

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
 Data File : BF089048.D
 Acq On : 16 Jul 2016 11:36
 Operator : UM/SJ
 Sample : H3951-16 5X
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LSS-SB-SB06(0-2in)

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-BF063016.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.770	14	16	48	rVB	1372386	2517045	74.41%	17.076%
2	2.170	48	51	59	rVB	23283	46597	1.38%	0.316%
3	4.776	277	279	282	rVB	30395	34491	1.02%	0.234%
4	5.244	318	320	323	rBV	207188	192335	5.69%	1.305%
5	6.307	411	413	415	rBV	258588	230509	6.81%	1.564%
6	6.422	421	423	426	rBV	177966	212081	6.27%	1.439%
7	6.662	441	444	446	rBV	397056	351045	10.38%	2.381%
8	6.810	455	457	460	rVB	169833	165980	4.91%	1.126%
9	7.222	491	493	495	rBV	182746	146567	4.33%	0.994%
10	7.942	554	556	559	rBV	402034	443069	13.10%	3.006%
11	8.719	621	624	626	rBV	28568	49127	1.45%	0.333%
12	9.028	648	651	653	rBV	297395	275356	8.14%	1.868%
13	9.428	683	686	687	rBV	59031	54971	1.62%	0.373%
14	9.702	707	710	712	rBV	480335	499520	14.77%	3.389%
15	9.942	725	731	733	rBV	67522	99073	2.93%	0.672%
16	10.479	777	778	780	rVB	115009	101414	3.00%	0.688%
17	10.879	810	813	817	rVV2	73859	134436	3.97%	0.912%
18	11.176	836	839	840	rBV	523842	463018	13.69%	3.141%
19	11.245	843	845	847	rBV	27618	37823	1.12%	0.257%
20	11.634	877	879	881	rBV	105921	217462	6.43%	1.475%
21	11.702	882	885	886	rVV2	109936	264713	7.83%	1.796%
22	11.771	886	891	896	rVB2	805248	1859337	54.96%	12.614%
23	12.388	942	945	947	rBV	166121	222659	6.58%	1.511%
24	12.479	947	953	954	rBV3	188201	481696	14.24%	3.268%
25	12.571	954	961	963	rVV	1328372	3382835	100.00%	22.949%
26	12.605	963	964	967	rVB	135233	204204	6.04%	1.385%
27	12.765	976	978	980	rBV	212029	198253	5.86%	1.345%
28	13.245	1018	1020	1022	rBV	206680	231556	6.85%	1.571%
29	13.657	1055	1056	1057	rBV	120590	133516	3.95%	0.906%
30	13.817	1067	1070	1071	rBV2	387633	513610	15.18%	3.484%
31	14.445	1123	1125	1127	rBV	239933	247170	7.31%	1.677%
32	15.120	1182	1184	1187	rBV	76155	119471	3.53%	0.810%
33	15.188	1187	1190	1191	rBV	165305	243412	7.20%	1.651%
34	16.457	1299	1301	1306	rVB	56401	104665	3.09%	0.710%

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSS-SB-SB06(0-2in)

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

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35	16.845	1332	1335	1338	rVB	51031	107236	3.17%	0.727%
36	17.383	1380	1382	1391	rVB5	60608	154289	4.56%	1.047%

