

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
 Data File : BF081467.D
 Acq On : 5 Sep 2015 16:19
 Operator : UM/IZ
 Sample : G3559-01
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP226BR-10-20

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	4.410	243	247	260	rVB	549712	1071114	50.40%	6.392%
2	4.913	288	291	293	rBV	1505552	1873672	88.16%	11.181%
3	6.033	384	389	391	rBV	1641426	2125376	100.00%	12.683%
4	6.124	395	397	399	rBV	1918671	1743827	82.05%	10.406%
5	6.353	415	417	420	rVB	390840	350223	16.48%	2.090%
6	6.513	428	431	433	rBV	1464249	1291050	60.74%	7.704%
7	6.936	465	468	470	rBV	1147737	1149890	54.10%	6.862%
8	7.644	528	530	532	rBV	544496	452749	21.30%	2.702%
9	8.730	622	625	627	rBV	1902665	1732384	81.51%	10.338%
10	9.130	658	660	663	rBV	318362	268426	12.63%	1.602%
11	9.382	680	682	685	rVB	473297	454744	21.40%	2.714%
12	10.170	748	751	753	rBV	1239508	1184599	55.74%	7.069%
13	10.319	762	764	767	rBV	22448	24840	1.17%	0.148%
14	10.845	808	810	813	rBV	446869	450393	21.19%	2.688%
15	11.428	859	861	866	rBV	52412	65353	3.07%	0.390%
16	12.296	934	937	939	rVB	124593	145101	6.83%	0.866%
17	12.365	942	943	946	rVB	36937	37158	1.75%	0.222%
18	12.433	946	949	952	rBV	1399570	1314870	61.87%	7.846%
19	12.994	996	998	1000	rBV	113255	105654	4.97%	0.630%
20	13.039	1000	1002	1003	rVV	25810	23924	1.13%	0.143%
21	13.359	1028	1030	1036	rBV	61922	114395	5.38%	0.683%
