

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041525\
 Data File : BM049928.D
 Acq On : 15 Apr 2025 10:36
 Operator : RC/JU
 Sample : PB167577BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB167577BL

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_M\Methods\8270-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049928.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.287	217	221	231	rBV	300522	420336	1.84%	0.443%
2	4.893	318	324	336	rBV	2236613	3173793	13.93%	3.344%
3	5.364	397	404	422	rBV	5933160	8858730	38.87%	9.334%
4	5.964	501	506	516	rBV	336523	500530	2.20%	0.527%
5	6.952	665	674	698	rBV	5504059	8812063	38.66%	9.285%
6	7.769	806	813	822	rBV	1237402	1948930	8.55%	2.054%
7	8.928	1001	1010	1030	rBV	3329192	5581228	24.49%	5.881%
8	10.563	1280	1288	1302	rBV	1378205	2400744	10.53%	2.530%
9	13.034	1701	1708	1727	rBV	9518829	13899705	60.98%	14.646%
10	14.416	1936	1943	1956	rBV	2169747	3227338	14.16%	3.401%
11	15.904	2189	2196	2218	rBV	7830208	11374351	49.90%	11.985%
12	17.157	2403	2409	2421	rBV	2520855	3796119	16.66%	4.000%
13	19.786	2850	2856	2869	rBV	19294604	22792024	100.00%	24.015%
14	21.398	3125	3130	3145	rBV	2740451	4006348	17.58%	4.221%
15	24.404	3633	3641	3653	rVB	1606288	4113446	18.05%	4.334%

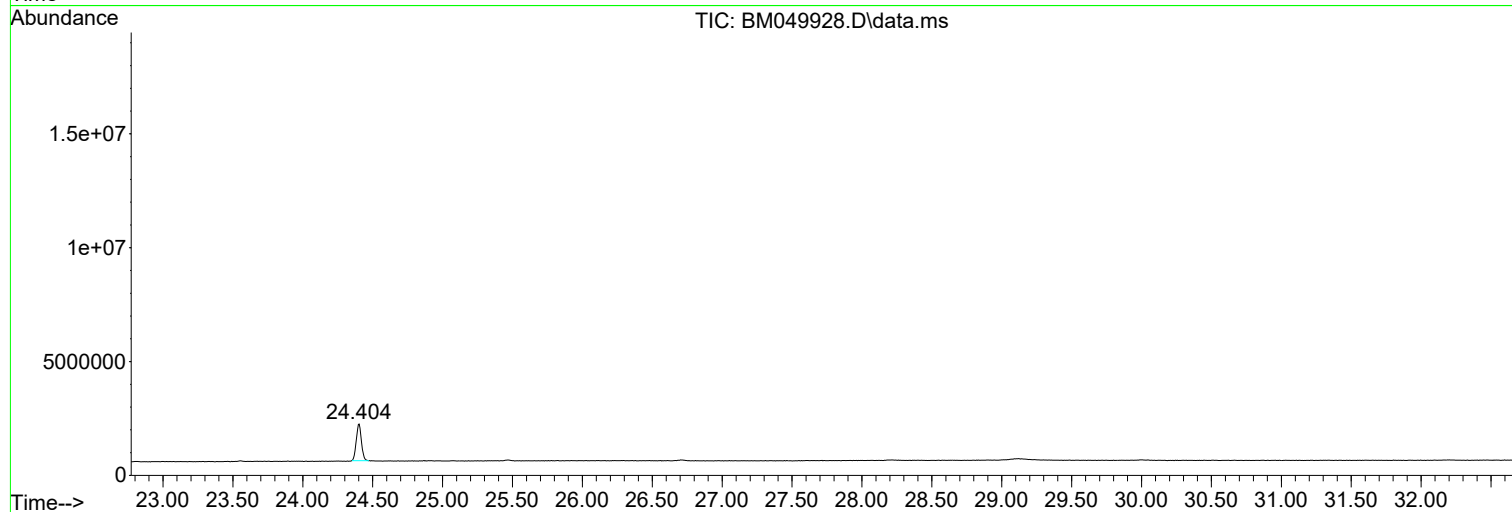
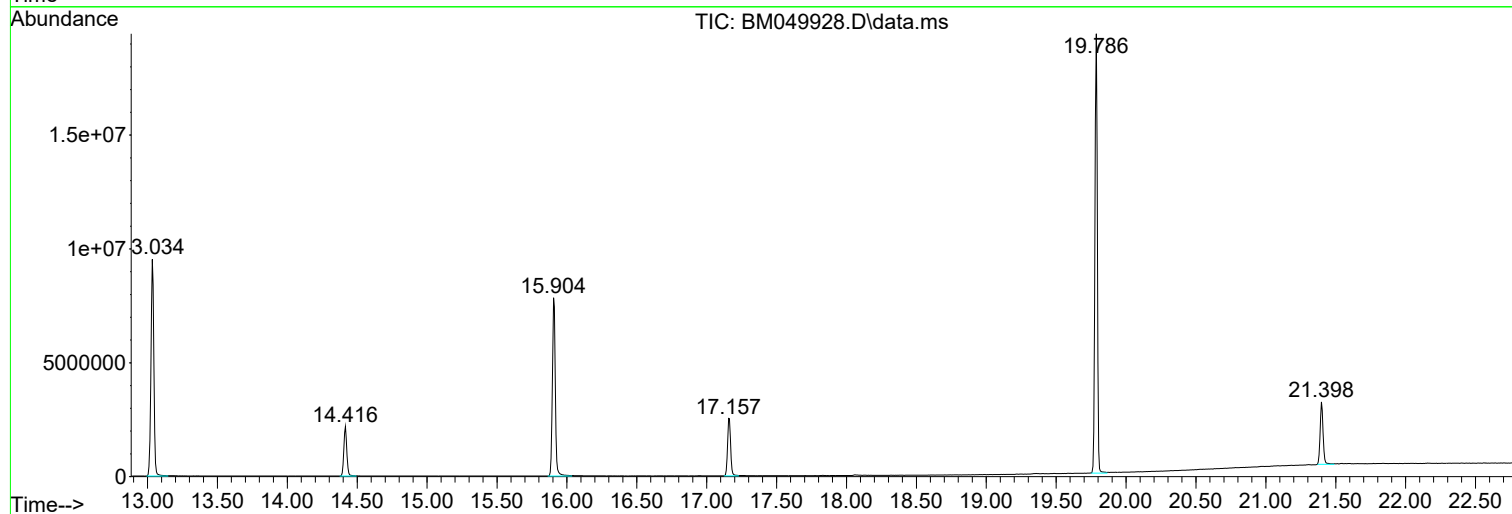
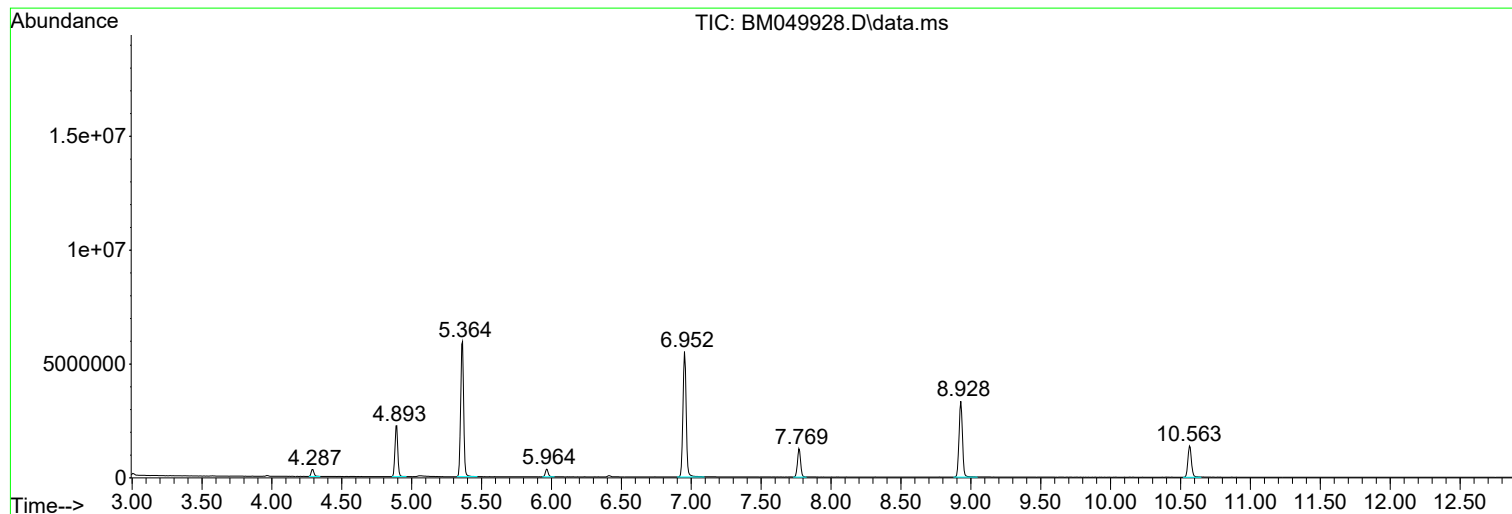
Sum of corrected areas: 94905685

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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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Instrument :
