LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

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_X\Method\SFAMXLM061322WMA.M
Title : VOC Analysis

Signal : TIC: VX029428.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	12	rVB3	2733	2969	0.20%	0.023%
2	1.288	30	33	40	rVV3	6013	9925	0.66%	0.077%
3	1.368	42	46	55	rVV	154680	204821	13.71%	1.587%
4	1.636	87	90	92	rBV	7380	9859	0.66%	0.076%
5	1.666	92	95	103	rVV	62645	94493	6.33%	0.732%
6	1.727	103	105	109	rVB4	4565	4891	0.33%	0.038%
7	2.179	176	179	189	rVB5	3275	6956	0.47%	0.054%
8	2.282	189	196	205	rBV	297881	488328	32.69%	3.783%
9	2.380	206	212	217	rBV3	3262	9173	0.61%	0.071%
10	2.794	274	280	285	rVB5	3932	8383	0.56%	0.065%
11	2.953	296	306	319	rBV	16599	52950	3.54%	0.410%
12	3.428	377	384	389	rVV4	3245	7843	0.53%	0.061%
13	4.507	549	561	589	rBV	66386	363634	24.34%	2.817%
14	5.062	640	652	671	rBV2	187181	593219	39.71%	4.595%
15	5.465	713	718	721	rBV4	1630	3687	0.25%	0.029%
16	5.971	789	801	819	rVV2	527147	1493692	100.00%	11.571%
17	6.379	858	868	890	rVV3	8670	31099	2.08%	0.241%
18	6.605	898	905	914	rVV5	3738	9753	0.65%	0.076%
19	6.763	921	931	951	rVV	443177	1073152	71.85%	8.313%
20	7.129	982	991	1001	rBV3	33096	82432	5.52%	0.639%
21	7.214	1001	1005	1013	rVV4	3874	11284	0.76%	0.087%
22	7.312	1013	1021	1039	rVB	299455	654334	43.81%	5.069%
23	7.482	1043	1049	1057	rBV6	1886	4148	0.28%	0.032%
24	7.964	1117	1128	1136	rBV7	5209	14197	0.95%	0.110%
25	8.269	1174	1178	1182	rVV5	2752	3845	0.26%	0.030%
26	8.330	1182	1188	1200	rVB	177701	293287	19.64%	2.272%
27	8.434	1201	1205	1211	rVB5	1694	3143	0.21%	0.024%
28	8.653	1228	1241	1248	rBV	750466	1220620	81.72%	9.456%
29	8.720	1248	1252	1256	rBV	14389	19881	1.33%	0.154%
30	8.848	1270	1273	1278	rVB6	1939	2899	0.19%	0.022%
31	8.909	1278	1283	1286	rBV2	12514	17652	1.18%	0.137%
32	8.952	1286	1290	1299	rVB	118290	186018	12.45%	1.441%
33	9.104	1308	1315	1320	rBV6	1948	3751	0.25%	0.029%
34	9.281	1338	1344	1350	rBV5	3125	5917	0.40%	0.046%
35	9.397	1357	1363	1377	rBV	330380	714778	47.85%	5.537%
36	9.531	1381	1385	1387	rBV2	10269	16102	1.08%	0.125%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

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_X\Method\SFAMXLM061322WMA.M
Title : VOC Analysis

