

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
 Data File : BF077072.D
 Acq On : 27 Jan 2015 4:14
 Operator : TP/IZ
 Sample : G1159-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-84(17-19)

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-BF011415.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	1.407	26	28	37	rVB	20432	46193	1.13%	0.304%
2	3.830	237	240	251	rVB	42256	109374	2.68%	0.720%
3	4.801	321	325	337	rVB	317887	654009	16.01%	4.302%
4	7.179	530	533	537	rBV	413420	660496	16.17%	4.345%
5	7.259	537	540	547	rVB	445647	726602	17.79%	4.780%
6	7.773	581	585	589	rBV	75581	131484	3.22%	0.865%
7	8.093	609	613	616	rBV	285440	502683	12.31%	3.307%
8	9.065	695	698	706	rBV	248683	421253	10.31%	2.771%
9	10.676	836	839	842	rBV	121376	185327	4.54%	1.219%
10	13.339	1068	1072	1075	rBV	414597	727087	17.80%	4.783%
11	14.803	1197	1200	1204	rBV	115844	201794	4.94%	1.328%
12	16.517	1348	1350	1356	rVB	317268	493104	12.07%	3.244%
13	17.637	1446	1448	1449	rBV	191195	205167	5.02%	1.350%
14	17.671	1449	1451	1454	rVV	169991	185736	4.55%	1.222%
15	17.751	1455	1458	1461	rVB	35832	43458	1.06%	0.286%
16	18.460	1517	1520	1522	rVB	758688	949787	23.25%	6.248%
17	18.643	1534	1536	1541	rBV	30474	45712	1.12%	0.301%
18	19.352	1593	1598	1600	rBV2	2600563	4084842	100.00%	26.872%
19	19.386	1600	1601	1603	rVB	2218953	1647896	40.34%	10.841%
20	19.500	1609	1611	1614	rVB	350253	405837	9.94%	2.670%
21	19.603	1618	1620	1623	rBV2	145948	216852	5.31%	1.427%
