

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111815\
 Data File : BF083020.D
 Acq On : 18 Nov 2015 20:58
 Operator : UM/IZ
 Sample : G4453-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CWC-MISC-2-20151116

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-BF110715.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	4.899	242	246	258	rVB	1828596	2949587	43.75%	4.299%
2	5.333	281	284	287	rBV	3372985	5006276	74.26%	7.297%
3	6.384	373	376	378	rBV	5557085	6463594	95.87%	9.421%
4	6.499	383	386	389	rBV	5433296	6416254	95.17%	9.352%
5	6.727	404	406	408	rBV	1781057	1445561	21.44%	2.107%
6	6.887	417	420	422	rBV	5648314	5062369	75.09%	7.378%
7	7.299	452	456	458	rBV	4523702	4926770	73.08%	7.181%
8	8.019	516	519	521	rBV	1893544	1904321	28.25%	2.776%
9	9.093	610	613	616	rBV	5569798	6741708	100.00%	9.826%
10	9.493	645	648	650	rBV	1569003	1381008	20.48%	2.013%
11	9.722	666	668	669	rBV	86461	91697	1.36%	0.134%
12	9.768	669	672	674	rBV	2338133	2102357	31.18%	3.064%
13	10.213	710	711	713	rVB	142555	114692	1.70%	0.167%
14	10.431	726	730	732	rBV3	47515	84274	1.25%	0.123%
15	10.556	738	741	743	rBV	4224529	4319574	64.07%	6.296%
16	10.682	750	752	757	rVB	141529	242651	3.60%	0.354%
17	11.013	776	781	783	rBV6	36284	99640	1.48%	0.145%
