

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010422\
 Data File : VN070470.D
 Acq On : 4 Jan 2022 17:58
 Operator : JC/MD
 Sample : M5251-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-6S

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_N\methods\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070470.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	81	92	100	rBV2	121404	255331	5.02%	0.903%
2	4.261	819	847	848	rBV3	53692	113894	2.24%	0.403%
3	4.580	942	966	992	rBV	44970	142240	2.80%	0.503%
4	5.077	1124	1151	1181	rBV3	132479	517939	10.19%	1.832%
5	5.613	1329	1351	1353	rBV	28982	54776	1.08%	0.194%
6	7.042	1865	1884	1901	rBV4	23639	68231	1.34%	0.241%
7	8.021	2224	2249	2260	rBV2	625958	1531840	30.14%	5.417%
8	8.083	2260	2272	2292	rVV	1196218	2756844	54.24%	9.749%
9	8.174	2295	2306	2331	rVB3	78616	192705	3.79%	0.681%
10	8.437	2383	2404	2429	rBV	800515	1857069	36.54%	6.567%
11	8.614	2455	2470	2495	rVB2	174794	444727	8.75%	1.573%
12	8.965	2581	2601	2630	rBV	1844086	3853171	75.81%	13.626%
13	9.880	2926	2942	2959	rVB3	69409	140411	2.76%	0.497%
14	10.011	2968	2991	3016	rBV4	81687	177107	3.48%	0.626%
15	10.440	3131	3151	3182	rBV	2709898	5082978	100.00%	17.975%
16	11.055	3362	3380	3402	rBV	173947	342113	6.73%	1.210%
17	11.741	3617	3636	3667	rBV	2358184	4315352	84.90%	15.261%
18	12.731	3984	4005	4031	rBV	1760751	3194881	62.85%	11.298%
19	13.672	4340	4356	4384	rBV	1615157	2867383	56.41%	10.140%
20	13.873	4407	4431	4450	rBV	155335	303419	5.97%	1.073%
21	14.327	4589	4600	4614	rVB2	40148	65485	1.29%	0.232%

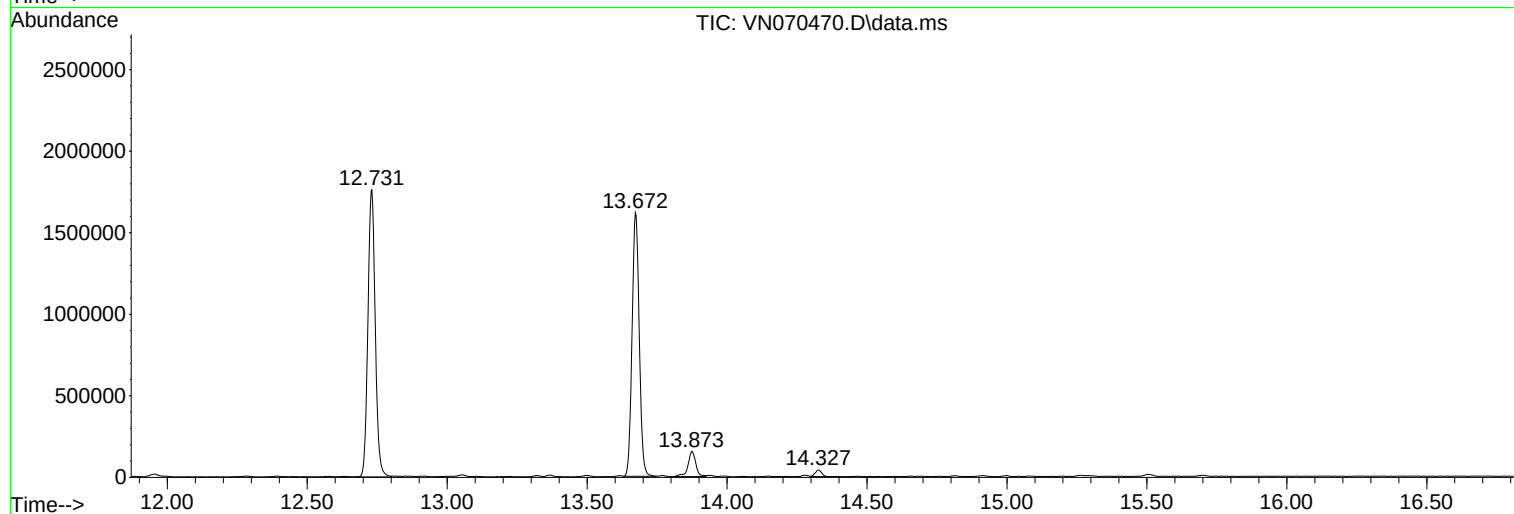
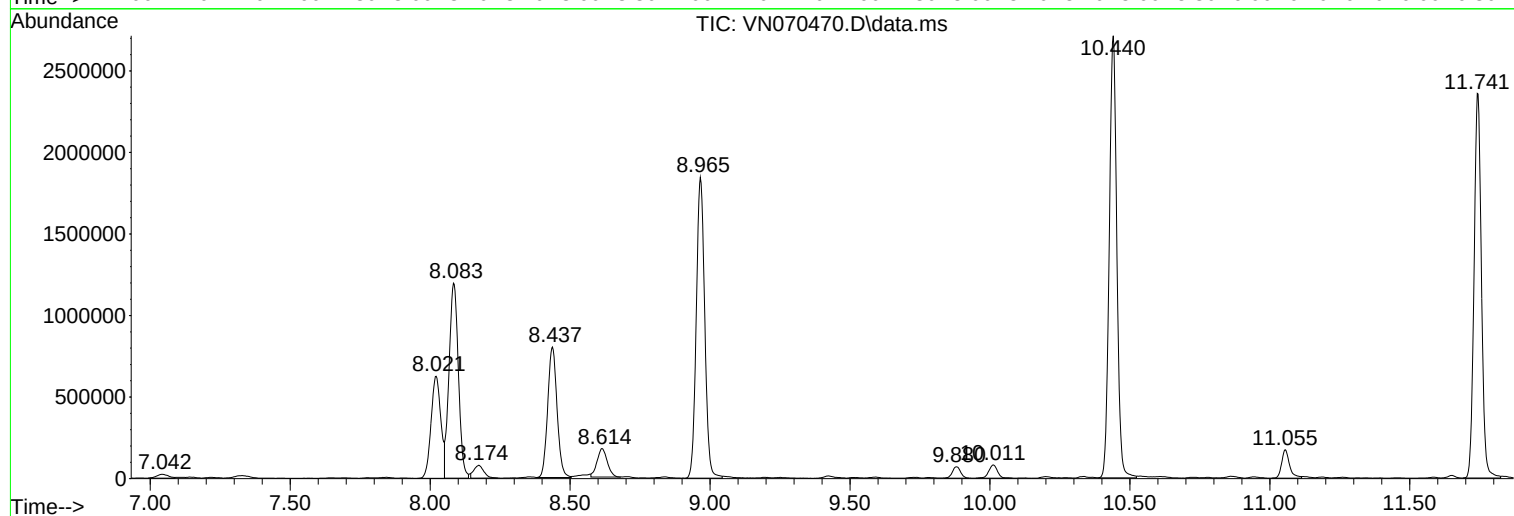
