

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063015\
 Data File : BF080262.D
 Acq On : 1 Jul 2015 7:24
 Operator : TP/IZ
 Sample : G2838-11
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-B11

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-BF061715.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	5.498	208	211	216	rVB	254036	250662	15.21%	1.893%
2	5.898	243	246	248	rBV	1261619	1184557	71.87%	8.946%
3	6.299	278	281	283	rVB	19421	19822	1.20%	0.150%
4	6.893	330	333	335	rBV	1499508	1230204	74.64%	9.290%
5	7.053	345	347	349	rBV	1545398	1264643	76.73%	9.550%
6	7.281	366	367	370	rVB	186977	202226	12.27%	1.527%
7	7.441	379	381	384	rVB	980977	924209	56.07%	6.980%
8	7.842	414	416	418	rBV	960898	761806	46.22%	5.753%
9	8.573	478	480	483	rBV	312632	285259	17.31%	2.154%
10	9.647	572	574	577	rBV	1147311	1390893	84.38%	10.504%
11	10.036	607	608	611	rBV	105901	120237	7.29%	0.908%
12	10.207	621	623	626	rBV	41383	34110	2.07%	0.258%
13	10.345	633	635	637	rBV	350448	332625	20.18%	2.512%
14	10.756	668	671	673	rBV	13176	16872	1.02%	0.127%