22	19.877	1642	1644	1647	rVB	516219	714504	17.49%	4.700%
23	20.060	1654	1660	1662	rBV	34821	52978	1.30%	0.349%
24	20.312	1679	1682	1685	rVB2	22741	47831	1.17%	0.315%
25	20.426	1689	1692	1696	rBV2	58261	96543	2.36%	0.635%
26	20.494	1696	1698	1702	rBV	42542	68126	1.67%	0.448%
27	20.677	1711	1714	1718	rBV3	68896	98956	2.42%	0.651%
28	20.952	1734	1738	1742	rVB3	44047	104604	2.56%	0.688%
29	21.146	1751	1755	1757	rBV2	280564	575772	14.10%	3.788%
30	21.180	1757	1758	1760	rVV	101588	81586	2.00%	0.537%
31	21.260	1764	1765	1770	rVV2	41003	70843	1.73%	0.466%
32	22.392	1861	1864	1870	rBV	101985	217929	5.34%	1.434%
33	22.678	1887	1889	1892	rVB	53208	69039	1.69%	0.454%
34	22.735	1892	1894	1897	rBV	79430	118705	2.91%	0.781%

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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-84(17-19)

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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.803	1897	1900	1904	rBV2	161518	238801	5.85%	1.571%
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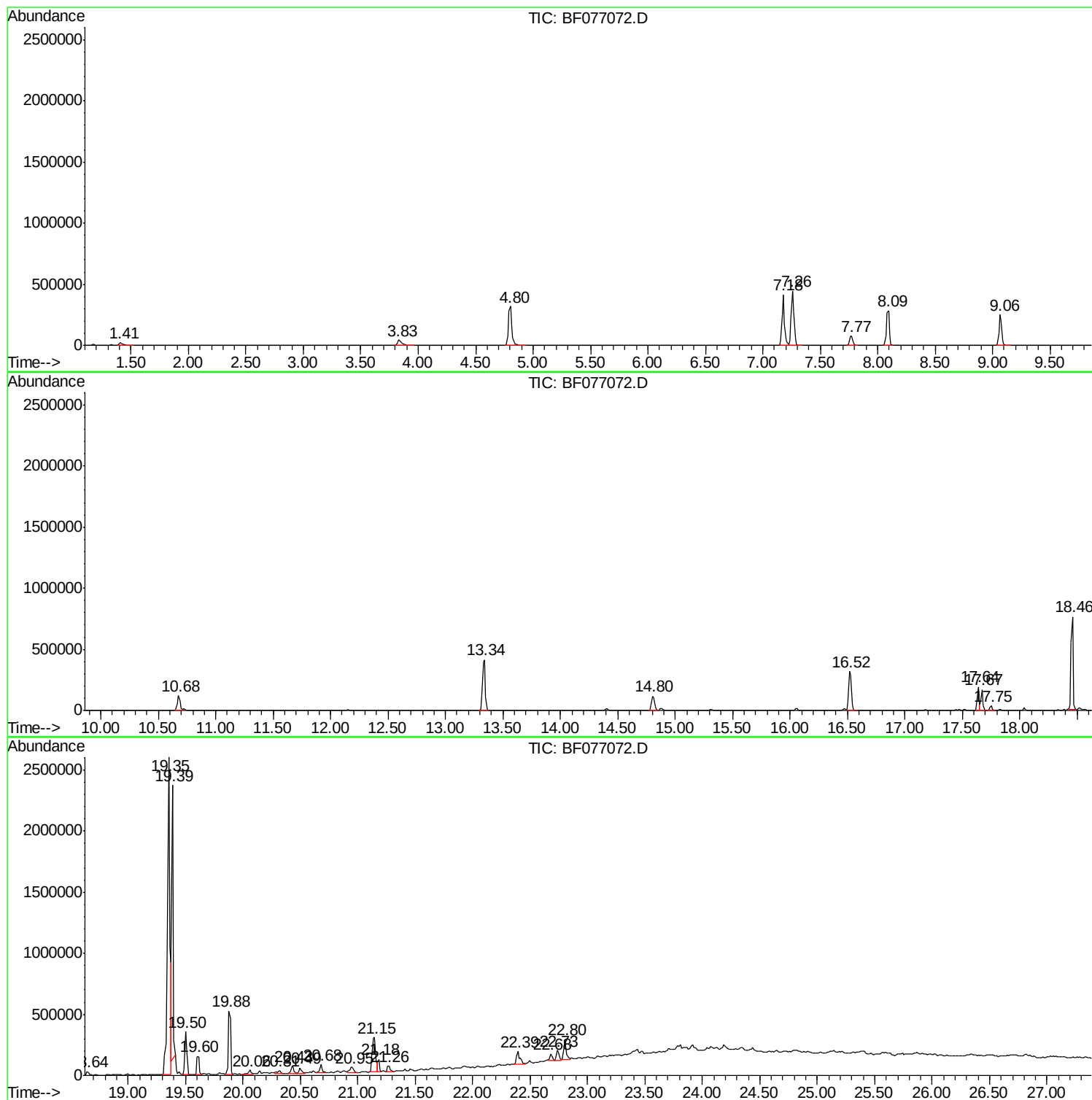
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
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Instrument :
BNA_F
ClientSampled :
SB-84(17-19)

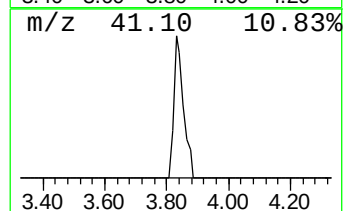
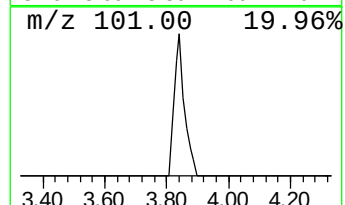
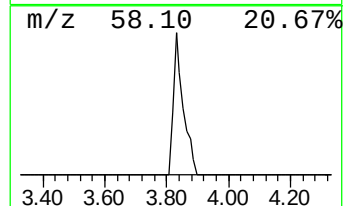
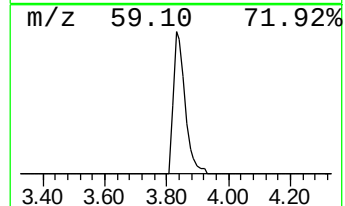
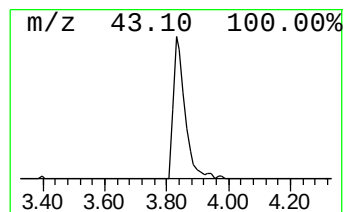