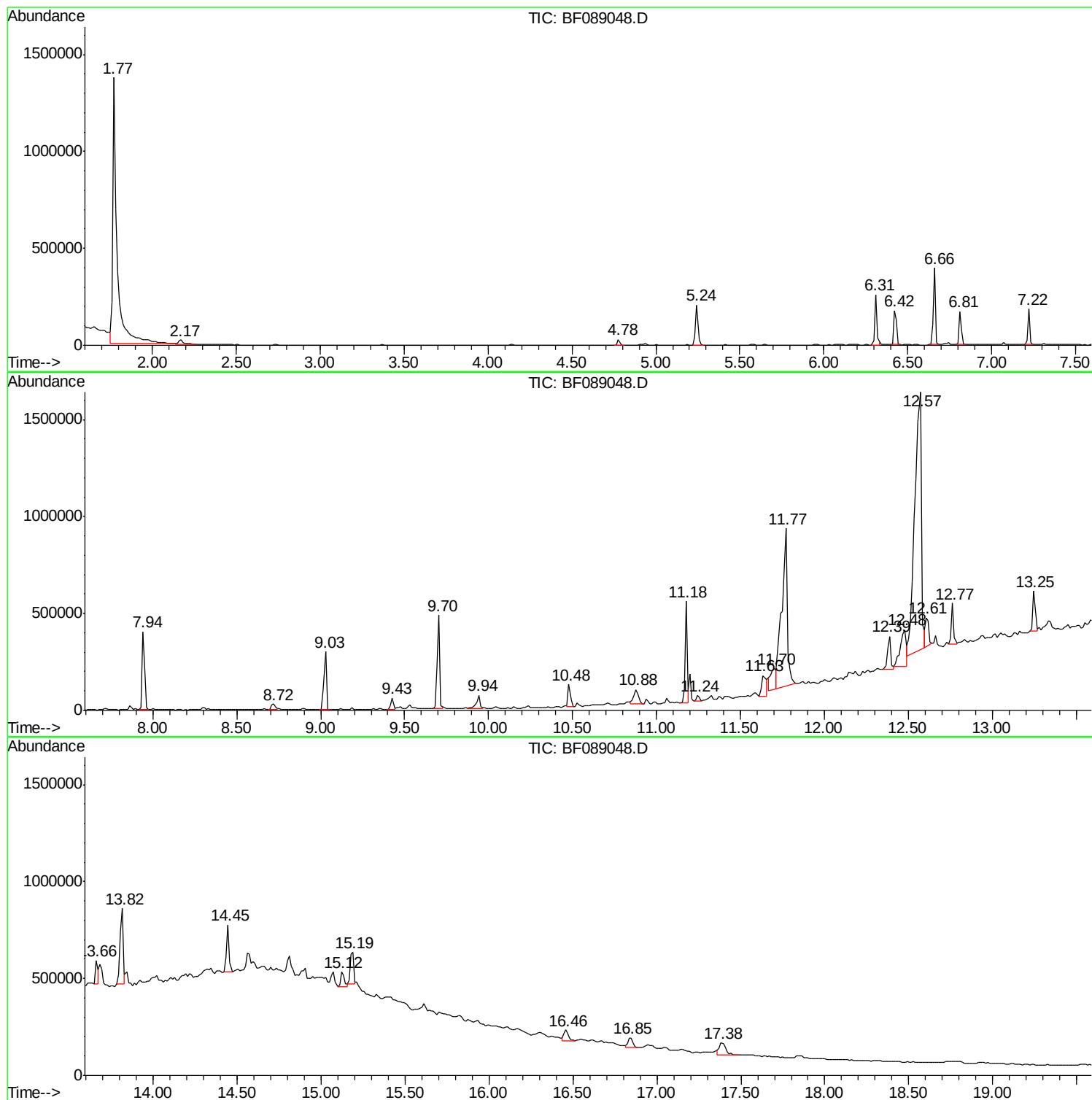
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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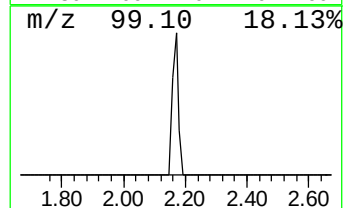
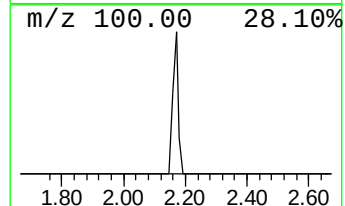
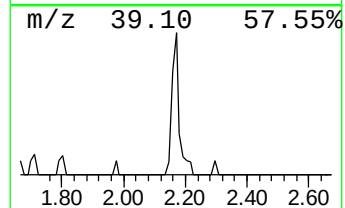
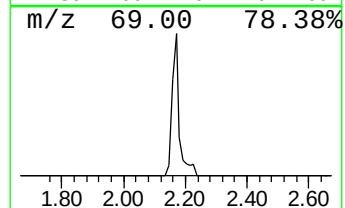
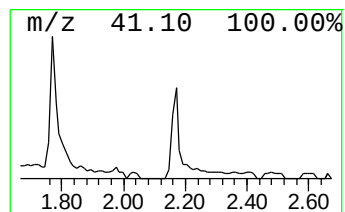
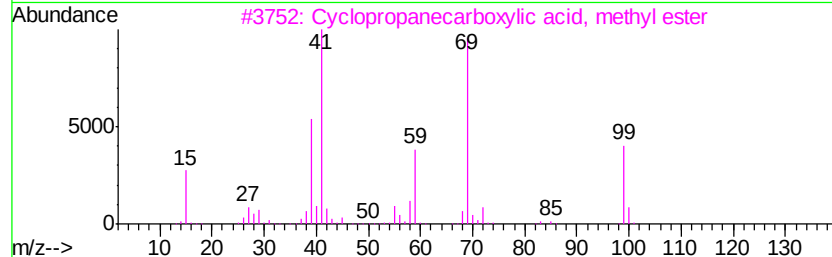
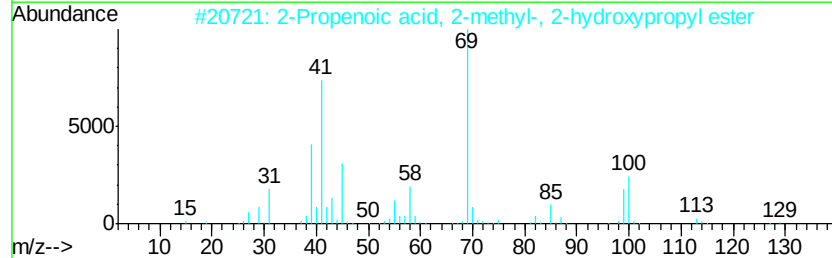
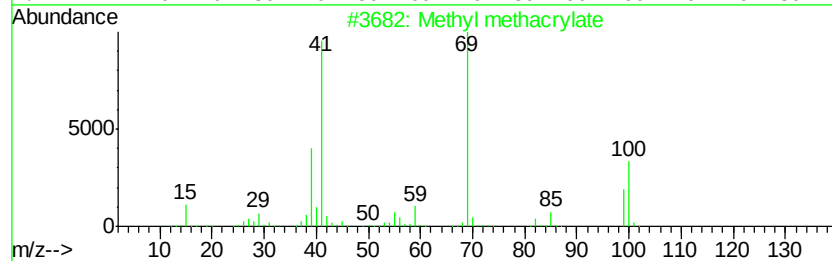
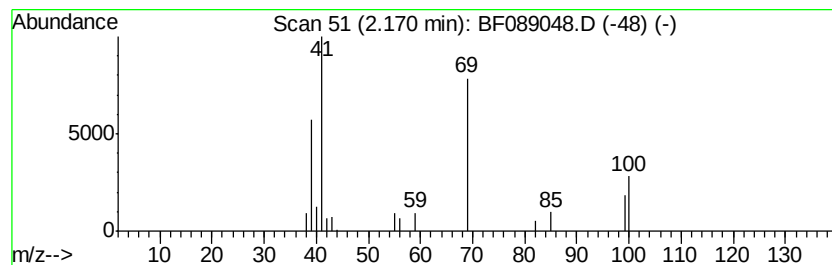
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Methyl methacrylate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.65 ng	46597	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl methacrylate	100	C5H8O2	000080-62-6	76
2			2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	72
3			Cyclopropanecarboxylic acid, met...	100	C5H8O2	002868-37-3	50
4			2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	25
5			Methyl 3-butenote	100	C5H8O2	003724-55-8	25