18	11.139	790	792	793	rBV	140200	169145	2.51%	0.247%
19	11.242	799	801	805	rBV2	2106564	2430320	36.05%	3.542%
20	11.311	805	807	809	rVB2	108030	165909	2.46%	0.242%
21	11.562	827	829	831	rVB2	93407	83776	1.24%	0.122%
22	11.745	840	845	846	rBV	147329	164219	2.44%	0.239%
23	11.768	846	847	850	rVV2	150235	204602	3.03%	0.298%
24	11.848	853	854	858	rVV	132009	267626	3.97%	0.390%
25	12.042	868	871	874	rVB3	198235	252429	3.74%	0.368%
26	12.191	881	884	885	rBV3	54299	69486	1.03%	0.101%
27	12.294	891	893	895	rBV	95525	107903	1.60%	0.157%
28	12.374	899	900	904	rVB2	63601	71574	1.06%	0.104%
29	12.454	904	907	909	rVB	977202	1077080	15.98%	1.570%
30	12.499	909	911	914	rBV3	41751	97435	1.45%	0.142%
31	12.602	916	920	922	rBV3	45048	117240	1.74%	0.171%
32	12.671	924	926	929	rBV	834383	1091975	16.20%	1.592%
33	12.728	929	931	934	rVB2	69366	93291	1.38%	0.136%
34	12.831	938	940	943	rVB	4785549	5260507	78.03%	7.667%

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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-BF110715.M
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35	12.899	943	946	952	rBV3	74861	138755	2.06%	0.202%
36	13.002	952	955	958	rVB	100011	195521	2.90%	0.285%
37	13.071	959	961	963	rBV2	75109	90575	1.34%	0.132%
38	13.105	963	964	970	rBV3	112451	203172	3.01%	0.296%
