

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
 Data File : BF088084.D
 Acq On : 16 Jun 2016 19:19
 Operator : UM/SJ
 Sample : H3571-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-27-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-BF060716.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	1.678	7	8	17	rVB	291141	467816	12.90%	1.539%
2	1.804	17	19	70	rVB	1564284	3627635	100.00%	11.935%
3	4.890	287	289	300	rBV	94916	147813	4.07%	0.486%
4	5.313	323	326	328	rBV	2008628	2242993	61.83%	7.380%
5	6.364	415	418	420	rBV	1943528	2207200	60.84%	7.262%
6	6.490	426	429	431	rBV	2022629	2423259	66.80%	7.973%
7	6.719	447	449	451	rBV	740588	694547	19.15%	2.285%
8	6.879	460	463	465	rVB	1377297	1902971	52.46%	6.261%
9	7.290	496	499	501	rBV	1425965	1691713	46.63%	5.566%
10	7.999	559	561	564	rBV	917924	950903	26.21%	3.129%
11	9.085	653	656	658	rBV	2693338	2900368	79.95%	9.542%
12	9.473	688	690	692	rVB	510720	569473	15.70%	1.874%
13	9.748	712	714	717	rVV	970143	1129798	31.14%	3.717%
14	10.193	751	753	755	rVB	115502	92122	2.54%	0.303%
15	10.411	769	772	775	rBV	36484	58554	1.61%	0.193%
16	10.536	781	783	786	rBV2	1253719	1665093	45.90%	5.478%
17	10.662	792	794	799	rVB	131283	146015	4.03%	0.480%
18	11.108	832	833	835	rBV	70062	63688	1.76%	0.210%
19	11.234	842	844	846	rBV	1266763	1182796	32.61%	3.891%
20	11.302	847	850	853	rVB	22769	40193	1.11%	0.132%
21	11.782	889	892	896	rBV	62458	129149	3.56%	0.425%
22	12.434	947	949	951	rBV	88002	90685	2.50%	0.298%
23	12.651	966	968	973	rBV2	138492	253484	6.99%	0.834%
24	12.822	980	983	985	rVB	2058893	2594546	71.52%	8.536%
25	13.348	1027	1029	1031	rBV	95398	84548	2.33%	0.278%
26	13.714	1059	1061	1071	rBV2	329019	432465	11.92%	1.423%
27	13.862	1071	1074	1076	rBV	895697	988232	27.24%	3.251%
28	14.034	1086	1089	1095	rBV5	15623	37094	1.02%	0.122%
29	14.342	1112	1116	1122	rBV5	42351	133673	3.68%	0.440%
30	14.617	1138	1140	1146	rBV2	62470	101237	2.79%	0.333%
31	14.697	1146	1147	1151	rVB2	24541	37941	1.05%	0.125%
32	14.765	1151	1153	1156	rVB2	49444	48466	1.34%	0.159%
