

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
 Data File : VV027067.D
 Acq On : 29 Jul 2022 04:35
 Operator : SY/MD
 Sample : N3790-14ME
 Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBUK8ME

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_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

Signal : TIC: VV027067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.207	48	52	57	rBV	10304	10050	0.43%	0.059%
2	1.301	74	81	120	rVB	221073	358129	15.21%	2.085%
3	1.558	156	161	185	rVB	104543	150016	6.37%	0.873%
4	2.079	312	323	338	rVB	578213	825926	35.08%	4.808%
5	2.436	424	434	444	rBV	19322	39274	1.67%	0.229%
6	2.609	477	488	503	rVB	19240	38061	1.62%	0.222%
7	2.789	541	544	547	rBV3	578	482	0.02%	0.003%
8	3.021	609	616	623	rVB5	1518	2089	0.09%	0.012%
9	3.182	660	666	671	rBV5	1366	1749	0.07%	0.010%
10	3.445	746	748	756	rVV2	592	526	0.02%	0.003%
11	3.783	848	853	856	rBV3	425	466	0.02%	0.003%
12	3.899	878	889	947	rBV	112275	550234	23.37%	3.203%
13	4.339	1010	1026	1060	rVB	362084	925934	39.33%	5.390%
14	4.693	1134	1136	1142	rVB3	543	432	0.02%	0.003%
15	4.805	1165	1171	1174	rBV	655	620	0.03%	0.004%
16	4.879	1190	1194	1198	rVB2	468	490	0.02%	0.003%
17	5.037	1226	1243	1279	rBV2	954722	2354527	100.00%	13.706%
18	5.233	1302	1304	1310	rVB4	934	786	0.03%	0.005%
19	5.339	1324	1337	1350	rBV5	12035	31211	1.33%	0.182%
20	5.548	1396	1402	1403	rBV4	1131	1022	0.04%	0.006%
21	5.609	1409	1421	1451	rBV	671582	1404635	59.66%	8.177%
22	5.725	1451	1457	1458	rBV4	4747	4463	0.19%	0.026%
23	5.902	1504	1512	1528	rVB5	18810	37456	1.59%	0.218%
24	6.063	1550	1562	1593	rVB	499578	1052749	44.71%	6.128%
25	6.542	1708	1711	1715	rVB2	609	462	0.02%	0.003%
26	6.635	1732	1740	1752	rBV8	5095	12559	0.53%	0.073%
27	6.809	1791	1794	1796	rBV3	456	367	0.02%	0.002%
28	6.902	1817	1823	1824	rBV2	605	507	0.02%	0.003%
29	6.982	1837	1848	1881	rBV	217167	427979	18.18%	2.491%
30	7.172	1903	1907	1908	rBV2	750	458	0.02%	0.003%
31	7.230	1923	1925	1929	rBV4	591	425	0.02%	0.002%
32	7.313	1938	1951	1978	rBV	1020977	1811196	76.92%	10.543%
33	7.619	2035	2046	2077	rBV	147670	292163	12.41%	1.701%
34	7.789	2095	2099	2111	rVV7	2180	3918	0.17%	0.023%
35	7.844	2114	2116	2122	rVB5	879	783	0.03%	0.005%
36	7.870	2122	2124	2128	rBV2	625	352	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
 Data File : VV027067.D
 Acq On : 29 Jul 2022 04:35
 Operator : SY/MD
 Sample : N3790-14ME
 Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBUK8ME

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_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

