

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
 Data File : BM039081.D
 Acq On : 21 Mar 2023 22:45
 Operator : CG/JU
 Sample : 02002-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 031023-3

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	294	300	311	rBV	1987217	2744343	28.88%	4.249%
2	5.522	373	380	393	rVB	4513260	6617349	69.64%	10.246%
3	7.128	644	653	669	rBV	4160513	6696178	70.47%	10.368%
4	7.963	788	795	803	rBV	1280382	1984520	20.88%	3.073%
5	9.134	986	994	1009	rBV	2630932	4260877	44.84%	6.597%
6	10.775	1265	1273	1281	rBV	1583387	2692848	28.34%	4.170%
7	13.233	1683	1691	1700	rBV	5877441	8405474	88.45%	13.015%
8	14.604	1916	1924	1932	rBV	2084805	3010128	31.68%	4.661%
9	15.963	2147	2155	2160	rBV	154541	221036	2.33%	0.342%
10	16.092	2170	2177	2195	rBV	3777302	5372690	56.54%	8.319%
11	17.351	2384	2391	2396	rBV	2172727	3124688	32.88%	4.838%
12	18.239	2538	2542	2552	rBV	384112	633943	6.67%	0.982%
13	19.404	2736	2740	2746	rVB	90188	129744	1.37%	0.201%
14	19.515	2755	2759	2763	rBV2	127511	182176	1.92%	0.282%
15	19.968	2830	2836	2841	rBV	8055010	9502818	100.00%	14.714%
16	21.227	3047	3050	3059	rBV	744465	1074900	11.31%	1.664%
17	21.527	3096	3101	3106	rBV	2888283	3741390	39.37%	5.793%
18	23.956	3508	3514	3522	rVB2	2111333	4188197	44.07%	6.485%

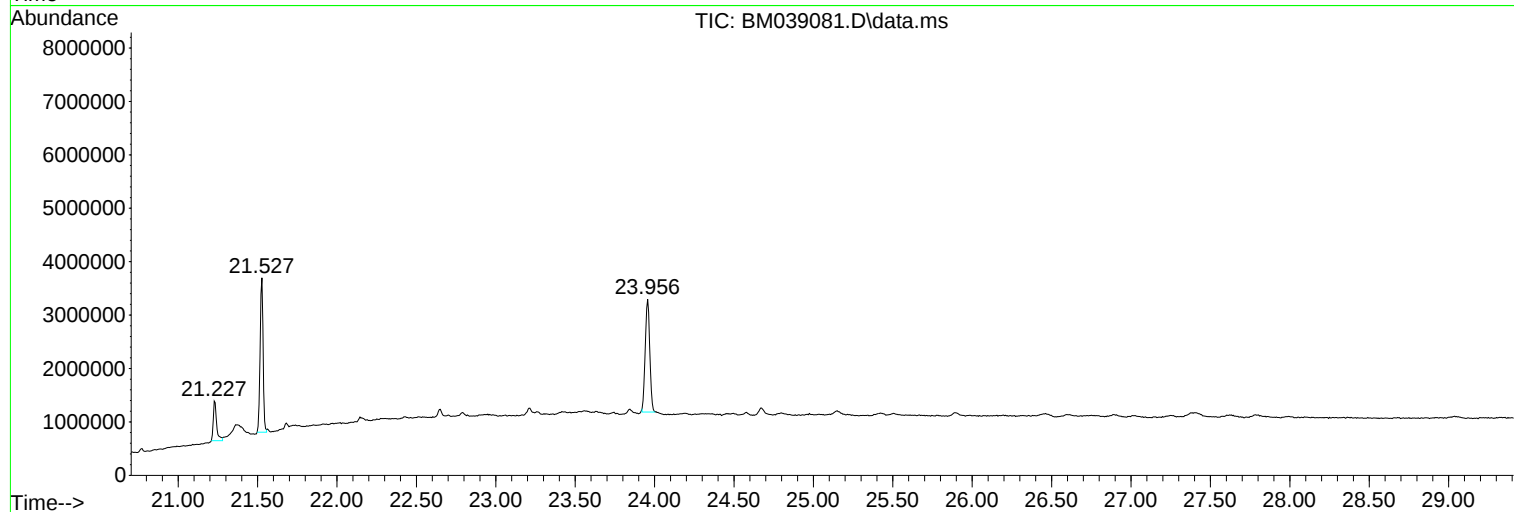
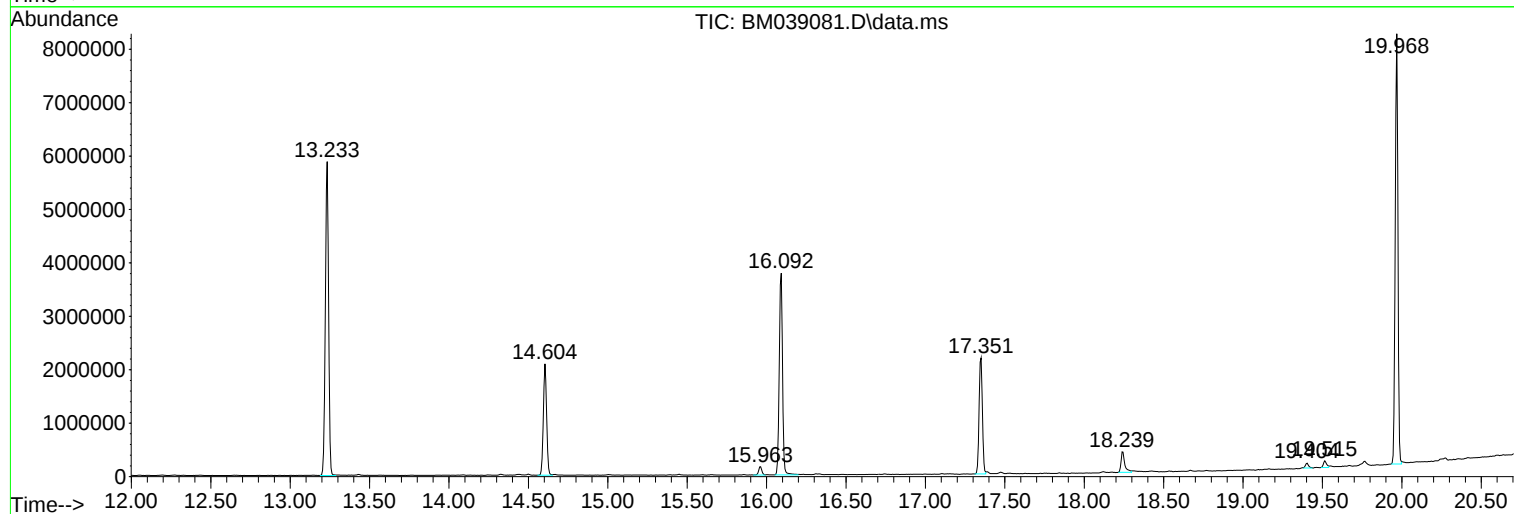
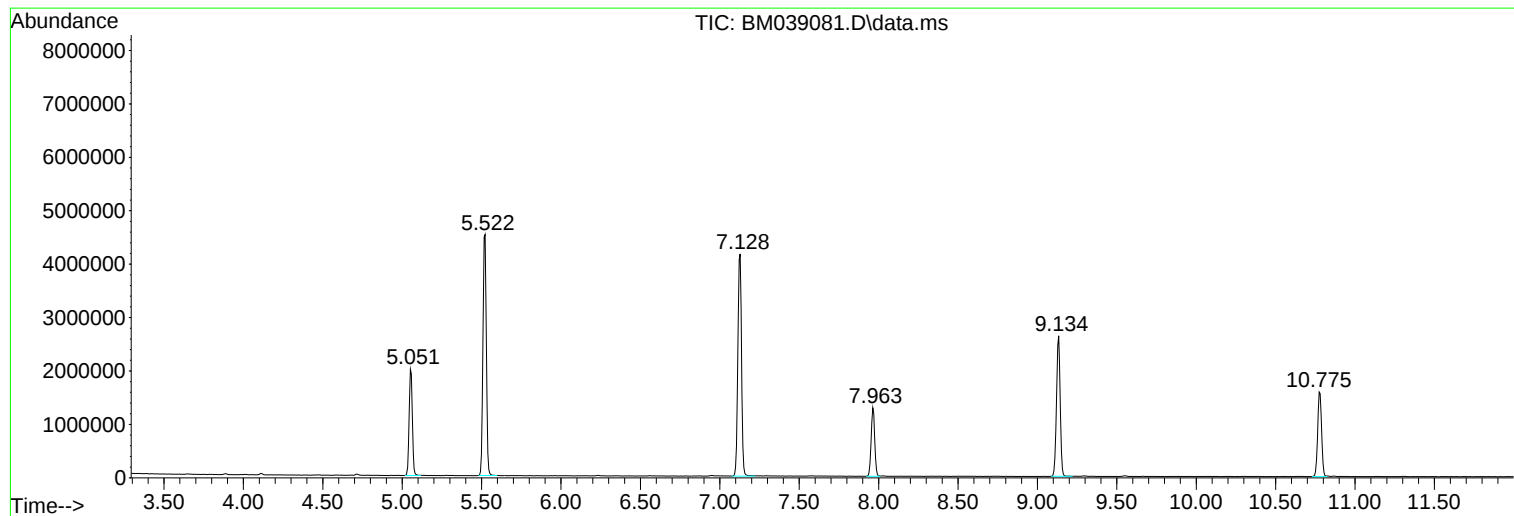
Sum of corrected areas: 64583299

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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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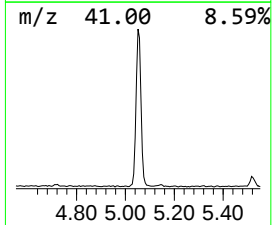