22	13.451	1036	1038	1041	rBV	320157	339064	15.95%	2.023%
23	13.679	1056	1058	1060	rBV	47525	45064	2.12%	0.269%
24	13.976	1082	1084	1087	rBV	36617	41038	1.93%	0.245%
25	14.274	1106	1110	1112	rBV	34611	39121	1.84%	0.233%
26	14.548	1132	1134	1137	rBV	20147	27005	1.27%	0.161%
27	14.765	1151	1153	1155	rBV	210637	242721	11.42%	1.448%
28	14.834	1157	1159	1162	rVB	19248	22377	1.05%	0.134%
29	15.154	1184	1187	1190	rBV	16565	21288	1.00%	0.127%

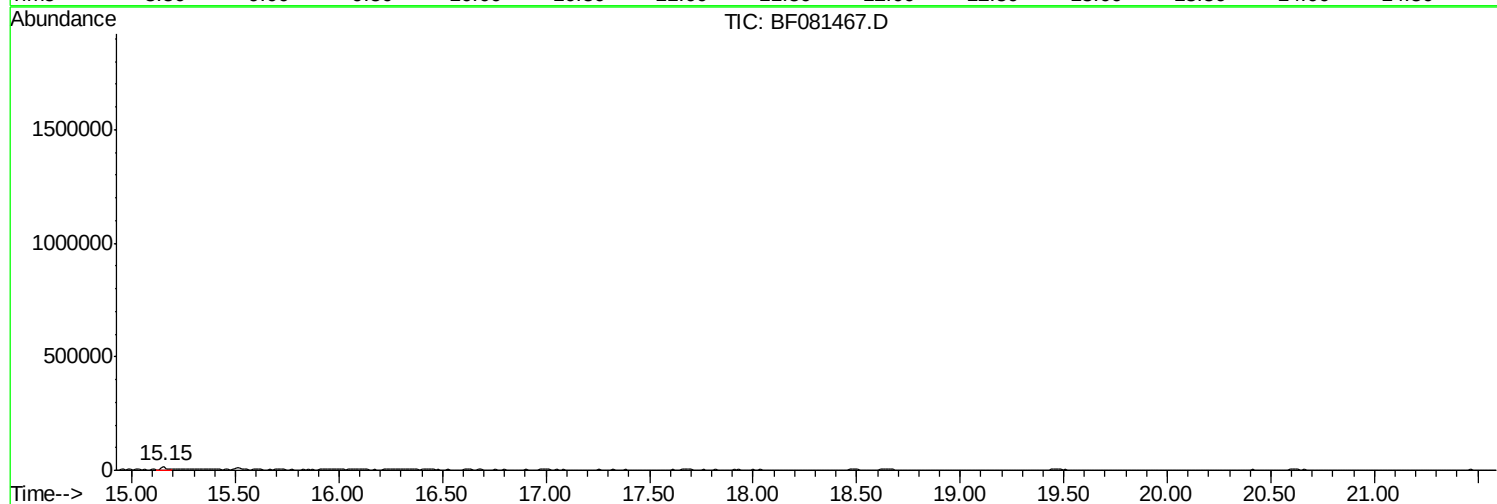
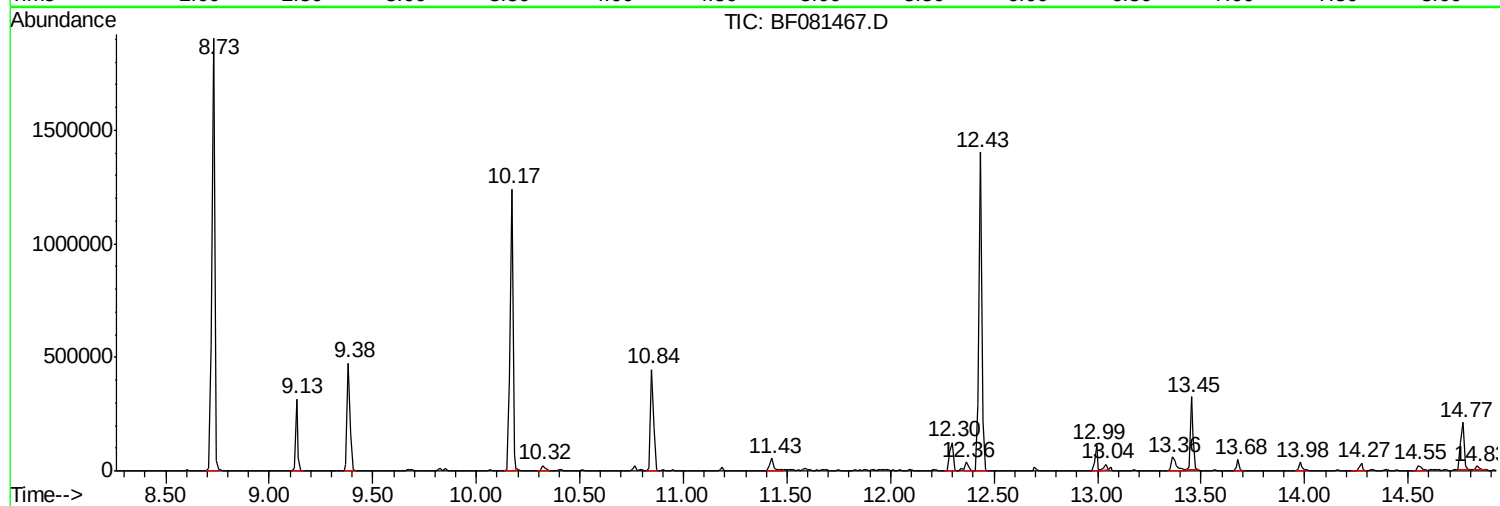
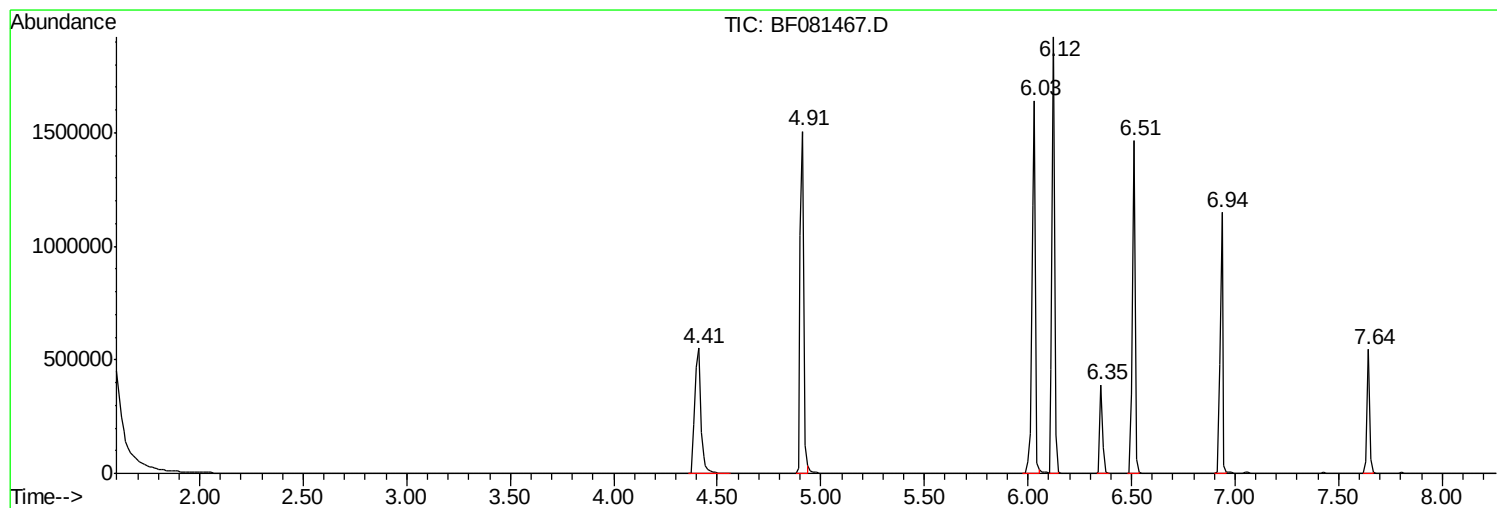
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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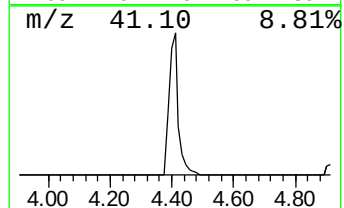
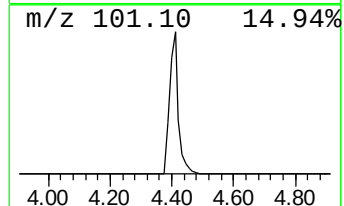
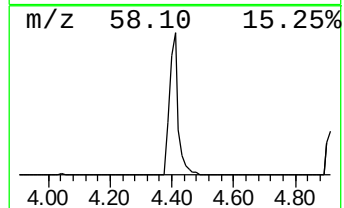
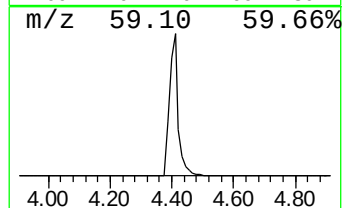
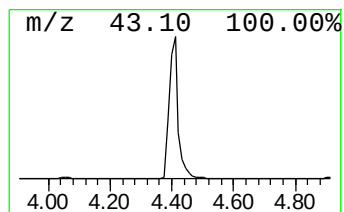
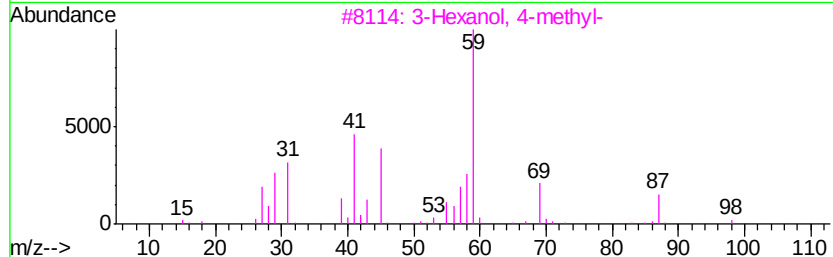
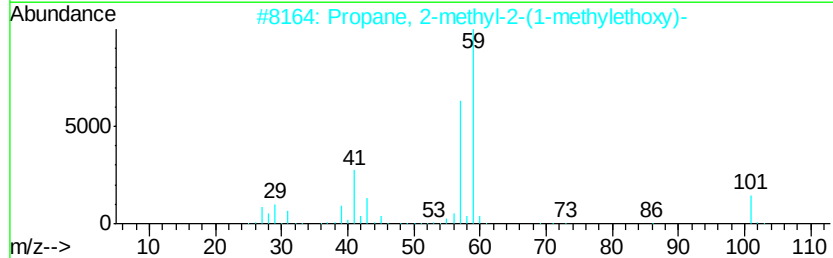
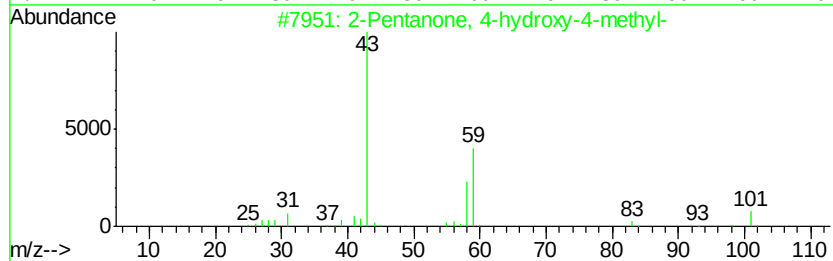
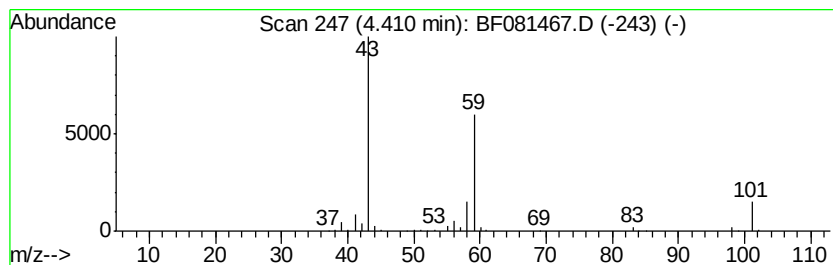
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	61.17 ng	1071110	1,4-Dichlorobenzene-d4	6.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Octanol	130	C8H18O	000589-98-0	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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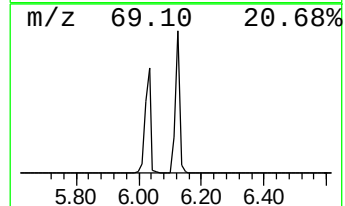
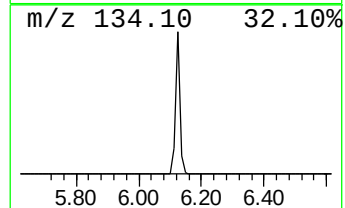
