

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
 Data File : BF135247.D
 Acq On : 14 Sep 2023 11:28
 Operator : CG\JU
 Sample : PB155361BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB155361BL

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	13	18	25	rVB	57878	75596	1.85%	0.297%
2	5.028	496	500	509	rVB	57779	85062	2.08%	0.334%
3	5.404	559	564	567	rBV	3218267	3548687	86.73%	13.940%
4	6.410	729	735	738	rBV	3249174	3533501	86.35%	13.881%
5	6.763	791	795	804	rVB	859564	686771	16.78%	2.698%
6	7.328	885	891	894	rBV	2222588	2360128	57.68%	9.271%
7	8.040	1007	1012	1016	rBV	1017852	903282	22.08%	3.548%
8	9.122	1190	1196	1199	rBV	3939543	3970070	97.02%	15.596%
9	9.798	1306	1311	1315	rBV	1262023	1034140	25.27%	4.062%
10	10.592	1442	1446	1450	rBV	2399111	2599150	63.52%	10.210%
11	11.292	1561	1565	1568	rBV	1313640	1127671	27.56%	4.430%
12	12.892	1832	1837	1840	rBV	3721680	4091861	100.00%	16.074%
13	13.945	2012	2016	2023	rBV	842555	720095	17.60%	2.829%
14	15.410	2260	2265	2280	rVB	479340	652698	15.95%	2.564%
15	17.057	2533	2545	2546	rBV	21913	67242	1.64%	0.264%

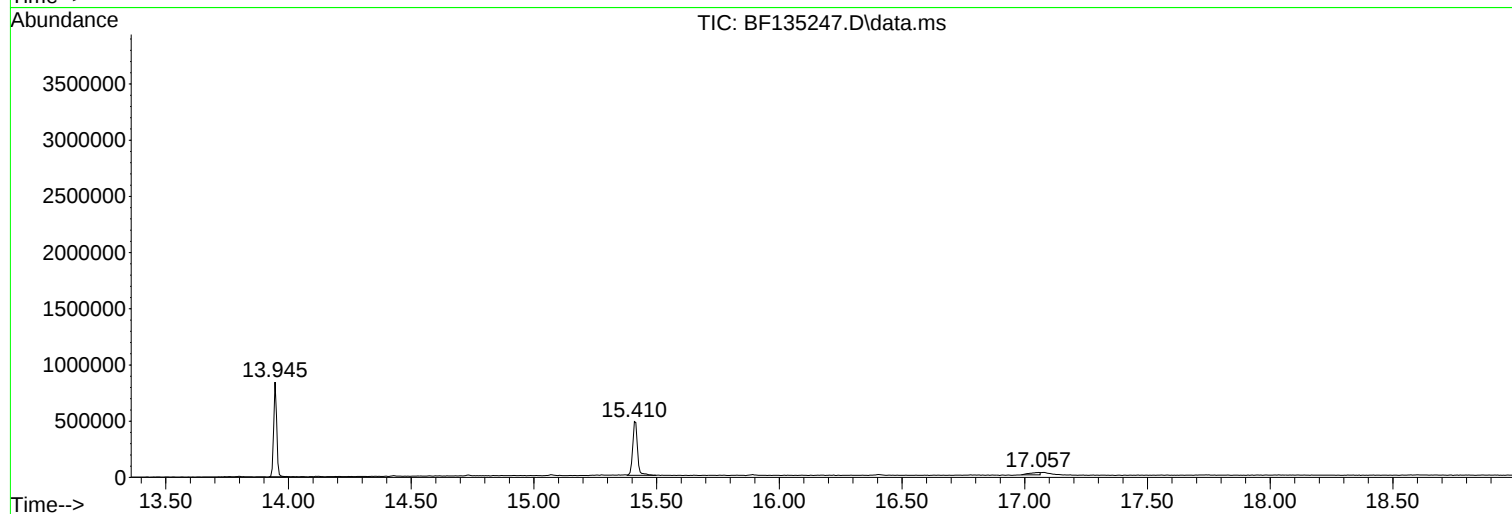
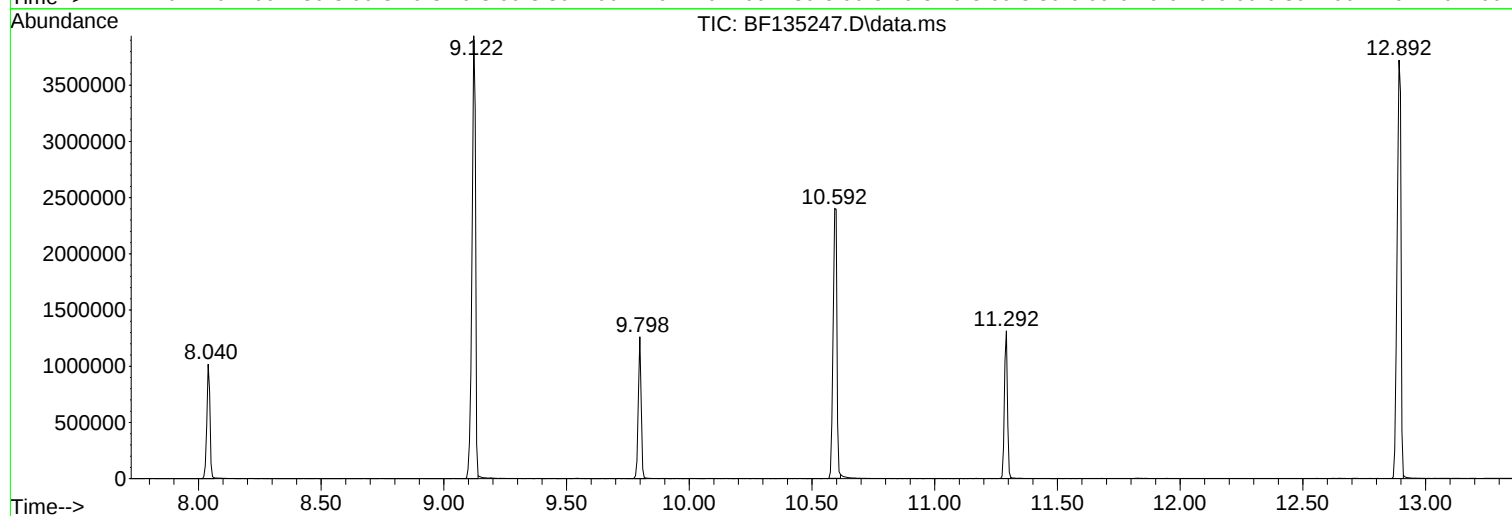
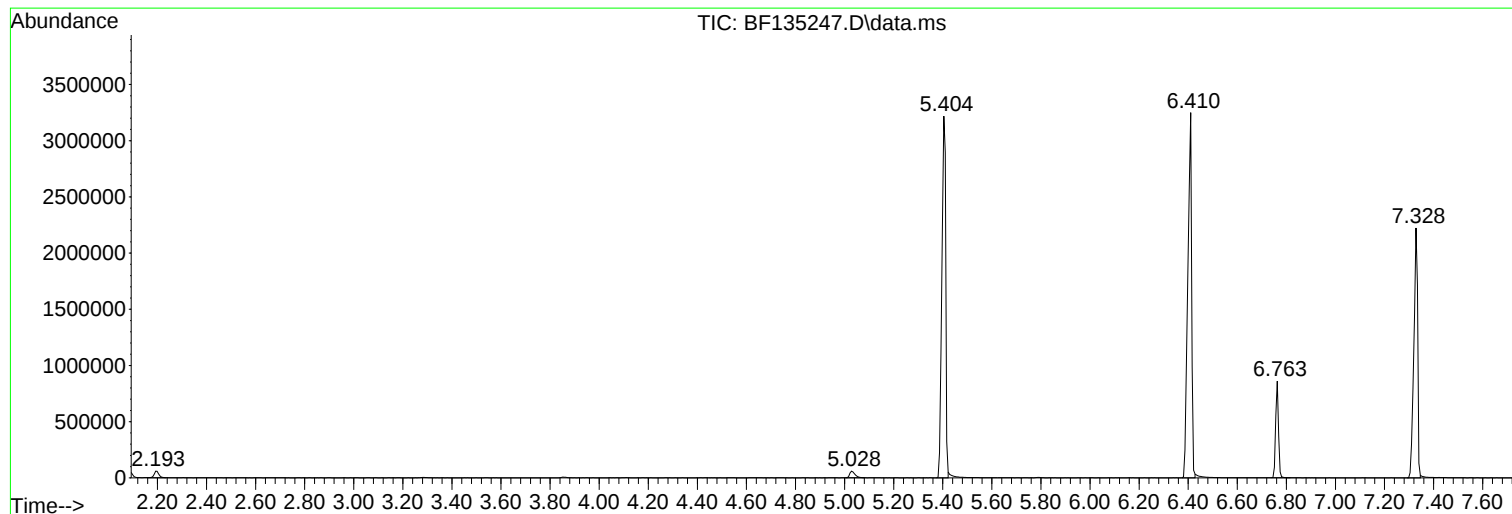
Sum of corrected areas: 25455954

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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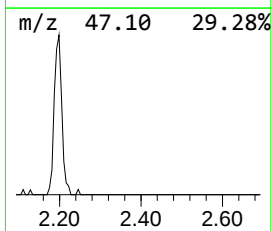
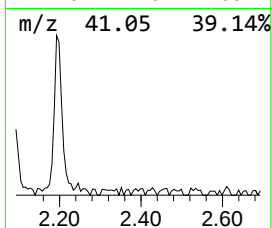
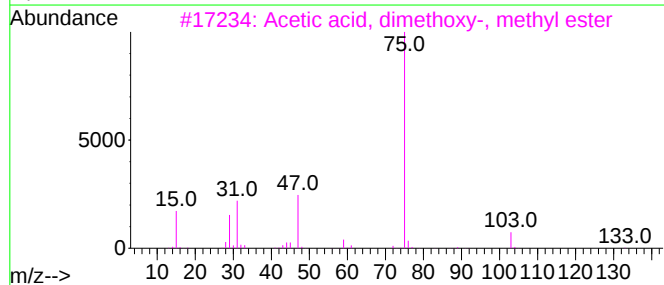
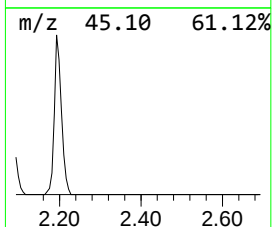