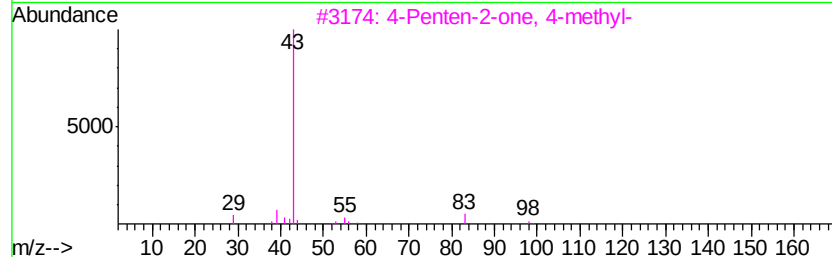
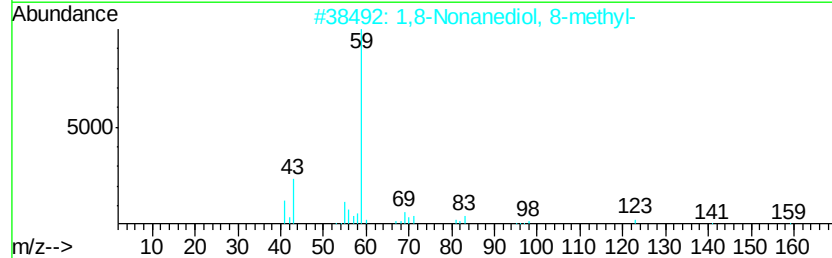
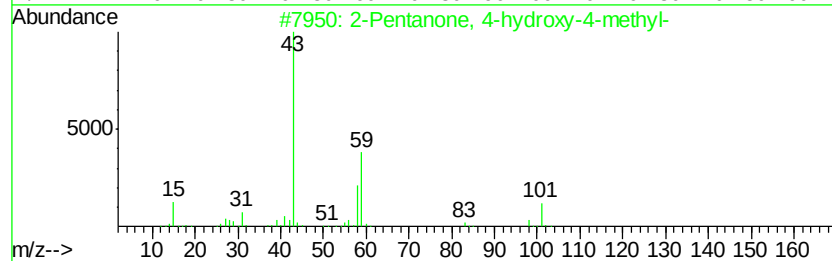
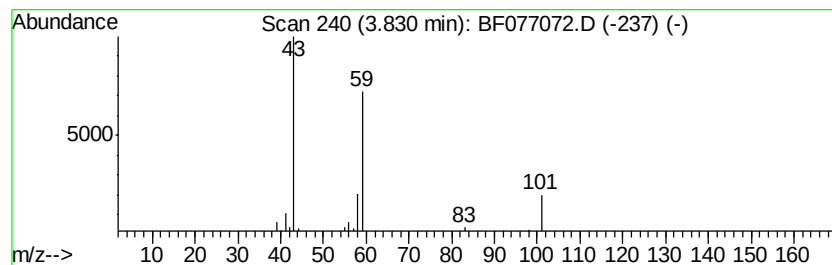
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.83	16.64 ng	109374	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4		Guanidine	59	CH5N3	000113-00-8	9
5		Acetone	58	C3H6O	000067-64-1	9



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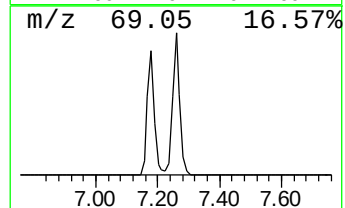
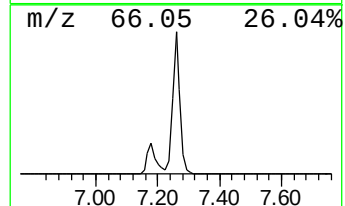
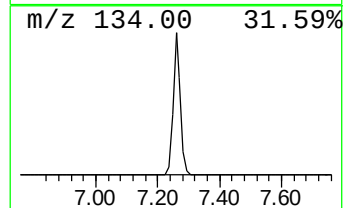
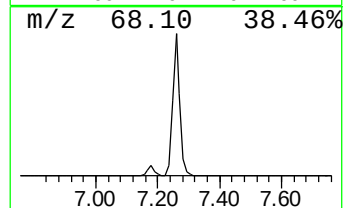
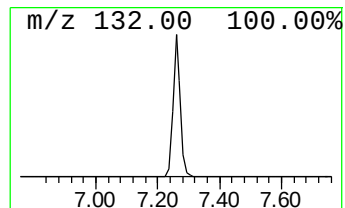
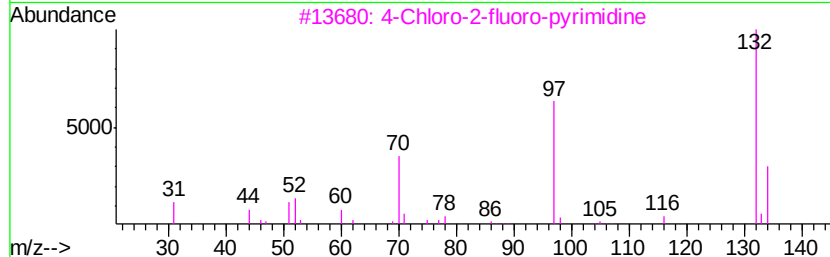
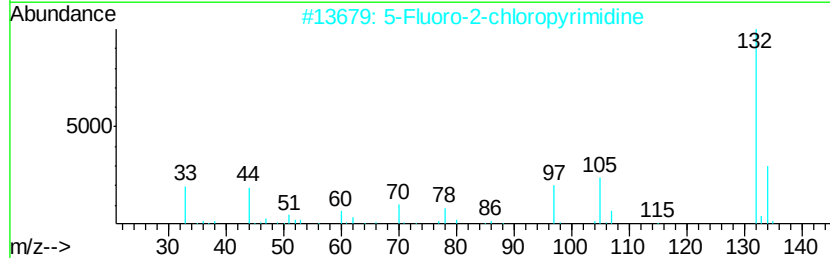
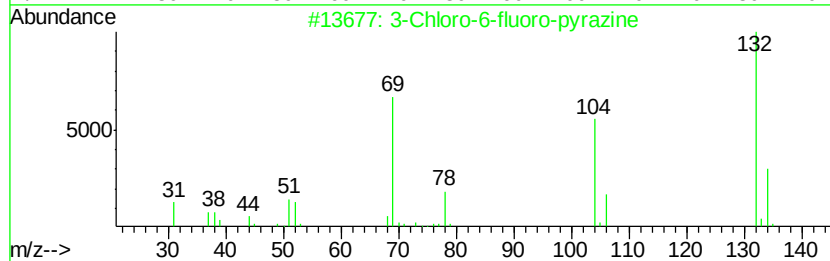
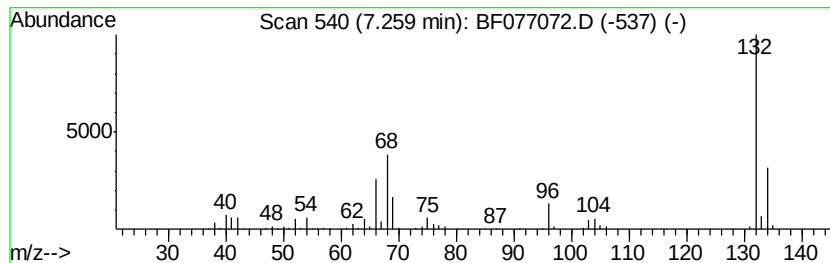
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	110.52 ng	726602	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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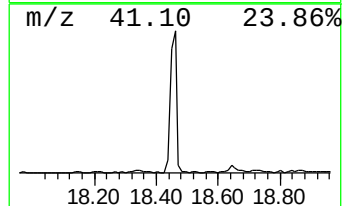
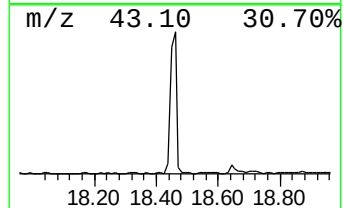
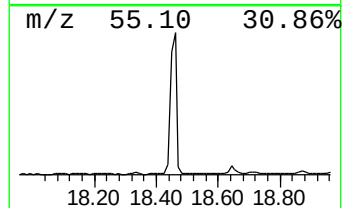
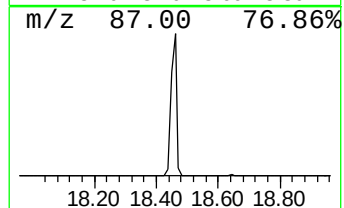
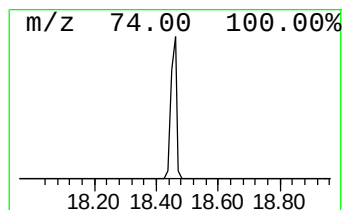
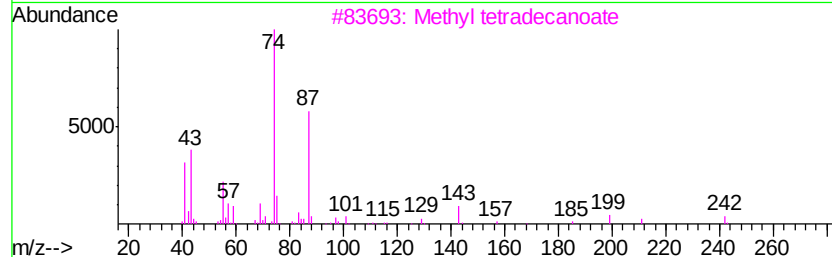
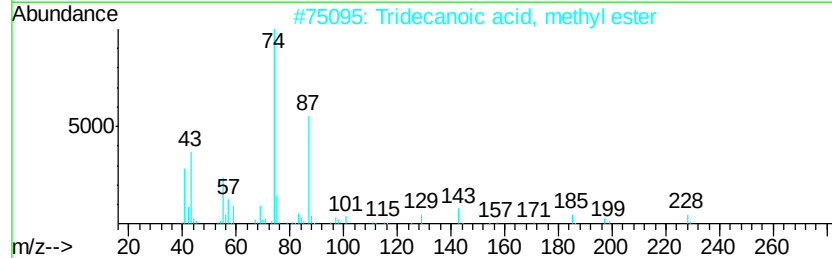
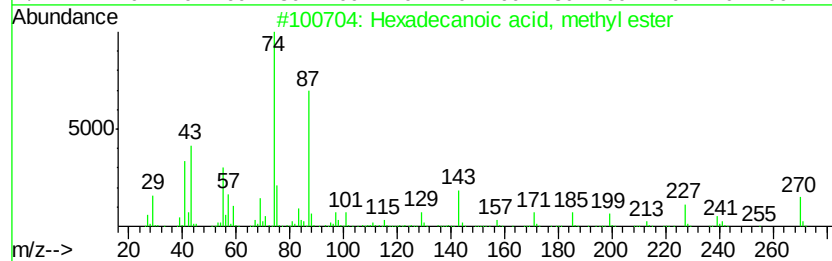
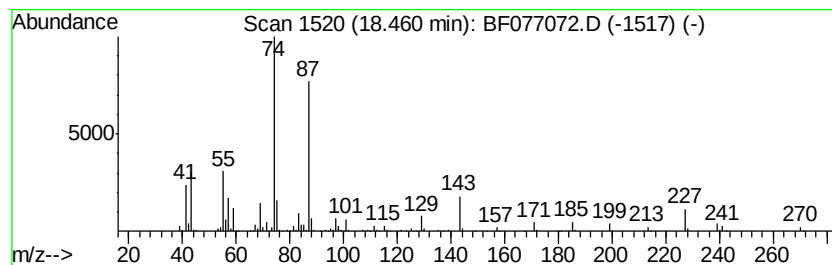
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TIC Library : C:\DATABASE\NIST02.L
