

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113020\
 Data File : BF122503.D
 Acq On : 30 Nov 2020 12:19
 Operator : JU/CG
 Sample : PB133297BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB133297BL

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	20	23	35	rVB	77148	117177	1.26%	0.205%
2	4.475	401	406	414	rBV	630306	695899	7.46%	1.216%
3	5.092	505	511	525	rVB	1540318	2232888	23.95%	3.901%
4	5.492	573	579	582	rBV	5458056	6641921	71.25%	11.605%
5	5.875	640	644	650	rBV	211878	171440	1.84%	0.300%
6	6.492	743	749	752	rBV	5073771	6785441	72.79%	11.855%
7	6.857	807	811	814	rBV	1862302	1493588	16.02%	2.610%
8	7.422	901	907	910	rBV	4053785	4473123	47.98%	7.815%
9	8.139	1024	1029	1046	rBV	2228758	2023368	21.70%	3.535%
10	9.222	1206	1213	1216	rBV	7443799	7874792	84.47%	13.759%
11	9.898	1322	1328	1347	rBV	2650834	2394647	25.69%	4.184%
12	10.692	1456	1463	1500	rBV	4548868	5663914	60.76%	9.896%
13	11.386	1575	1581	1588	rBV	2386924	2487939	26.69%	4.347%
14	12.980	1844	1852	1855	rBV	8253665	9322286	100.00%	16.288%
15	14.027	2025	2030	2049	rBV	2519536	2477067	26.57%	4.328%
16	15.498	2274	2280	2295	rBV	1482636	2237351	24.00%	3.909%
17	16.962	2520	2529	2542	rBV4	32162	142789	1.53%	0.249%

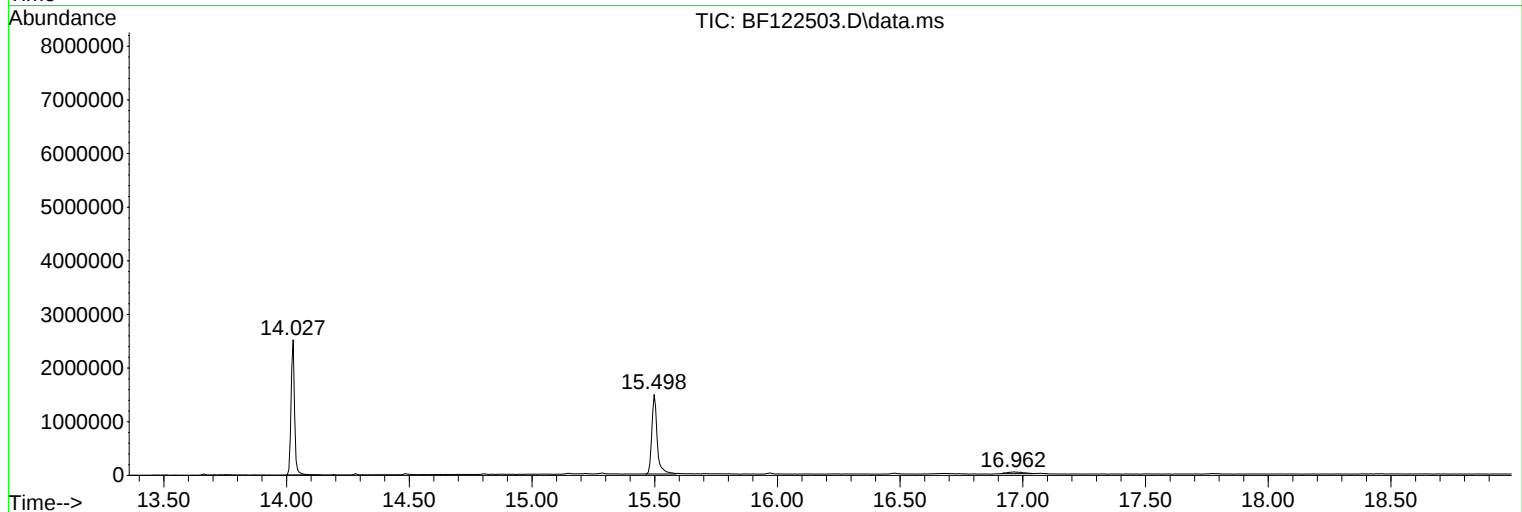
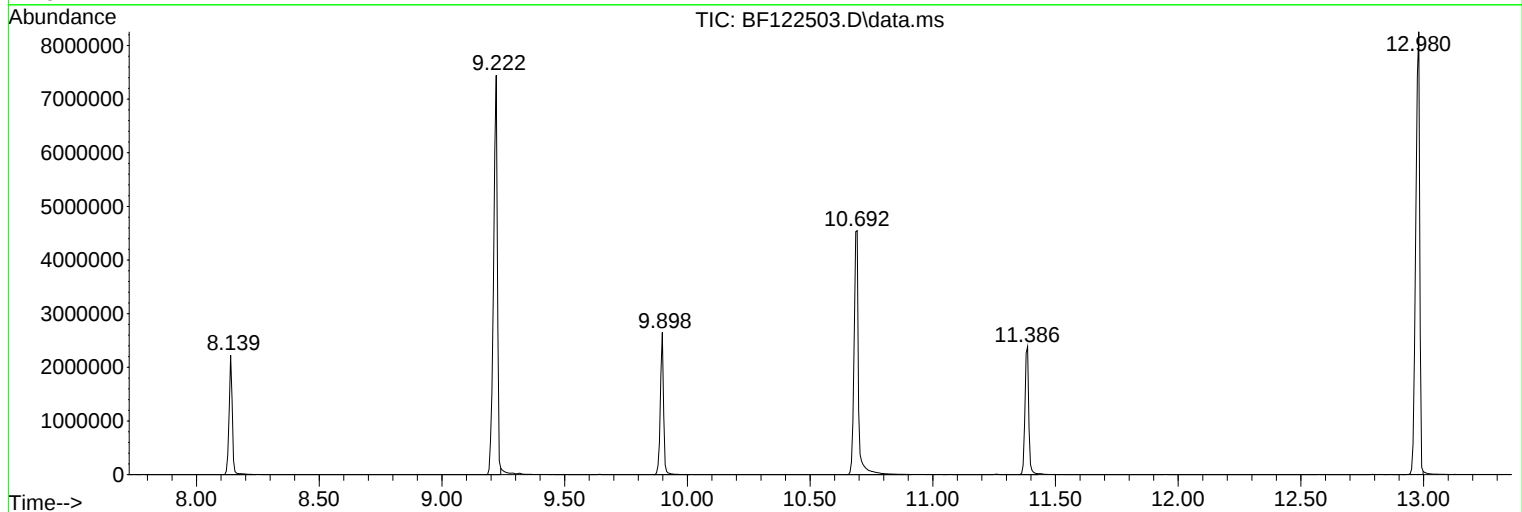
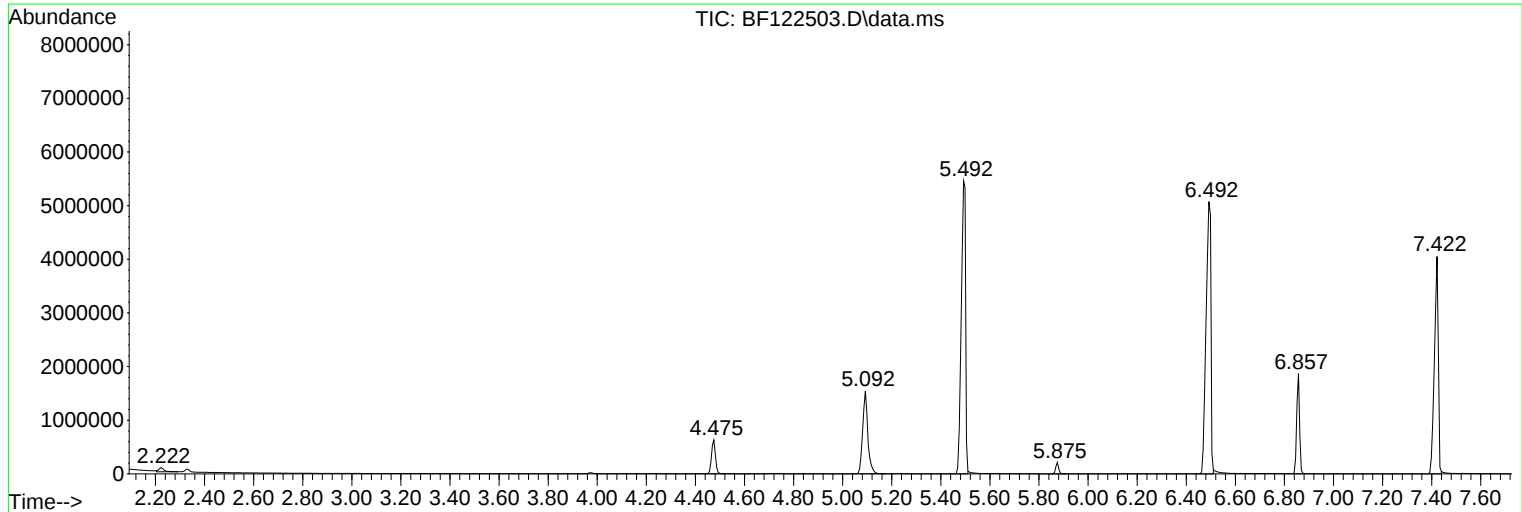
Sum of corrected areas: 57235630

