

Data Path : Z:\HPCHEM1\BNA F\DATA\BF090315\
 Data File : BF081417.D
 Acq On : 4 Sep 2015 12:32
 Operator : UM/IZ
 Sample : G3491-01
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-EF-01-004-ABCD

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-BF090115.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	3.541	169	171	178	rBB	17928	35385	1.72%	0.188%
2	4.364	240	243	245	rBV	29318	43931	2.13%	0.233%
3	4.421	245	248	263	rVB	697113	1494339	72.55%	7.938%
4	4.924	290	292	295	rBV	1825119	2059643	100.00%	10.941%
5	5.347	327	329	332	rBV	28925	26806	1.30%	0.142%
6	6.044	387	390	392	rBV	1900382	2041095	99.10%	10.842%
7	6.136	396	398	401	rVV	1792257	2038484	98.97%	10.828%
8	6.364	416	418	421	rVB	355189	339893	16.50%	1.805%
9	6.524	429	432	434	rBV	1722070	1498793	72.77%	7.961%
10	6.947	466	469	471	rBV	1311388	1306423	63.43%	6.940%
11	7.096	479	482	484	rBV	19633	21348	1.04%	0.113%
12	7.656	529	531	534	rBV	512520	445269	21.62%	2.365%
13	8.742	623	626	629	rBV	2017003	1819087	88.32%	9.663%
14	9.142	659	661	664	rBV	244732	230751	11.20%	1.226%
15	9.393	681	683	685	rVB	342780	413852	20.09%	2.198%
16	10.182	749	752	755	rBV	1248250	1211962	58.84%	6.438%
17	10.331	763	765	768	rBV	32596	38804	1.88%	0.206%
18	10.776	802	804	805	rBV	29588	24759	1.20%	0.132%
