LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

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\SFAMULM052924WMA.M
Title : VOC Analysis

Signal : TIC: VU059374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	65	rBV2	1656	1734	0.25%	0.033%
2	1.592	86	94	117	rVB	39257	63168	8.97%	1.215%
3	1.817	133	164	165	rBV8	43765	150564	21.37%	2.895%
4	2.354	329	331	341	rVB9	1264	1929	0.27%	0.037%
5	2.538	376	388	406	rVB	94515	152071	21.58%	2.924%
6	2.631	411	417	419	rBV3	822	853	0.12%	0.016%
7	2.933	508	511	515	rVB2	320	218	0.03%	0.004%
8	2.969	516	522	525	rBV	249	310	0.04%	0.006%
9	3.030	532	541	550	rBV4	3407	6328	0.90%	0.122%
10	3.107	562	565	569	rBV	302	244	0.03%	0.005%
11	3.174	578	586	594	rVB3	899	1774	0.25%	0.034%
12	3.284	617	620	625	rVB2	237	231	0.03%	0.004%
13	3.415	654	661	665	rBV	269	253	0.04%	0.005%
14	3.444	666	670	676	rVV2	275	238	0.03%	0.005%
15	3.997	837	842	845	rBV2	321	379	0.05%	0.007%
16	4.049	852	858	862	rBV	246	352	0.05%	0.007%
17	4.097	866	873	878	rBV	231	335	0.05%	0.006%
18	4.319	938	942	947	rBV	271	288	0.04%	0.006%
19	4.621	1027	1036	1085	rBV2	43305	137569	19.53%	2.645%
20	4.965	1140	1143	1146	rVB2	281	219	0.03%	0.004%
21	5.052	1155	1170	1192	rBV2	92305	208900	29.65%	4.017%
22	5.357	1261	1265	1271	rBV2	201	256	0.04%	0.005%
23	5.644	1346	1354	1357	rVB2	278	333	0.05%	0.006%
24	5.711	1357	1375	1398	rBV2	198106	526277	74.70%	10.120%
25	5.833	1410	1413	1420	rVB2	293	333	0.05%	0.006%
26	5.972	1449	1456	1458	rBV2	768	750	0.11%	0.014%
27	6.020	1468	1471	1478	rBV3	211	214	0.03%	0.004%
28	6.120	1499	1502	1507	rVB2	361	295	0.04%	0.006%
29	6.238	1527	1539	1563	rBV	276478	538323	76.41%	10.352%
30	6.322	1563	1565	1571	rVB2	1240	945	0.13%	0.018%
31	6.528	1617	1629	1638	rBV7	3704	6447	0.92%	0.124%
32	6.599	1643	1651	1660	rVV5	1268	2614	0.37%	0.050%
33	6.682	1663	1677	1700	rVB	121059	239789	34.03%	4.611%
34	6.811	1714	1717	1721	rVB2	398	336	0.05%	0.006%
35	6.846	1723	1728	1732	rVB	277	276	0.04%	0.005%
36	6.869	1732	1735	1739	rBV2	294	289	0.04%	0.006%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

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\SFAMULM052924WMA.M
Title : VOC Analysis