37	7.937	2142	2145	2148	rVB3	785	528	0.02%	0.003%
38	7.976	2148	2157	2169	rBV10	3475	5458	0.23%	0.032%
39	8.098	2184	2195	2198	rBV	260633	404969	17.20%	2.357%
40	8.503	2318	2321	2329	rVB4	818	843	0.04%	0.005%
41	8.599	2346	2351	2361	rVB6	982	1369	0.06%	0.008%
42	8.664	2364	2371	2373	rBV6	1363	1568	0.07%	0.009%
43	8.799	2409	2413	2417	rBV4	389	355	0.02%	0.002%
44	8.850	2417	2429	2460	rBV	978077	1738041	73.82%	10.117%
45	9.146	2518	2521	2524	rBV2	511	375	0.02%	0.002%
46	9.368	2587	2590	2594	rVB3	475	370	0.02%	0.002%
47	9.513	2631	2635	2638	rBV3	415	431	0.02%	0.003%
48	9.551	2643	2647	2648	rBV2	470	377	0.02%	0.002%
49	9.564	2648	2651	2655	rVB3	499	378	0.02%	0.002%
50	9.680	2682	2687	2690	rVB2	485	360	0.02%	0.002%
51	9.757	2704	2711	2720	rVB6	2192	2741	0.12%	0.016%
52	9.902	2746	2756	2768	rVB2	31113	51414	2.18%	0.299%
53	10.027	2792	2795	2799	rBV2	329	350	0.01%	0.002%
54	10.053	2800	2803	2806	rVB2	824	481	0.02%	0.003%
55	10.217	2834	2854	2885	rBV	639304	1127240	47.88%	6.562%
56	10.580	2957	2967	2976	rVV7	11300	18282	0.78%	0.106%
57	10.693	2996	3002	3008	rVB5	677	933	0.04%	0.005%
58	10.853	3049	3052	3057	rBV3	1084	911	0.04%	0.005%
59	10.898	3063	3066	3070	rVB	568	363	0.02%	0.002%
60	10.924	3070	3074	3078	rBV	618	472	0.02%	0.003%
61	11.191	3147	3157	3163	rBV8	2605	3262	0.14%	0.019%
62	11.252	3163	3176	3194	rBV	996676	1573903	66.85%	9.162%
63	11.371	3211	3213	3217	rVB3	802	570	0.02%	0.003%
64	11.455	3234	3239	3243	rVB4	794	772	0.03%	0.004%
65	11.532	3259	3263	3265	rBV2	806	704	0.03%	0.004%
66	11.625	3279	3292	3312	rBV	950885	1503335	63.85%	8.751%
67	11.963	3391	3397	3401	rBV3	482	594	0.03%	0.003%
68	12.242	3476	3484	3498	rVB3	5704	8952	0.38%	0.052%
69	12.352	3511	3518	3520	rVV6	1695	1755	0.07%	0.010%
70	12.374	3523	3525	3534	rVB5	2270	2943	0.12%	0.017%
71	12.660	3610	3614	3619	rBV3	474	460	0.02%	0.003%
72	12.885	3678	3684	3692	rBV7	2834	3857	0.16%	0.022%
73	12.956	3704	3706	3711	rVB2	450	370	0.02%	0.002%
74	13.004	3716	3721	3723	rBV3	420	385	0.02%	0.002%
75	13.069	3730	3741	3752	rBV6	5222	8253	0.35%	0.048%
76	13.268	3799	3803	3805	rBV3	533	433	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
 Data File : VV027067.D
 Acq On : 29 Jul 2022 04:35
 Operator : SY/MD
 Sample : N3790-14ME
 Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBUK8ME

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_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

77	13.381	3836	3838	3843	rBV	365	367	0.02%	0.002%
78	13.435	3848	3855	3864	rVV5	4650	6778	0.29%	0.039%
79	13.506	3868	3877	3889	rBV	15118	25376	1.08%	0.148%
80	13.693	3927	3935	3936	rBV2	572	521	0.02%	0.003%
81	13.747	3949	3952	3956	rVB2	602	507	0.02%	0.003%
82	13.776	3956	3961	3962	rBV3	435	393	0.02%	0.002%
83	13.898	3992	3999	4007	rBV4	6926	8758	0.37%	0.051%
84	13.963	4014	4019	4020	rBV	679	558	0.02%	0.003%
85	14.336	4129	4135	4138	rBV6	2578	2289	0.10%	0.013%
86	14.413	4149	4159	4177	rBV	111721	166183	7.06%	0.967%
87	14.638	4224	4229	4237	rBV6	3321	4428	0.19%	0.026%
88	14.731	4255	4258	4261	rVB3	703	388	0.02%	0.002%
89	14.818	4280	4285	4297	rBV6	2719	4344	0.18%	0.025%
90	14.985	4332	4337	4342	rBV7	1879	2270	0.10%	0.013%
91	15.104	4372	4374	4377	rBV4	706	495	0.02%	0.003%
92	15.178	4389	4397	4407	rBV4	6427	10274	0.44%	0.060%
93	15.258	4418	4422	4423	rBV3	2326	1510	0.06%	0.009%
94	15.496	4484	4496	4510	rBV3	16150	32138	1.36%	0.187%
95	15.590	4519	4525	4534	rBV8	6356	10343	0.44%	0.060%
96	15.721	4559	4566	4576	rVB9	15327	26559	1.13%	0.155%
97	15.898	4618	4621	4625	rBV3	2827	2994	0.13%	0.017%
98	16.120	4684	4690	4701	rVB7	11938	17578	0.75%	0.102%
99	16.178	4702	4708	4715	rBV7	10023	15274	0.65%	0.089%
100	16.300	4740	4746	4757	rVB7	17509	26833	1.14%	0.156%