39	13.197	970	972	974	rBV2	77984	109199	1.62%	0.159%
40	13.391	986	989	991	rBV2	79821	166466	2.47%	0.243%
41	13.505	998	999	1001	rBV	65376	73885	1.10%	0.108%
42	13.619	1007	1009	1011	rBV	105985	169984	2.52%	0.248%
43	13.654	1011	1012	1016	rVV4	78678	165571	2.46%	0.241%
44	13.722	1016	1018	1019	rVV2	80809	120908	1.79%	0.176%
45	13.745	1019	1020	1028	rVV3	126962	314175	4.66%	0.458%
46	13.871	1028	1031	1037	rVV2	1707020	2434316	36.11%	3.548%
47	14.168	1055	1057	1060	rBV3	57910	103310	1.53%	0.151%
48	14.225	1060	1062	1063	rBV	64707	78706	1.17%	0.115%
49	14.877	1116	1119	1124	rVB	356546	699889	10.38%	1.020%
50	15.151	1141	1143	1145	rVB	209721	267210	3.96%	0.389%
51	15.197	1145	1147	1150	rVV	249184	388539	5.76%	0.566%
52	15.265	1150	1153	1156	rVB	845538	1143498	16.96%	1.667%
53	16.294	1241	1243	1249	rVB6	53896	131599	1.95%	0.192%
54	16.568	1264	1267	1272	rVB2	99141	196142	2.91%	0.286%
55	16.957	1298	1301	1308	rVB	73697	157452	2.34%	0.229%
56	19.540	1518	1527	1529	rBV9	31955	184542	2.74%	0.269%

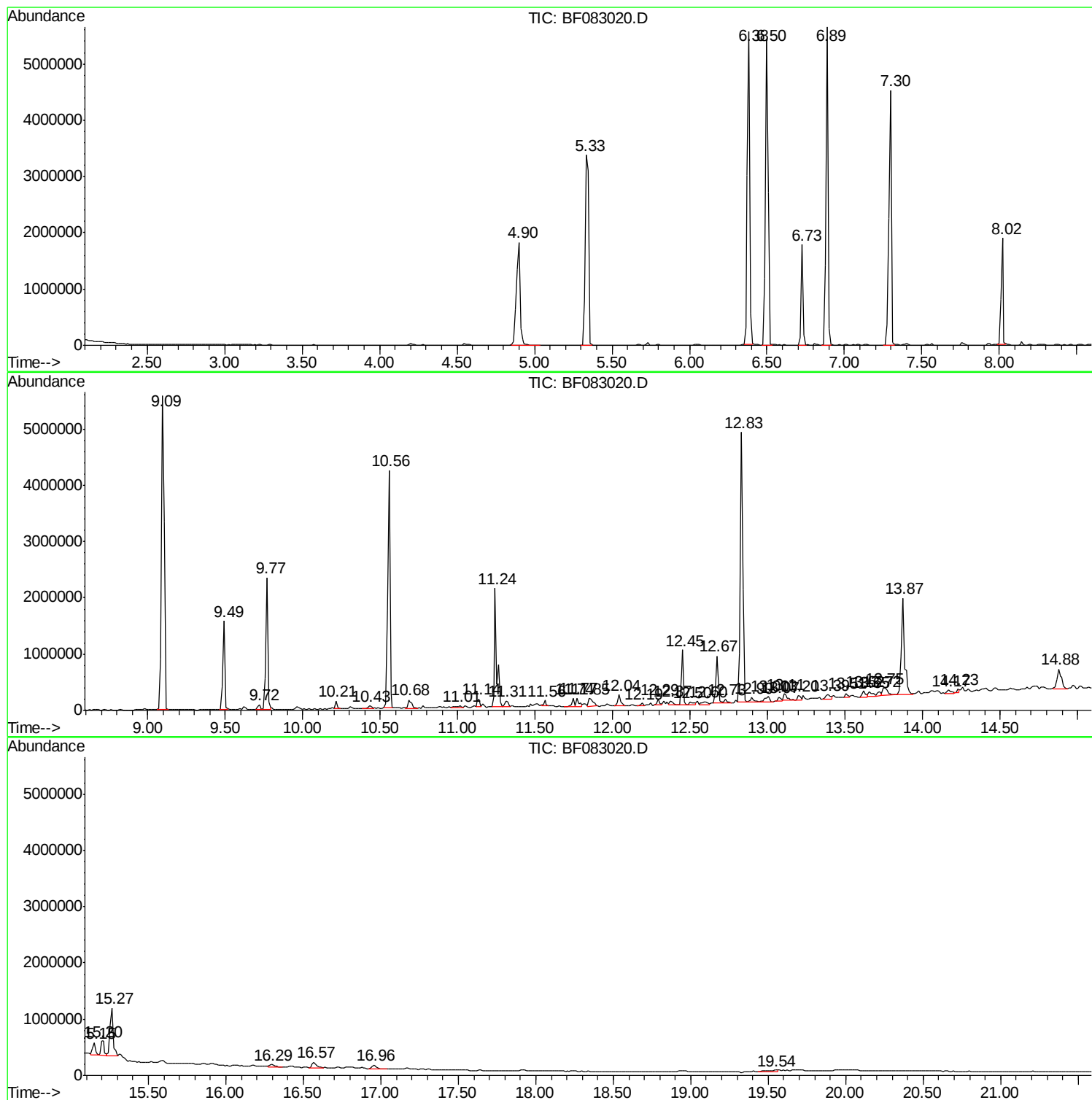
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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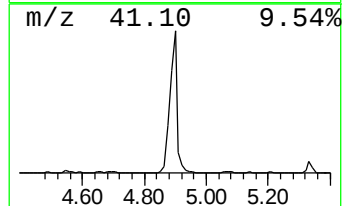
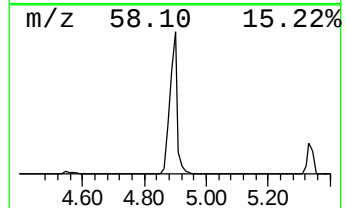
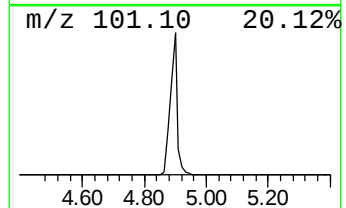
