LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

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\82N091024W.M
Title : SW846 8260

Signal : TIC: VN083917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1046	1056	1060	rBV2	114998	278455	4.65%	0.501%
2	8.218	1060	1065	1077	rVB	223863	496324	8.29%	0.893%
3	8.577	1116	1126	1137	rBV	138963	308304	5.15%	0.554%
4	9.100	1206	1215	1228	rBV	307200	634059	10.59%	1.140%
5	10.565	1456	1464	1479	rBV	468476	864625	14.44%	1.555%
6	11.641	1639	1647	1659	rVV5	45145	116619	1.95%	0.210%
7	11.741	1659	1664	1670	rVB2	47325	75345	1.26%	0.136%
8	11.865	1678	1685	1697	rVB	410861	727149	12.15%	1.308%
9	12.071	1710	1720	1724	rBV	205398	355126	5.93%	0.639%
10	12.371	1764	1771	1773	rBV4	79468	149028	2.49%	0.268%
11	12.482	1784	1790	1795	rVB	110057	180565	3.02%	0.325%
12	12.594	1795	1809	1822	rBV9	100263	467493	7.81%	0.841%
13	12.741	1822	1834	1835	rVV8	79569	207005	3.46%	0.372%
14	12.771	1835	1839	1841	rVV	147168	249794	4.17%	0.449%
15	12.794	1841	1843	1847	rVV	139969	167435	2.80%	0.301%
16	12.847	1847	1852	1862	rVV2	348229	754504	12.60%	1.357%
17	13.018	1877	1881	1887	rVB3	61776	115064	1.92%	0.207%
18	13.094	1887	1894	1898	rBV2	179509	346001	5.78%	0.622%
19	13.159	1898	1905	1913	rVB3	941207	1685146	28.15%	3.031%
20	13.223	1913	1916	1921	rVB2	106865	155800	2.60%	0.280%
21	13.312	1922	1931	1932	rBV4	100756	171003	2.86%	0.308%
22	13.394	1941	1945	1951	rVB2	279981	433712	7.25%	0.780%
23	13.482	1956	1960	1964	rVV	128964	197277	3.30%	0.355%
24	13.518	1964	1966	1971	rVB2	80364	93166	1.56%	0.168%
25	13.576	1971	1976	1979	rBV4	96489	154283	2.58%	0.277%
26	13.671	1986	1992	1997	rBV4	292220	650693	10.87%	1.170%
27	13.718	1997	2000	2003	rVV2	262727	375626	6.28%	0.676%
28	13.747	2003	2005	2007	rVV	158071	171255	2.86%	0.308%
29	13.788	2007	2012	2020	rVB3	584449	1097049	18.33%	1.973%
30	13.853	2020	2023	2030	rVB2	264722	395198	6.60%	0.711%
31	13.941	2030	2038	2041	rBV6	118340	306588	5.12%	0.551%
32	13.982	2041	2045	2048	rBV2	214244	315775	5.28%	0.568%
33	14.023	2048	2052	2057	rVB3	196453	362664	6.06%	0.652%
34	14.106	2060	2066	2072	rBV	1868147	3147512	52.58%	5.661%
35	14.265	2087	2093	2098	rBV3	229381	487416	8.14%	0.877%
36	14.323	2099	2103	2107	rBV3	260281	382314	6.39%	0.688%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

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\82N091024W.M
Title : SW846 8260

37	14.365	2107	2110	2116	rVB4	251852	413902	6.91%	0.744%
38	14.435	2116	2122	2128	rBV3	354219	716713	11.97%	1.289%
39	14.500	2129	2133	2139	rVB7	140149	277664	4.64%	0.499%
40	14.582	2141	2147	2150	rBV4	447845	872490	14.58%	1.569%
41	14.623	2150	2154	2158	rVV2	841566	1248626	20.86%	2.246%
42	14.659	2158	2160	2164	rVV	367431	401414	6.71%	0.722%
43	14.729	2168	2172	2176	rBV2	557555	701546	11.72%	1.262%
44	14.788	2176	2182	2187	rVB4	282536	620710	10.37%	1.116%
45	14.847	2187	2192	2194	rBV2	224574	395812	6.61%	0.712%
46	14.959	2202	2211	2218	rBV2	2671748	4513746	75.41%	8.118%
47	15.076	2219	2231	2241	rVV5	958466	4093334	68.38%	7.362%
48	15.217	2250	2255	2260	rVB2	382188	801645	13.39%	1.442%
49	15.270	2260	2264	2267	rBV6	163071	254602	4.25%	0.458%
50	15.317	2267	2272	2277	rVV5	424711	762679	12.74%	1.372%
51	15.429	2284	2291	2300	rBV6	404386	1579844	26.39%	2.841%
52	15.506	2300	2304	2313	rVB5	618763	1413932	23.62%	2.543%
53	15.588	2313	2318	2328	rVB	1123490	2295297	38.35%	4.128%
54	15.694	2329	2336	2340	rBV3	350491	894767	14.95%	1.609%
55	15.741	2341	2344	2348	rVV2	280034	388426	6.49%	0.699%
56	15.829	2354	2359	2370	rVB	3167724	5985850	100.00%	10.766%
57	15.947	2370	2379	2385	rBV5	724166	2224741	37.17%	4.001%
58	16.017	2388	2391	2401	rVB3	432484	839448	14.02%	1.510%
59	16.164	2412	2416	2427	rVB4	766933	1584715	26.47%	2.850%
60	16.312	2437	2441	2444	rBV4	369642	686497	11.47%	1.235%
61	16.459	2461	2466	2467	rBV	421564	631318	10.55%	1.135%
62	16.541	2477	2480	2487	rVB5	572900	1064782	17.79%	1.915%
63	16.611	2488	2492	2500	rVB	594505	1056461	17.65%	1.900%
64	16.706	2502	2508	2515	rBV2	838284	1804956	30.15%	3.246%

