

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060516\
 Data File : BF087708.D
 Acq On : 5 Jun 2016 15:19
 Operator : UM/SJ
 Sample : H3378-17
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.770	15	16	26	rVB	310793	529764	9.75%	1.764%
2	1.907	26	28	88	rVB	2294191	5433633	100.00%	18.094%
3	5.039	300	302	308	rVB	56887	71452	1.31%	0.238%
4	5.130	308	310	312	rBV	84368	83339	1.53%	0.278%
5	5.450	335	338	341	rBV	1486193	1408501	25.92%	4.690%
6	6.479	425	428	430	rBV	1051736	906216	16.68%	3.018%
7	6.627	438	441	443	rBV	2486949	2744984	50.52%	9.141%
8	6.856	459	461	464	rBV	785138	686156	12.63%	2.285%
9	7.016	472	475	477	rVB	2614694	2408307	44.32%	8.020%
10	7.427	507	511	513	rBV	1824204	2211372	40.70%	7.364%
11	8.148	571	574	576	rBV	834952	927202	17.06%	3.088%
12	9.222	665	668	671	rBV	2879545	3555323	65.43%	11.839%
13	9.896	725	727	730	rVB	1134337	1031175	18.98%	3.434%
14	10.685	793	796	799	rBV	1990106	2071300	38.12%	6.897%
15	11.382	854	857	859	rBV	1131546	1068409	19.66%	3.558%
16	12.799	978	981	983	rBV	136609	165141	3.04%	0.550%
17	12.971	993	996	998	rBV	3035214	3100110	57.05%	10.323%
18	13.497	1040	1042	1045	rBV	73467	81129	1.49%	0.270%
19	14.011	1084	1087	1089	rBV	1004997	898995	16.55%	2.994%
20	15.440	1209	1212	1215	rBV	548489	647726	11.92%	2.157%

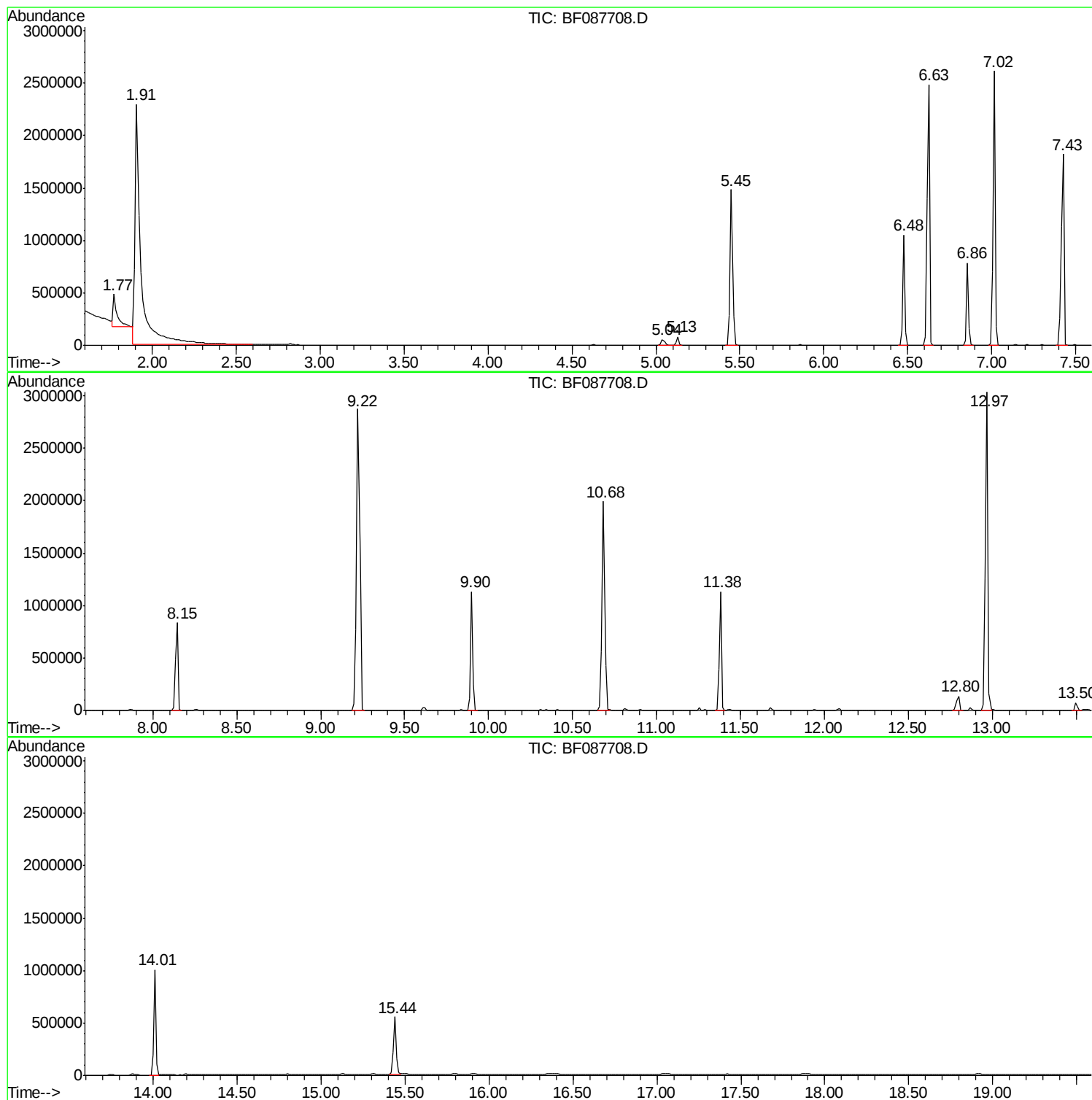
Sum of corrected areas: 30030234

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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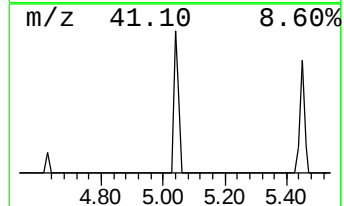
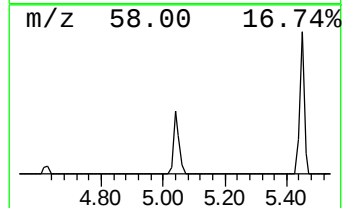
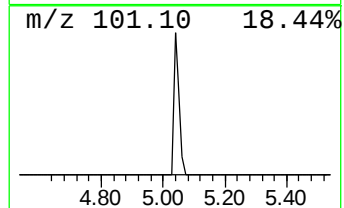
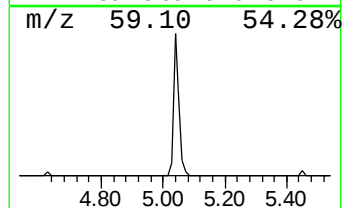
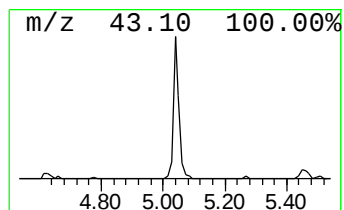