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 Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.46	92.59 ng	949787	Phenanthrene-d10	17.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	91
5		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87



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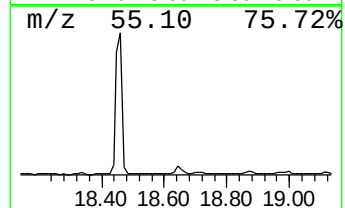
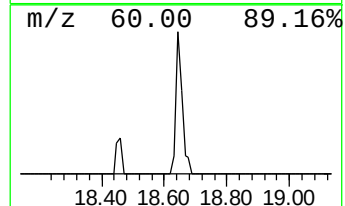
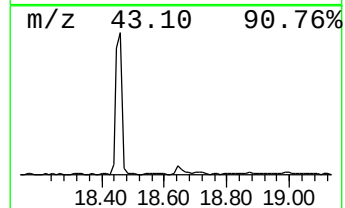
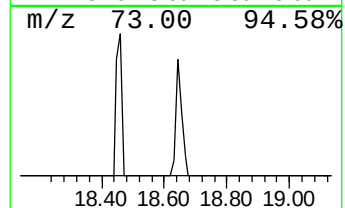
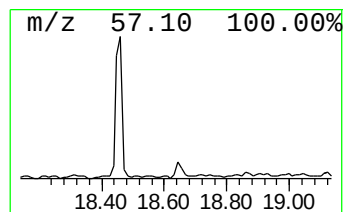
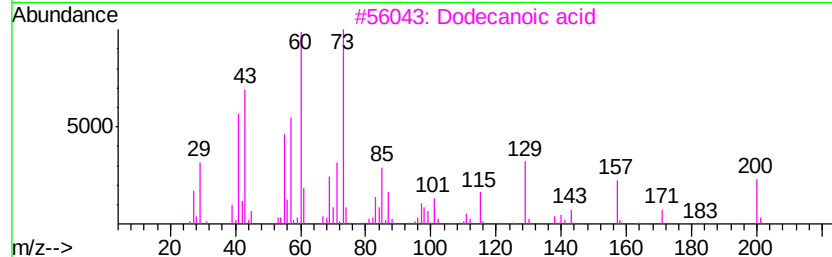
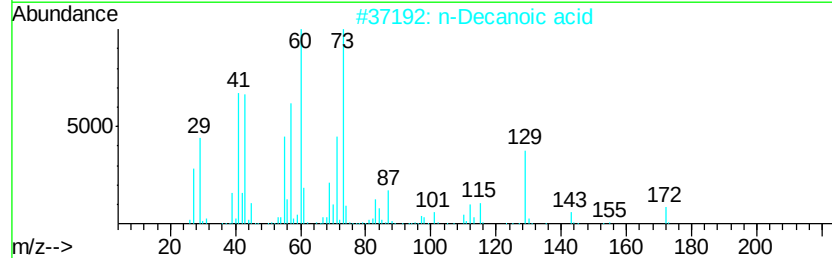
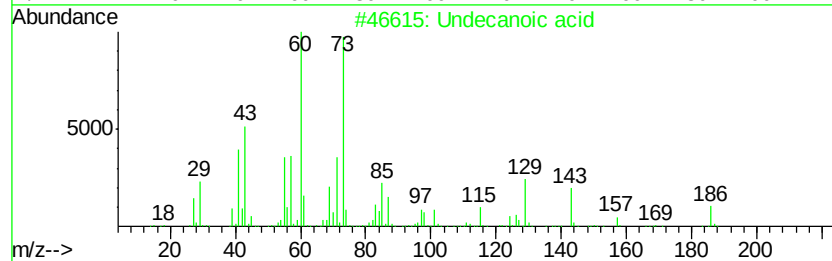
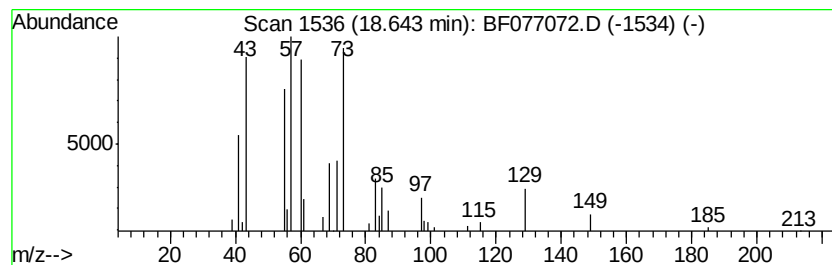
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.64	4.46 ng	45712	Phenanthrene-d10		17.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	72
2			n-Decanoic acid	172	C10H20O2	000334-48-5	59
3			Dodecanoic acid	200	C12H24O2	000143-07-7	59
4			Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	50
5			.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22



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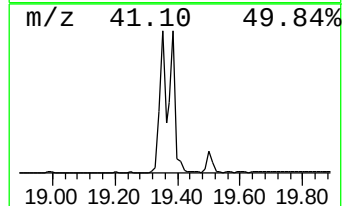
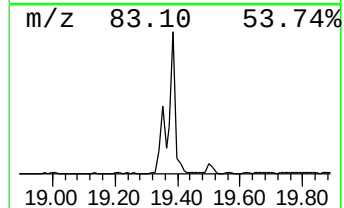
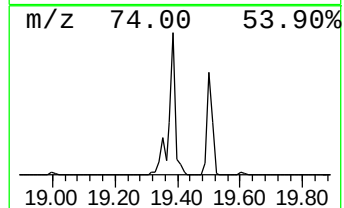
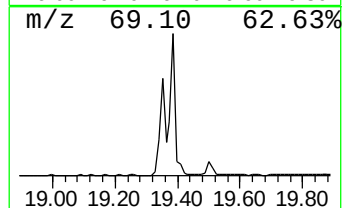
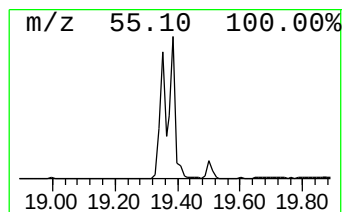
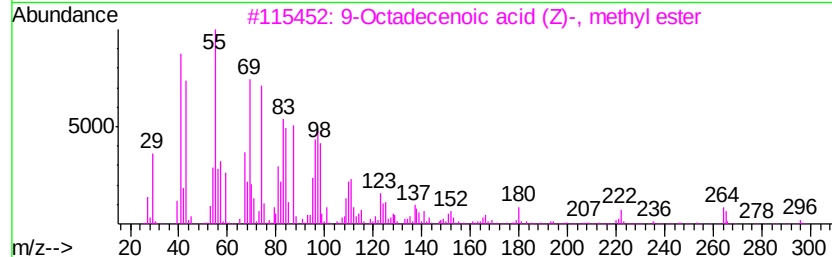
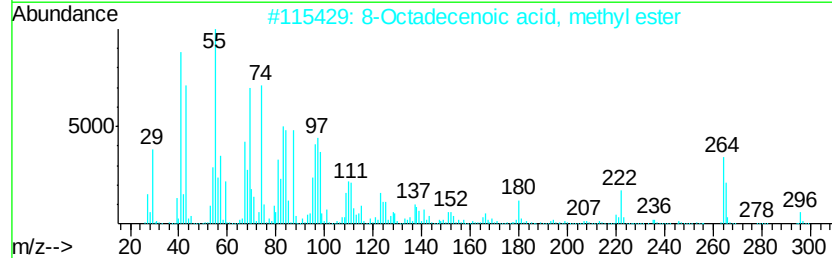
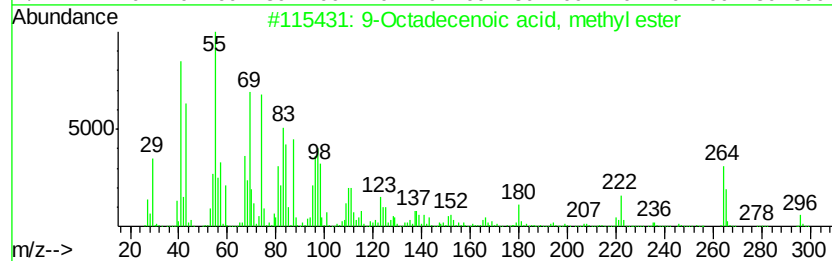
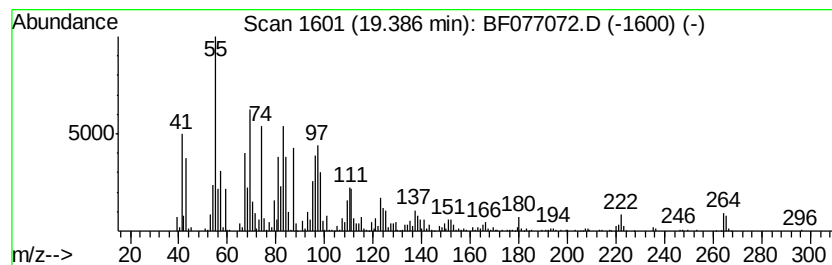
