

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030316\
 Data File : BF085196.D
 Acq On : 4 Mar 2016 9:45
 Operator : SJ/UM
 Sample : H1661-01 5X
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-45-COMP

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-BF030316.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	5.167	249	252	255	rBV	156627	153157	12.33%	1.249%
2	5.578	285	288	290	rBV	469472	654170	52.65%	5.335%
3	6.596	374	377	378	rBV	562767	744934	59.96%	6.076%
4	6.619	378	379	382	rVB	22030	17864	1.44%	0.146%
5	6.676	382	384	387	rBV	12826	30990	2.49%	0.253%
6	6.744	387	390	392	rBV	665206	714957	57.55%	5.831%
7	6.973	408	410	413	rBV	701386	903411	72.71%	7.368%
8	7.133	422	424	426	rVB	799431	654304	52.66%	5.337%
9	7.533	457	459	462	rBV	574442	491107	39.53%	4.005%
10	8.264	520	523	525	rBV	1494269	1242401	100.00%	10.133%
11	8.779	563	568	574	rBV3	4927	18070	1.45%	0.147%
12	9.339	614	617	619	rBV	1084008	920243	74.07%	7.506%
13	9.727	649	651	656	rVB	184777	169534	13.65%	1.383%
14	9.945	668	670	674	rBV	33346	30413	2.45%	0.248%
15	10.025	674	677	679	rBV	992451	1208495	97.27%	9.856%
16	10.253	694	697	700	rBV2	20268	35006	2.82%	0.286%