19	10.868	809	812	815	rBV	328000	481643	23.38%	2.558%
20	10.936	815	818	824	rVB	27086	36178	1.76%	0.192%
21	11.131	834	835	839	rBV	19466	26641	1.29%	0.142%
22	11.199	839	841	844	rVB	26896	22612	1.10%	0.120%
23	11.439	860	862	864	rBV	126265	135106	6.56%	0.718%
24	12.056	914	916	918	rBV	146694	124722	6.06%	0.663%
25	12.274	933	935	939	rBV2	95543	141161	6.85%	0.750%
26	12.445	948	950	953	rBV	1317985	1257748	61.07%	6.681%
27	12.616	960	965	967	rBV2	13494	23647	1.15%	0.126%
28	13.005	996	999	1000	rBV	26531	27749	1.35%	0.147%
29	13.371	1028	1031	1037	rBV	125230	196833	9.56%	1.046%
30	13.462	1037	1039	1044	rVV2	246096	428925	20.83%	2.278%
31	13.691	1056	1059	1062	rBV4	15005	34574	1.68%	0.184%
32	13.999	1084	1086	1089	rVB	24371	33478	1.63%	0.178%
33	14.342	1115	1116	1120	rVB	60348	65140	3.16%	0.346%
34	14.457	1123	1126	1130	rVV	57897	124441	6.04%	0.661%

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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35	14.594	1134	1138	1140	rVV3	20266	68352	3.32%	0.363%
36	14.685	1144	1146	1148	rVV	46270	56703	2.75%	0.301%
37	14.731	1148	1150	1152	rVV	39985	47152	2.29%	0.250%
38	14.777	1152	1154	1158	rVV	222081	266644	12.95%	1.416%
39	15.177	1187	1189	1191	rBV2	25236	45369	2.20%	0.241%
40	15.611	1225	1227	1232	rVB4	29065	59029	2.87%	0.314%