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 9-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	160.64 ng	1647900	Phenanthrene-d10	17.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2		8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	98
3		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
4		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
5		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91



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Misc :
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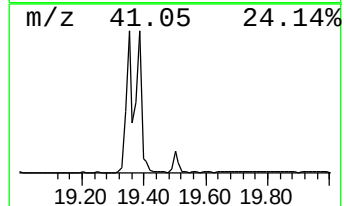
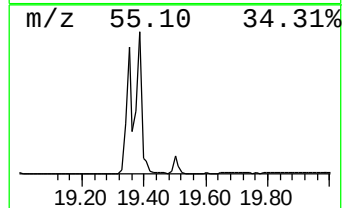
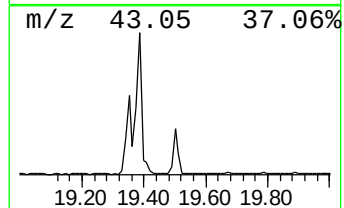
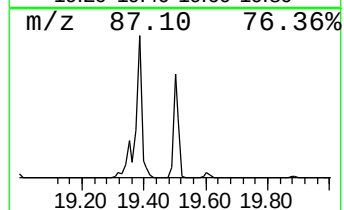
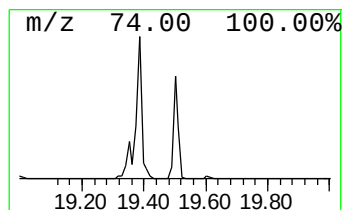
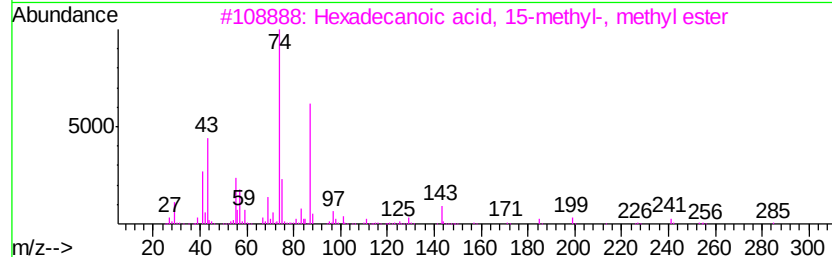
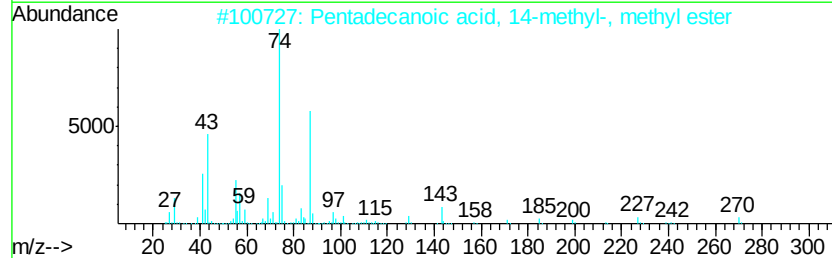
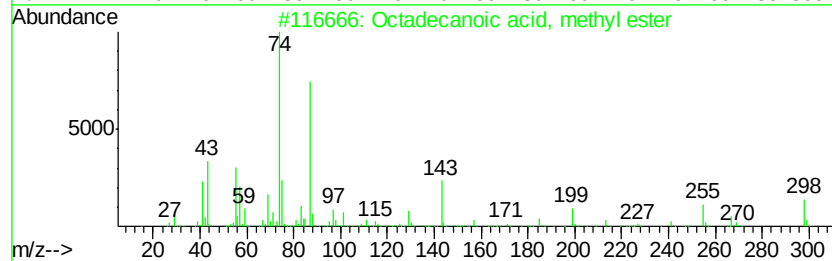
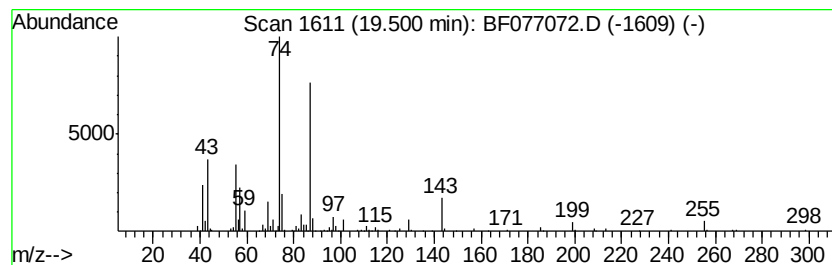
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BNA_F
ClientSampleId :
SB-84(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.50	14.10 ng	405837	Chrysene-d12	21.15		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, methyl ester	298	C19H38O2	000112-61-8	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077072.D
Acq On : 27 Jan 2015 4:14
Operator : TP/IZ
Sample : G1159-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-84(17-19)

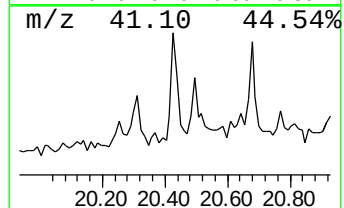
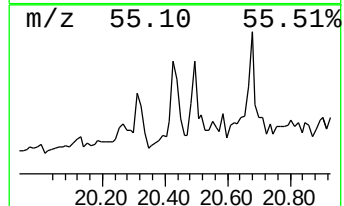
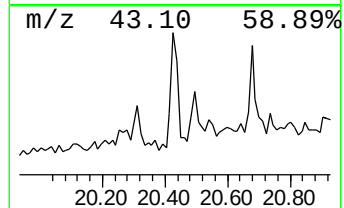