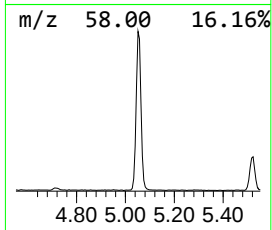
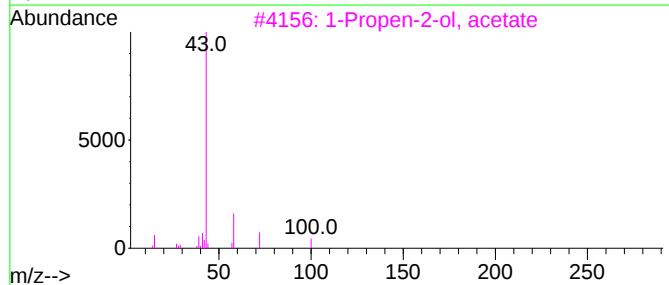
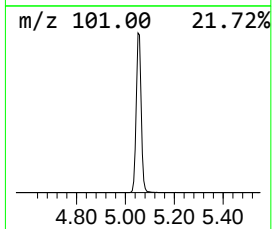
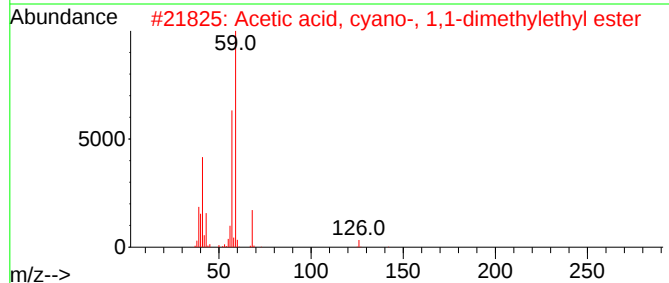
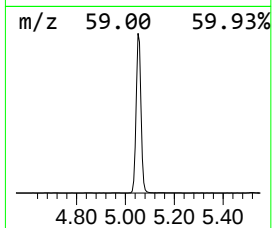
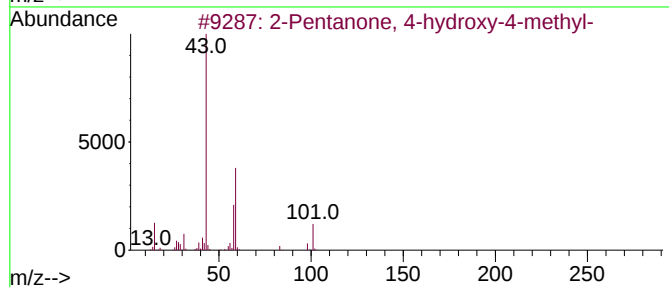
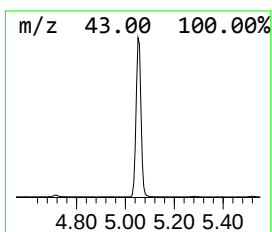
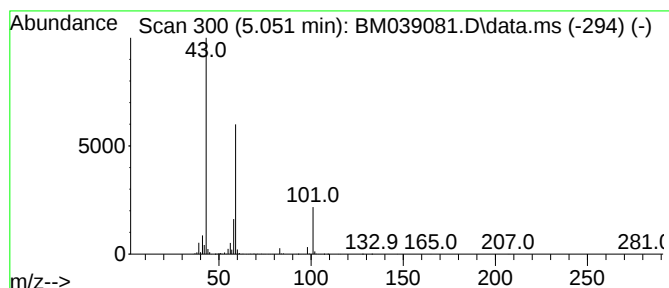
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.051	27.66 ng	2744340	1,4-Dichlorobenzene-d4	7.963

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			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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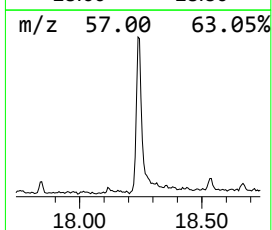
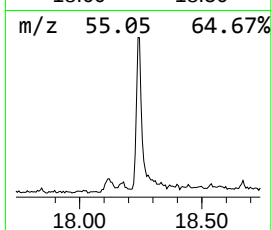
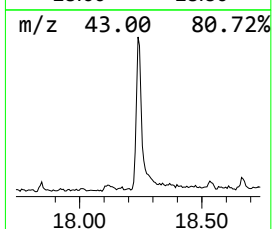
