

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120617\
 Data File : BF101166.D
 Acq On : 6 Dec 2017 14:37
 Operator : SJ/JU
 Sample : I6642-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PENN-1-E(4-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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	5.075	505	508	522	rBB	47641	66463	4.87%	0.610%
2	5.469	571	575	578	rBV	1128510	1039768	76.21%	9.539%
3	6.481	742	747	761	rVB	1077695	1107769	81.19%	10.163%
4	6.616	766	770	773	rBV	1274653	1130864	82.89%	10.375%
5	6.845	805	809	814	rBB	343180	274396	20.11%	2.517%
6	7.004	831	836	839	rBV	945468	889071	65.17%	8.156%
7	7.410	900	905	908	rBV	690863	681909	49.98%	6.256%
8	8.128	1023	1027	1042	rBV	445698	367964	26.97%	3.376%
9	9.204	1205	1210	1213	rBV	1594910	1364333	100.00%	12.516%
10	9.598	1273	1277	1283	rVB	104335	106560	7.81%	0.978%
11	9.804	1308	1312	1316	rBV	32889	27783	2.04%	0.255%
12	9.880	1321	1325	1338	rVB	434506	425543	31.19%	3.904%
13	10.304	1393	1397	1400	rVB	31873	24684	1.81%	0.226%
14	10.675	1456	1460	1471	rVB	858630	787288	57.70%	7.223%
15	10.775	1474	1477	1484	rVB	28606	26775	1.96%	0.246%
16	11.375	1575	1579	1582	rBV	515272	454986	33.35%	4.174%
17	12.957	1844	1848	1852	rBV	1379447	1344879	98.57%	12.338%
18	13.151	1876	1881	1884	rBV	19748	17388	1.27%	0.160%
19	13.839	1994	1998	2006	rBV	126044	132684	9.73%	1.217%
20	14.016	2024	2028	2038	rVB	389446	359446	26.35%	3.298%
21	15.492	2274	2279	2289	rBV2	182634	251421	18.43%	2.307%
22	15.968	2355	2360	2367	rBV4	9701	18439	1.35%	0.169%

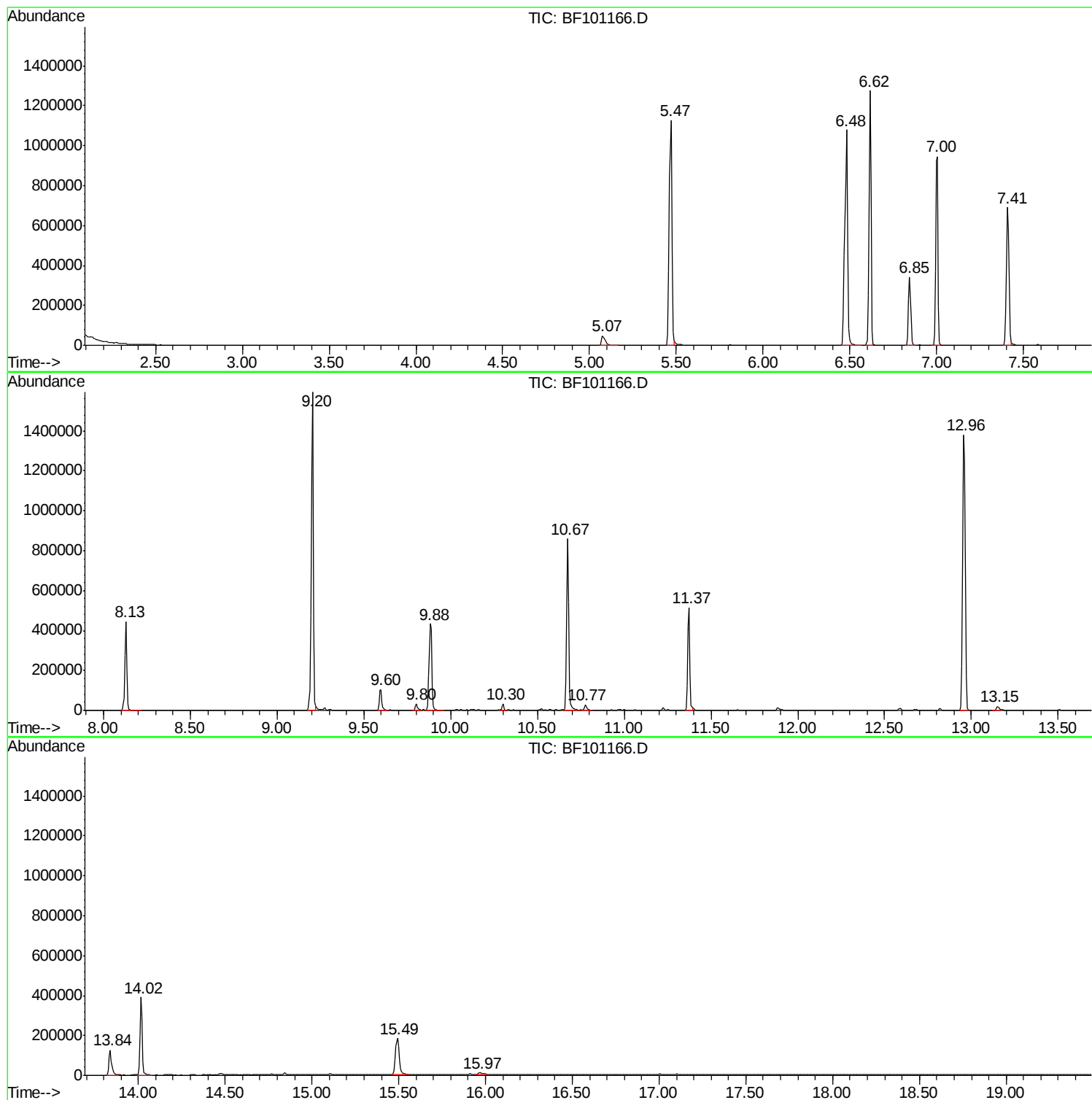
Sum of corrected areas: 10900413

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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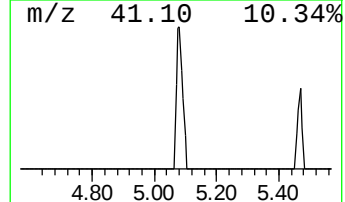
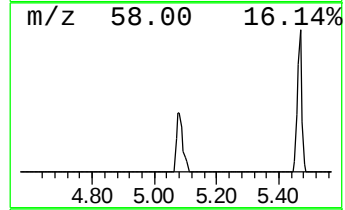