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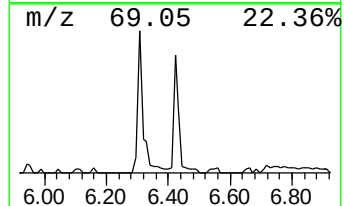
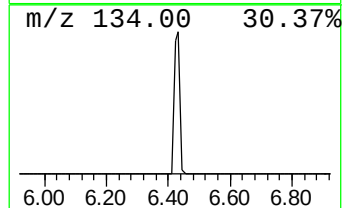
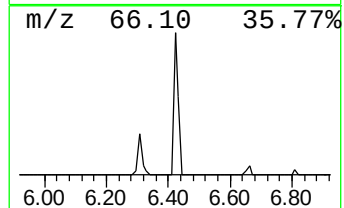
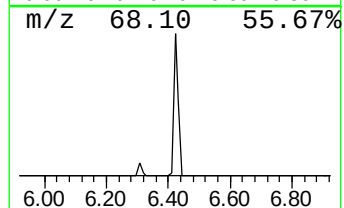
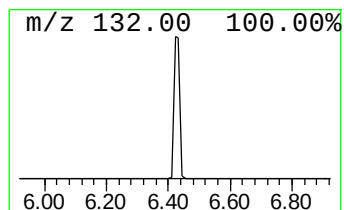
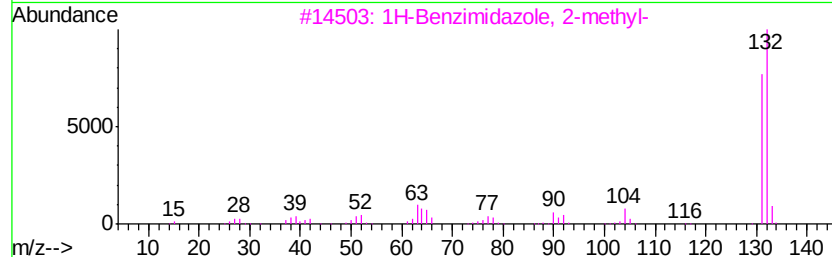
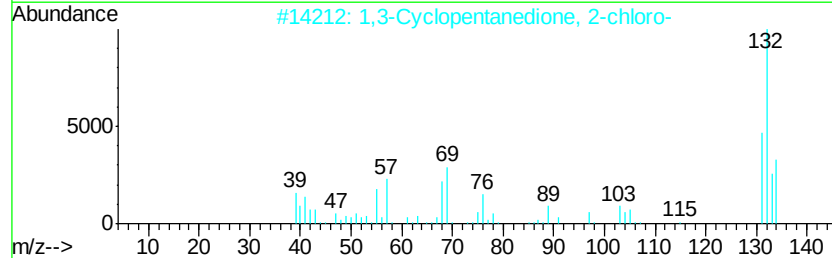
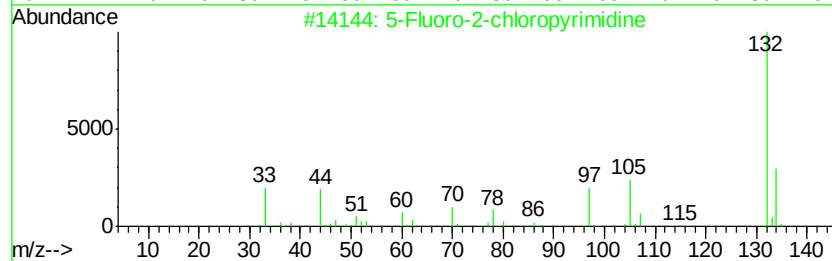
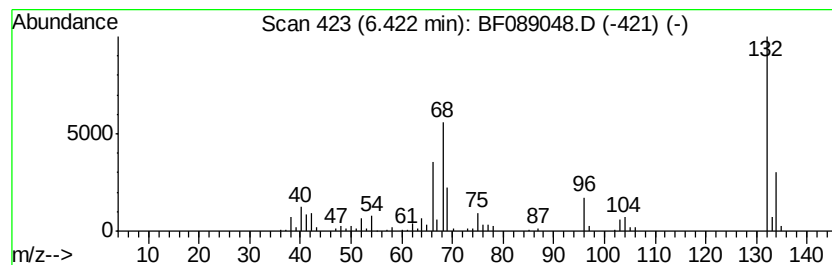
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.42 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	12.08 ng	212081	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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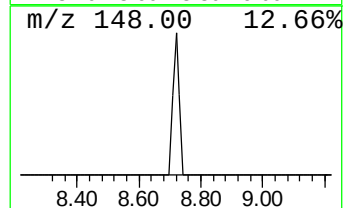
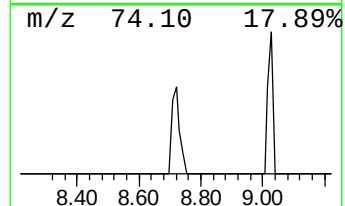
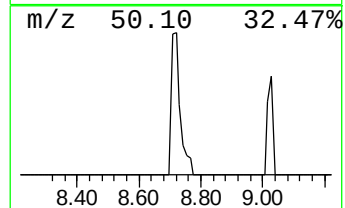
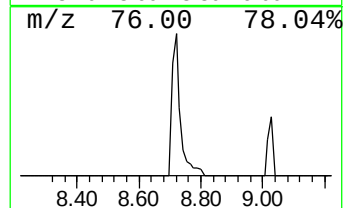
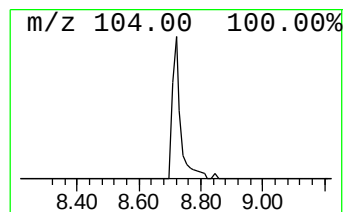
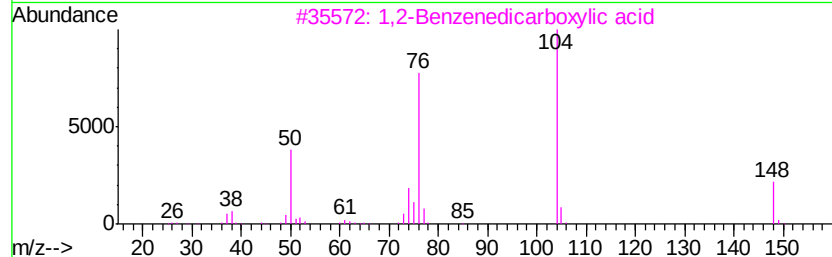
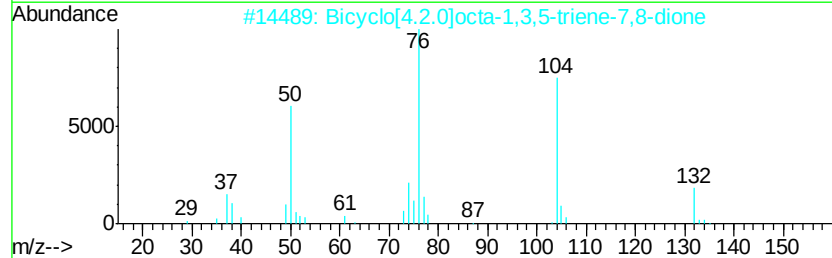
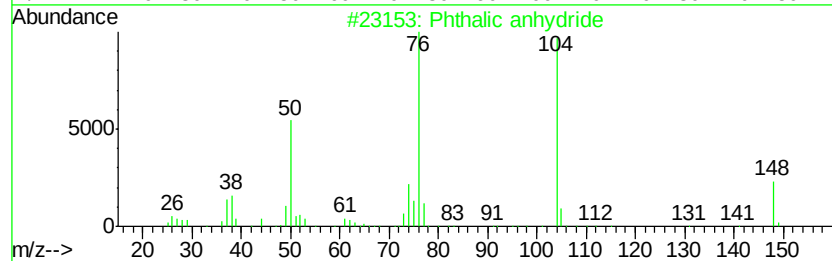
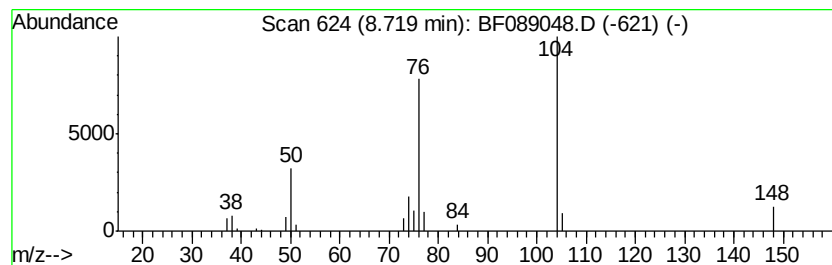
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Phthalic anhydride Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.22 ng	49127	Naphthalene-d8	7.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	94
2			Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	83
3			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
4			Phthalamic acid	165	C8H7NO3	000088-97-1	83
5			1H-Isoindole-1,3(2H)-dione, 2-(2...	201	C11H7NO3	004616-63-1	64