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ClientSampleId :
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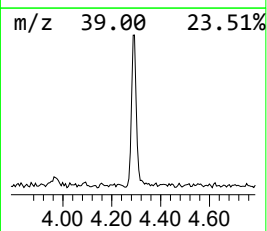
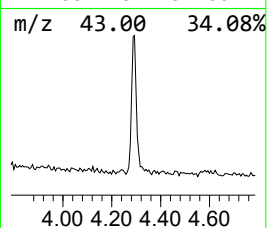
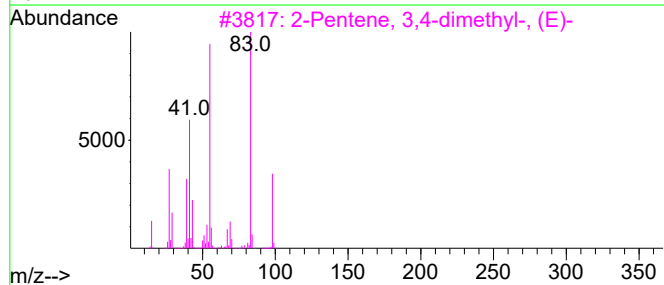
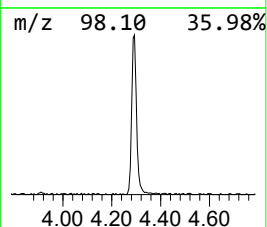
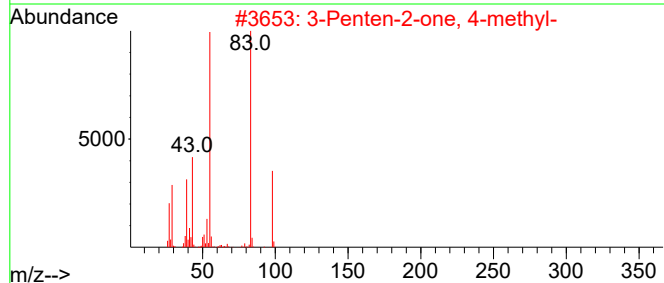
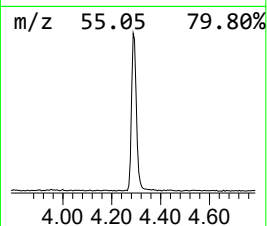
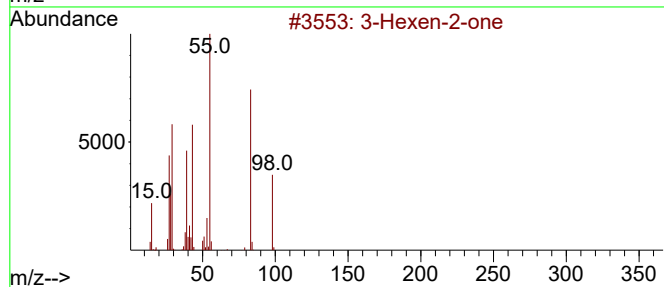
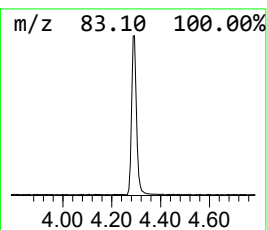
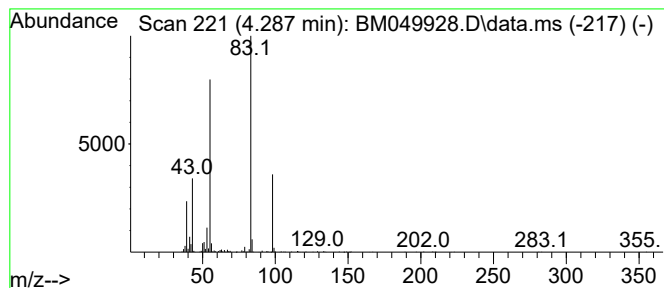
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.287	4.31 ng	420336	1,4-Dichlorobenzene-d4	7.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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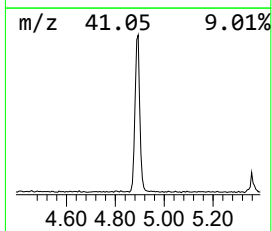
