

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
 Data File : BF131774.D
 Acq On : 22 Dec 2022 13:19
 Operator : CG\JU
 Sample : PB149691BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149691BL

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131774.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	17	rVB	54611	69385	1.84%	0.325%
2	2.269	26	31	40	rVB	47243	58369	1.55%	0.273%
3	5.075	503	508	519	rBV	271871	393908	10.47%	1.844%
4	5.475	571	576	579	rBV	2756623	2700615	71.78%	12.644%
5	6.486	742	748	751	rBV	2482876	2718425	72.25%	12.728%
6	6.851	806	810	814	rBV	633322	493454	13.12%	2.310%
7	7.422	901	907	910	rBV	1641469	1767991	46.99%	8.278%
8	8.139	1025	1029	1033	rBV	717648	652487	17.34%	3.055%
9	9.227	1207	1214	1217	rBV	3594484	3332298	88.57%	15.602%
10	9.904	1324	1329	1332	rBV	994578	800619	21.28%	3.749%
11	10.698	1458	1464	1467	rBV	2507530	2227032	59.19%	10.427%
12	11.398	1579	1583	1586	rBV	1092356	872180	23.18%	4.084%
13	12.992	1849	1854	1857	rBV	4097887	3762370	100.00%	17.616%
14	14.045	2029	2033	2037	rBV	847338	708907	18.84%	3.319%
15	15.168	2219	2224	2228	rVB	32545	39160	1.04%	0.183%
16	15.533	2281	2286	2297	rBV	432232	568527	15.11%	2.662%
17	15.998	2360	2365	2370	rBV	36300	54685	1.45%	0.256%
18	16.521	2448	2454	2460	rBV2	30927	53493	1.42%	0.250%
19	17.127	2550	2557	2563	rBV3	19260	39489	1.05%	0.185%
20	17.845	2669	2679	2688	rBV5	15642	44868	1.19%	0.210%