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Instrument :
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ClientSampleId :
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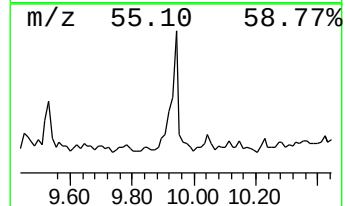
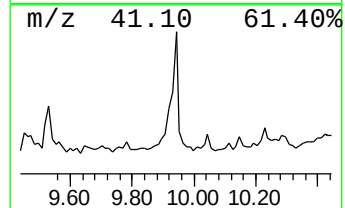
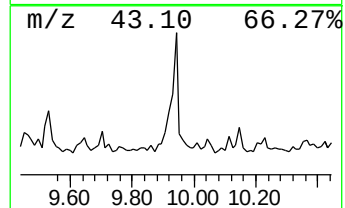
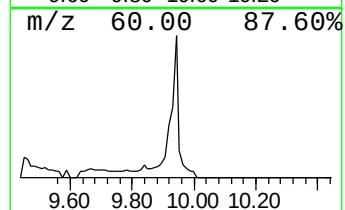
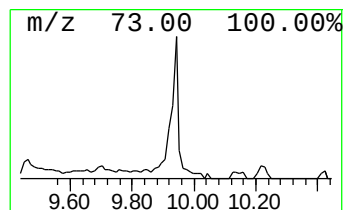
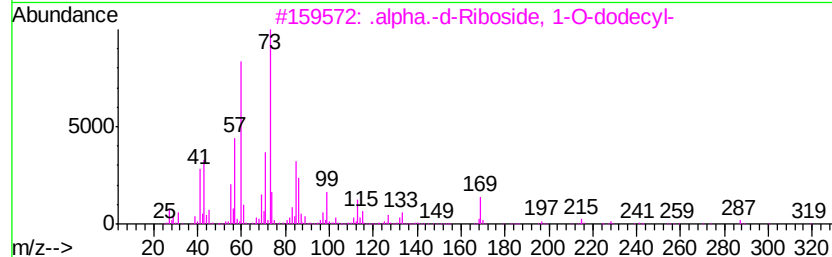
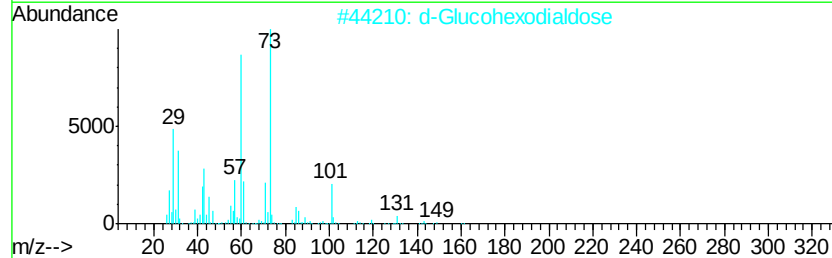
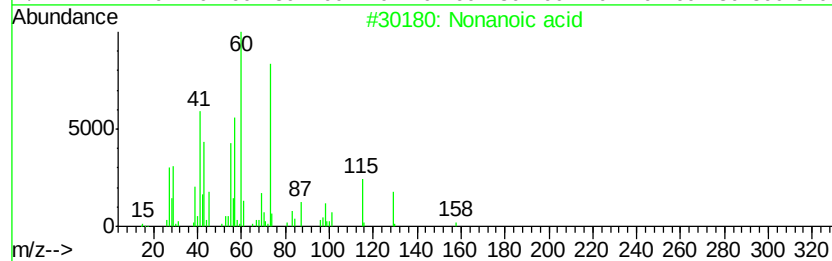
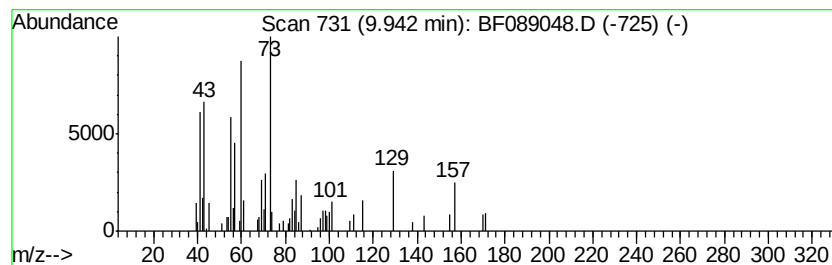
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown9.94 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	3.97 ng	99073	Acenaphthene-d10	9.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	43
2		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	43
3		.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	38
4		Alpha-l-rhamnopyranose	164	C6H12O5	035810-56-1	38
5		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38



