LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\METHOD\SOMULM103119WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.610	76	84	99	rVB	287140	353672	13.45%	1.276%
2	1.890	166	171	180	rVB	264131	289659	11.01%	1.045%
3	2.559	366	379	394	rBV	487503	801632	30.48%	2.891%
4	2.999	506	516	528	rBV2	11079	20522	0.78%	0.074%
5	3.131	555	557	561	rVB2	682	411	0.02%	0.001%
6	3.166	565	568	571	rBV2	924	733	0.03%	0.003%
7	3.221	573	585	601	rBV2	15963	39584	1.51%	0.143%
8	3.375	621	633	644	rVB3	8161	16270	0.62%	0.059%
9	3.587	696	699	702	rBV	1033	588	0.02%	0.002%
10	3.652	717	719	724	rVB3	552	418	0.02%	0.002%
11	3.706	730	736	738	rBV4	2430	2257	0.09%	0.008%
12	3.761	750	753	758	rVB4	690	468	0.02%	0.002%
13	3.787	758	761	765	rVB2	1034	603	0.02%	0.002%
14	3.851	779	781	784	rVB2	855	453	0.02%	0.002%
15	3.935	801	807	809	rBV3	419	377	0.01%	0.001%
16	3.986	821	823	828	rVB3	604	492	0.02%	0.002%
17	4.012	828	831	835	rBV3	688	609	0.02%	0.002%
18	4.060	842	846	849	rBV2	698	630	0.02%	0.002%
19	4.099	852	858	860	rBV2	545	564	0.02%	0.002%
20	4.147	867	873	875	rBV2	602	549	0.02%	0.002%
21	4.234	895	900	902	rBV	590	570	0.02%	0.002%
22	4.247	902	904	908	rVB	713	393	0.01%	0.001%
23	4.282	908	915	917	rBV3	509	442	0.02%	0.002%
24	4.501	980	983	985	rBV3	552	387	0.01%	0.001%
25	4.552	996	999	1003	rBV2	1174	1124	0.04%	0.004%
26	4.636	1020	1025	1027	rBV3	705	604	0.02%	0.002%
27	4.710	1027	1048	1080	rBV2	880174	2208061	83.96%	7.964%
28	4.903	1106	1108	1111	rVB3	793	452	0.02%	0.002%
29	4.983	1129	1133	1136	rBV4	1040	869	0.03%	0.003%
30	5.112	1155	1173	1196	rVV	444696	1043339	39.67%	3.763%
31	5.259	1215	1219	1229	rVB7	1721	2350	0.09%	0.008%
32	5.327	1235	1240	1248	rBV7	1973	2780	0.11%	0.010%
33	5.404	1256	1264	1266	rBV4	3451	4039	0.15%	0.015%
34	5.478	1285	1287	1290	rBV3	521	403	0.02%	0.001%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\METHOD\SOMULM103119WMA.M
Title : VOC Analysis

35	5.526	1298	1302	1306	rVB4	429	458	0.02%	0.002%
36	5.555	1310	1311	1318	rVB3	841	738	0.03%	0.003%
37	5.616	1325	1330	1341	rVB8	1616	2712	0.10%	0.010%
38	5.661	1341	1344	1348	rBV3	588	462	0.02%	0.002%
39	5.681	1348	1350	1354	rVB2	898	465	0.02%	0.002%
40	5.761	1354	1375	1398	rBV2	1058791	2629987	100.00%	9.485%
41	5.992	1444	1447	1450	rVB5	752	428	0.02%	0.002%
42	6.021	1451	1456	1458	rBV4	955	832	0.03%	0.003%
43	6.134	1487	1491	1492	rBV	891	634	0.02%	0.002%
44	6.163	1492	1500	1507	rVV10	4873	7752	0.29%	0.028%
45	6.208	1511	1514	1518	rVV3	640	499	0.02%	0.002%
46	6.288	1524	1539	1559	rBV	824728	1622130	61.68%	5.850%
47	6.481	1597	1599	1602	rBV3	730	397	0.02%	0.001%
48	6.504	1604	1606	1609	rVB3	1250	652	0.02%	0.002%
49	6.520	1609	1611	1613	rBV2	925	411	0.02%	0.001%
50	6.578	1613	1629	1646	rBV	970266	1843366	70.09%	6.648%
51	6.732	1662	1677	1705	rBV	604211	1236833	47.03%	4.461%
52	7.057	1775	1778	1781	rVB4	794	524	0.02%	0.002%
53	7.073	1781	1783	1786	rBV3	677	497	0.02%	0.002%
54	7.095	1786	1790	1792	rVV3	1184	757	0.03%	0.003%
55	7.230	1818	1832	1852	rBV9	13809	35309	1.34%	0.127%
56	7.378	1875	1878	1884	rVB4	913	720	0.03%	0.003%
57	7.443	1894	1898	1900	rBV3	645	477	0.02%	0.002%
58	7.529	1912	1925	1932	rBV7	2888	6137	0.23%	0.022%
59	7.603	1934	1948	1967	rBV	313754	586840	22.31%	2.117%
60	7.771	1998	2000	2003	rBV3	769	603	0.02%	0.002%
61	7.822	2009	2016	2017	rBV7	2201	2114	0.08%	0.008%
62	7.883	2030	2035	2037	rBV4	10870	10706	0.41%	0.039%
63	7.931	2038	2050	2066	rVB	1113093	1961951	74.60%	7.076%
64	8.160	2114	2121	2126	rVB4	9299	11772	0.45%	0.042%
65	8.217	2127	2139	2151	rBV2	219776	421642	16.03%	1.521%
66	8.398	2184	2195	2205	rBV5	17348	31165	1.18%	0.112%
67	8.462	2208	2215	2220	rVV8	2583	3430	0.13%	0.012%
68	8.584	2238	2253	2267	rBV	1006687	1740546	66.18%	6.278%
69	8.687	2271	2285	2311	rBV	749690	1597019	60.72%	5.760%
70	8.825	2322	2328	2341	rVB7	35296	66813	2.54%	0.241%
71	8.893	2343	2349	2357	rVB4	29289	43758	1.66%	0.158%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\METHOD\SOMULM103119WMA.M
Title : VOC Analysis