37	7.116	1808	1812	1815	rBV	250	253	0.04%	0.005%
38	7.200	1828	1838	1841	rBV4	1468	2237	0.32%	0.043%
39	7.560	1938	1950	1970	rBV2	58469	107864	15.31%	2.074%
40	7.631	1970	1972	1976	rVB	547	371	0.05%	0.007%
41	7.711	1985	1997	2006	rBV4	1048	1919	0.27%	0.037%
42	7.891	2040	2053	2073	rBV	224668	393068	55.79%	7.558%
43	8.071	2106	2109	2114	rVB2	373	383	0.05%	0.007%
44	8.174	2132	2141	2170	rBV	39450	71602	10.16%	1.377%
45	8.344	2189	2194	2196	rBV2	327	257	0.04%	0.005%
46	8.357	2196	2198	2202	rVB	279	229	0.03%	0.004%
47	8.390	2202	2208	2211	rBV	264	328	0.05%	0.006%
48	8.496	2237	2241	2244	rBV	283	323	0.05%	0.006%
49	8.550	2250	2258	2266	rBV6	2050	3143	0.45%	0.060%
50	8.637	2270	2285	2323	rBV	127873	291946	41.44%	5.614%
51	8.917	2370	2372	2375	rBV	324	228	0.03%	0.004%
52	8.988	2392	2394	2400	rVB2	273	250	0.04%	0.005%
53	9.078	2419	2422	2427	rBV2	255	291	0.04%	0.006%
54	9.370	2508	2513	2514	rBV	270	234	0.03%	0.004%
55	9.412	2514	2526	2561	rVV	401886	704565	100.00%	13.548%
56	9.621	2585	2591	2593	rBV3	406	431	0.06%	0.008%
57	9.692	2607	2613	2615	rBV2	1043	1173	0.17%	0.023%
58	9.743	2626	2629	2634	rVB2	435	265	0.04%	0.005%
59	9.782	2639	2641	2645	rVB2	390	299	0.04%	0.006%
60	9.888	2669	2674	2679	rVB2	274	291	0.04%	0.006%
61	9.914	2679	2682	2685	rBV	378	223	0.03%	0.004%
62	9.930	2685	2687	2692	rVB2	513	419	0.06%	0.008%
63	10.113	2739	2744	2749	rVB3	385	420	0.06%	0.008%
64	10.299	2797	2802	2808	rBV2	321	381	0.05%	0.007%
65	10.328	2808	2811	2815	rBV2	275	287	0.04%	0.006%
66	10.647	2906	2910	2914	rBV2	284	235	0.03%	0.005%
67	10.753	2931	2943	2967	rVV	200569	330215	46.87%	6.350%
68	10.840	2967	2970	2973	rVB	306	213	0.03%	0.004%
69	11.200	3078	3082	3085	rBV2	385	349	0.05%	0.007%
70	11.254	3094	3099	3101	rBV2	268	295	0.04%	0.006%
71	11.528	3179	3184	3188	rVB3	328	340	0.05%	0.007%
72	11.586	3198	3202	3204	rBV2	317	268	0.04%	0.005%
73	11.672	3226	3229	3233	rVB3	441	309	0.04%	0.006%
74	11.746	3250	3252	3258	rBV3	584	652	0.09%	0.013%
75	11.807	3260	3271	3294	rBV	422984	694984	98.64%	13.364%
76	12.007	3330	3333	3338	rVB3	471	265	0.04%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

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\SFAMULM052924WMA.M
Title : VOC Analysis

77	12.100	3360	3362	3366	rVB2	475	259	0.04%	0.005%
78	12.190	3375	3390	3409	rBV	246317	410375	58.25%	7.891%
79	12.573	3506	3509	3513	rVB5	655	482	0.07%	0.009%
80	12.614	3518	3522	3525	rBV3	777	719	0.10%	0.014%
81	13.129	3678	3682	3685	rBV4	759	738	0.10%	0.014%
82	13.257	3719	3722	3723	rBV2	511	270	0.04%	0.005%
83	13.373	3754	3758	3760	rBV4	534	395	0.06%	0.008%
84	13.399	3763	3766	3768	rBV3	529	414	0.06%	0.008%
85	13.505	3797	3799	3804	rBV5	460	401	0.06%	0.008%
86	13.743	3870	3873	3880	rBV5	669	644	0.09%	0.012%
87	13.811	3890	3894	3896	rBV4	1189	846	0.12%	0.016%
88	14.045	3964	3967	3969	rBV3	769	615	0.09%	0.012%
89	14.444	4086	4091	4099	rBV6	4018	5681	0.81%	0.109%
90	14.537	4118	4120	4123	rBV3	916	465	0.07%	0.009%
91	14.778	4192	4195	4196	rBV3	681	342	0.05%	0.007%
92	14.933	4241	4243	4246	rBV3	909	533	0.08%	0.010%
93	15.007	4264	4266	4274	rBV7	888	919	0.13%	0.018%
94	15.135	4304	4306	4316	rVB9	1688	2181	0.31%	0.042%
95	15.174	4316	4318	4320	rBV3	818	324	0.05%	0.006%
96	15.206	4321	4328	4333	rVV8	3023	4286	0.61%	0.082%
97	15.392	4378	4386	4395	rBV4	10654	16172	2.30%	0.311%
98	15.971	4560	4566	4579	rVB6	9389	13624	1.93%	0.262%
99	16.286	4656	4664	4672	rBV3	23148	33755	4.79%	0.649%
100	17.125	4918	4925	4937	rVB2	33308	48694	6.91%	0.936%