33	14.868	1159	1162	1166	rBV	64810	125508	3.46%	0.413%
34	14.960	1166	1170	1174	rBV2	53481	134860	3.72%	0.444%

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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-BF060716.M
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35	15.131	1184	1185	1189	rVB	29801	42880	1.18%	0.141%
36	15.188	1189	1190	1193	rVB	45271	64453	1.78%	0.212%
37	15.245	1193	1195	1198	rBV	601226	729869	20.12%	2.401%
38	15.668	1229	1232	1234	rBV	34985	51237	1.41%	0.169%
39	16.571	1308	1311	1314	rBV	30738	61611	1.70%	0.203%
40	16.971	1343	1346	1349	rBV	22258	47945	1.32%	0.158%

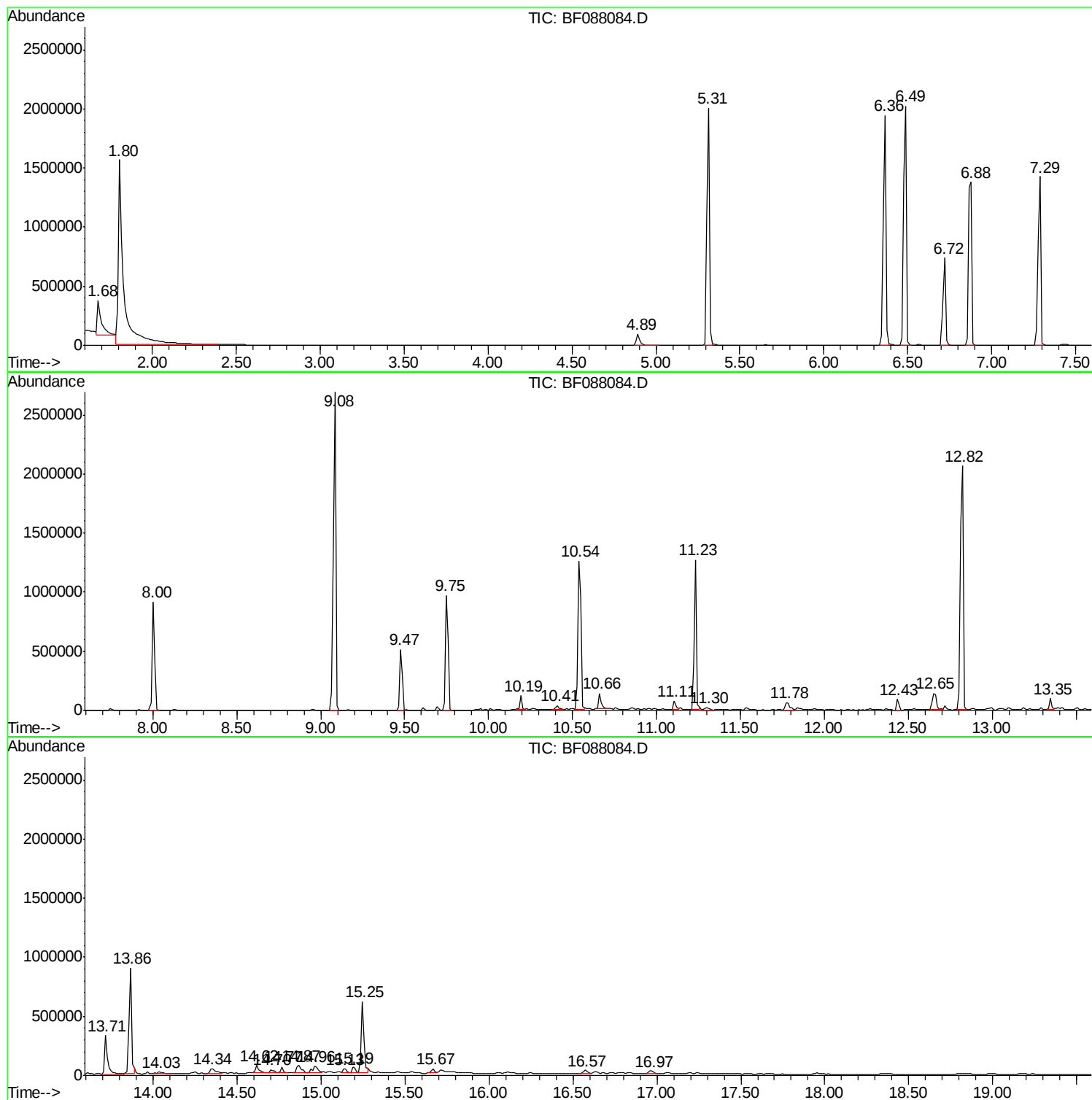
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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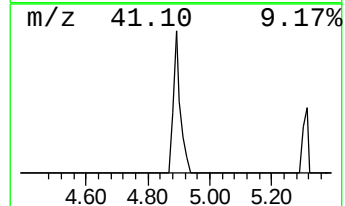
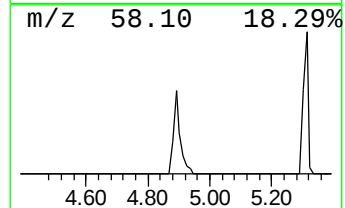
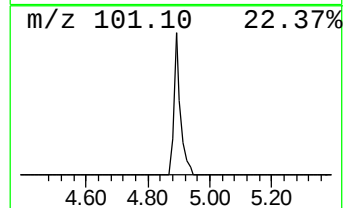
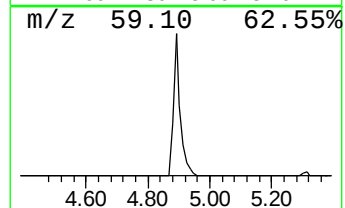
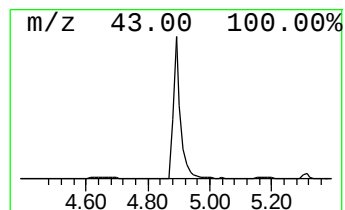
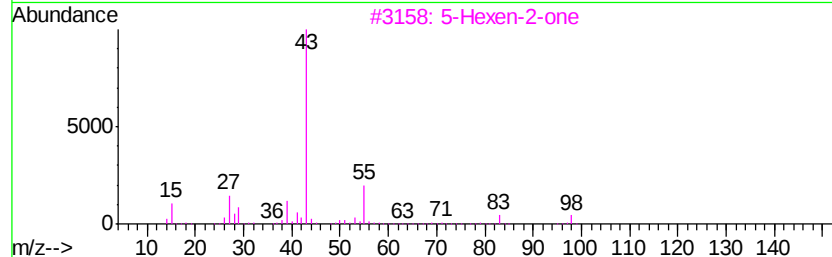
