

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
 Data File : BG048475.D
 Acq On : 23 Mar 2021 18:30
 Operator : CG/JU
 Sample : M1779-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-6B1-(3.0-3.5)

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_G\METHODS\8270-BG031821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048475.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.177	308	313	321	rVB	35534	55473	1.35%	0.317%
2	5.653	387	394	406	rVB	922788	1450066	35.23%	8.284%
3	7.251	658	666	677	rBV	934267	1640556	39.86%	9.373%
4	8.103	804	811	817	rBV	151046	258555	6.28%	1.477%
5	9.272	1000	1010	1019	rBV	580483	1060845	25.77%	6.061%
6	10.929	1282	1292	1301	rBV	192639	351849	8.55%	2.010%
7	13.367	1700	1707	1714	rBV	1500445	2277539	55.33%	13.012%
8	14.184	1842	1846	1851	rBV2	40337	62311	1.51%	0.356%
9	14.742	1934	1941	1949	rVB	336279	521313	12.67%	2.978%
10	16.234	2187	2195	2203	rBV	1580868	2396458	58.22%	13.691%
11	17.492	2403	2409	2416	rBV	488569	723637	17.58%	4.134%
12	18.373	2554	2559	2570	rBV2	242219	357464	8.68%	2.042%
13	19.642	2771	2775	2783	rVB3	45345	60882	1.48%	0.348%
14	19.907	2816	2820	2825	rBV2	45796	58068	1.41%	0.332%
15	20.106	2847	2854	2859	rBV	3014760	4116023	100.00%	23.515%
16	20.888	2983	2987	2991	rVB2	59196	63819	1.55%	0.365%
17	21.417	3072	3077	3087	rBV2	207740	497903	12.10%	2.845%
18	21.781	3133	3139	3148	rVB	468418	799040	19.41%	4.565%
19	25.118	3697	3707	3717	rVB3	260631	751977	18.27%	4.296%

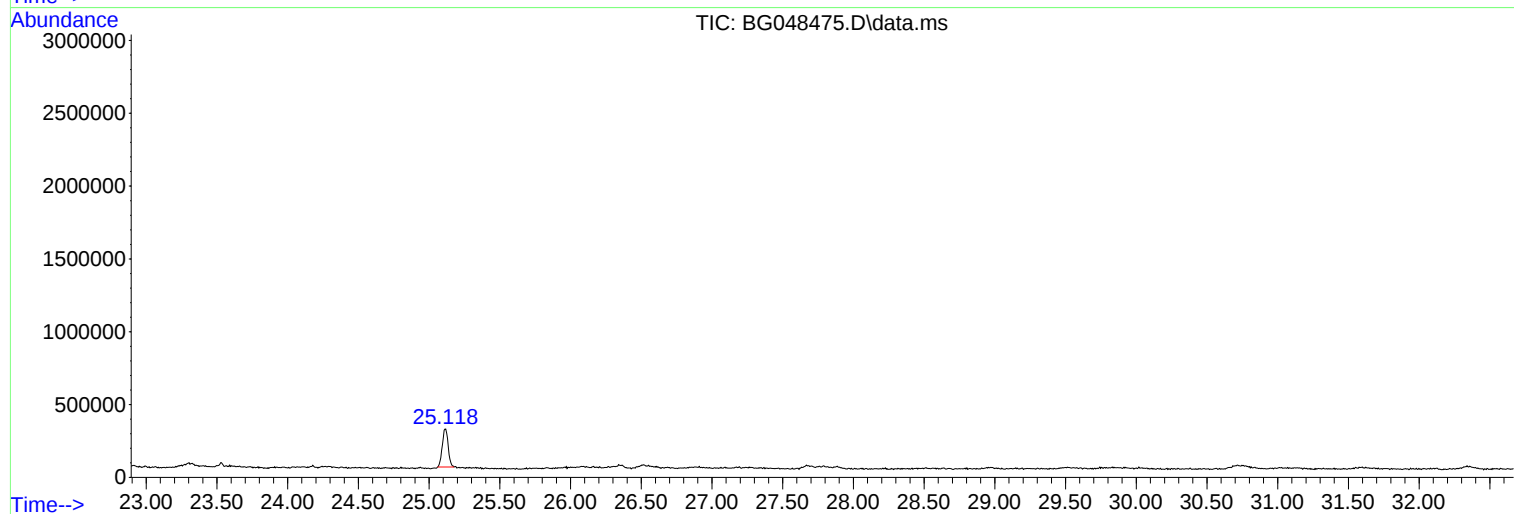
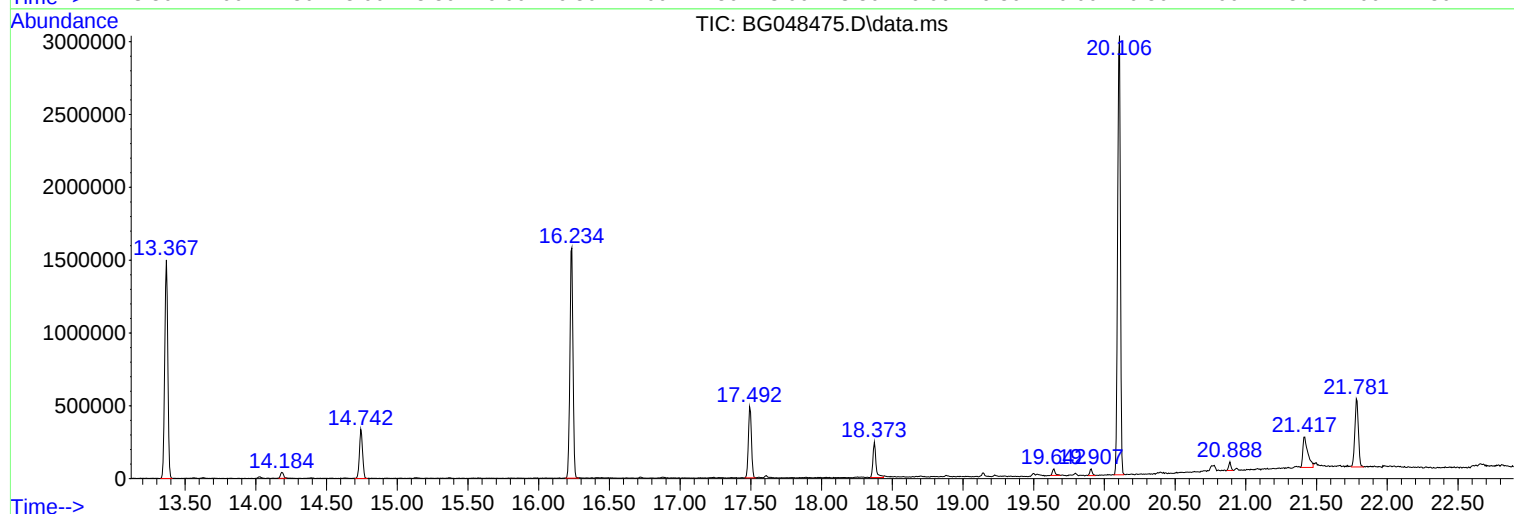
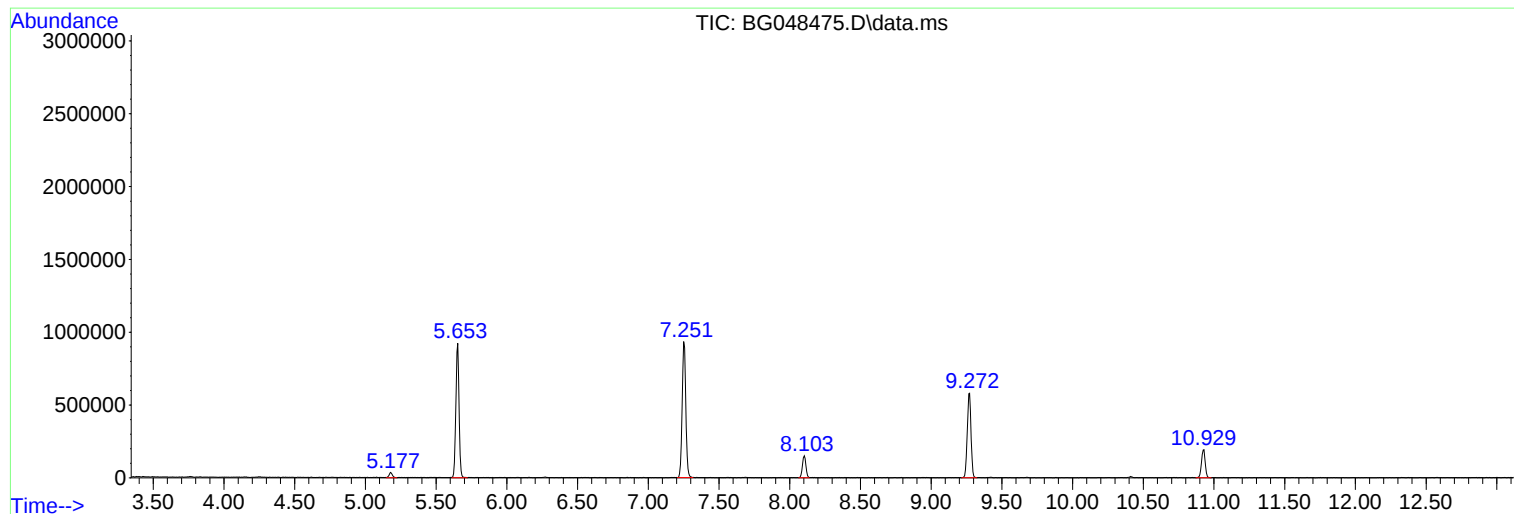
Sum of corrected areas: 17503778