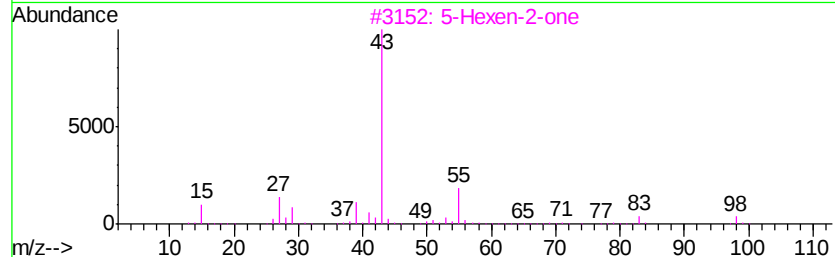
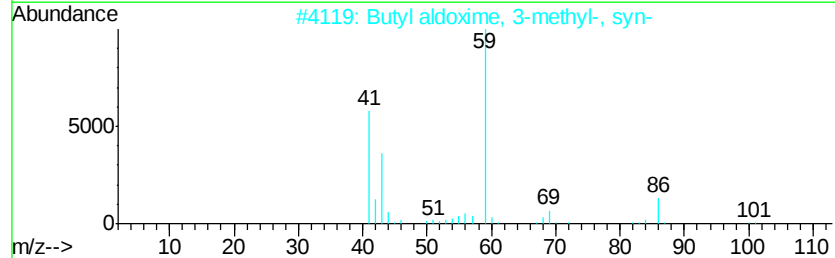
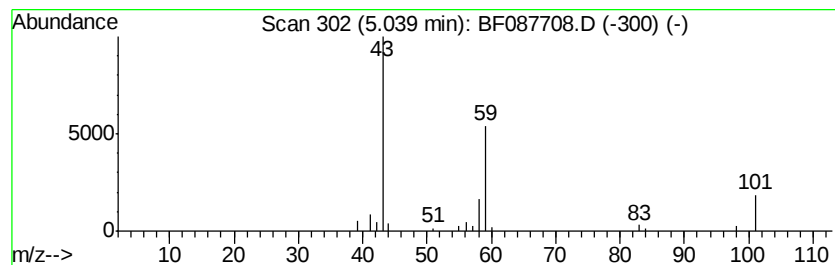
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.08 ng	71452	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9	
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9	



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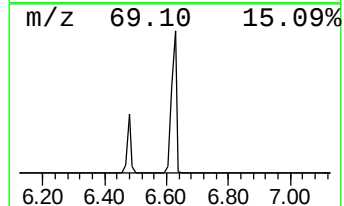
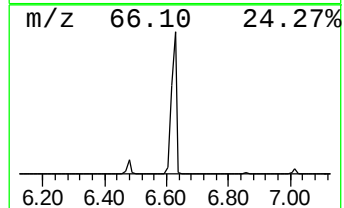
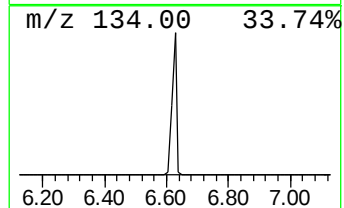
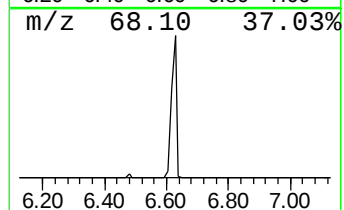
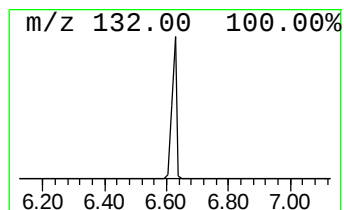
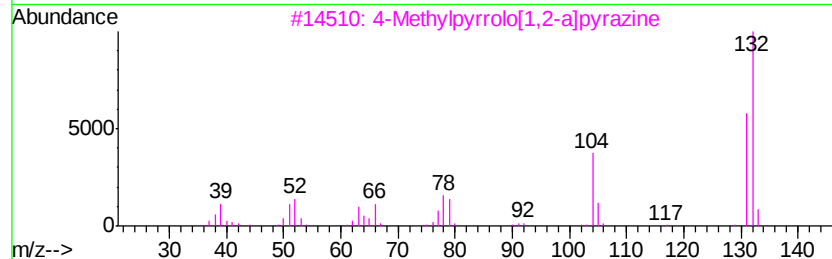
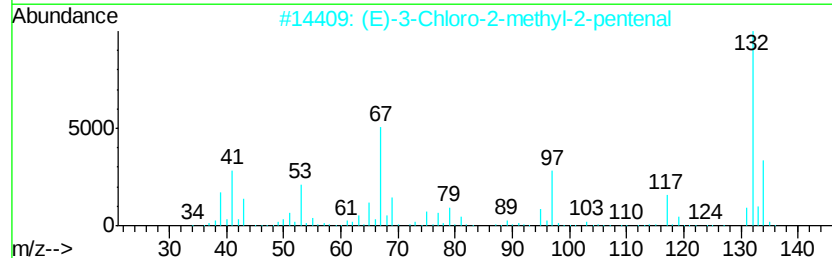
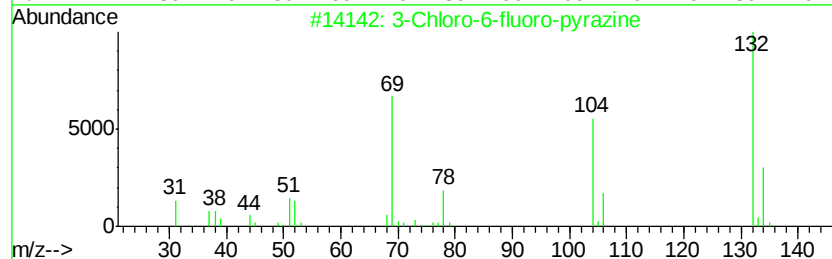
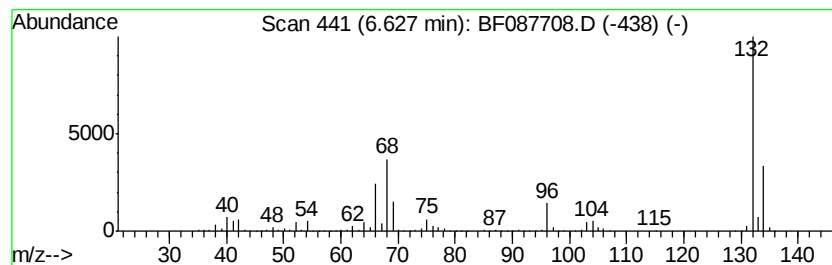
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Peak Number 5 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.01 ng	2744980	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9