15	11.145	703	705	707	rBV	973854	941777	57.14%	7.112%
16	11.236	711	713	719	rVB	24697	31731	1.93%	0.240%
17	11.865	765	768	769	rBV	435060	373926	22.69%	2.824%
18	11.888	769	770	772	rVV	57981	47539	2.88%	0.359%
19	11.945	772	775	777	rVV	29017	29688	1.80%	0.224%
20	12.036	779	783	785	rBV2	11881	19100	1.16%	0.144%
21	12.436	816	818	820	rBV2	12186	18614	1.13%	0.141%
22	12.528	823	826	829	rVB	16226	29431	1.79%	0.222%
23	13.191	882	884	887	rBV	130839	119207	7.23%	0.900%
24	13.465	904	908	910	rBV	98754	134540	8.16%	1.016%
25	13.625	919	922	924	rBV	1610979	1648274	100.00%	12.448%
26	13.854	935	942	944	rBV	23190	46491	2.82%	0.351%
27	14.768	1019	1022	1029	rVB2	59244	122569	7.44%	0.926%
28	14.974	1037	1040	1042	rBV2	411548	528171	32.04%	3.989%
29	15.511	1085	1087	1089	rVB	15359	19414	1.18%	0.147%
30	15.648	1097	1099	1101	rBV3	18149	25143	1.53%	0.190%
31	16.059	1132	1135	1137	rBV2	34613	45500	2.76%	0.344%
32	16.197	1145	1147	1150	rBV	52677	81545	4.95%	0.616%
33	16.414	1163	1166	1172	rBV	60242	176329	10.70%	1.332%
