LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

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\SFAMULM032422WMA.M
Title : VOC Analysis

Signal : TIC: VU047924.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	115	rVB	157247	316952	12.12%	1.506%
2	1.896	168	173	197	rBV	94583	192935	7.38%	0.916%
3	2.546	362	375	388	rBV	433457	748047	28.60%	3.553%
4	2.899	482	485	490	rBV3	362	401	0.02%	0.002%
5	2.960	499	504	506	rBV4	1587	1570	0.06%	0.007%
6	3.038	520	528	535	rBV7	2432	3853	0.15%	0.018%
7	3.176	566	571	573	rBV3	489	403	0.02%	0.002%
8	3.536	678	683	689	rVV3	440	494	0.02%	0.002%
9	3.597	698	702	706	rBV3	359	354	0.01%	0.002%
10	4.147	869	873	876	rBV2	588	449	0.02%	0.002%
11	4.642	1011	1027	1081	rBV	190016	704648	26.94%	3.347%
12	5.063	1140	1158	1180	rVV	436415	983978	37.62%	4.674%
13	5.292	1226	1229	1235	rVB3	573	531	0.02%	0.003%
14	5.369	1251	1253	1256	rBV3	611	471	0.02%	0.002%
15	5.529	1299	1303	1306	rBV2	373	381	0.01%	0.002%
16	5.719	1337	1362	1398	rBV2	959029	2615228	100.00%	12.423%
17	5.919	1422	1424	1428	rVB2	896	458	0.02%	0.002%
18	6.246	1512	1526	1552	rVV	385092	759916	29.06%	3.610%
19	6.526	1603	1613	1621	rBV5	3238	5618	0.21%	0.027%
20	6.597	1631	1635	1637	rBV3	469	387	0.01%	0.002%
21	6.690	1649	1664	1690	rBV	554205	1135364	43.41%	5.393%
22	6.809	1694	1701	1707	rVV5	1846	2650	0.10%	0.013%
23	7.047	1772	1775	1779	rVV2	584	511	0.02%	0.002%
24	7.195	1810	1821	1844	rBV5	7588	23011	0.88%	0.109%
25	7.497	1906	1915	1916	rBV5	1516	1650	0.06%	0.008%
26	7.568	1923	1937	1965	rVB	270815	523566	20.02%	2.487%
27	7.693	1969	1976	1984	rBV4	2486	4320	0.17%	0.021%
28	7.822	2011	2016	2018	rBV2	365	355	0.01%	0.002%
29	7.899	2025	2040	2055	rBV	1124616	1998854	76.43%	9.495%
30	7.970	2057	2062	2087	rVB2	35095	69621	2.66%	0.331%
31	8.182	2115	2128	2150	rVV	174948	361583	13.83%	1.718%
32	8.372	2181	2187	2189	rVV4	536	564	0.02%	0.003%
33	8.391	2192	2193	2201	rVB4	770	595	0.02%	0.003%
34	8.471	2214	2218	2219	rBV	682	415	0.02%	0.002%
35	8.581	2244	2252	2259	rBV4	2779	4954	0.19%	0.024%
36	8.658	2260	2276	2315	rVV	804504	1635862	62.55%	7.770%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

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\SFAMULM032422WMA.M
Title : VOC Analysis