41	16.034	1262	1264	1266	rBV2	20117	31227	1.52%	0.166%

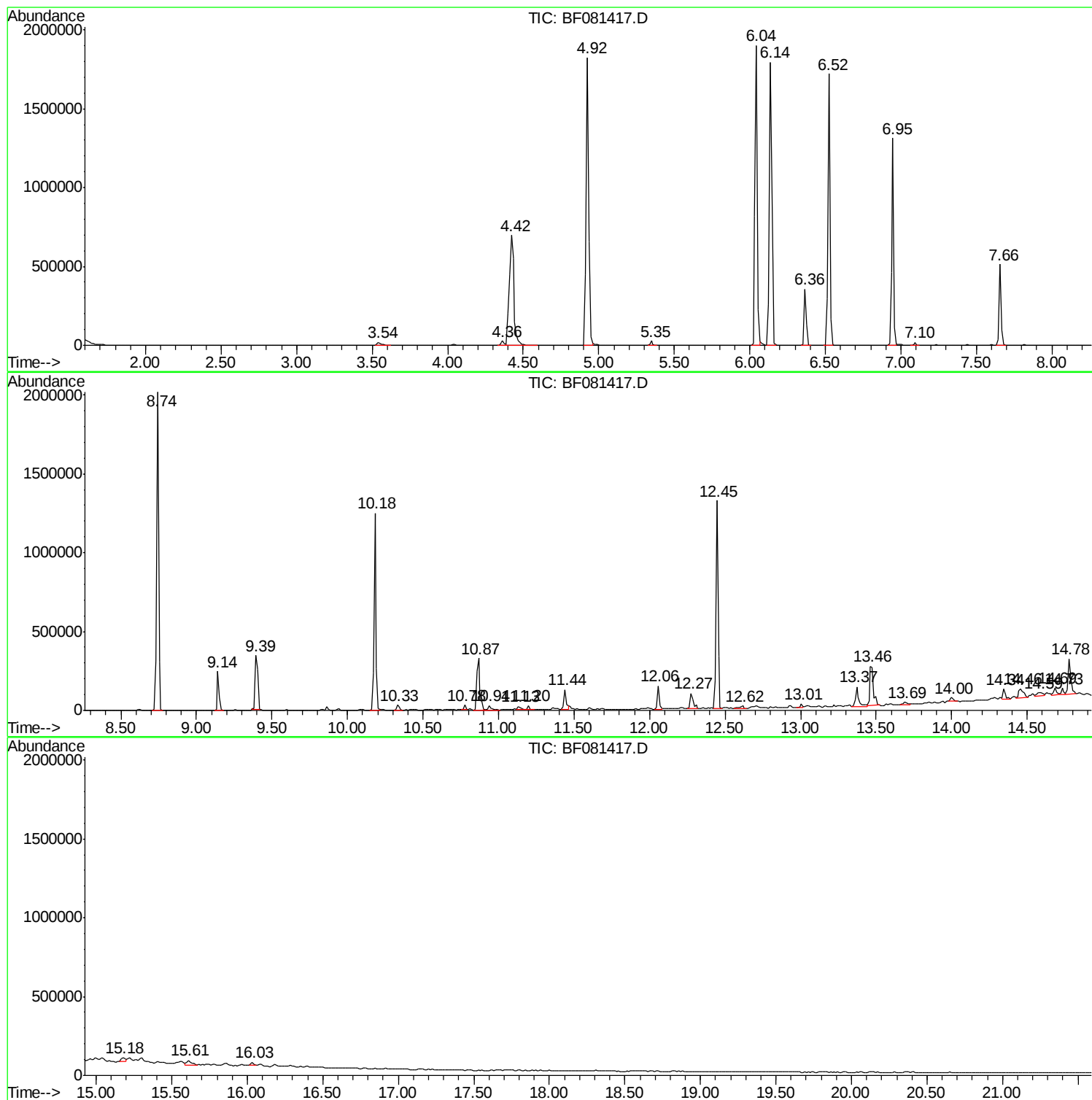
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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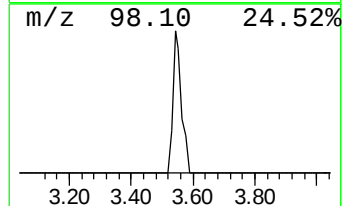
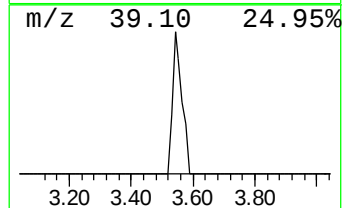
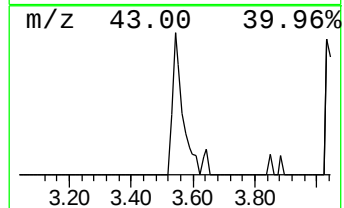
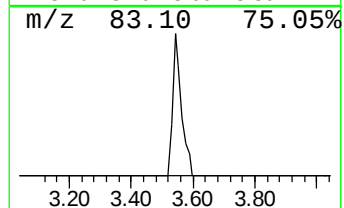
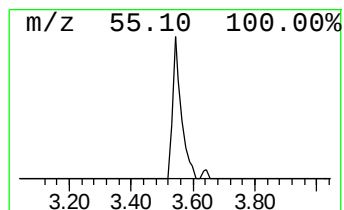
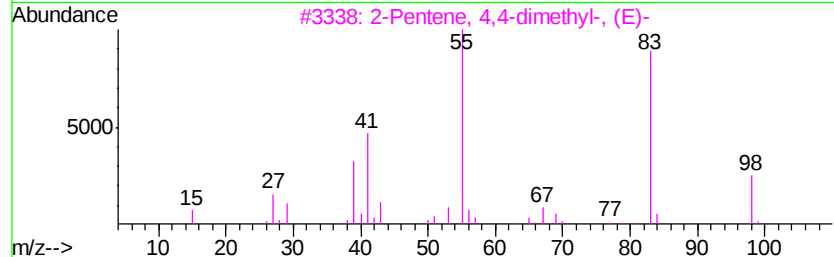
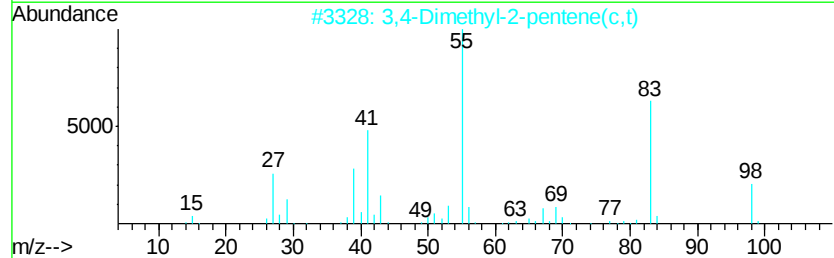
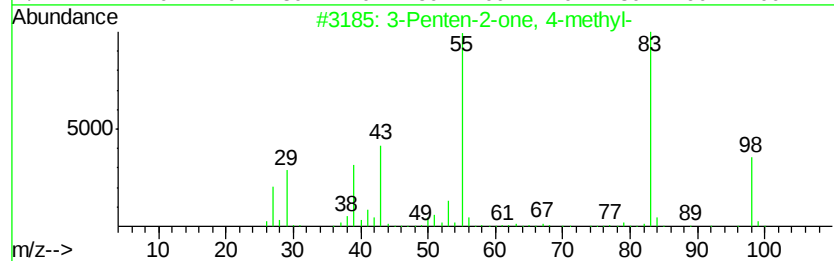
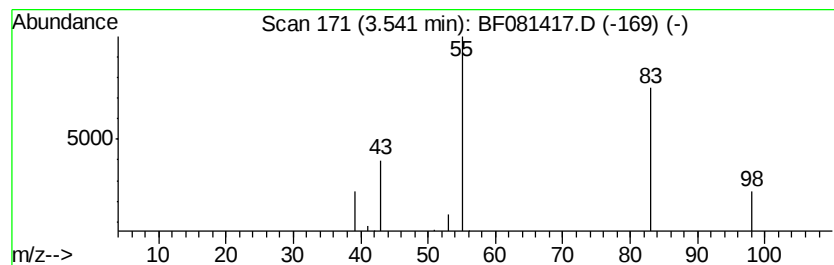
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	2.08 ng	35385	1,4-Dichlorobenzene-d4	6.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	83
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	83
4			Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	78
5			3-Hexen-2-one	98	C6H10O	000763-93-9	78



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ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-004-ABCD

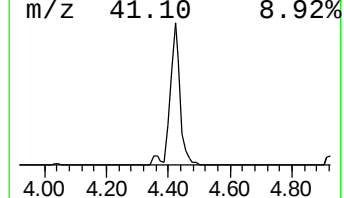
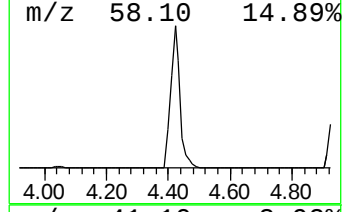
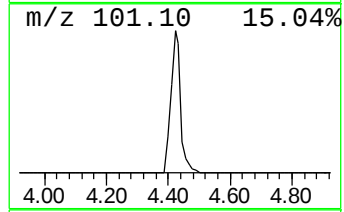
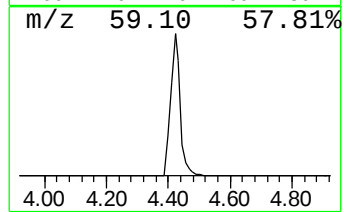
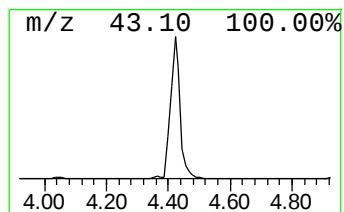
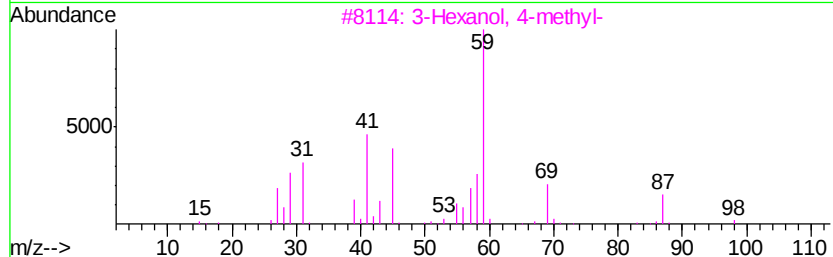
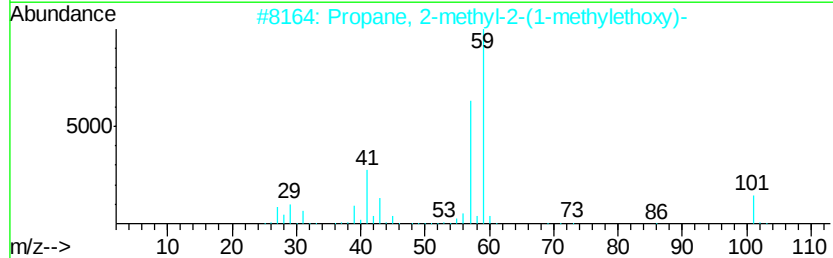
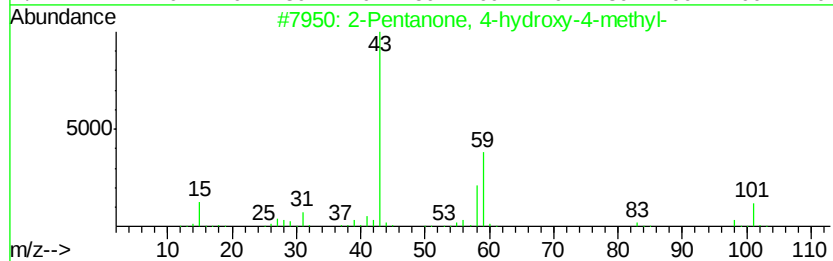