34	16.551	1176	1178	1181	rVB	22980	32289	1.96%	0.244%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	16.791	1197	1199	1203	rBV	44117	65499	3.97%	0.495%
36	16.871	1203	1206	1208	rBV	55942	80910	4.91%	0.611%
37	16.951	1210	1213	1216	rBV	296762	421499	25.57%	3.183%
38	17.865	1291	1293	1302	rVB9	14202	46892	2.84%	0.354%
39	18.803	1371	1375	1381	rVB2	27772	72114	4.38%	0.545%
40	19.351	1419	1423	1427	rBV	24494	65352	3.96%	0.494%

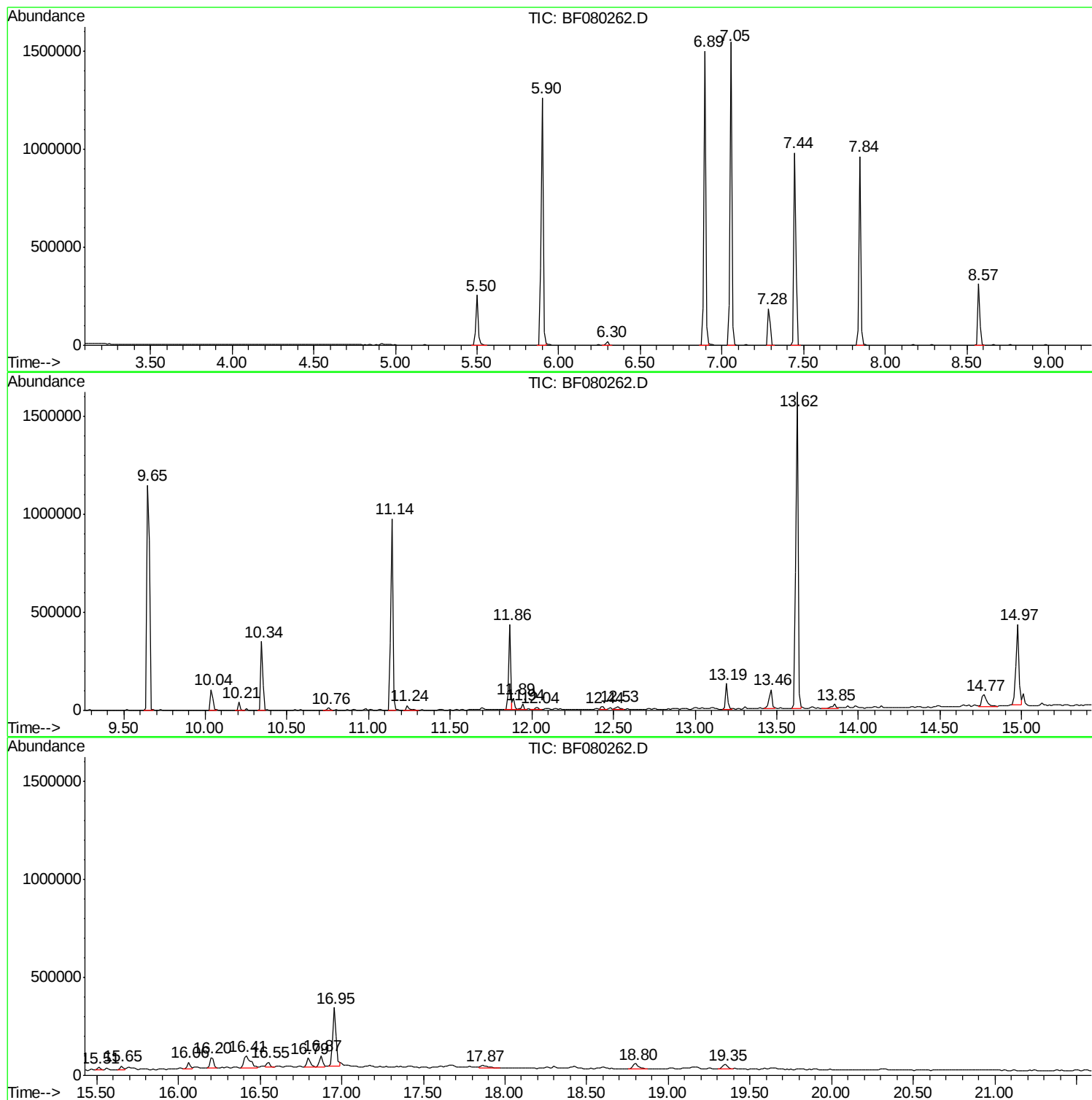
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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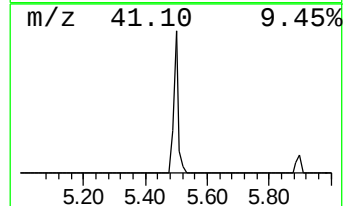
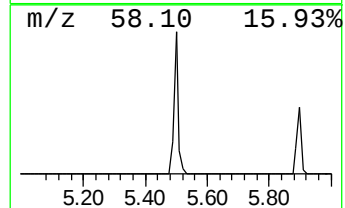
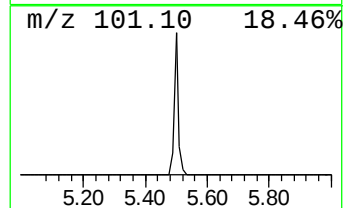
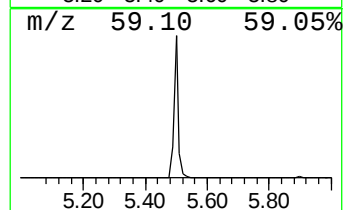
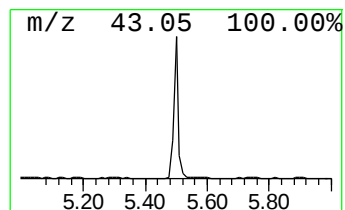
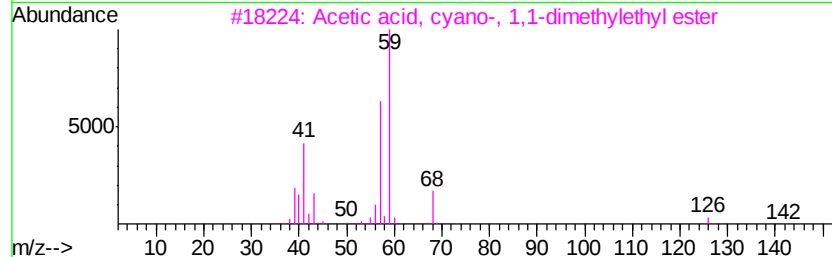
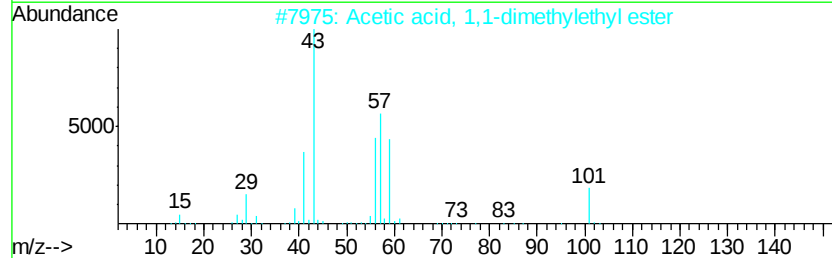
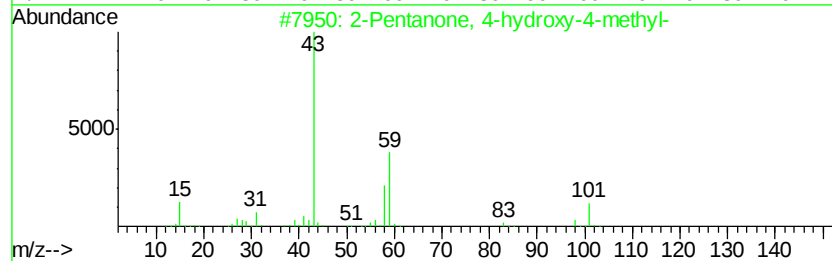
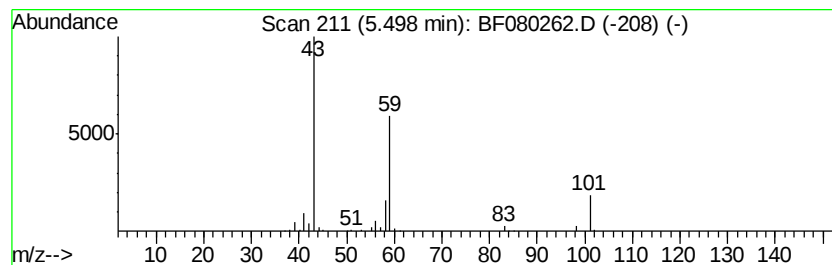