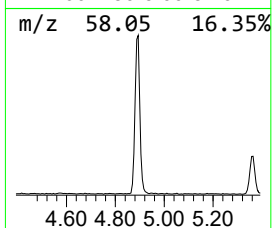
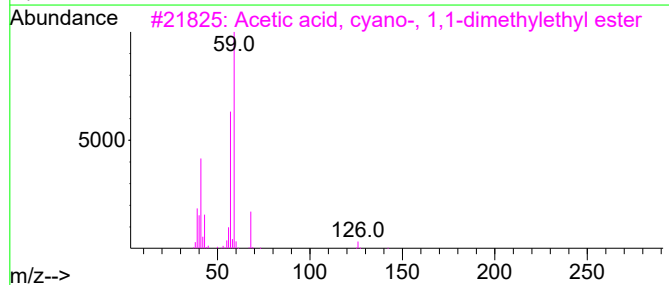
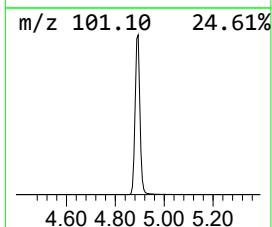
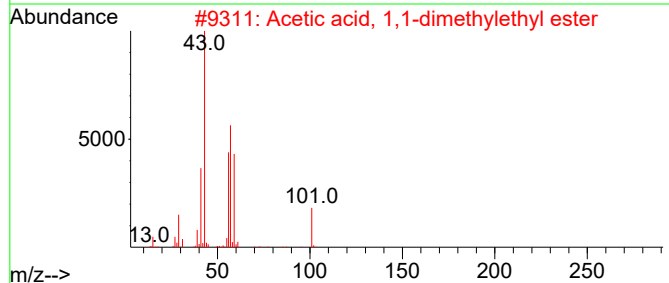
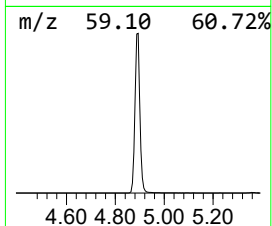
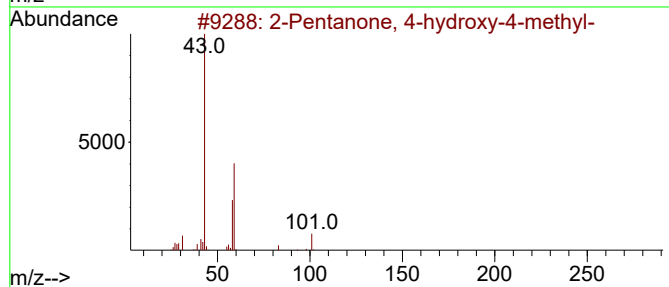
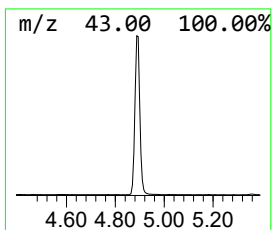
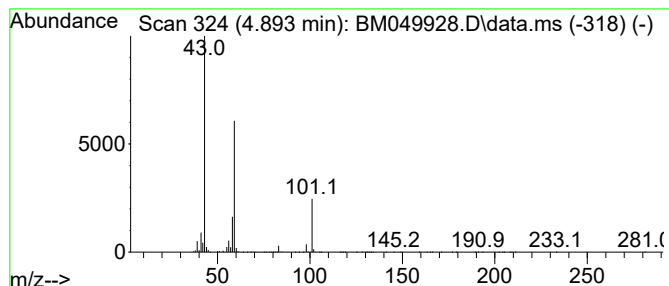
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.893	32.57 ng	3173790	1,4-Dichlorobenzene-d4	7.769	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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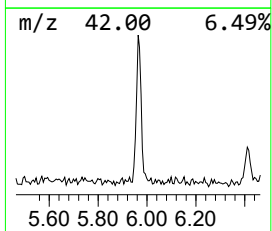
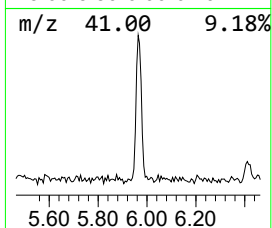
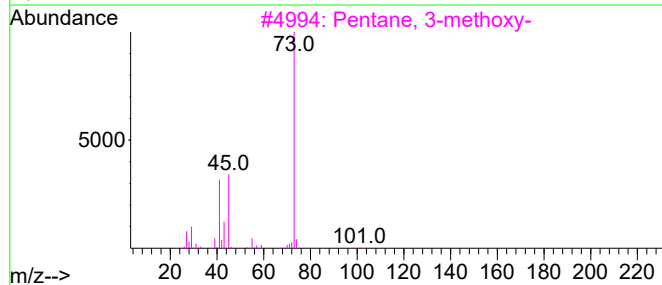
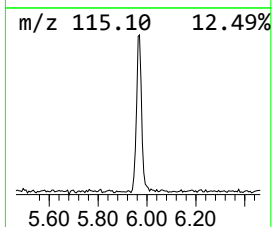