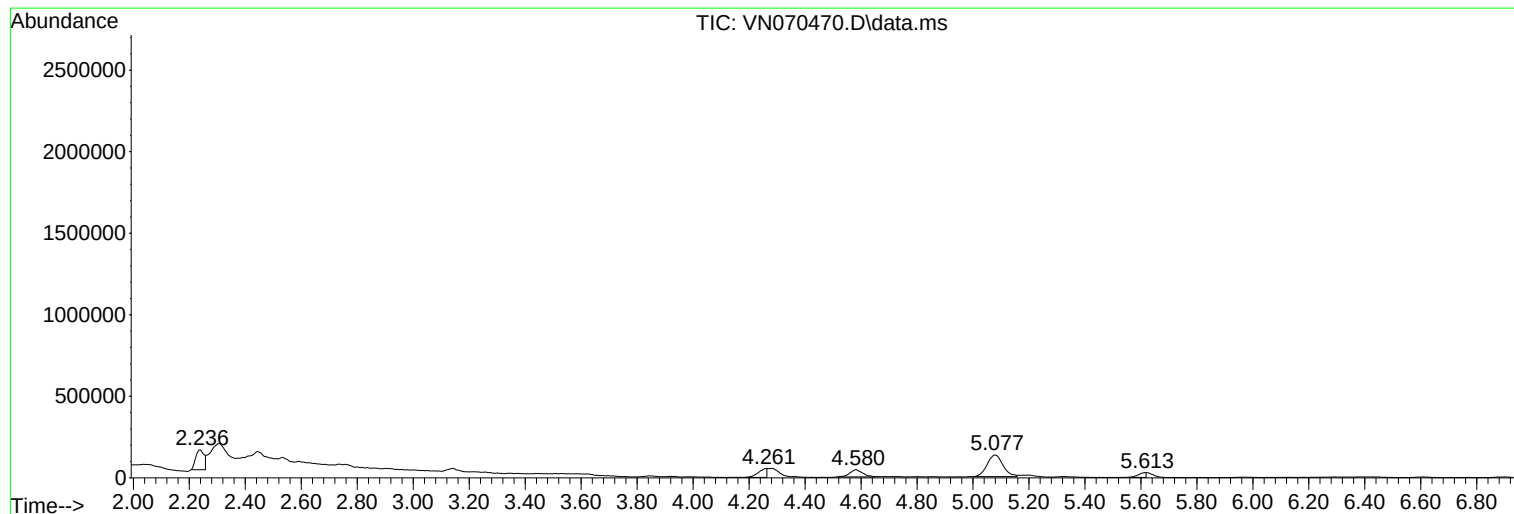
Sum of corrected areas: 28277896

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Quant Title : SW846 8260

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



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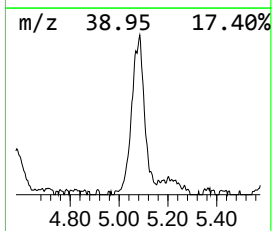
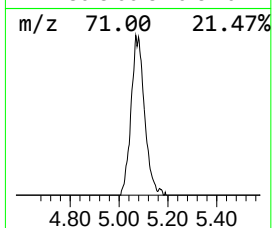
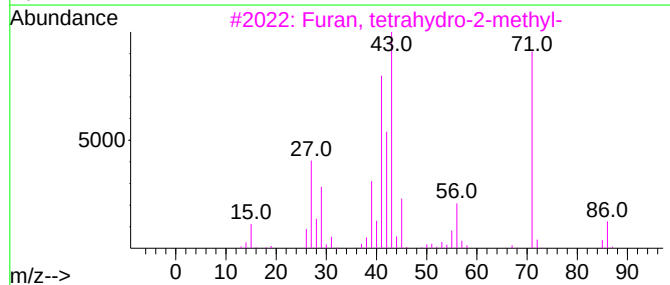
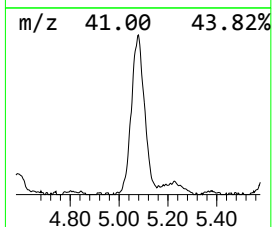
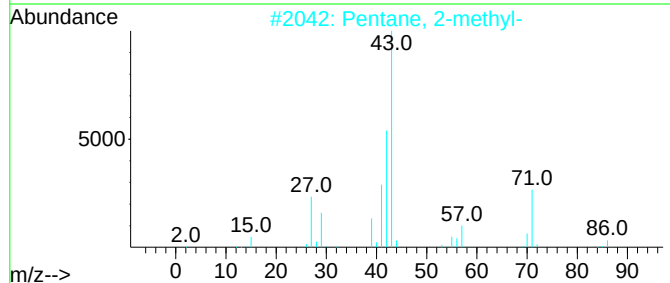
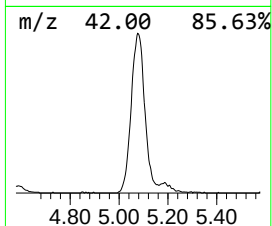
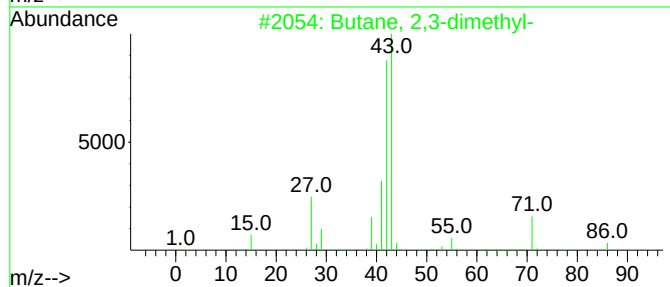
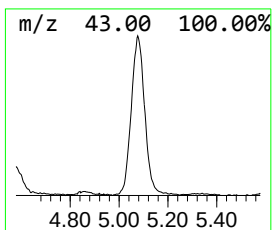
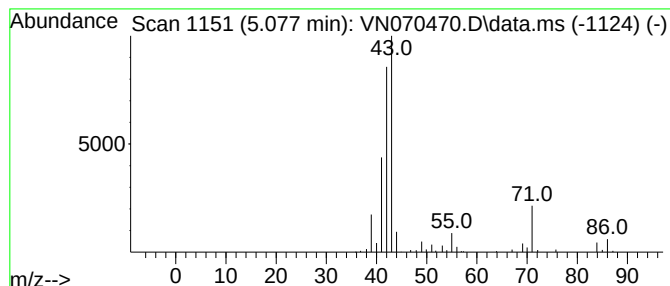
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.077	9.39 ug/l	517939	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	28
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