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.50	24.79 ng	250662	1,4-Dichlorobenzene-d4	7.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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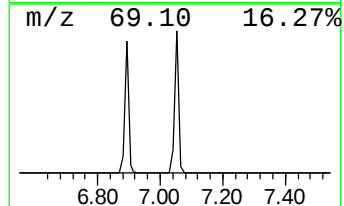
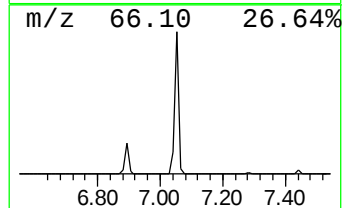
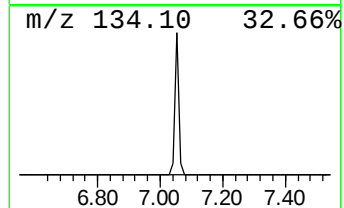
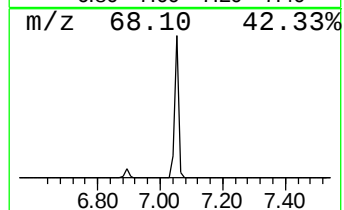
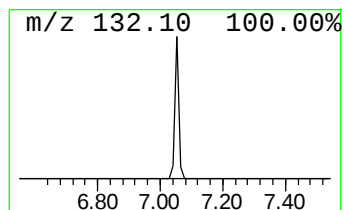
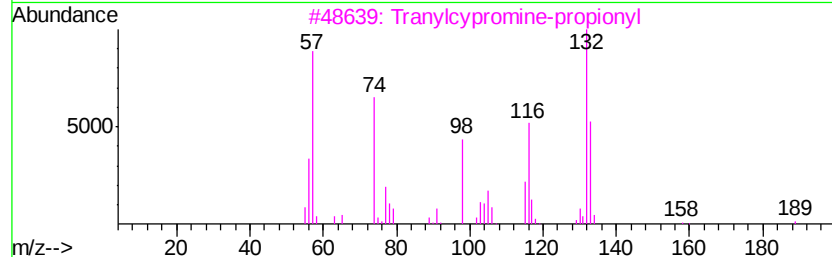
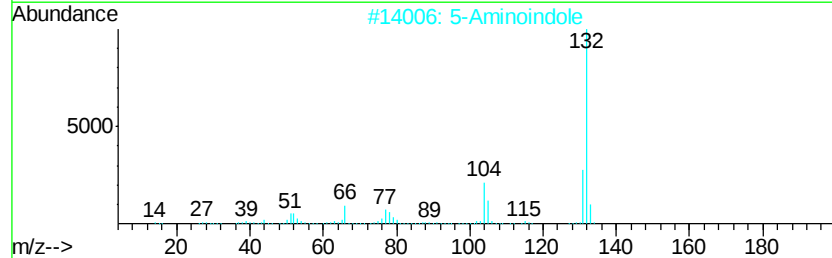
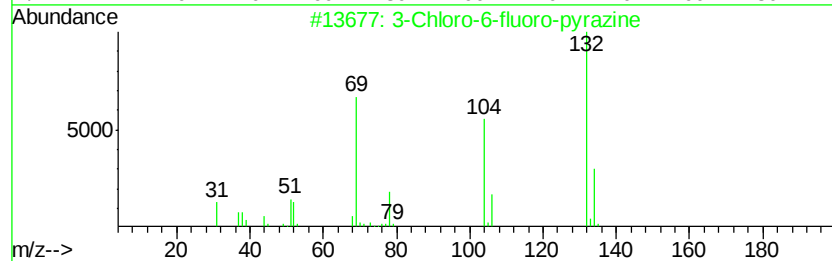
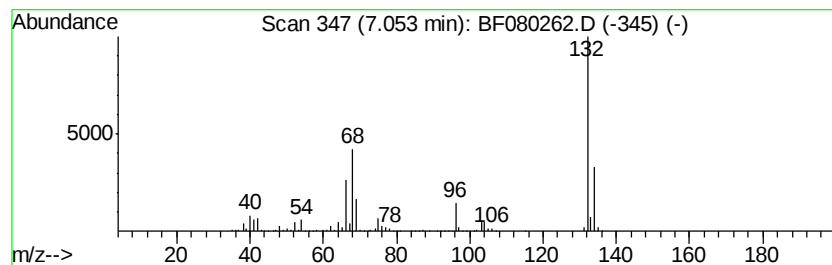
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Peak Number 2 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	125.07 ng	1264640	1,4-Dichlorobenzene-d4	7.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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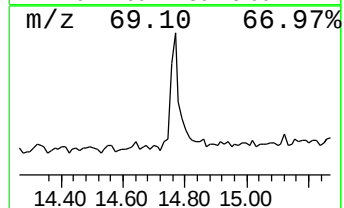
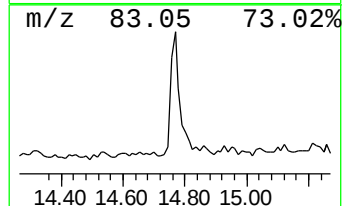
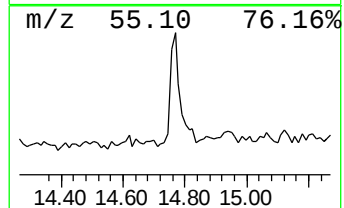
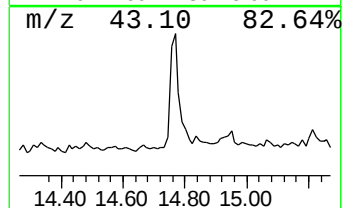
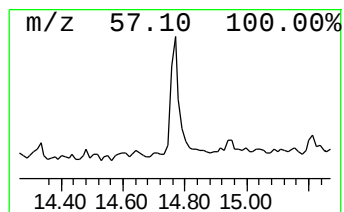
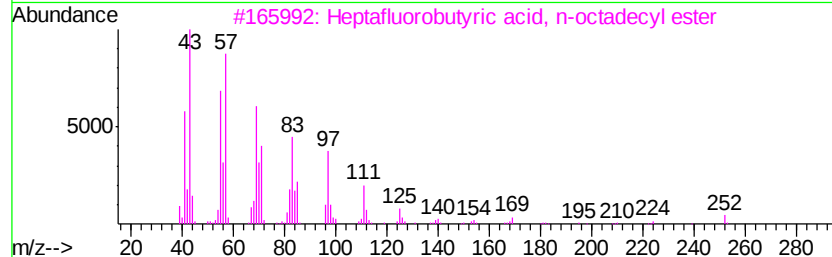
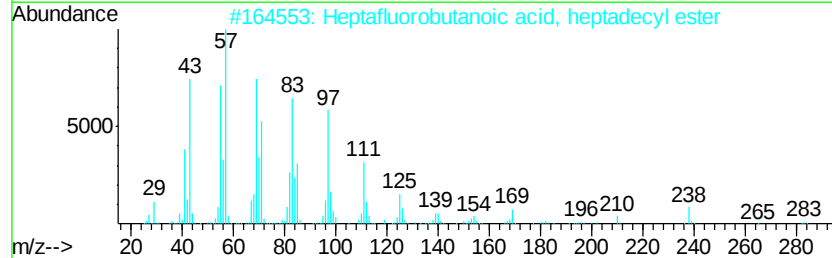
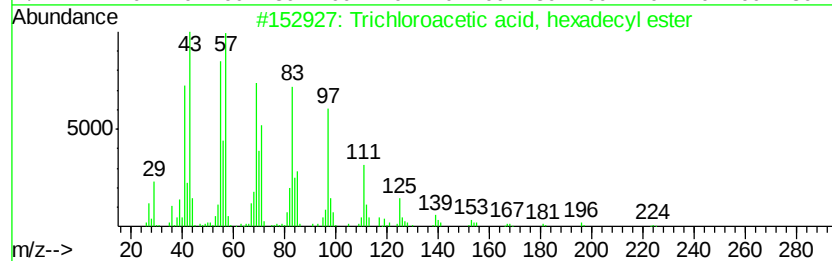