Sum of corrected areas: 55601289

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Sample : P3936-01
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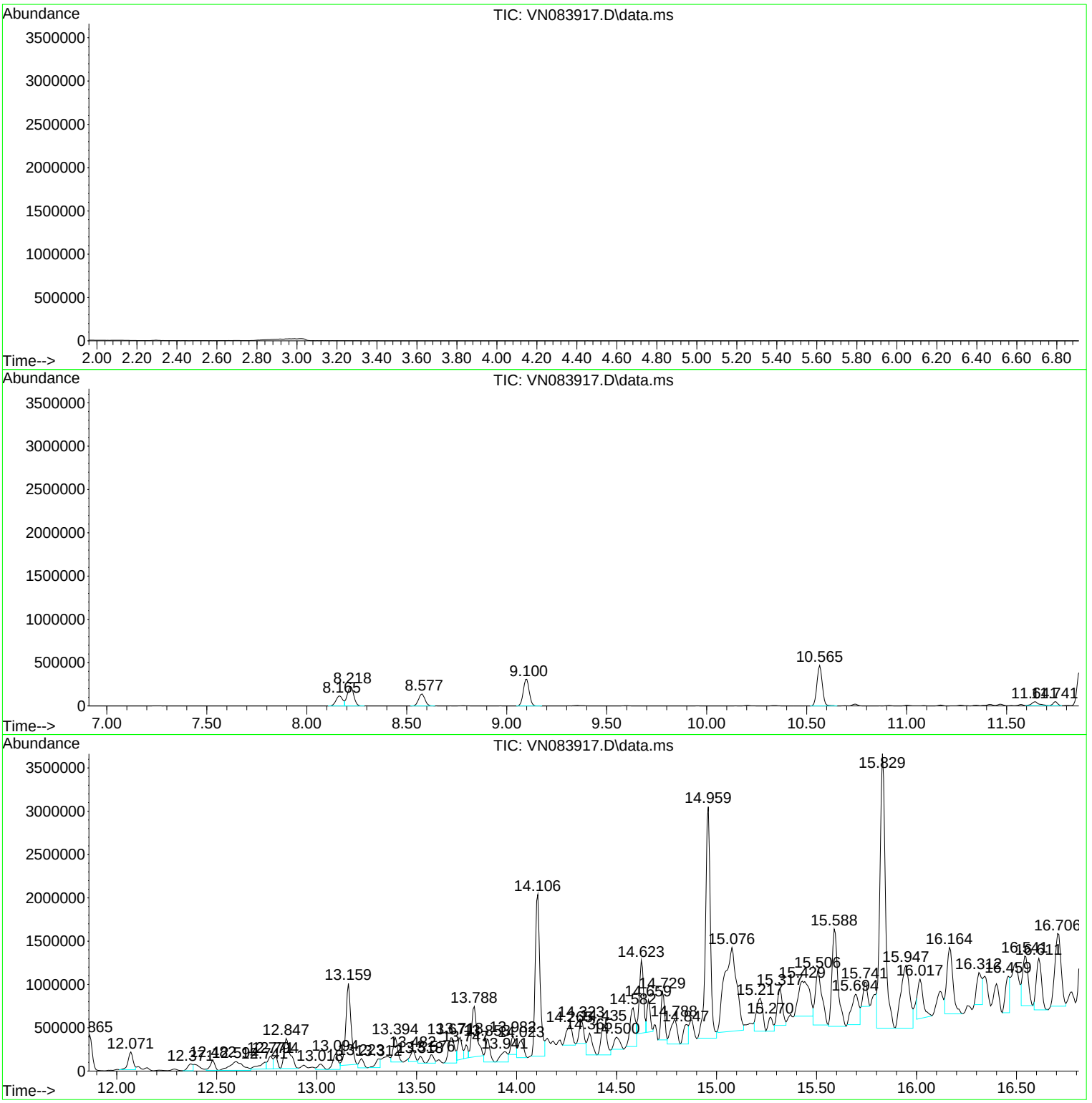
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
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MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

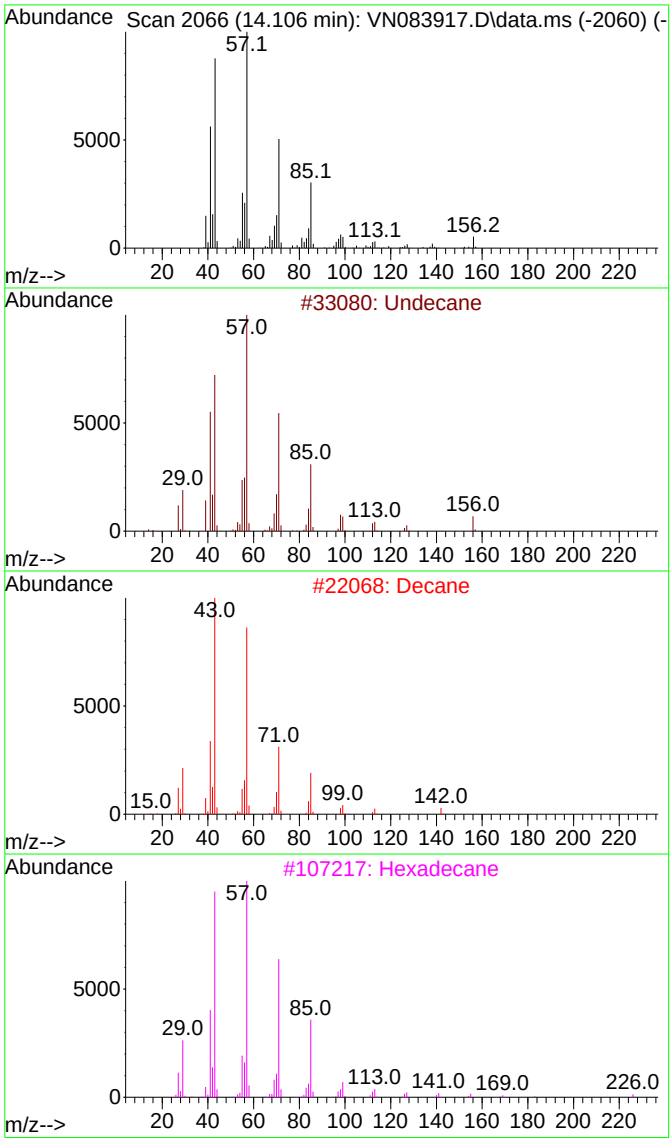
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