37	8.967	2366	2372	2373	rBV2	489	410	0.02%	0.002%
38	9.037	2386	2394	2398	rVB3	617	628	0.02%	0.003%
39	9.182	2431	2439	2449	rVB4	3061	4959	0.19%	0.024%
40	9.365	2485	2496	2502	rBV2	19209	31022	1.19%	0.147%
41	9.423	2502	2514	2519	rBV	555871	1040050	39.77%	4.940%
42	9.578	2555	2562	2580	rVB7	7378	13639	0.52%	0.065%
43	9.700	2588	2600	2611	rVB2	3958	6137	0.23%	0.029%
44	9.844	2637	2645	2658	rVB4	1033	1996	0.08%	0.009%
45	9.947	2673	2677	2684	rBV3	487	617	0.02%	0.003%
46	10.105	2719	2726	2737	rVB7	1872	3101	0.12%	0.015%
47	10.430	2823	2827	2836	rBV	468	579	0.02%	0.003%
48	10.552	2861	2865	2870	rBV	346	366	0.01%	0.002%
49	10.671	2890	2902	2912	rVB7	5330	10735	0.41%	0.051%
50	10.764	2915	2931	2952	rBV	920842	1519177	58.09%	7.216%
51	10.867	2956	2963	2968	rBV6	810	1189	0.05%	0.006%
52	10.973	2990	2996	3000	rBV2	1437	1898	0.07%	0.009%
53	11.102	3028	3036	3039	rBV5	1270	2015	0.08%	0.010%
54	11.253	3078	3083	3092	rBV5	2037	2959	0.11%	0.014%
55	11.295	3092	3096	3107	rVV3	1229	1566	0.06%	0.007%
56	11.340	3107	3110	3114	rVB3	437	343	0.01%	0.002%
57	11.417	3129	3134	3138	rBV4	1027	927	0.04%	0.004%
58	11.468	3139	3150	3164	rVB2	5539	10798	0.41%	0.051%
59	11.581	3179	3185	3195	rVB5	931	1294	0.05%	0.006%
60	11.700	3215	3222	3231	rVB5	2204	3012	0.12%	0.014%
61	11.751	3233	3238	3244	rVB	2050	2041	0.08%	0.010%
62	11.815	3245	3258	3273	rBV	687289	1074989	41.10%	5.106%
63	11.883	3275	3279	3291	rVB9	5800	9189	0.35%	0.044%
64	11.954	3294	3301	3306	rBV6	3910	6293	0.24%	0.030%
65	12.021	3317	3322	3332	rVB9	2818	4501	0.17%	0.021%
66	12.079	3332	3340	3345	rBV6	996	1517	0.06%	0.007%
67	12.108	3345	3349	3351	rBV4	626	444	0.02%	0.002%
68	12.121	3351	3353	3358	rVB4	559	402	0.02%	0.002%
69	12.198	3358	3377	3396	rBV	1249174	2001810	76.54%	9.509%
70	12.323	3413	3416	3430	rVB8	1866	3097	0.12%	0.015%
71	12.375	3430	3432	3436	rBV5	612	466	0.02%	0.002%
72	12.401	3436	3440	3448	rVV5	1012	1240	0.05%	0.006%
73	12.471	3453	3462	3478	rVV5	26685	42831	1.64%	0.203%
74	12.709	3526	3536	3545	rVV2	19762	30336	1.16%	0.144%
75	12.876	3581	3588	3595	rVV5	4271	6073	0.23%	0.029%
76	12.973	3606	3618	3636	rVB2	57735	98137	3.75%	0.466%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

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\SFAMULM032422WMA.M
Title : VOC Analysis

77	13.066	3644	3647	3649	rBV	563	388	0.01%	0.002%
78	13.163	3667	3677	3687	rBV2	16706	25949	0.99%	0.123%
79	13.211	3687	3692	3694	rBV4	1176	1004	0.04%	0.005%
80	13.330	3722	3729	3732	rBV3	4161	5141	0.20%	0.024%
81	13.378	3732	3744	3760	rVB	898628	1324051	50.63%	6.289%
82	13.619	3815	3819	3827	rBV7	1414	1986	0.08%	0.009%
83	13.780	3862	3869	3873	rBV7	1869	2820	0.11%	0.013%
84	13.844	3883	3889	3898	rVB7	2967	4041	0.15%	0.019%
85	13.986	3931	3933	3937	rVB3	637	351	0.01%	0.002%
86	14.044	3949	3951	3953	rBV2	698	416	0.02%	0.002%
87	14.095	3959	3967	3975	rVB2	3935	5779	0.22%	0.027%
88	14.282	4020	4025	4029	rBV6	536	663	0.03%	0.003%
89	14.333	4035	4041	4042	rBV5	1821	1572	0.06%	0.007%
90	14.429	4061	4071	4081	rBV3	62789	99320	3.80%	0.472%
91	14.494	4081	4091	4109	rVB2	115213	194308	7.43%	0.923%
92	14.616	4127	4129	4135	rVB4	734	463	0.02%	0.002%
93	14.950	4226	4233	4244	rVB7	8212	13446	0.51%	0.064%
94	15.166	4294	4300	4309	rBV8	2088	2992	0.11%	0.014%
95	15.214	4312	4315	4320	rVB5	1015	932	0.04%	0.004%
96	15.285	4329	4337	4341	rBV4	12555	17497	0.67%	0.083%
97	15.317	4341	4347	4356	rVB5	17119	27388	1.05%	0.130%
98	15.397	4369	4372	4373	rBV3	1289	862	0.03%	0.004%
99	15.545	4405	4418	4437	rBV	745296	1146996	43.86%	5.448%
100	16.391	4670	4681	4693	rBV2	79390	130238	4.98%	0.619%

