

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
 Data File : VY019206.D
 Acq On : 22 Aug 2024 07:45
 Operator : SY/MD
 Sample : P3671-12
 Misc : 8.20g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-903-J-SO-0.5-1.0-081924

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_Y\methods\82Y081524S.M
 Title : SW846 8260

Signal : TIC: VY019206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.610	465	474	485	rBV3	12230	35959	5.08%	0.937%
2	7.628	960	969	975	rBV	81699	192307	27.18%	5.011%
3	7.701	975	981	994	rVB	129645	297676	42.07%	7.757%
4	8.055	1030	1039	1052	rVB2	59337	139171	19.67%	3.627%
5	8.609	1122	1130	1142	rBV	193605	379477	53.62%	9.889%
6	8.859	1163	1171	1180	rVB3	18833	37294	5.27%	0.972%
7	10.109	1367	1376	1387	rBV	324079	563652	79.65%	14.688%
8	10.646	1457	1464	1474	rVB	35520	60813	8.59%	1.585%
9	11.420	1583	1591	1600	rBV	295001	484126	68.41%	12.616%
10	11.597	1600	1620	1621	rBV7	32323	127741	18.05%	3.329%
11	12.261	1722	1729	1739	rBV	448021	707650	100.00%	18.441%
12	12.407	1747	1753	1762	rBV	215016	339184	47.93%	8.839%
13	12.511	1762	1770	1779	rBV4	28760	66590	9.41%	1.735%
14	12.816	1815	1820	1827	rVB3	12834	20945	2.96%	0.546%
15	13.352	1901	1908	1914	rVB	210104	322730	45.61%	8.410%
16	13.724	1963	1969	1983	rVB	8854	28592	4.04%	0.745%
17	13.889	1990	1996	2002	rBV2	8215	12948	1.83%	0.337%
18	14.078	2017	2027	2028	rBV3	6352	12853	1.82%	0.335%
19	14.096	2028	2030	2035	rVB5	5111	7711	1.09%	0.201%

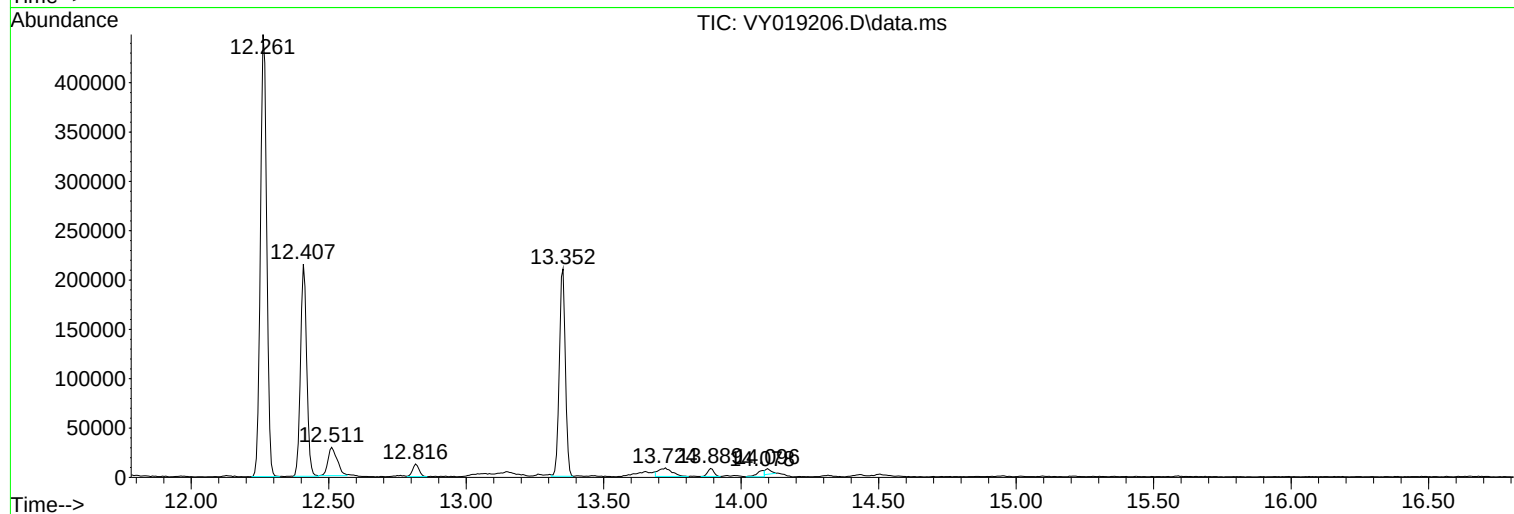
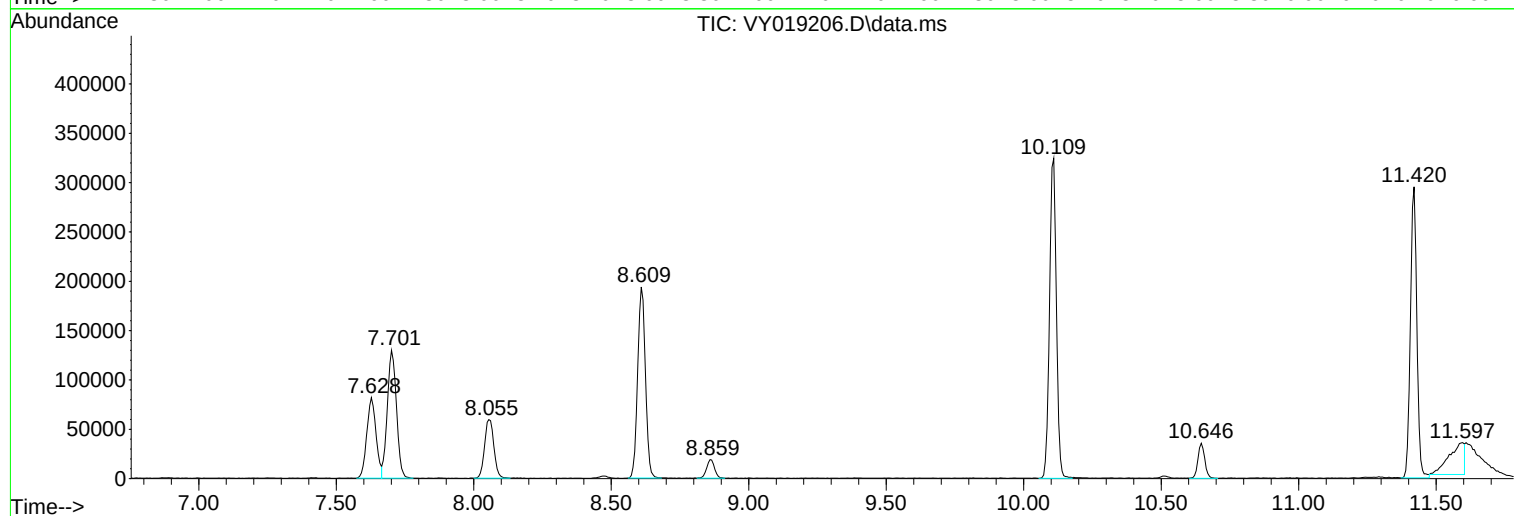
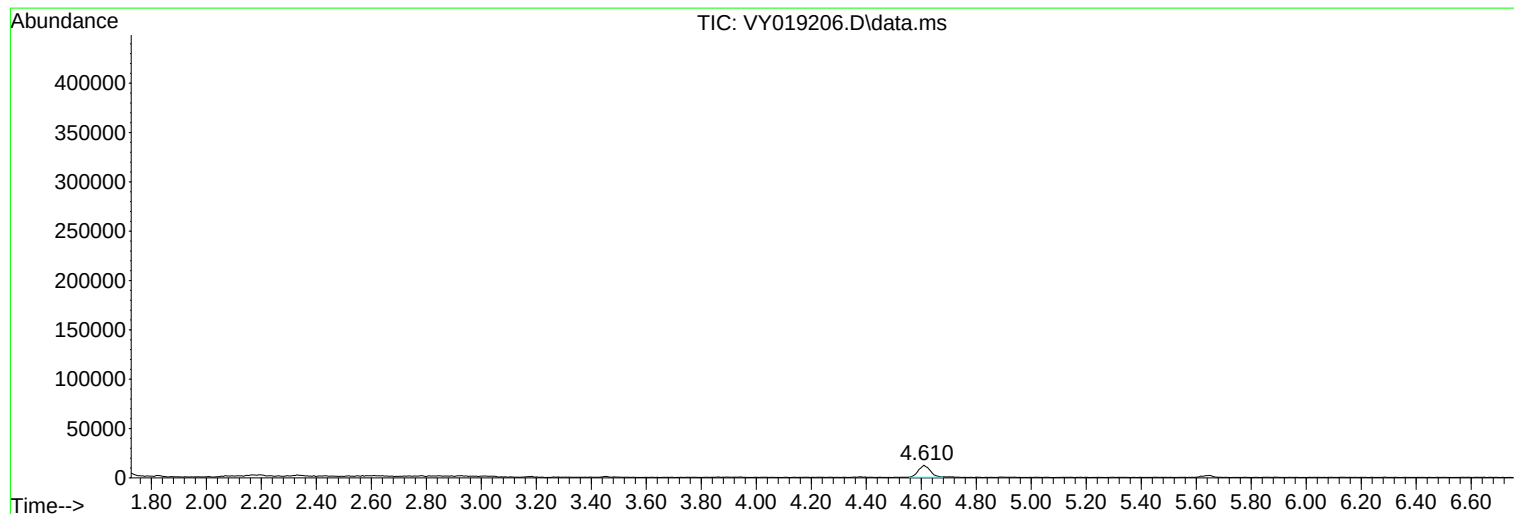
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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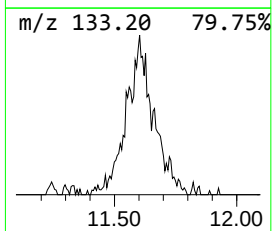
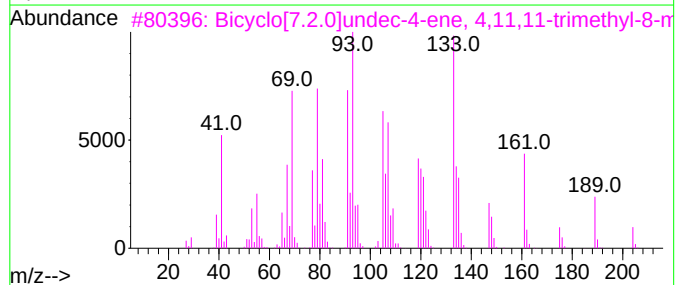