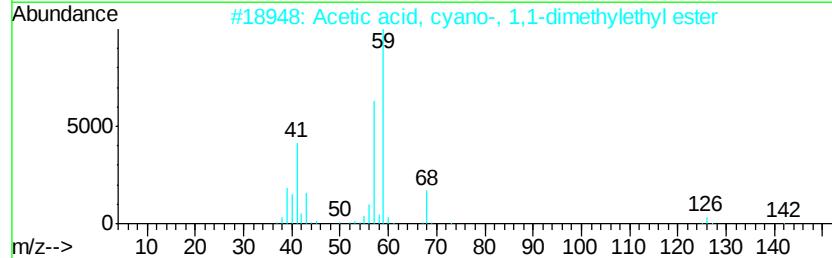
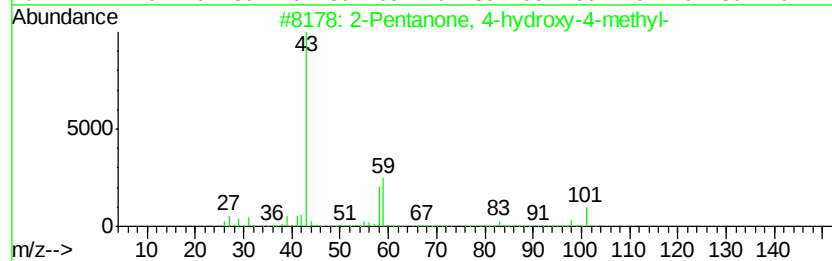
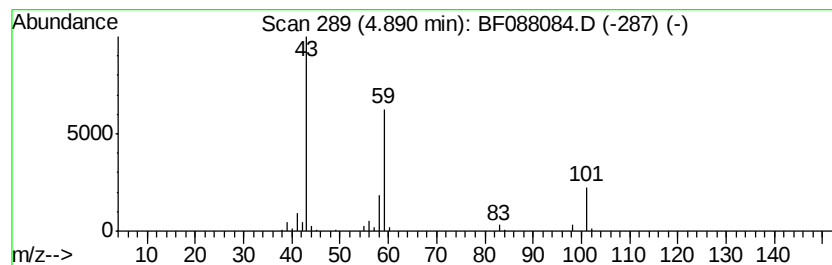
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	4.26 ng	147813	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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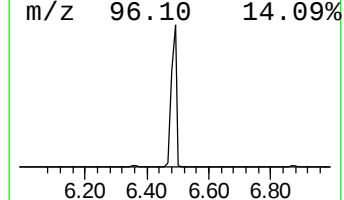
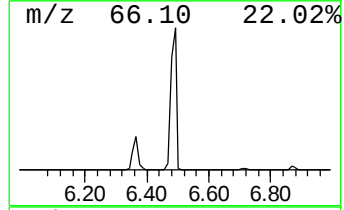
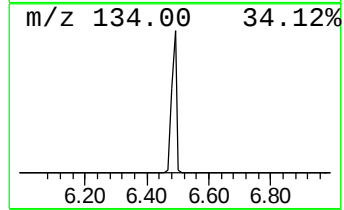
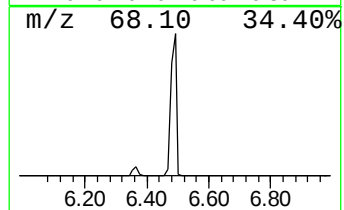
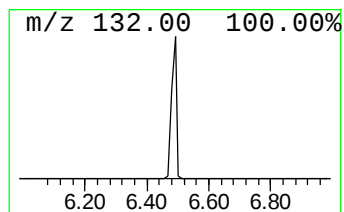
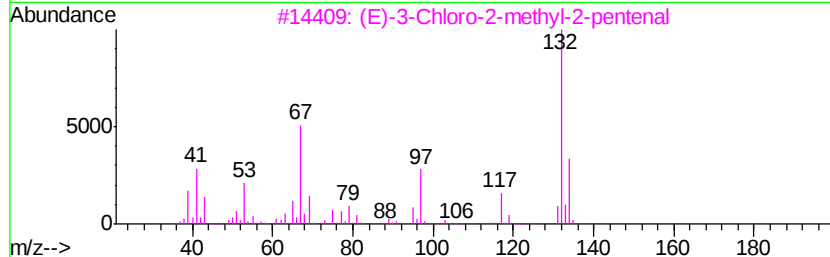
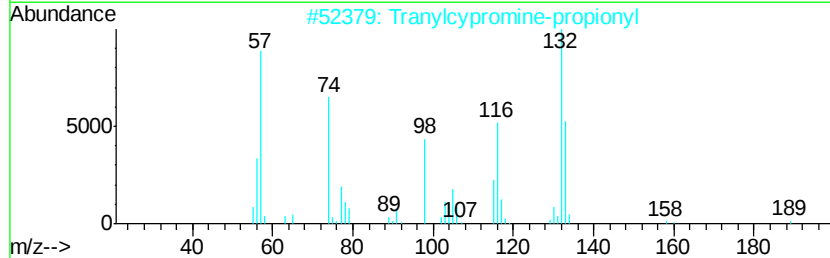
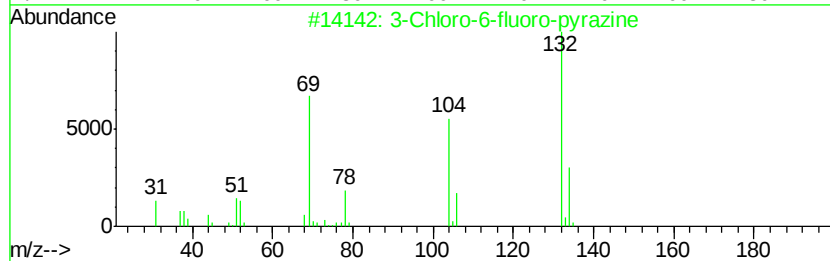
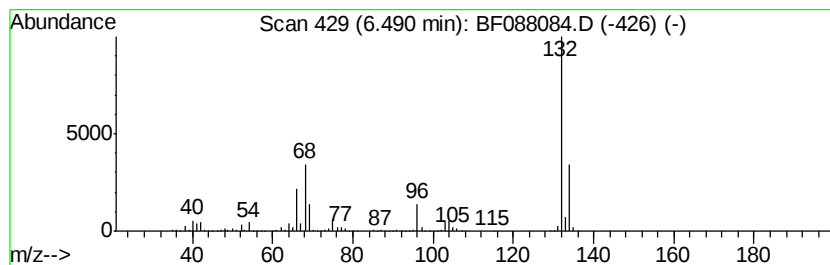
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	69.78 ng	2423260	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Xenon	132	Xe	007440-63-3	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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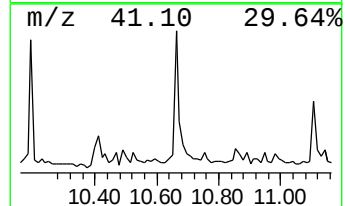
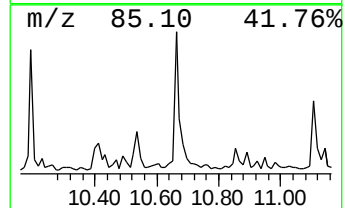
