

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040618\
Data File : BF104340.D
Acq On : 7 Apr 2018 6:46
Operator : JU/SJ
Sample : J2225-15
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
040218-SIDI-F-U-M

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.004	492	496	501	rVB	205637	227225	5.29%	0.906%
2	5.404	560	564	568	rBV	1438522	1280544	29.81%	5.108%
3	6.416	732	736	745	rVB	876463	801805	18.67%	3.198%
4	6.569	757	762	765	rBV	2569156	2314137	53.88%	9.231%
5	6.804	798	802	805	rBV	1043563	867570	20.20%	3.461%
6	6.963	824	829	832	rBV	3226720	3000303	69.85%	11.968%
7	7.369	892	898	901	rBV	2312428	2575552	59.96%	10.273%
8	8.086	1016	1020	1023	rBV	1407304	1155012	26.89%	4.607%
9	9.169	1198	1204	1207	rBV	4064309	4295220	100.00%	17.133%
10	9.839	1313	1318	1322	rVB2	1378465	1228639	28.60%	4.901%
11	10.275	1385	1392	1394	rBV2	47775	47727	1.11%	0.190%
12	10.628	1447	1452	1455	rBV	1760717	1573981	36.64%	6.278%
13	11.327	1567	1571	1574	rBV	1185523	960574	22.36%	3.832%
14	12.739	1808	1811	1814	rVB	100033	72840	1.70%	0.291%
15	12.921	1837	1842	1845	rBV	3170848	3041306	70.81%	12.131%
16	13.445	1927	1931	1934	rBV	59017	45429	1.06%	0.181%
17	13.816	1990	1994	2000	rBV	70264	80474	1.87%	0.321%
18	13.968	2016	2020	2024	rBV	935181	790887	18.41%	3.155%
19	15.427	2263	2268	2272	rBV	606924	710798	16.55%	2.835%

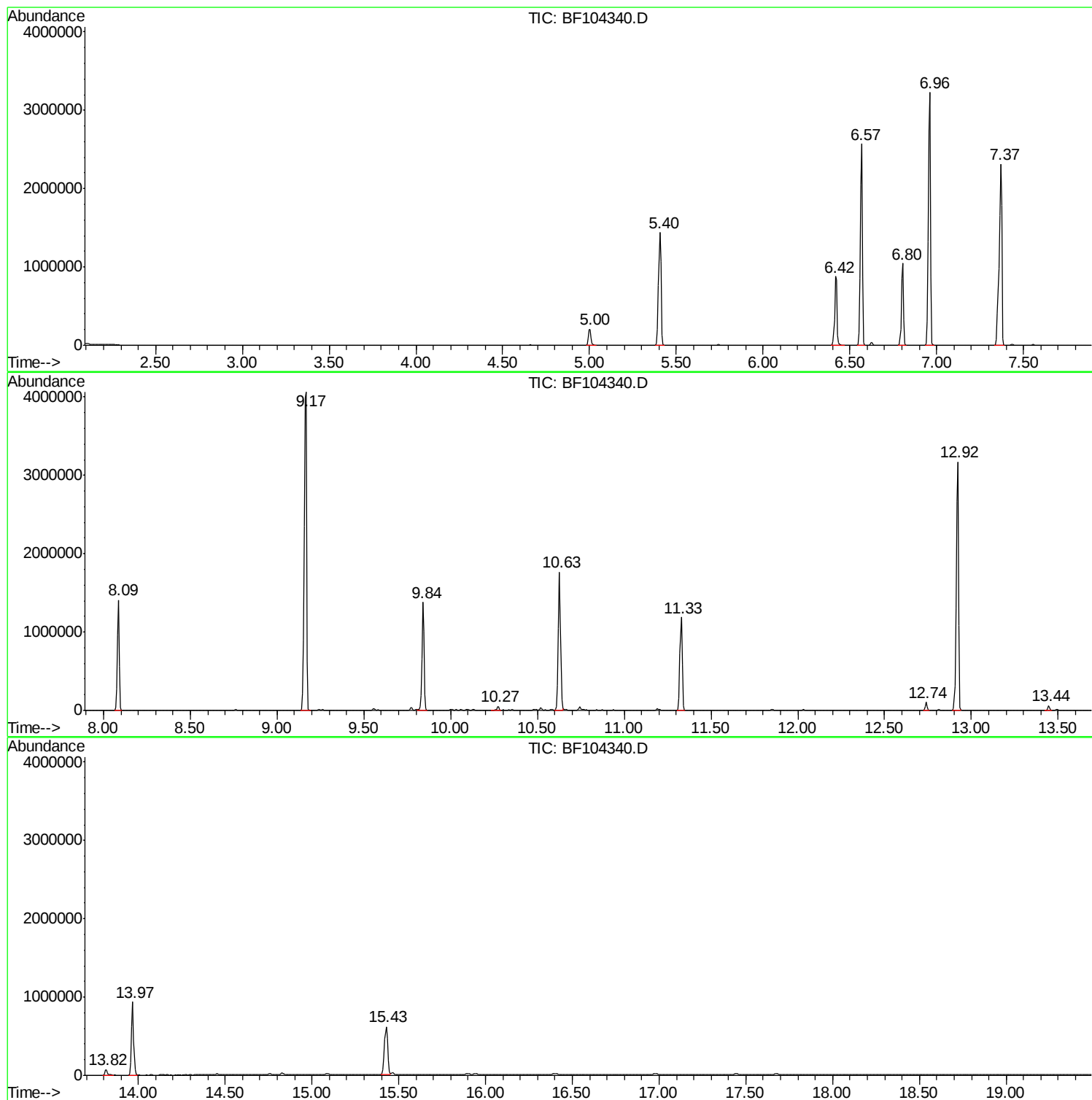
Sum of corrected areas: 25070023

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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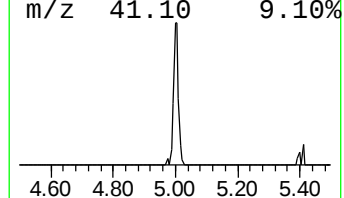
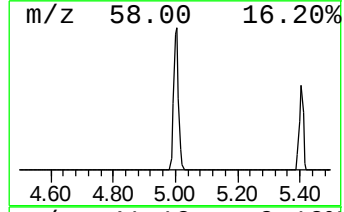
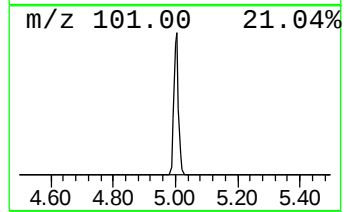