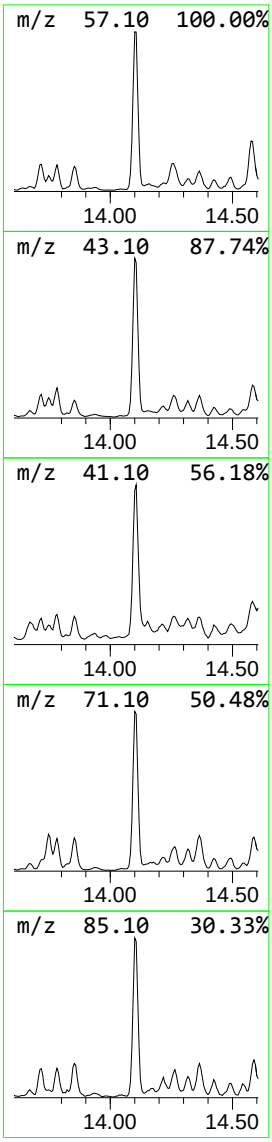
****

Peak Number 1 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	143.45 ug/l	3147510	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Decane	142	C10H22	000124-18-5	78
3	Hexadecane	226	C16H34	000544-76-3	64
4	Tridecane	184	C13H28	000629-50-5	64
5	Tetradecane	198	C14H30	000629-59-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

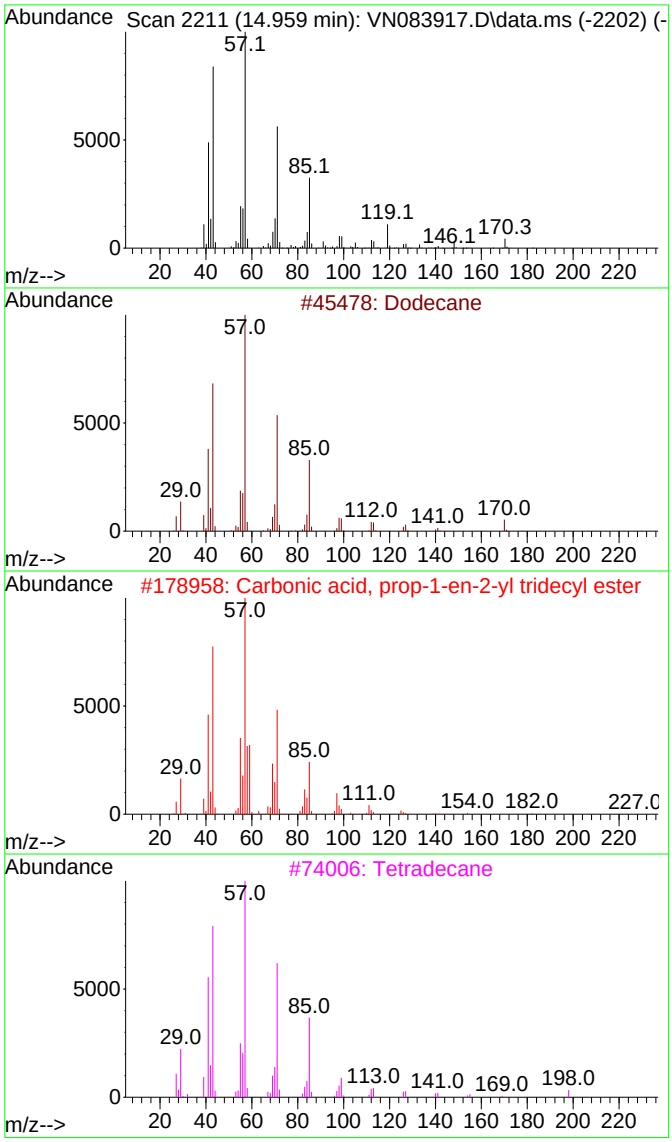
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

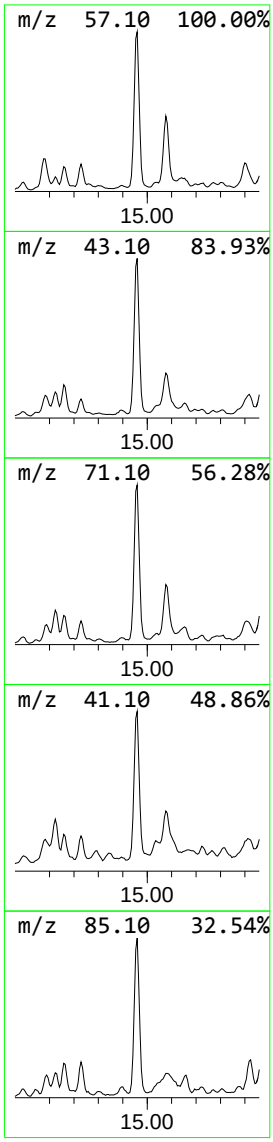
****

Peak Number 2 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	205.72 ug/l	4513750	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	95
2	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Undecane	156	C11H24	001120-21-4	80
5	Hexadecane	226	C16H34	000544-76-3	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