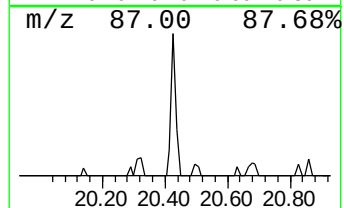
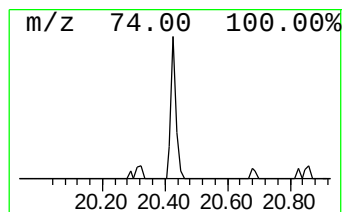
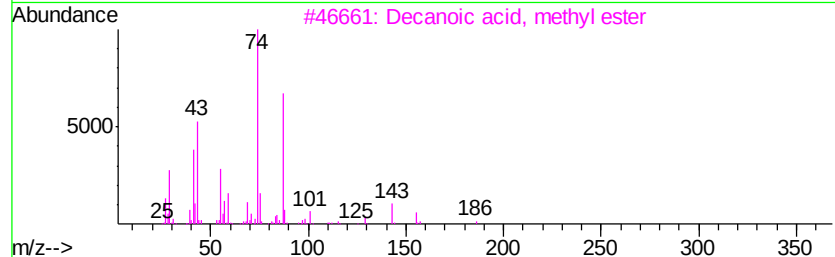
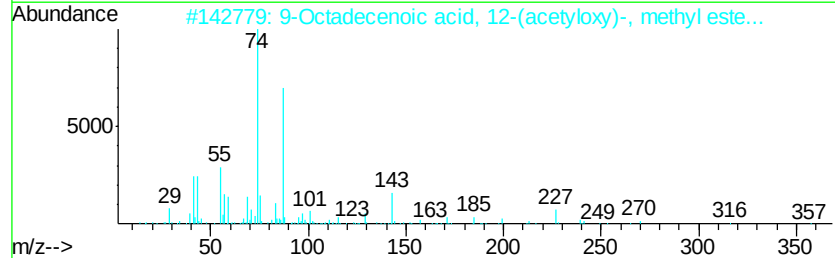
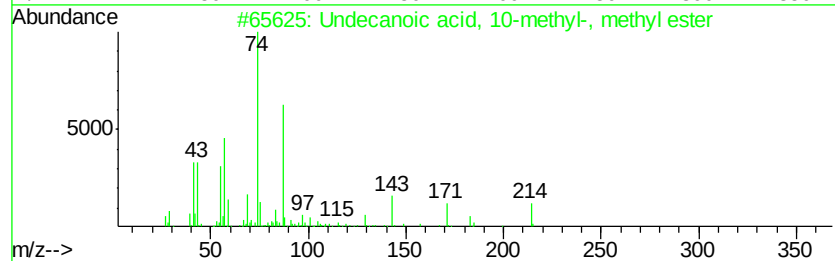
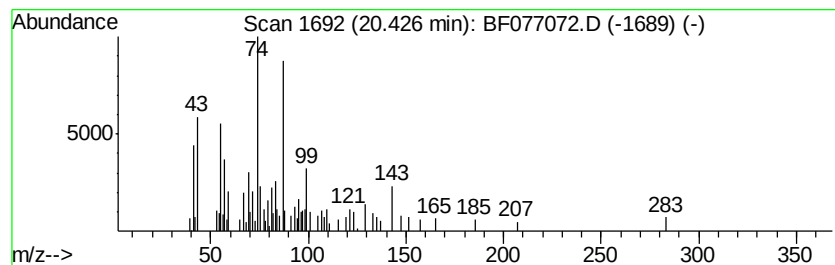
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Undecanoic acid, 10-methyl-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	3.35 ng	96543	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	59
2		9-Octadecenoic acid, 12-(acetylo...	354	C21H38O4	000140-03-4	59
3		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	53
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	53
5		Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
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Acq On : 27 Jan 2015 4:14
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Sample : G1159-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

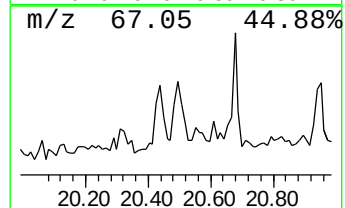
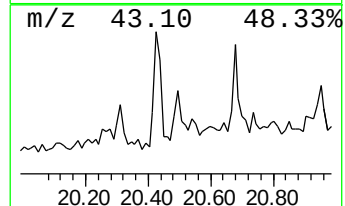
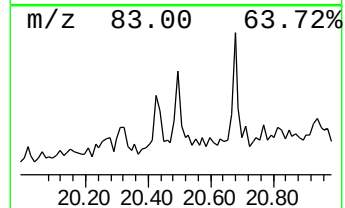
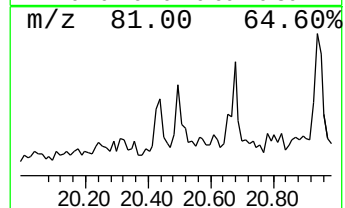
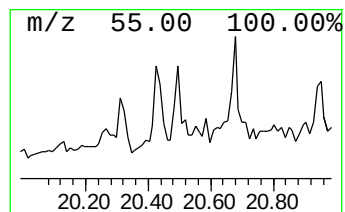
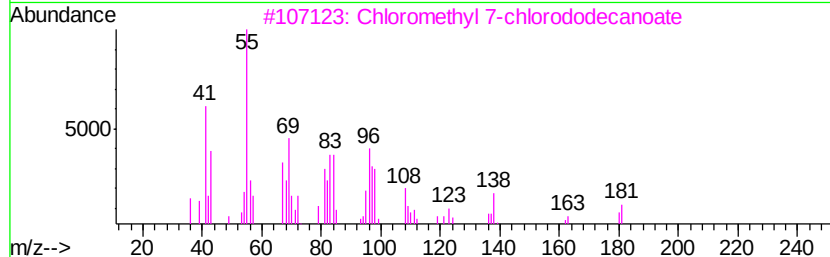
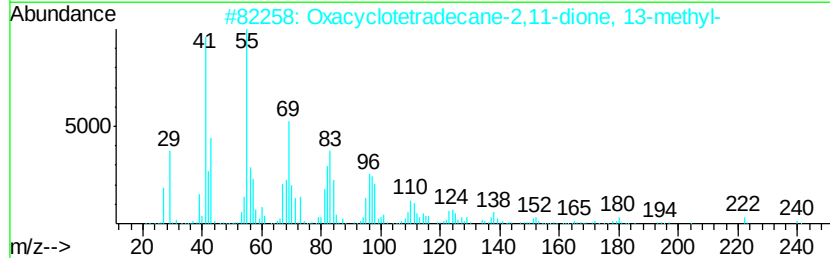
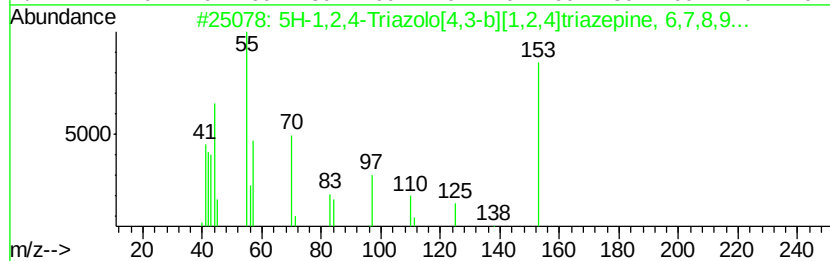
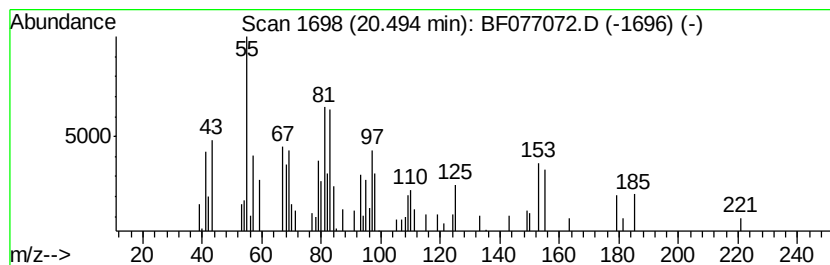
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ClientSampleId :
SB-84(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.49 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.		