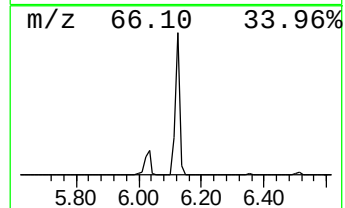
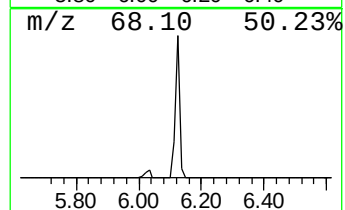
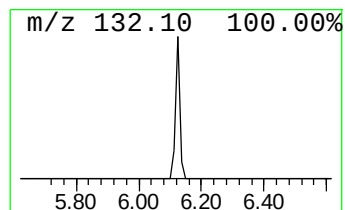
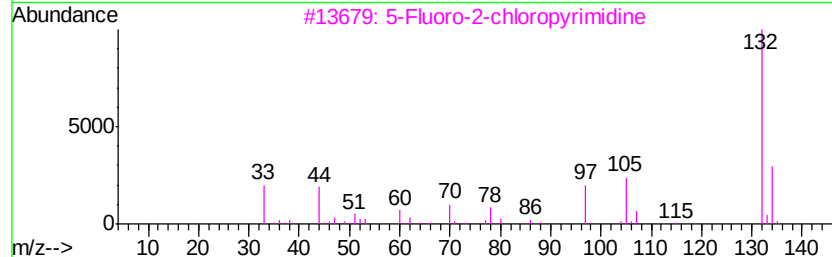
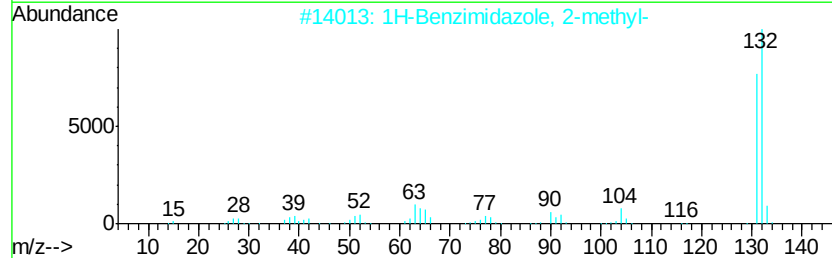
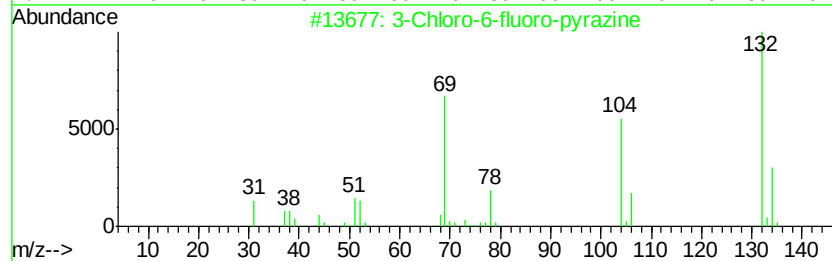
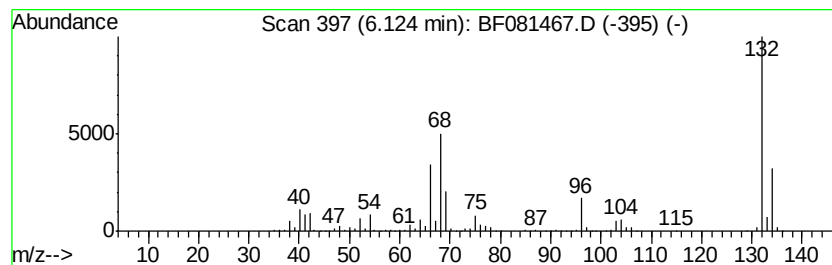
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Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	99.58 ng	1743830	1,4-Dichlorobenzene-d4	6.35

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	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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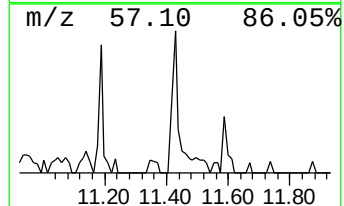
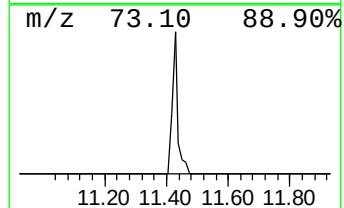
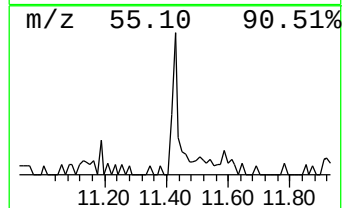
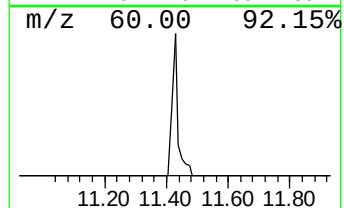
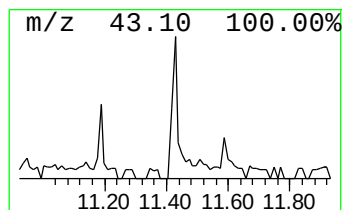
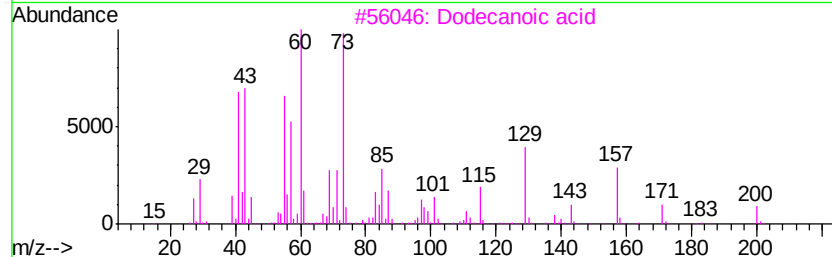
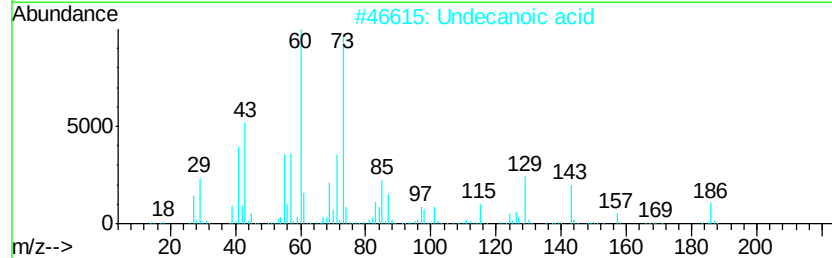
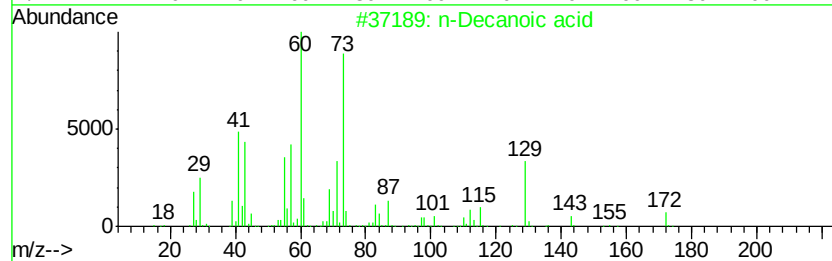
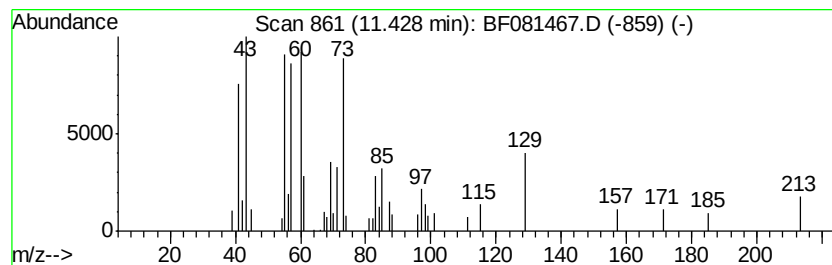
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Peak Number 4 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.43	2.90 ng	65353	Phenanthrene-d10	10.84		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	50	
2	Undecanoic acid	186	C11H22O2	000112-37-8	50	
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50	
4	3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	43	
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	43	



