

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047611.D
Acq On : 23 Sep 2024 19:44
Operator : RC/JU
Sample : PB163606BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB163606BL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047611.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.357	209	216	232	rVB	28643875	43145873	100.00%	21.491%
2	4.957	310	318	329	rBV	12788143	18072854	41.89%	9.002%
3	5.416	389	396	407	rBV	12070259	16970835	39.33%	8.453%
4	6.028	494	500	510	rVB	2146068	3115356	7.22%	1.552%
5	7.004	657	666	675	rBV	12091266	19023247	44.09%	9.475%
6	7.839	800	808	815	rBV	1978751	3154348	7.31%	1.571%
7	8.992	995	1004	1015	rBV	6552086	10651698	24.69%	5.306%
8	10.633	1275	1283	1291	rVB	2587262	4218945	9.78%	2.101%
9	13.092	1694	1701	1713	rBV	14916585	21448629	49.71%	10.683%
10	14.468	1928	1935	1943	rBV	3187898	4619833	10.71%	2.301%
11	15.951	2178	2187	2205	rBV	10472323	14383186	33.34%	7.164%
12	17.204	2393	2400	2410	rBV	3659099	4925202	11.42%	2.453%
13	19.821	2839	2845	2850	rBV	23472624	27270301	63.20%	13.583%
14	21.427	3113	3118	3125	rBV2	3345275	4891051	11.34%	2.436%
15	24.450	3624	3632	3640	rBV	1891439	4874363	11.30%	2.428%

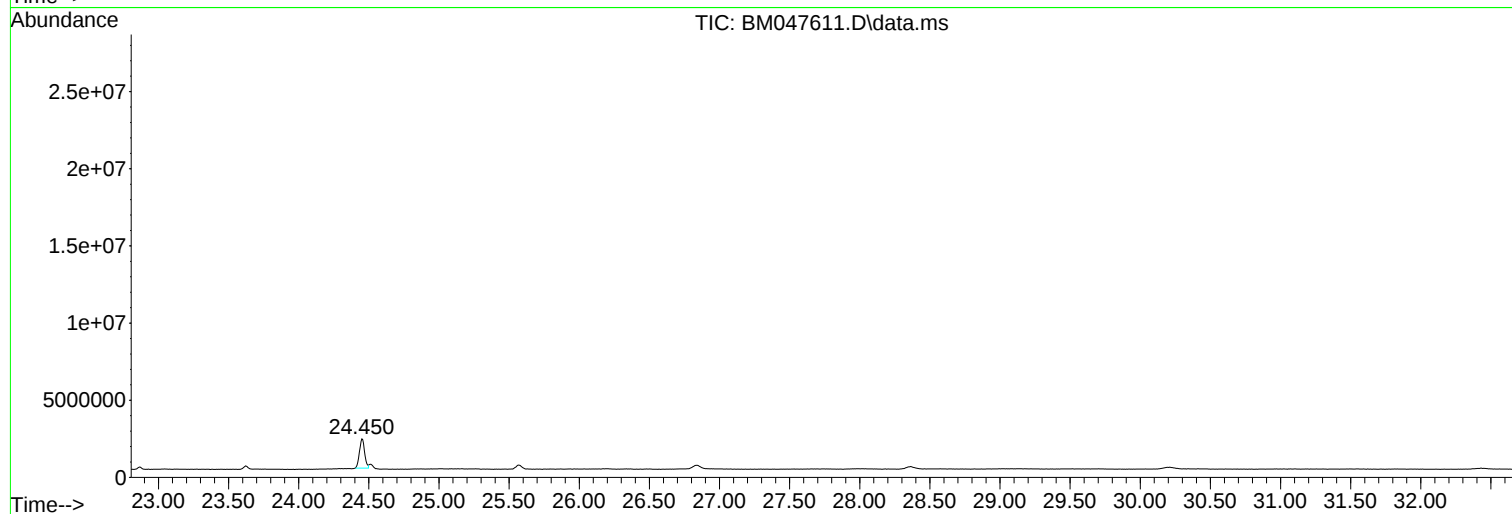
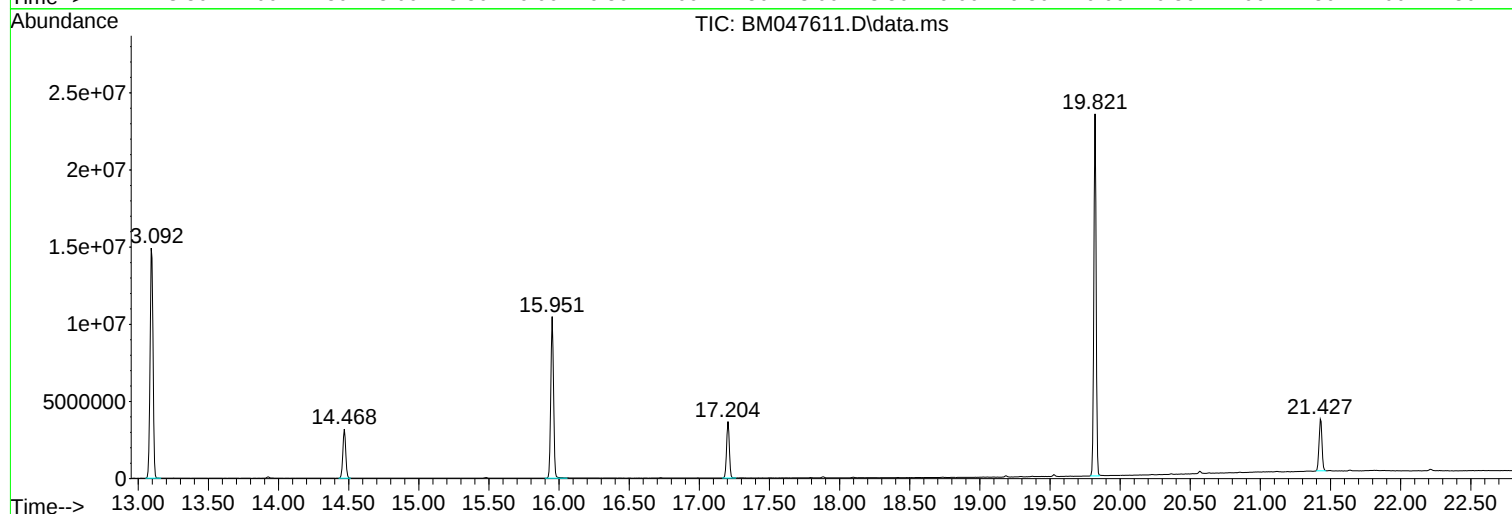
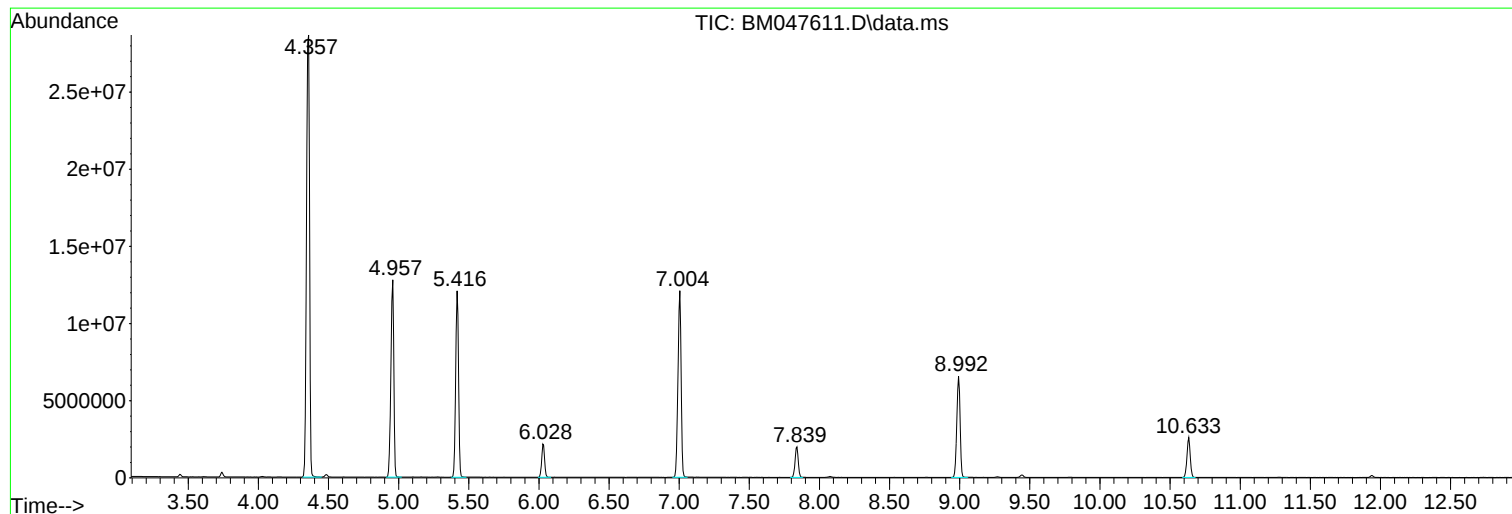
Sum of corrected areas: 200765721