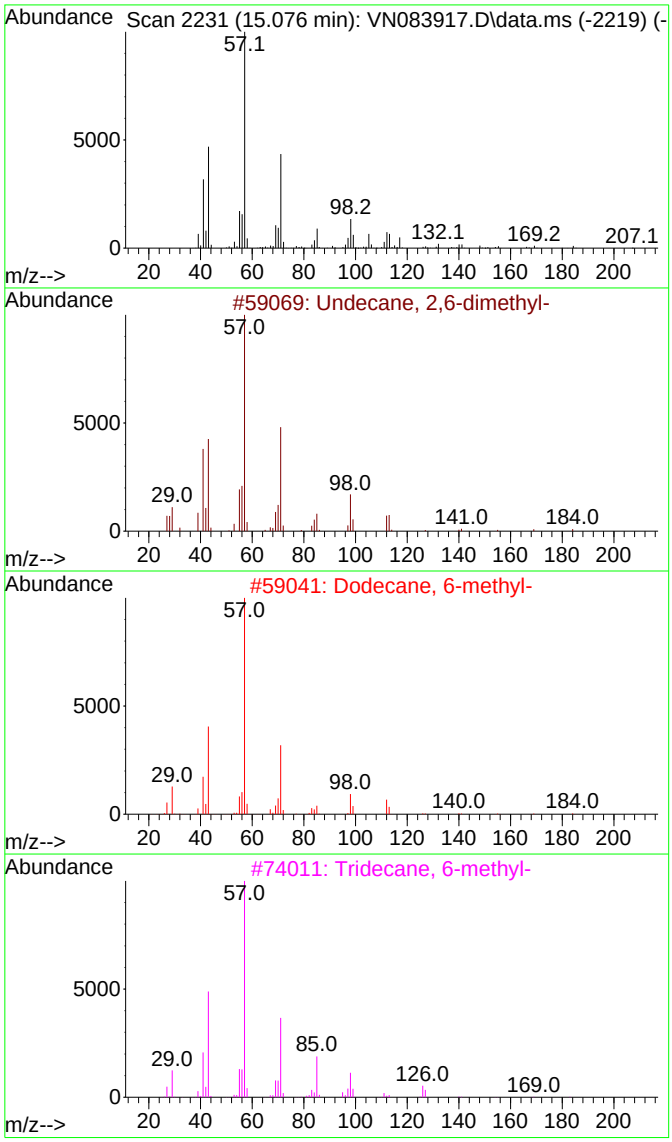
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

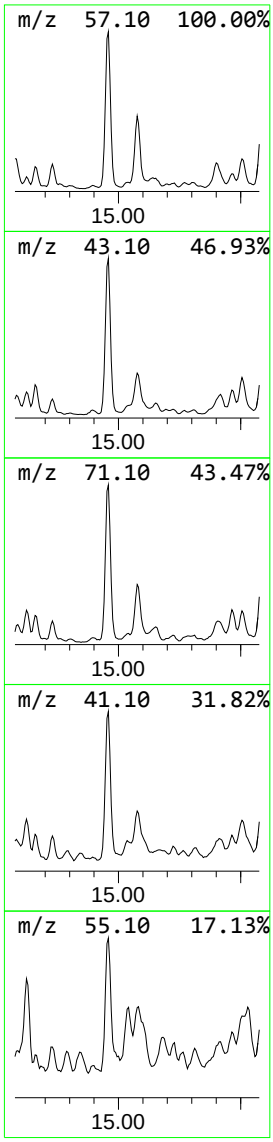
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Undecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.076	186.56 ug/l	4093330	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	94
2	Dodecane, 6-methyl-	184	C13H28	006044-71-9	64
3	Tridecane, 6-methyl-	198	C14H30	013287-21-3	59
4	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	58
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

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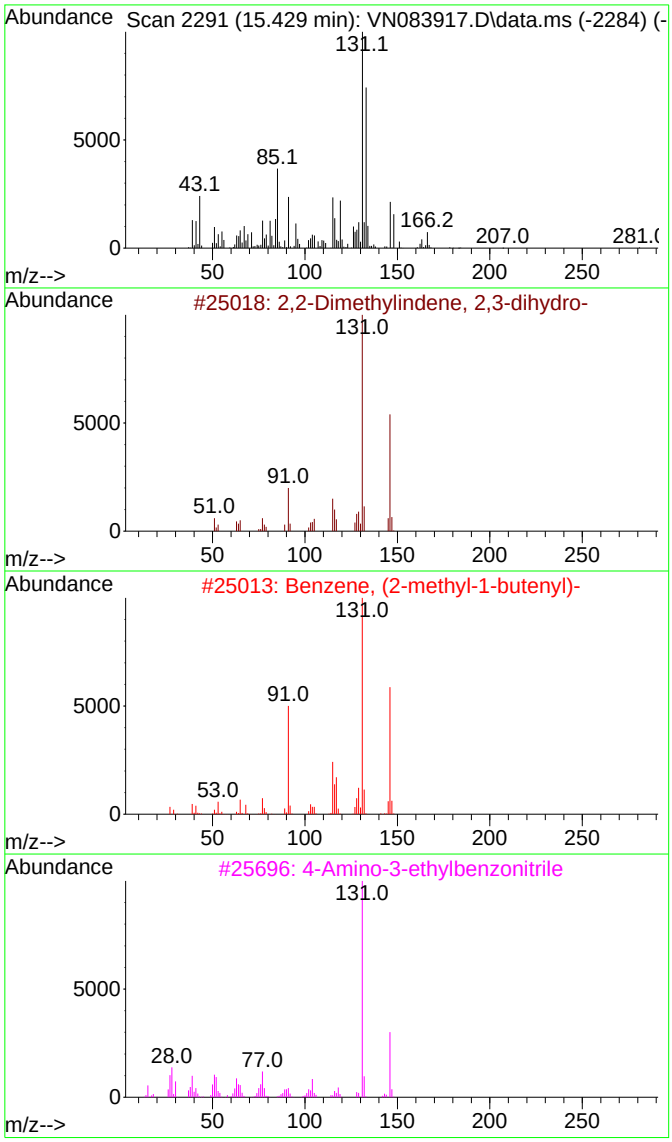
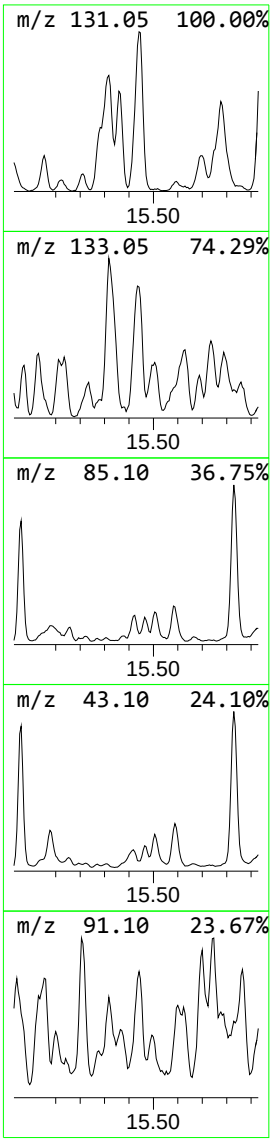
Peak Number 4 unknown15.429 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.429	72.00 ug/l	1579840	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	46
2	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	46
3	4-Amino-3-ethylbenzonitrile	146	C9H10N2	170230-87-2	42
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	41
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	41