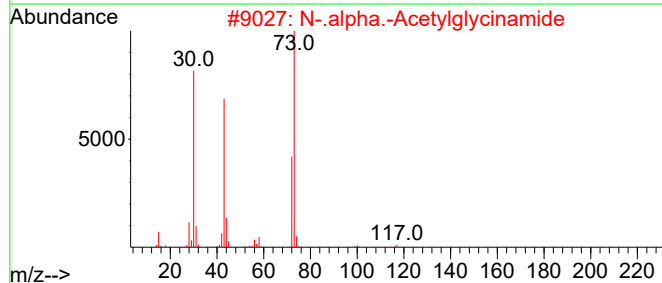
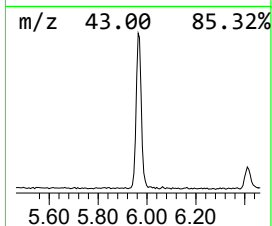
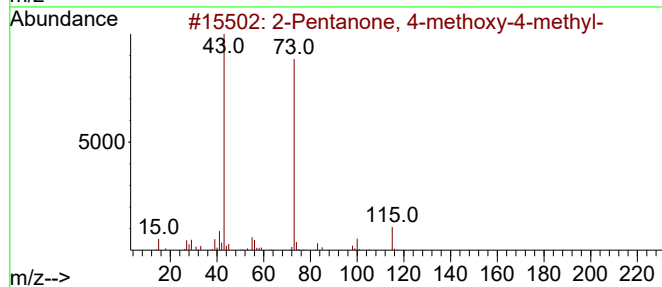
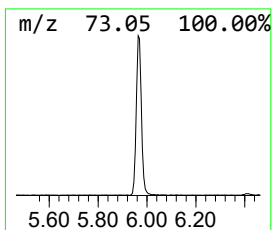
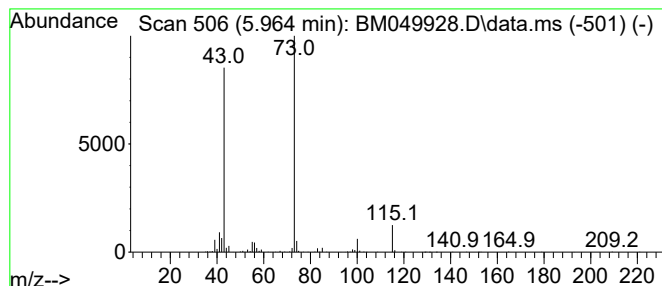
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.964	5.14 ng	500530	1,4-Dichlorobenzene-d4			7.769
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	Pentane, 3-methoxy-		102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-(1-methylethyl)-		116	C6H12O2	000822-83-3	10
5	Borane, dimethoxy-		74	C2H7BO2	004542-61-4	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.287	4.3	ng	420336	1	7.769	1948930	20.0
2-Pentanone, 4-...	4.893	32.6	ng	3173790	1	7.769	1948930	20.0
2-Pentanone, 4-...	5.964	5.1	ng	500530	1	7.769	1948930	20.0