17	10.448	707	714	716	rBV	46431	57563	4.63%	0.469%
18	10.665	730	733	736	rBV2	11730	19014	1.53%	0.155%
19	10.802	743	745	748	rVB	152357	131530	10.59%	1.073%
20	10.916	753	755	760	rVB	38929	49611	3.99%	0.405%
21	11.110	770	772	777	rVB3	10041	22436	1.81%	0.183%
22	11.362	792	794	797	rBV	12986	24819	2.00%	0.202%
23	11.499	804	806	809	rBV2	883747	1039326	83.65%	8.477%
24	12.048	849	854	861	rBV4	12207	44627	3.59%	0.364%
25	12.402	882	885	886	rBV2	9623	17073	1.37%	0.139%
26	12.436	886	888	896	rVV5	25124	74752	6.02%	0.610%
27	12.551	896	898	906	rVB4	9787	29235	2.35%	0.238%
28	12.905	927	929	931	rVB	38515	33202	2.67%	0.271%
29	13.088	942	945	947	rBV	575183	616700	49.64%	5.030%
30	13.316	960	965	968	rVB5	8960	21594	1.74%	0.176%
31	13.614	988	991	992	rBV	21848	24830	2.00%	0.203%
32	13.979	1021	1023	1028	rVB3	18563	28010	2.25%	0.228%
33	14.139	1034	1037	1039	rBV	995447	885067	71.24%	7.219%
34	14.299	1049	1051	1054	rBV3	9528	17720	1.43%	0.145%

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35	14.608	1076	1078	1080	rBV3	12318	20398	1.64%	0.166%
36	14.768	1090	1092	1094	rBV	72819	85740	6.90%	0.699%
37	14.894	1100	1103	1107	rBV3	69879	97196	7.82%	0.793%