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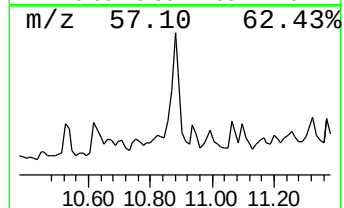
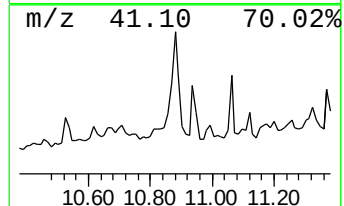
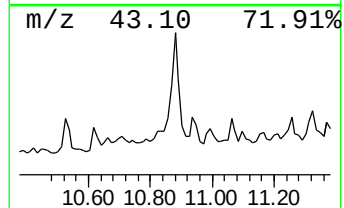
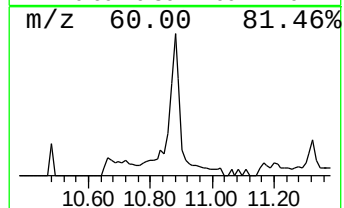
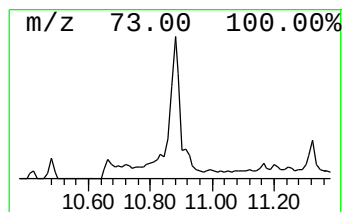
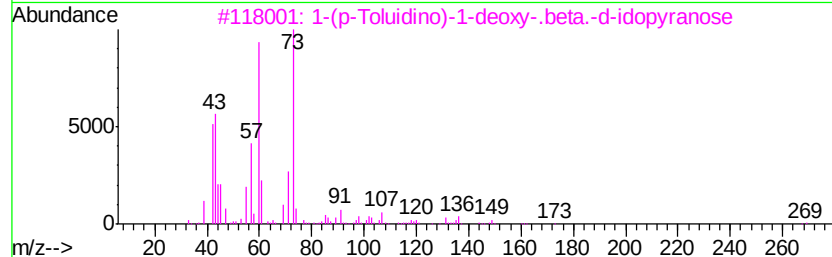
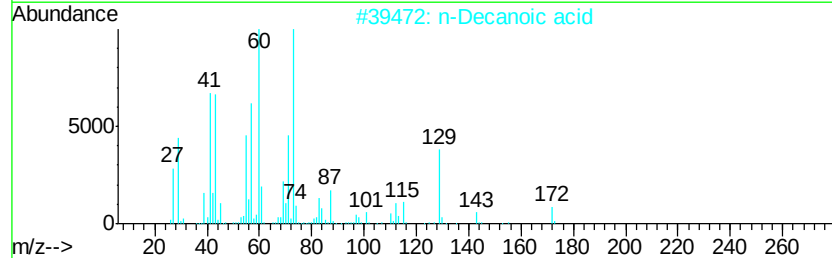
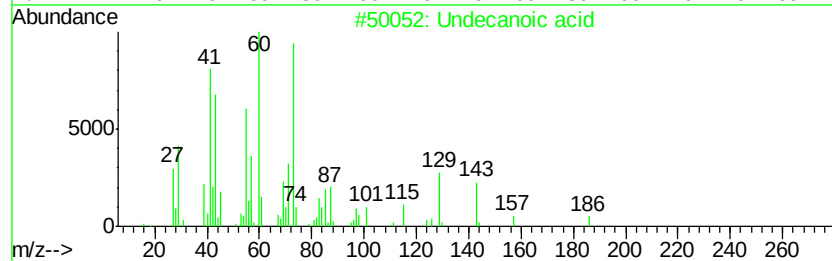
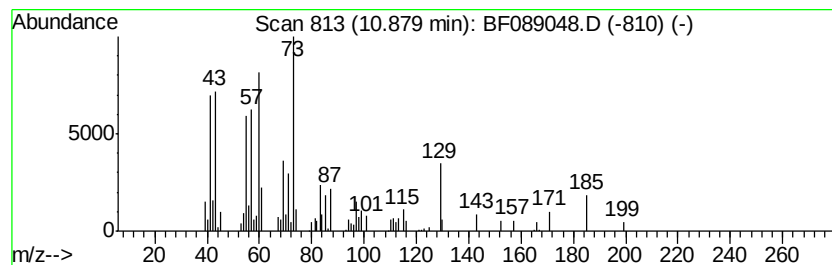
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Peak Number 7 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.88	5.81 ng	134436	Phenanthrene-d10		11.18
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	47
4	Methyl .beta.-d-galactopyranoside	194	C7H14O6	1000126-04-6	47
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	43



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LSS-SB-SB06(0-2in)

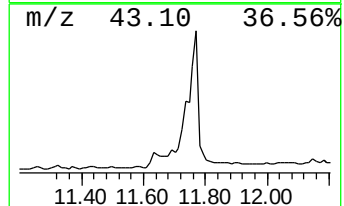
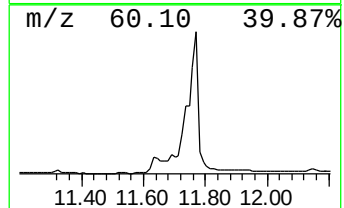
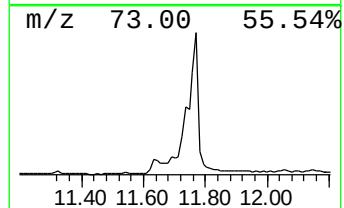
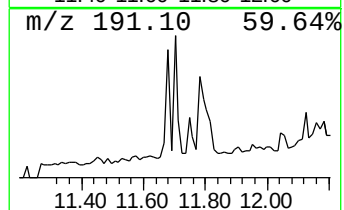
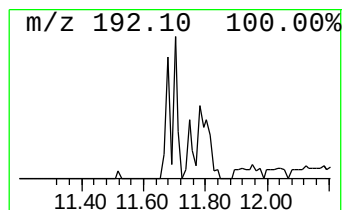
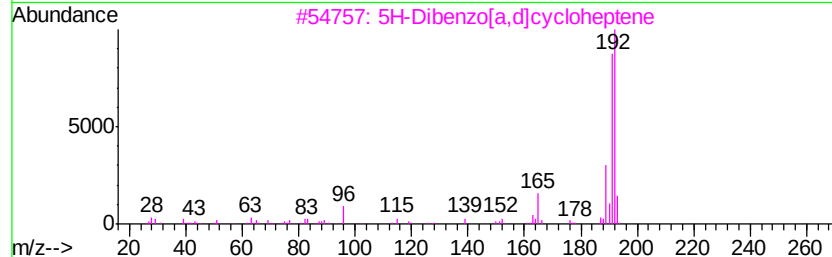
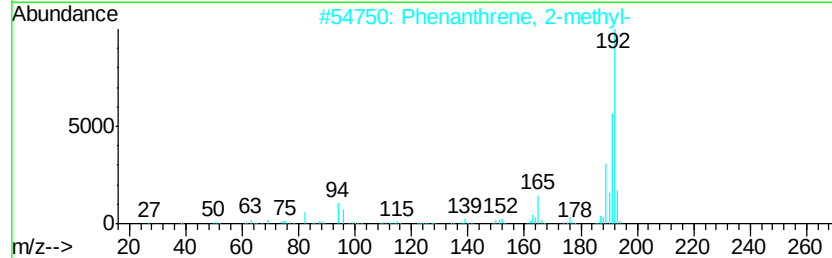
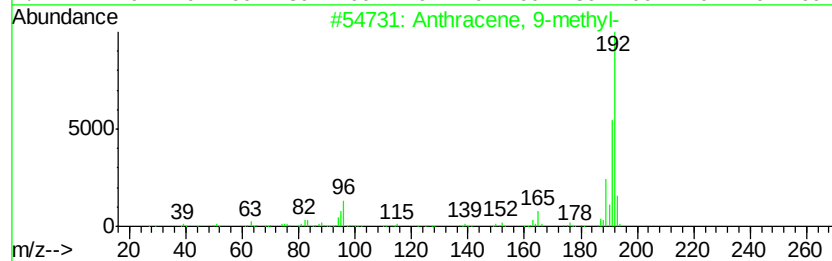
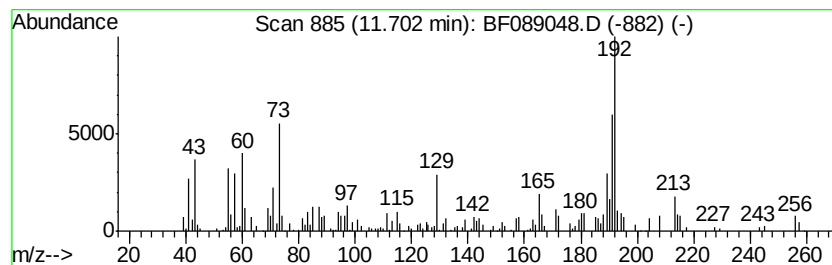
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Anthracene, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	11.43 ng	264713	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
3		5H-Dibenzof[a,d]cycloheptene	192	C15H12	000256-81-5	55
4		1H-Cyclopropa[all]phenanthrene, 1a,...	192	C15H12	000949-41-7	55
5		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	55