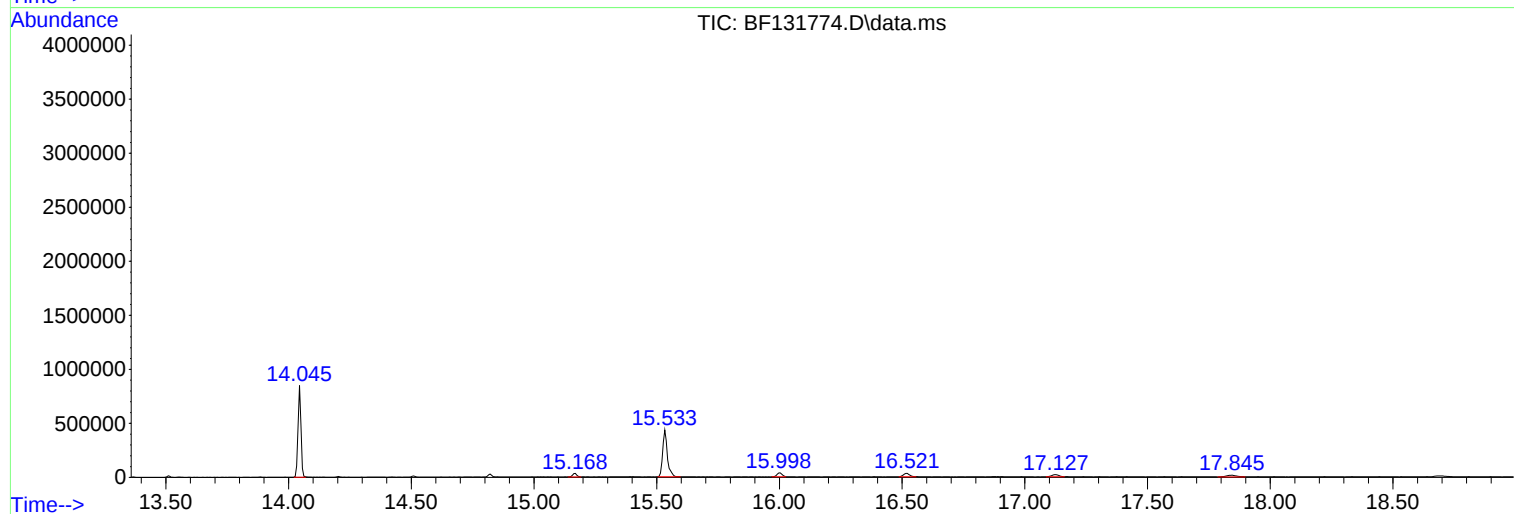
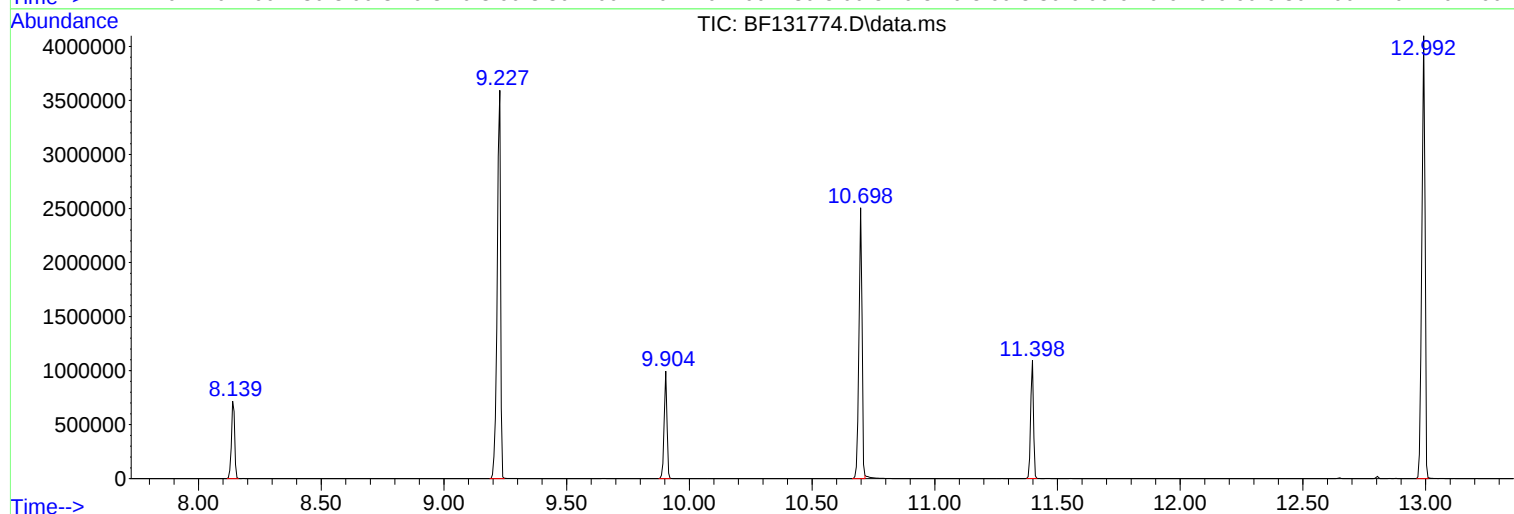
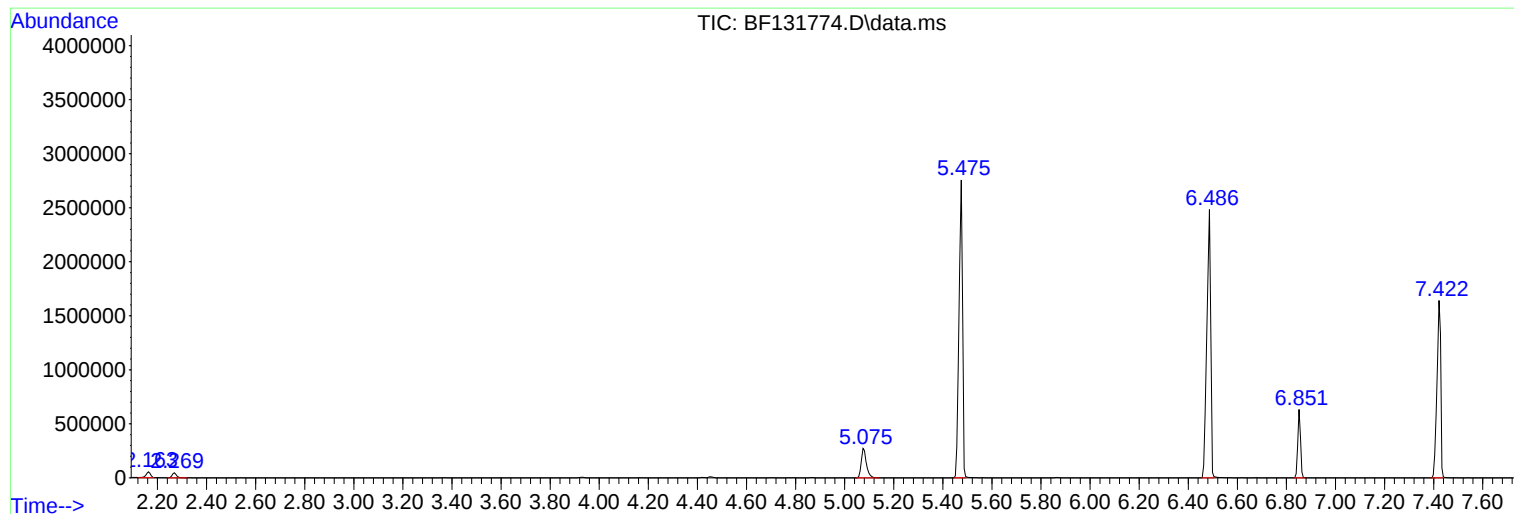
Sum of corrected areas: 21358262

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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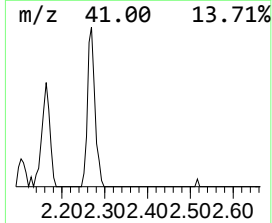
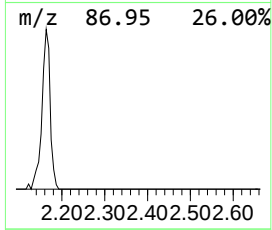
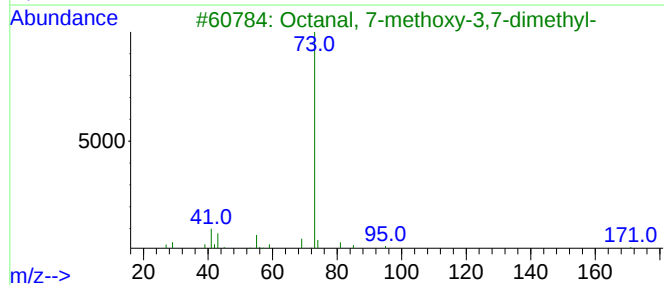
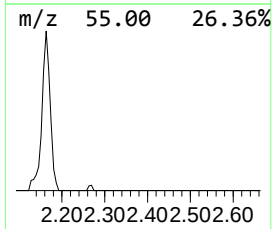
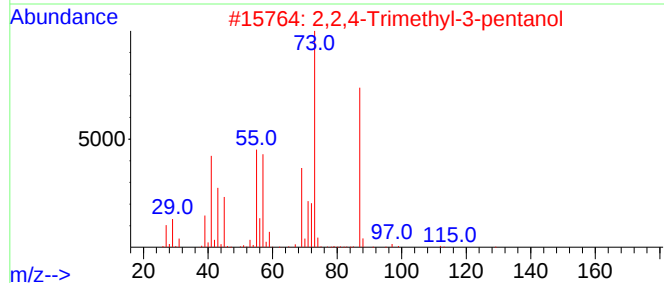
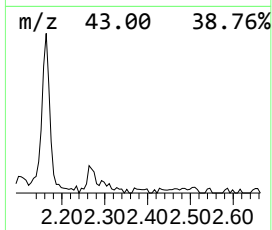
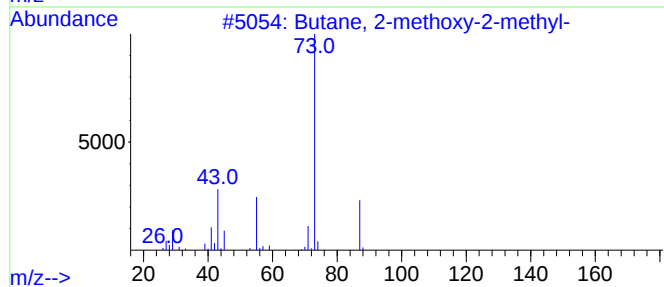
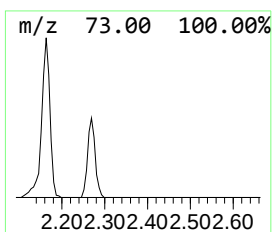
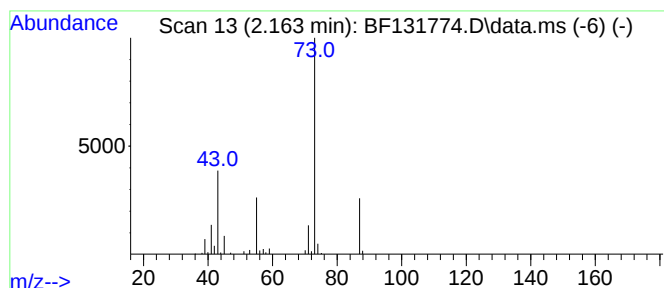