20.49	2.37 ng	68126	Chrysene-d12		21.15		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-1,2,4-Triazolo[4,3-b][1,2,4]t...	153	C6H11N5	062170-16-5	27		
2	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	25		
3	Chloromethyl 7-chlorododecanoate	282	C13H24Cl2O2	080419-03-0	22		
4	1,19-Eicosadiene	278	C20H38	014811-95-1	16		
5	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	14		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077072.D
Acq On : 27 Jan 2015 4:14
Operator : TP/IZ
Sample : G1159-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-84(17-19)

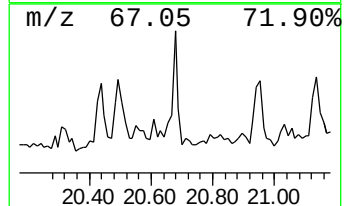
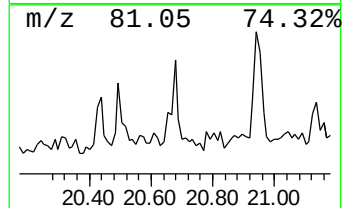
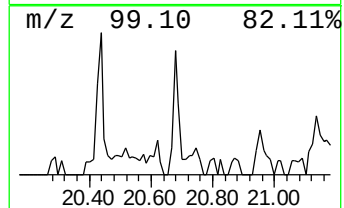
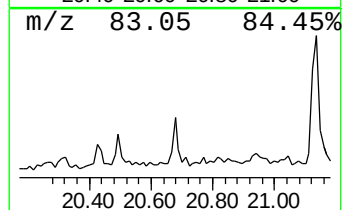
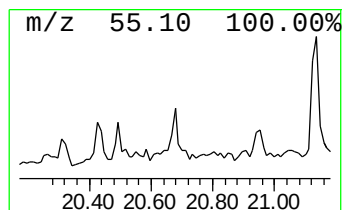
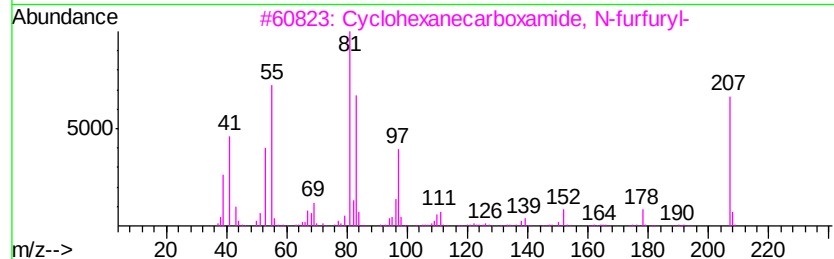
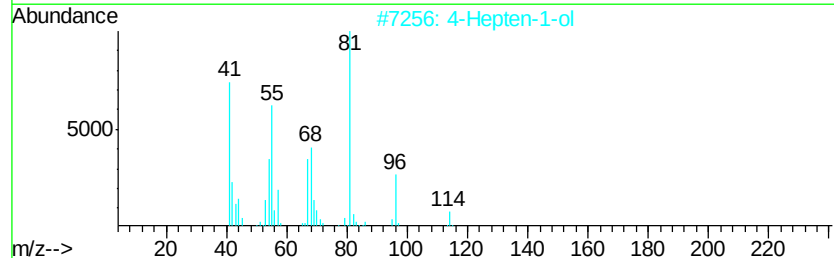
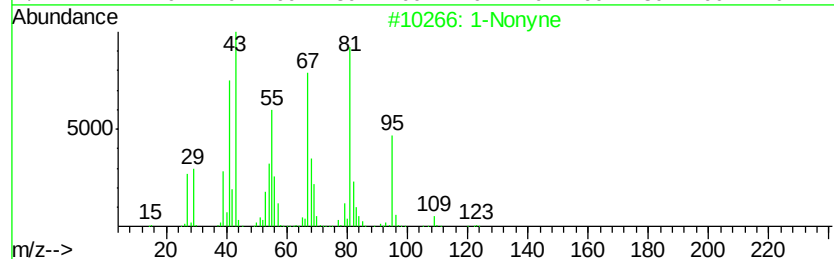
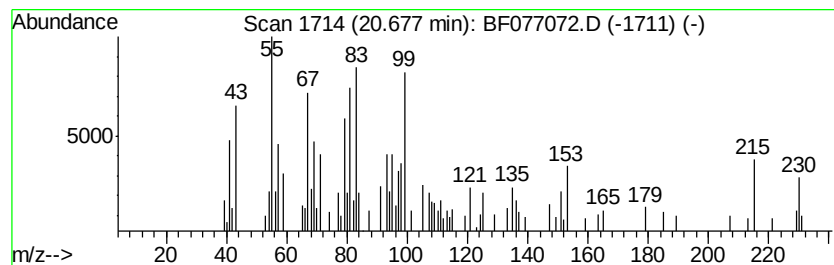
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown20.68 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.68	3.44 ng	98956	Chrysene-d12	21.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonyne			124	C9H16	003452-09-3	18
2	4-Hepten-1-ol			114	C7H14O	020851-55-2	15
3	Cyclohexanecarboxamide, N-furfuryl-			207	C12H17NO2	006341-32-8	14
4	Cyclohexane, ethenyl-			110	C8H14	000695-12-5	11
5	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077072.D