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089048.D
Acq On : 16 Jul 2016 11:36
Operator : UM/SJ
Sample : H3951-16 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSS-SB-SB06(0-2in)

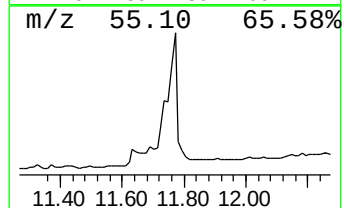
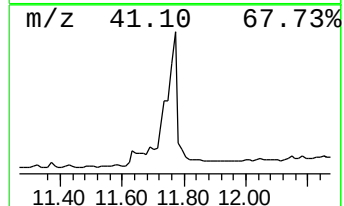
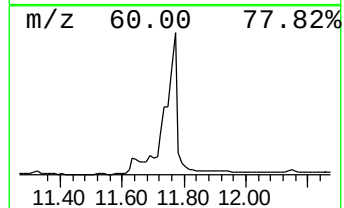
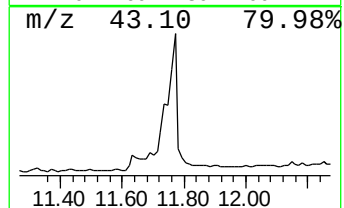
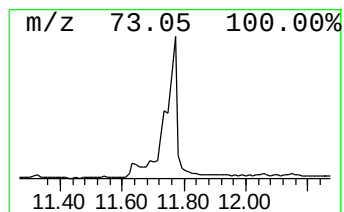
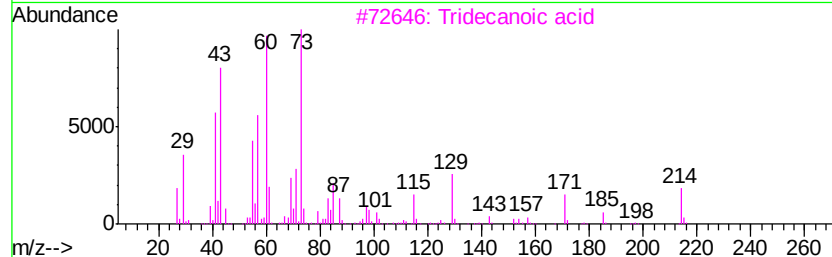
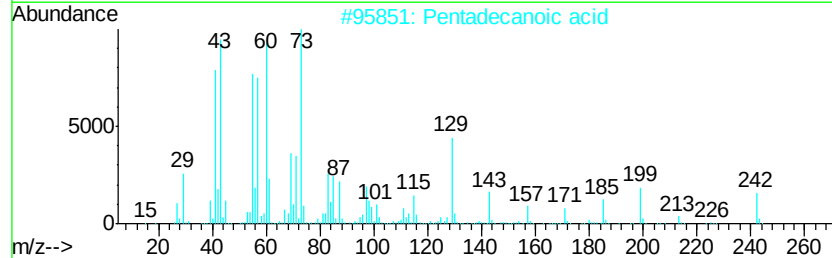
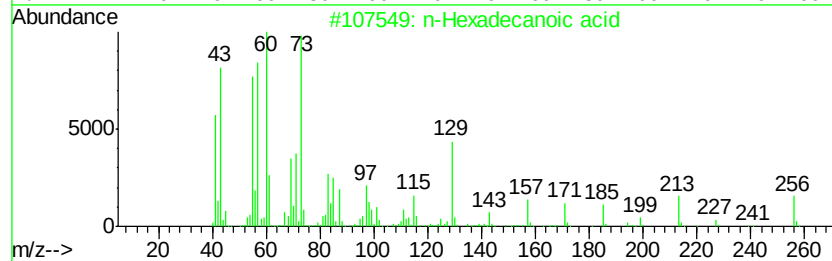
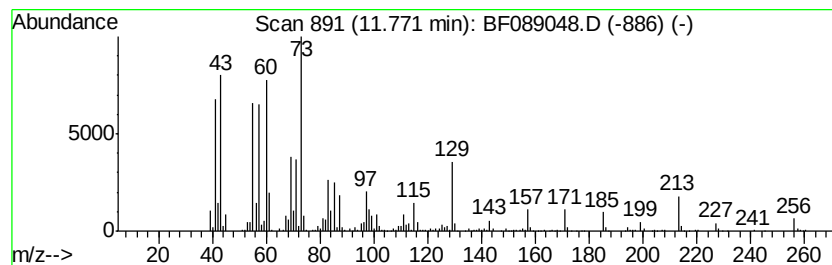
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	80.31 ng	1859340	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089048.D
Acq On : 16 Jul 2016 11:36
Operator : UM/SJ
Sample : H3951-16 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-SB-SB06(0-2in)