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

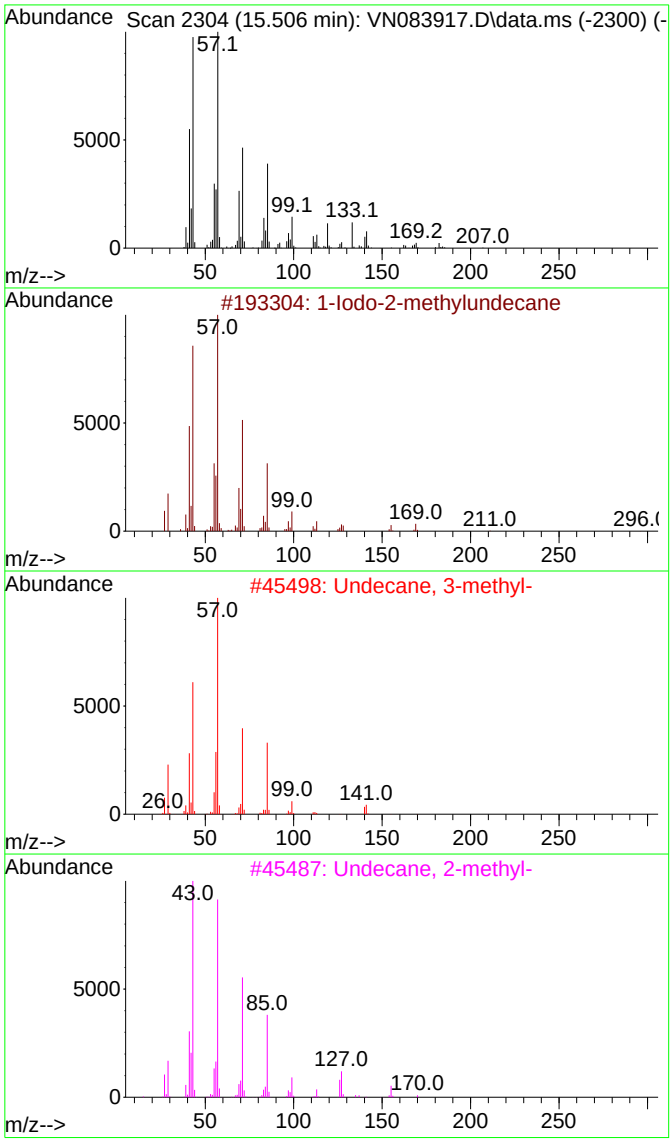
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

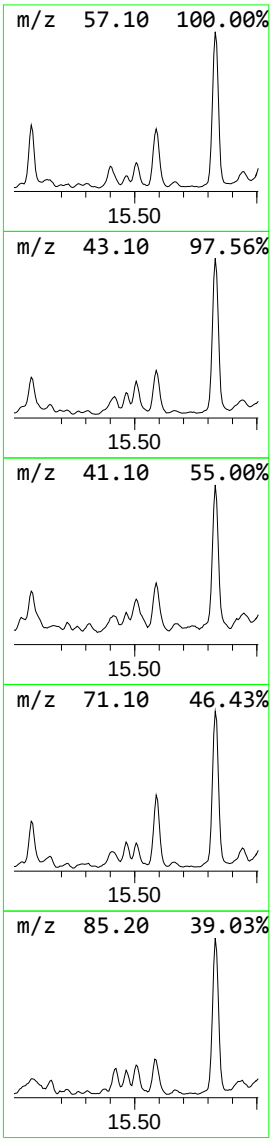
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Iodo-2-methylundecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.506	64.44 ug/l	1413930	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	64
2	Undecane, 3-methyl-	170	C12H26	001002-43-3	64
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	59
4	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	59
5	Octadecane	254	C18H38	000593-45-3	59





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Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

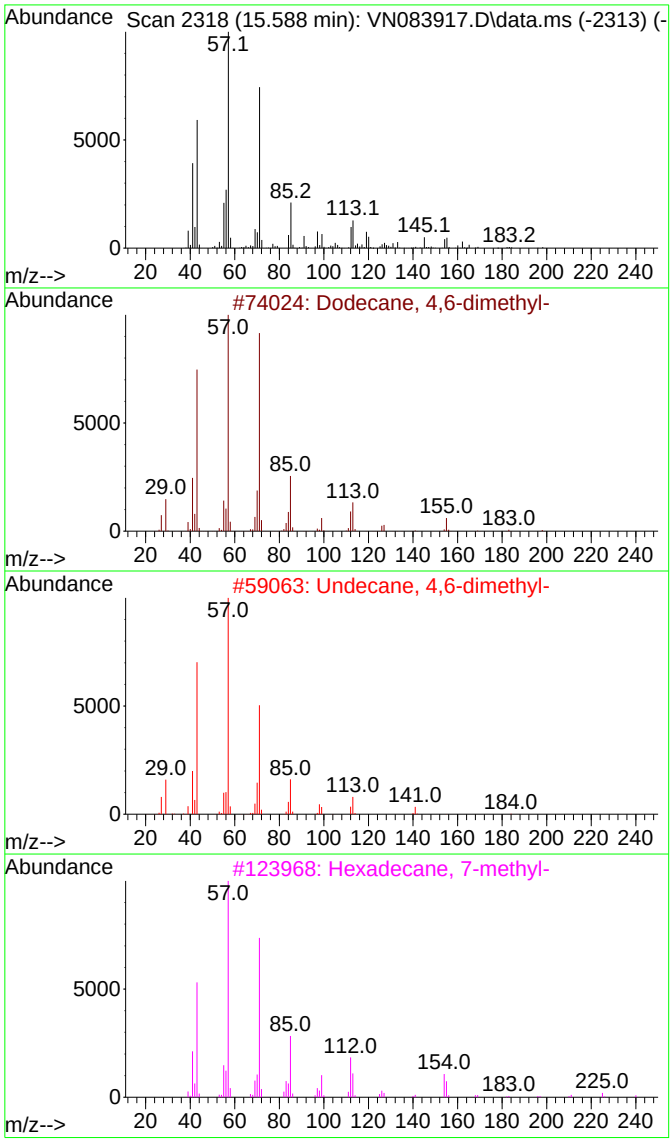
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