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	2.81 ng	69385	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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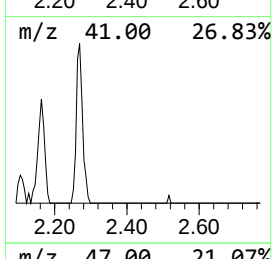
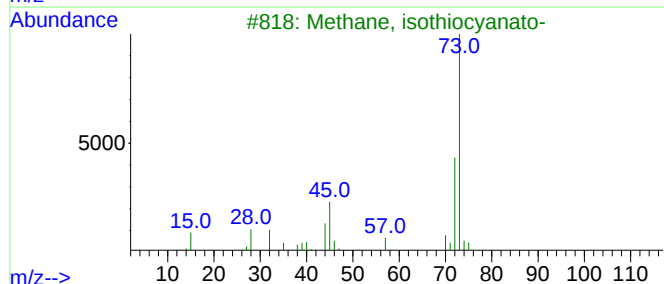
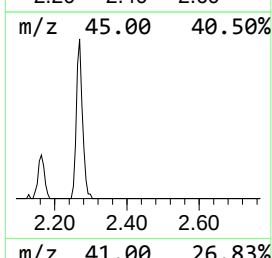
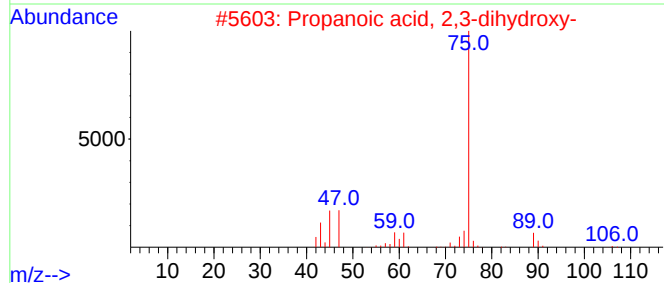
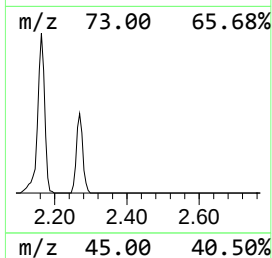
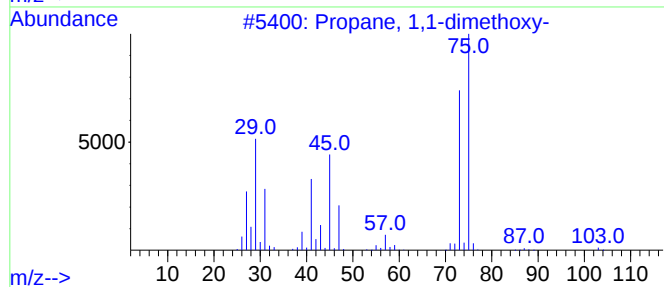
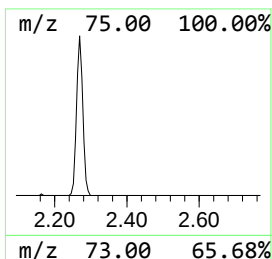
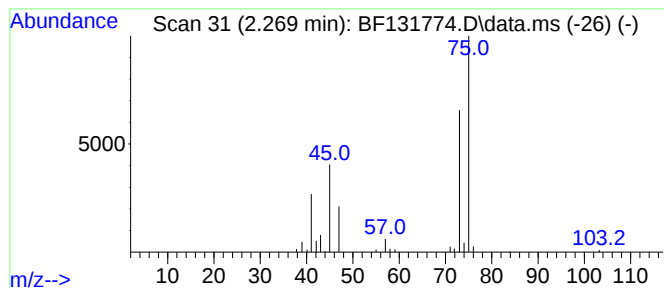
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.37 ng	58369	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	36
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4			Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9
5			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	9