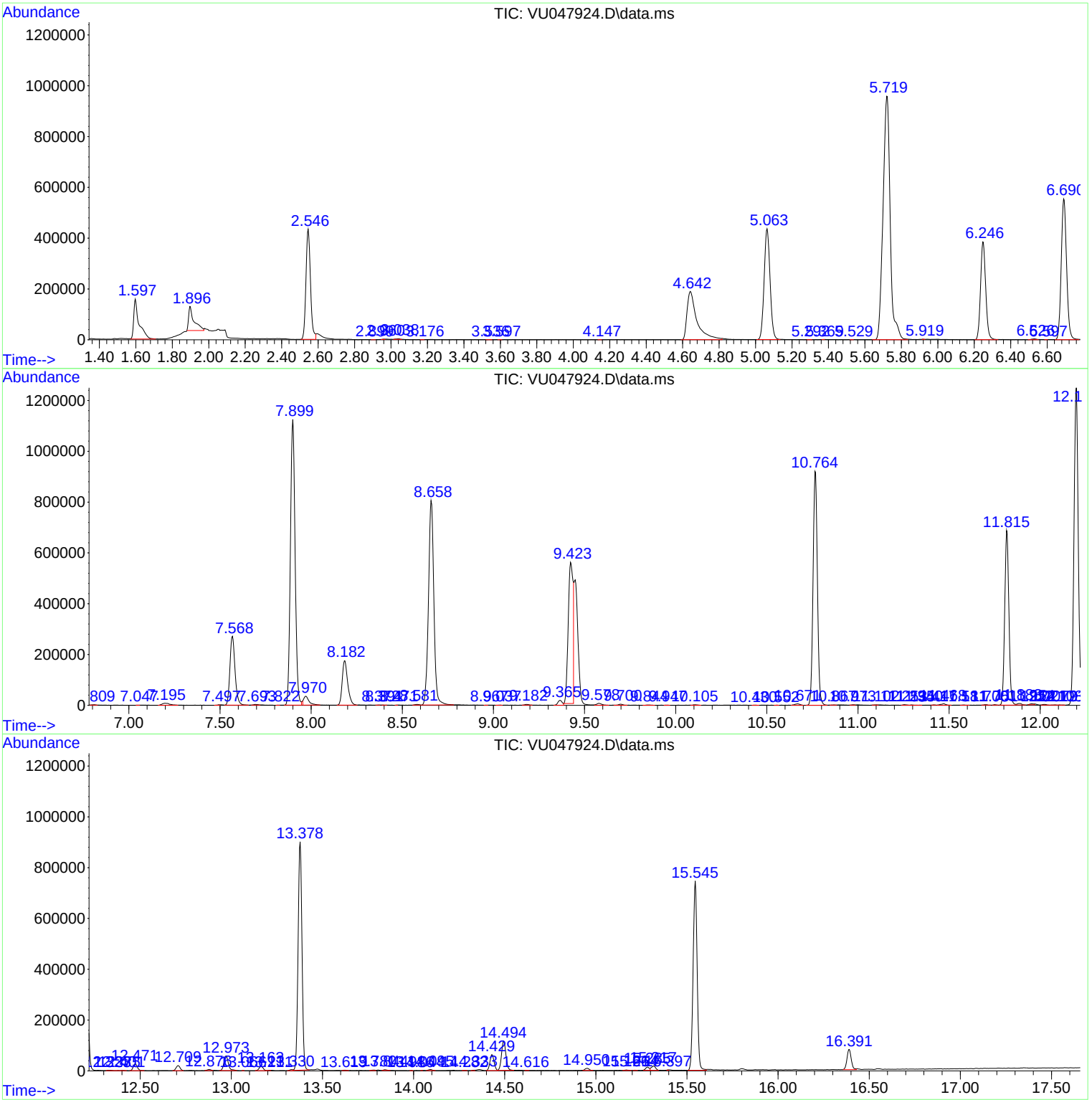
Sum of corrected areas: 21052335

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

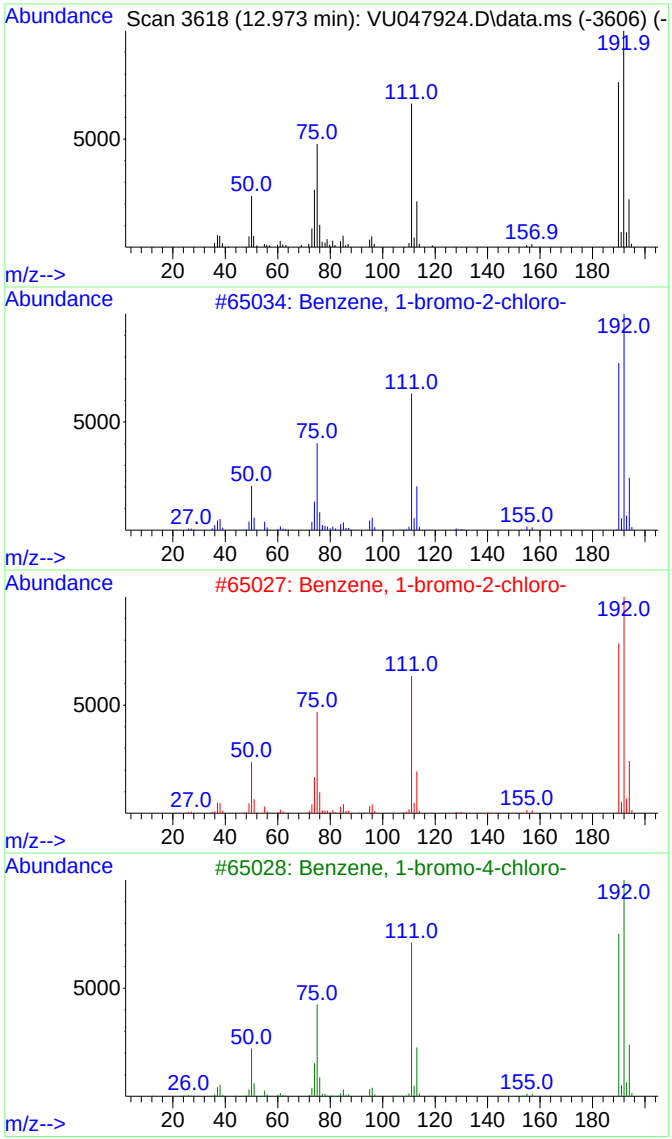
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

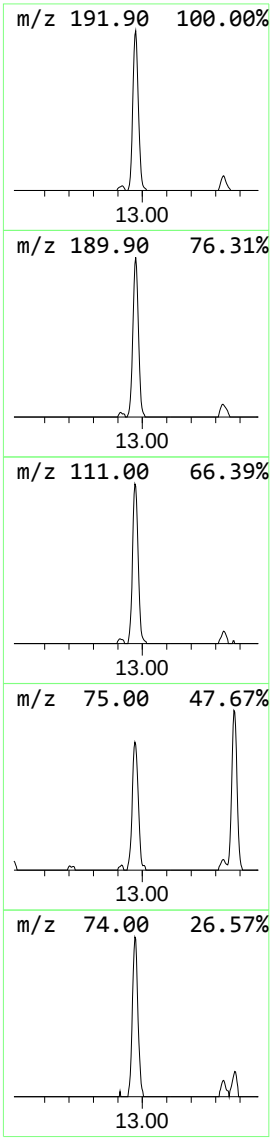
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-bromo-2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.973	