72	8.954	2358	2368	2377	rBV4	62503	113394	4.31%	0.409%
73	9.098	2404	2413	2420	rBV6	13362	22465	0.85%	0.081%
74	9.147	2421	2428	2433	rVV3	14851	21470	0.82%	0.077%
75	9.192	2433	2442	2450	rVV4	74709	130804	4.97%	0.472%
76	9.240	2451	2457	2471	rVB4	61212	99514	3.78%	0.359%
77	9.320	2475	2482	2484	rBV5	3424	4444	0.17%	0.016%
78	9.359	2485	2494	2504	rBV2	47421	74314	2.83%	0.268%
79	9.452	2510	2523	2544	rBV	1232595	2147582	81.66%	7.746%
80	9.597	2556	2568	2579	rBV4	90254	174338	6.63%	0.629%
81	9.658	2580	2587	2591	rBV5	20385	31006	1.18%	0.112%
82	9.722	2600	2607	2617	rBV2	160062	277336	10.55%	1.000%
83	9.906	2651	2664	2678	rBV10	18091	46897	1.78%	0.169%
84	9.973	2682	2685	2695	rVB8	4689	6976	0.27%	0.025%
85	10.060	2697	2712	2722	rBV7	53969	142128	5.40%	0.513%
86	10.131	2726	2734	2747	rVB	117209	208924	7.94%	0.754%
87	10.272	2769	2778	2793	rBV3	64380	135792	5.16%	0.490%
88	10.491	2839	2846	2858	rVB3	18981	37129	1.41%	0.134%
89	10.574	2859	2872	2882	rBV9	32057	81475	3.10%	0.294%
90	10.790	2927	2939	2950	rBV	875902	1519743	57.79%	5.481%
91	10.973	2991	2996	3006	rBV3	15226	22346	0.85%	0.081%
92	11.134	3040	3046	3062	rVB4	114174	203570	7.74%	0.734%
93	11.436	3133	3140	3148	rVB2	64809	88035	3.35%	0.318%
94	11.838	3254	3265	3279	rBV	1003512	1719075	65.36%	6.200%
95	12.221	3371	3384	3398	rBV	965911	1640114	62.36%	5.915%
96	12.346	3417	3423	3434	rVB2	41429	55095	2.09%	0.199%
97	12.909	3592	3598	3604	rBV6	7711	9820	0.37%	0.035%
98	13.452	3760	3767	3772	rBV7	7702	12267	0.47%	0.044%
99	13.864	3889	3895	3900	rBV8	5977	8023	0.31%	0.029%
100	14.105	3963	3970	3978	rBV2	16839	24735	0.94%	0.089%