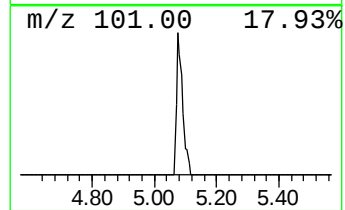
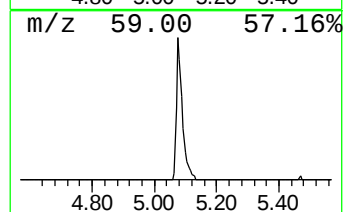
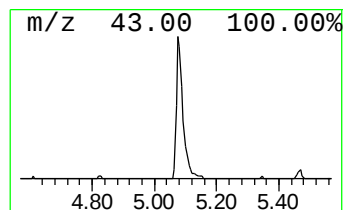
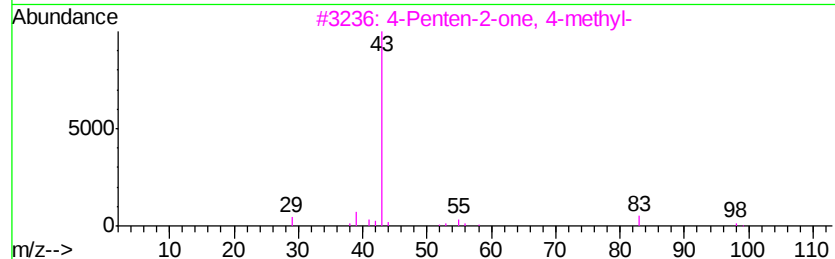
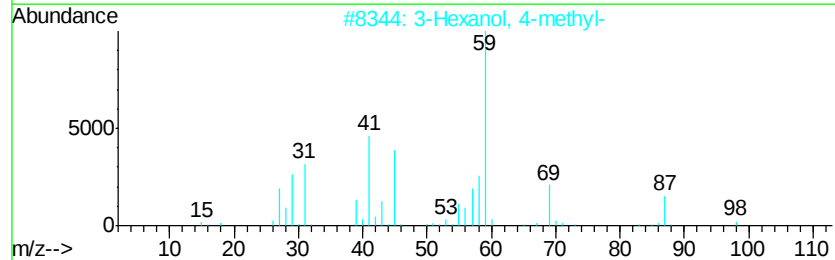
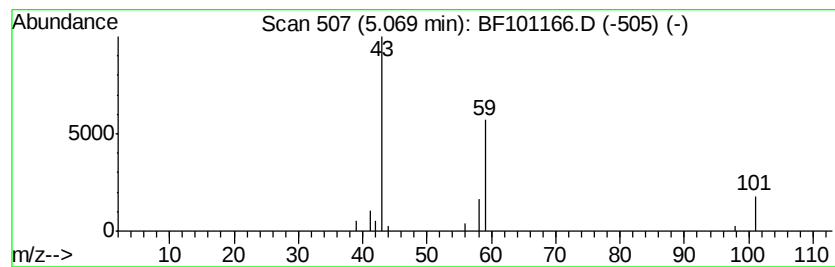
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	4.84 ng	66463	1,4-Dichlorobenzene-d4	6.85

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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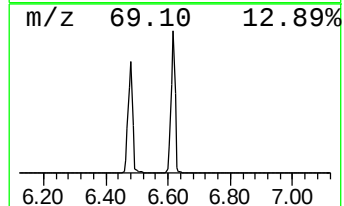
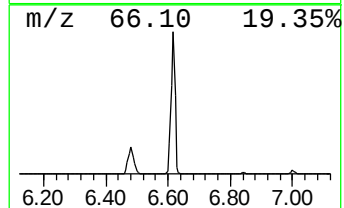
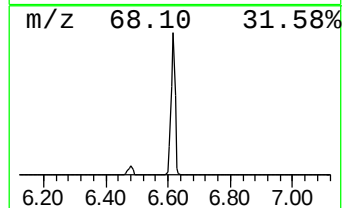
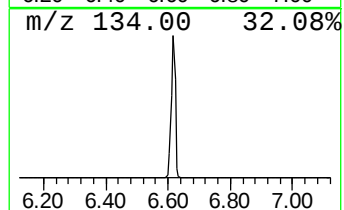
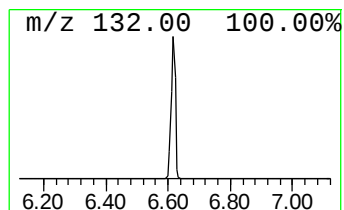
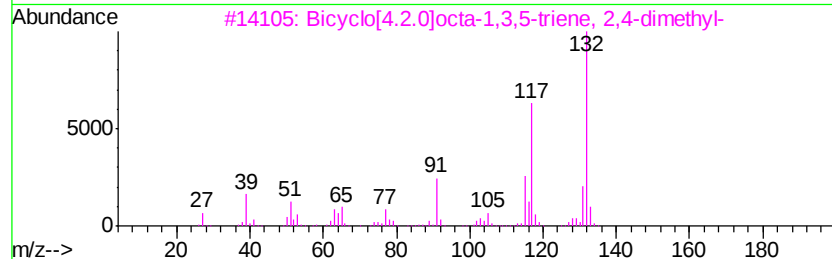
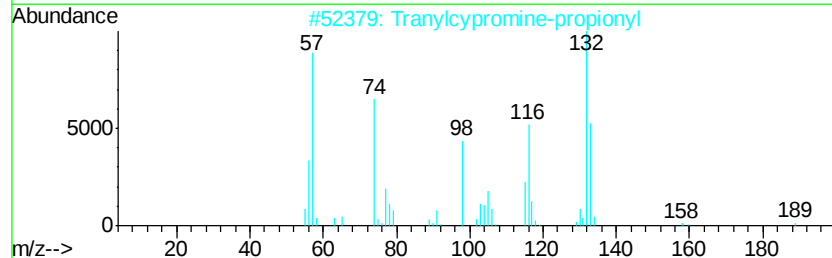
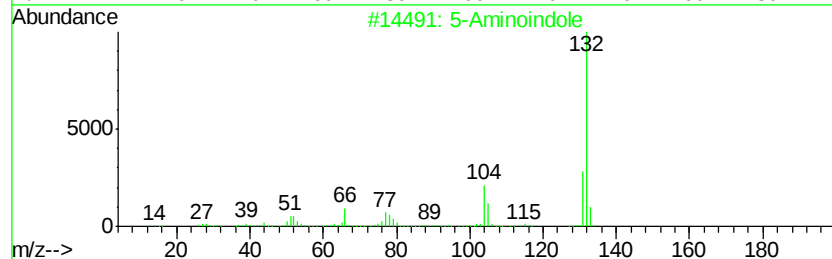
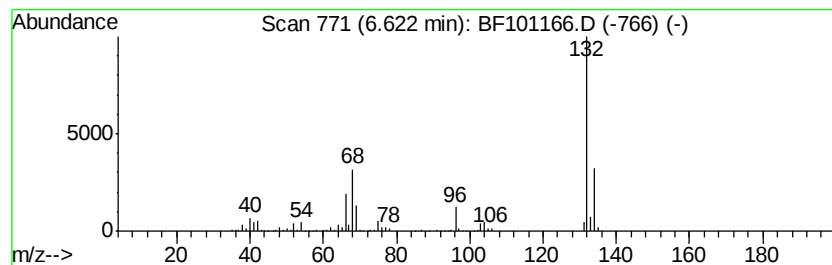