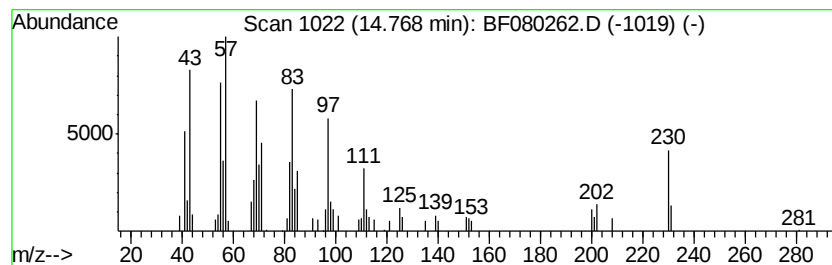
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	4.64 ng	122569	Chrysene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	92
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	70
4			11-Tricosene	322	C23H46	052078-56-5	70
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	70



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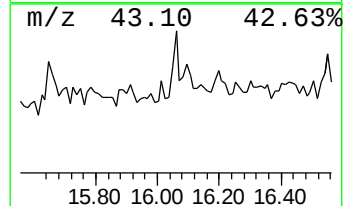
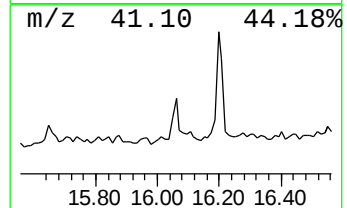
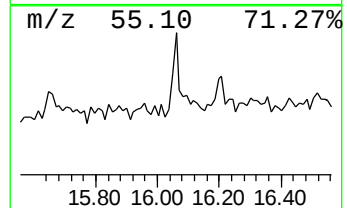
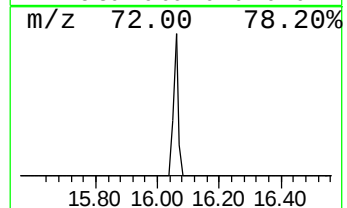
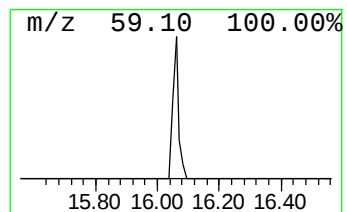
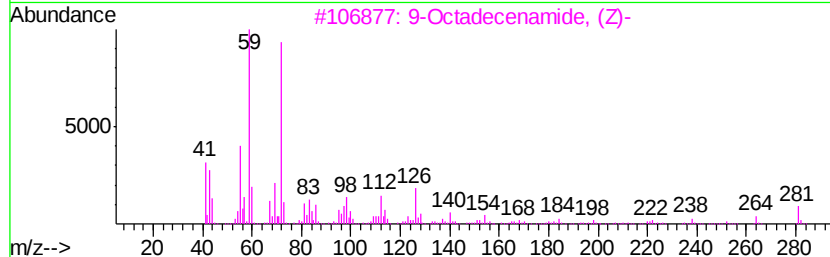
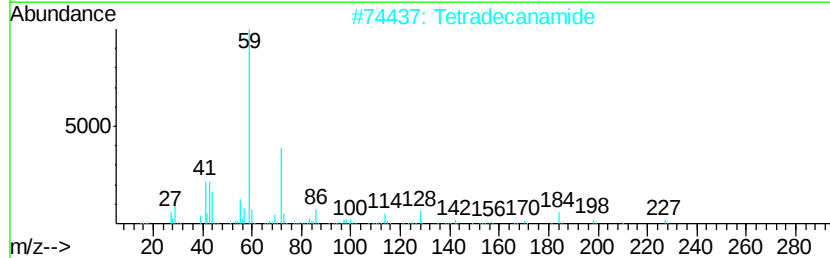
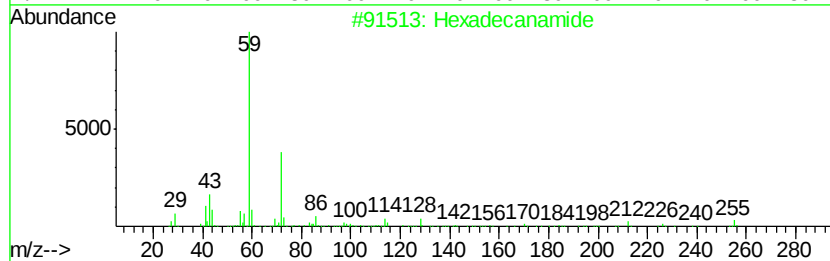
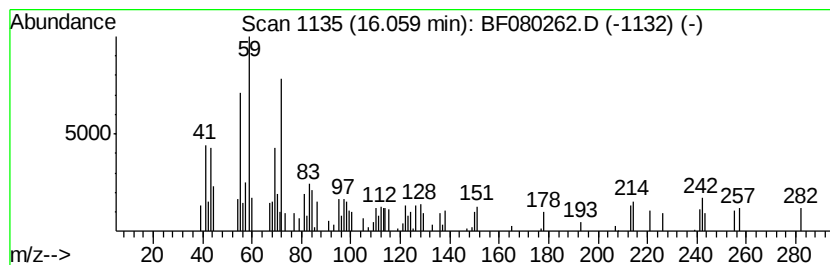
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Peak Number 5 Hexadecanamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.06	2.16 ng	45500	Perylene-d12	16.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	53
2	Tetradecanamide	227	C14H29NO	000638-58-4	50