Sum of corrected areas: 27726651

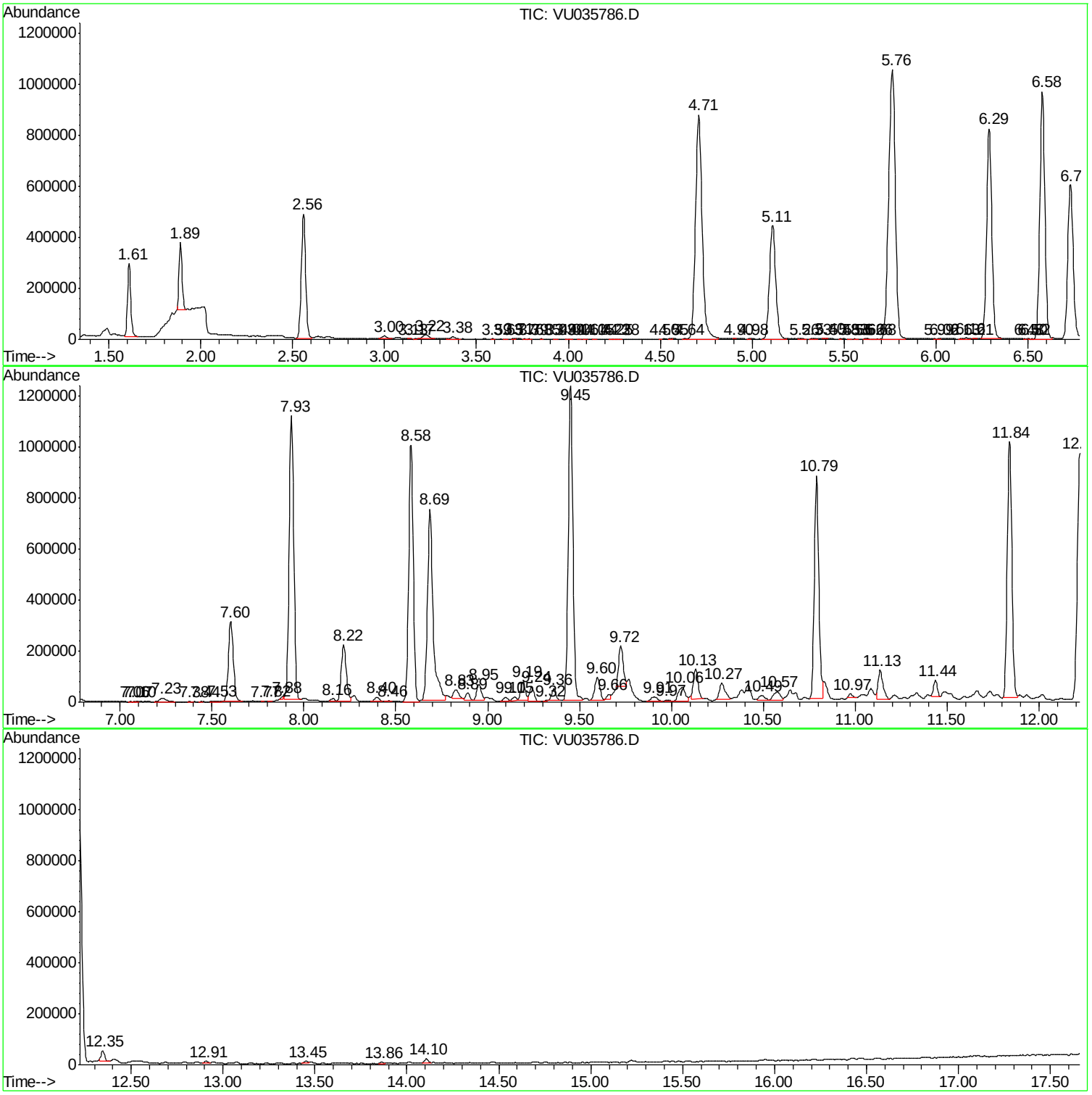
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

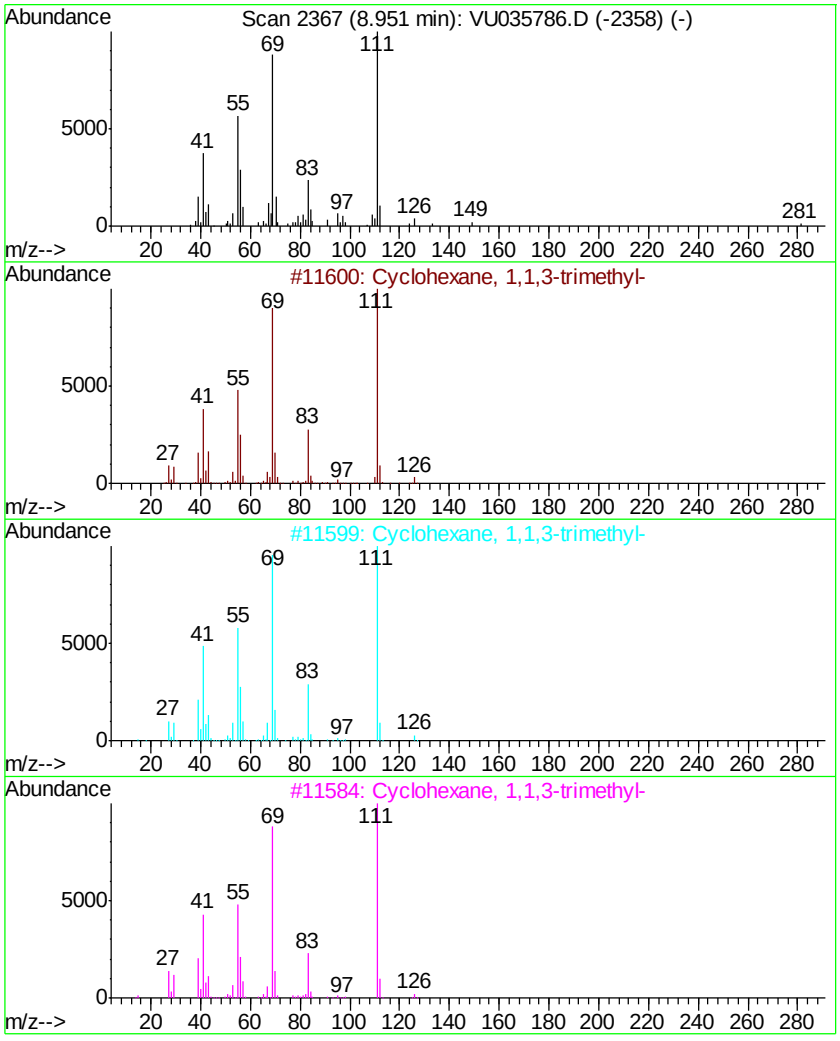
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