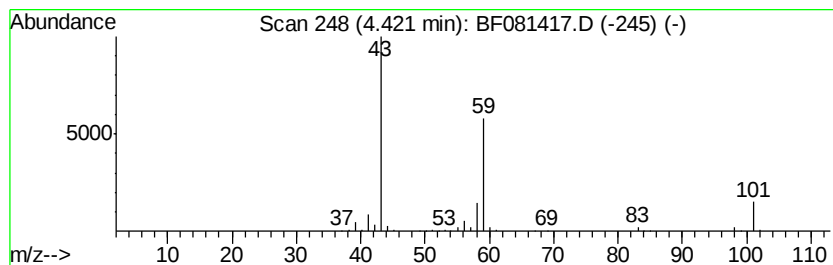
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	87.93 ng	1494340	1,4-Dichlorobenzene-d4	6.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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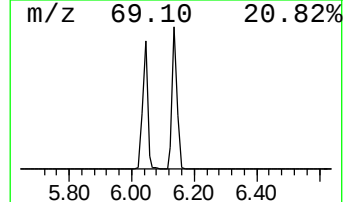
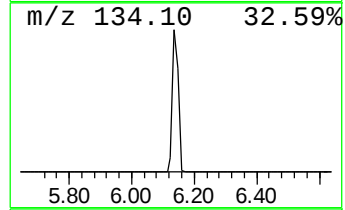
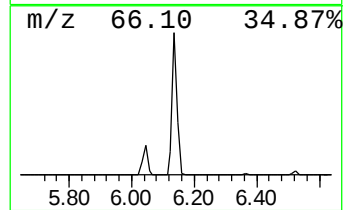
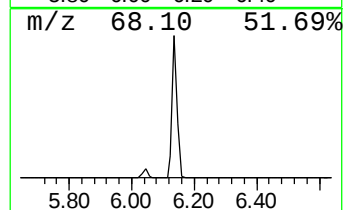
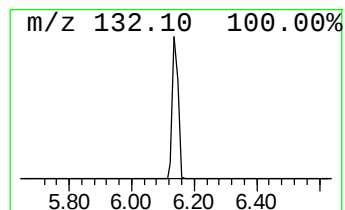
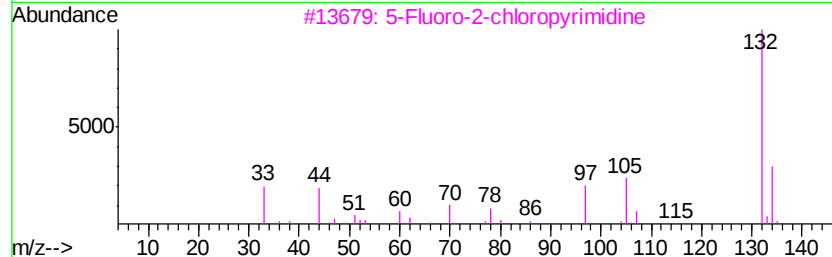
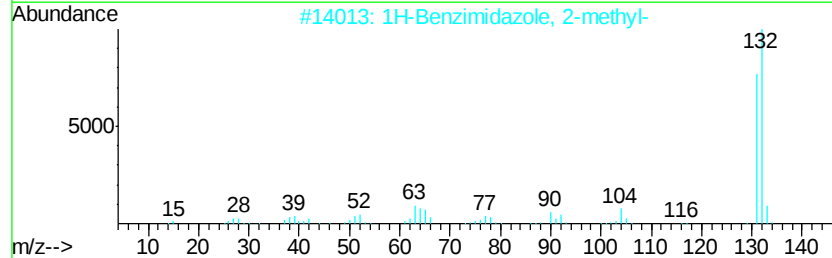
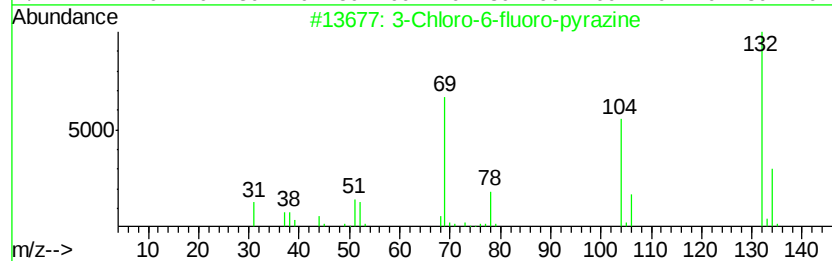
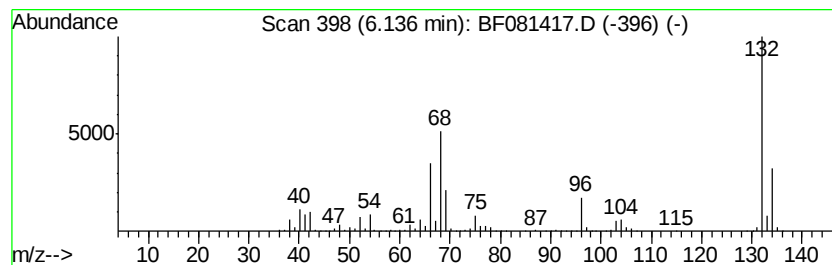
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.14 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	119.95 ng	2038480	1,4-Dichlorobenzene-d4	6.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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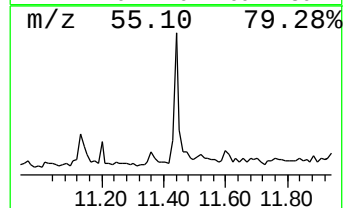
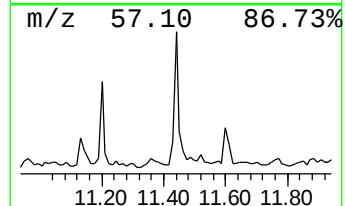
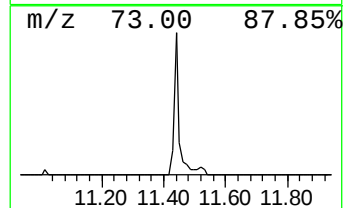
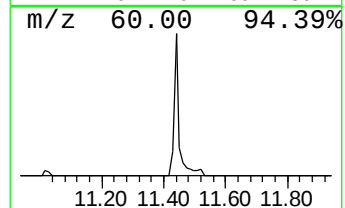
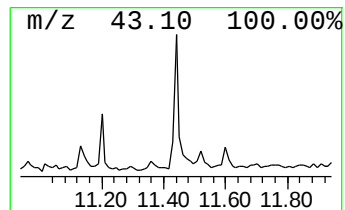
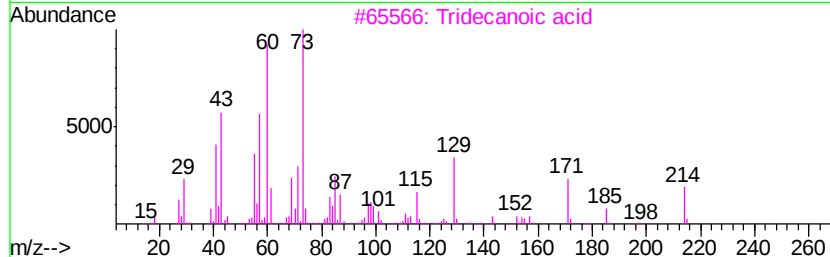
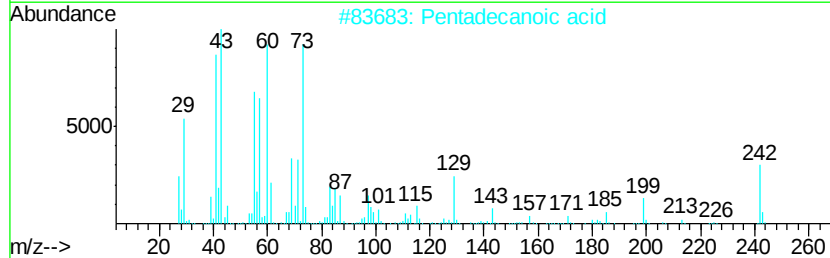
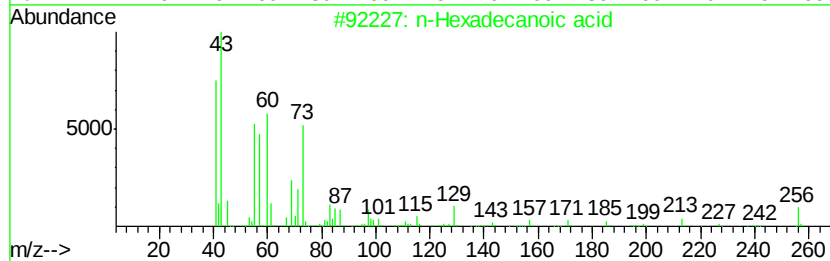
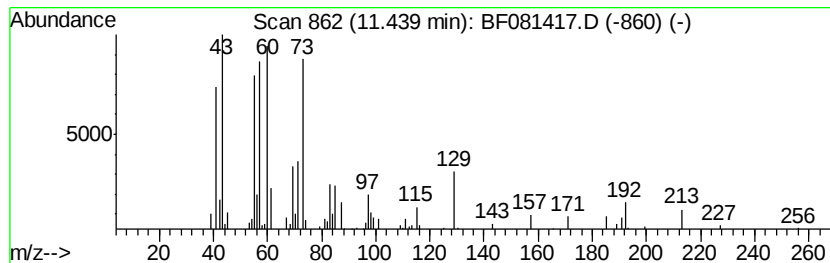