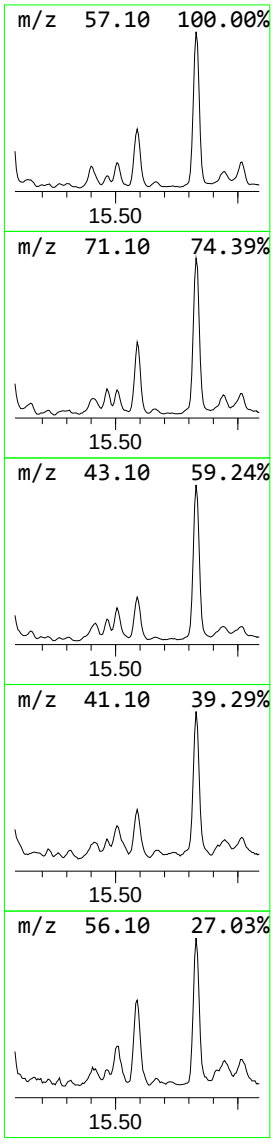
****

Peak Number 6 Dodecane, 4,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.588	104.61 ug/l	2295300	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	89
2	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	74
3	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	72
4	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

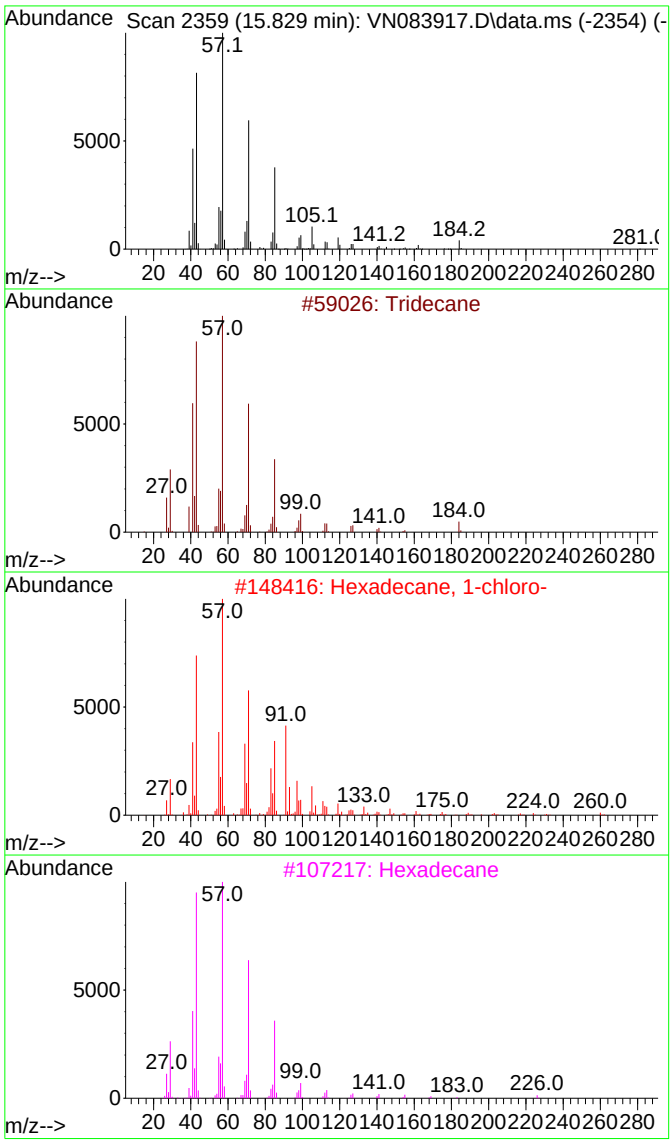
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

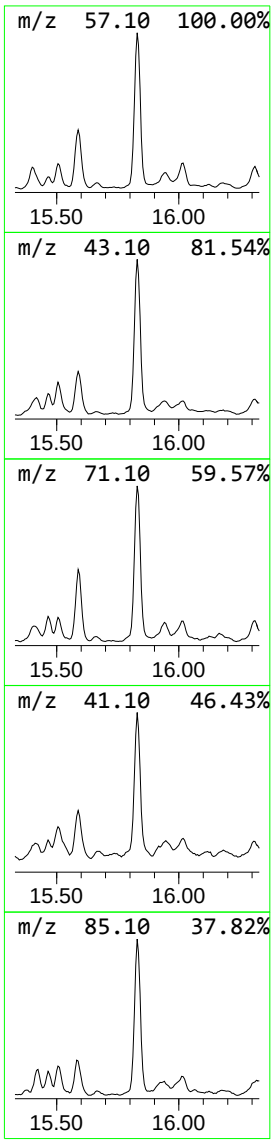
****

Peak Number 7 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	272.82 ug/l	5985850	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	83
3	Hexadecane	226	C16H34	000544-76-3	74
4	Tetradecane	198	C14H30	000629-59-4	74
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