4.56 ug/L	98137	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
2	Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
3	Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
4	4-Chlorophenylselenol	192	C6H5ClSe	016645-10-6	97
5	Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

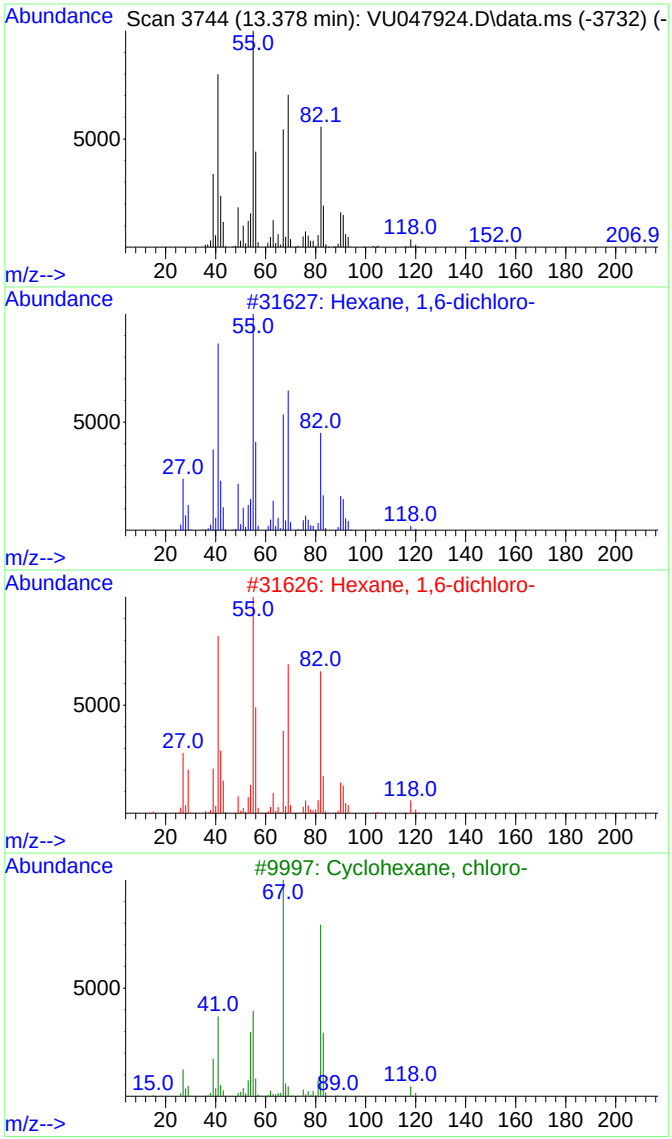
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