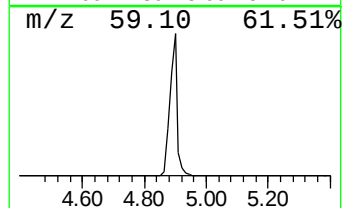
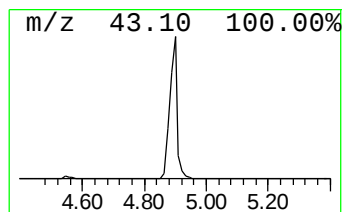
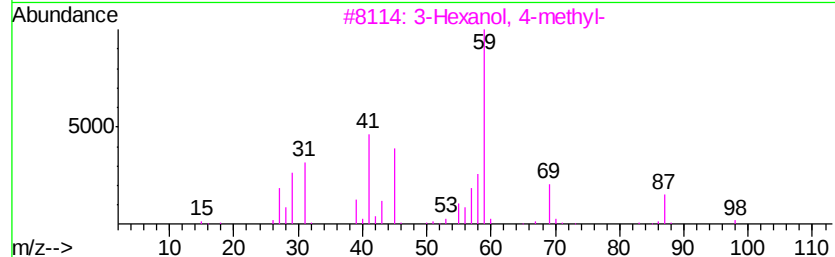
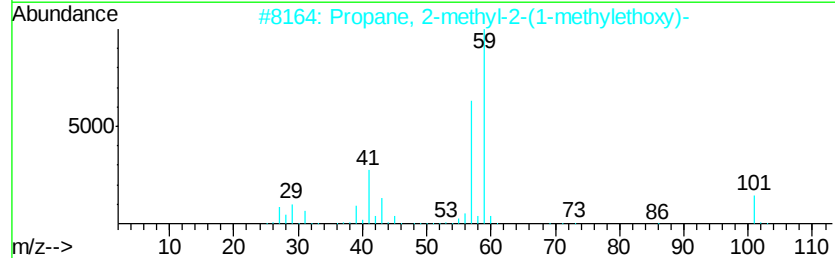
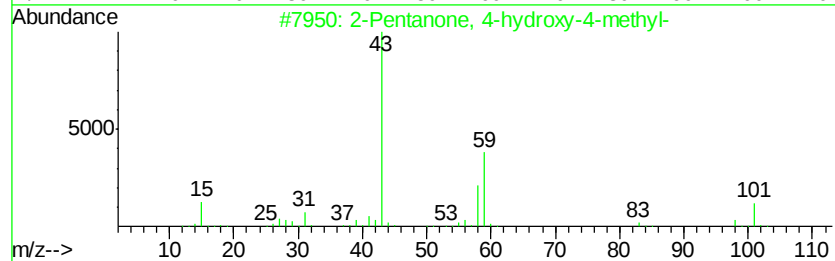
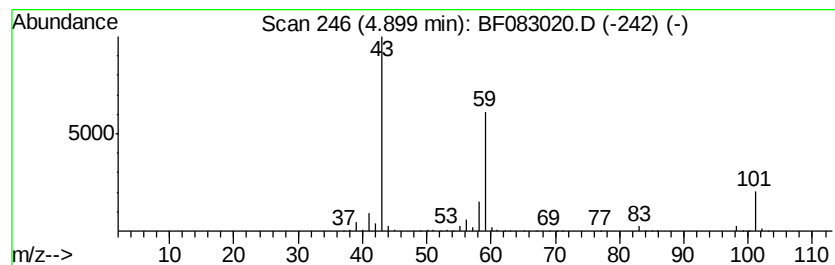
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	40.81 ng	2949590	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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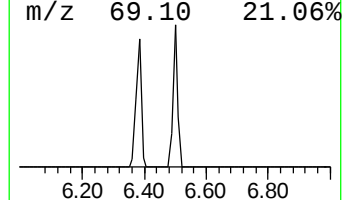
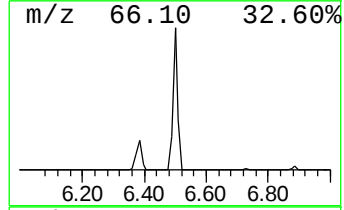
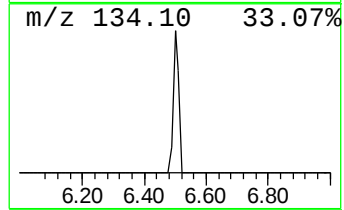
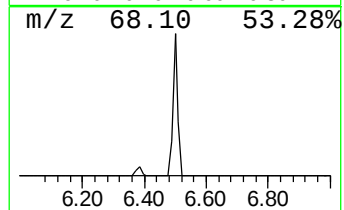
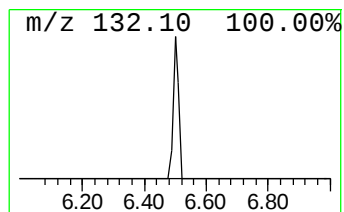
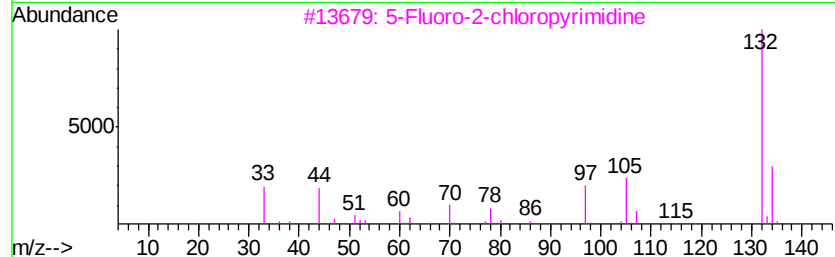
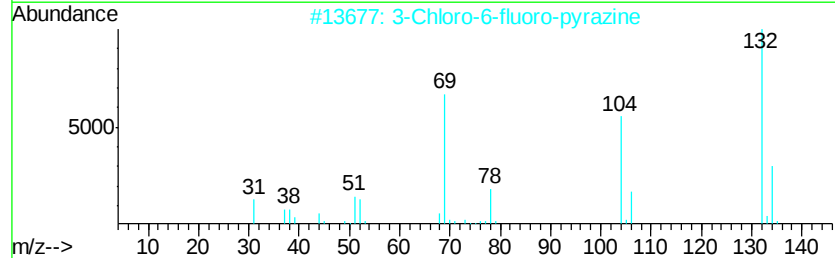
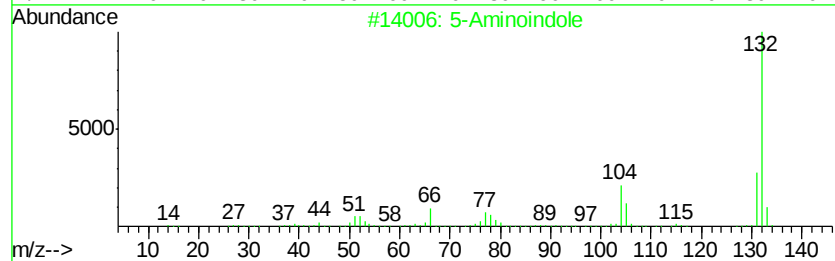
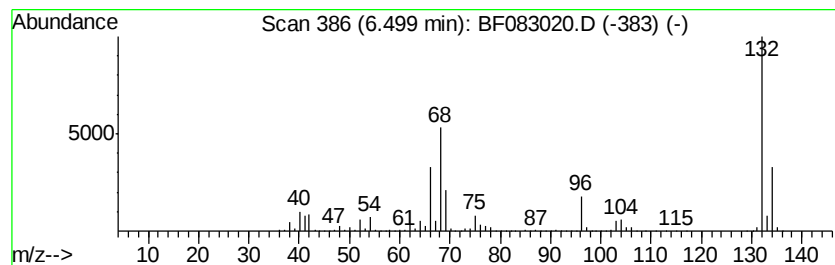
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	88.77 ng	6416250	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminoindole	132	C8H8N2	005192-03-0	27
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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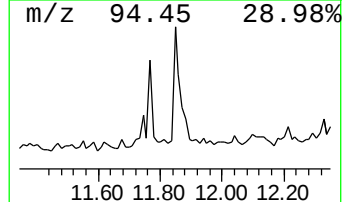
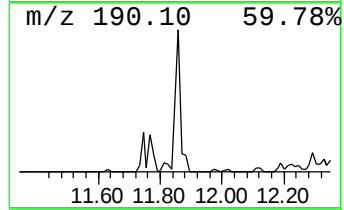
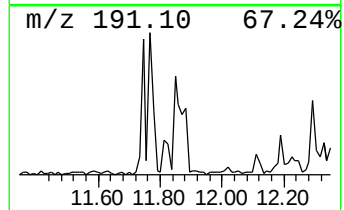
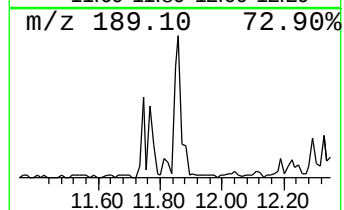
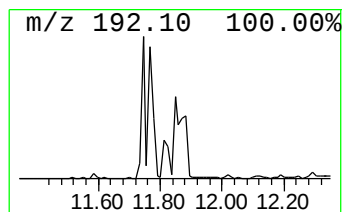