Sum of corrected areas: 5200373

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
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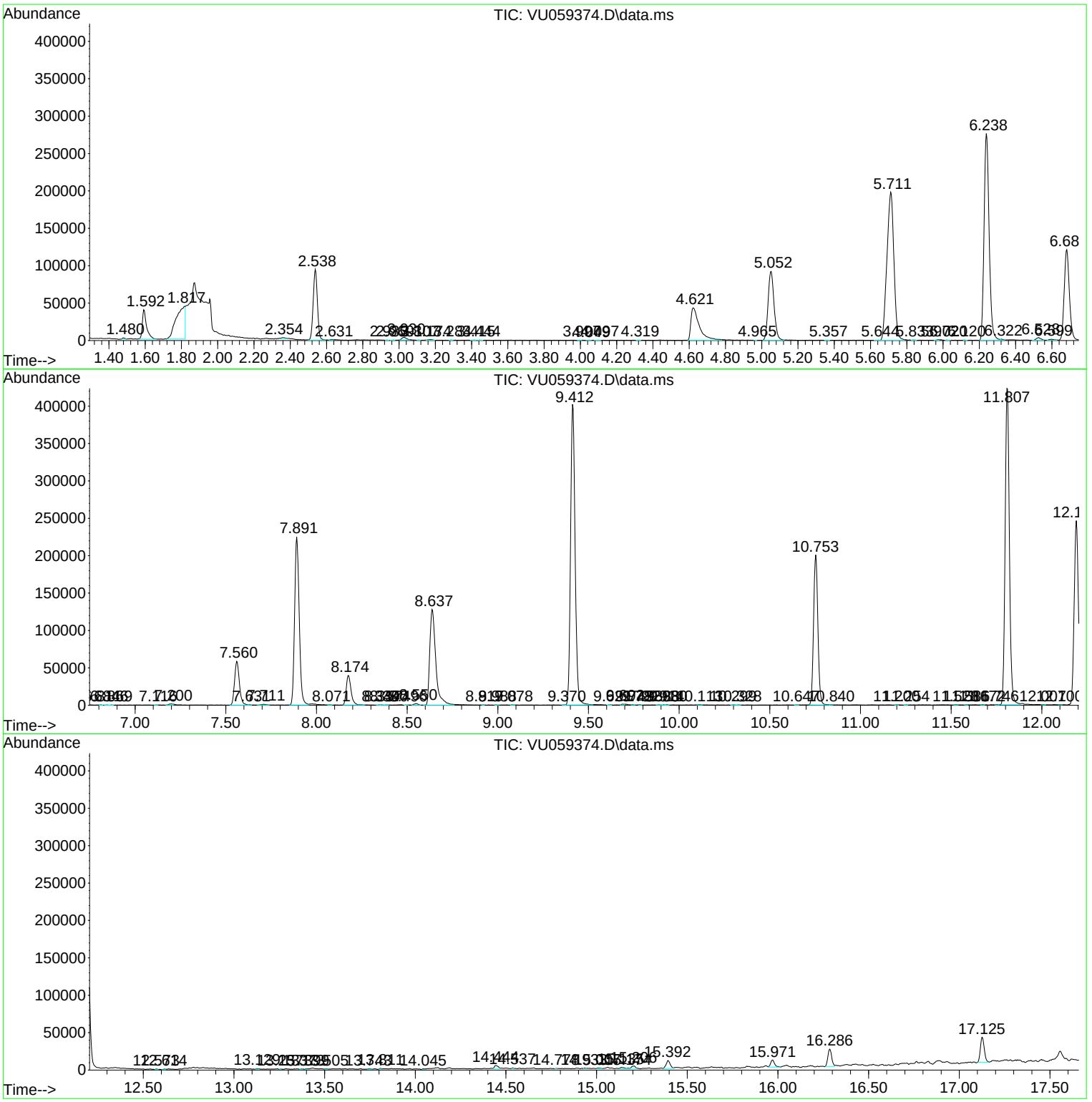
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