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	50
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	38
5	Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	35



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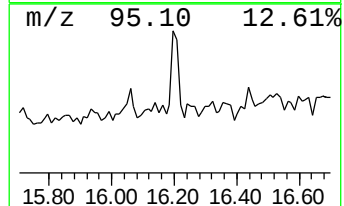
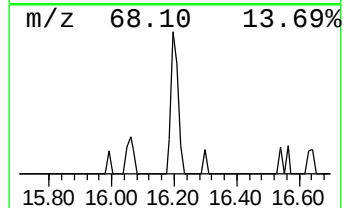
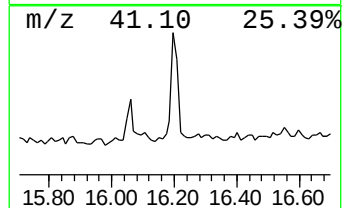
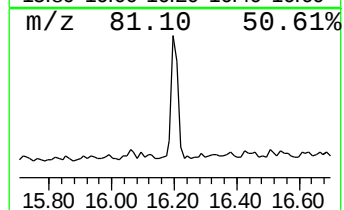
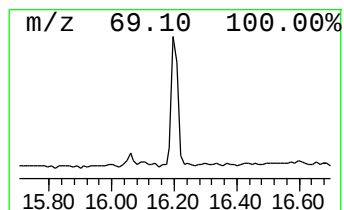
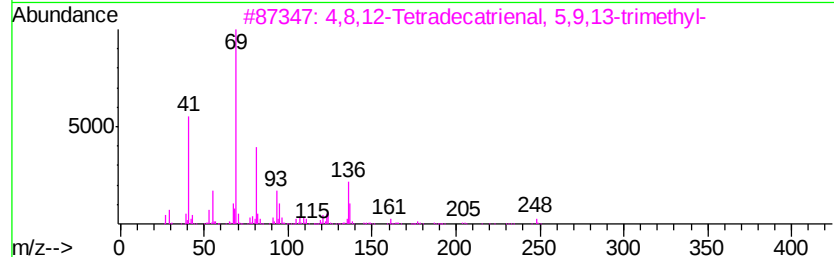
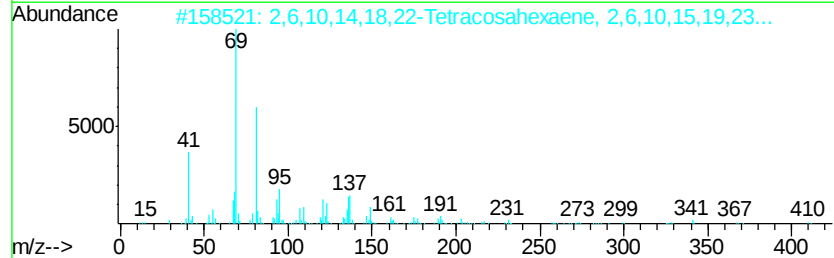
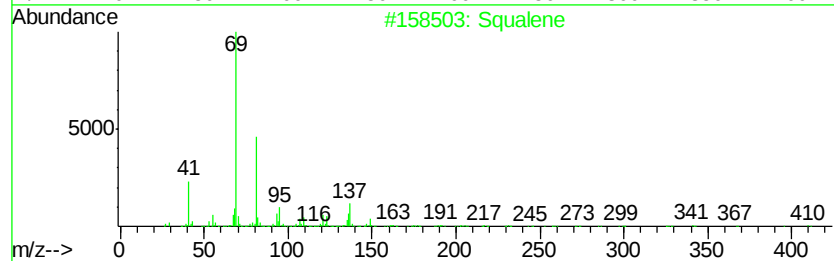
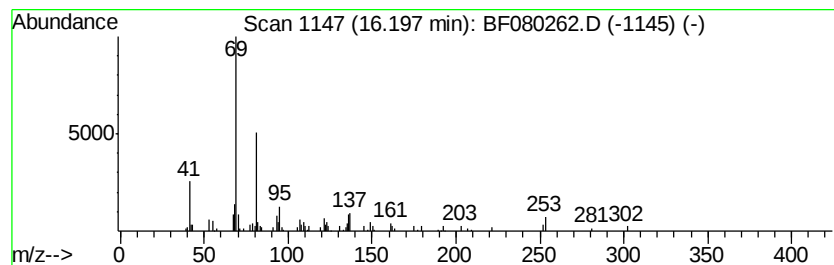
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	3.87 ng	81545	Perylene-d12	16.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	74
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063015\
Data File : BF080262.D
Acq On : 1 Jul 2015 7:24
Operator : TP/IZ
Sample : G2838-11
Misc :
ALS Vial : 30 Sample Multiplier: 1

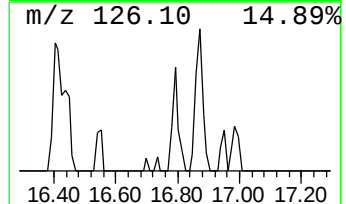
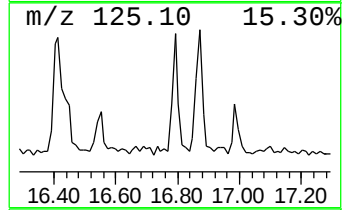
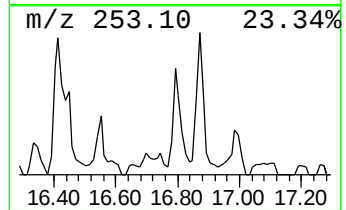
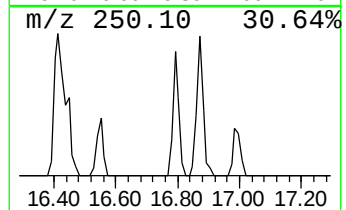