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	5.61 ng	135106	Phenanthrene-d10	10.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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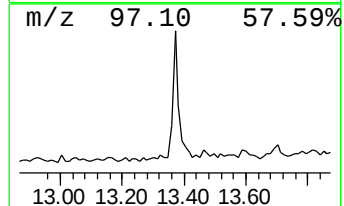
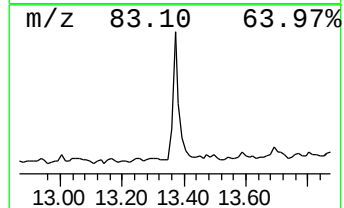
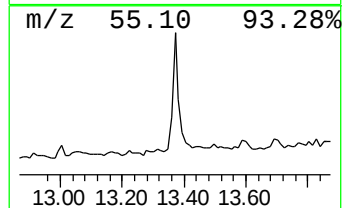
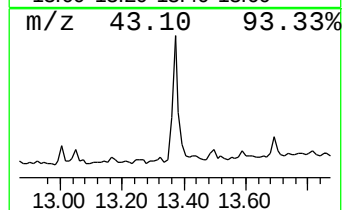
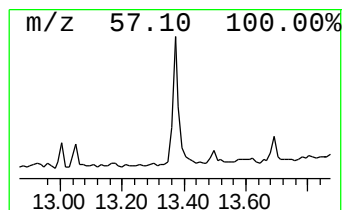
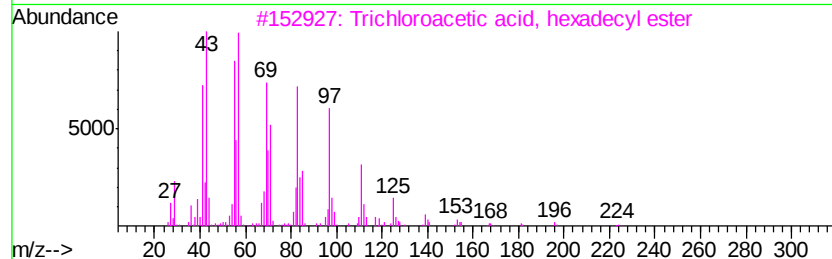
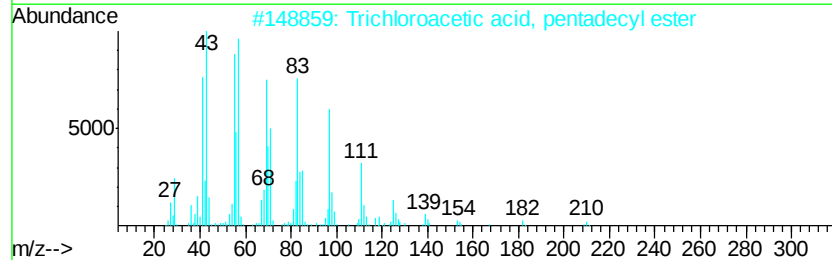
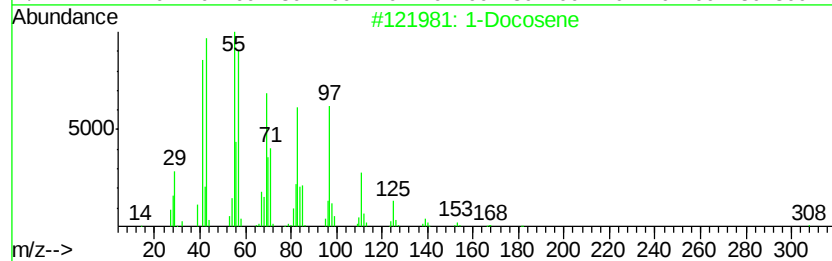
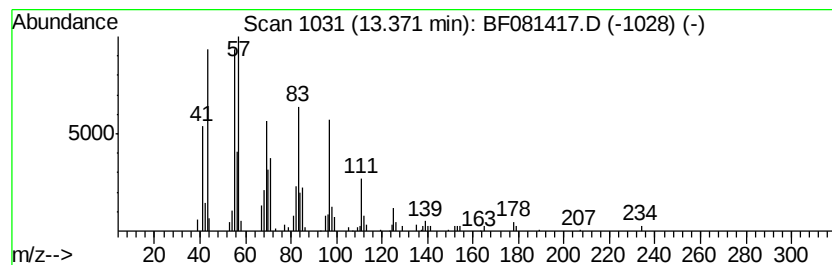
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	9.18 ng	196833	Chrysene-d12	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF090315\
 Data File : BF081417.D
 Acq On : 4 Sep 2015 12:32
 Operator : UM/IZ
 Sample : G3491-01
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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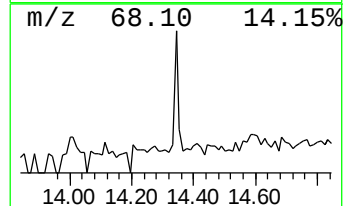
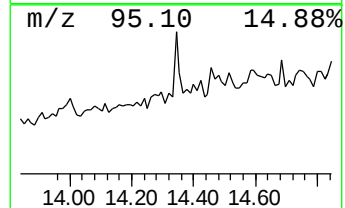
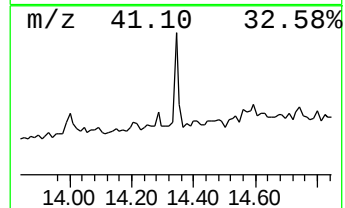
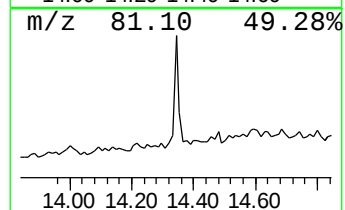
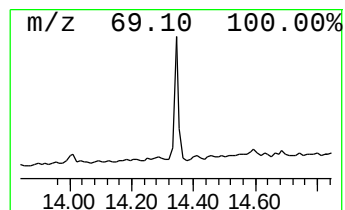
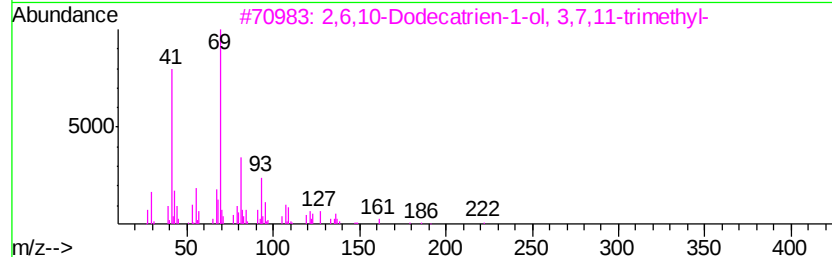
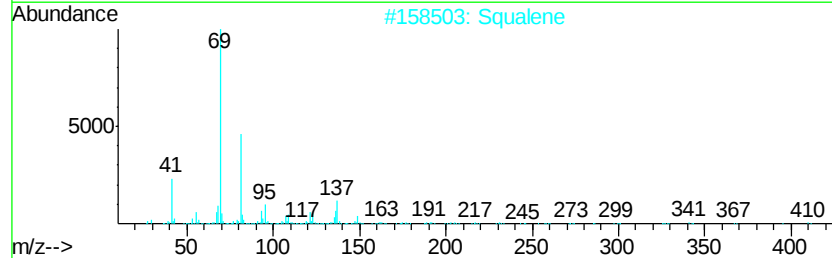
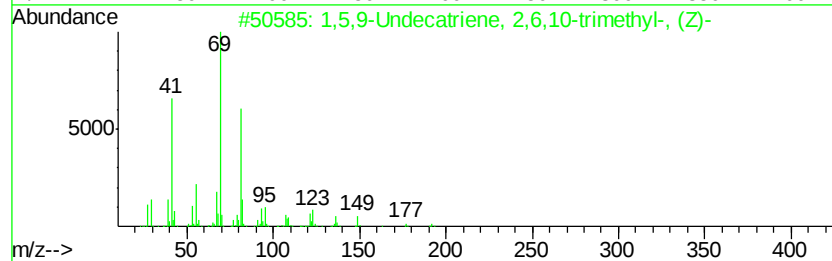
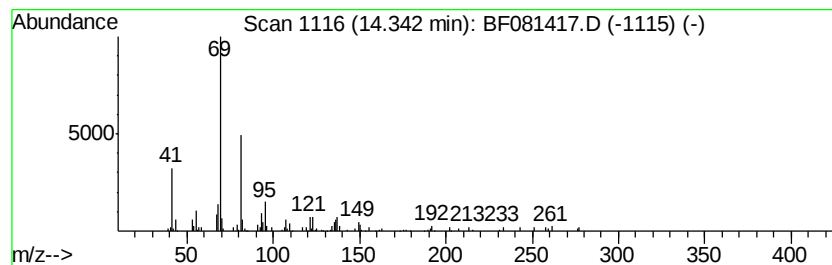