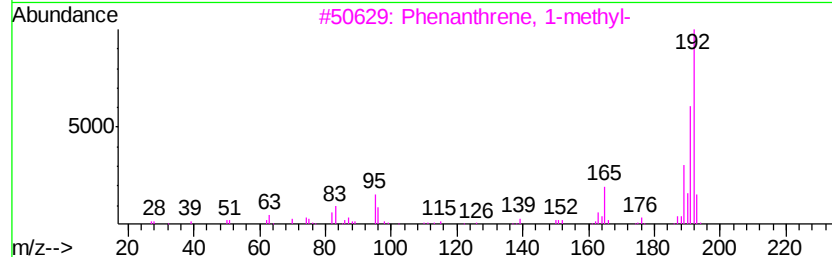
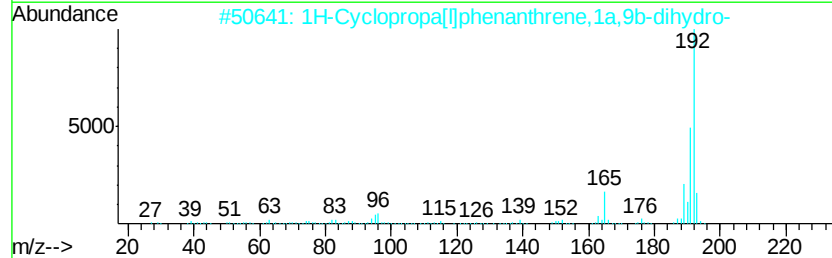
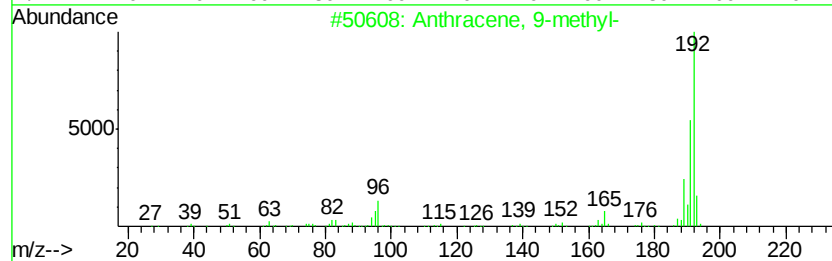
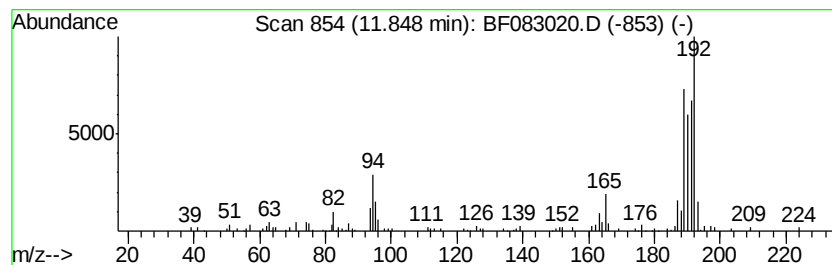
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Anthracene, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	2.20 ng	267626	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	64
2	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	60
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	55
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	55



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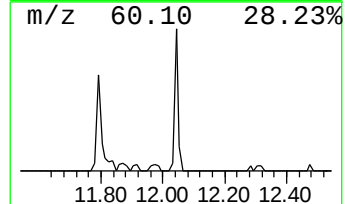
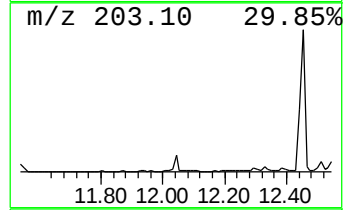
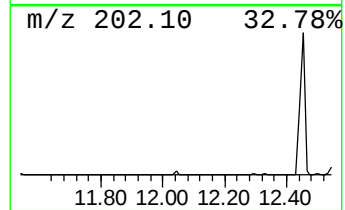
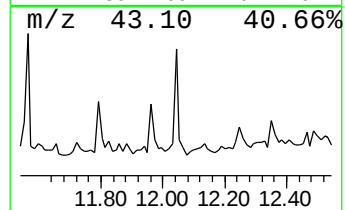
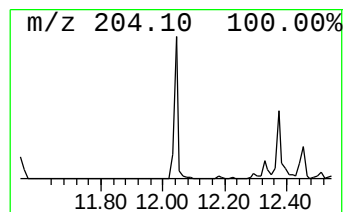
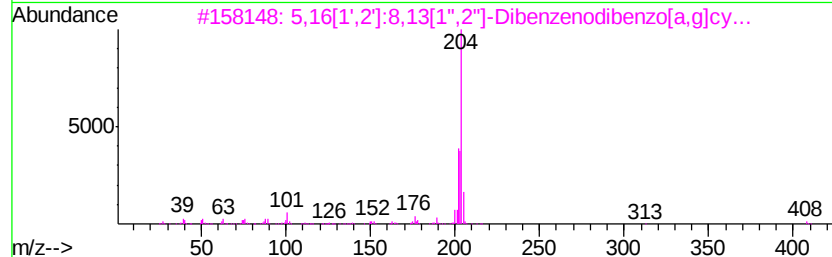
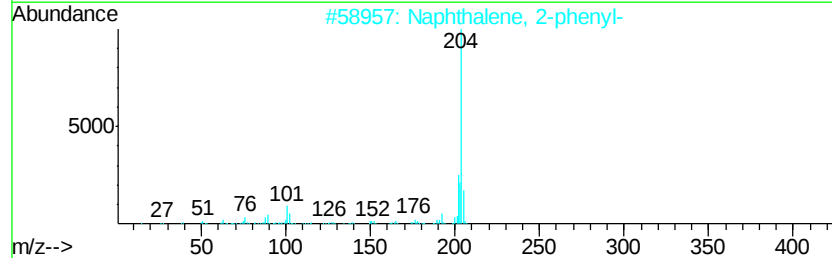
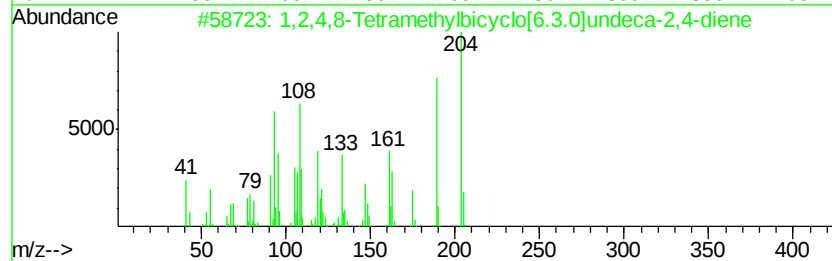
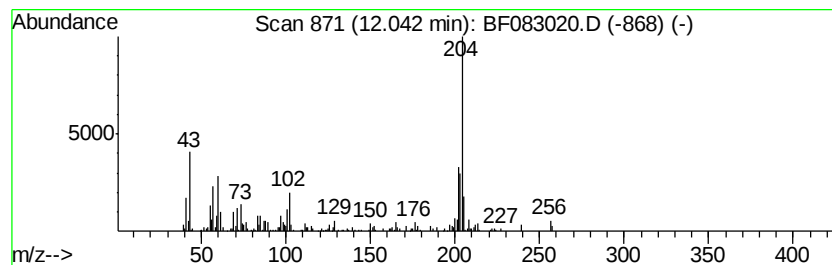
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,2,4,8-Tetramethylbicyclo[...] Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.08 ng	252429	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24		137235-51-9	93
2	Naphthalene, 2-phenyl-	204	C16H12		000612-94-2	60