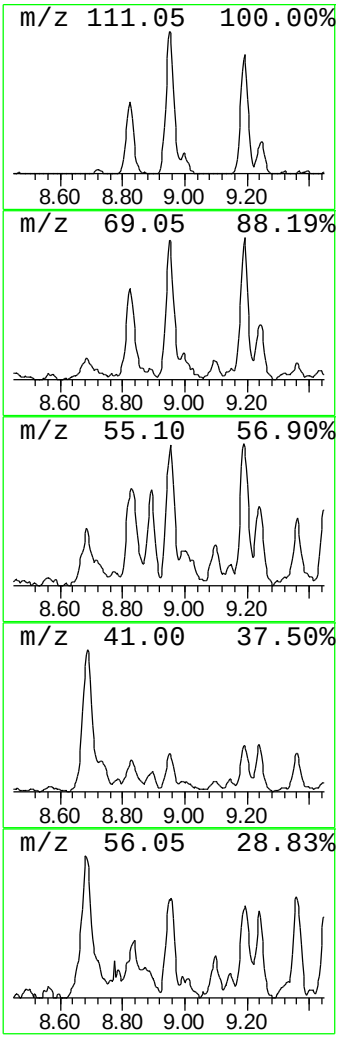
****

Peak Number 2 (DEL) Alkane: Cyclic8.95 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	2.64 ug/L	113394	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	94
2	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	93
3	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	93
4	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
5	Cyclooctane, butyl-	168	C12H24	016538-93-5	78





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

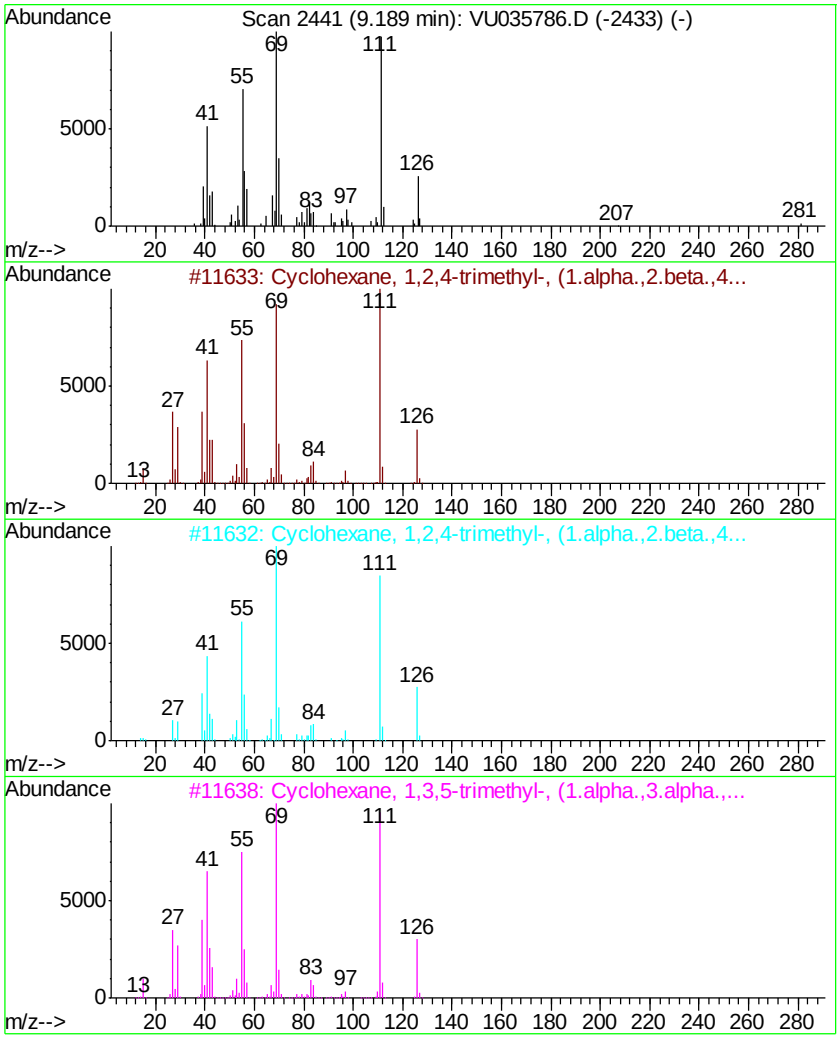
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