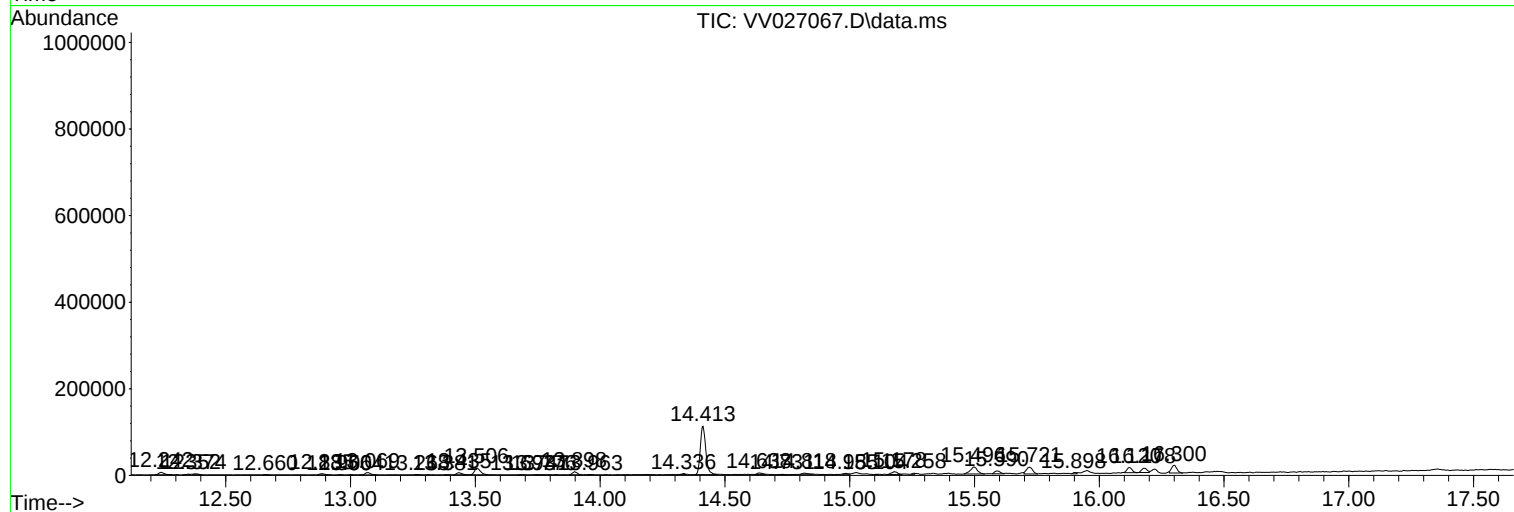
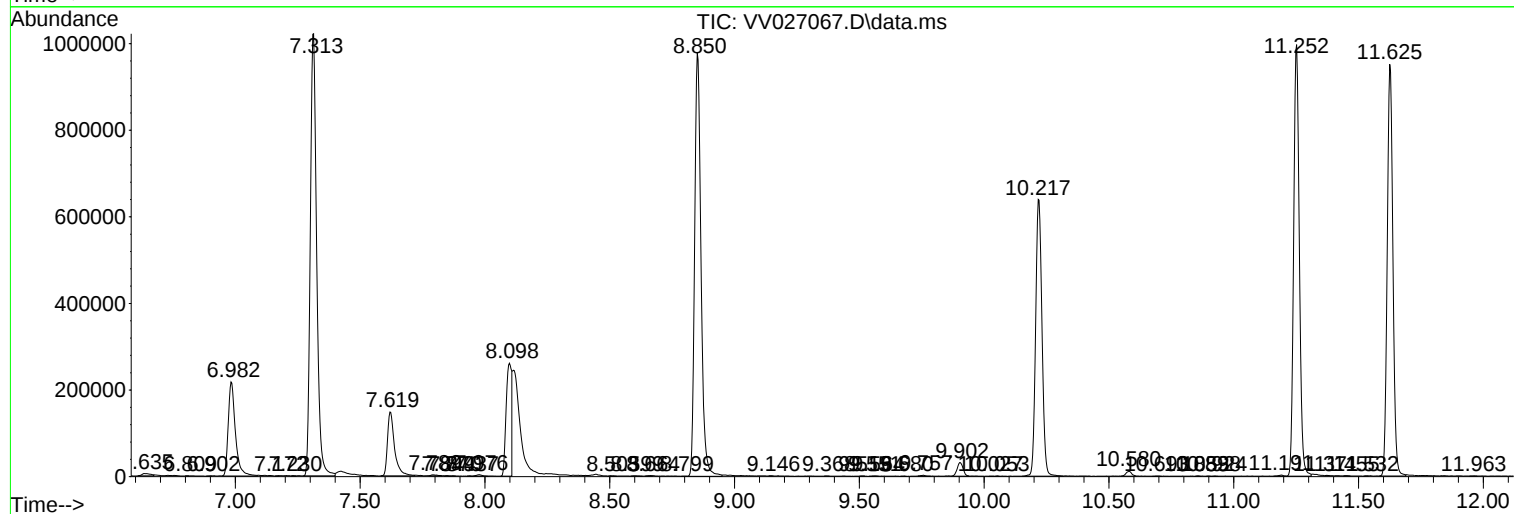