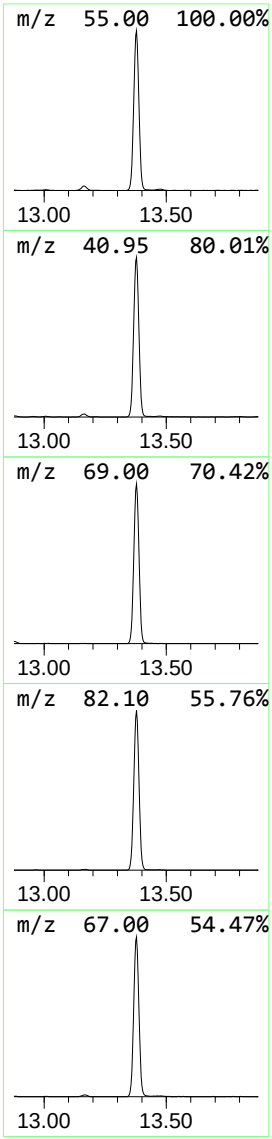
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexane, 1,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.378	61.58 ug/L	1324050	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	91
2	Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	59
3	Cyclohexane, chloro-	118	C6H11Cl	000542-18-7	50
4	6-Oxabicyclo[3.1.0]hexane	84	C5H8O	000285-67-6	35
5	cis-3-Hexenyl crotonate	168	C10H16O2	1000429-17-4	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

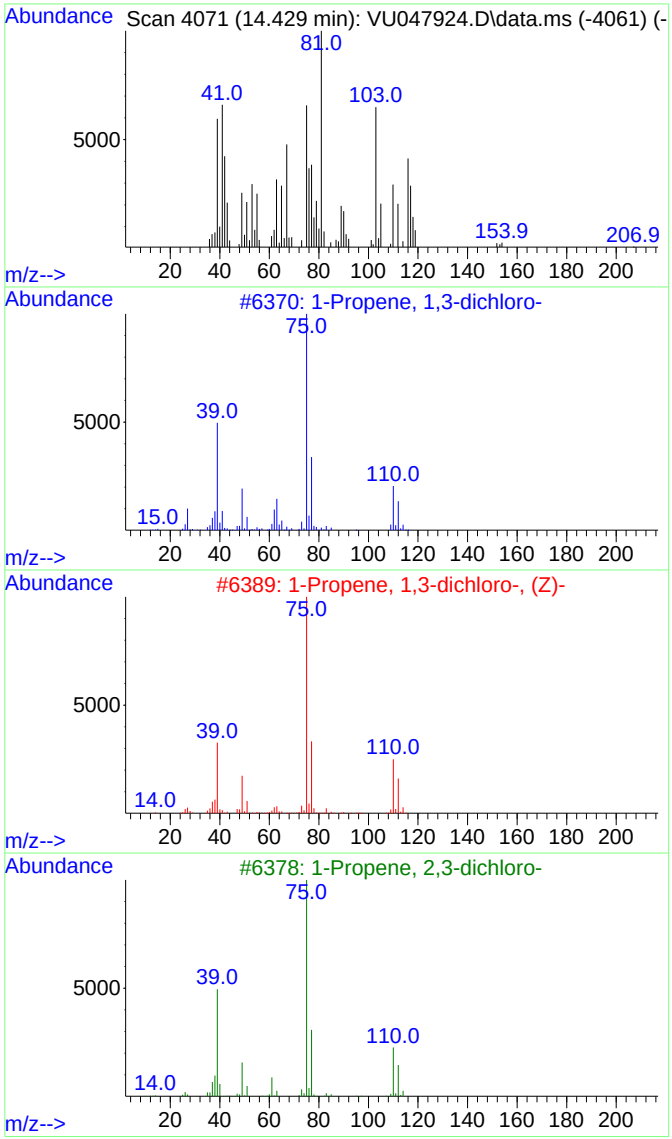
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