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.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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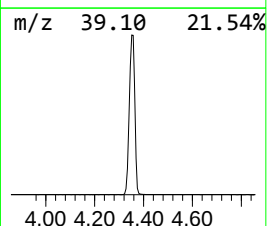
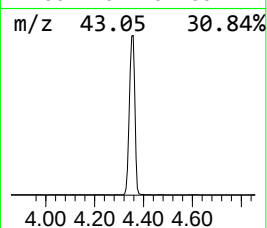
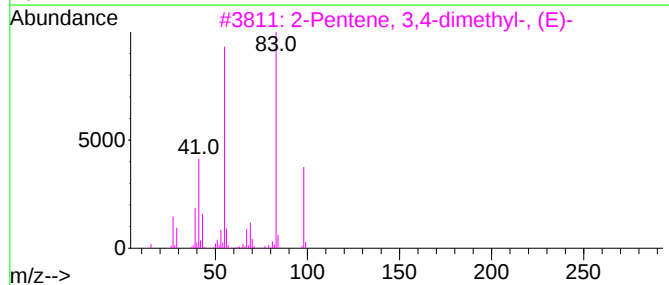
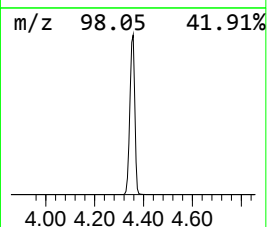
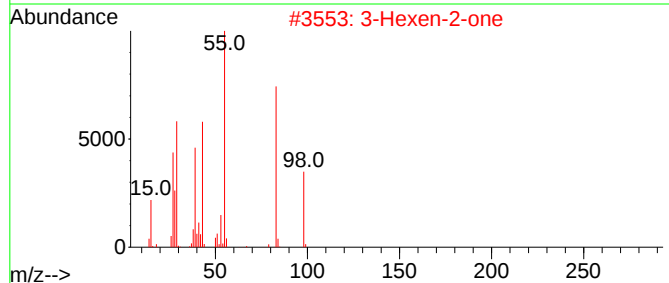
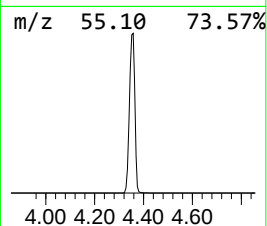
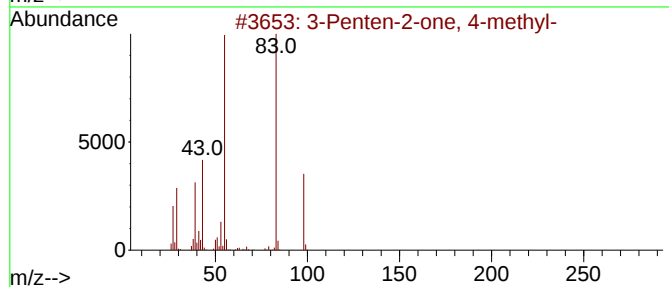
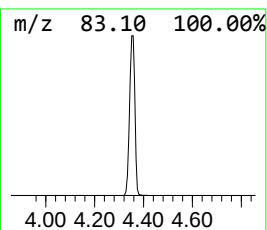
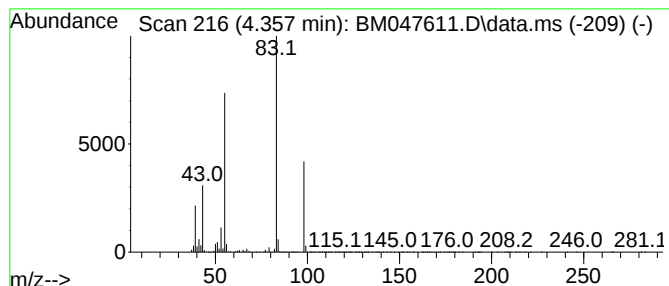
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.357	273.56 ng	43145900	1,4-Dichlorobenzene-d4	7.839

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	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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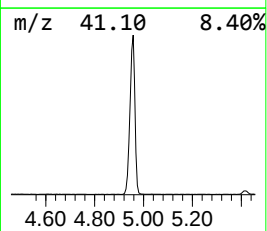