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	82.43 ng	1130860	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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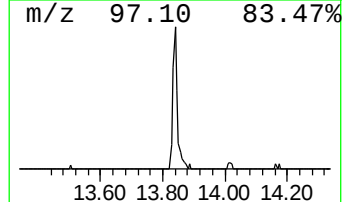
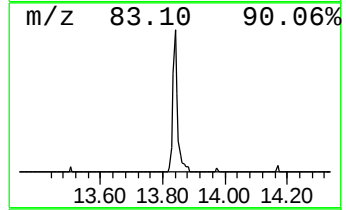
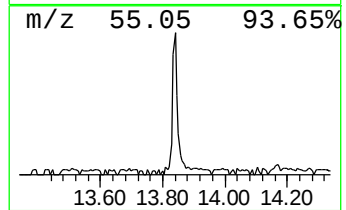
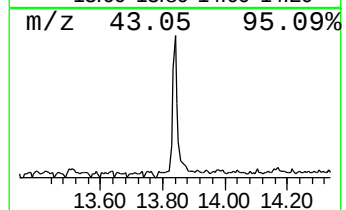
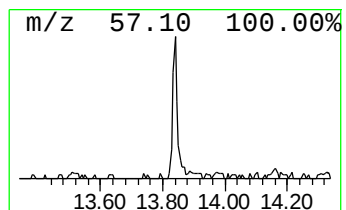
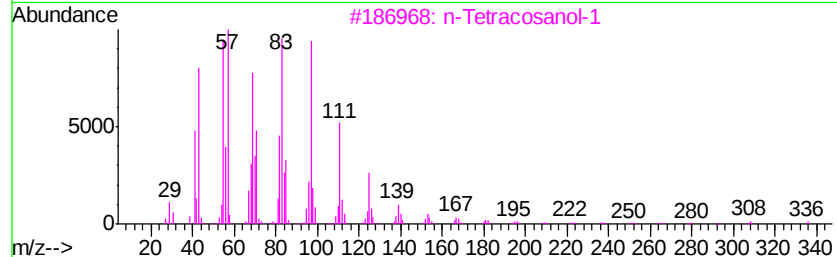
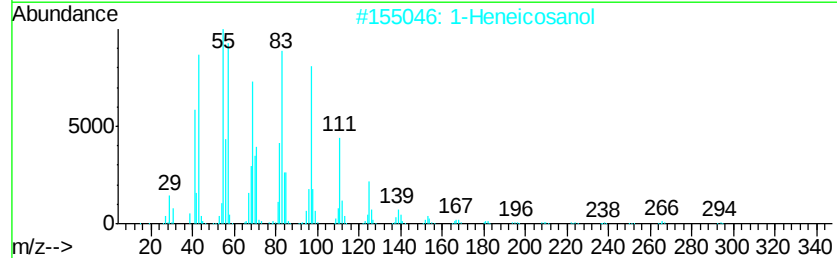
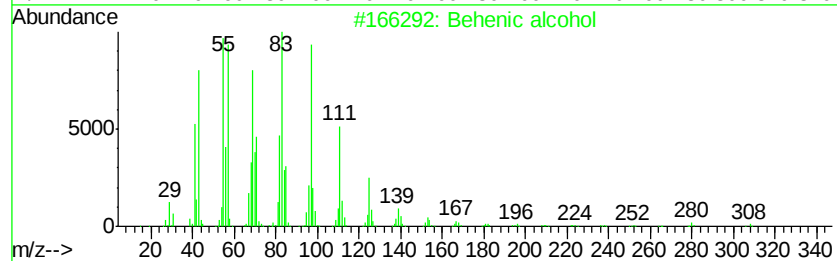
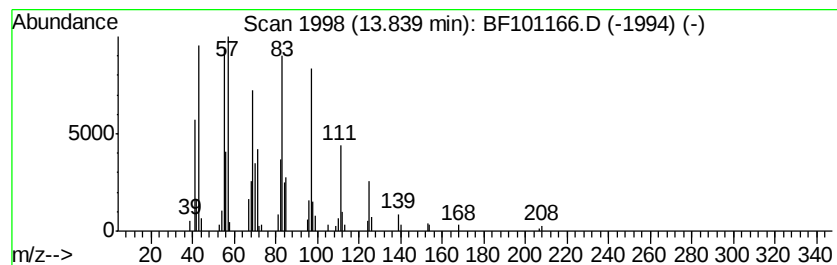
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Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.84	7.38 ng	132684	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Docosene	308	C22H44	001599-67-3	91
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	4.8	ng	66463	1	6.85	274396	20.0
unknown6.62	6.62	82.4	ng	1130860	1	6.85	274396	20.0
Behenic alcohol	13.84	7.4	ng	132684	5	14.02	359446	20.0