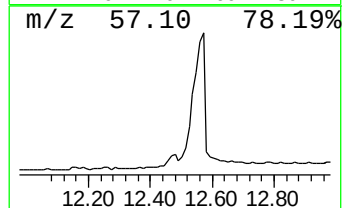
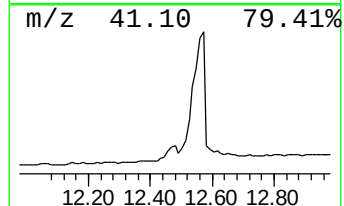
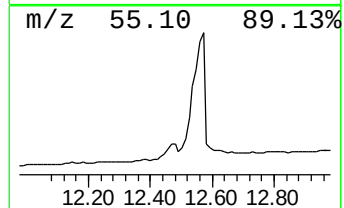
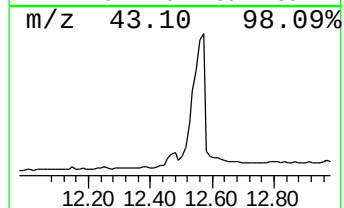
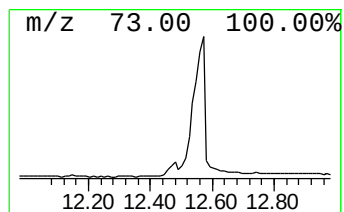
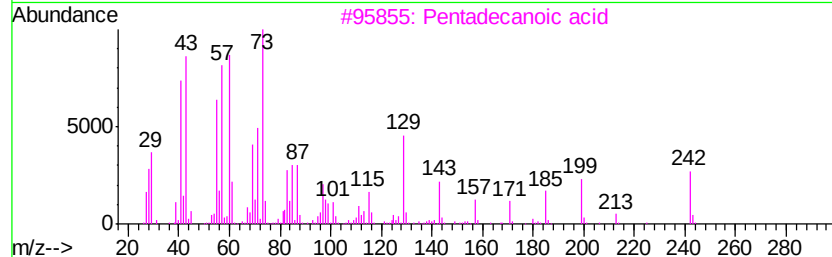
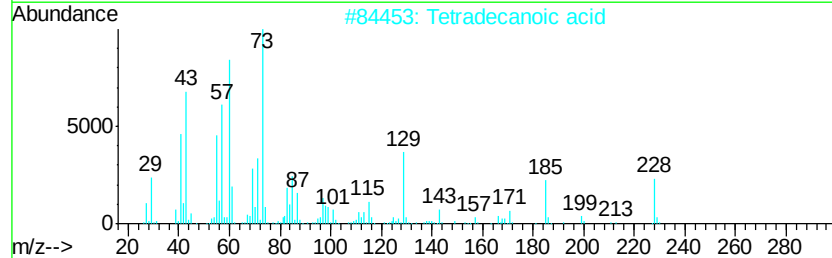
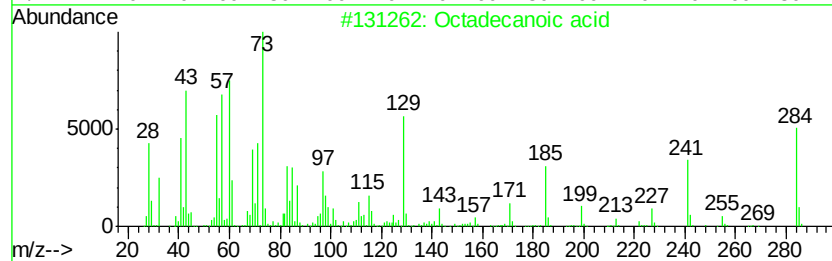
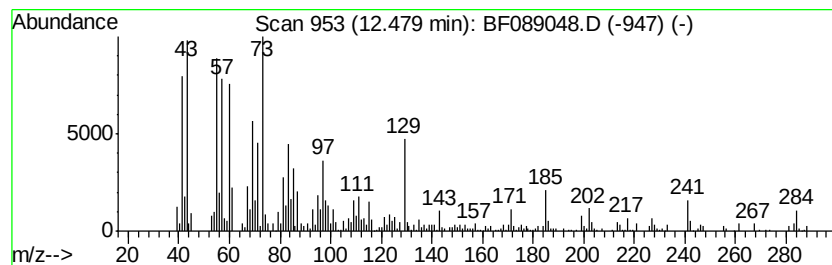
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	20.81 ng	481696	Phenanthrene-d10	11.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5		Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089048.D
Acq On : 16 Jul 2016 11:36
Operator : UM/SJ
Sample : H3951-16 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSS-SB-SB06(0-2in)

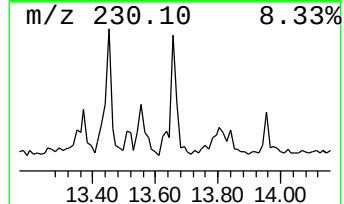
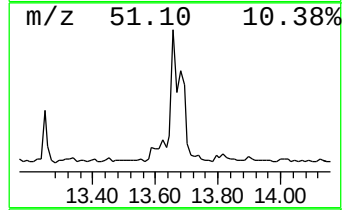
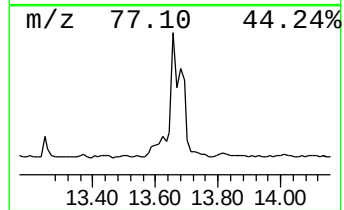
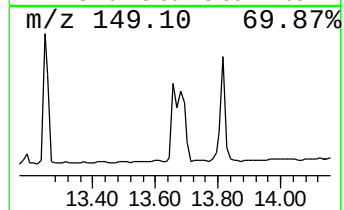
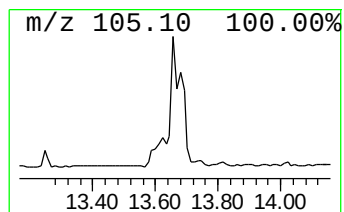
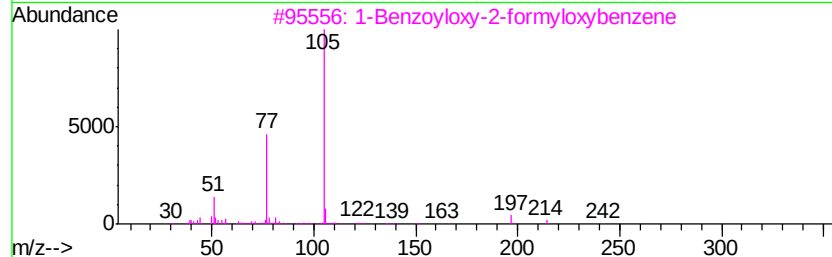
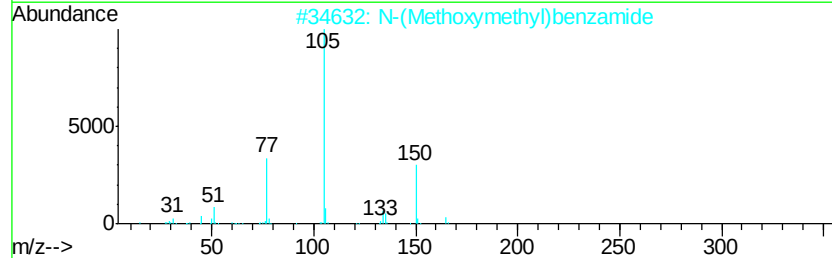
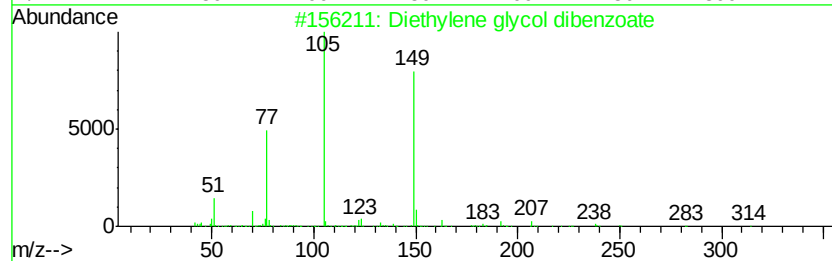
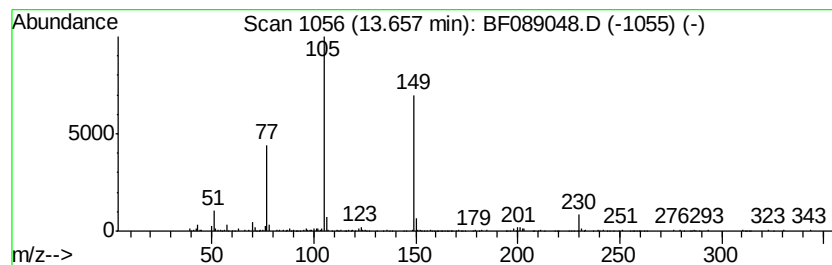
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	5.20 ng	133516	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2		N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	47
3		1-Benzoyloxy-2-formyloxybenzene	242	C14H10O4	079792-93-1	43
4		Pentanediamide, N,N'-di-benzoyloxy-	370	C19H18N2O6	1000253-26-3	43
5		1,2-Bis(benzoyloxy)benzene	318	C20H14O4	000643-94-7	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089048.D
Acq On : 16 Jul 2016 11:36
Operator : UM/SJ
Sample : H3951-16 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSS-SB-SB06(0-2in)