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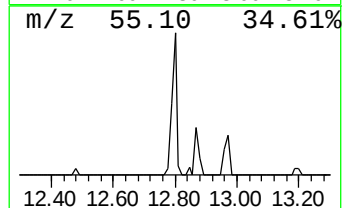
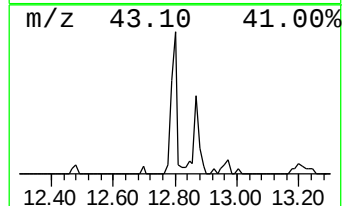
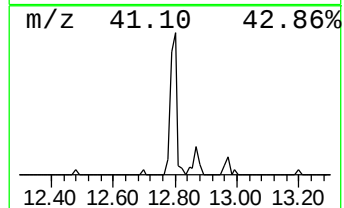
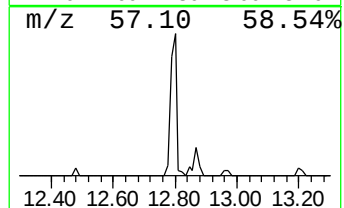
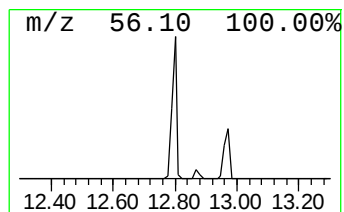
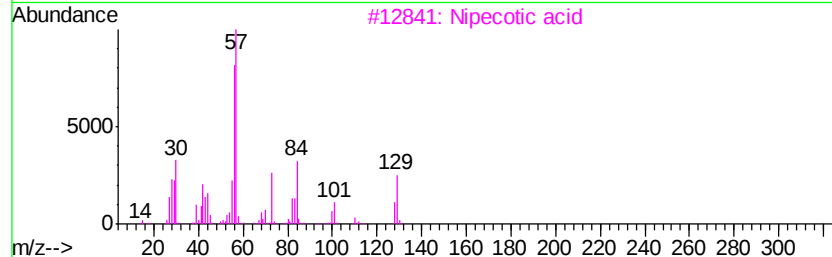
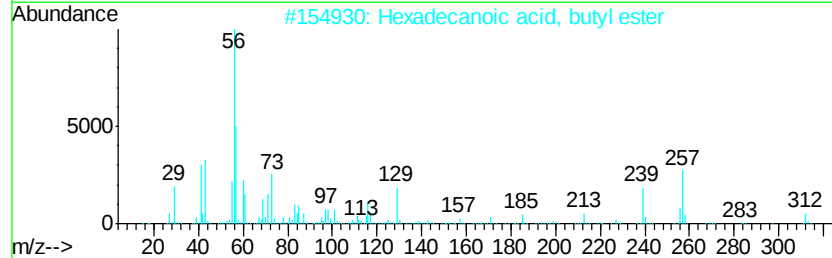
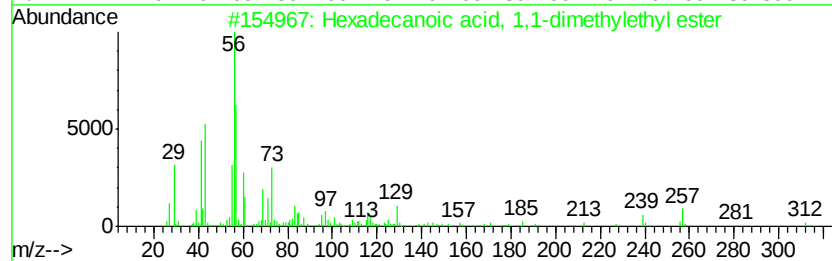
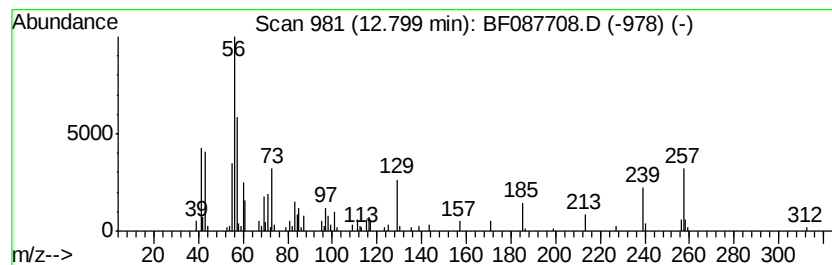
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Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	3.67 ng	165141	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	2.1	ng	71452	1	6.86	686156	20.0
unknown6.63	6.63	80.0	ng	2744980	1	6.86	686156	20.0
Hexadecanoic acid...	12.80	3.7	ng	165141	5	14.01	898995	20.0