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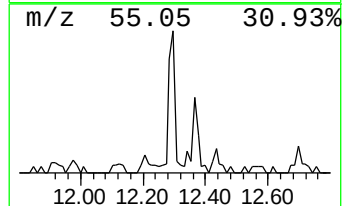
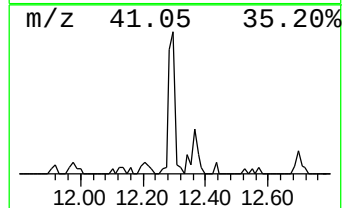
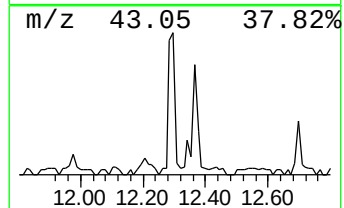
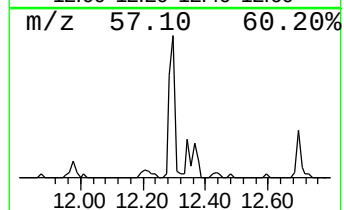
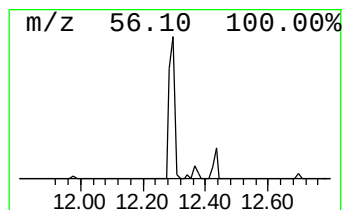
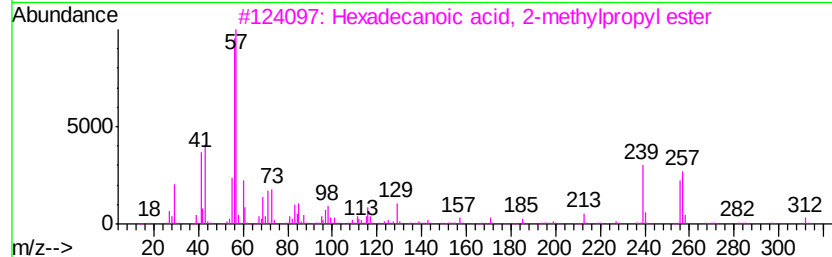
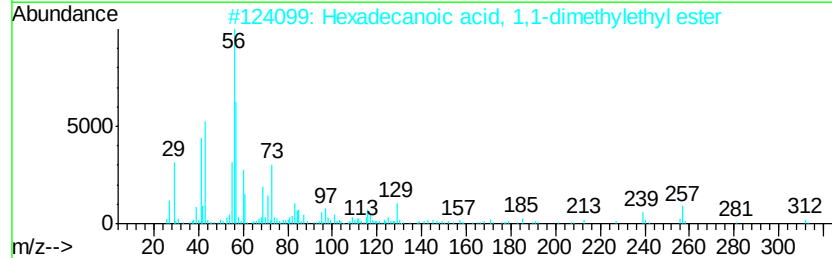
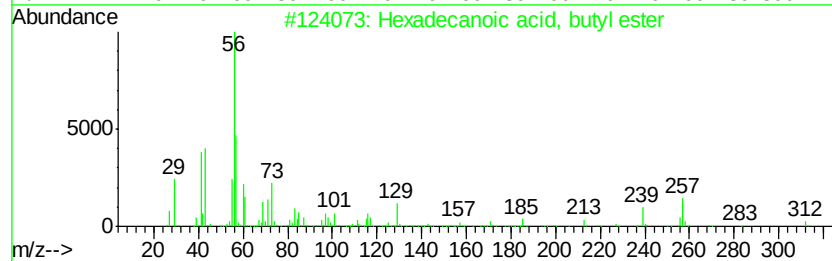
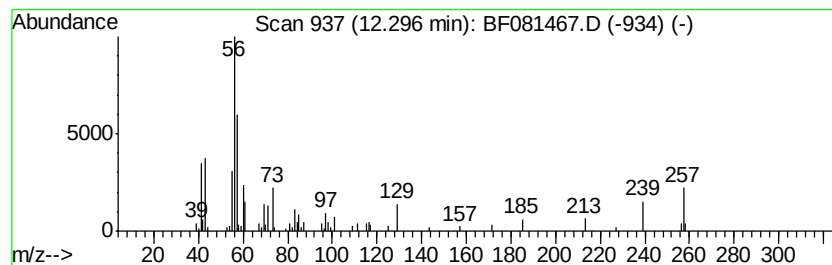
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	8.56 ng	145101	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	80
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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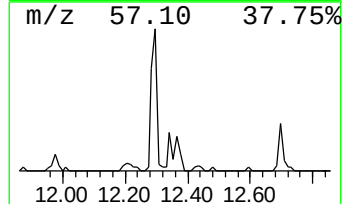
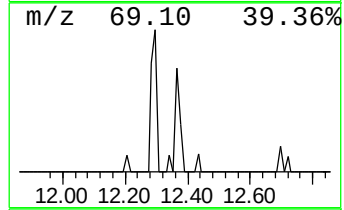
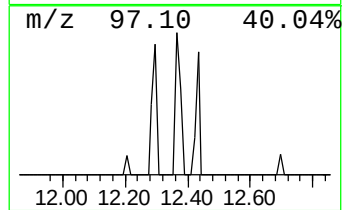
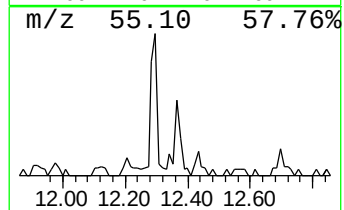
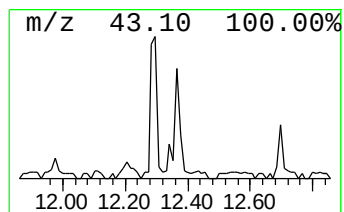
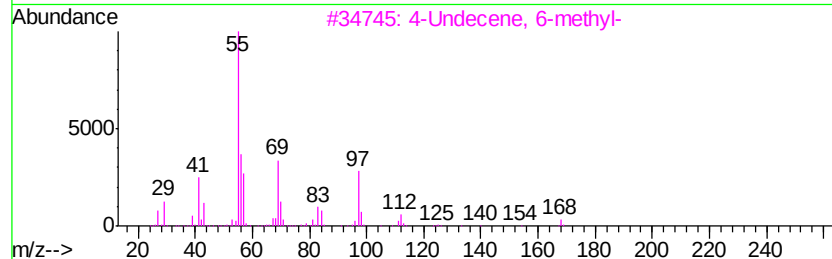
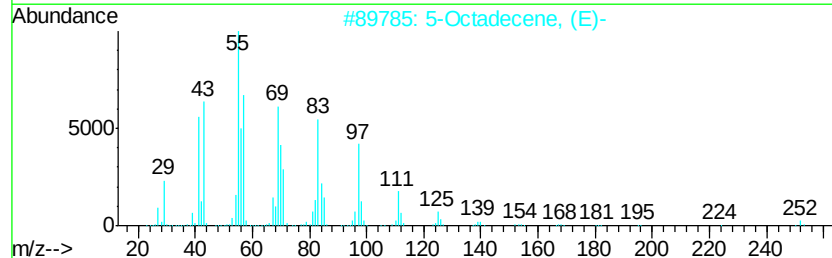
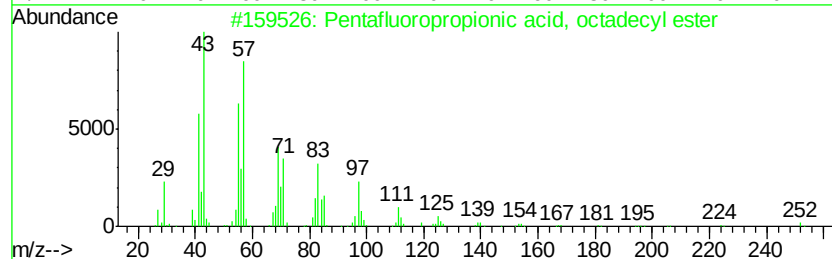
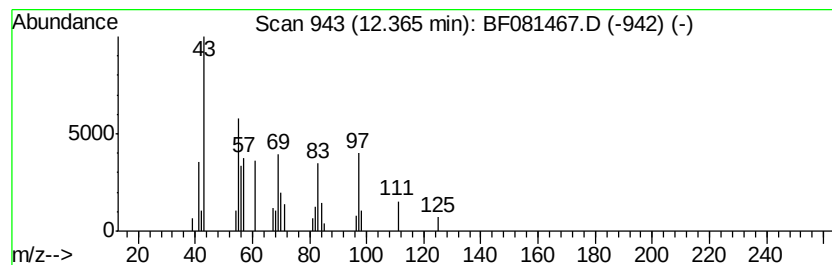
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	2.19 ng	37158	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	59
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	58
3		4-Undecene, 6-methyl-	168	C12H24	1000061-85-4	53
4		Cycloheptane, methyl-	112	C8H16	004126-78-7	53
5		Cyclotetradecane	196	C14H28	000295-17-0	52



