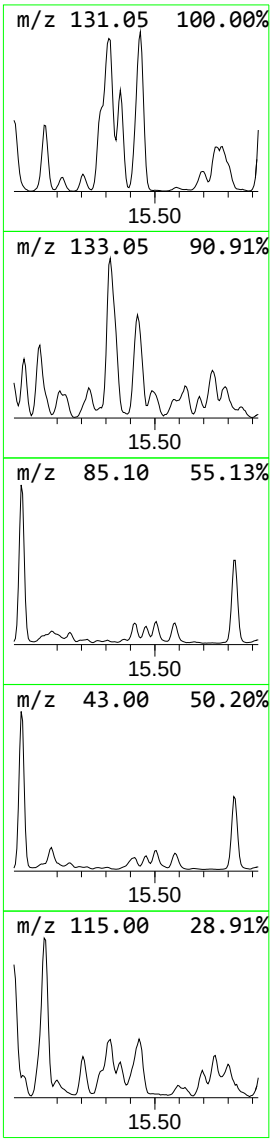
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.423	66.08 ug/l	1911080	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	80
2	Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	38
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	38
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	38
5	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

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

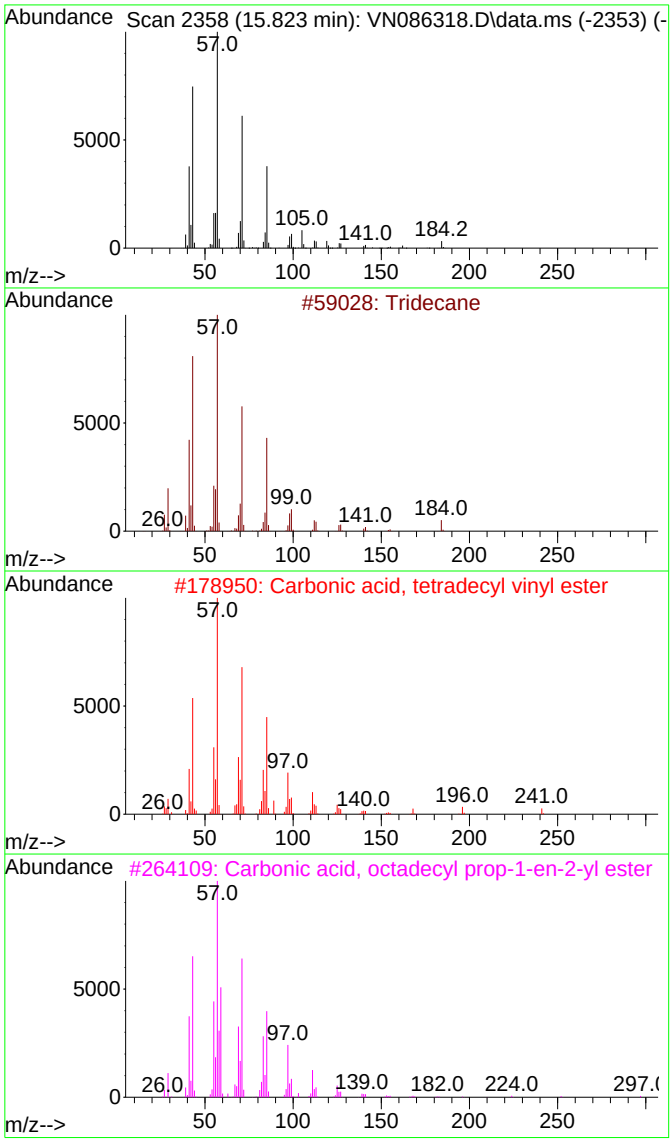
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

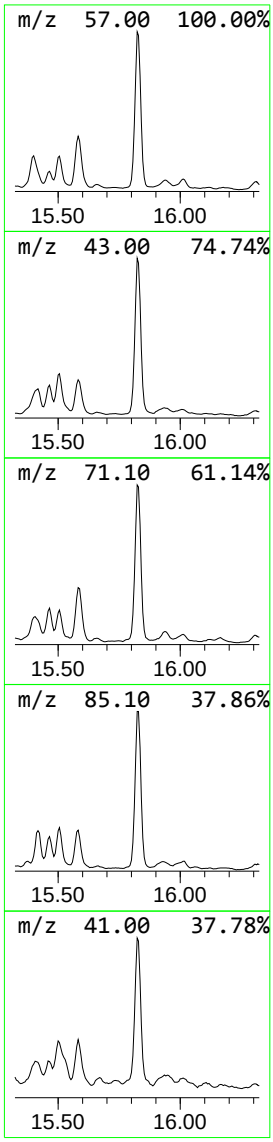
****

Peak Number 9 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	174.31 ug/l	5041180	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	95
2	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Tetradecane	198	C14H30	000629-59-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
288