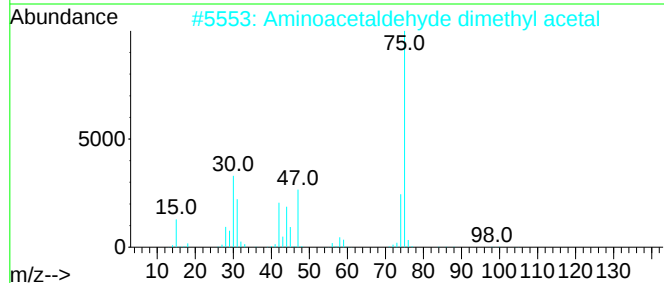
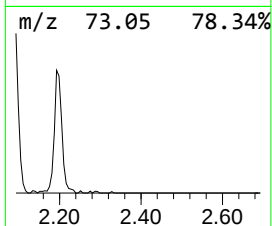
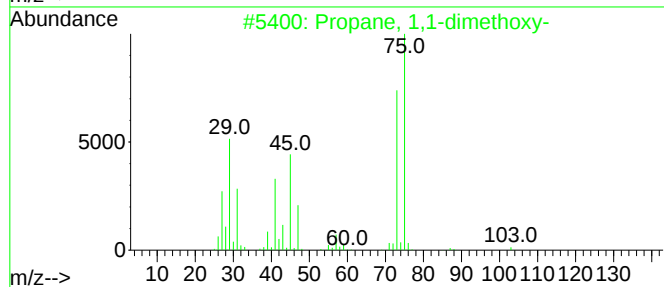
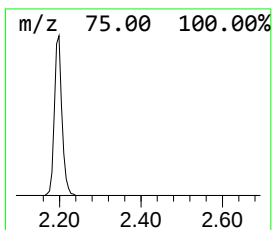
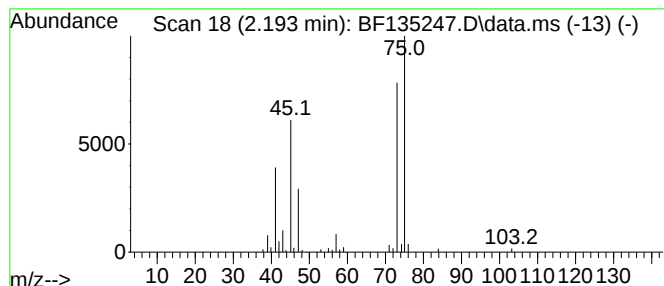
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	2.20 ng	75596	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
4			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
5			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	12



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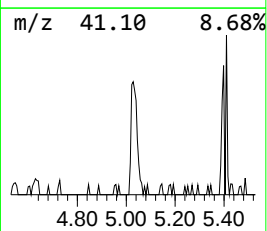
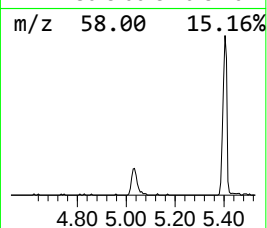
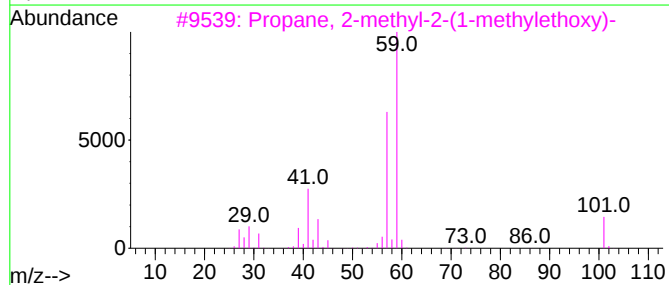
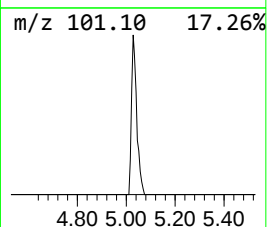
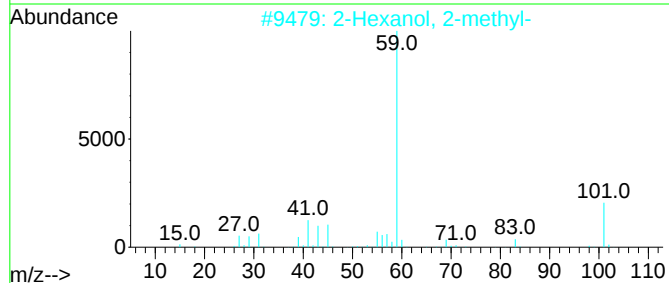
