

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051922\
 Data File : BF128345.D
 Acq On : 19 May 2022 19:26
 Operator : CG\JU
 Sample : N2934-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-220512

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.098	474	478	487	rVB	56340	69089	1.97%	0.364%
2	5.492	541	545	556	rBV	1939735	1822693	51.84%	9.595%
3	6.492	711	715	728	rBV	1526410	1475438	41.97%	7.767%
4	6.863	774	778	785	rBV	604230	494233	14.06%	2.602%
5	7.433	869	875	878	rBV	2060521	2117243	60.22%	11.145%
6	8.145	992	996	1004	rVB	725546	629860	17.92%	3.316%
7	8.704	1088	1091	1101	rBV	61664	68640	1.95%	0.361%
8	9.222	1174	1179	1182	rBV	3525028	3515736	100.00%	18.507%
9	9.904	1289	1295	1298	rBV	829442	737340	20.97%	3.881%
10	10.698	1425	1430	1445	rBV	2347765	2365792	67.29%	12.454%
11	10.986	1463	1479	1490	rBV4	12160	57939	1.65%	0.305%
12	11.398	1545	1549	1552	rBV	767161	697936	19.85%	3.674%
13	11.768	1609	1612	1616	rVB	143328	109292	3.11%	0.575%
14	12.986	1814	1819	1822	rBV	3470221	3155358	89.75%	16.610%
15	14.045	1995	1999	2004	rBV	474245	452157	12.86%	2.380%
16	14.786	2121	2125	2134	rBV	692495	724361	20.60%	3.813%
17	15.533	2247	2252	2261	rVB	392785	503834	14.33%	2.652%

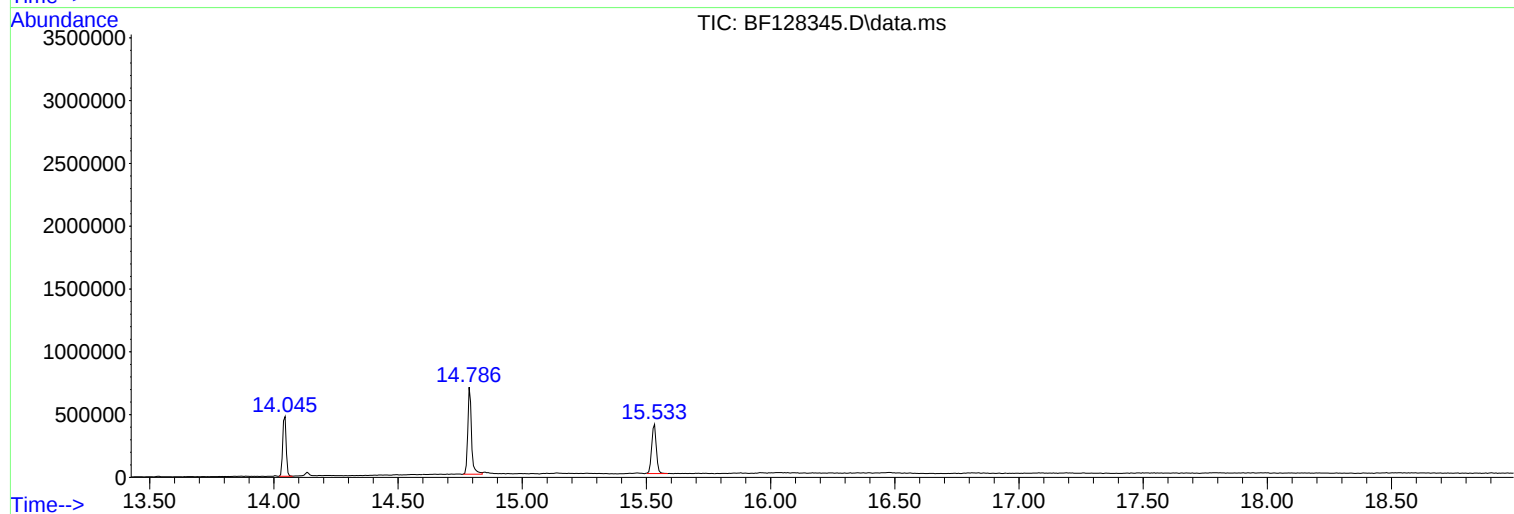
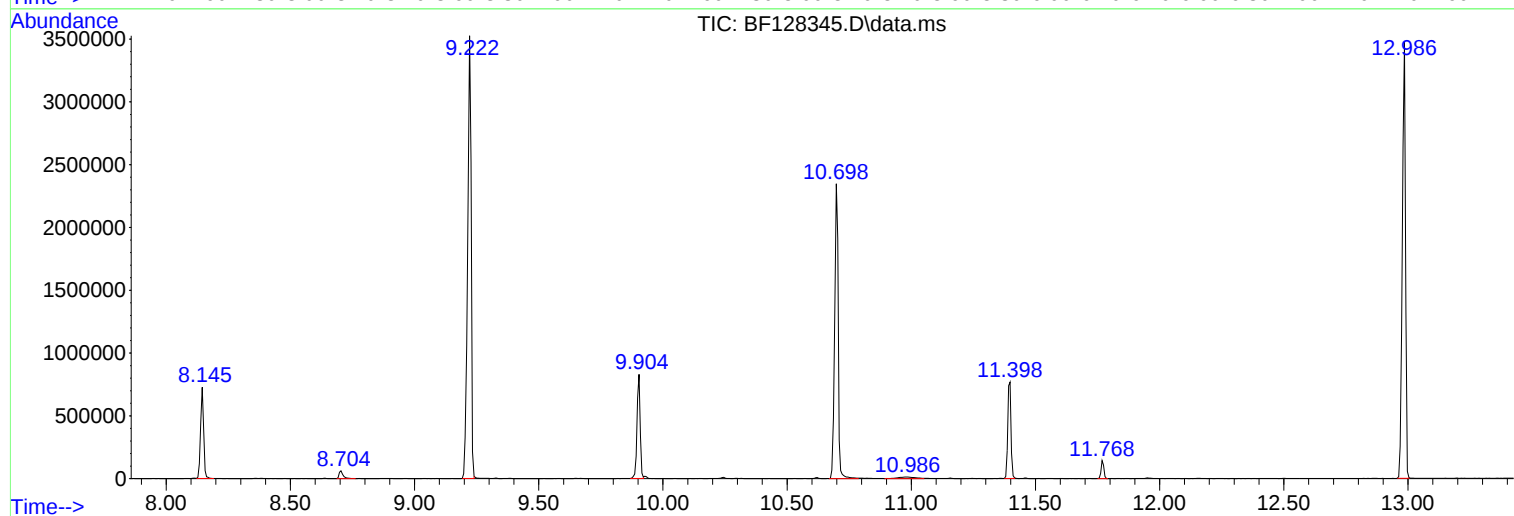
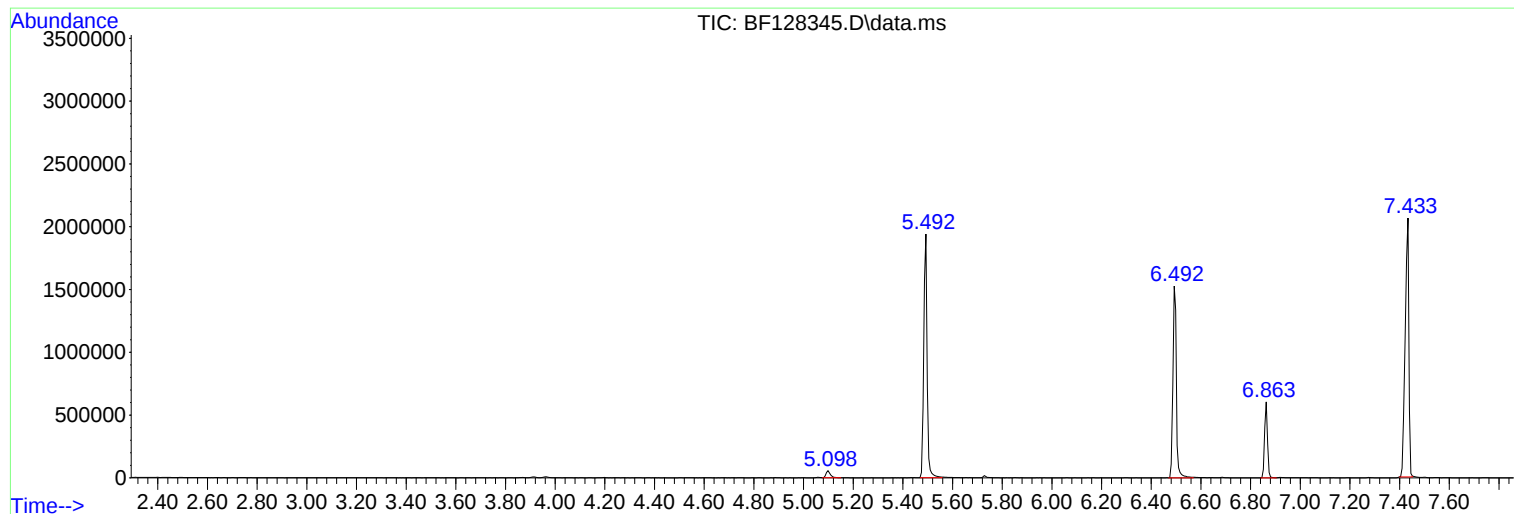
Sum of corrected areas: 18996941

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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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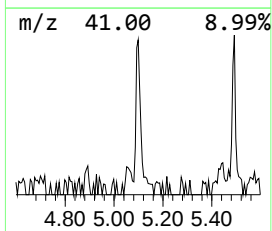
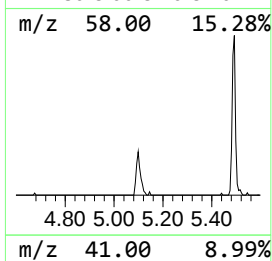