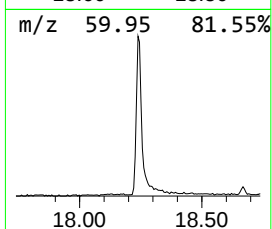
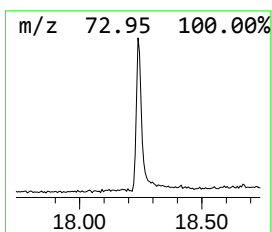
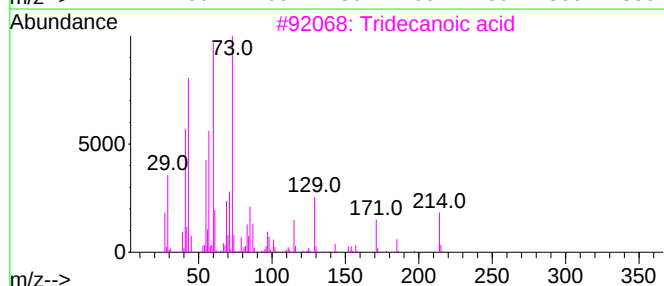
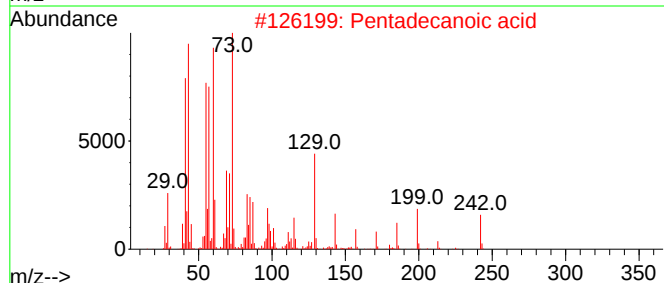
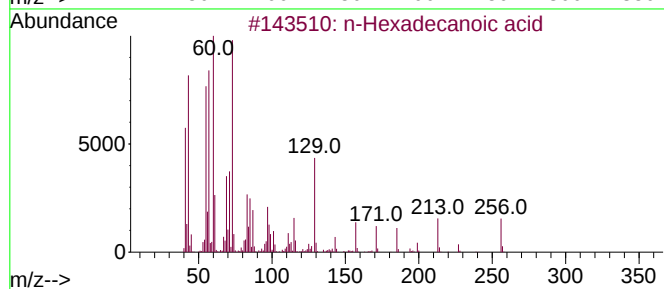
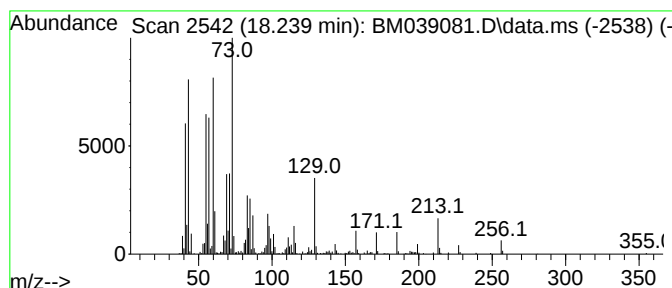
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	4.06 ng	633943	Phenanthrene-d10	17.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Octadecanoic acid	284	C18H36O2	000057-11-4	74
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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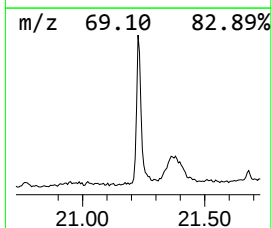
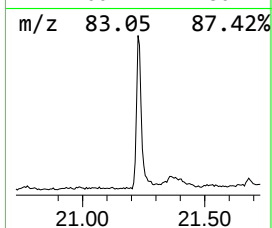
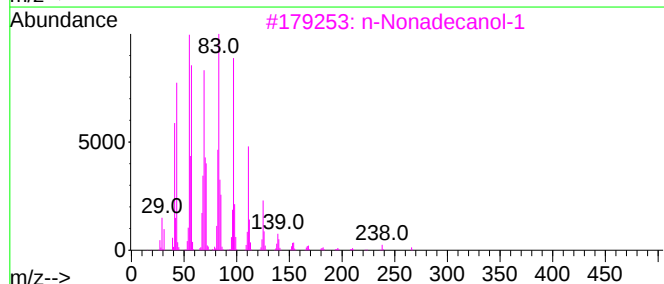
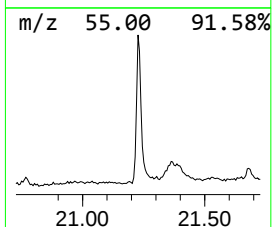
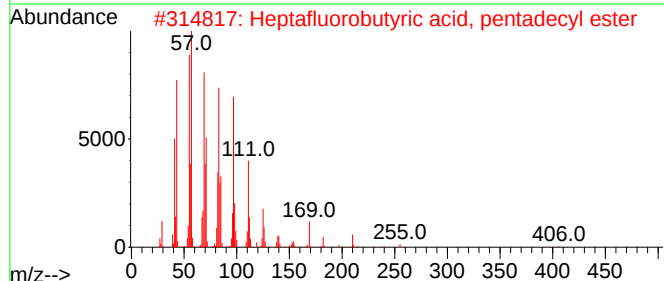
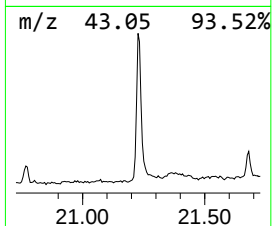