4			Pentane	72	C5H12	000109-66-0	9
5			1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	7



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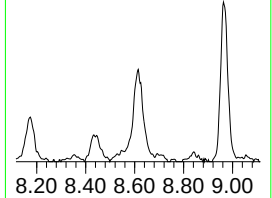
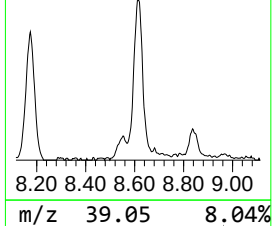
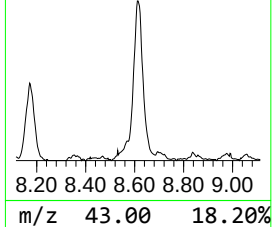
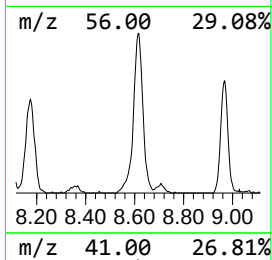
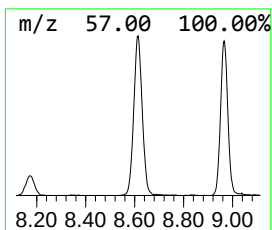
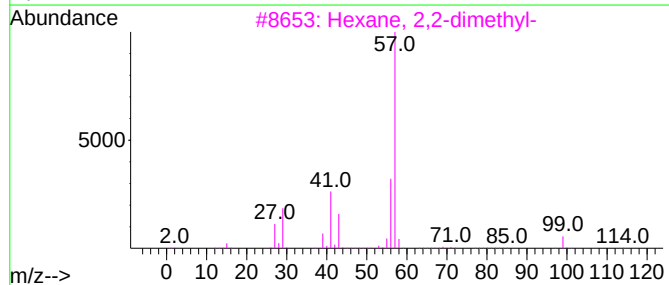
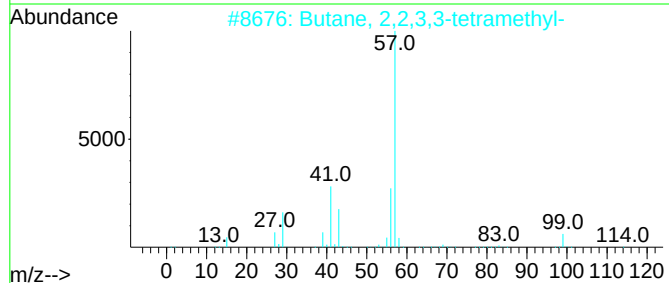
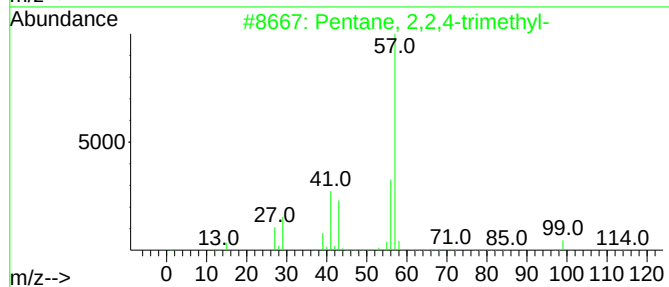
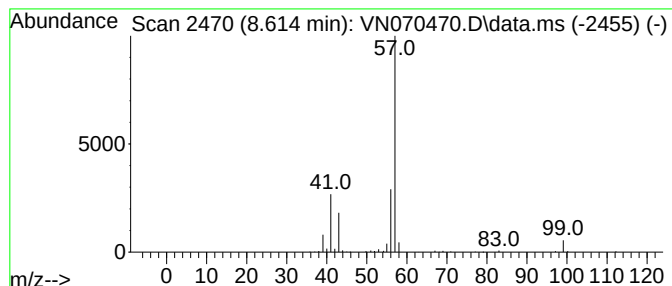
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	5.77 ug/l	444727	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



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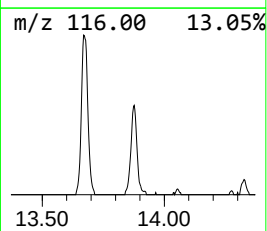
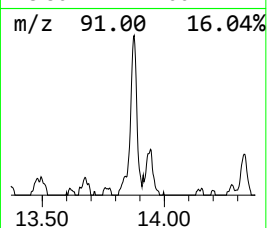