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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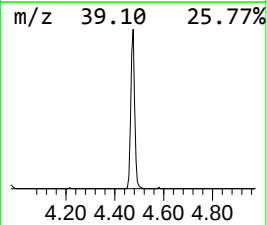
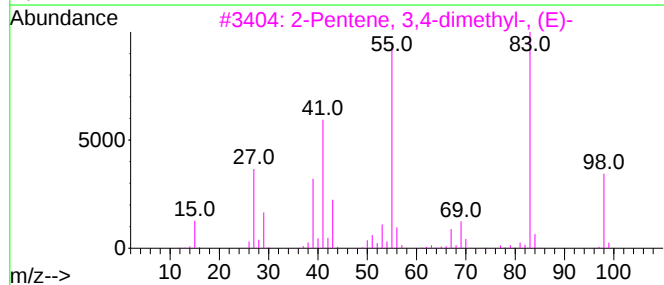
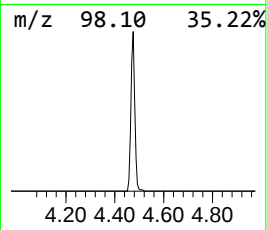
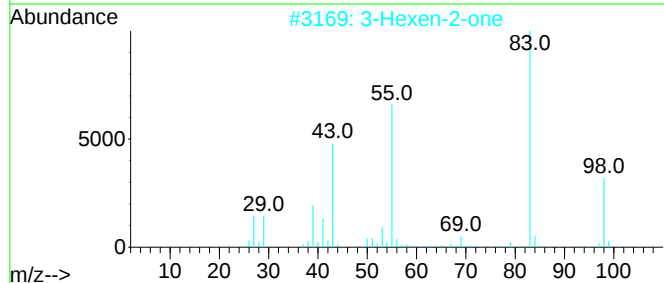
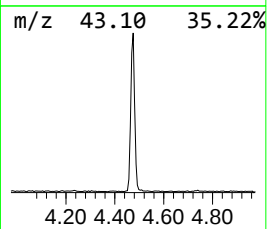
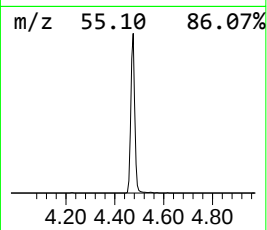
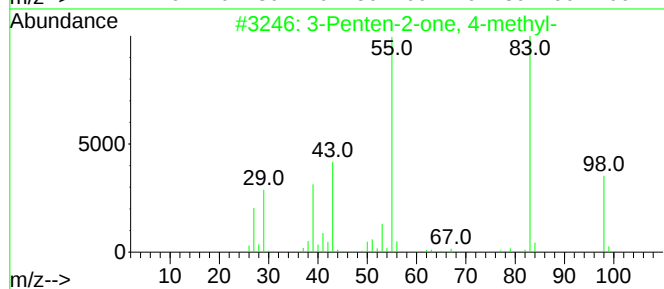
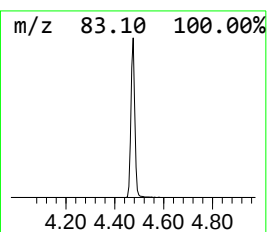
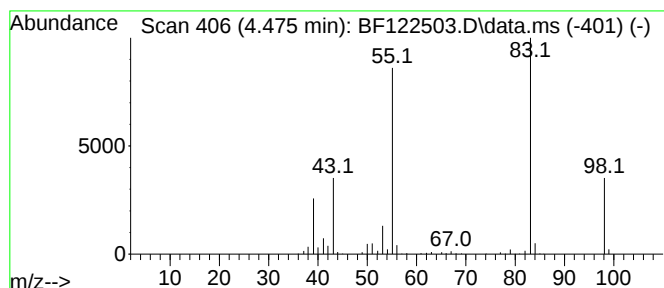
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	9.32 ng	695899	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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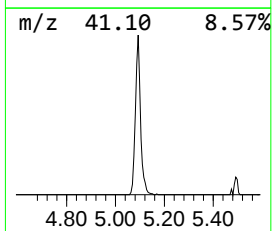