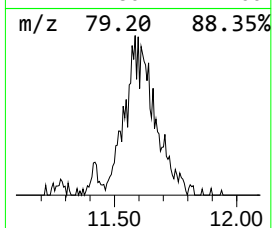
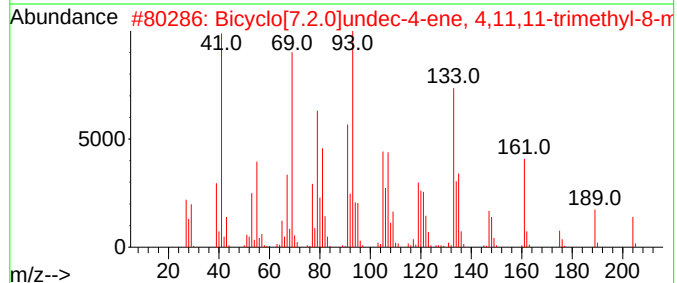
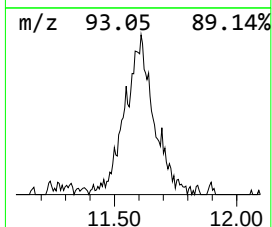
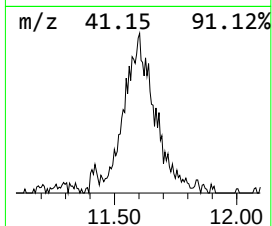
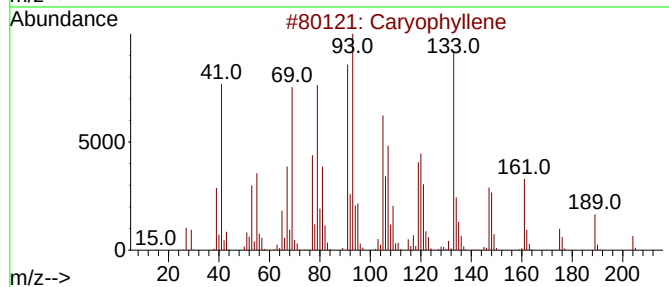
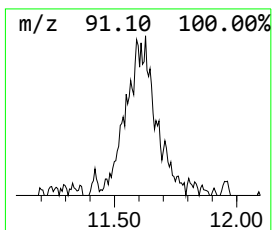
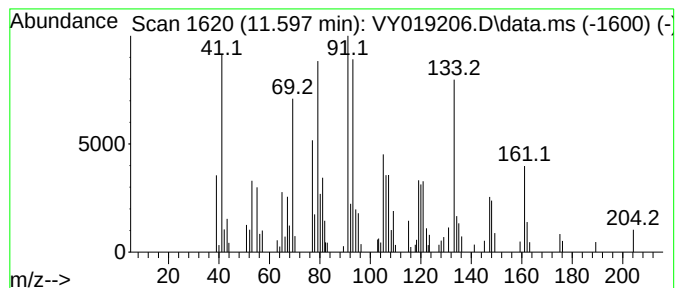
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.597	13.19 ug/l	127741	Chlorobenzene-d5	11.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	99
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	89
3			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	89
4			1R,3Z,9S-4,11,11-Trimethyl-8-met...	204	C15H24	1000159-39-4	83
5			Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	70



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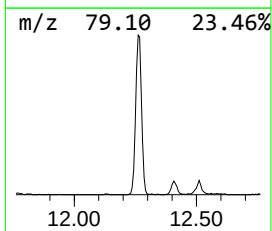
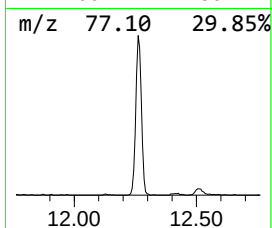
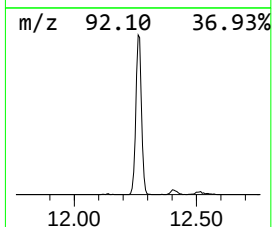
