

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092922\
 Data File : BF130466.D
 Acq On : 29 Sep 2022 14:40
 Operator : CG\JU
 Sample : N4860-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-01

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-BF091422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.151	345	351	356	rBV	34215	45628	1.08%	0.215%
2	4.816	460	464	475	rBV	448527	559307	13.19%	2.631%
3	5.240	532	536	548	rBV	1632221	1680757	39.64%	7.907%
4	5.645	601	605	614	rBV	101558	92651	2.19%	0.436%
5	6.275	708	712	724	rBV	1207025	1122294	26.47%	5.280%
6	6.639	770	774	777	rBV	690605	630988	14.88%	2.969%
7	7.210	865	871	874	rBV	1975942	2160546	50.96%	10.164%
8	7.922	987	992	995	rBV	867256	831790	19.62%	3.913%
9	8.998	1169	1175	1178	rBV	4297080	4239767	100.00%	19.946%
10	9.669	1281	1289	1293	rBV	1153371	933573	22.02%	4.392%
11	10.210	1374	1381	1390	rBV2	26903	49384	1.16%	0.232%
12	10.463	1418	1424	1427	rBV	3010359	2741046	64.65%	12.895%
13	11.151	1537	1541	1544	rBV	1080966	894013	21.09%	4.206%
14	11.686	1627	1632	1636	rBV	73329	84740	2.00%	0.399%
15	12.739	1806	1811	1814	rBV	4116056	3747285	88.38%	17.629%
16	13.310	1904	1908	1912	rVB	292202	270577	6.38%	1.273%
17	13.780	1984	1988	1992	rBV	760408	640242	15.10%	3.012%
18	13.886	2003	2006	2014	rVB	43403	59032	1.39%	0.278%
19	15.168	2220	2224	2228	rBV	429284	472490	11.14%	2.223%

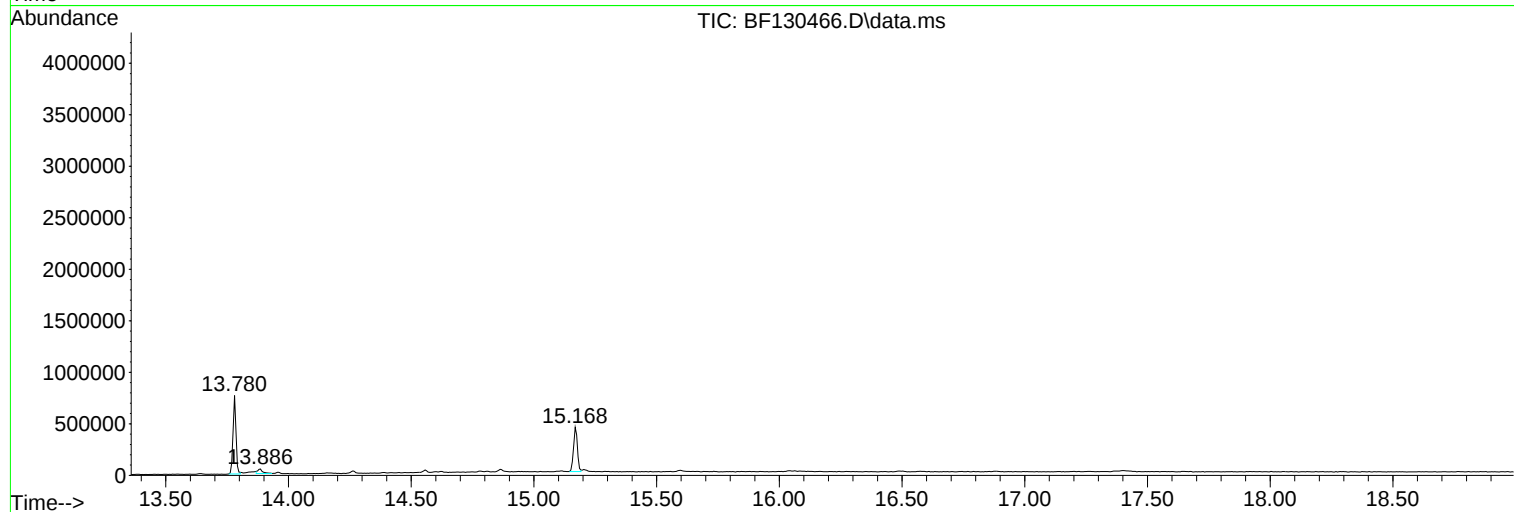
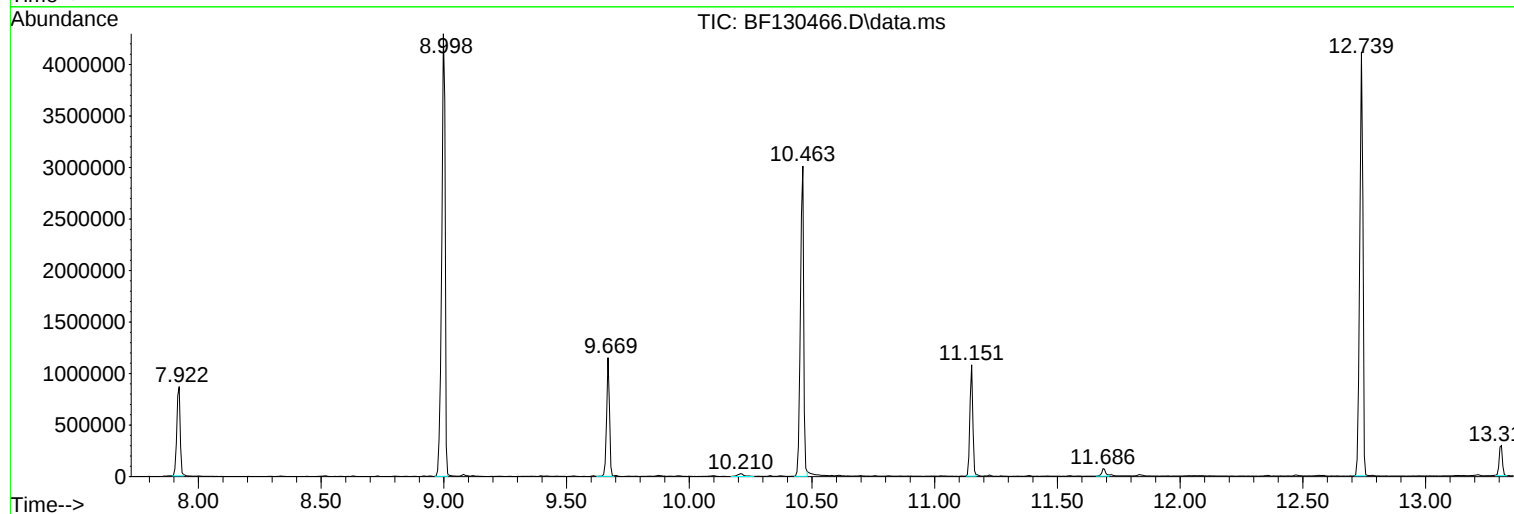
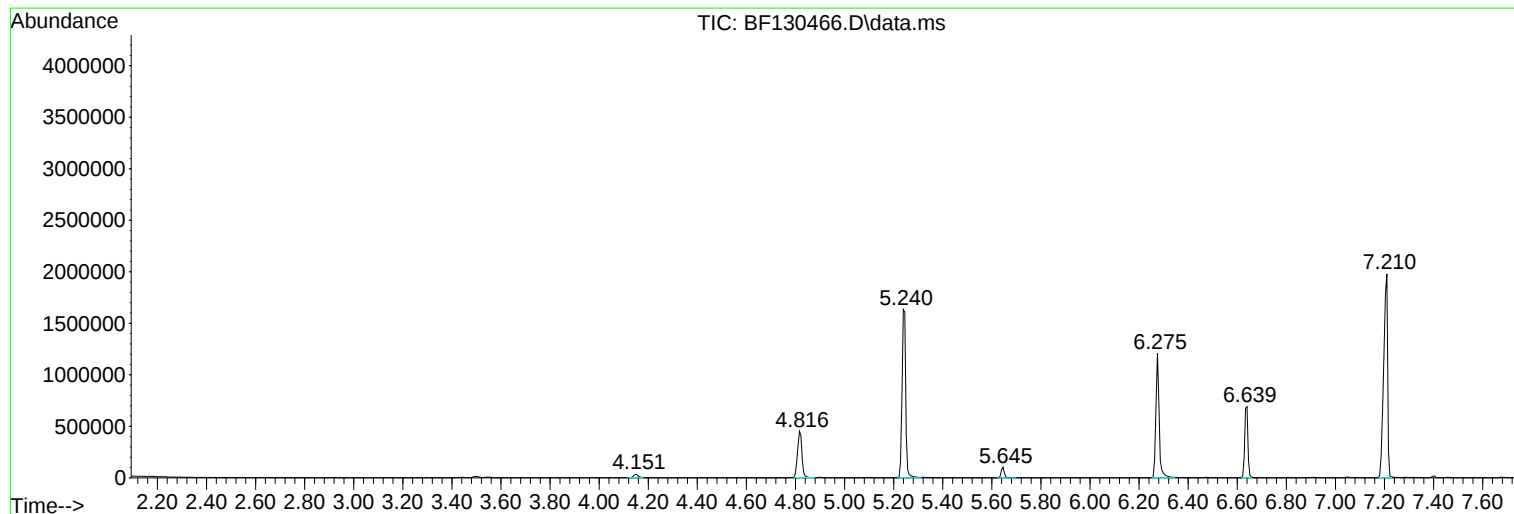
Sum of corrected areas: 21256110

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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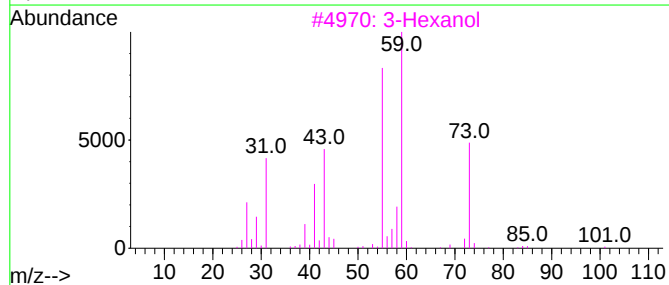