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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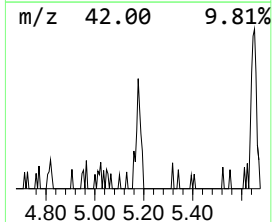
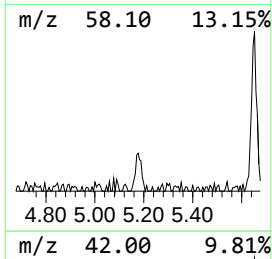
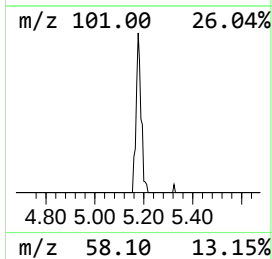
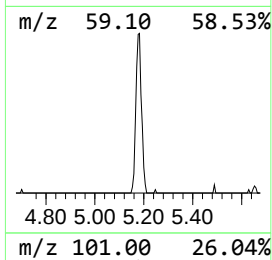
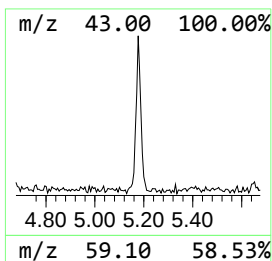
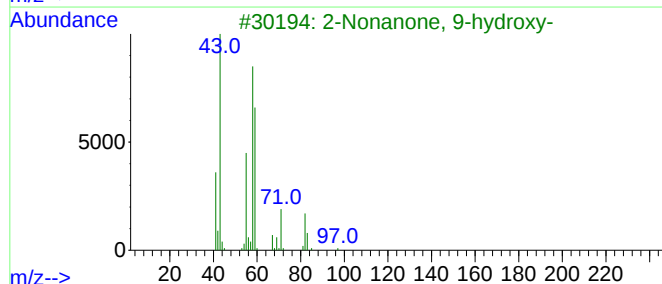
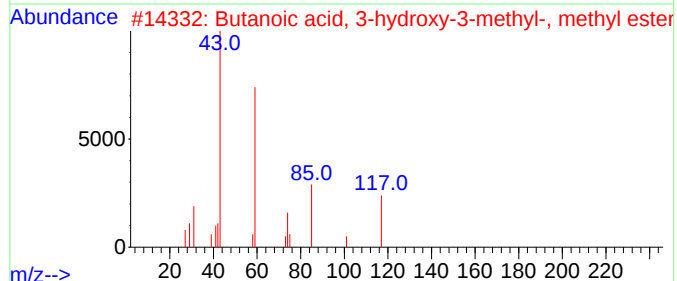
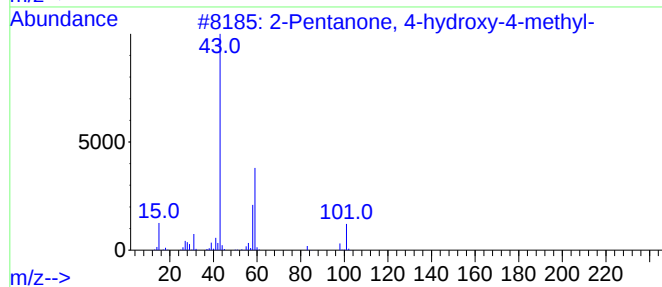
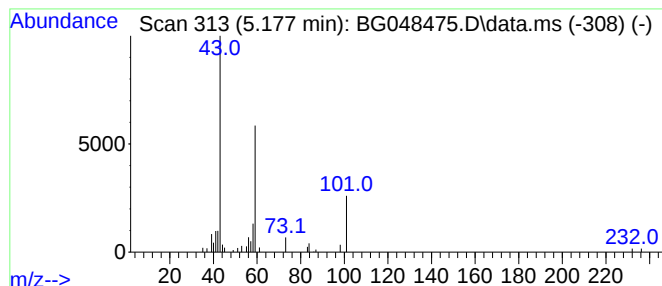
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	4.29 ng	55473	1,4-Dichlorobenzene-d4	8.103

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36	
2	Butanoic acid, 3-hydroxy-3-methyl...	132	C6H12O3	006149-45-7	33	
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28	
4	Undecanol-3	172	C11H24O	006929-08-4	25	
5	3-Heptadecanol	256	C17H36O	084534-30-5	25	