37	9.616	1395	1399	1409	rVB2	6469	12830	0.86%	0.099%
38	9.720	1411	1416	1419	rBV4	2945	4235	0.28%	0.033%
39	9.763	1419	1423	1428	rVB5	1845	3392	0.23%	0.026%
40	9.817	1428	1432	1436	rBV5	2021	3874	0.26%	0.030%
41	9.903	1442	1446	1451	rVB2	4292	6799	0.46%	0.053%
42	10.006	1457	1463	1466	rBV3	4676	7816	0.52%	0.061%
43	10.055	1466	1471	1482	rVB	883829	1209963	81.00%	9.373%
44	10.201	1490	1495	1502	rVB5	2026	4179	0.28%	0.032%
45	10.281	1502	1508	1509	rBV4	2253	4097	0.27%	0.032%
46	10.305	1509	1512	1517	rVB2	5787	8516	0.57%	0.066%
47	10.360	1517	1521	1530	rVB2	13221	18614	1.25%	0.144%
48	10.458	1530	1537	1543	rBV4	2263	3410	0.23%	0.026%
49	10.592	1552	1559	1562	rBV6	2169	3868	0.26%	0.030%
50	10.659	1565	1570	1571	rBV2	2160	3371	0.23%	0.026%
51	10.781	1582	1590	1594	rBV2	10406	15651	1.05%	0.121%
52	10.866	1599	1604	1607	rBV4	9038	15678	1.05%	0.121%
53	10.957	1614	1619	1624	rVB5	2263	3633	0.24%	0.028%
54	11.031	1628	1631	1635	rVV4	3080	3988	0.27%	0.031%
55	11.085	1635	1640	1642	rVV4	7131	9667	0.65%	0.075%
56	11.116	1642	1645	1650	rVB3	7744	12602	0.84%	0.098%
57	11.195	1650	1658	1667	rBV	499641	690501	46.23%	5.349%
58	11.390	1687	1690	1693	rVV5	2560	3410	0.23%	0.026%
59	11.427	1693	1696	1700	rVV4	3603	6201	0.42%	0.048%
60	11.476	1700	1704	1711	rVB	43990	55758	3.73%	0.432%
61	11.634	1726	1730	1734	rVB6	3838	5175	0.35%	0.040%
62	11.683	1734	1738	1740	rBV3	3575	4777	0.32%	0.037%
63	11.713	1740	1743	1746	rVV	23665	27301	1.83%	0.211%
64	11.750	1746	1749	1759	rVB5	11006	23238	1.56%	0.180%
65	11.841	1759	1764	1767	rBV4	3923	6953	0.47%	0.054%
66	11.890	1770	1772	1776	rVB4	7017	7595	0.51%	0.059%
67	11.933	1776	1779	1784	rBV4	18504	27643	1.85%	0.214%
68	12.024	1789	1794	1800	rVV	977004	1207413	80.83%	9.353%
69	12.073	1800	1802	1804	rVV2	8982	9447	0.63%	0.073%
70	12.104	1804	1807	1812	rVV3	9925	13824	0.93%	0.107%
71	12.165	1812	1817	1822	rVB5	8255	19094	1.28%	0.148%
72	12.244	1826	1830	1831	rBV4	2384	3301	0.22%	0.026%
73	12.323	1837	1843	1849	rBV	798312	994404	66.57%	7.703%
74	12.427	1855	1860	1864	rBV	88491	98218	6.58%	0.761%
75	12.549	1877	1880	1882	rBV3	3184	4100	0.27%	0.032%
76	12.585	1883	1886	1891	rVB5	8691	13758	0.92%	0.107%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

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_X\Method\SFAMXLM061322WMA.M
Title : VOC Analysis

77	12.634	1891	1894	1897	rVB5	2714	3311	0.22%	0.026%
78	12.683	1898	1902	1906	rBV4	10308	12872	0.86%	0.100%
79	12.860	1927	1931	1934	rBV2	60071	75163	5.03%	0.582%
80	12.945	1943	1945	1947	rBV3	5474	5251	0.35%	0.041%
81	12.975	1947	1950	1955	rVB3	12135	13540	0.91%	0.105%
82	13.042	1958	1961	1966	rBV4	10342	13102	0.88%	0.101%
83	13.268	1994	1998	2002	rBV	100207	117727	7.88%	0.912%
84	13.384	2014	2017	2021	rBV	42674	53626	3.59%	0.415%
85	13.536	2039	2042	2044	rBV4	3381	3578	0.24%	0.028%
86	13.701	2063	2069	2072	rBV5	17371	30755	2.06%	0.238%
87	13.768	2078	2080	2083	rBV3	6314	6315	0.42%	0.049%
88	13.798	2083	2085	2088	rVV4	9519	10299	0.69%	0.080%
89	13.841	2088	2092	2096	rVB2	22309	31516	2.11%	0.244%
90	14.042	2121	2125	2128	rVB	76005	85779	5.74%	0.665%
91	14.103	2133	2135	2138	rBV3	9361	8552	0.57%	0.066%
92	14.268	2158	2162	2164	rBV4	5140	7156	0.48%	0.055%
93	14.615	2216	2219	2222	rBV2	15092	16941	1.13%	0.131%
94	14.670	2226	2228	2234	rVB7	7738	9426	0.63%	0.073%
95	14.756	2239	2242	2246	rVB	38670	41174	2.76%	0.319%
96	15.134	2302	2304	2308	rVB2	6161	6764	0.45%	0.052%
97	15.213	2315	2317	2320	rVB4	7346	6335	0.42%	0.049%
98	15.493	2359	2363	2368	rVB2	16477	23754	1.59%	0.184%
99	15.646	2384	2388	2393	rVB4	7205	12843	0.86%	0.099%
100	16.383	2504	2509	2516	rVB10	5218	11595	0.78%	0.090%