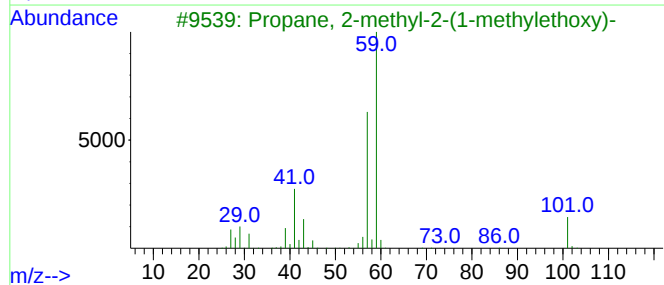
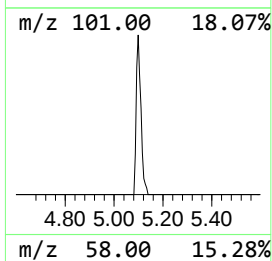
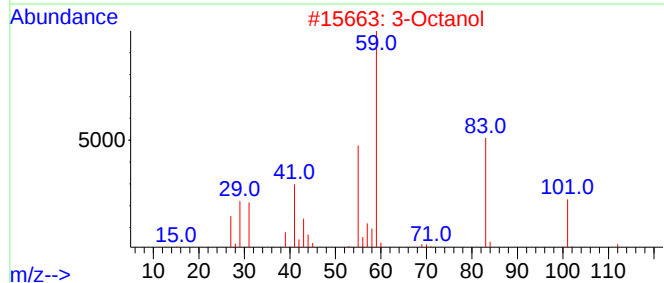
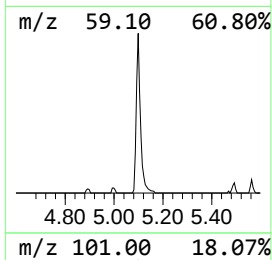
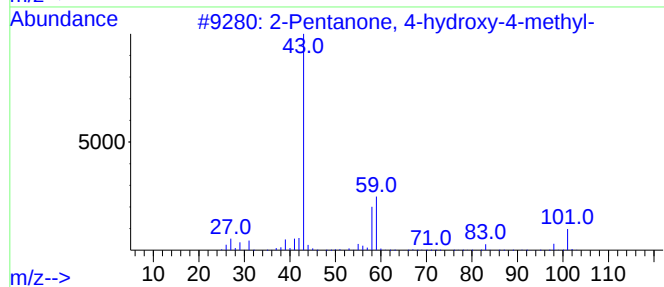
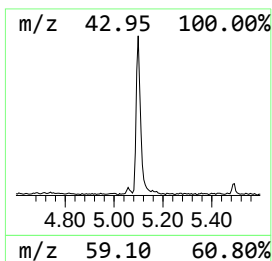
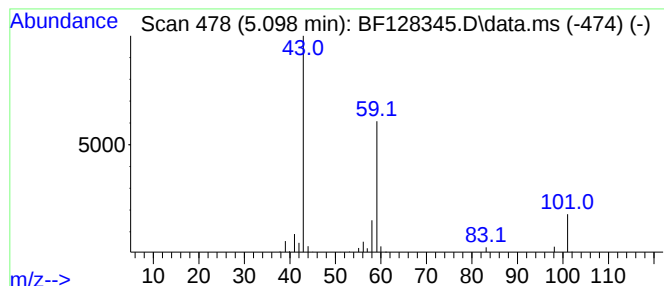
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.098	2.80 ng	69089	1,4-Dichlorobenzene-d4			6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	3-Octanol	130	C8H18O		000589-98-0	36
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	36
4	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	35
5	2-Hexanol, 2-methyl-	116	C7H16O		000625-23-0	28



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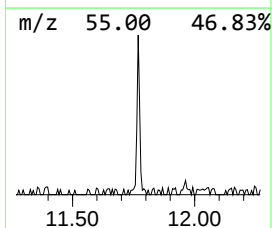
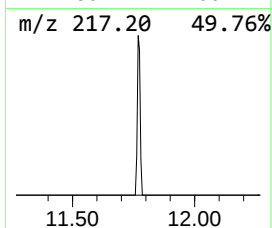