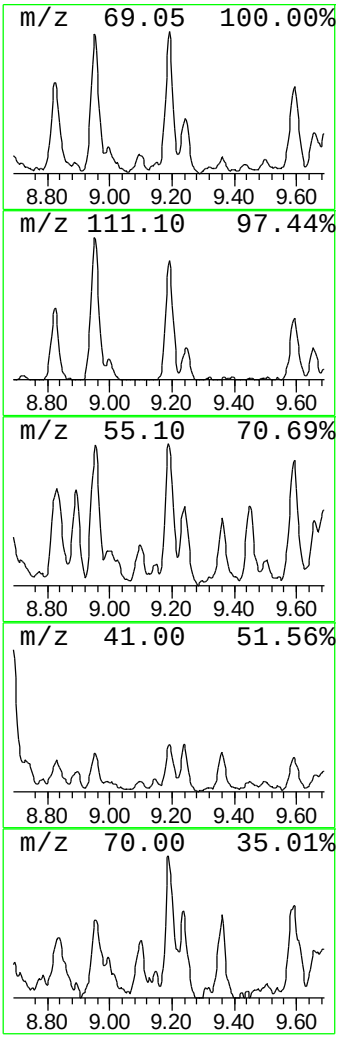
****

Peak Number 3 (DEL) Alkane: Cyclic9.19 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	3.05 ug/L	130804	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	94
2	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	94
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	90
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	83
5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	83





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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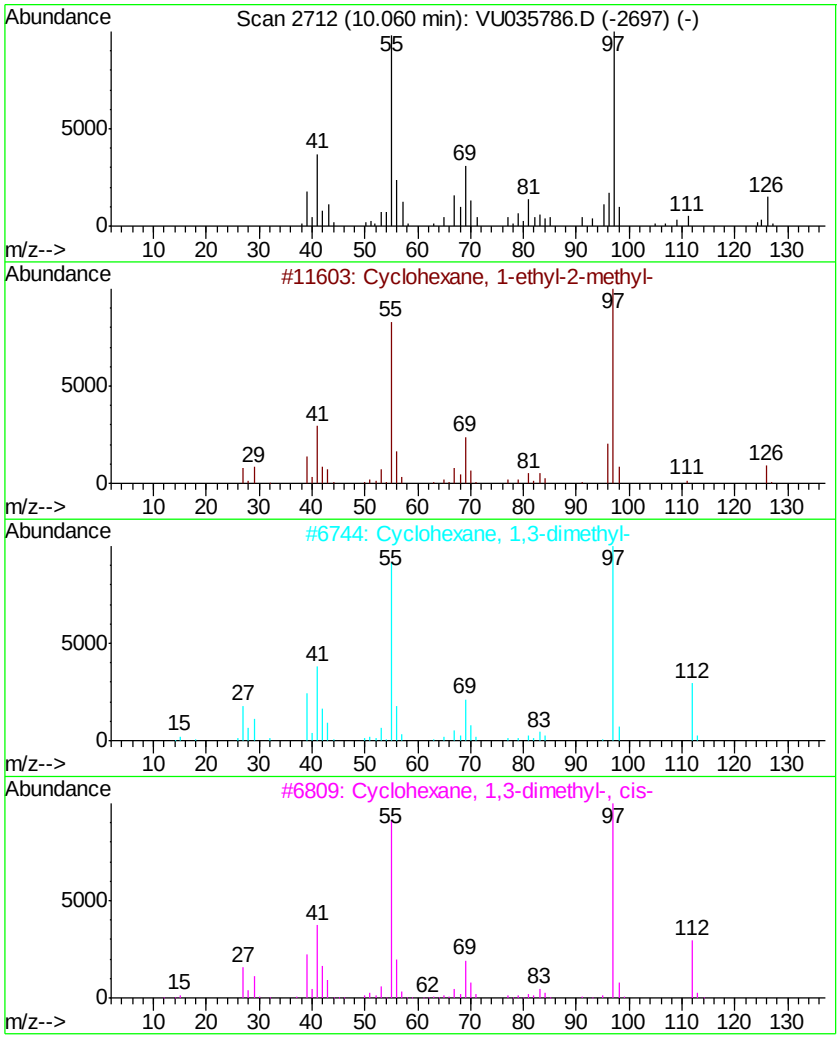
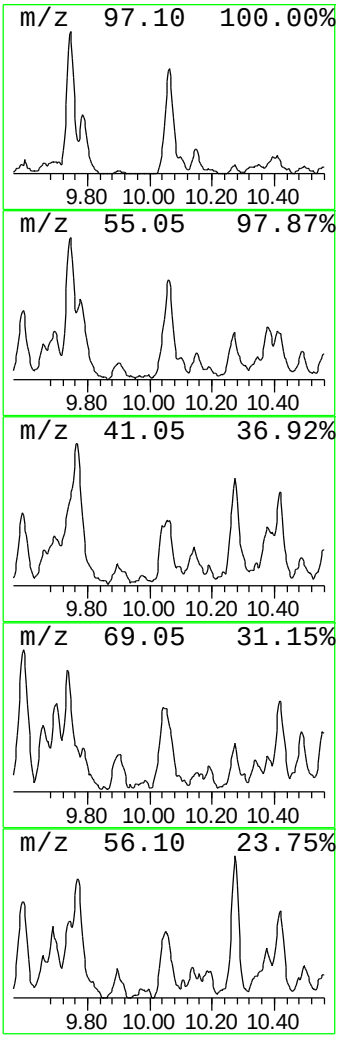
Peak Number 4 (DEL) Alkane: Cyclic10.06 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	3.31 ug/L	142128	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	87
2	Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	64
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	64
4	4-Octen-3-one	126	C8H14O	014129-48-7	58
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