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.89 ng	65140	Perylene-d12	14.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
2			Squalene	410	C30H50	007683-64-9	72
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081417.D
Acq On : 4 Sep 2015 12:32
Operator : UM/IZ
Sample : G3491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-004-ABCD

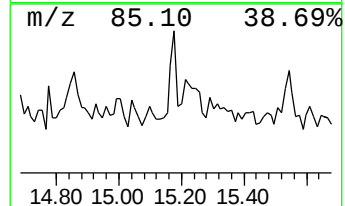
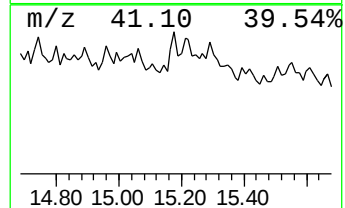
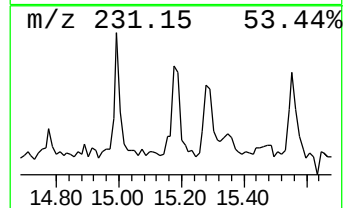
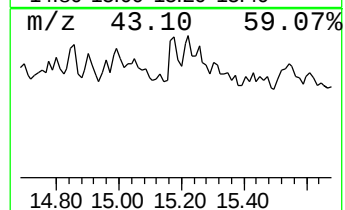
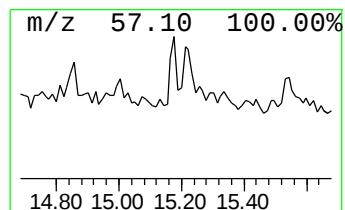
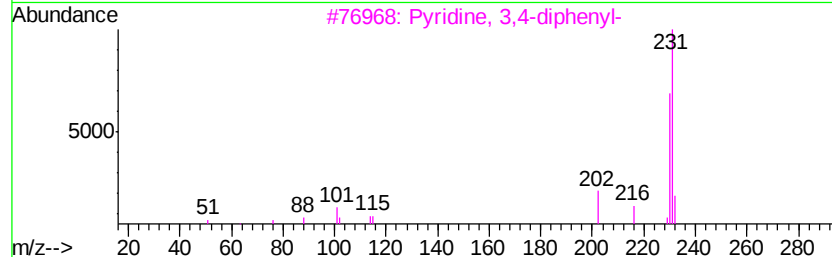
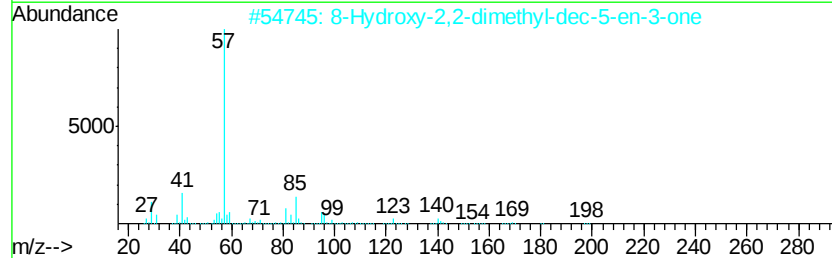
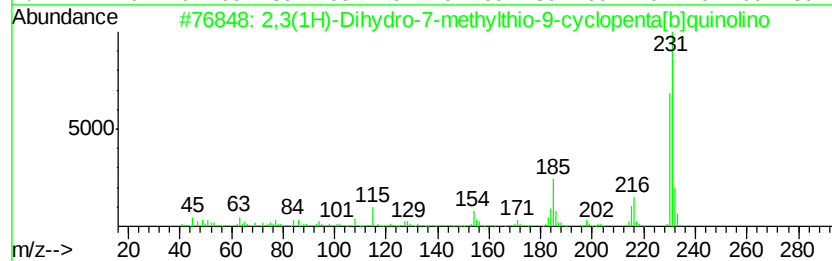
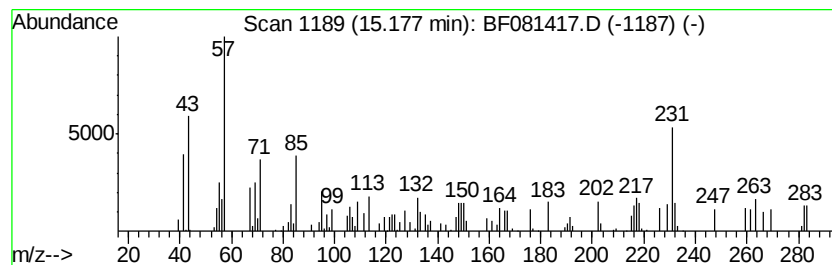
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.18 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	3.40 ng	45369	Perylene-d12	14.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3(1H)-Dihydro-7-methylthio-9-c...	231	C13H13NOS	1000257-08-5	22		
2	8-Hydroxy-2,2-dimethyl-dec-5-en-...	198	C12H22O2	1000193-60-0	22		
3	Pyrindine, 3,4-diphenyl-	231	C17H13N	005216-04-6	22		
4	10H-Phenothiazine, 5,5-dioxide	231	C12H9N02S	001209-66-1	18		
5	Phosphinic acid, diphenyl-, meth...	232	C13H13O2P	001706-90-7	14		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081417.D
Acq On : 4 Sep 2015 12:32
Operator : UM/IZ