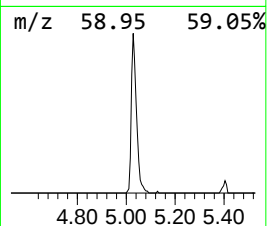
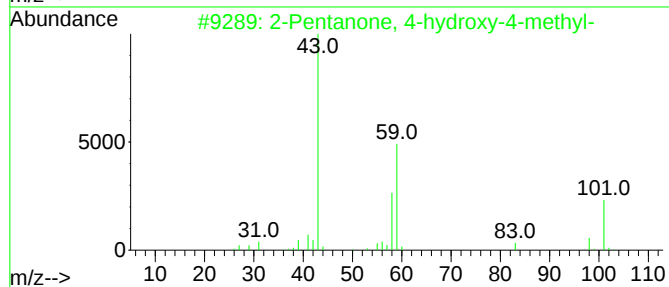
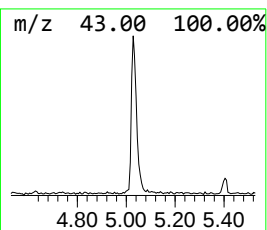
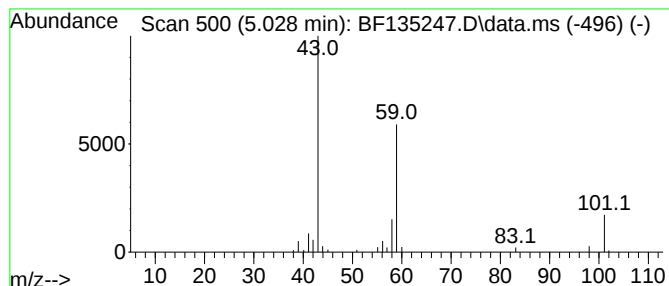
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.028	2.48 ng	85062	1,4-Dichlorobenzene-d4	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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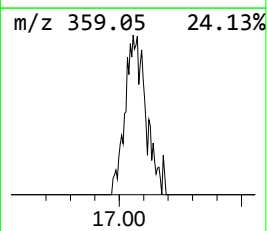
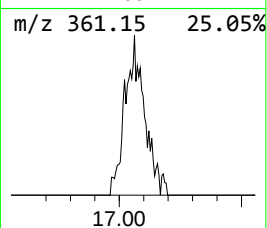
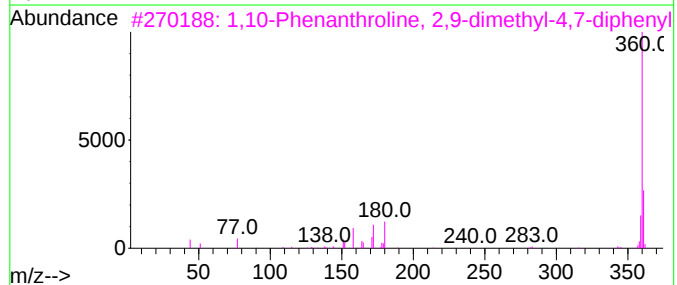
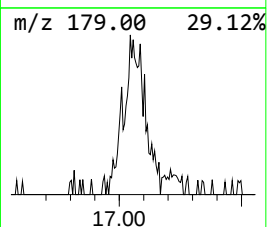
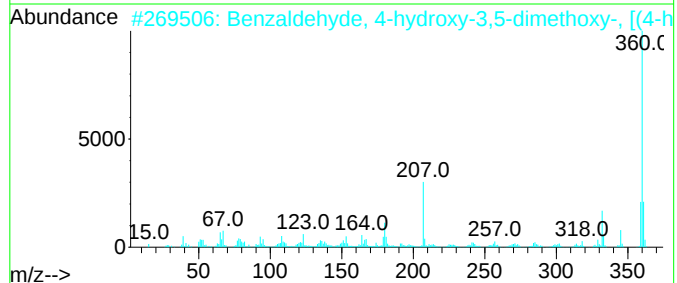
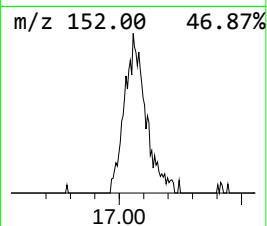
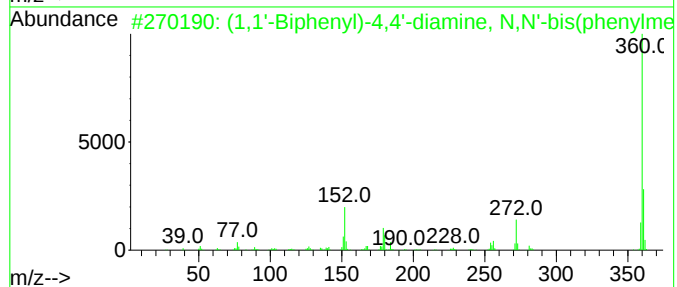
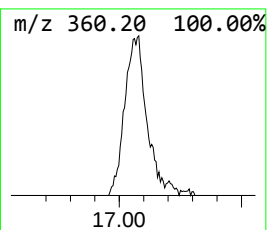
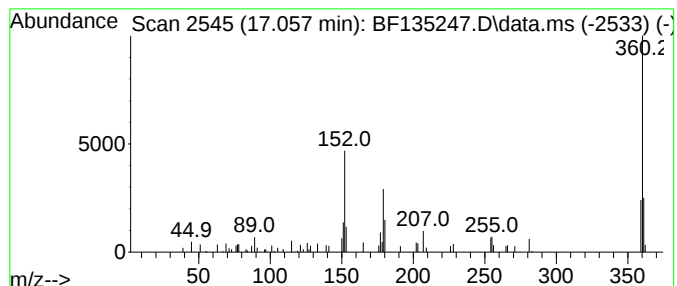
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Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.057	2.06 ng	67242	Perylene-d12	15.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N'-dimethyl-	360	C26H20N2	006311-48-4	81
2	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	360	C18H20N2O6	014414-32-5	50
3	1,10-Phenanthroline, 2,9-dimethyl-	360	C26H20N2	004733-39-5	47
4	Androst-4-ene-3,17-dione, 12-hydroxy-	360	C21H32N2O3	069688-31-9	43
5	Jaceidin	360	C18H16O8	010173-01-0	43



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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
Propane, 1,1-di...	2.193	2.2	ng	75596	1	6.763	686771	20.0
2-Pentanone, 4-...	5.028	2.5	ng	85062	1	6.763	686771	20.0
(1,1'-Biphenyl)...	17.057	2.1	ng	67242	6	15.416	652698	20.0