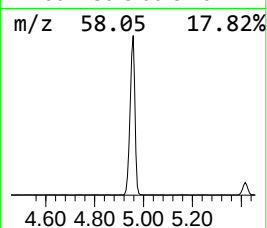
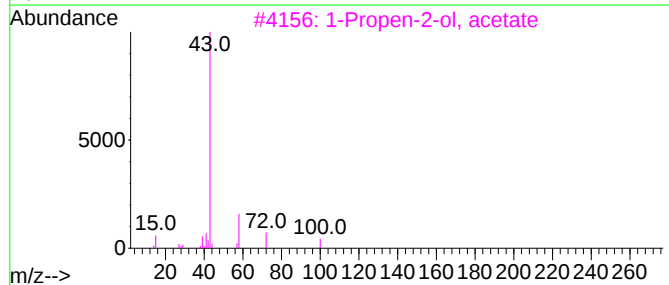
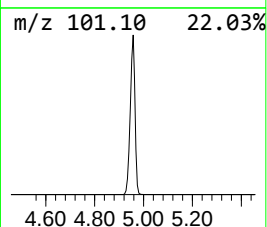
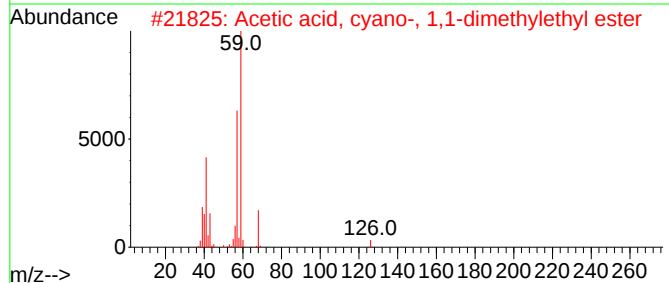
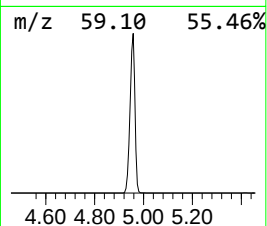
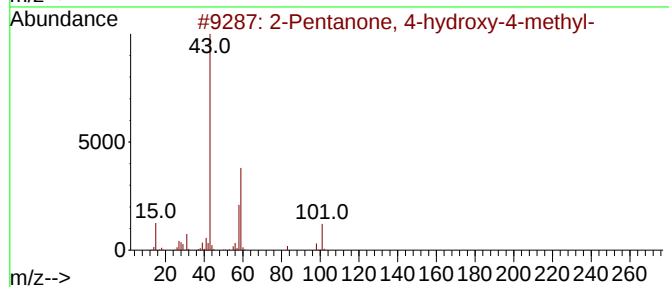
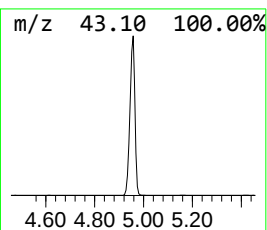
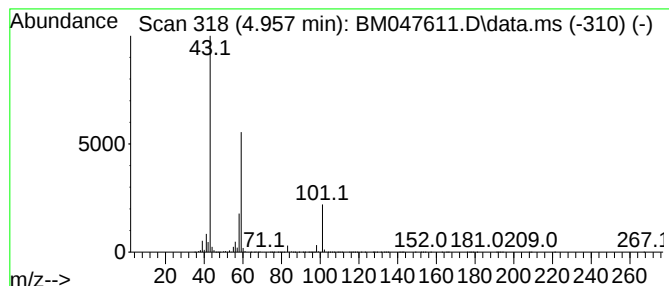
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	114.59 ng	18072900	1,4-Dichlorobenzene-d4	7.839

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	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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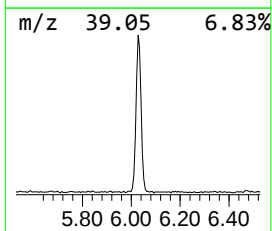