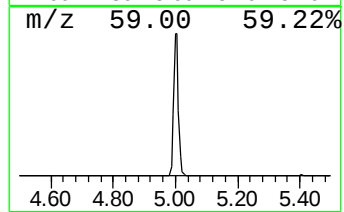
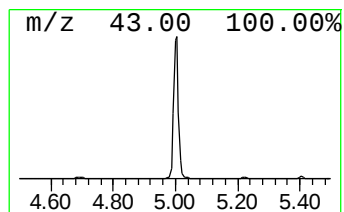
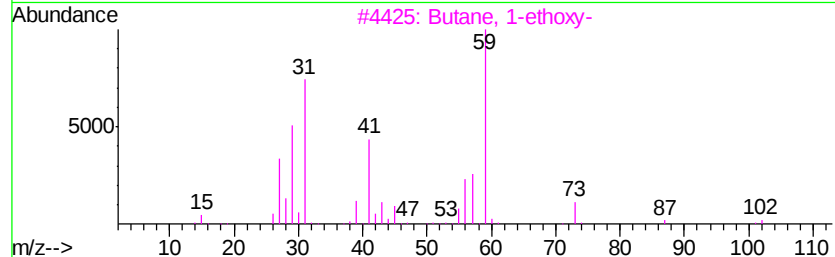
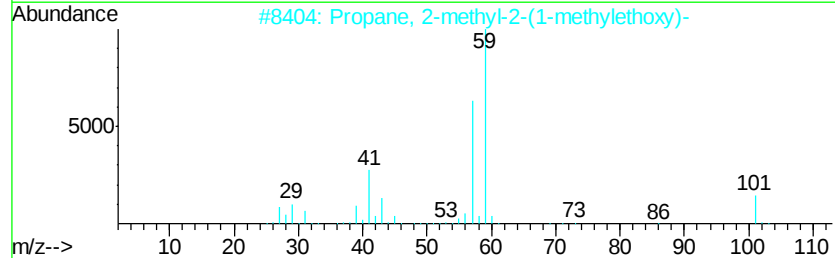
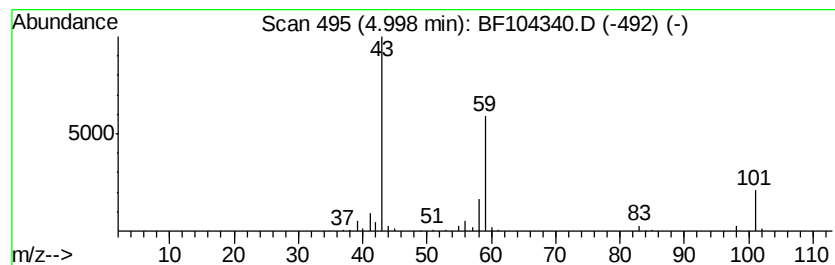
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.24 ng	227225	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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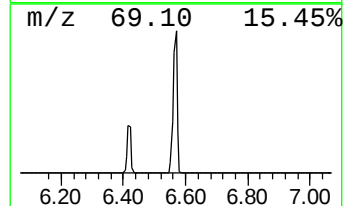
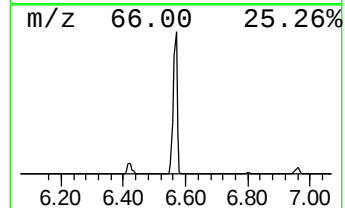
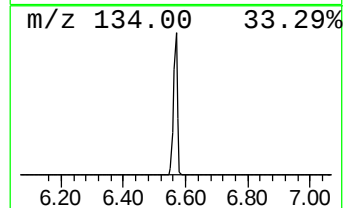
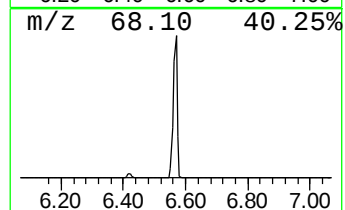
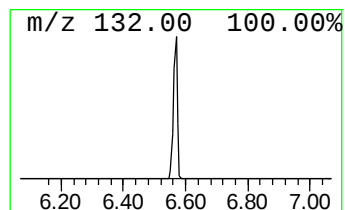
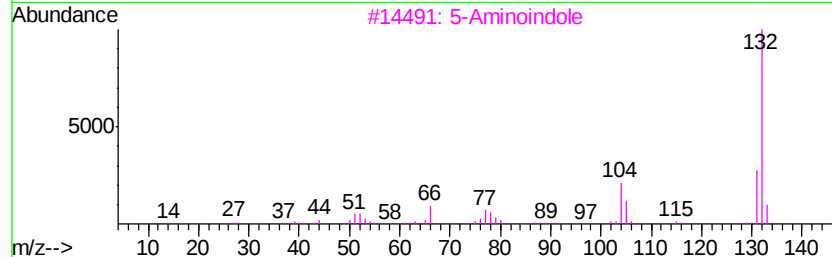
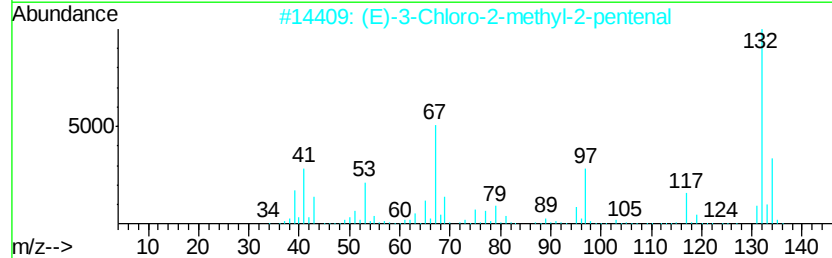
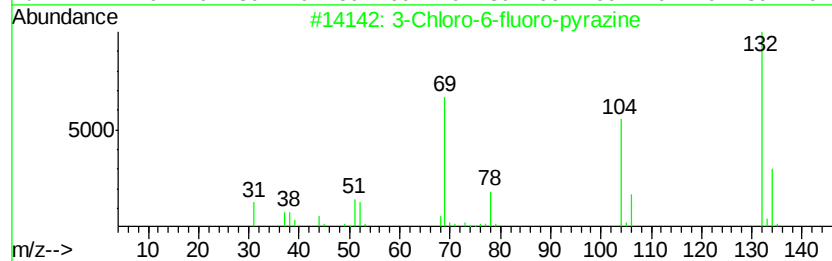
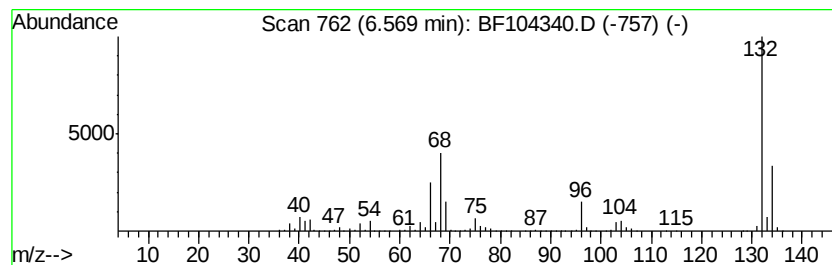