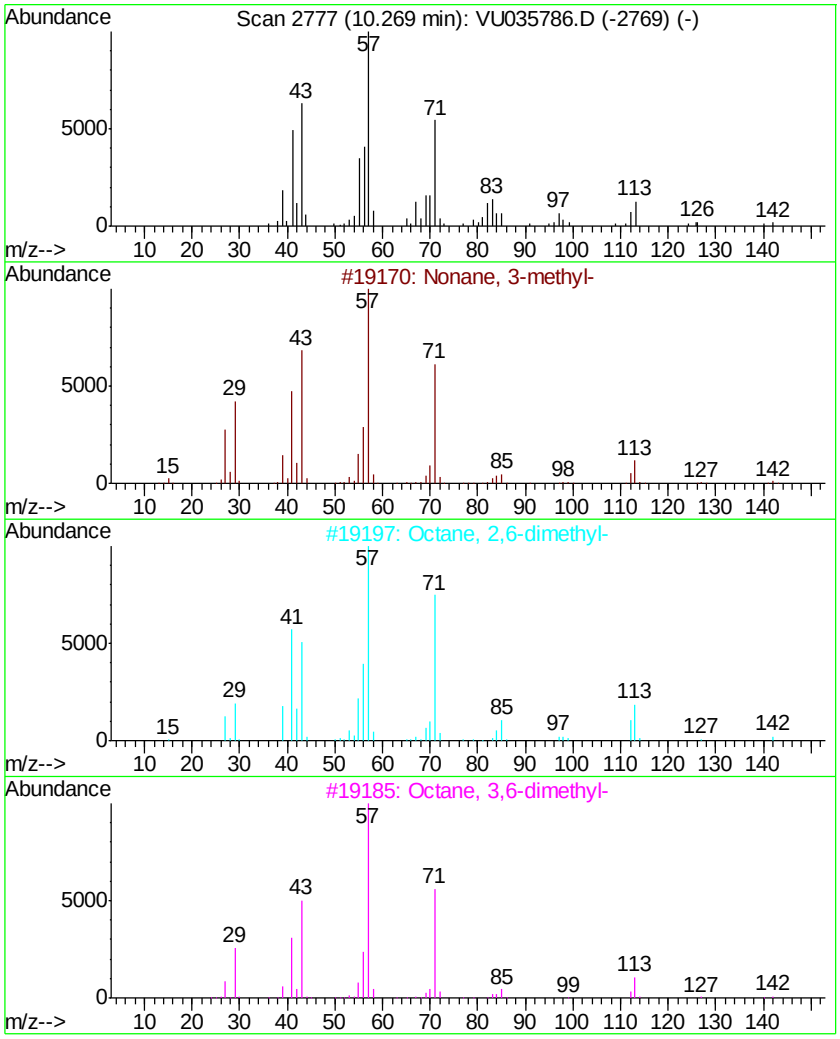
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

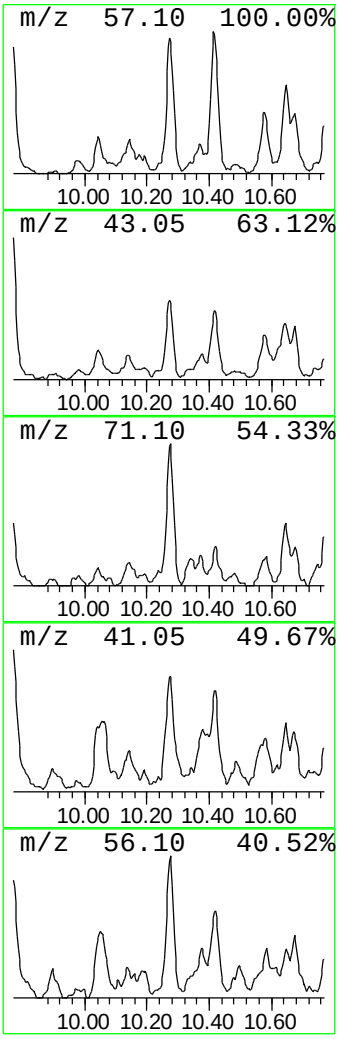
****

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	3.16 ug/L	135792	Chlorobenzene-d5	9.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	70
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	58
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	53
5	Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