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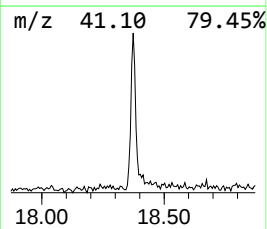
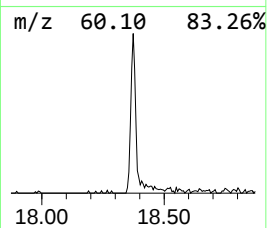
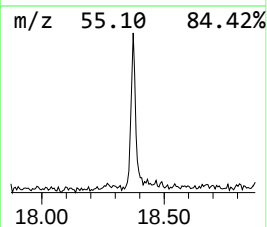
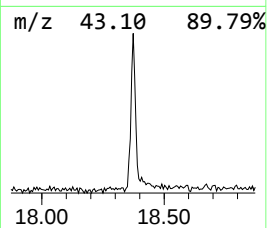
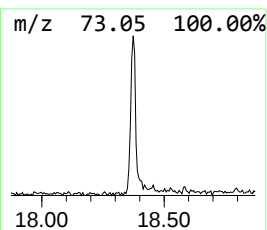
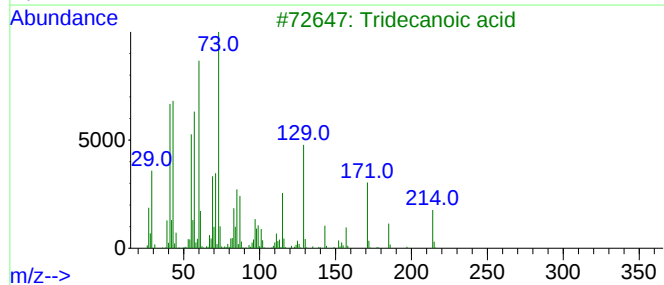
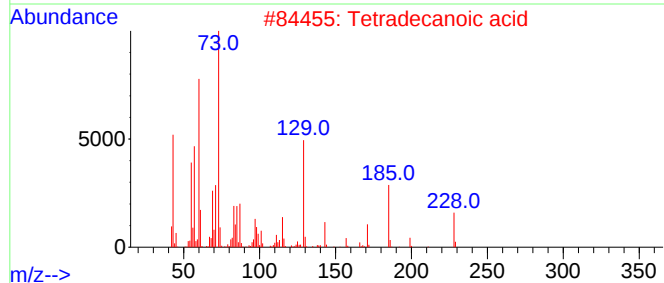
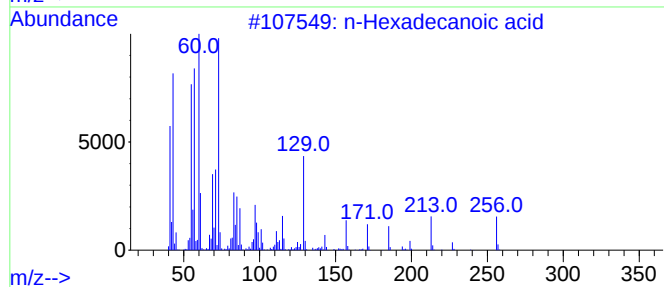
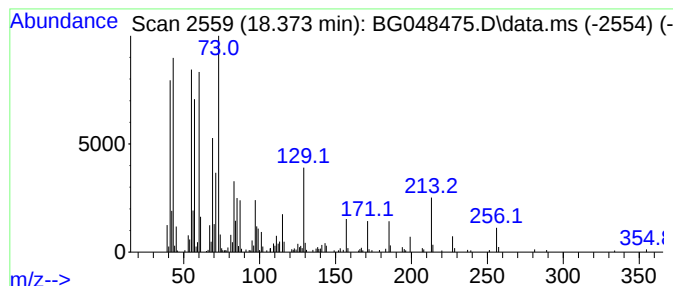
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	9.88 ng	357464	Phenanthrene-d10	17.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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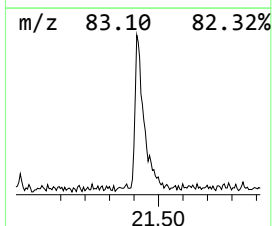
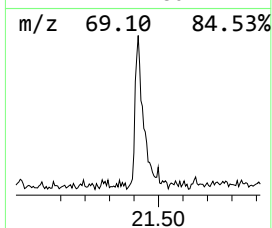
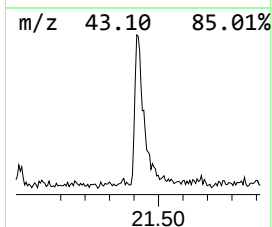
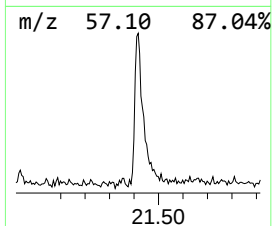