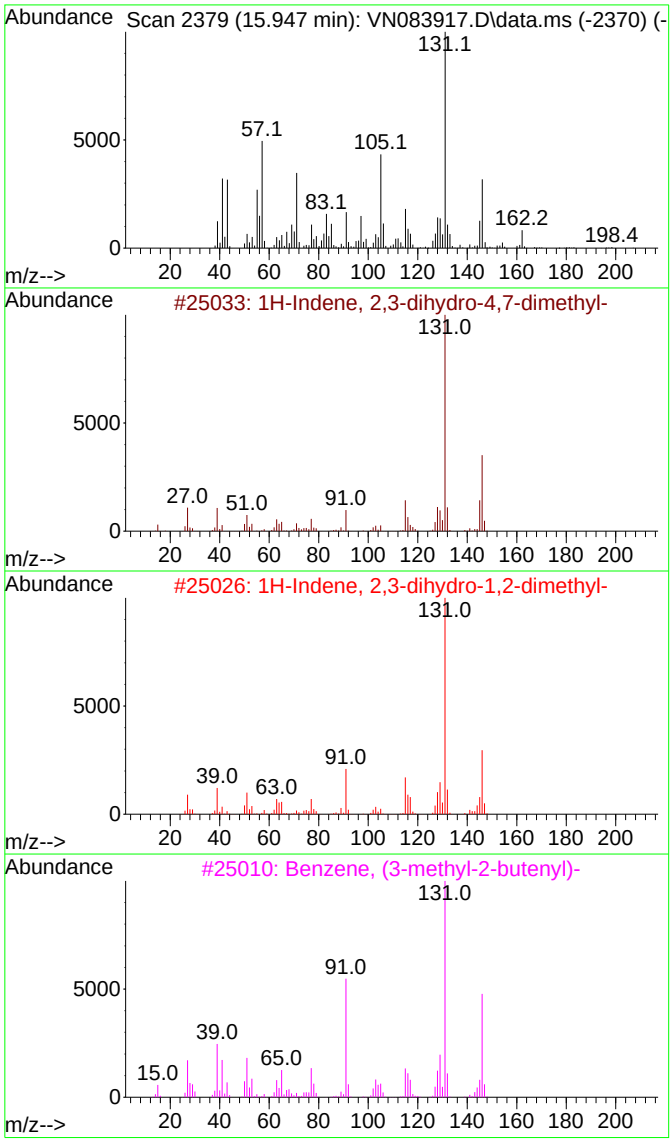
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

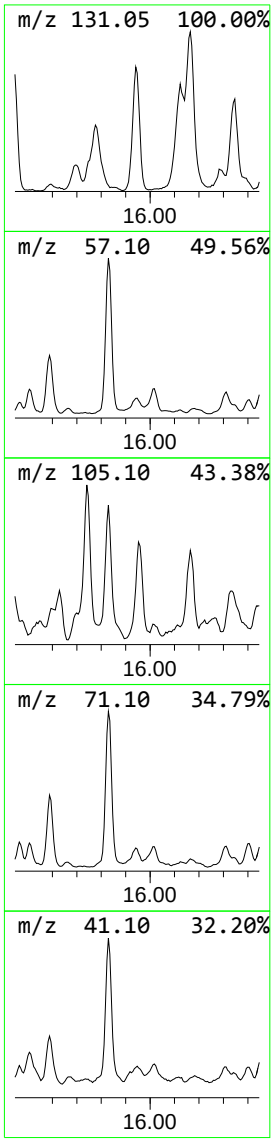
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	101.40 ug/l	2224740	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	86
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	86
3	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

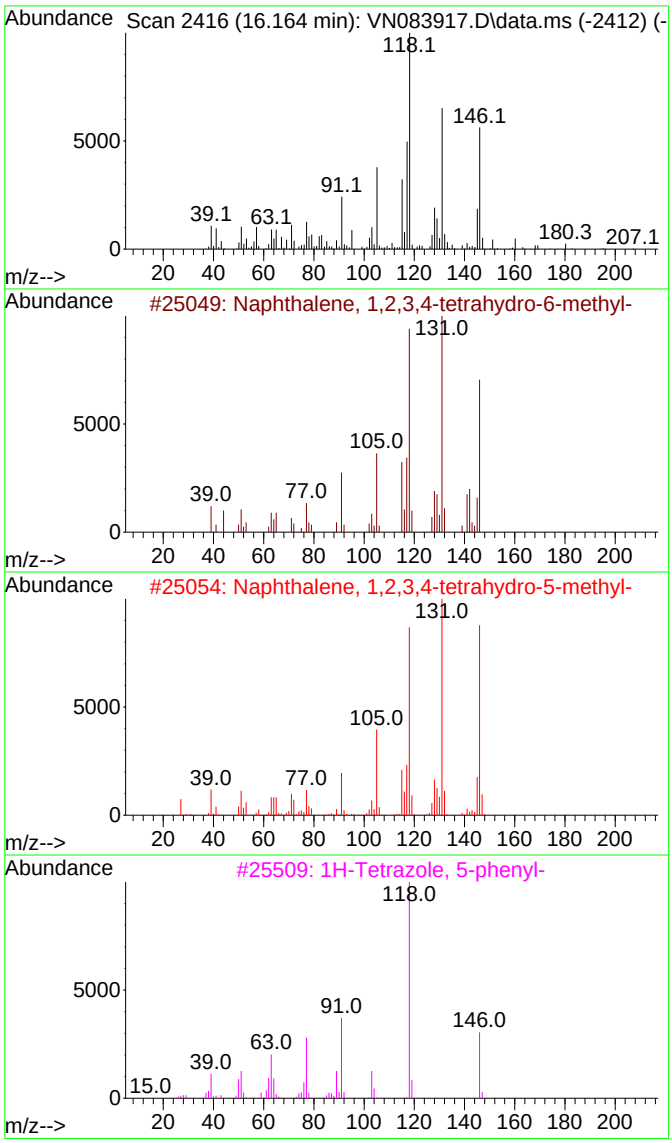
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