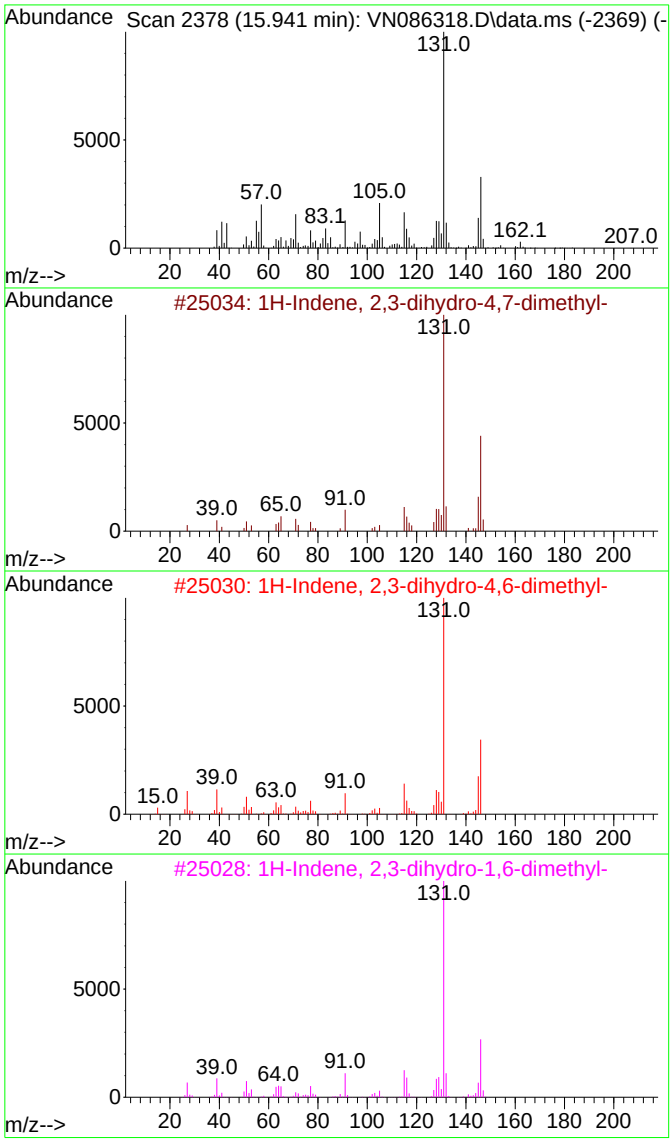
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

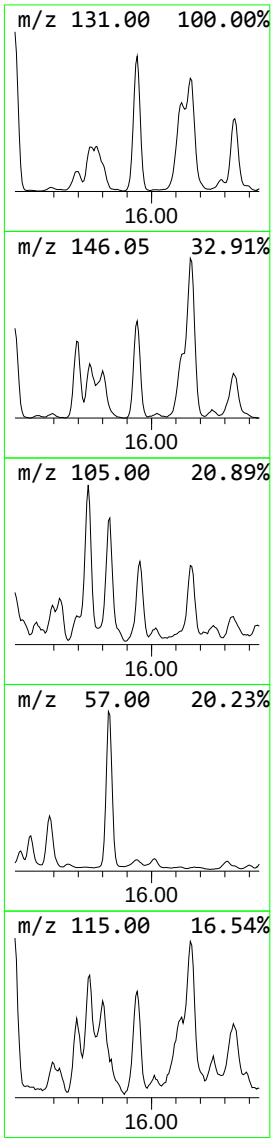
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	59.03 ug/l	1707290	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	94
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	90
5	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086318.D
Acq On : 17 Apr 2025 13:41
Operator : JC\MD
Sample : Q1824-03
Misc : 1.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1-ethy...	13.094	77.0	ug/l	2227600	4	13.788	1446060	50.0
unknown14.576	14.576	59.7	ug/l	1725560	4	13.788	1446060	50.0
unknown14.623	14.623	85.1	ug/l	2462200	4	13.788	1446060	50.0
Undecane, 2-met...	14.659	64.9	ug/l	1877070	4	13.788	1446060	50.0
Undecane, 3-met...	14.729	57.9	ug/l	1673680	4	13.788	1446060	50.0
Dodecane	14.953	323.6	ug/l	9358740	4	13.788	1446060	50.0
1H-Indene, 2,3-...	15.047	205.2	ug/l	5934830	4	13.788	1446060	50.0
Benzene, (2-met...	15.423	66.1	ug/l	1911080	4	13.788	1446060	50.0
Tridecane	15.823	174.3	ug/l	5041180	4	13.788	1446060	50.0
1H-Indene, 2,3-...	15.941	59.0	ug/l	1707290	4	13.788	1446060	50.0