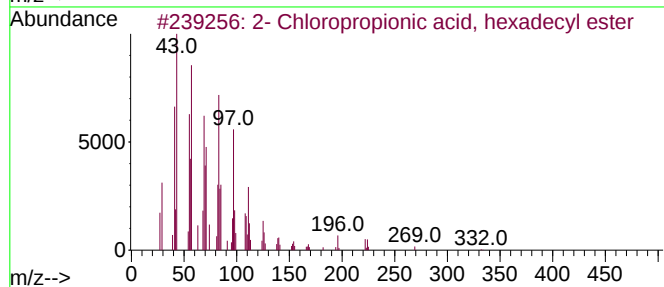
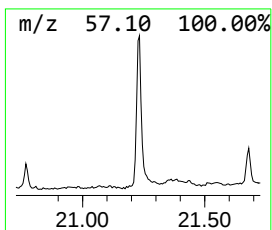
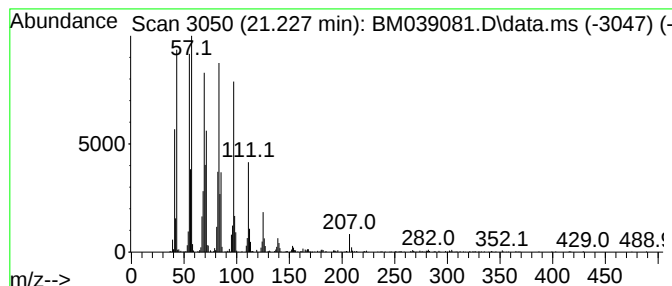
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Peak Number 3 2- Chloropropionic acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	5.75 ng	1074900	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91	
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91		
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91		
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91		
5	1-Hexacosene	364	C26H52	018835-33-1	91		



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	27.7	ng	2744340	1	7.963	1984520	20.0
n-Hexadecanoic ...	18.239	4.1	ng	633943	4	17.351	3124690	20.0
2- Chloropropio...	21.227	5.8	ng	1074900	5	21.527	3741390	20.0