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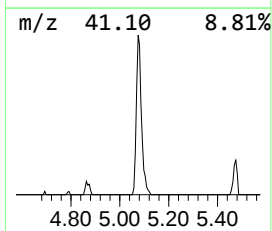
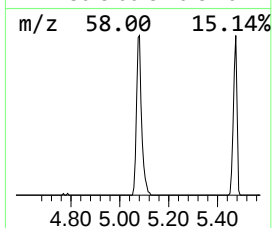
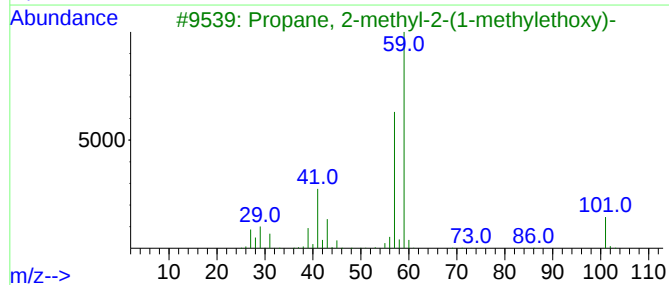
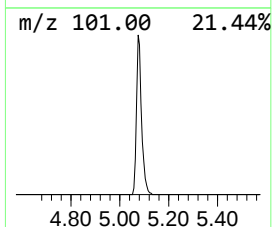
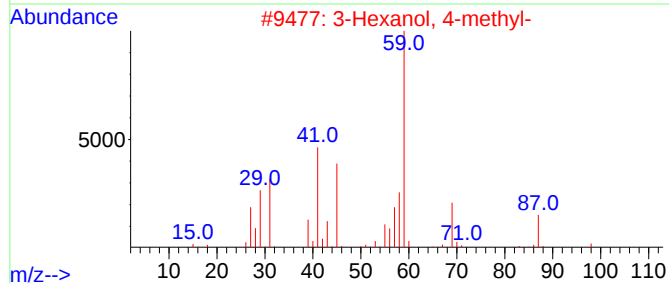
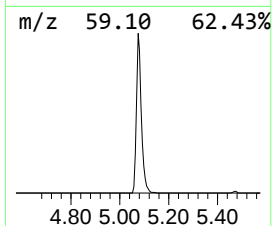
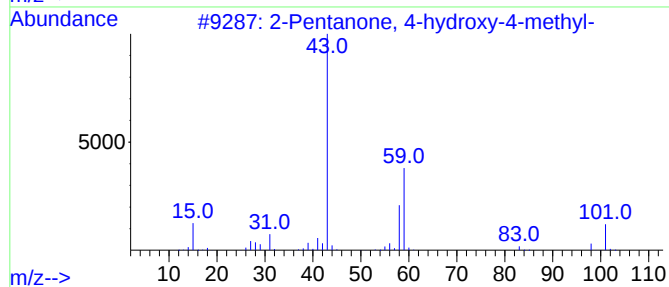
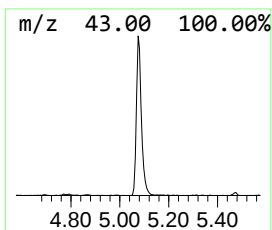
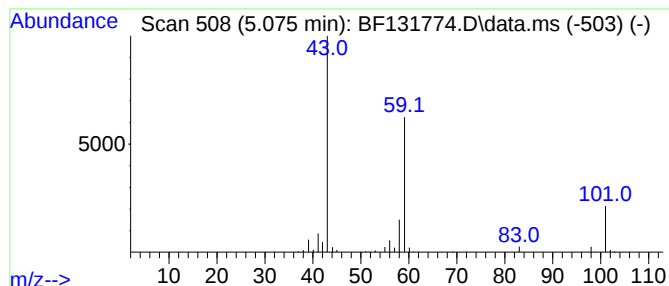
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	15.97 ng	393908	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	2.8	ng	69385	1	6.851	493454	20.0
Propane, 1,1-di...	2.269	2.4	ng	58369	1	6.851	493454	20.0
2-Pentanone, 4-...	5.075	16.0	ng	393908	1	6.851	493454	20.0