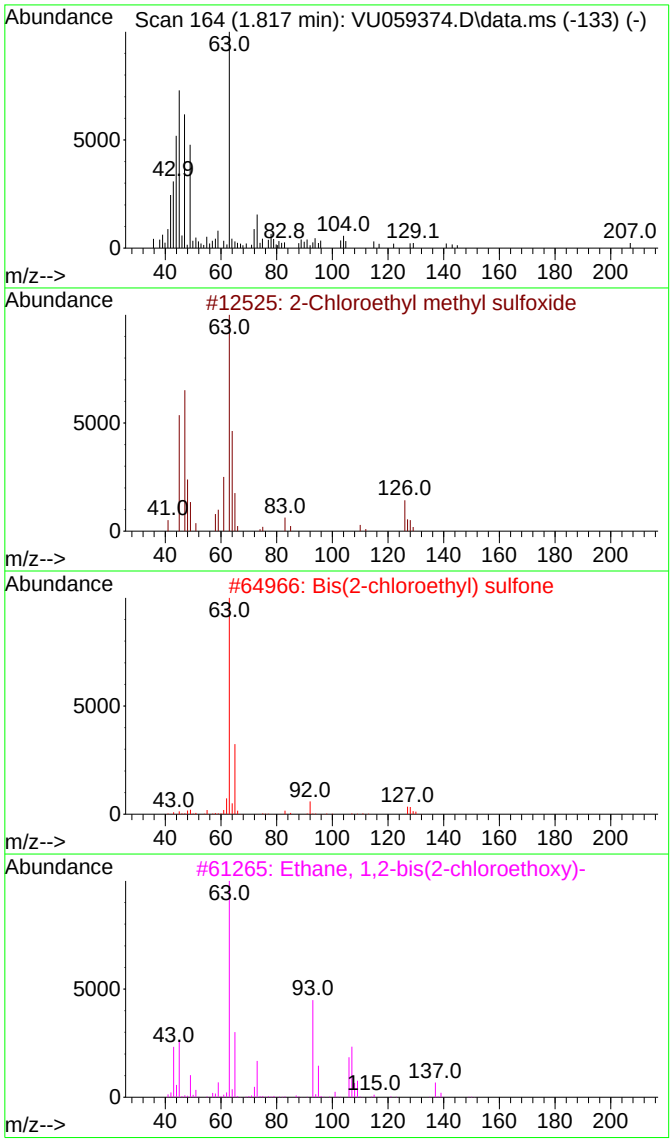
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

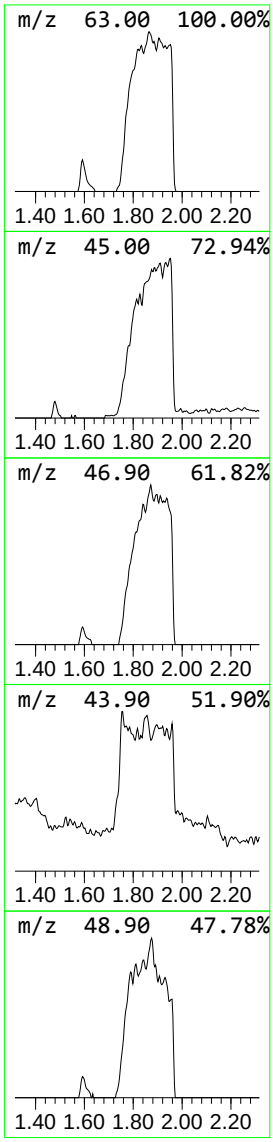
****

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.817	13.98 ug/L	150564	1,4-Difluorobenzene	6.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	38
2	Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	32
3	Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	25
4	Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	23
5	Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	077287-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
Misc : 2.55g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