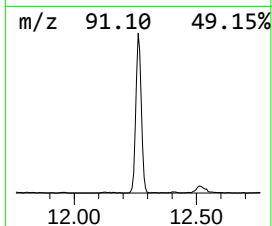
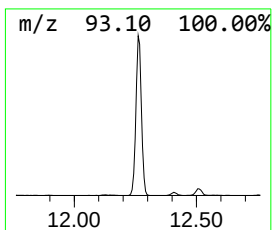
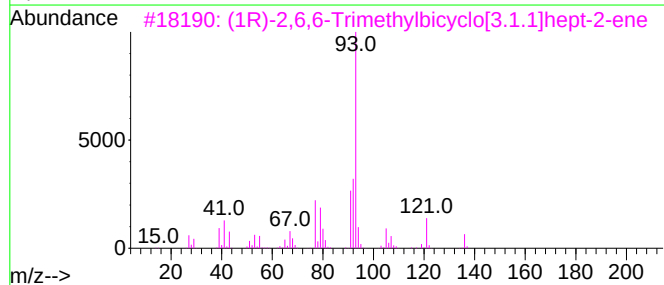
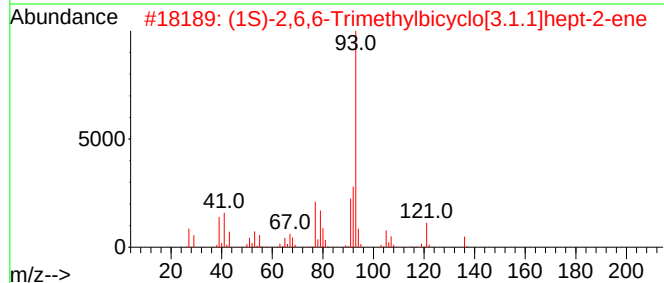
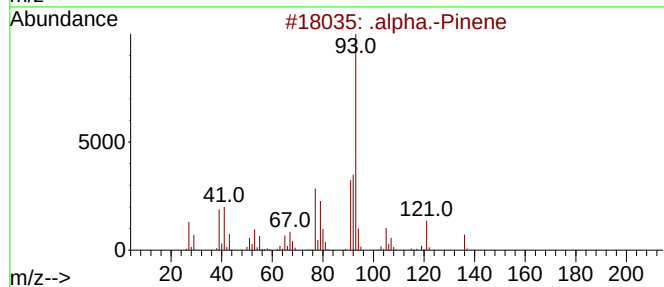
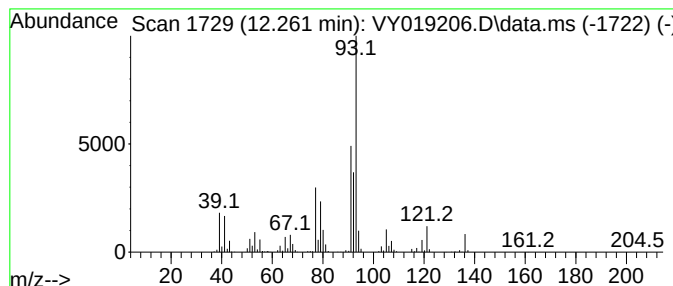
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Peak Number 3 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.261	73.09 ug/l	707650	Chlorobenzene-d5	11.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	97
2			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	95
3			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
4			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
5			.gamma.-Terpinene	136	C10H16	000099-85-4	91



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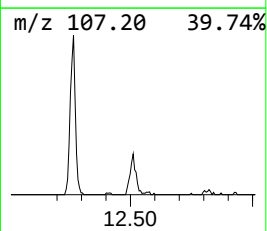
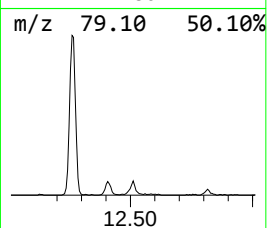
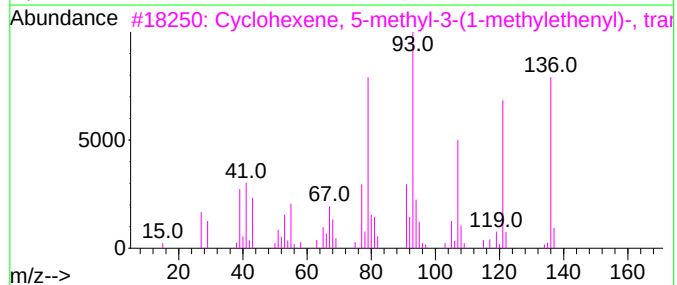
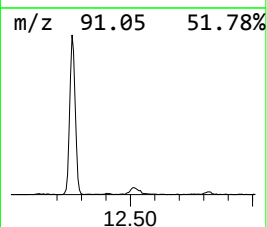