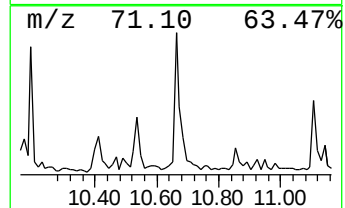
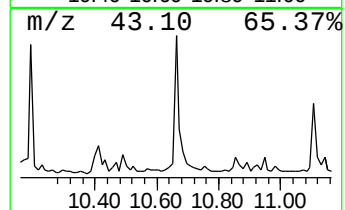
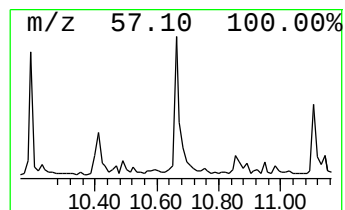
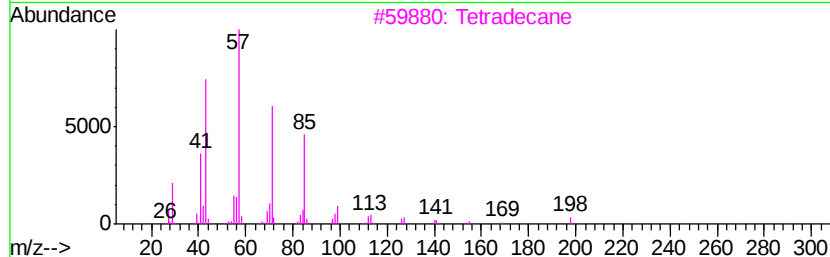
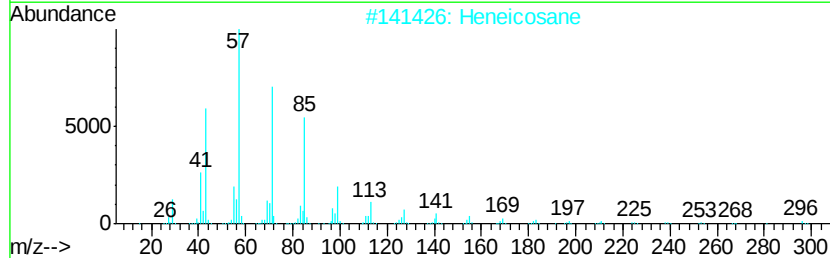
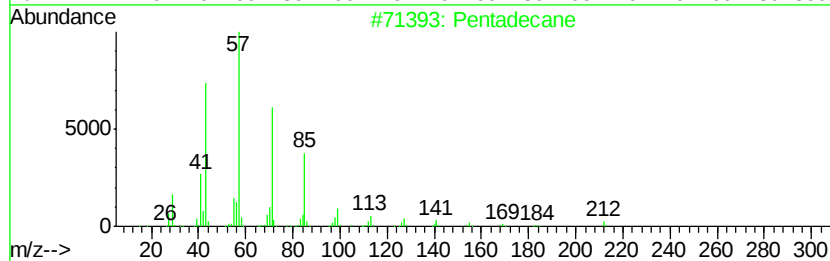
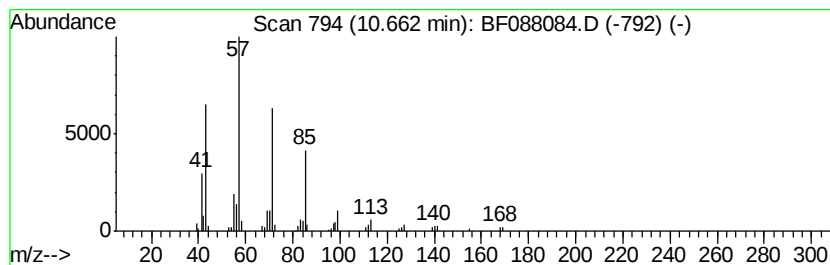
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.47 ng	146015	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Heneicosane		296	C21H44	000629-94-7	90
3	Tetradecane		198	C14H30	000629-59-4	87
4	Nonadecane		268	C19H40	000629-92-5	86
5	Hexadecane		226	C16H34	000544-76-3	83



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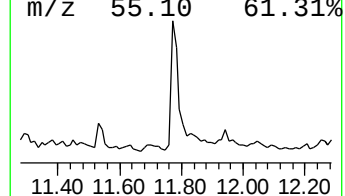
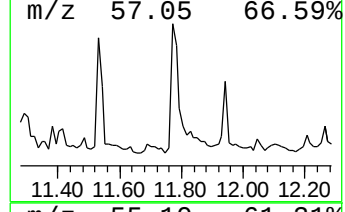
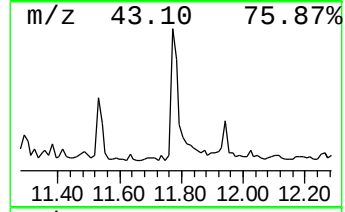
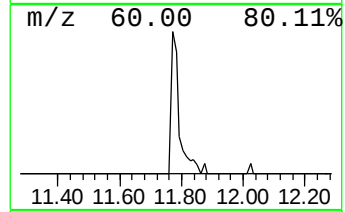
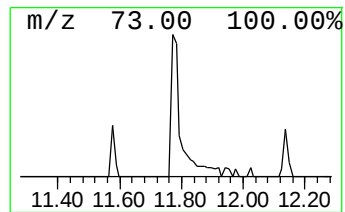
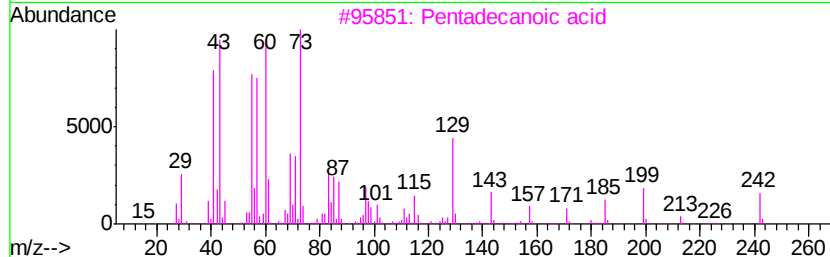
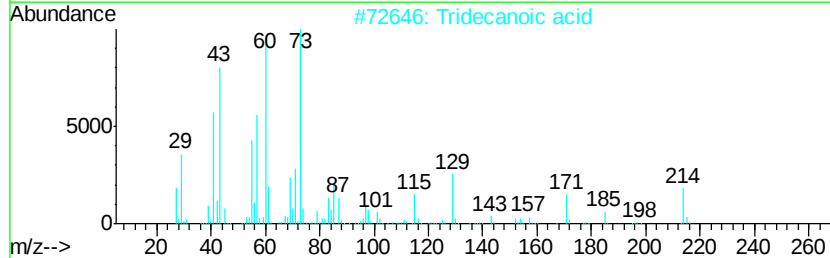
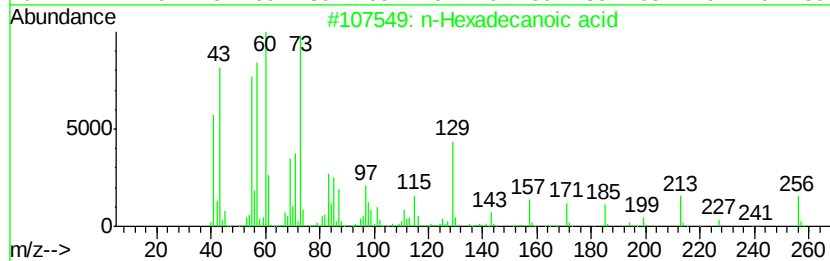
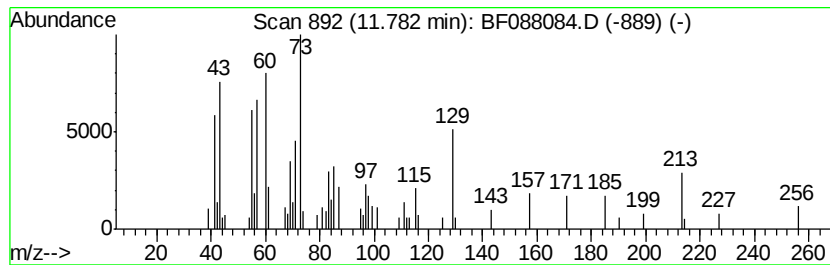