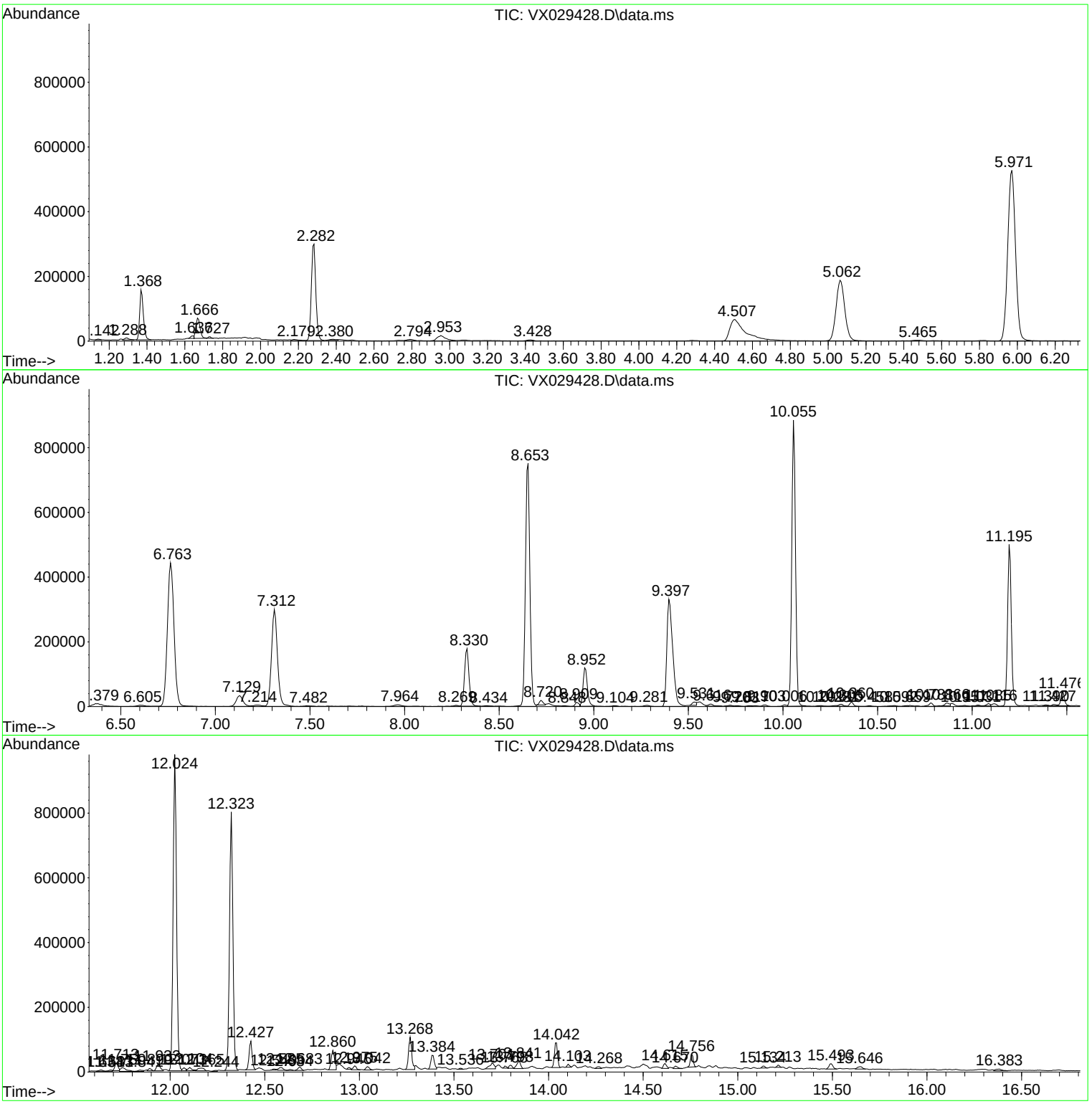
Sum of corrected areas: 12908783

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

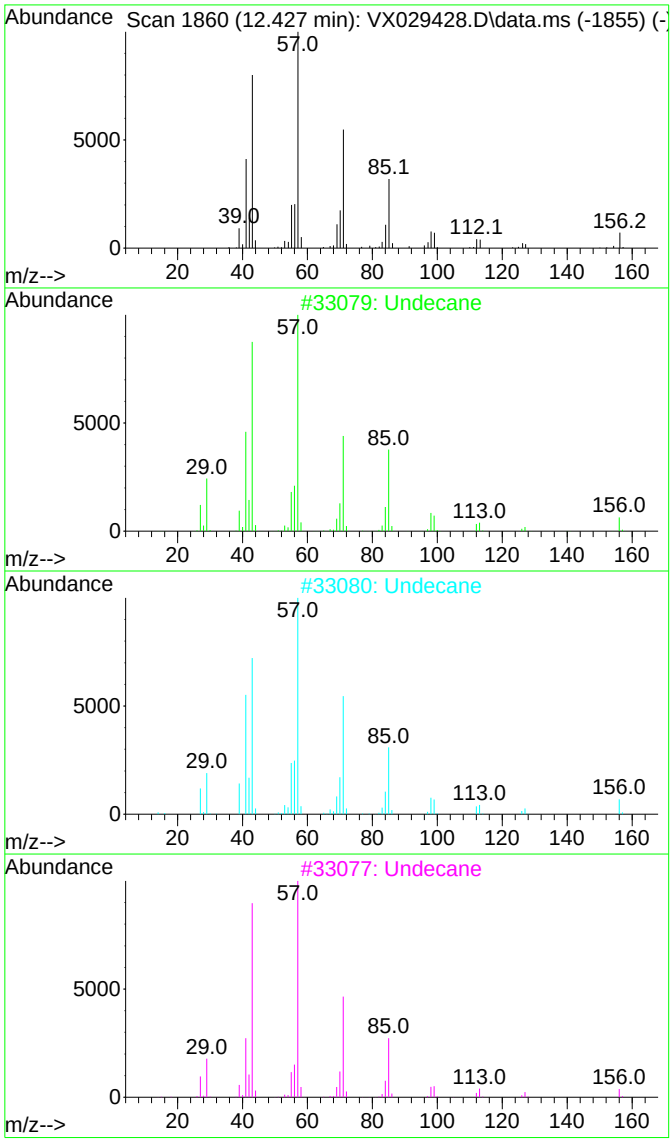
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

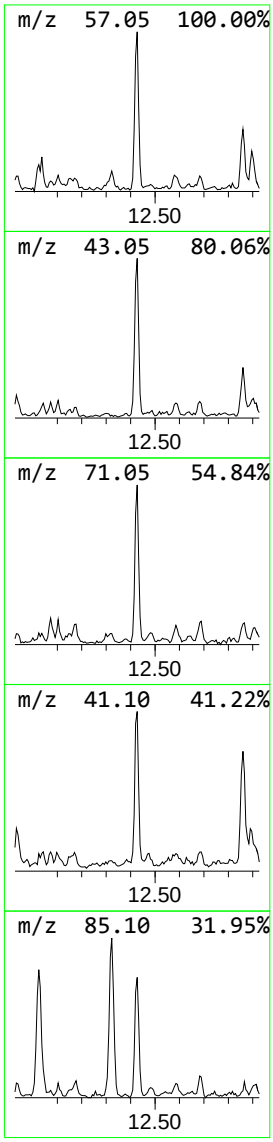
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	4.07 ug/L	98218	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	95
2	Undecane	156	C11H24	001120-21-4	94
3	Undecane	156	C11H24	001120-21-4	91
4	Tetradecane	198	C14H30	000629-59-4	86
5	Undecane	156	C11H24	001120-21-4	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