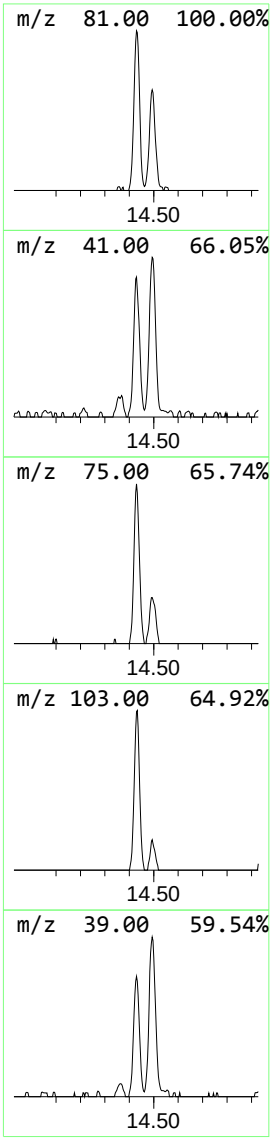
****

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.429	4.62 ug/L	99320	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 1,3-dichloro-	110	C3H4Cl2	000542-75-6	42
2	1-Propene, 1,3-dichloro-, (Z)-	110	C3H4Cl2	010061-01-5	38
3	1-Propene, 2,3-dichloro-	110	C3H4Cl2	000078-88-6	30
4	1-Propene, 1,3-dichloro-, (Z)-	110	C3H4Cl2	010061-01-5	30
5	1-Propene, 1,3-dichloro-, (E)-	110	C3H4Cl2	010061-02-6	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

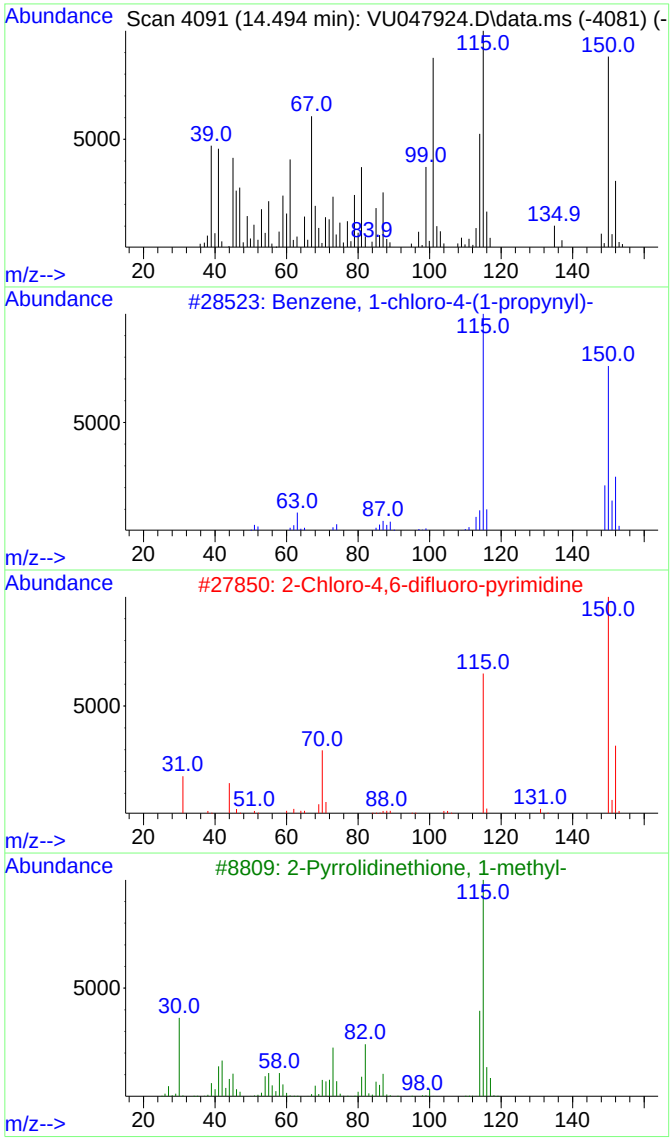
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