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.35 ng	2314140	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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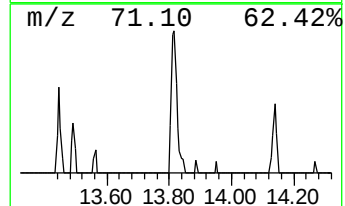
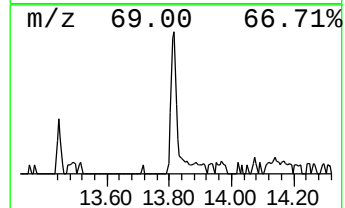
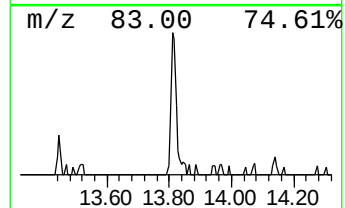
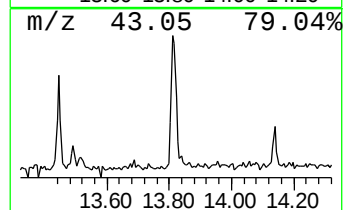
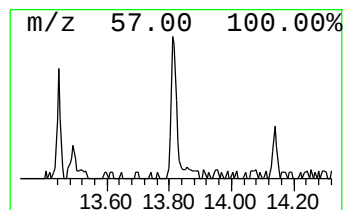
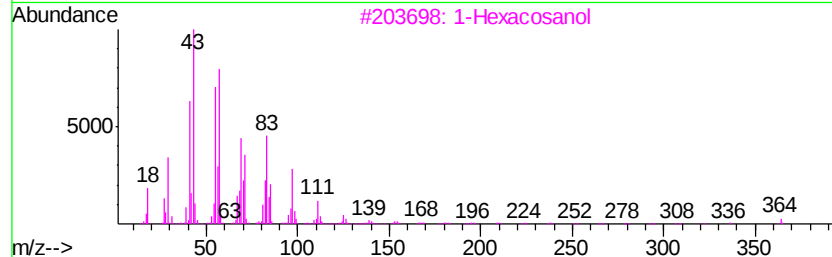
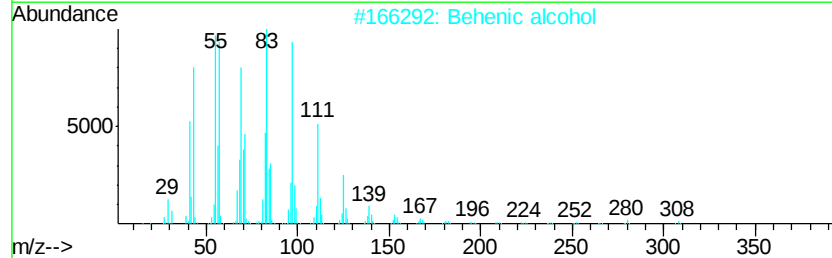
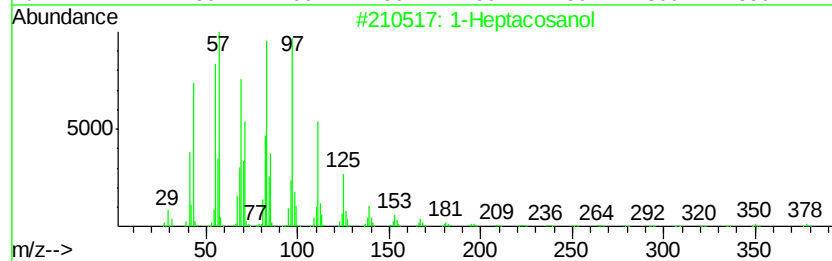
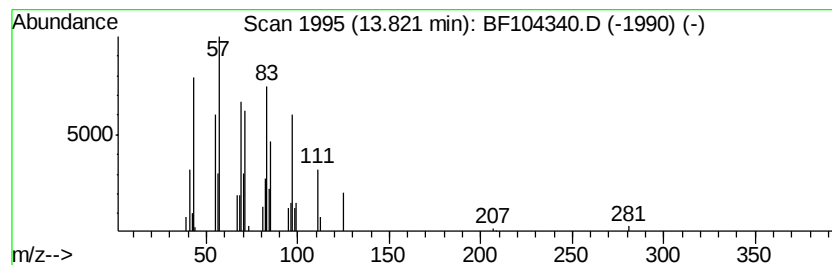
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Peak Number 4 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.04 ng	80474	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	5.2	ng	227225	1	6.80	867570	20.0
unknown6.57	6.57	53.4	ng	2314140	1	6.80	867570	20.0
1-Heptacosanol	13.82	2.0	ng	80474	5	13.97	790887	20.0