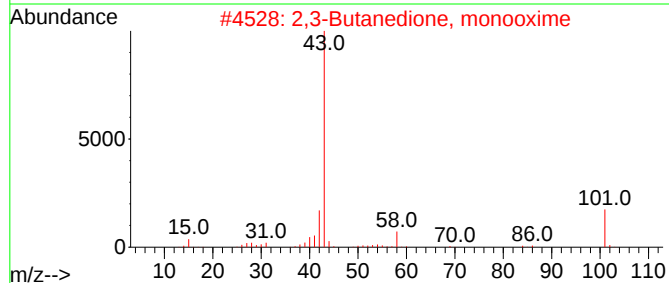
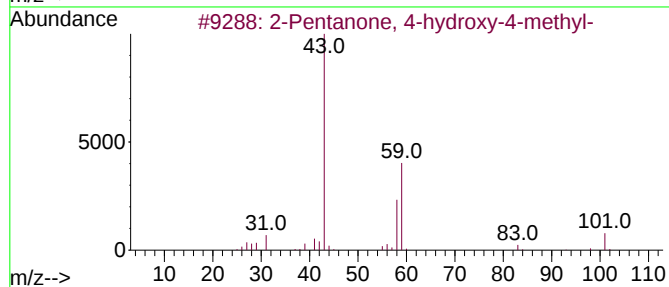
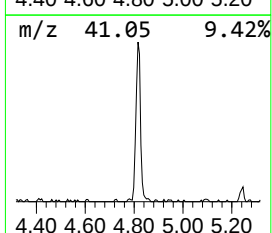
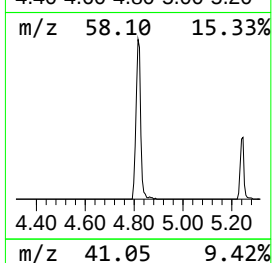
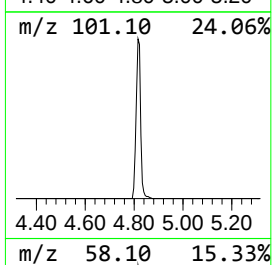
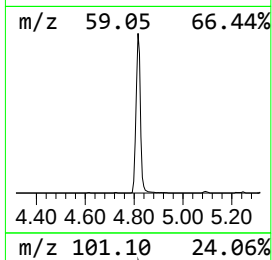
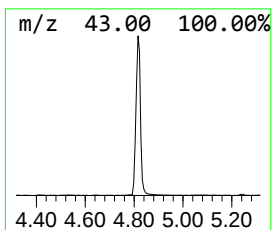
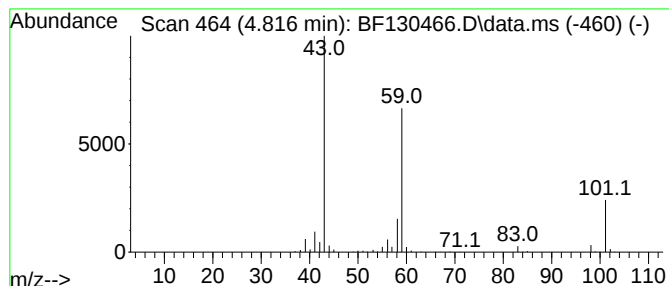
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	17.73 ng	559307	1,4-Dichlorobenzene-d4	6.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
3	3-Hexanol	102	C6H14O	000623-37-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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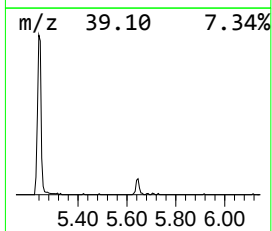
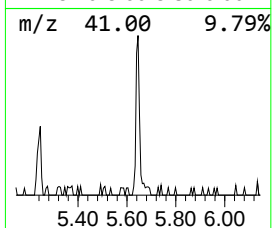
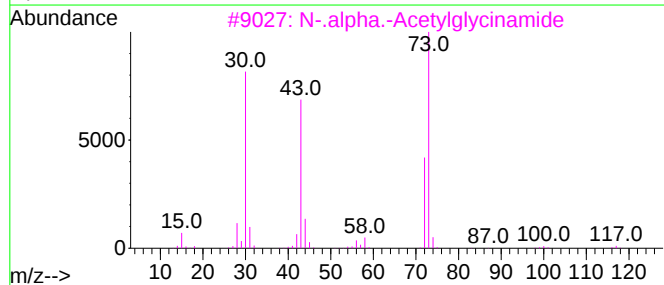