Sample : G3491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-004-ABCD

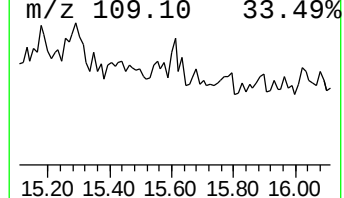
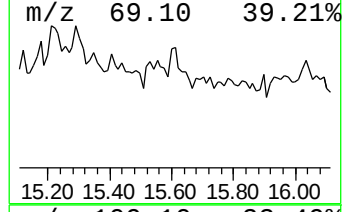
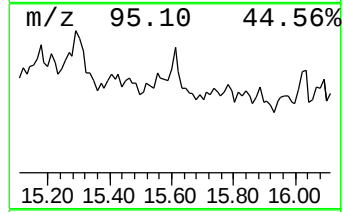
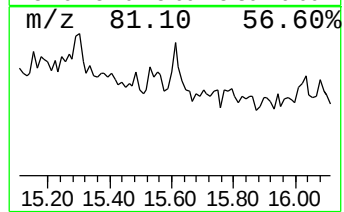
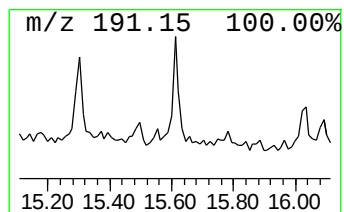
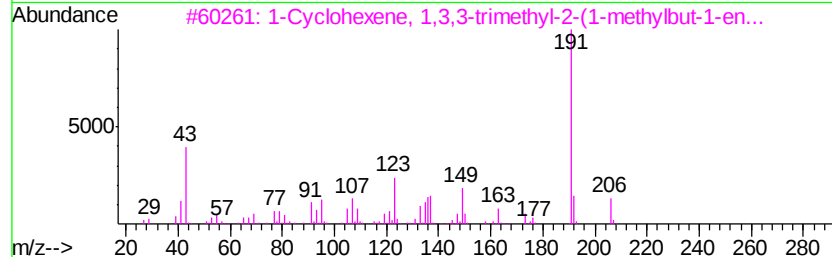
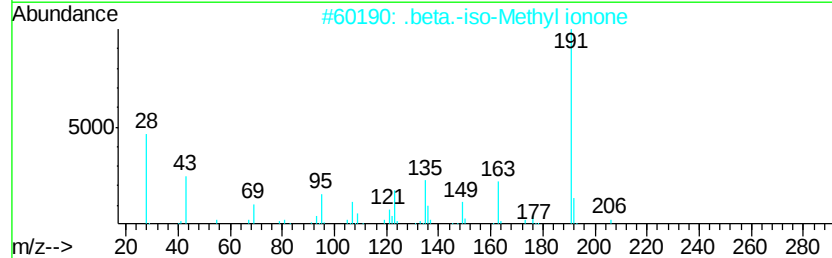
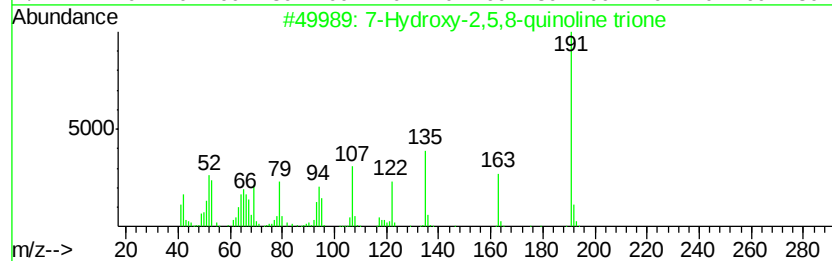
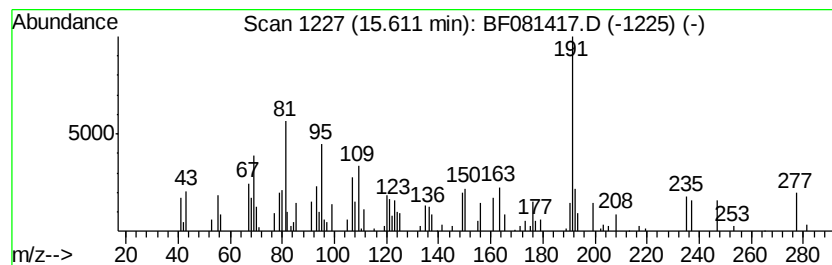
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.61 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	4.43 ng	59029	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Hydroxy-2,5,8-quinoline trione	191	C9H5NO4	015544-54-4	38
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4		Spiro[4-oxatricyclo[5.3.0.0(2,6)...]	276	C18H28O2	1000156-82-9	37
5		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF090315\
Data File : BF081417.D
Acq On : 4 Sep 2015 12:32
Operator : UM/IZ
Sample : G3491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-004-ABCD

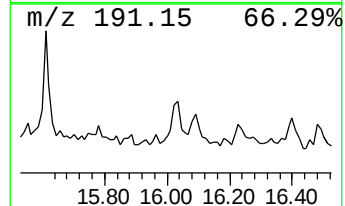
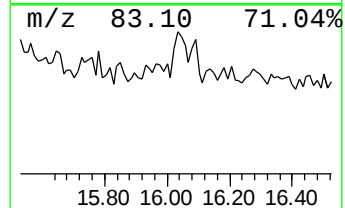
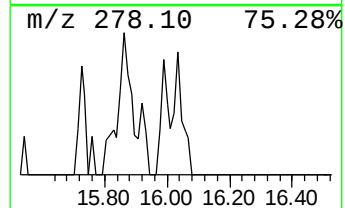
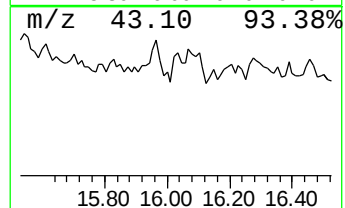
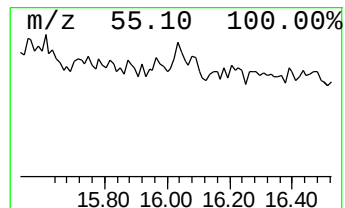
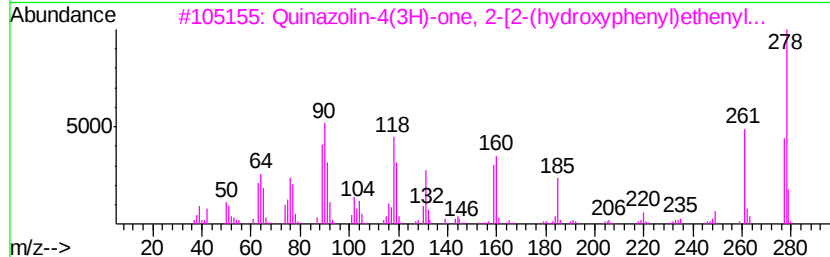
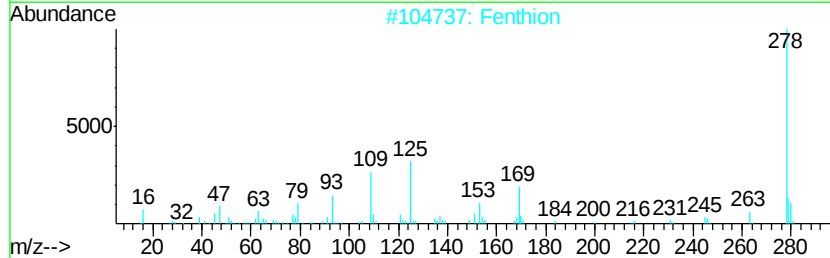