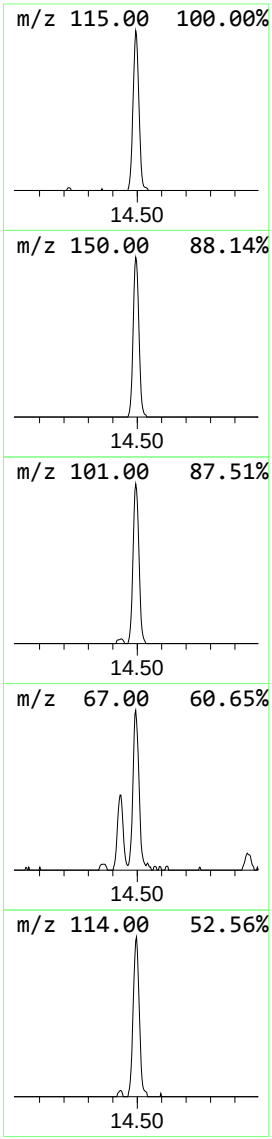
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.494	9.04 ug/L	194308	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	43
2	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	27
3	2-Pyrrolidinethione, 1-methyl-	115	C5H9NS	010441-57-3	18
4	Silane, ethenylethoxydimethyl-	130	C6H14OSi	005356-83-2	12
5	Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	11





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

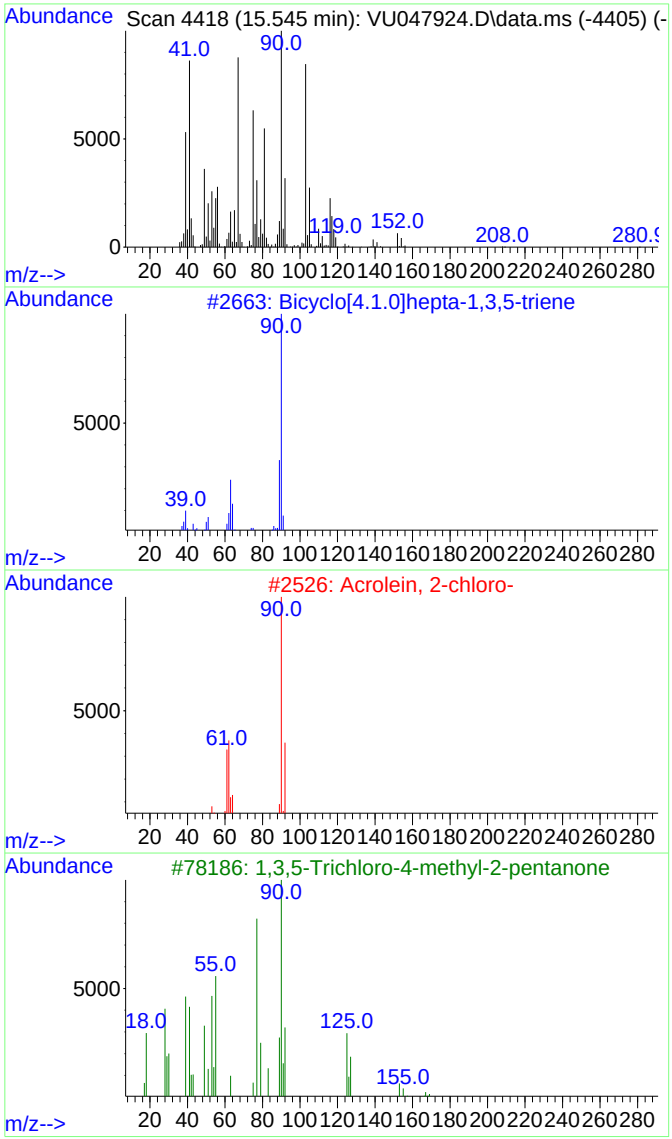
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

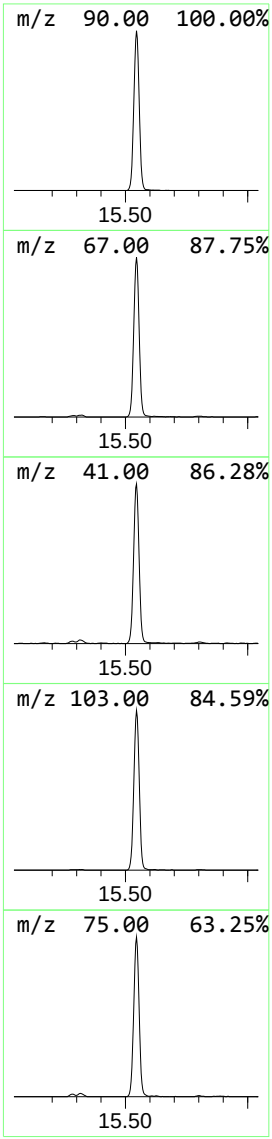
****

Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	53.35 ug/L	1147000	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
2	Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
3	1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	25
4	Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	25
5	2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