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	2.18 ng	129149	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	15



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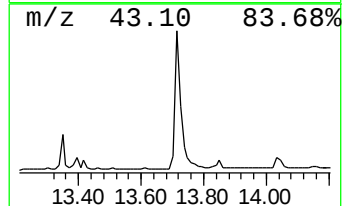
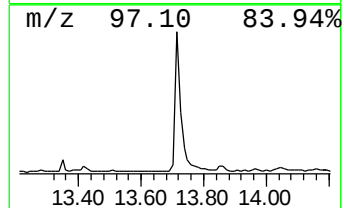
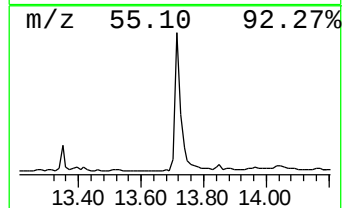
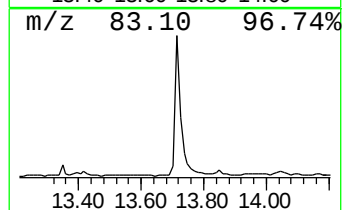
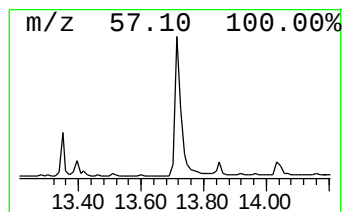
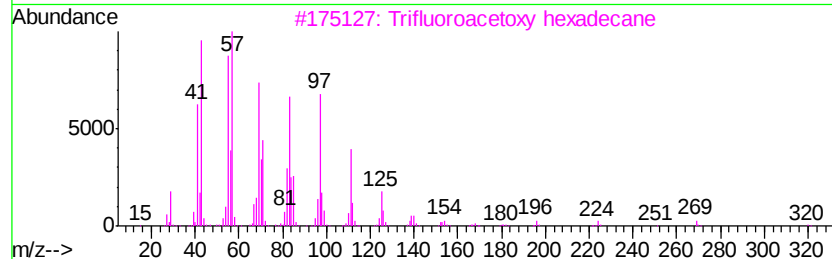
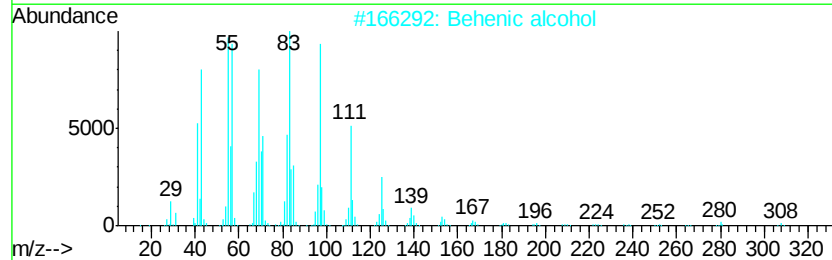
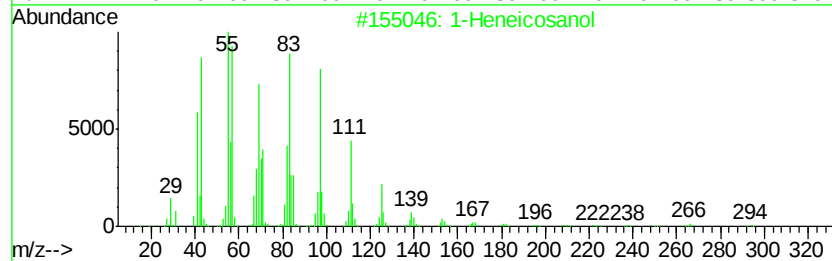
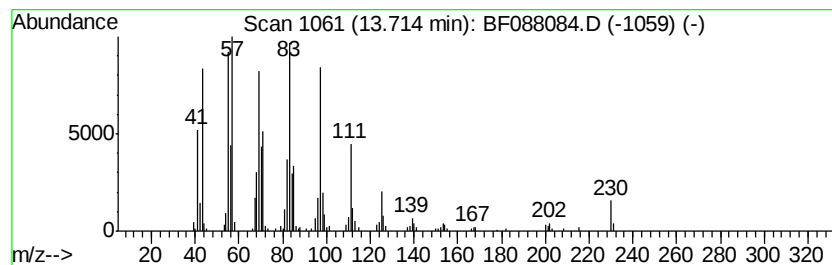
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Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	8.75 ng	432465	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
Data File : BF088084.D
Acq On : 16 Jun 2016 19:19
Operator : UM/SJ
Sample : H3571-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-27-COMP

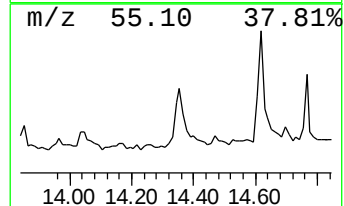
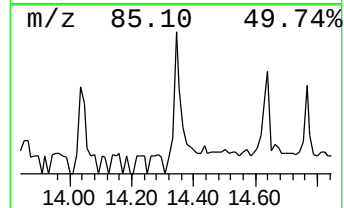
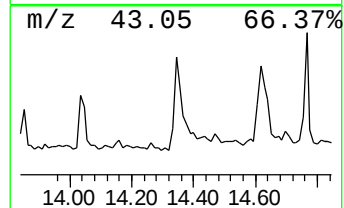