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24		005672-97-9	52
4	6-Phenylbenzocyclohepten-7-one	232	C17H12O		093327-56-1	52
5	6-Cyanophenanthridine	204	C14H8N2		002176-28-5	45



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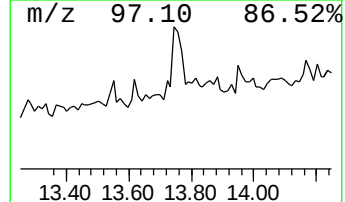
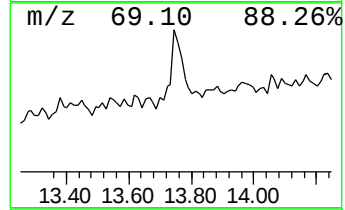
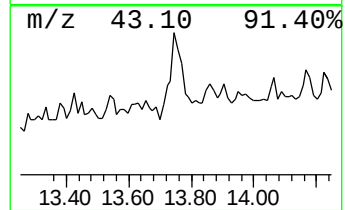
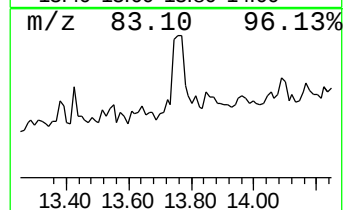
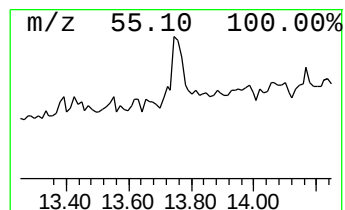
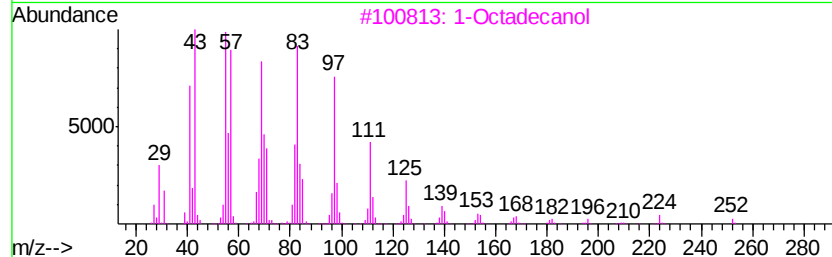
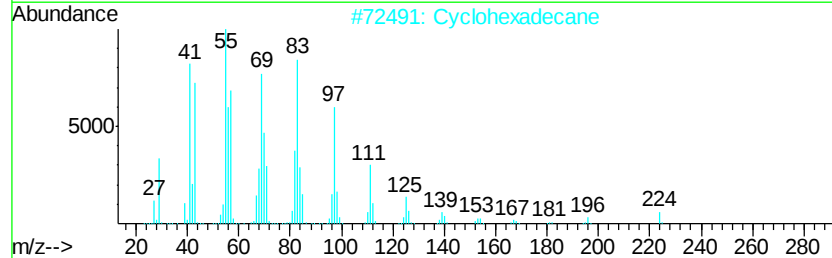
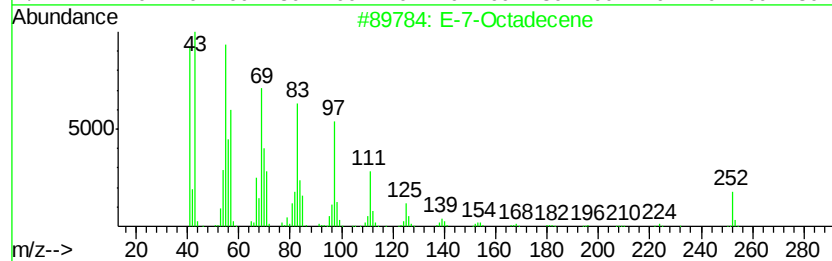
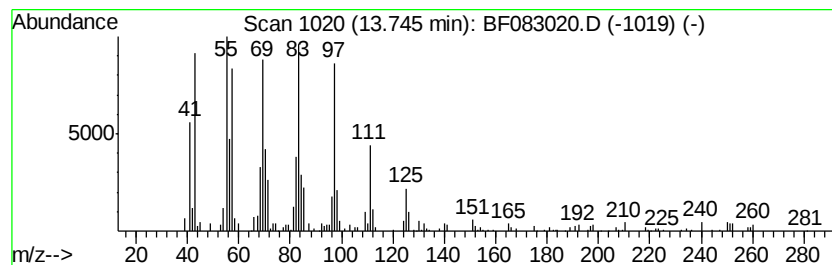
Instrument :
BNA_F
ClientSampleId :
CWC-MISC-2-20151116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 E-7-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	2.58 ng	314175	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-7-Octadecene	252	C18H36	1000130-92-0	93
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
5	Cyclopentadecane	210	C15H30	000295-48-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111815\
Data File : BF083020.D
Acq On : 18 Nov 2015 20:58
Operator : UM/IZ
Sample : G4453-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

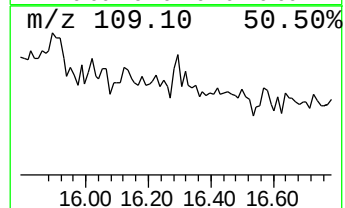
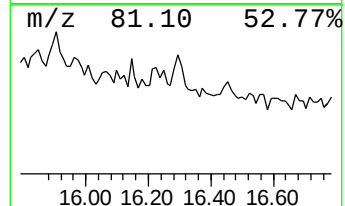
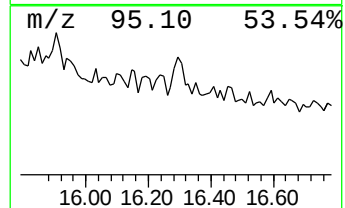