38	15.614	1163	1166	1172	rVB	665126	863042	69.47%	7.039%
39	15.820	1182	1184	1188	rBV4	11622	17186	1.38%	0.140%
40	16.082	1205	1207	1210	rBV2	11991	19902	1.60%	0.162%
41	16.585	1249	1251	1256	rVB3	16745	31282	2.52%	0.255%

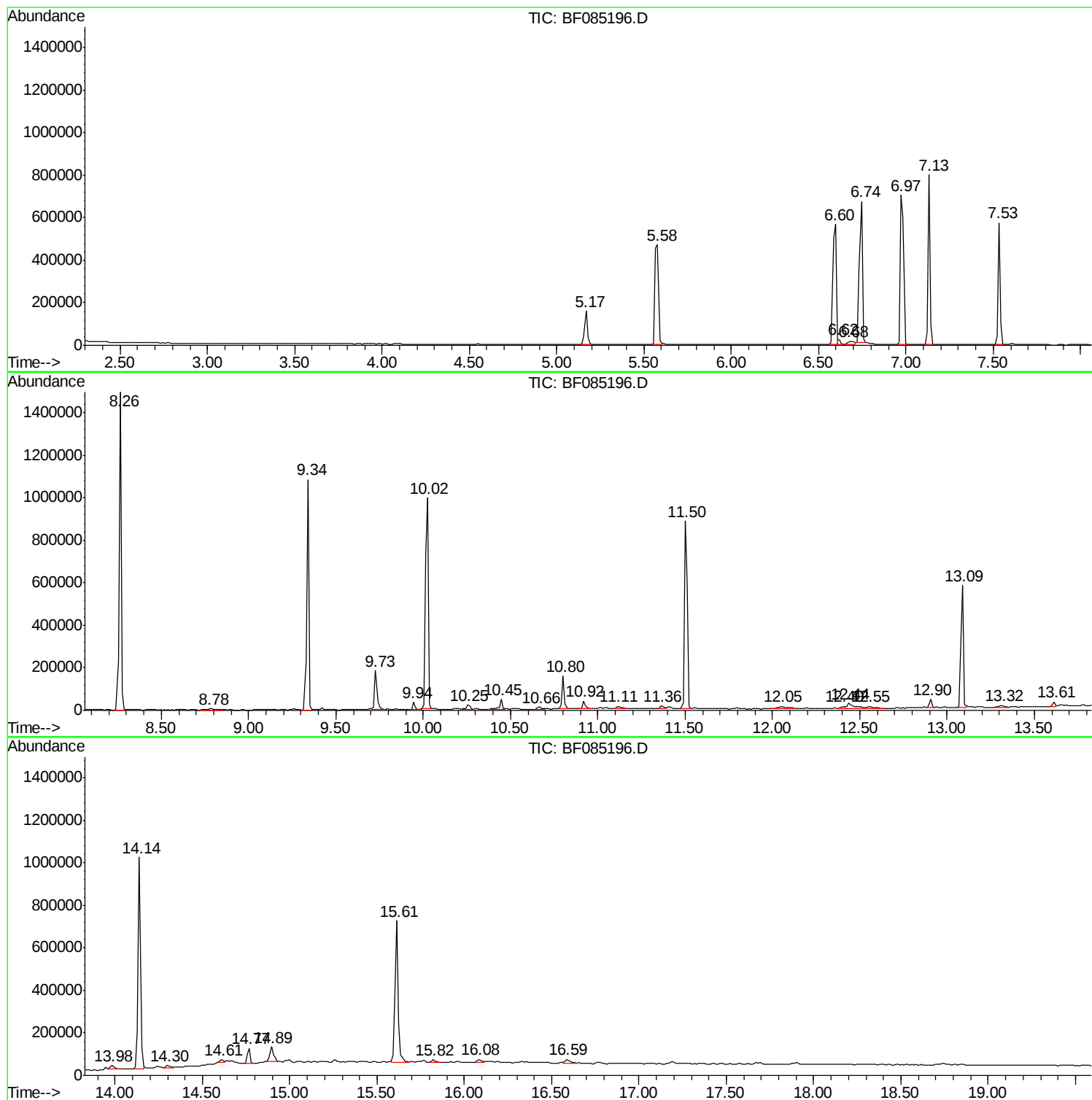
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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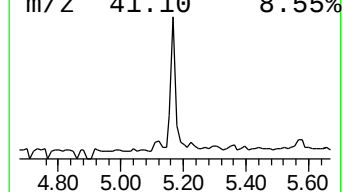
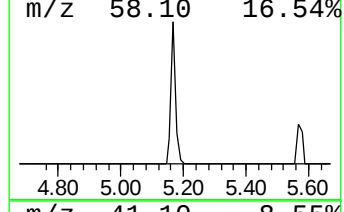
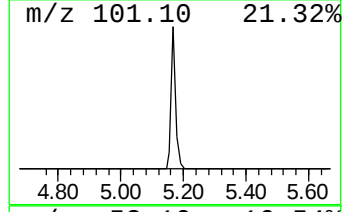
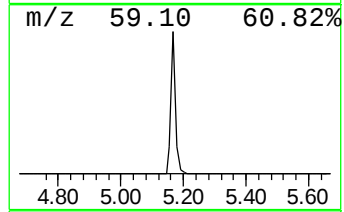
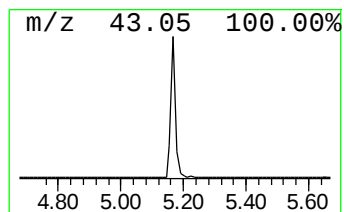
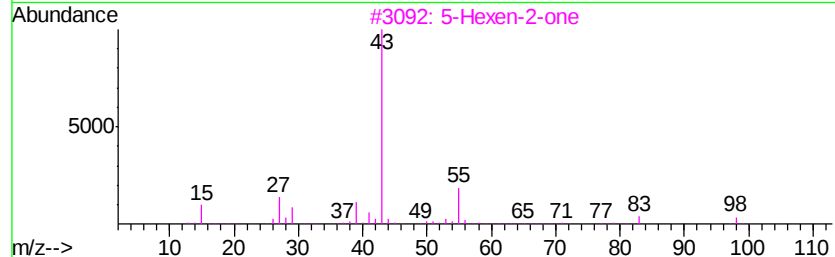
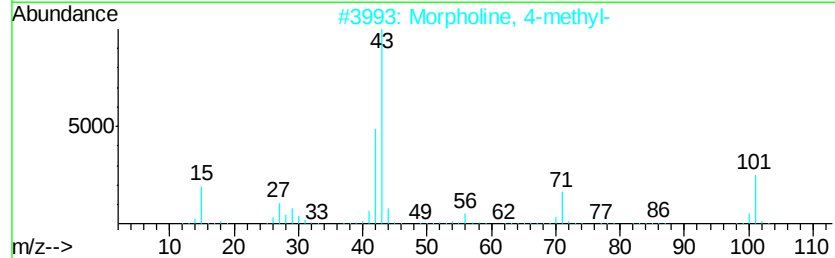
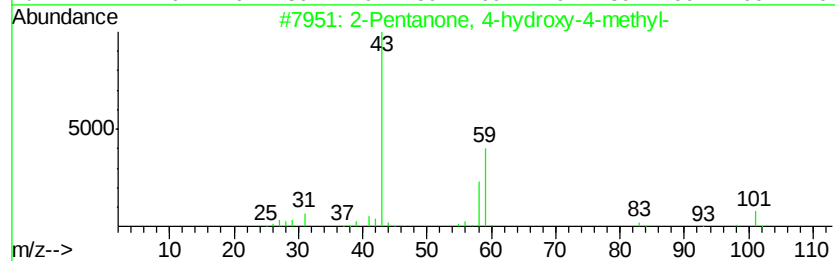
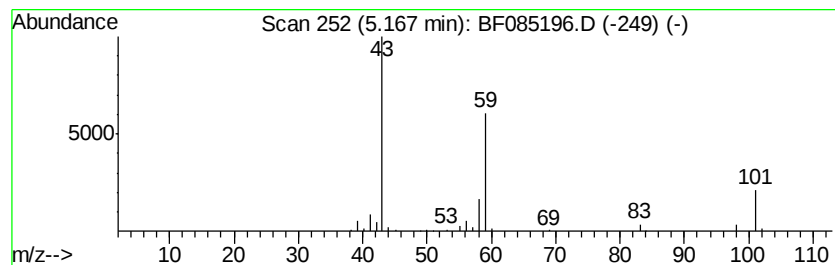
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.39 ng	153157	1,4-Dichlorobenzene-d4	6.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9



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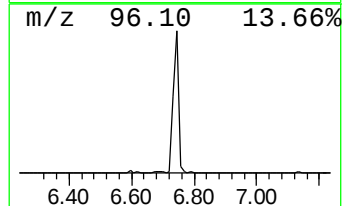
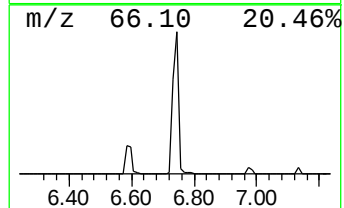
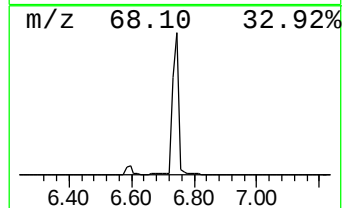
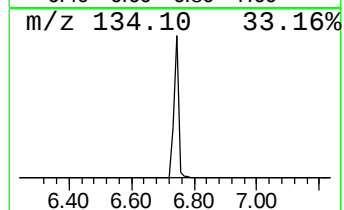
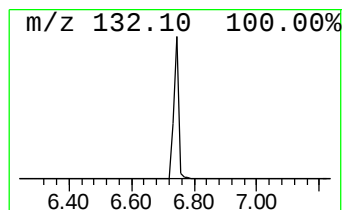
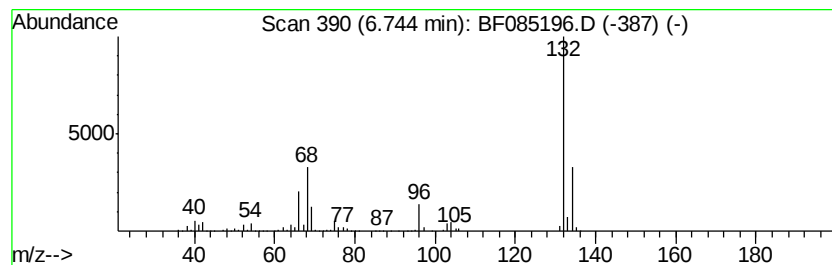