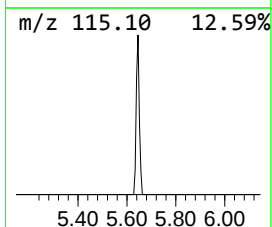
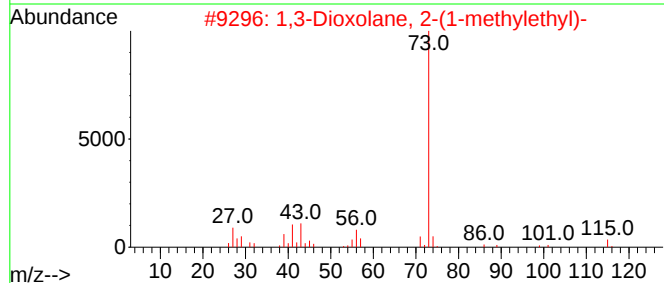
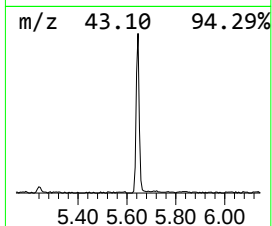
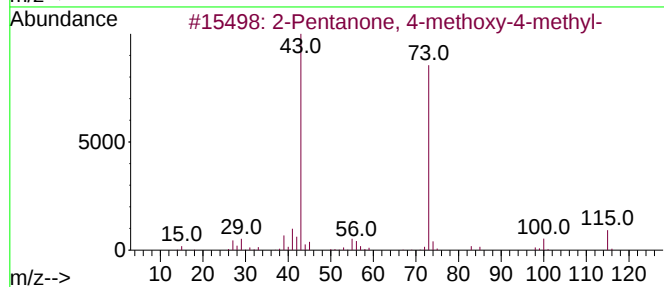
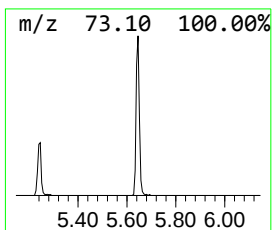
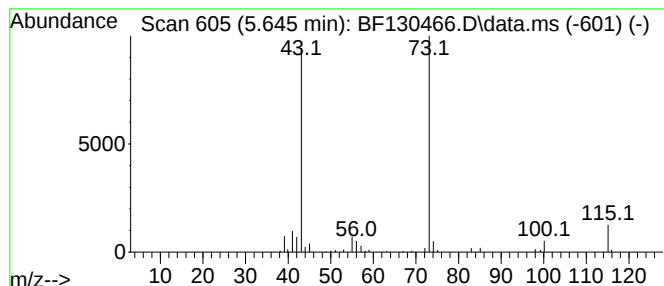
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.645	2.94 ng	92651	1,4-Dichlorobenzene-d4	6.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
3			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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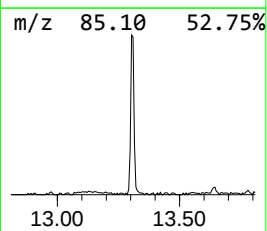
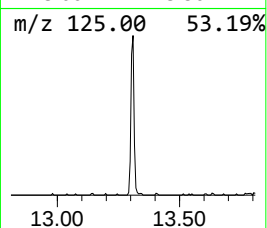
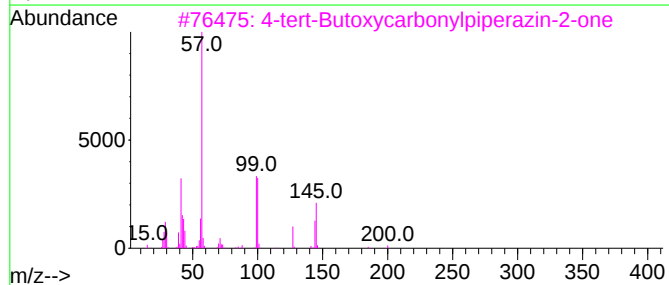
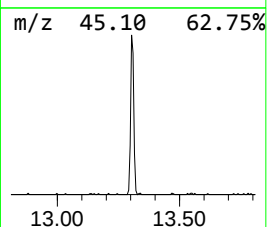
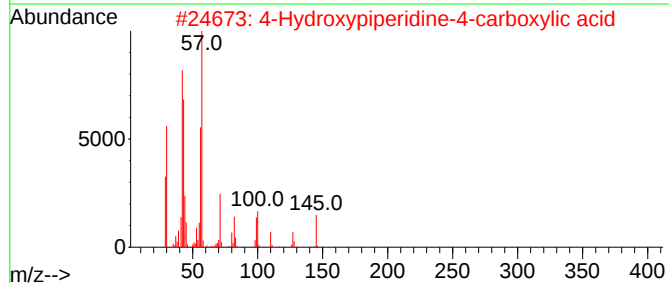
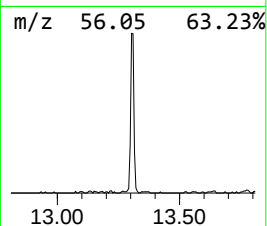
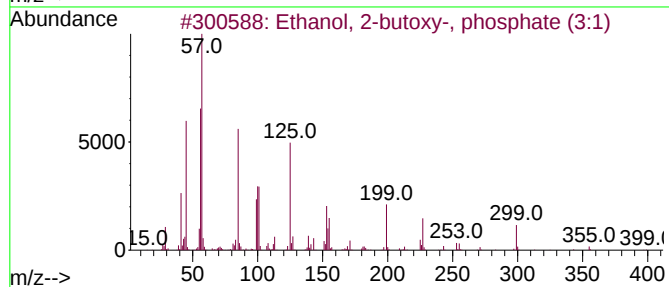