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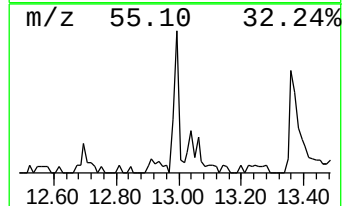
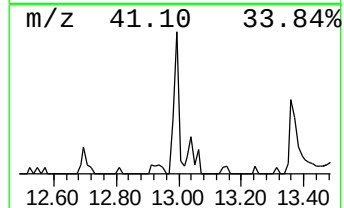
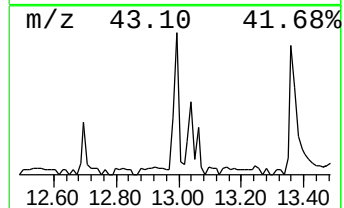
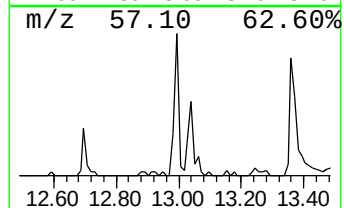
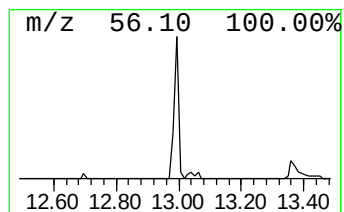
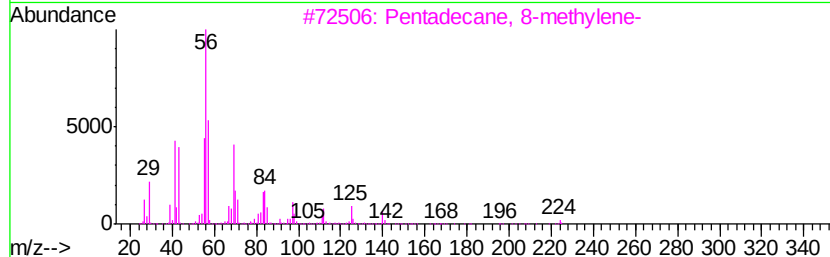
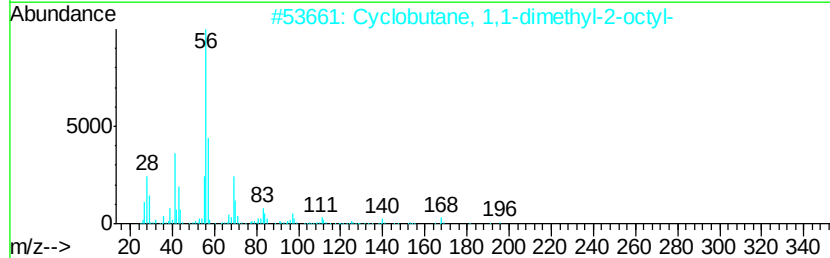
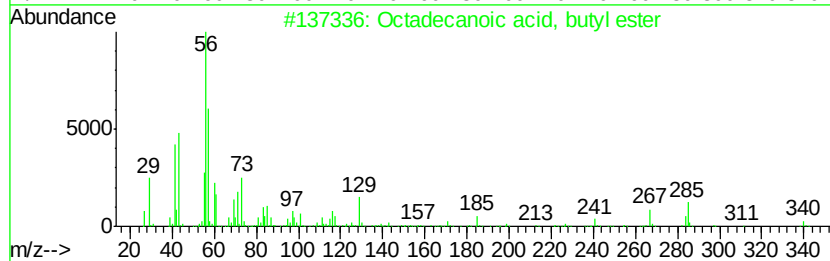
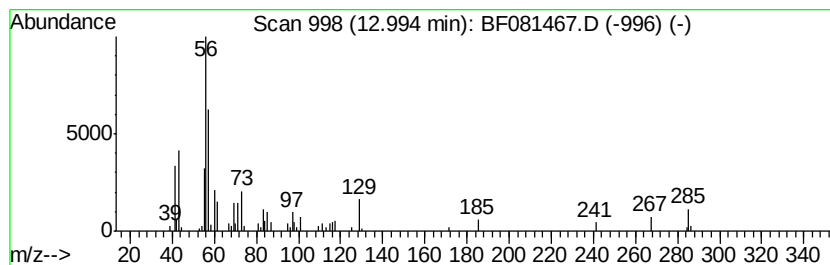
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	6.23 ng	105654	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
3		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081467.D
Acq On : 5 Sep 2015 16:19
Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-10-20

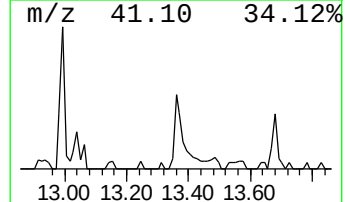
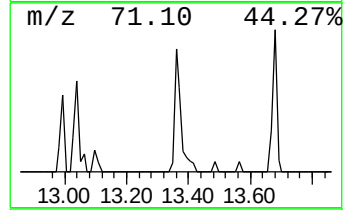
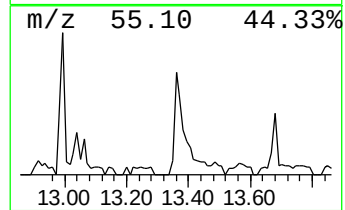
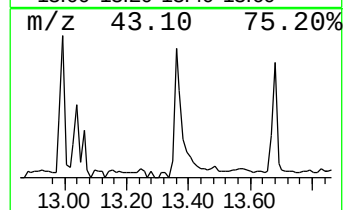
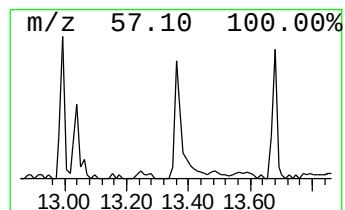
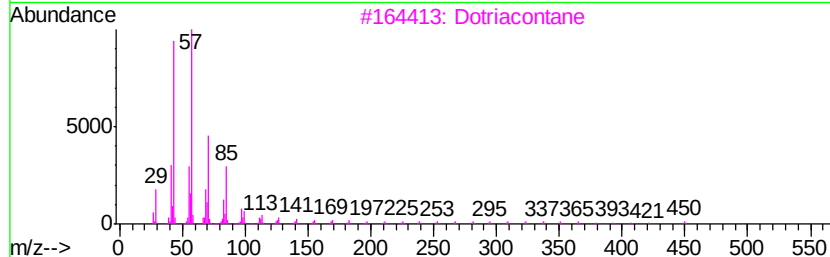
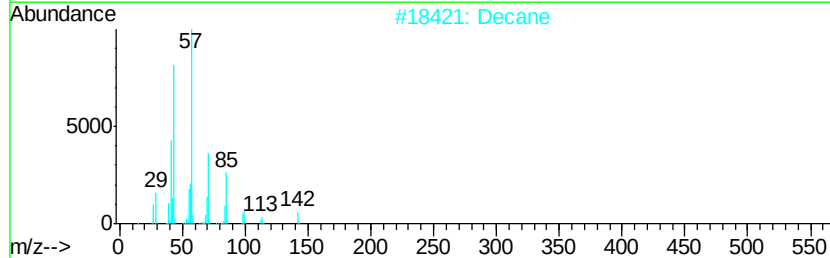
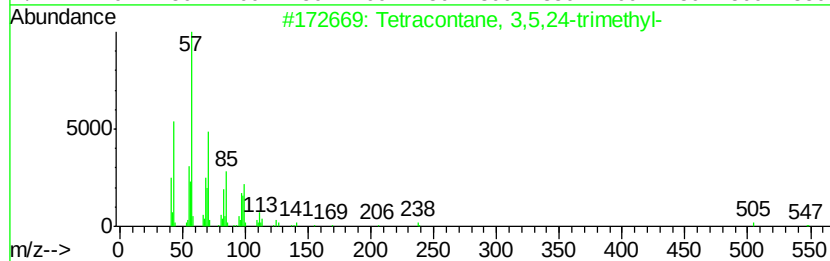
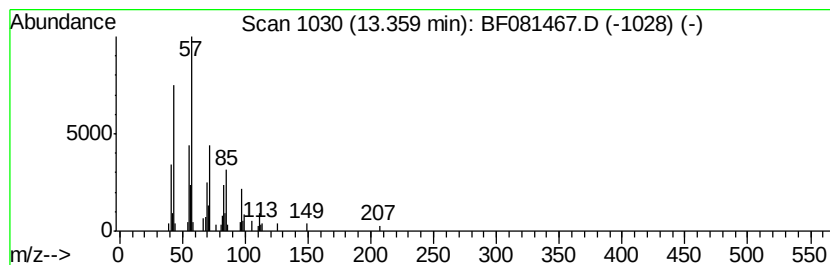
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracontane, 3,5,24-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	6.75 ng	114395	Chrysene-d12	13.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	90
2		Decane	142	C10H22	000124-18-5	52
3		Dotriacontane	451	C32H66	000544-85-4	50
4		10-Methylnonadecane	282	C20H42	056862-62-5	50