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	15.83 ng	714957	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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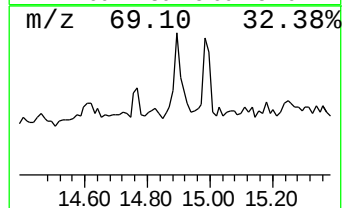
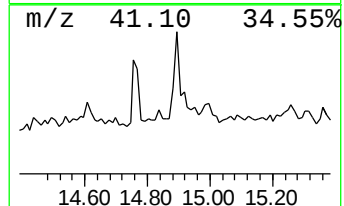
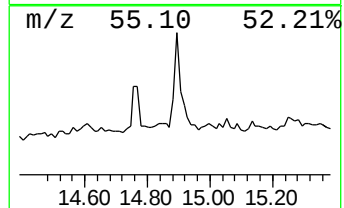
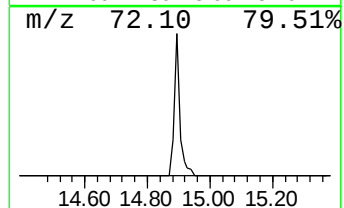
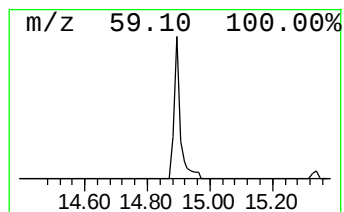
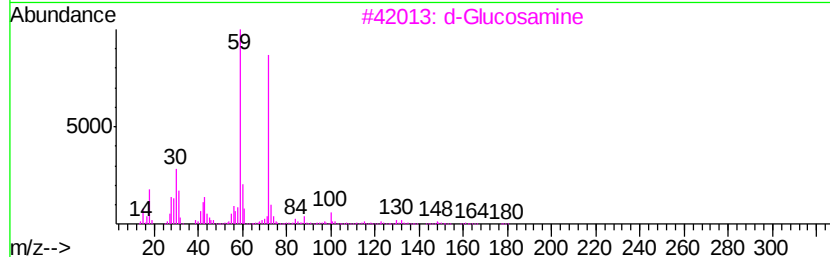
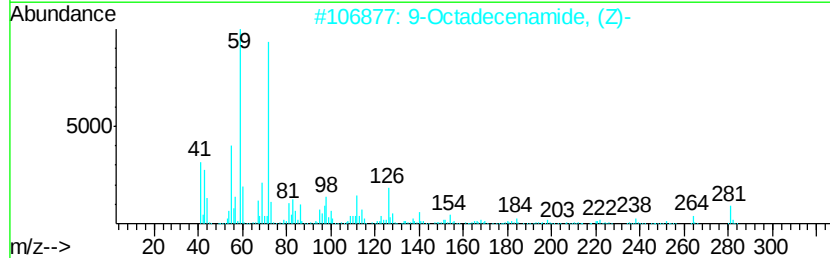
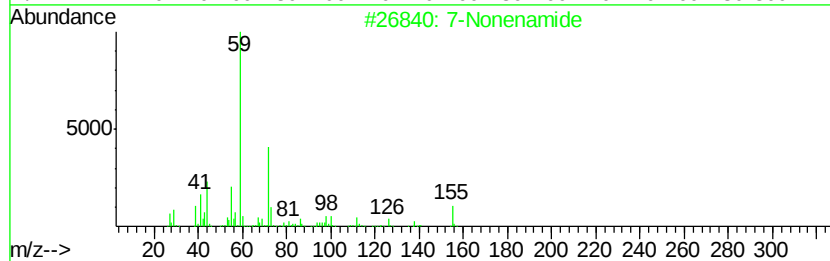
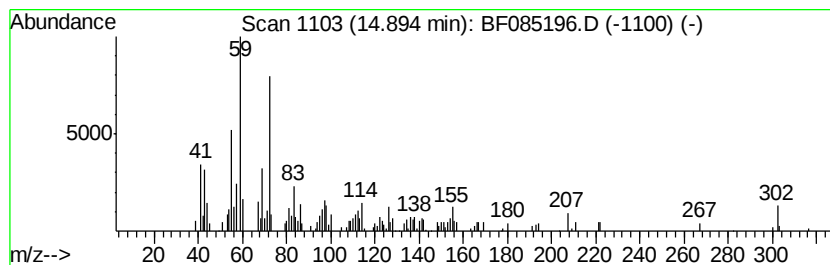
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Peak Number 4 7-Nonenamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.25 ng	97196	Perylene-d12	15.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide		155	C9H17NO	090949-53-4	74
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	59
3	d-Glucosamine		179	C6H13NO5	000090-77-7	53
4	Tetradecanamide		227	C14H29NO	000638-58-4	43
5	Pentanamide, 4-methyl-		115	C6H13NO	001119-29-5	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	3.4	ng	153157	1	6.98	903411	20.0
unknown6.74	6.74	15.8	ng	714957	1	6.98	903411	20.0
7-Nonenamide	14.89	2.3	ng	97196	6	15.61	863042	20.0