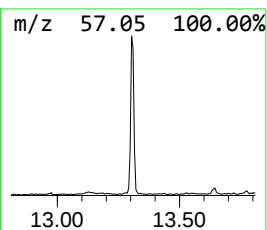
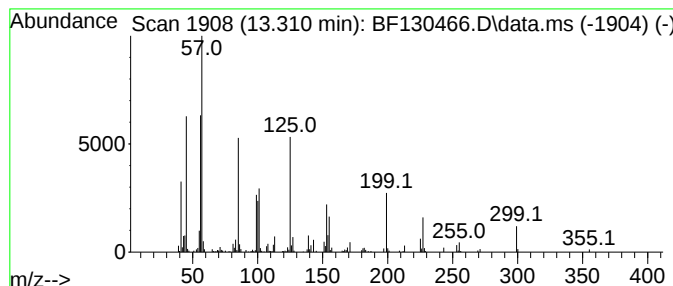
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Peak Number 3 Ethanol, 2-butoxy-, phospho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.310	8.45 ng	270577	Chrysene-d12	13.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	90
2			4-Hydroxypiperidine-4-carboxylic...	145	C6H11NO3	050289-06-0	14
3			4-tert-Butoxycarbonylpiperazin-2...	200	C9H16N2O3	076003-29-7	10
4			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	10
5			2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	10



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.816	17.7	ng	559307	1	6.639	630988	20.0
2-Pentanone, 4-...	5.645	2.9	ng	92651	1	6.639	630988	20.0
Ethanol, 2-buto...	13.310	8.4	ng	270577	5	13.780	640242	20.0