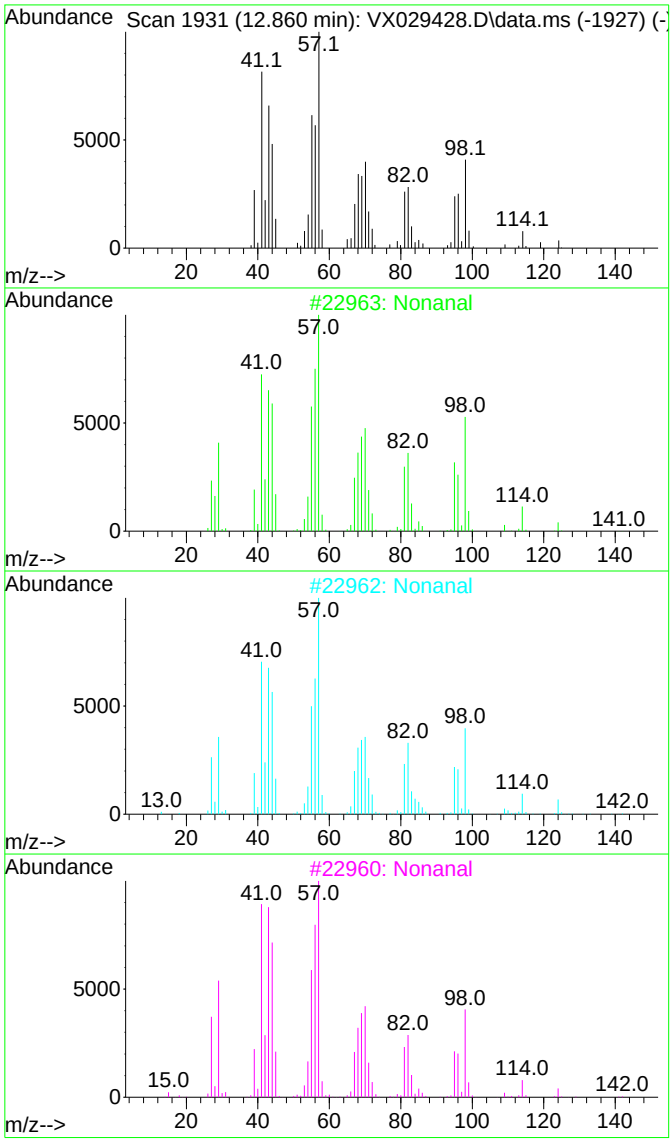
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

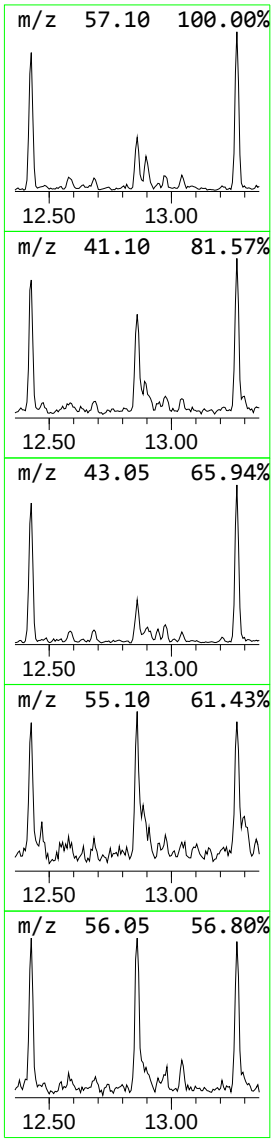
****

Peak Number 4 Nonanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	3.11 ug/L	75163	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	91
3	Nonanal	142	C9H18O	000124-19-6	90
4	Nonanal	142	C9H18O	000124-19-6	87
5	Cycloheptane	98	C7H14	000291-64-5	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