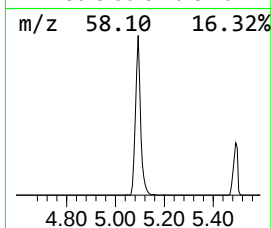
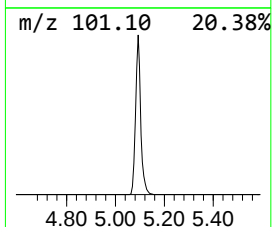
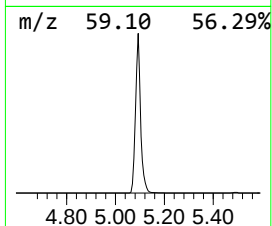
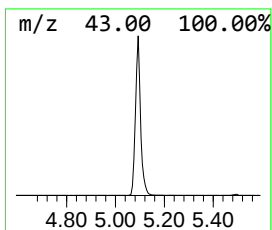
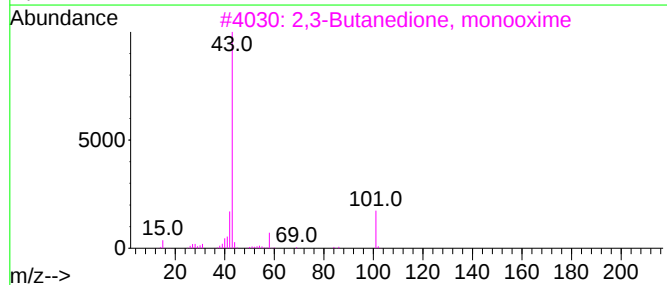
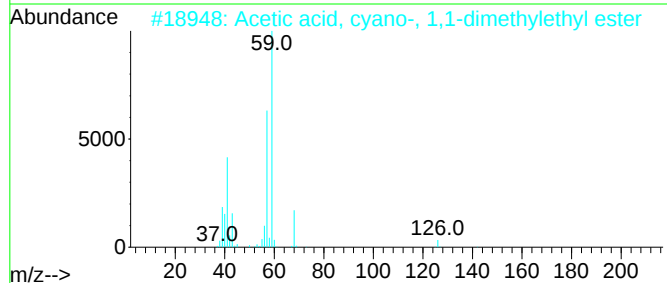
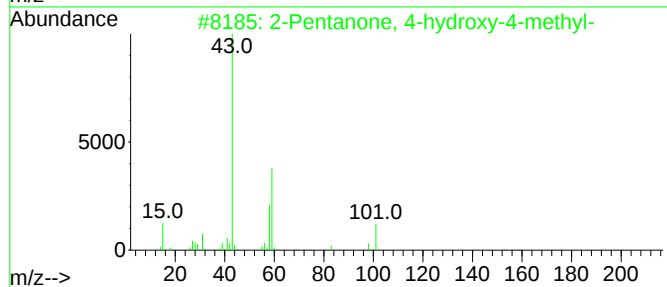
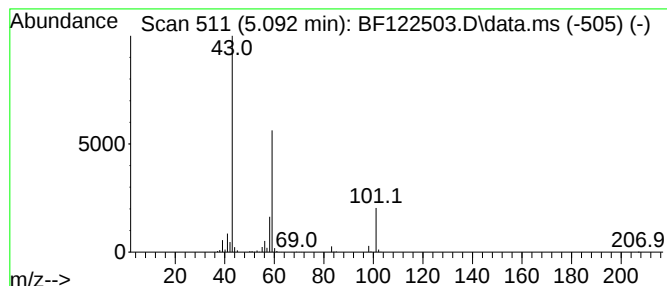
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	29.90 ng	2232890	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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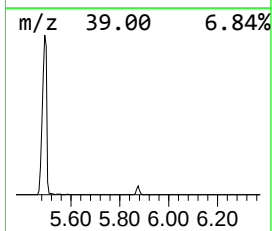
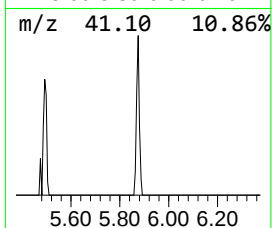
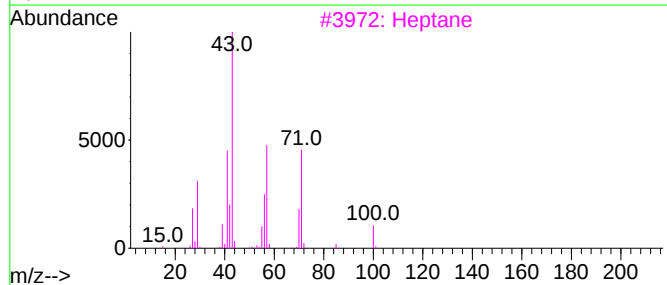
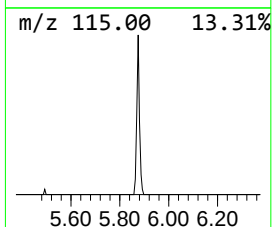