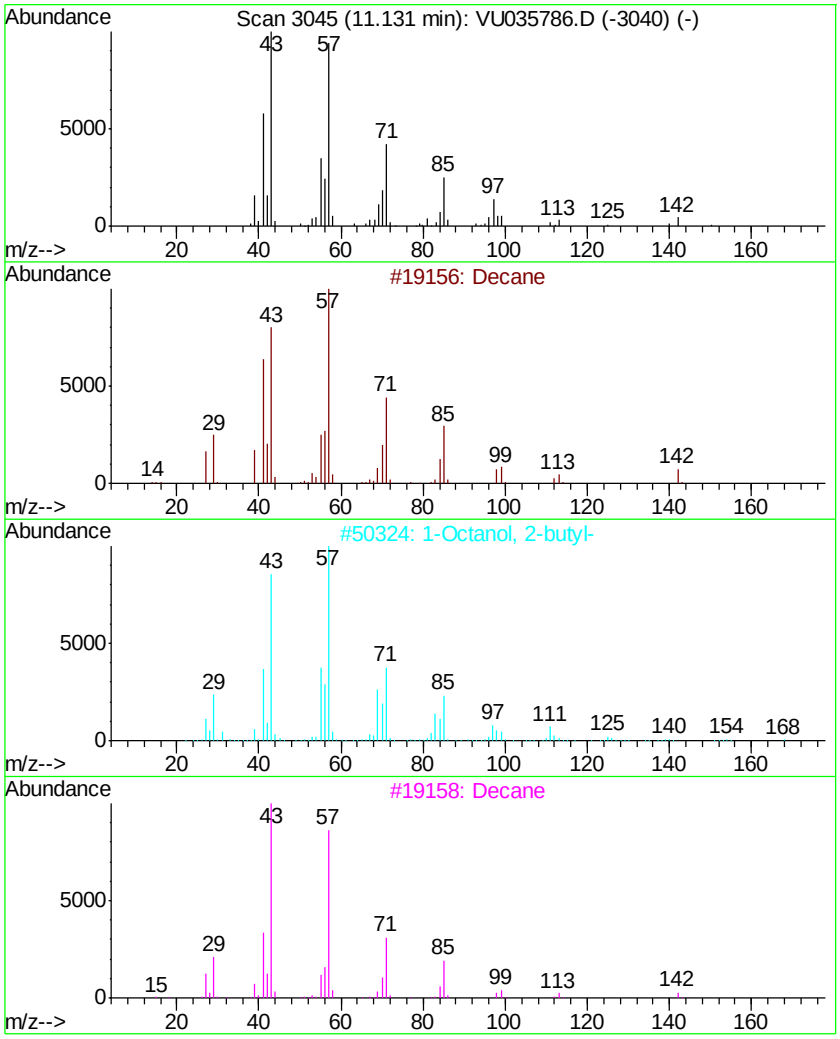
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

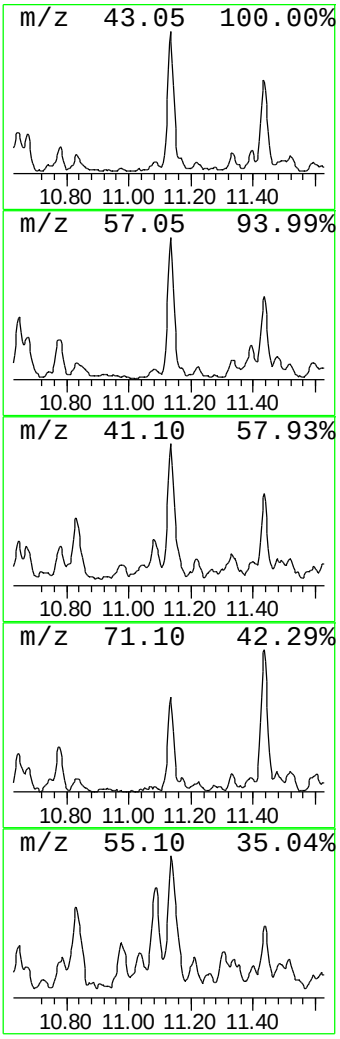
****

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	5.92 ug/L	203570	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	90
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	83
3	Decane	142	C10H22	000124-18-5	81
4	Decane	142	C10H22	000124-18-5	78
5	Undecane	156	C11H24	001120-21-4	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