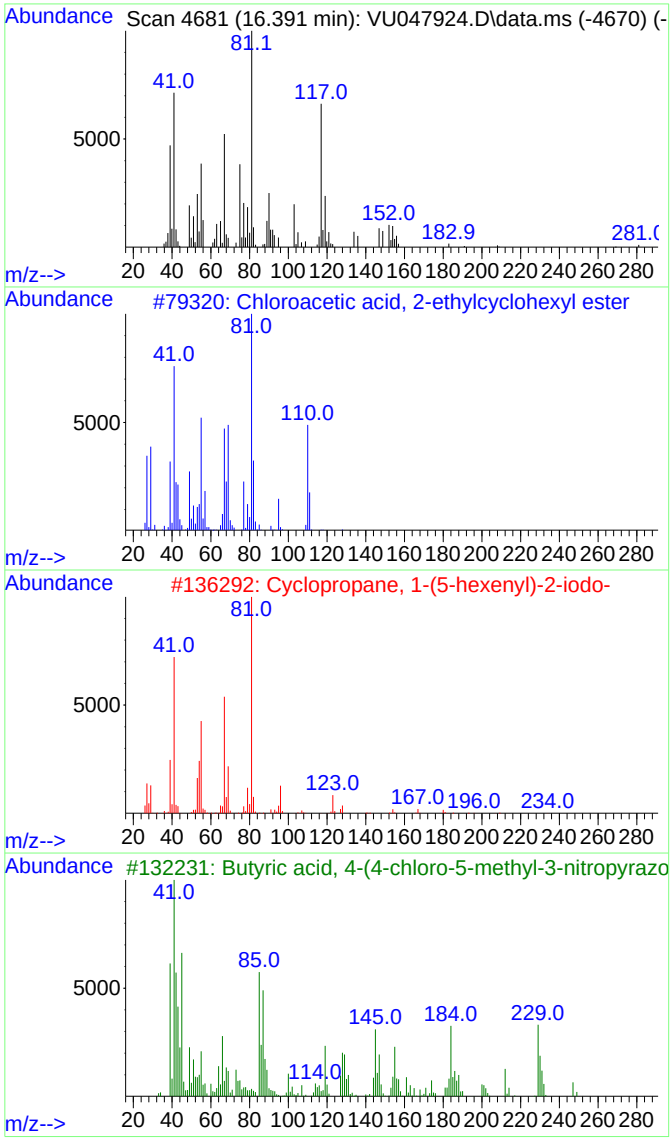
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

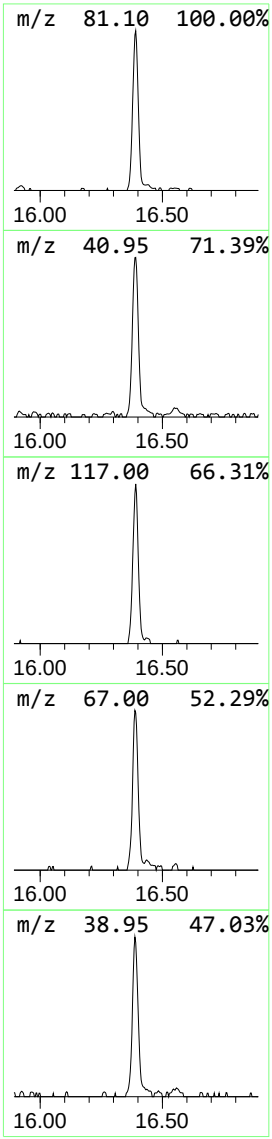
****

Peak Number 7 unknown-04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	6.06 ug/L	130238	1,4-Dichlorobenzene-d4	11.815

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, 2-ethylcycloh...	204	C10H17ClO2	1000279-89-1	37
2	Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
3	Butyric acid, 4-(4-chloro-5-meth...	247	C8H10ClN3O4	1000304-30-9	10
4	1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	10
5	1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047924.D
Acq On : 11 Apr 2022 22:37
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
Benzene, 1-brom...	12.973	4.6	ug/L	98137	3	11.815	1074990	50.0
Hexane, 1,6-dic...	13.378	61.6	ug/L	1324050	3	11.815	1074990	50.0
unknown-01	14.429	4.6	ug/L	99320	3	11.815	1074990	50.0
unknown-02	14.494	9.0	ug/L	194308	3	11.815	1074990	50.0
unknown-03	15.545	53.4	ug/L	1147000	3	11.815	1074990	50.0
unknown-04	16.391	6.1	ug/L	130238	3	11.815	1074990	50.0