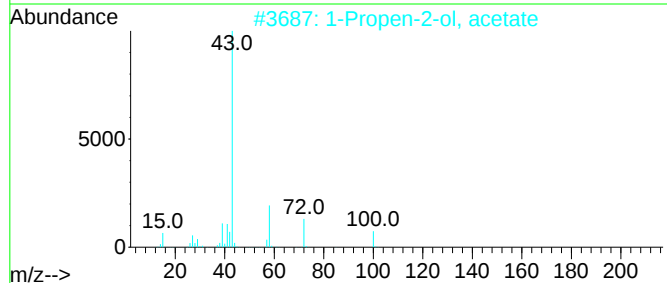
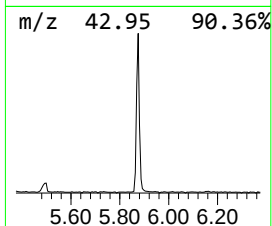
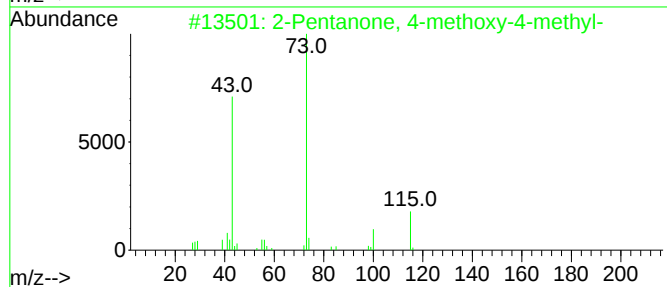
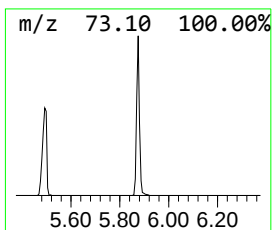
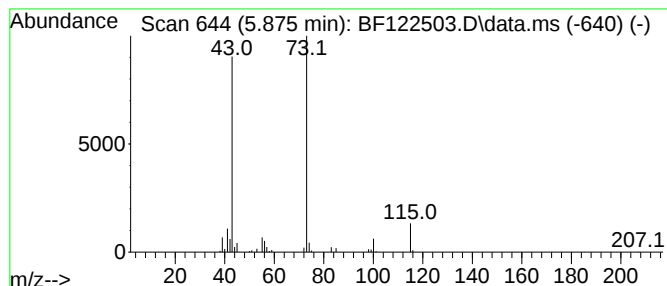
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	2.30 ng	171440	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Heptane	100	C7H16	000142-82-5	9
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
5		Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	9



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.475	9.3	ng	695899	1	6.857	1493590	20.0
2-Pentanone, 4-...	5.092	29.9	ng	2232890	1	6.857	1493590	20.0
2-Pentanone, 4-...	5.875	2.3	ng	171440	1	6.857	1493590	20.0