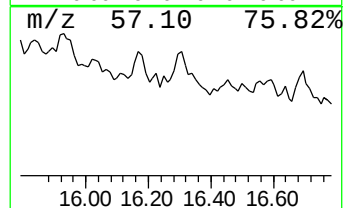
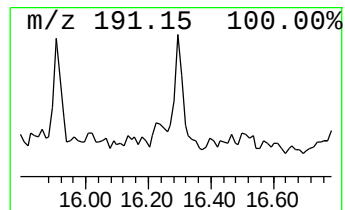
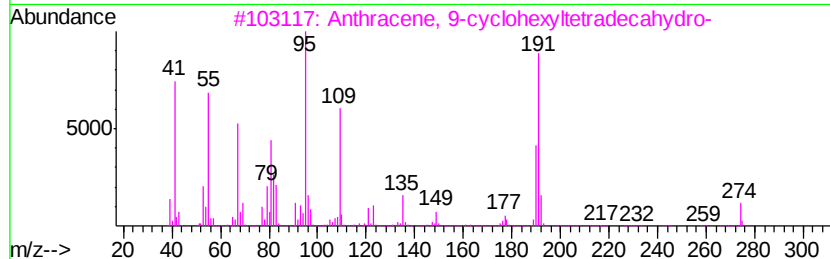
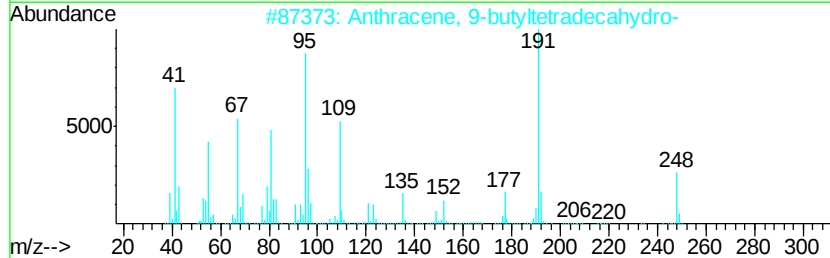
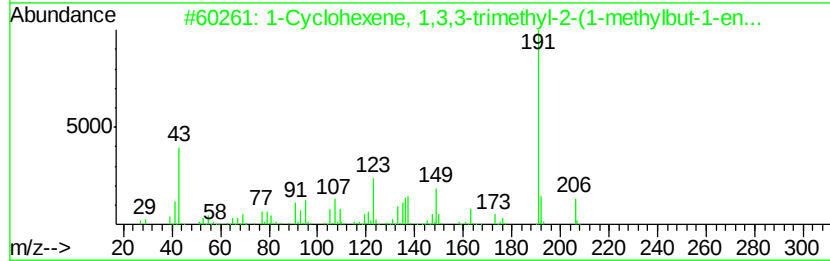
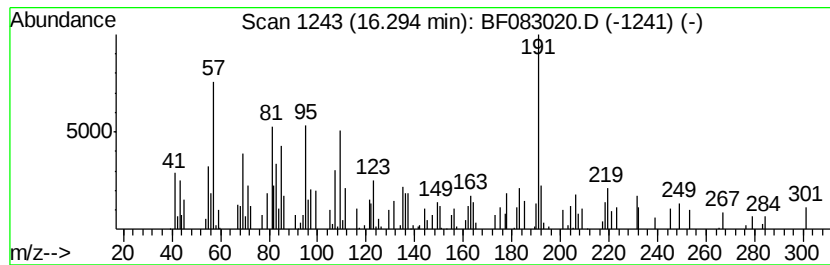
Instrument :
BNA_F
ClientSampleId :
CWC-MISC-2-20151116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.29 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	2.30 ng	131599	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Cyclohexene, 1,3,3-trimethyl-2...	206 C14H22O	1000197-08-4 41
2		Anthracene, 9-butyldodecahydro-	248 C18H32	055133-89-6 38
3		Anthracene, 9-cyclohexyldodec...	274 C20H34	055255-70-4 38
4		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206 C14H22O	1000195-40-9 38
5		.beta.-iso-Methyl ionone	206 C14H22O	1000285-40-2 32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111815\
Data File : BF083020.D
Acq On : 18 Nov 2015 20:58
Operator : UM/IZ
Sample : G4453-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CWC-MISC-2-20151116

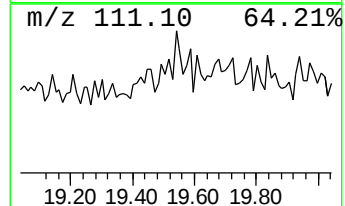
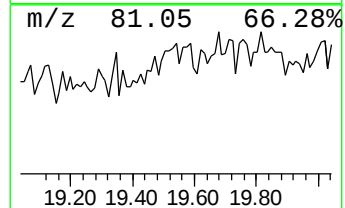
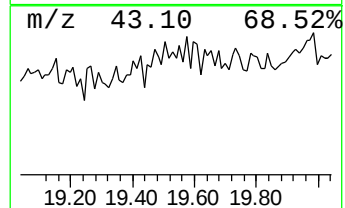
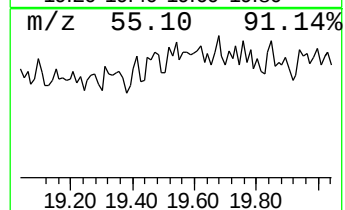
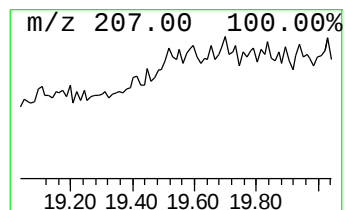
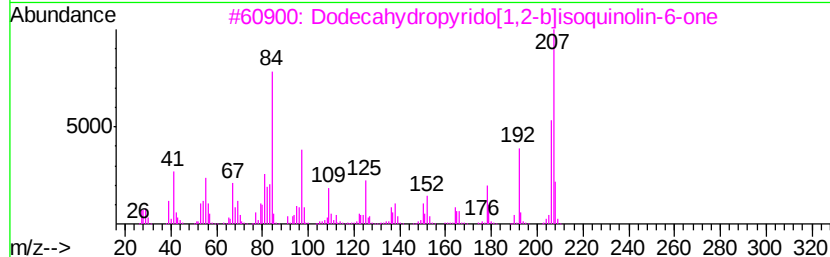