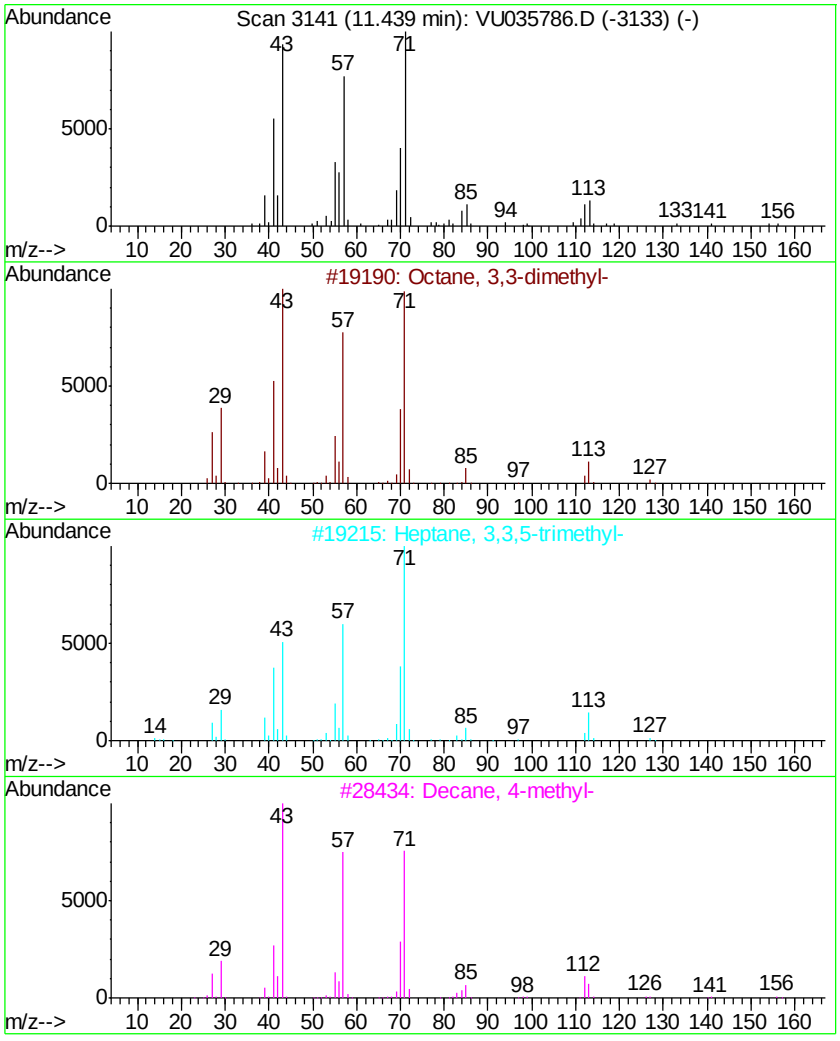
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

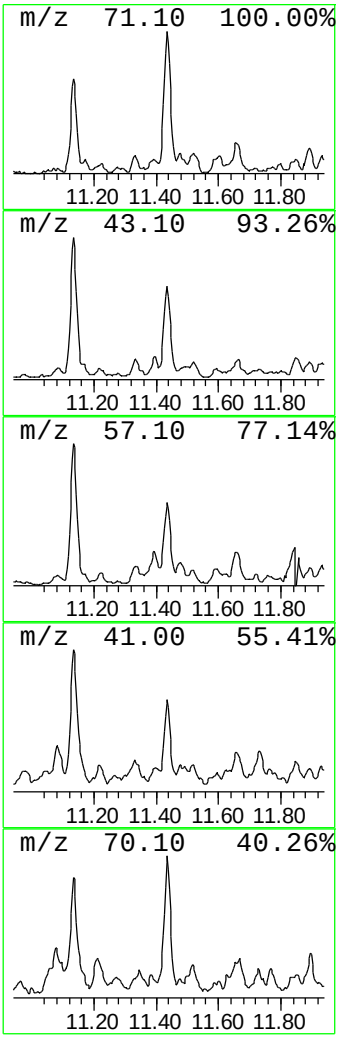
****

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	2.56 ug/L	88035	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
2	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
3	Decane, 4-methyl-	156	C11H24	002847-72-5	68
4	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
5	Decane, 4-methyl-	156	C11H24	002847-72-5	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU112019\
Data File : VU035786.D
Acq On : 20 Nov 2019 13:54
Operator : JC/SP
Sample : K5811-03ME
Misc : 5.83g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : ETOP1ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM103119WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Cyc...	8.95	2.6	ug/L	113394	2	9.45	2147580	50.0
(DEL) Alkane: Cyc...	9.19	3.0	ug/L	130804	2	9.45	2147580	50.0
(DEL) Alkane: Cyc...	10.06	3.3	ug/L	142128	2	9.45	2147580	50.0
(DEL) Alkane: Str...	10.27	3.2	ug/L	135792	2	9.45	2147580	50.0
(DEL) Alkane: Str...	11.13	5.9	ug/L	203570	3	11.84	1719080	50.0
(DEL) Alkane: Str...	11.44	2.6	ug/L	88035	3	11.84	1719080	50.0