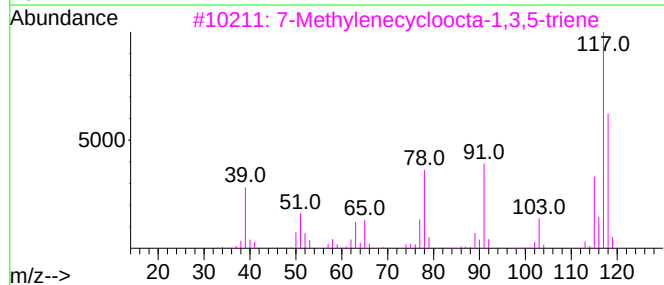
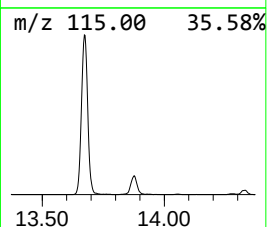
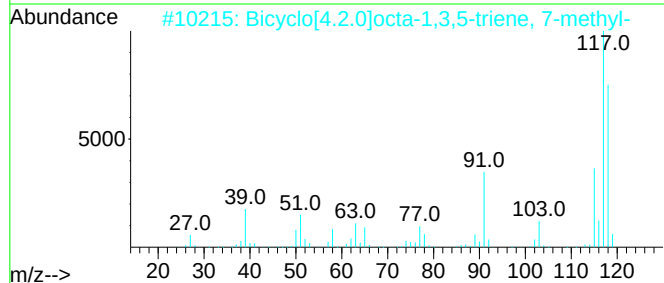
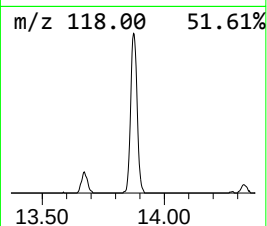
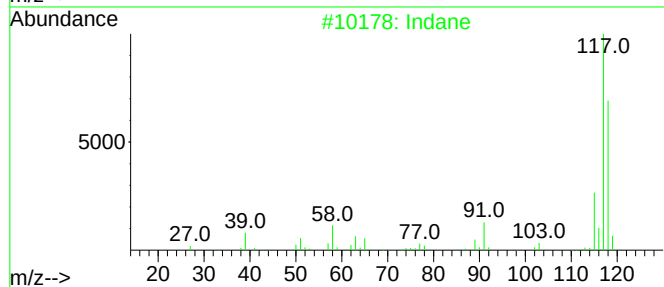
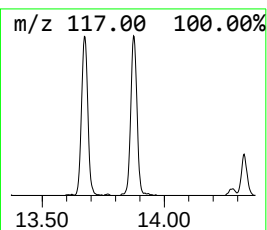
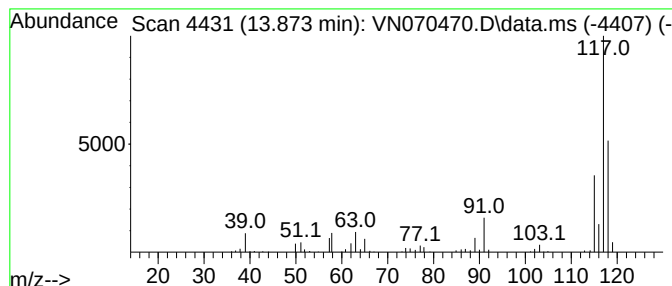
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Peak Number 3 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	5.29 ug/l	303419	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
3			7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	64
4			Deltacyclene	118	C9H10	007785-10-6	59
5			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2,3-dim...	5.077	9.4	ug/l	517939	1	8.086	2756840	50.0
Pentane, 2,2,4-...	8.614	5.8	ug/l	444727	2	8.965	3853170	50.0
Indane	13.873	5.3	ug/l	303419	4	13.672	2867380	50.0