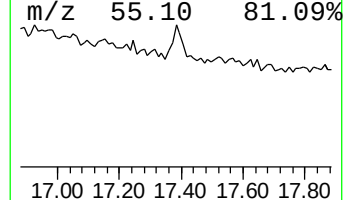
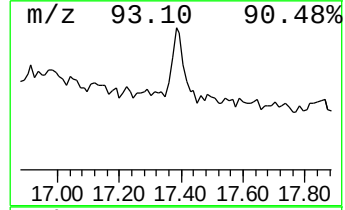
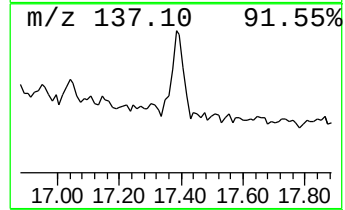
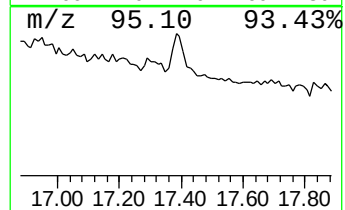
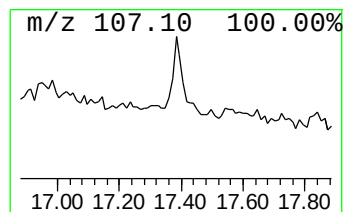
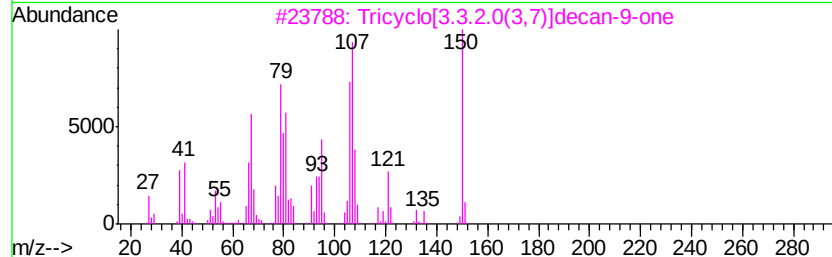
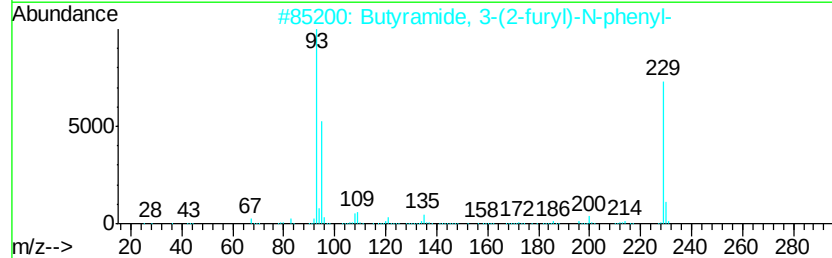
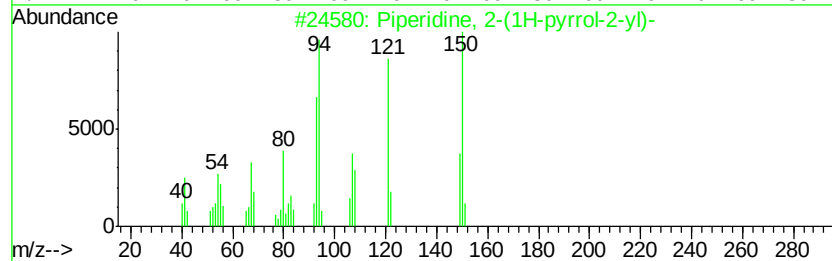
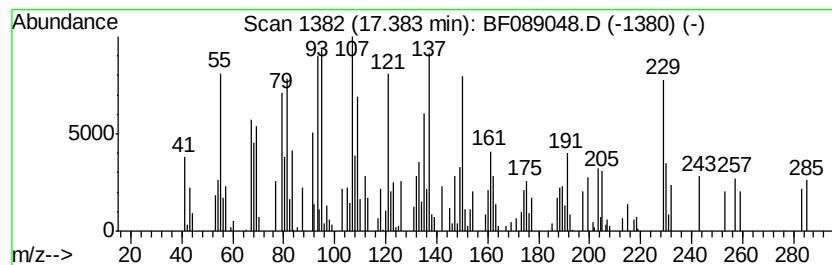
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.38 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	12.68 ng	154289	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Piperidine, 2-(1H-pyrrol-2-yl)-	150	C9H14N2	054966-12-0	47
2		Butyramide, 3-(2-furyl)-N-phenyl-	229	C14H15NO2	1000156-94-9	35
3		Tricyclo[3.3.2.0(3,7)]decan-9-one	150	C10H14O	071382-31-5	35
4		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	25
5		Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	000080-57-9	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089048.D
Acq On : 16 Jul 2016 11:36
Operator : UM/SJ
Sample : H3951-16 5X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSS-SB-SB06(0-2in)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.42	6.42	12.1	ng	212081	1	6.66	351045	20.0
Phthalic anhydride	8.72	2.2	ng	49127	2	7.94	443069	20.0
unknown9.94	9.94	4.0	ng	99073	3	9.70	499520	20.0
Undecanoic acid	10.88	5.8	ng	134436	4	11.18	463018	20.0
Anthracene, 9-met...	11.70	11.4	ng	264713	4	11.18	463018	20.0
n-Hexadecanoic acid	11.77	80.3	ng	1859340	4	11.18	463018	20.0
Octadecanoic acid	12.48	20.8	ng	481696	4	11.18	463018	20.0
Diethylene glycol...	13.66	5.2	ng	133516	5	13.82	513610	20.0
unknown17.38	17.38	12.7	ng	154289	6	15.19	243412	20.0