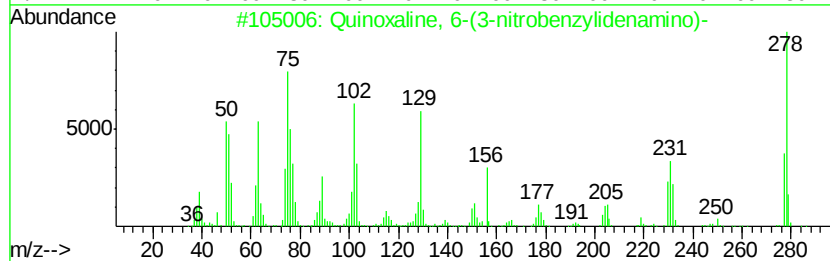
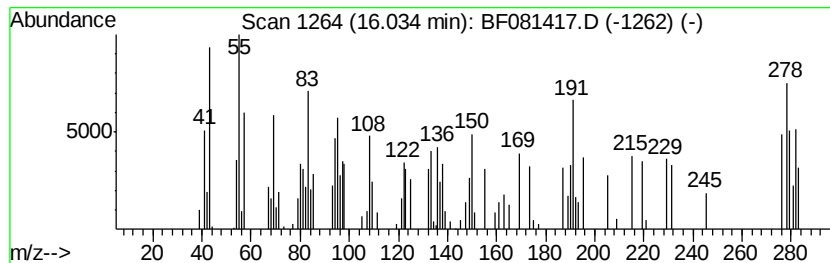
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.34 ng	31227	Perylene-d12	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoxaline, 6-(3-nitrobenzylidene...	278	C15H10N4O2	302800-55-1	11
2		Fenthion	278	C10H15O3PS2	000055-38-9	11
3		Quinazolin-4(3H)-one, 2-[2-(hydr...	278	C17H14N2O2	050830-07-4	11
4		[4,5'-Bipyrимidine]-2,2',4',6(1H...	278	C12H14N4O4	062880-87-9	11
5		Aspidospermidine, 1,2,6,7-tetrad...	278	C19H22N2	032975-46-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090315\
Data File : BF081417.D
Acq On : 4 Sep 2015 12:32
Operator : UM/IZ
Sample : G3491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-004-ABCD

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
3-Penten-2-one, 4...	3.54	2.1 ng		35385	1	6.36	339893	20.0
2-Pentanone, 4-hy...	4.42	87.9 ng		1494340	1	6.36	339893	20.0
unknown6.14	6.14	120.0 ng		2038480	1	6.36	339893	20.0
n-Hexadecanoic acid	11.44	5.6 ng		135106	4	10.87	481643	20.0
1-Docosene	13.37	9.2 ng		196833	5	13.47	428925	20.0
1,5,9-Undecatrien...	14.34	4.9 ng		65140	6	14.78	266644	20.0
unknown15.18	15.18	3.4 ng		45369	6	14.78	266644	20.0
unknown15.61	15.61	4.4 ng		59029	6	14.78	266644	20.0
unknown16.03	16.03	2.3 ng		31227	6	14.78	266644	20.0