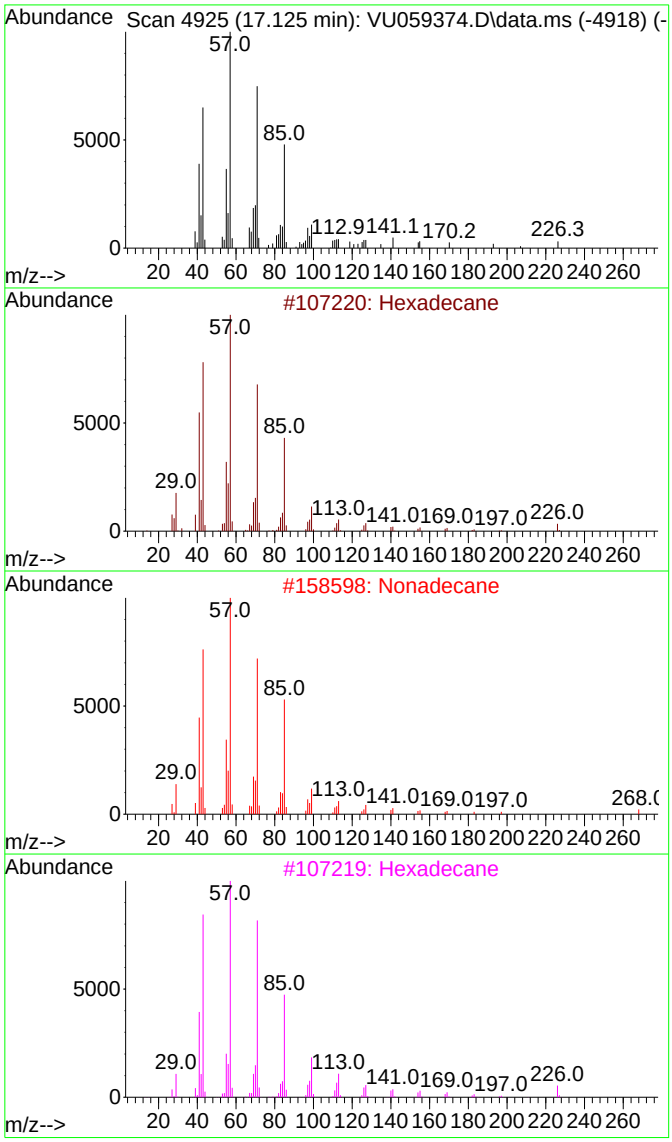
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

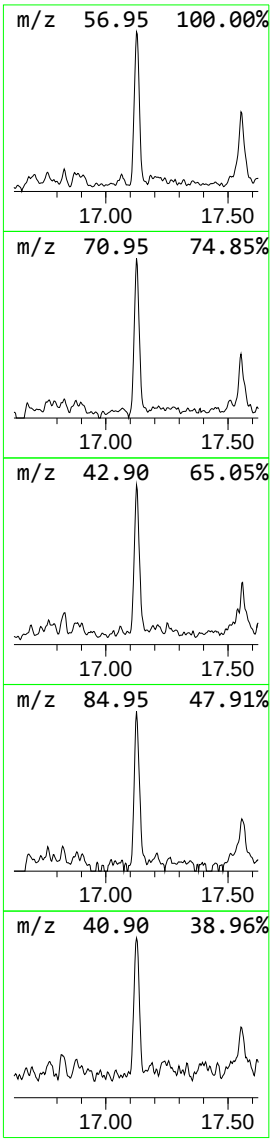
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.125	3.50 ug/L	48694	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Hexadecane	226	C16H34	000544-76-3	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Dodecane	170	C12H26	000112-40-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059374.D
Acq On : 20 Jun 2024 12:54
Operator : MD/SY
Sample : P2897-12ME
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T59ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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
unknown-01	1.817	14.0	ug/L	150564	1	6.238	538323	50.0
(DEL) Alkane: S...	17.125	3.5	ug/L	48694	3	11.811	694984	50.0