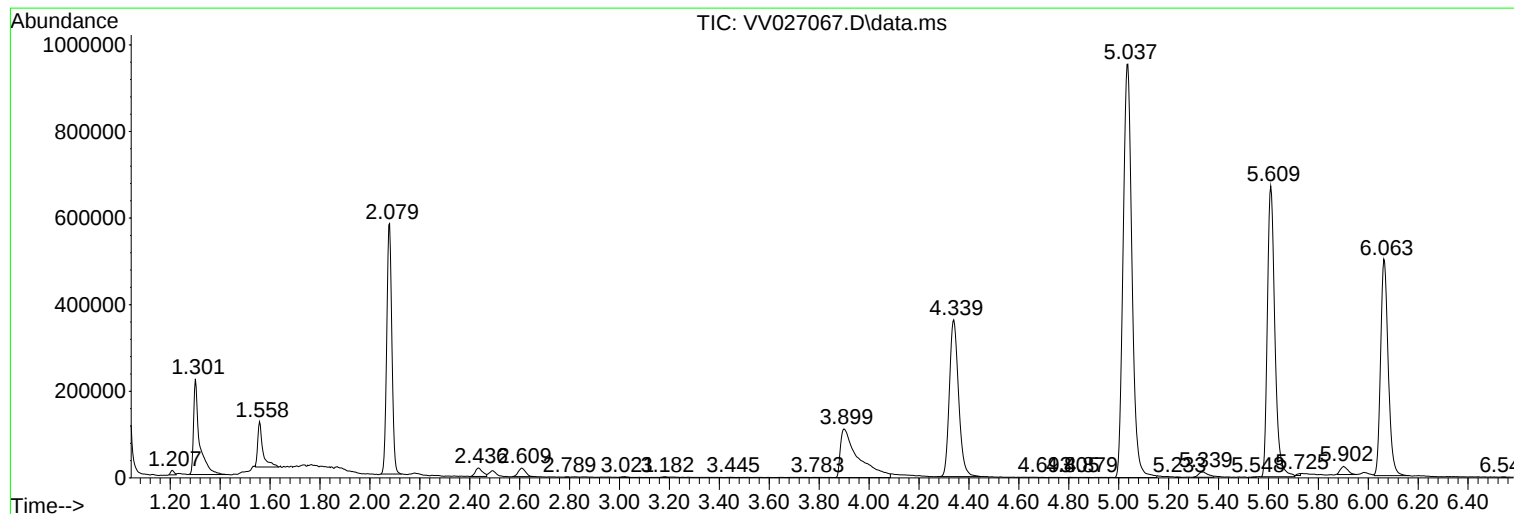
Sum of corrected areas: 17178811