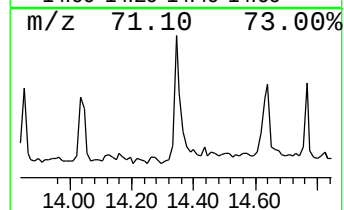
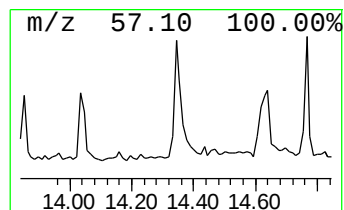
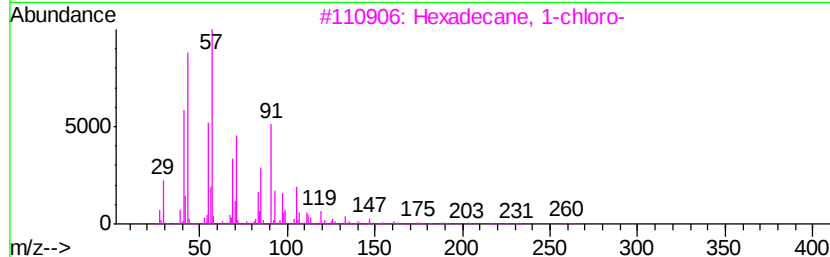
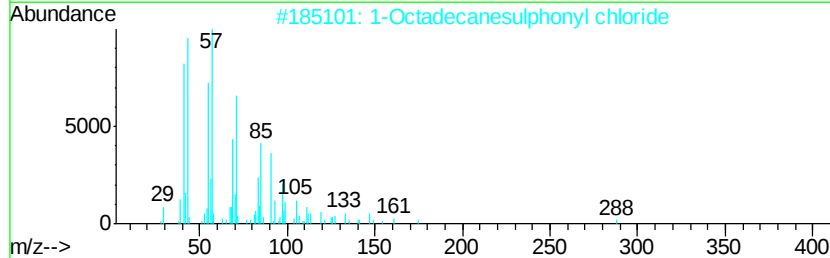
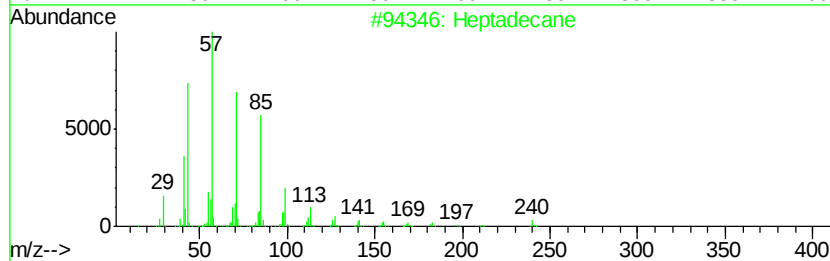
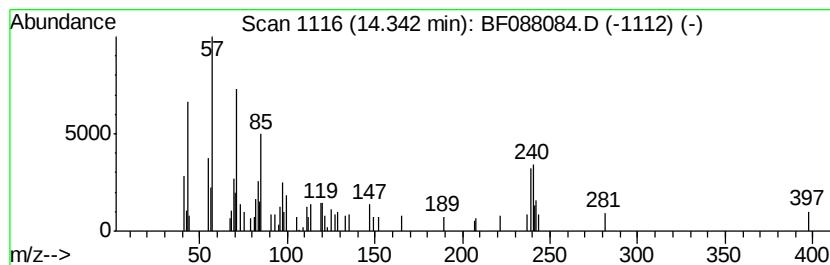
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.34 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.71 ng	133673	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	49
2		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	46
3		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	46
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	46
5		Tetratetracontane	619	C44H90	007098-22-8	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088084.D
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Sample : H3571-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-27-COMP

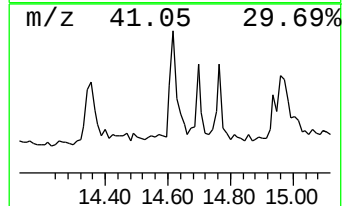
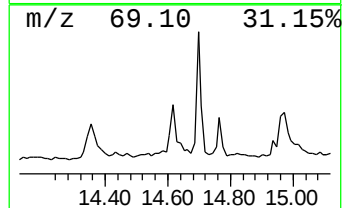
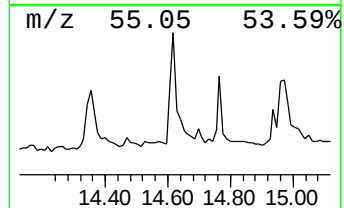
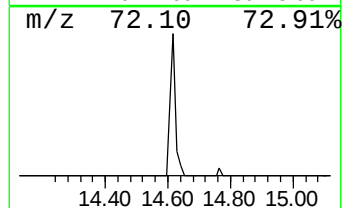