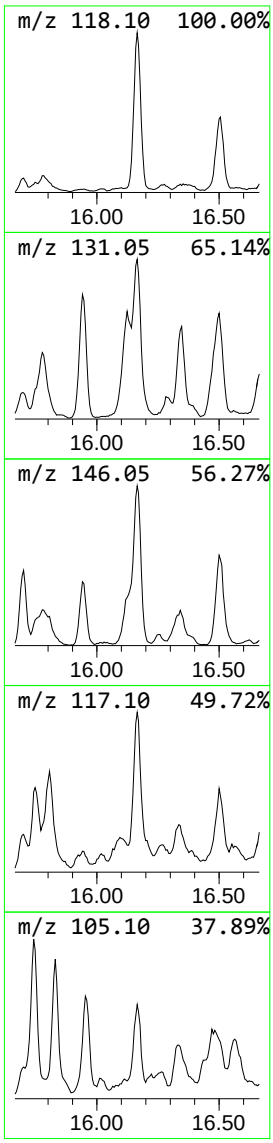
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.165	72.23 ug/l	1584720	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	91
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	72
3	1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	38
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	38
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

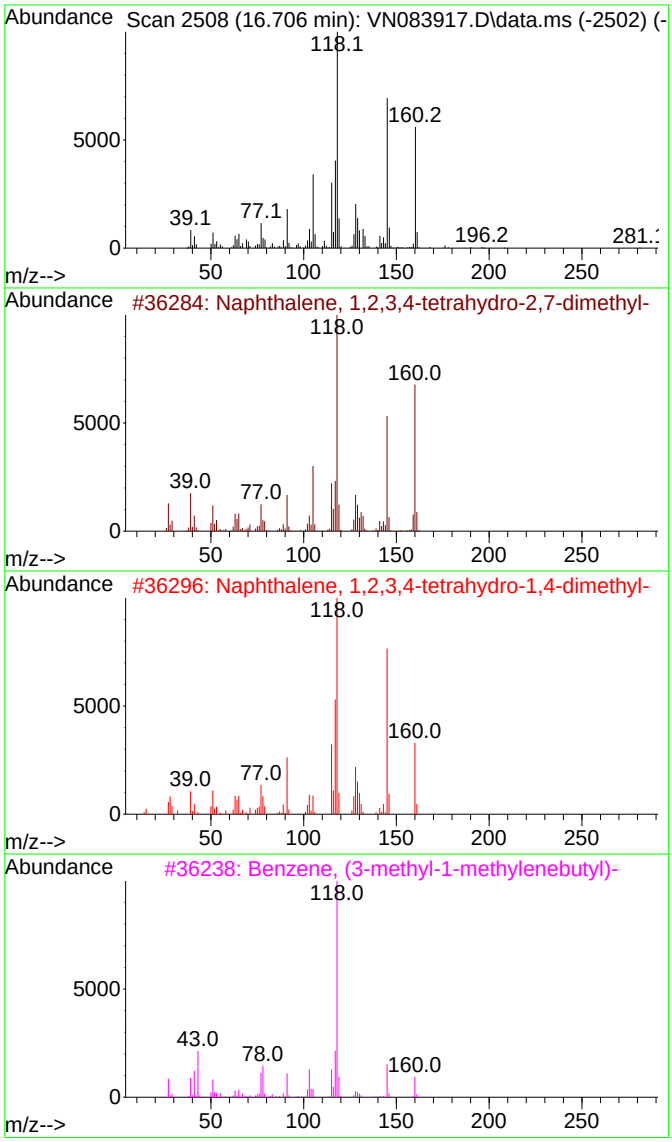
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

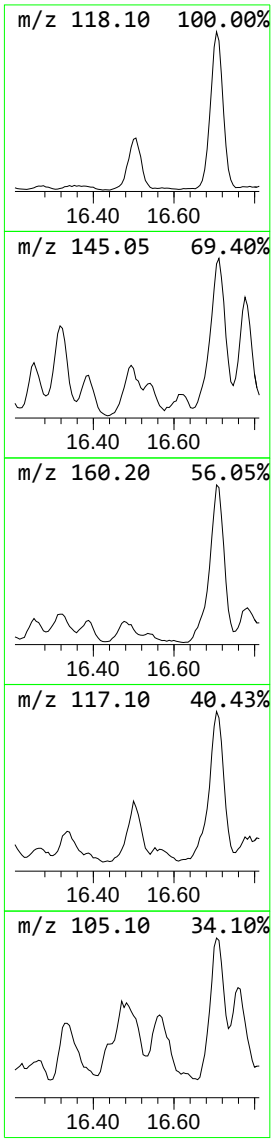
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.706	82.26 ug/l	1804960	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	83
3	Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	70
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	70
5	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091624\
Data File : VN083917.D
Acq On : 16 Sep 2024 15:03
Operator : JC\MD
Sample : P3936-01
Misc : 4.11g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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
Undecane	14.106	143.4	ug/l	3147510	4	13.794	1097050	50.0
Dodecane	14.959	205.7	ug/l	4513750	4	13.794	1097050	50.0
Undecane, 2,6-d...	15.076	186.6	ug/l	4093330	4	13.794	1097050	50.0
unknown15.429	15.429	72.0	ug/l	1579840	4	13.794	1097050	50.0
1-Iodo-2-methyl...	15.506	64.4	ug/l	1413930	4	13.794	1097050	50.0
Dodecane, 4,6-d...	15.588	104.6	ug/l	2295300	4	13.794	1097050	50.0
Tridecane	15.829	272.8	ug/l	5985850	4	13.794	1097050	50.0
1H-Indene, 2,3-...	15.947	101.4	ug/l	2224740	4	13.794	1097050	50.0
Naphthalene, 1,...	16.165	72.2	ug/l	1584720	4	13.794	1097050	50.0
Naphthalene, 1,...	16.706	82.3	ug/l	1804960	4	13.794	1097050	50.0