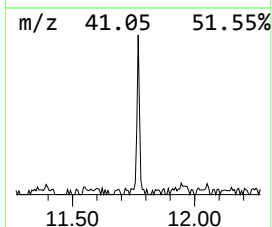
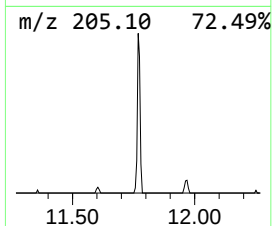
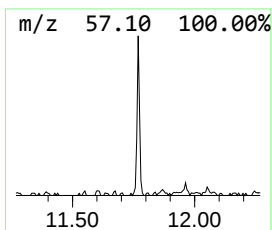
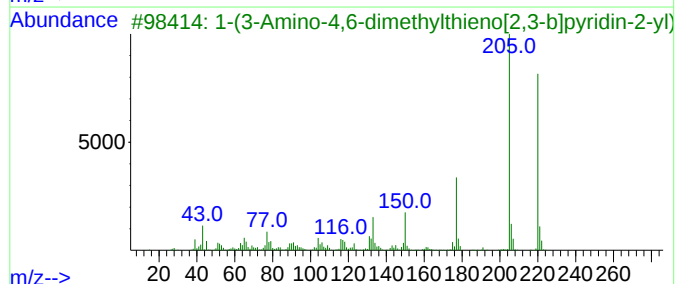
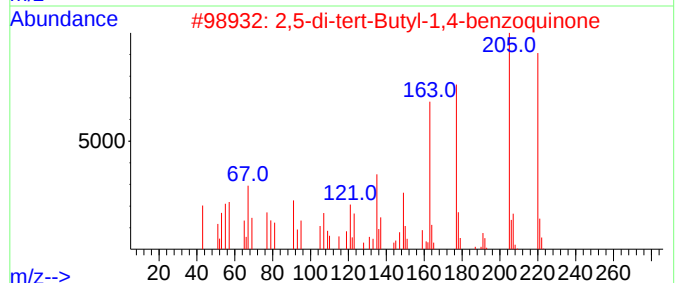
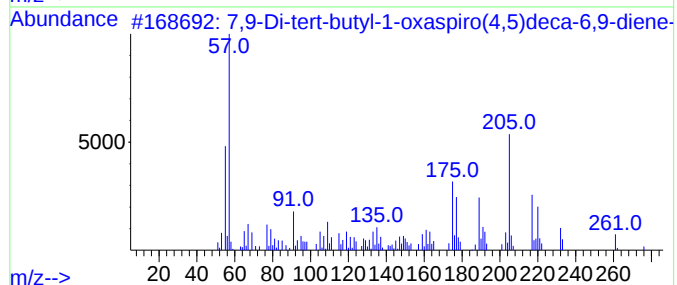
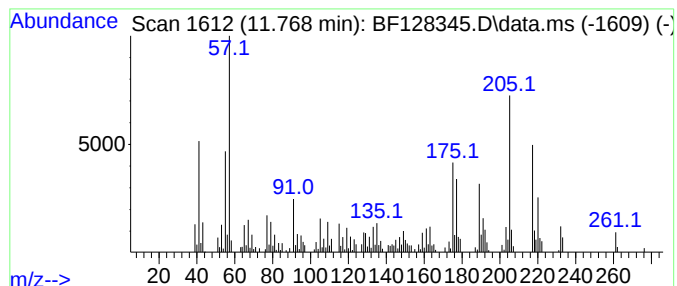
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Peak Number 2 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	3.13 ng	109292	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	48		
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	42		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38		
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	35		



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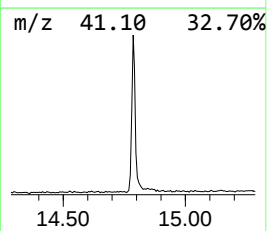
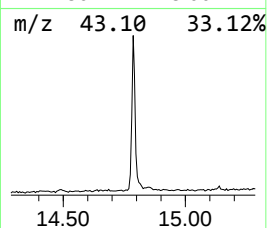