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027067.D
Acq On : 29 Jul 2022 04:35
Operator : SY/MD
Sample : N3790-14ME
Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027067.D
Acq On : 29 Jul 2022 04:35
Operator : SY/MD
Sample : N3790-14ME
Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK8ME

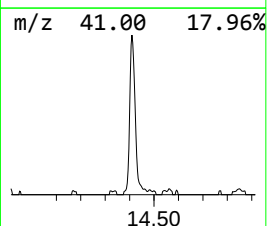
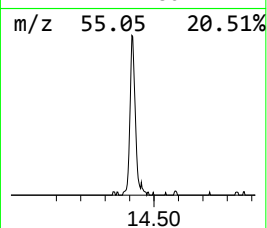
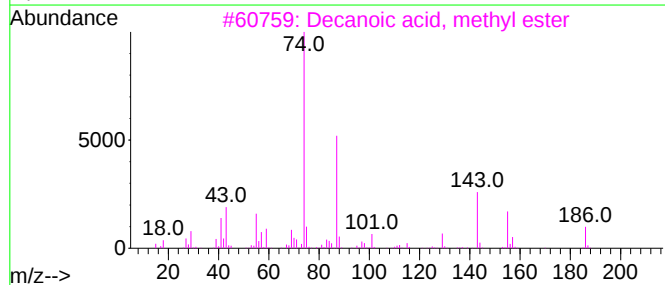
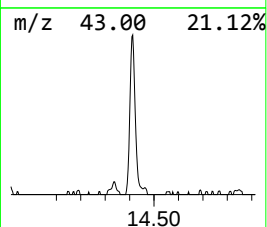
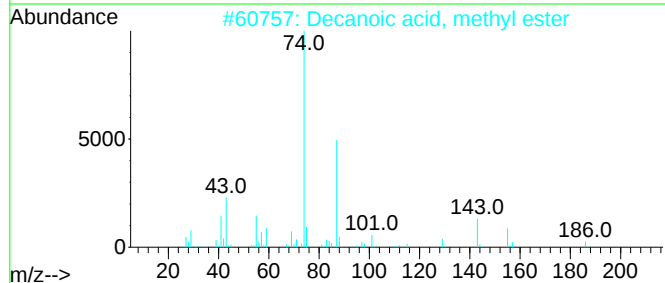
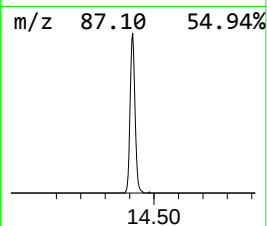
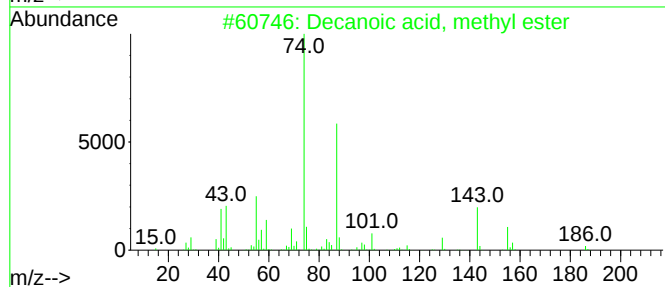
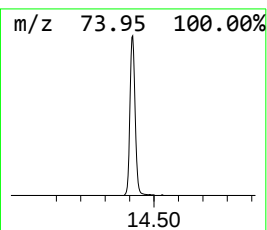
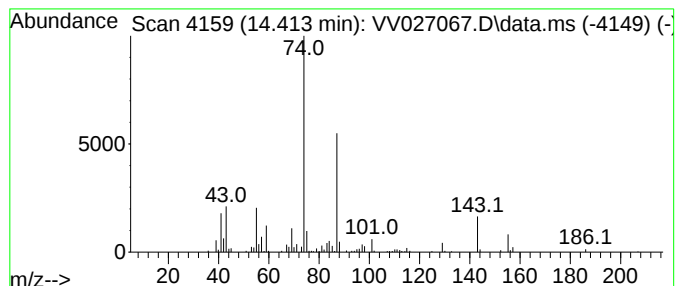
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Decanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.413	5.28 ug/L	166183	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	97
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	91
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83
4			Undecanoic acid, 11-bromo-, meth...	278	C12H23BrO2	006287-90-7	78
5			Undecanoic acid, 11-bromo-, meth...	278	C12H23BrO2	006287-90-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072822\
Data File : VV027067.D
Acq On : 29 Jul 2022 04:35
Operator : SY/MD
Sample : N3790-14ME
Misc : 3.46g/5.0mL/100uL/5mL/MSVOA_V/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decanoic acid, ...	14.413	5.3	ug/L	166183	3	11.252	1573900	50.0