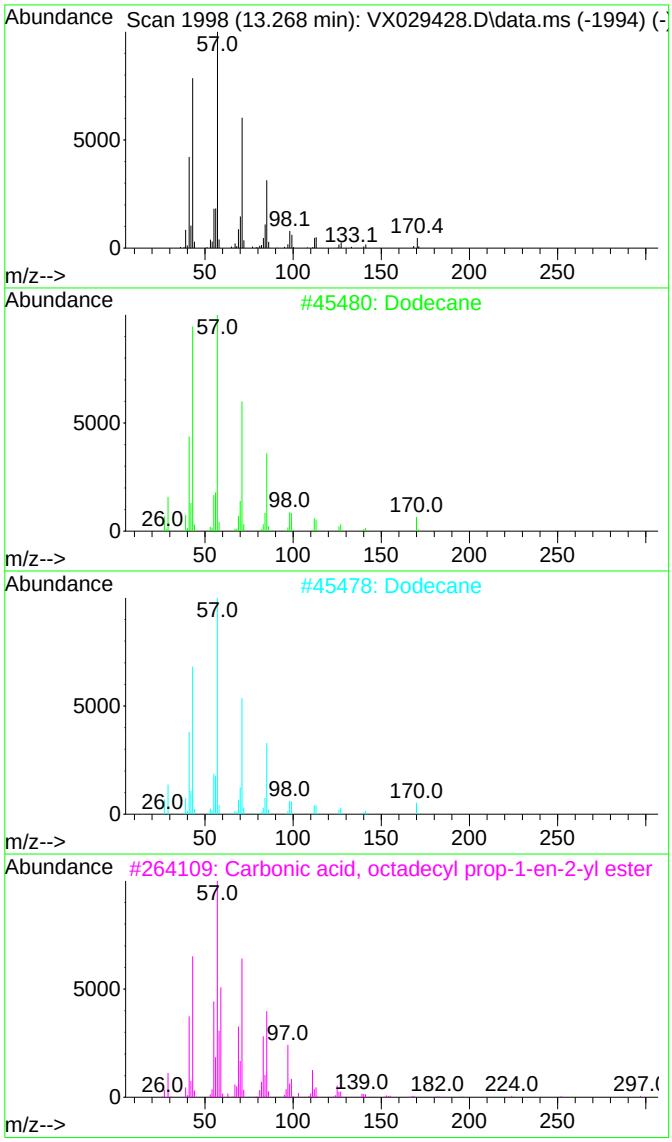
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

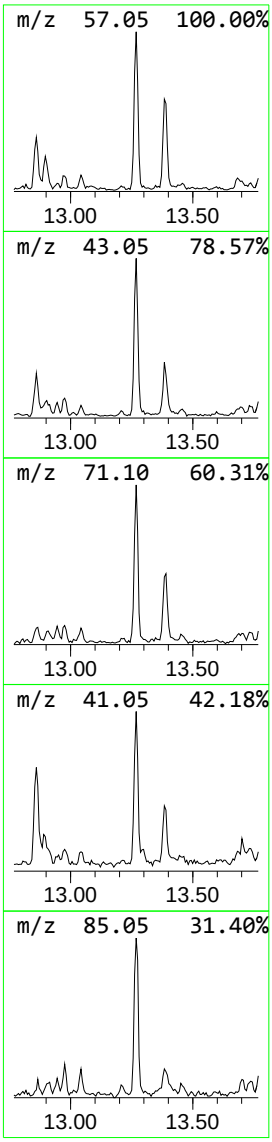
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	4.88 ug/L	117727	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Dodecane	170	C12H26	000112-40-3	96
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	90
5	Tetradecane	198	C14H30	000629-59-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