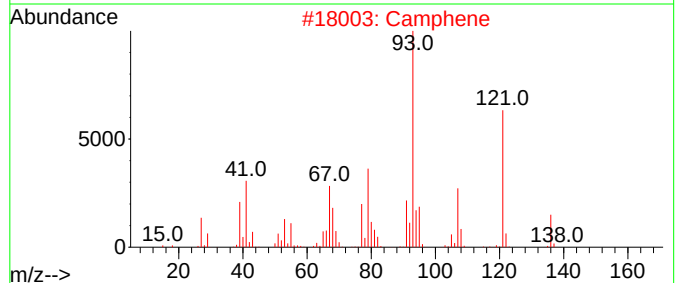
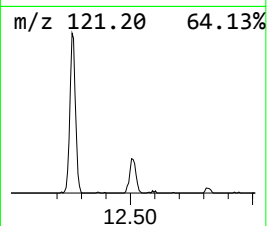
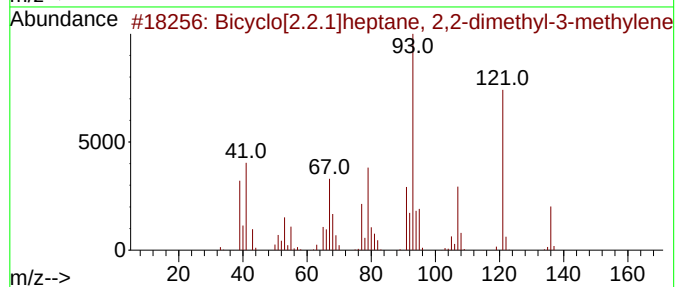
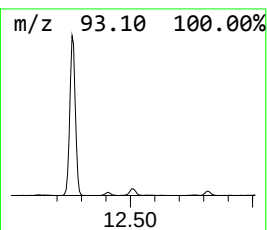
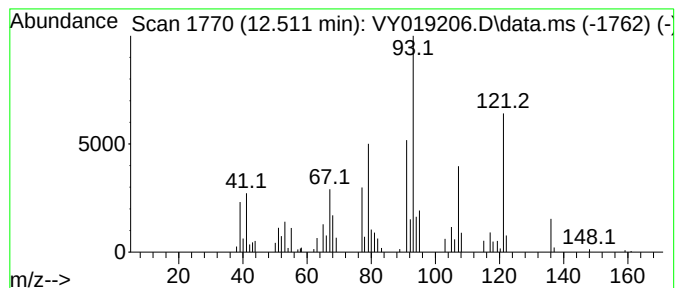
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Peak Number 4 Bicyclo[2.2.1]heptane, 2,2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.511	10.32 ug/l	66590	1,4-Dichlorobenzene-d4	13.352

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	94
2			Camphene	136	C10H16	000079-92-5	93
3			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	93
4			1,3,6-Heptatriene, 2,5,6-trimethyl-	136	C10H16	042123-66-0	91
5			1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Caryophyllene	11.597	13.2	ug/l	127741	3	11.420	484126	50.0
.alpha.-Pinene	12.261	73.1	ug/l	707650	3	11.420	484126	50.0
Bicyclo[2.2.1]h...	12.511	10.3	ug/l	66590	4	13.352	322730	50.0