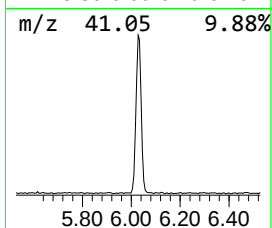
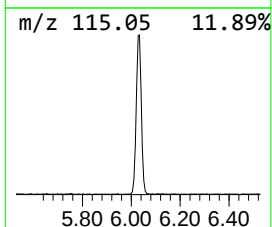
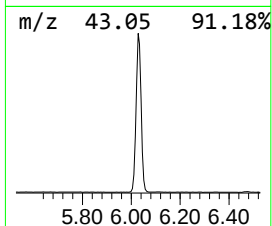
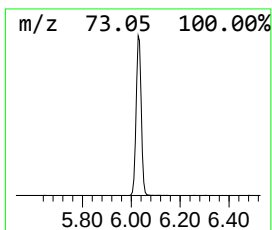
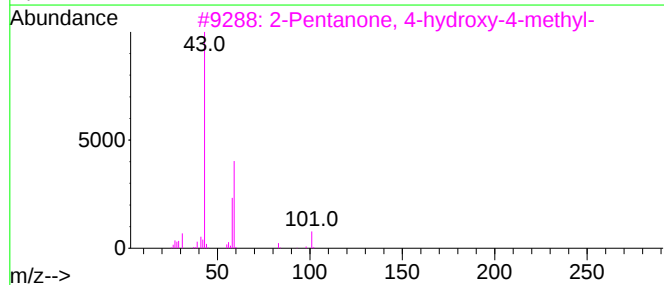
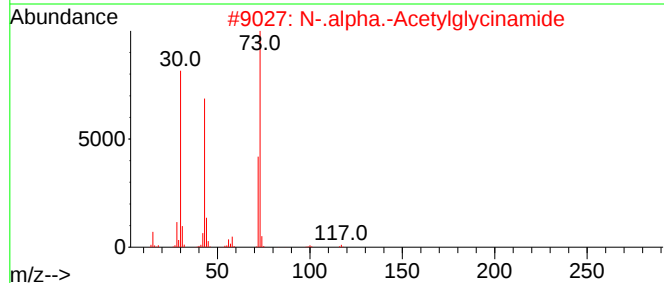
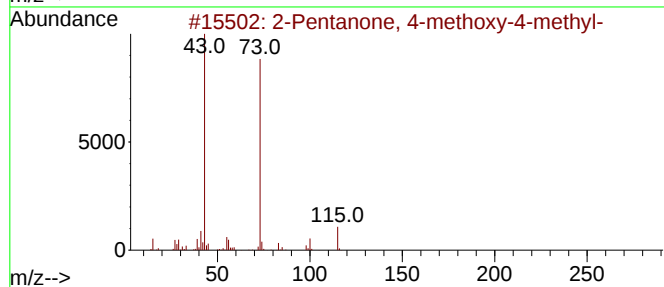
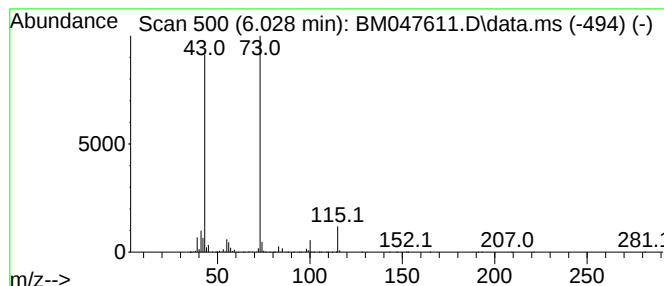
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.028	19.75 ng	3115360	1,4-Dichlorobenzene-d4	7.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.357	273.6	ng	43145900	1	7.839	3154350	20.0
2-Pentanone, 4-...	4.957	114.6	ng	18072900	1	7.839	3154350	20.0
2-Pentanone, 4-...	6.028	19.8	ng	3115360	1	7.839	3154350	20.0