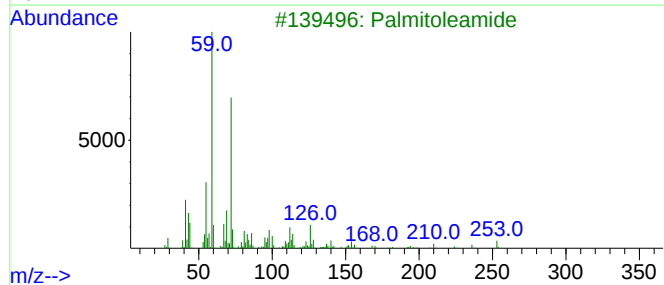
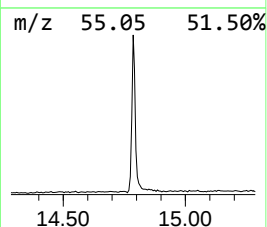
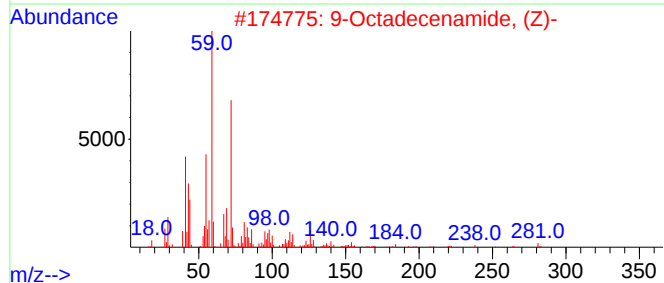
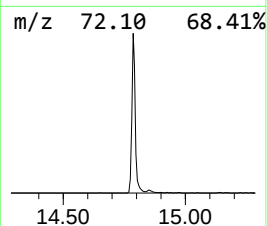
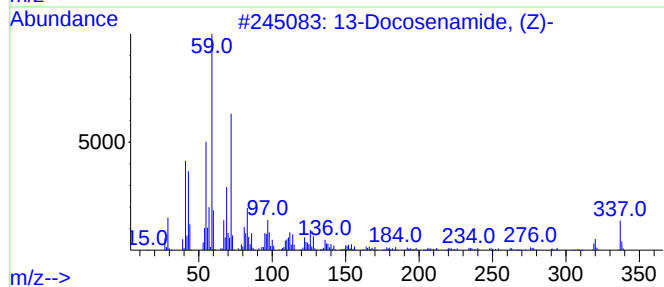
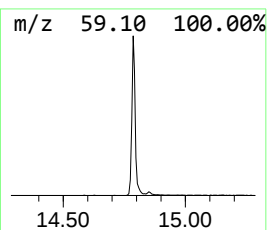
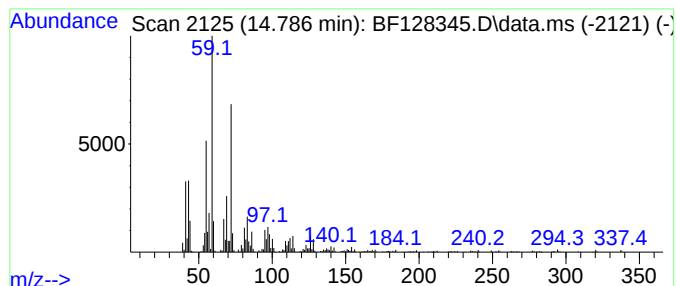
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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	32.04 ng	724361	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Palmitoleamide	253	C16H31NO	106010-22-4	64
4			Octanamide	143	C8H17NO	000629-01-6	53
5			Dodecanamide	199	C12H25NO	001120-16-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.098	2.8	ng	69089	1	6.863	494233	20.0
7,9-Di-tert-but...	11.769	3.1	ng	109292	4	11.398	697936	20.0
13-Docosenamide...	14.786	32.0	ng	724361	5	14.045	452157	20.0