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
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Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

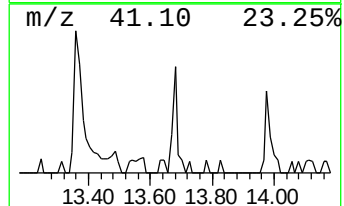
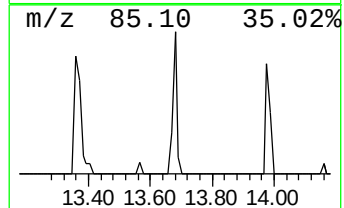
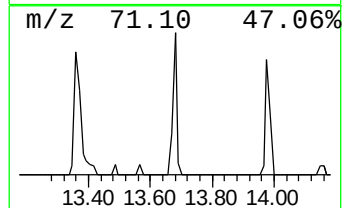
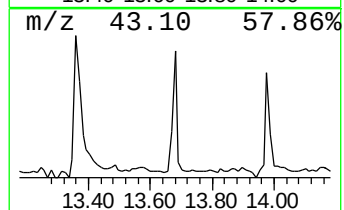
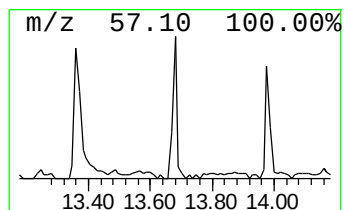
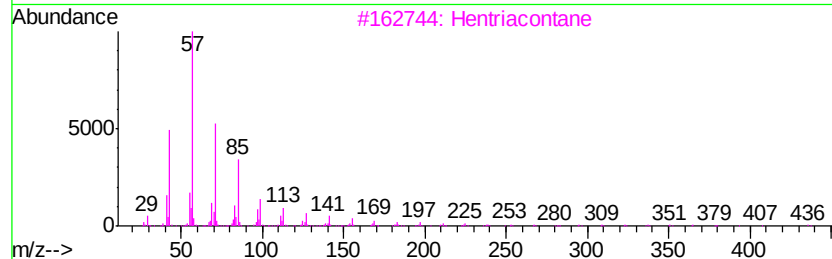
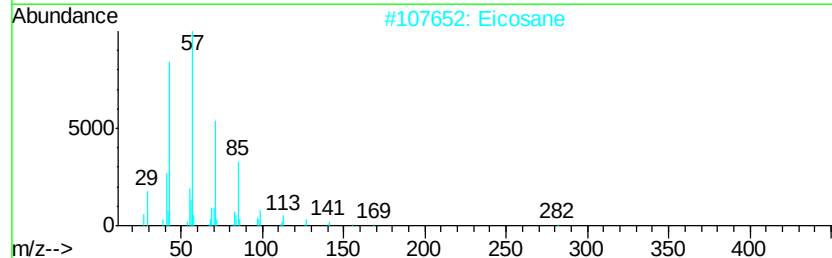
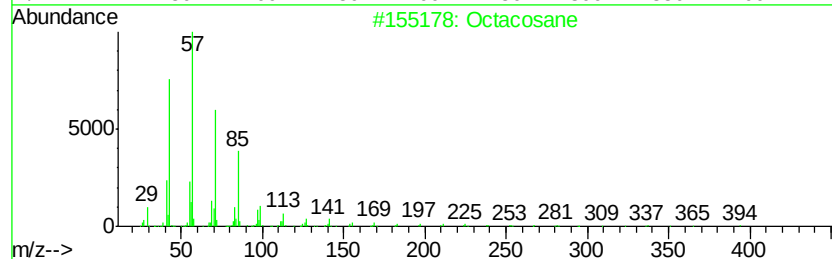
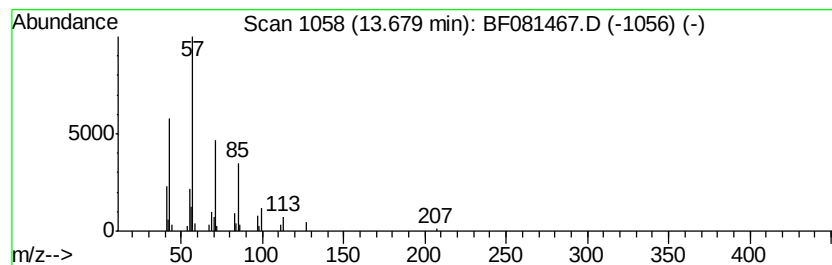
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.66 ng	45064	Chrysene-d12	13.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	91
2	Eicosane	282 C20H42	000112-95-8	90
3	Hentriacontane	437 C31H64	000630-04-6	90
4	Heptacosane	380 C27H56	000593-49-7	90
5	Tetratetracontane	619 C44H90	007098-22-8	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081467.D
Acq On : 5 Sep 2015 16:19
Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

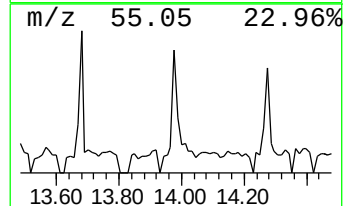
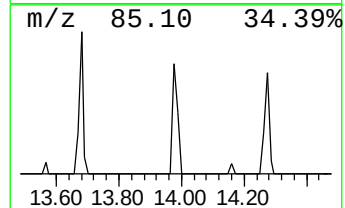
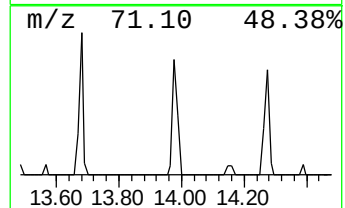
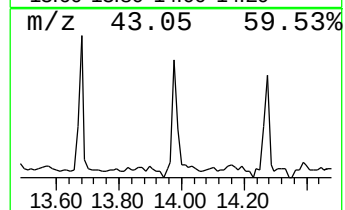
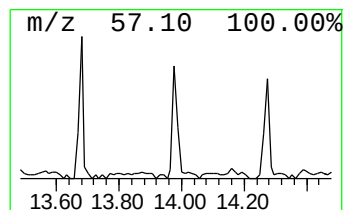
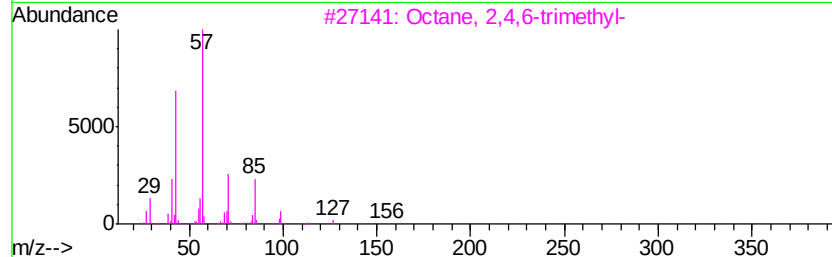
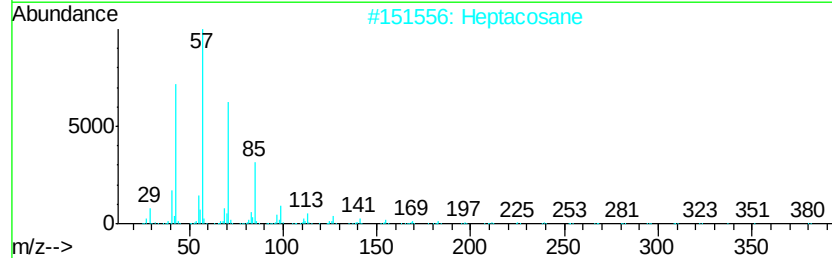
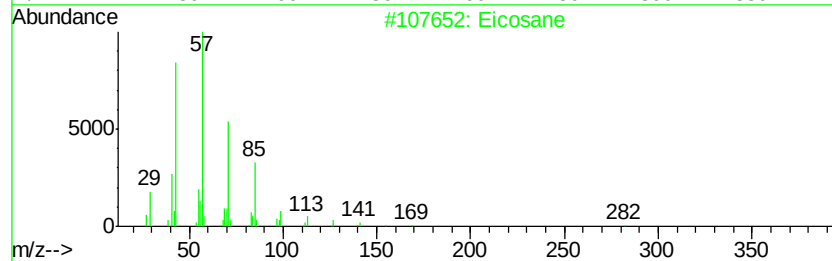
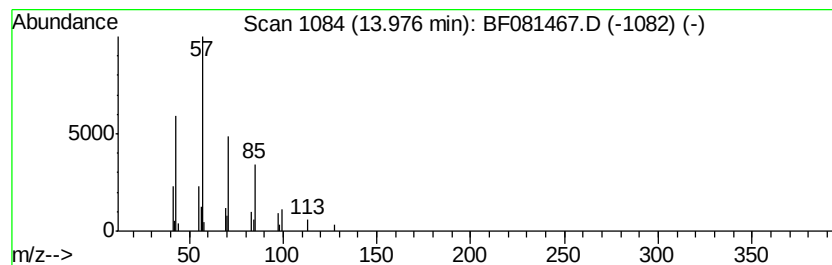