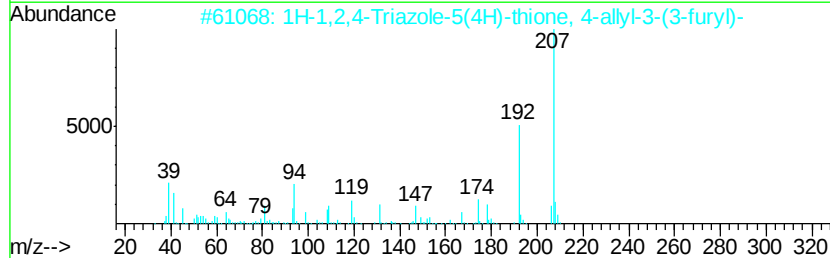
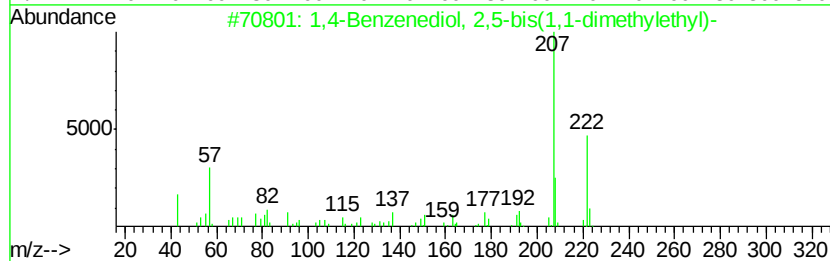
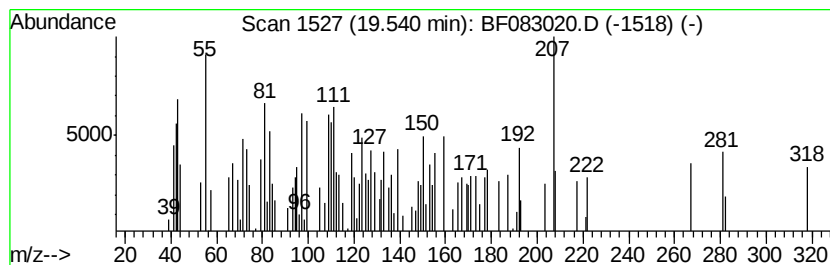
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown19.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	3.23 ng	184542	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2,5-bis(1,1-dim...	222	C14H22O2	000088-58-4	30
2		1H-1,2,4-Triazole-5(4H)-thione, ...	207	C9H9N3OS	1000277-38-2	22
3		Dodecahydropyrido[1,2-b]isoquino...	207	C13H21NO	108873-36-5	16
4		1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	16
5		Perhydro-htx-2-one, 2-depentyl-,...	281	C16H27NO3	080090-53-5	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111815\
Data File : BF083020.D
Acq On : 18 Nov 2015 20:58
Operator : UM/IZ
Sample : G4453-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CWC-MISC-2-20151116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	4.90	40.8	ng	2949590	1	6.73	1445560	20.0
unknown6.50	6.50	88.8	ng	6416250	1	6.73	1445560	20.0
Anthracene, 9-met...	11.85	2.2	ng	267626	4	11.24	2430320	20.0
1,2,4,8-Tetrameth...	12.04	2.1	ng	252429	4	11.24	2430320	20.0
E-7-Octadecene	13.75	2.6	ng	314175	5	13.87	2434320	20.0
unknown16.29	16.29	2.3	ng	131599	6	15.27	1143500	20.0
unknown19.54	19.54	3.2	ng	184542	6	15.27	1143500	20.0