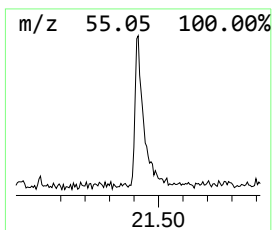
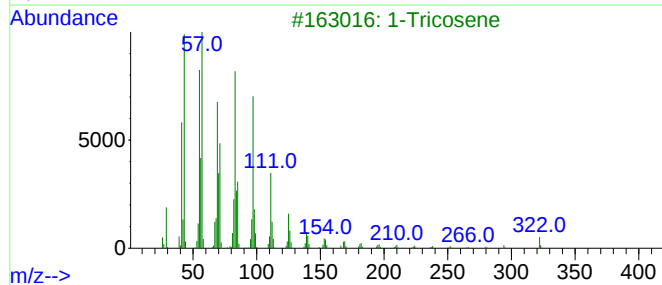
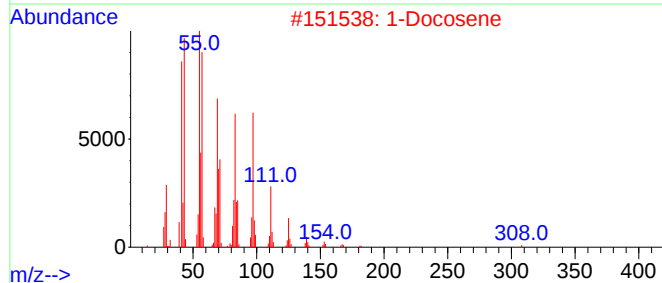
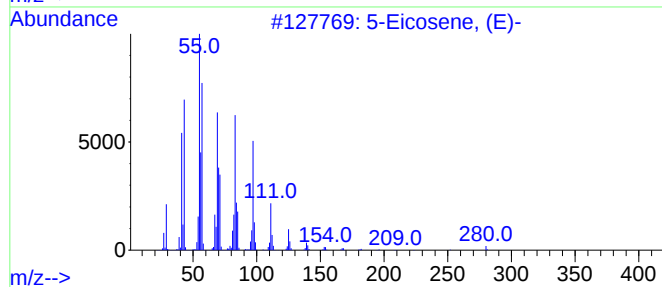
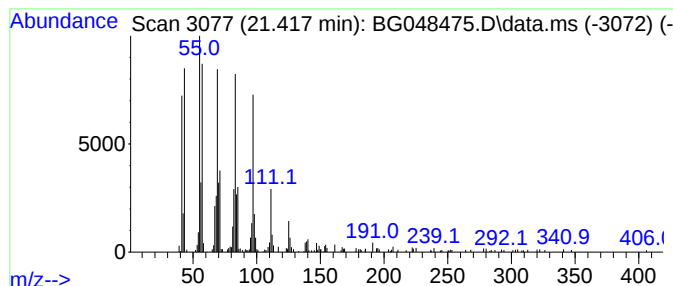
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Peak Number 3 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.417	12.46 ng	497903	Chrysene-d12	21.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Docosene		308	C22H44	001599-67-3	95
3	1-Tricosene		322	C23H46	018835-32-0	92
4	Bromoacetic acid, hexadecyl ester		362	C18H35BrO2	005454-48-8	91
5	Tetradecyl trifluoroacetate		310	C16H29F3O2	006222-02-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.177	4.3	ng	55473	1	8.103	258555	20.0
n-Hexadecanoic ...	18.373	9.9	ng	357464	4	17.492	723637	20.0
5-Eicosene, (E)-	21.417	12.5	ng	497903	5	21.781	799040	20.0