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.42 ng	41038	Chrysene-d12	13.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	90
2	Heptacosane	380 C27H56	000593-49-7	72
3	Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9	72
4	Hexadecane	226 C16H34	000544-76-3	64
5	Pentadecane	212 C15H32	000629-62-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081467.D
Acq On : 5 Sep 2015 16:19
Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP226BR-10-20

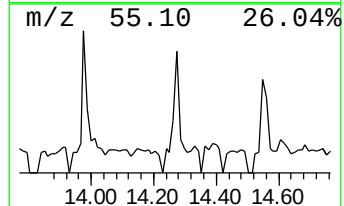
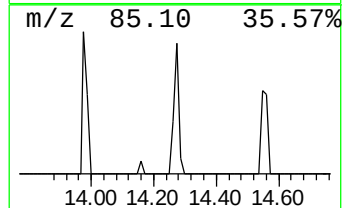
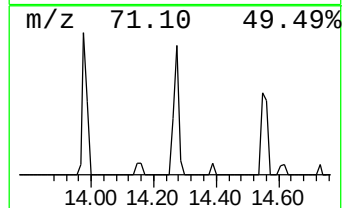
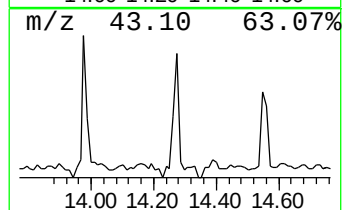
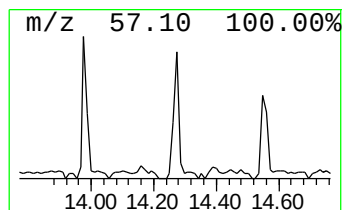
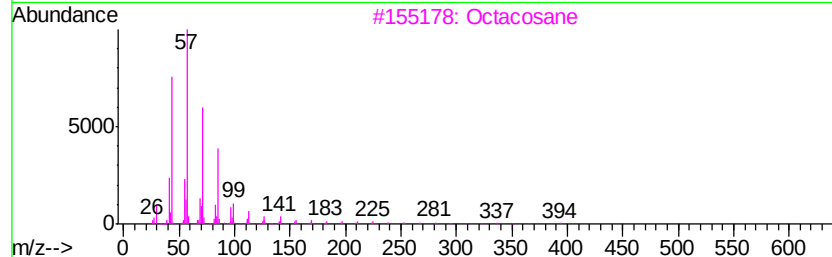
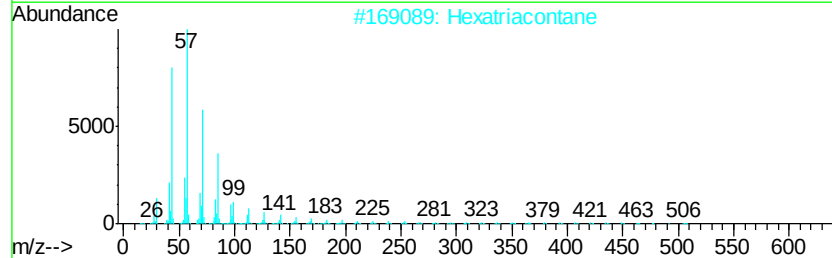
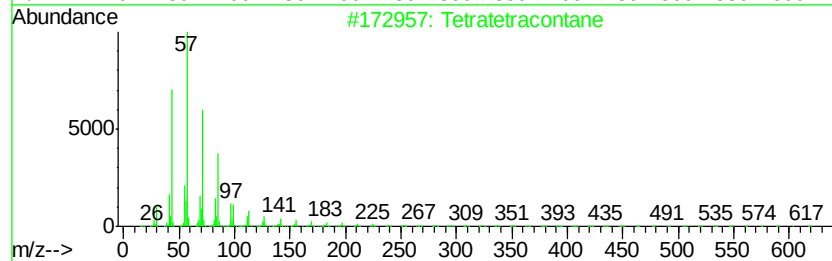
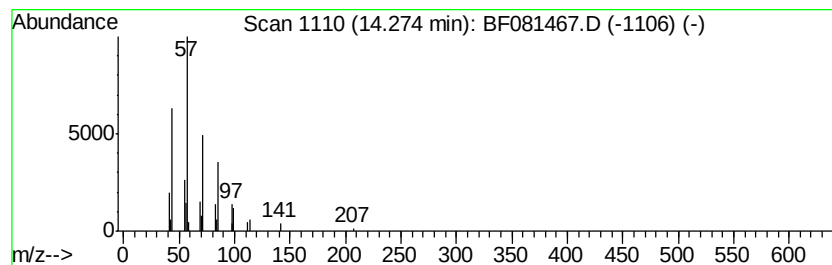
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	3.22 ng	39121	Perylene-d12	14.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hexatriacontane	507	C36H74	000630-06-8	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetratriacontane	479	C34H70	014167-59-0	86
5			Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081467.D
Acq On : 5 Sep 2015 16:19
Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MGP226BR-10-20

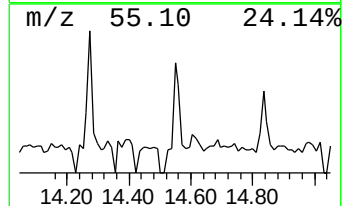
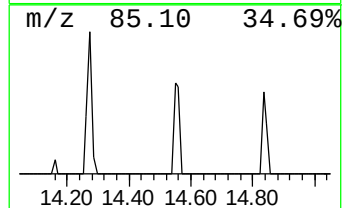
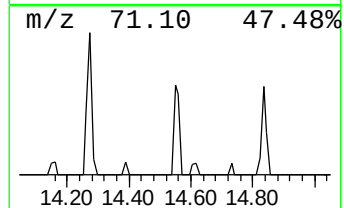
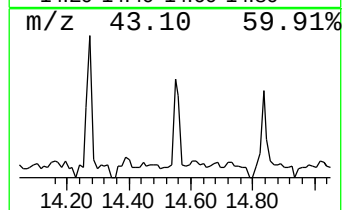