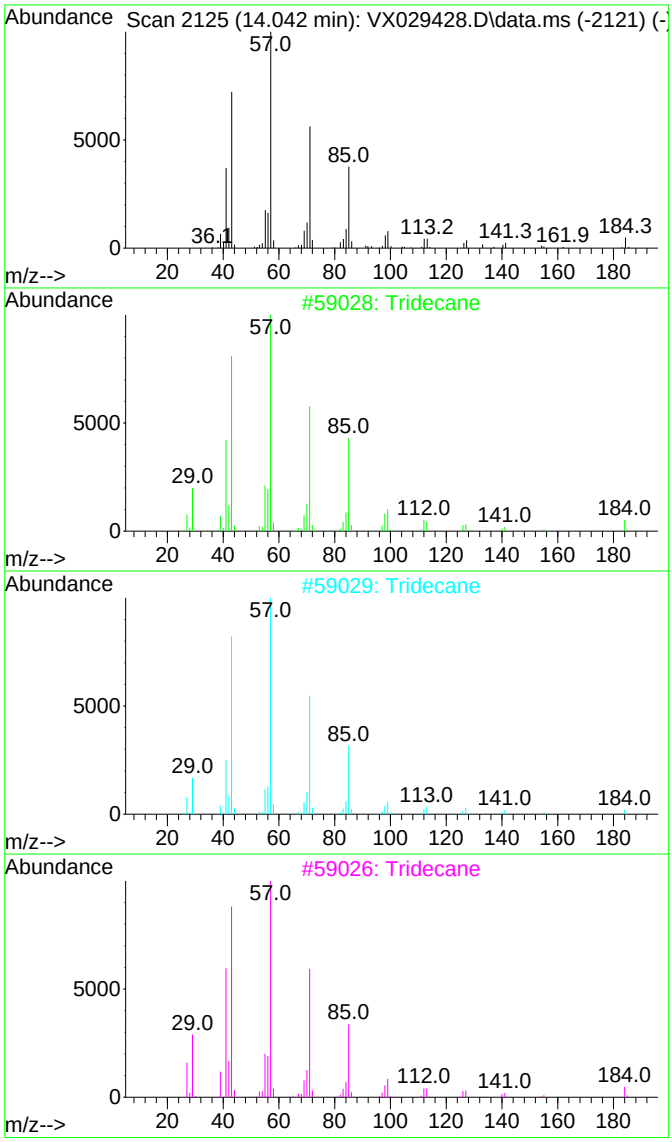
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

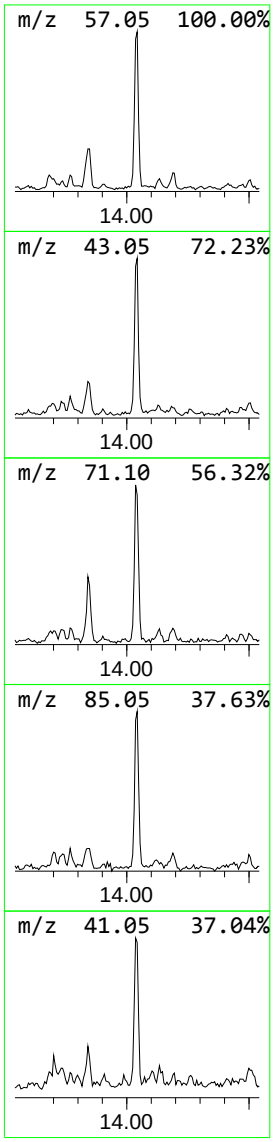
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.042	3.55 ug/L	85779	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	98
2	Tridecane	184	C13H28	000629-50-5	95
3	Tridecane	184	C13H28	000629-50-5	94
4	Tridecane	184	C13H28	000629-50-5	91
5	Tetradecane	198	C14H30	000629-59-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061322\
Data File : VX029428.D
Acq On : 13 Jun 2022 21:16
Operator : JC/MD
Sample : N3226-03ME
Misc : 6.62g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4L4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM061322WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	12.427	4.1	ug/L	98218	3	12.024	1207410	50.0
Nonanal	12.860	3.1	ug/L	75163	3	12.024	1207410	50.0
(DEL) Alkane: S...	13.268	4.9	ug/L	117727	3	12.024	1207410	50.0
(DEL) Alkane: S...	14.042	3.5	ug/L	85779	3	12.024	1207410	50.0