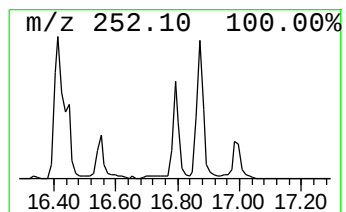
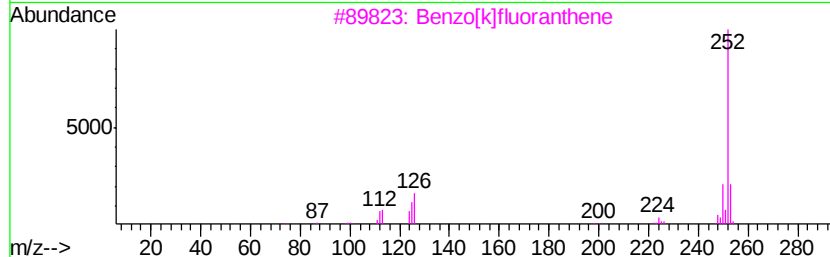
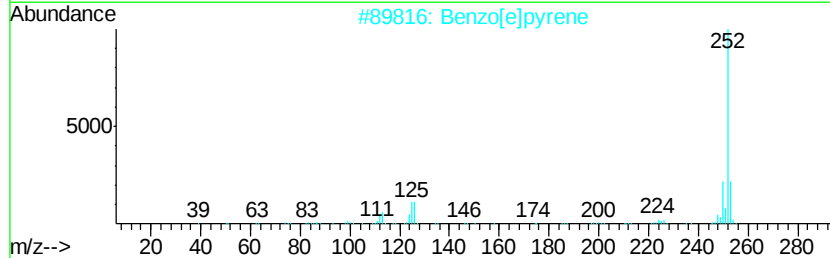
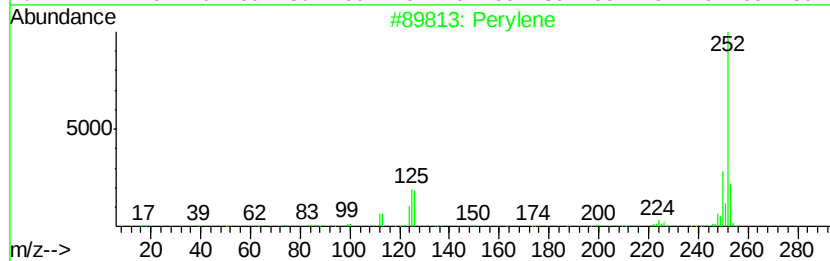
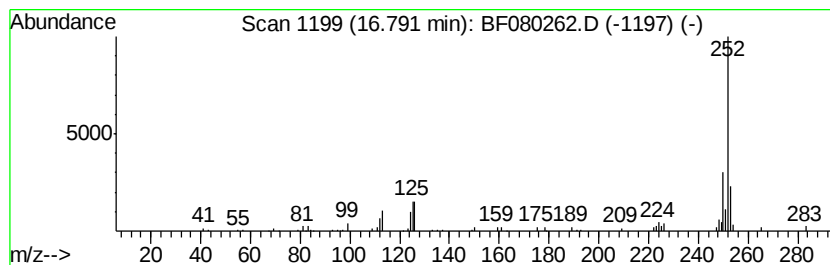
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BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.79	3.11 ng	65499	Perylene-d12	16.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	97
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063015\
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Acq On : 1 Jul 2015 7:24
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Sample : G2838-11
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-B11

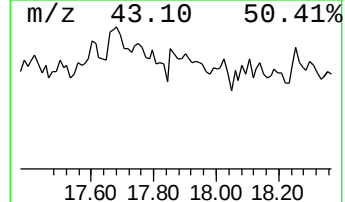
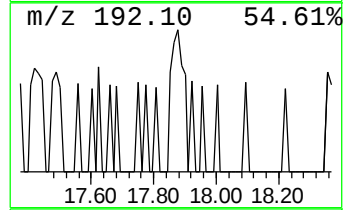
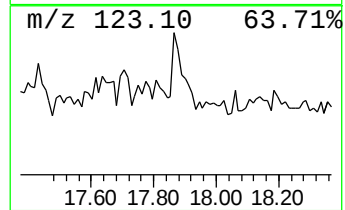
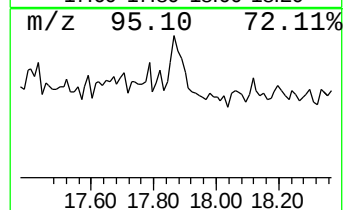
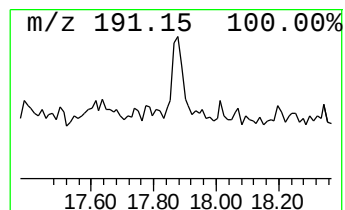
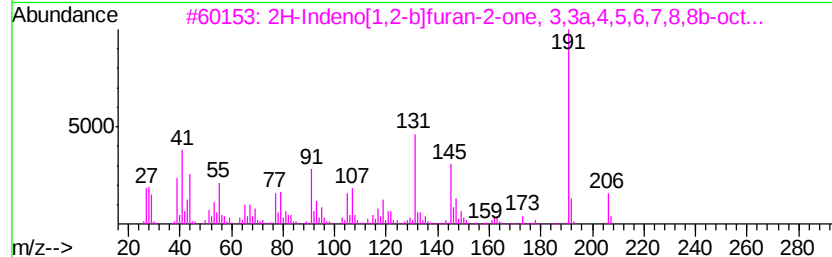
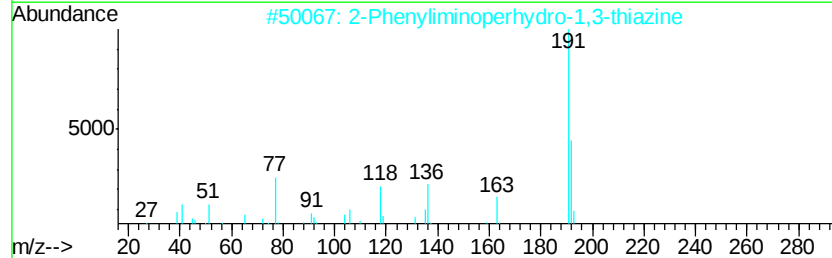
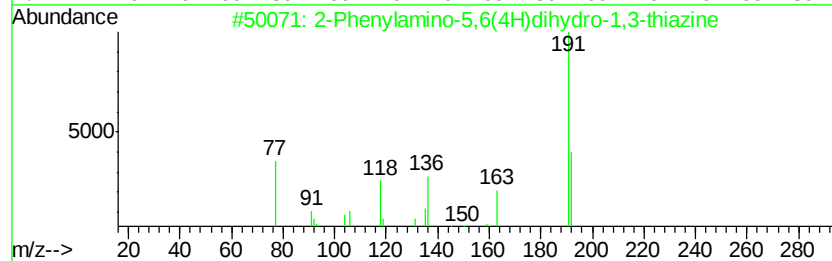
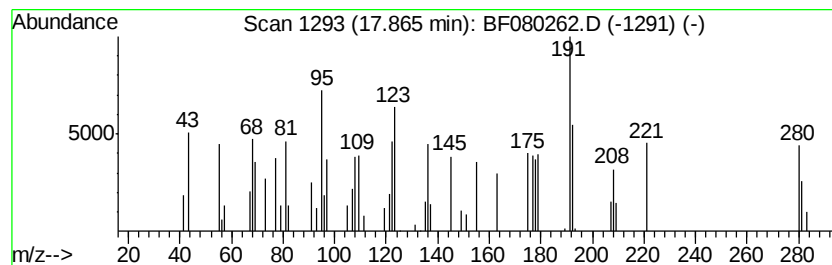
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.87 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.23 ng	46892	Perylene-d12	16.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	18
2		2-Phenyliminoperhydro-1,3-thiazine	192	C10H12N2S	1000138-91-3	14
3		2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	10
4		5-Amino-2-thiocyanoacetophenone	192	C9H8N2OS	014428-51-4	10
5		1H-Pyrrolo[3,4-c]pyridine-1,3,(2...	191	C9H9N3O2	298688-32-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063015\
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Sample : G2838-11
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-B11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.50	24.8	ng	250662	1	7.28	202226	20.0
unknown7.05	7.05	125.1	ng	1264640	1	7.28	202226	20.0
Trichloroacetic a...	14.77	4.6	ng	122569	5	14.97	528171	20.0
Hexadecanamide	16.06	2.2	ng	45500	6	16.95	421499	20.0
Squalene	16.20	3.9	ng	81545	6	16.95	421499	20.0
Perylene	16.79	3.1	ng	65499	6	16.95	421499	20.0
unknown17.87	17.87	2.2	ng	46892	6	16.95	421499	20.0