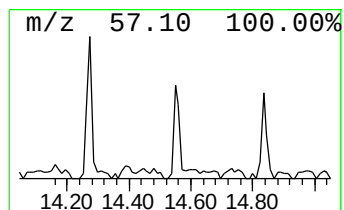
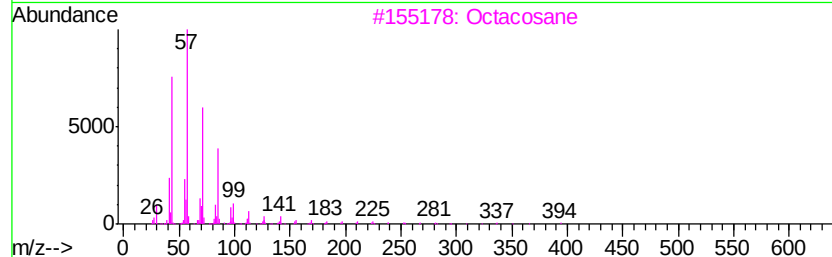
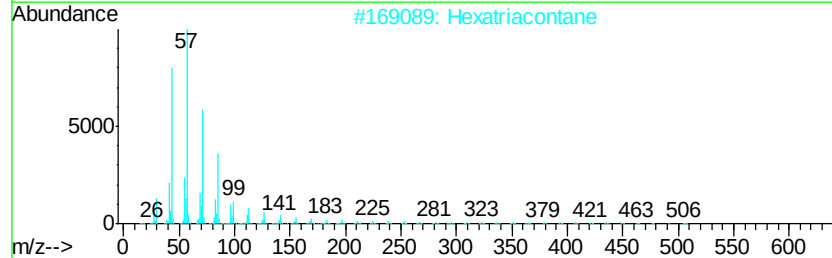
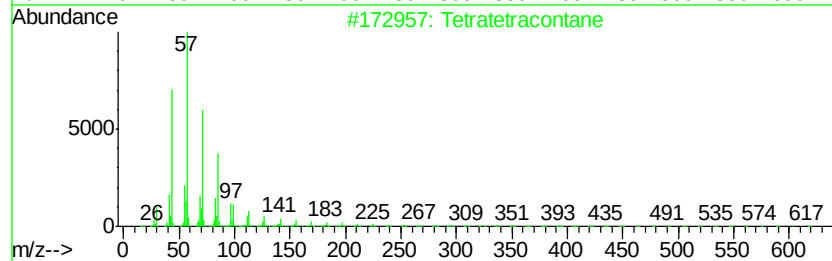
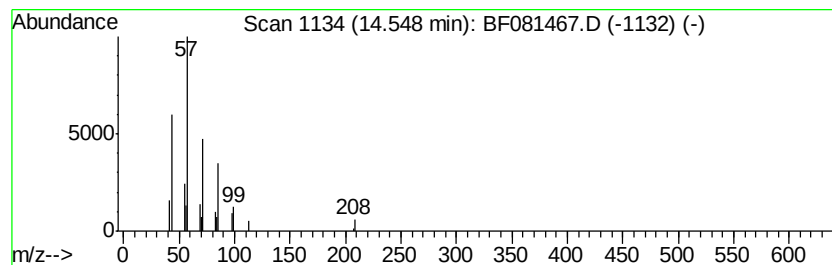
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexatriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.23 ng	27005	Perylene-d12	14.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Hexatriacontane	507	C36H74	000630-06-8	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Tetracosane	338	C24H50	000646-31-1	80
5		Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081467.D
Acq On : 5 Sep 2015 16:19
Operator : UM/IZ
Sample : G3559-01
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MGP226BR-10-20

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
2-Pentanone, 4-hy...	4.41	61.2	ng	1071110	1	6.35	350223	20.0
unknown6.12	6.12	99.6	ng	1743830	1	6.35	350223	20.0
n-Decanoic acid	11.43	2.9	ng	65353	4	10.84	450393	20.0
Hexadecanoic acid...	12.30	8.6	ng	145101	5	13.45	339064	20.0
Pentafluoropropio...	12.36	2.2	ng	37158	5	13.45	339064	20.0
Octadecanoic acid...	12.99	6.2	ng	105654	5	13.45	339064	20.0
Tetracontane, 3,5...	13.36	6.8	ng	114395	5	13.45	339064	20.0
Octacosane	13.68	2.7	ng	45064	5	13.45	339064	20.0
Eicosane	13.98	2.4	ng	41038	5	13.45	339064	20.0
Tetratetracontane	14.27	3.2	ng	39121	6	14.77	242721	20.0
Hexatriacontane	14.55	2.2	ng	27005	6	14.77	242721	20.0