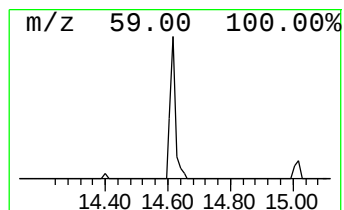
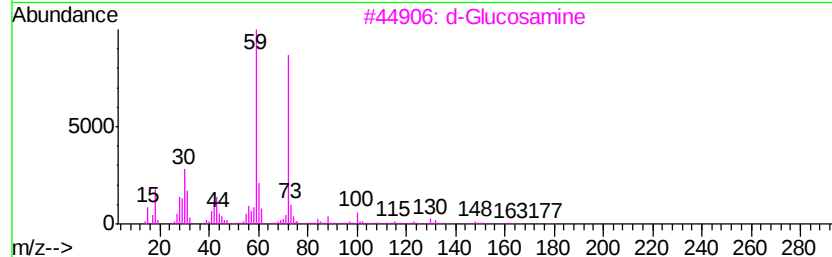
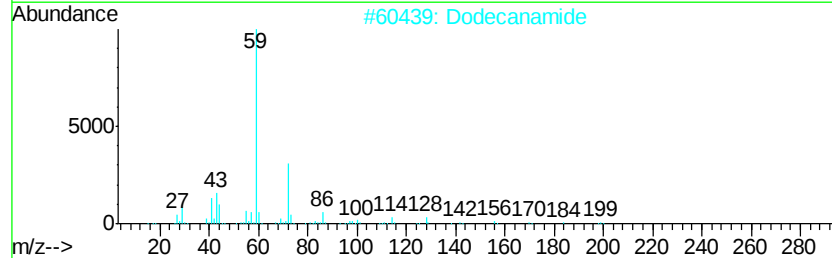
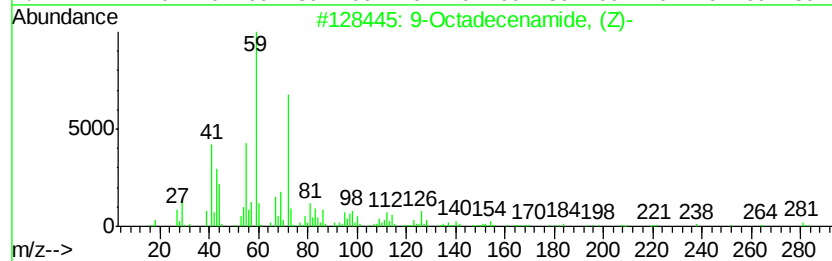
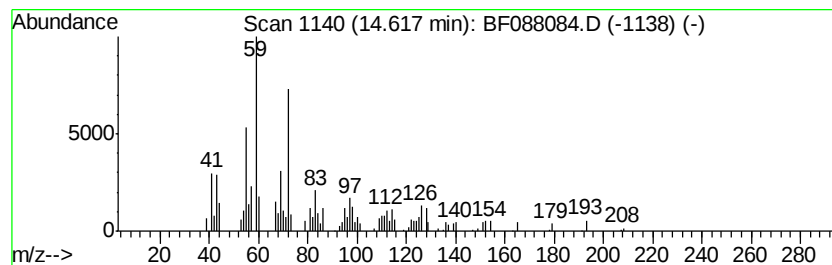
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.77 ng	101237	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Dodecanamide	199	C12H25NO	001120-16-7	59
3		d-Glucosamine	179	C6H13NO5	000090-77-7	47
4		N'-(4-Nitrobenzylidene)-2-pentyl...	303	C16H21N3O3	339027-09-7	43
5		6,8-Dichlorooctanamide	211	C8H15Cl2NO	003579-00-8	43



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-27-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	4.3	ng	147813	1	6.72	694547	20.0
unknown6.49	6.49	69.8	ng	2423260	1	6.72	694547	20.0
Pentadecane	10.66	2.5	ng	146015	4	11.23	1182800	20.0
n-Hexadecanoic acid	11.78	2.2	ng	129149	4	11.23	1182800	20.0
1-Heneicosanol	13.71	8.8	ng	432465	5	13.86	988232	20.0
unknown14.34	14.34	2.7	ng	133673	5	13.86	988232	20.0
9-Octadecenamide, ...	14.62	2.8	ng	101237	6	15.25	729869	20.0