Acq On : 27 Jan 2015 4:14
Operator : TP/IZ
Sample : G1159-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-84(17-19)

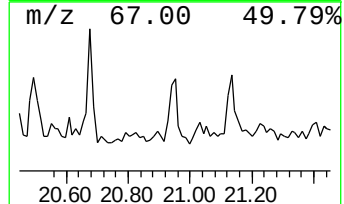
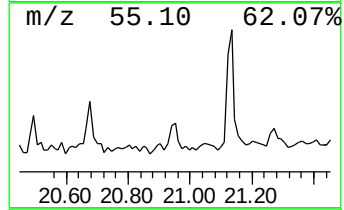
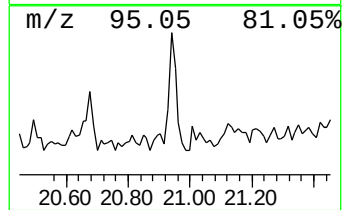
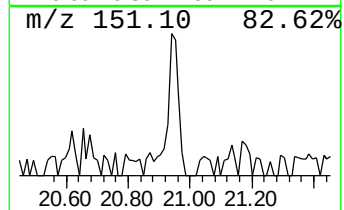
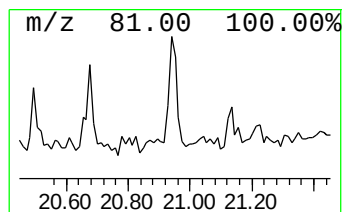
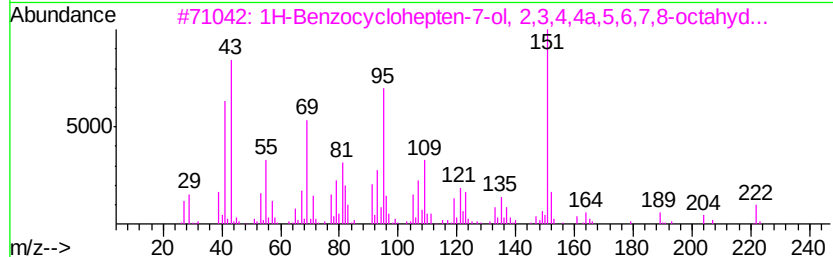
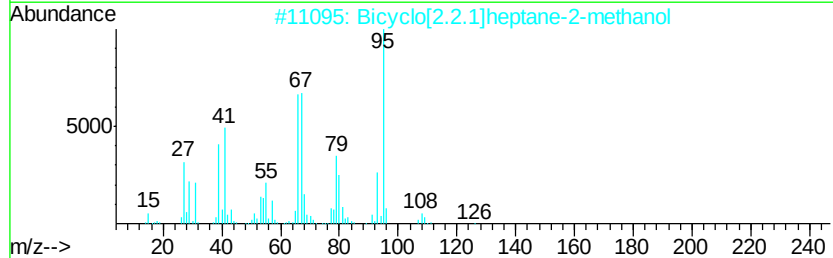
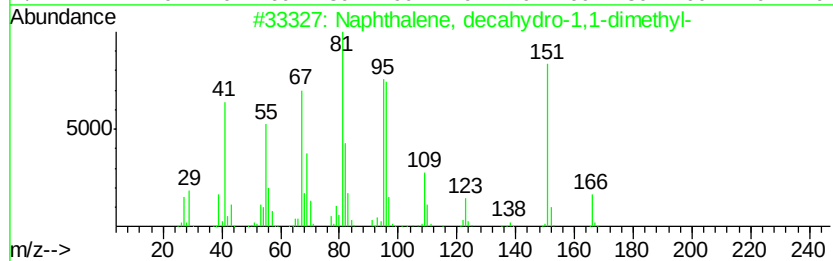
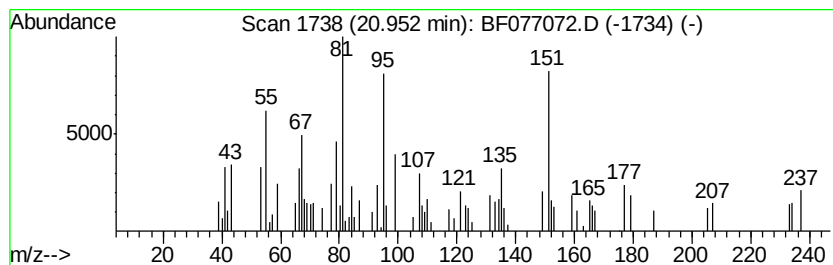
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown20.95 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	3.63 ng	104604	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-1,1-dimet...	166	C12H22	035431-04-0	38
2		Bicyclo[2.2.1]heptane-2-methanol	126	C8H14O	005240-72-2	22
3		1H-Benzocyclohepten-7-ol, 2,3,4,...	222	C15H26O	006892-80-4	22
4		2-Furanone, 4-methyl-5-(1-butene...	206	C13H18O2	1000154-19-4	22
5		Cedrol	222	C15H26O	000077-53-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077072.D
Acq On : 27 Jan 2015 4:14
Operator : TP/IZ
Sample : G1159-04
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ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
SB-84(17-19)

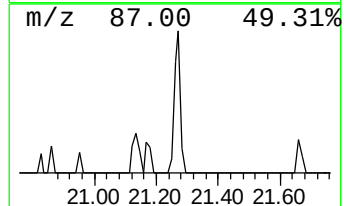
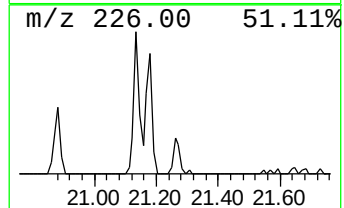
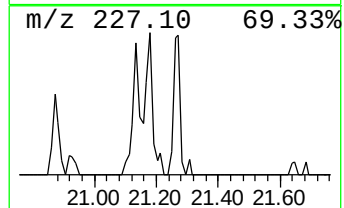
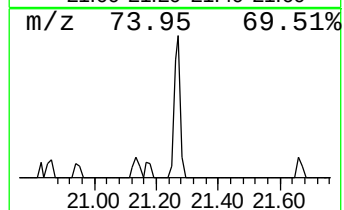
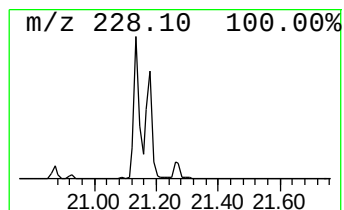
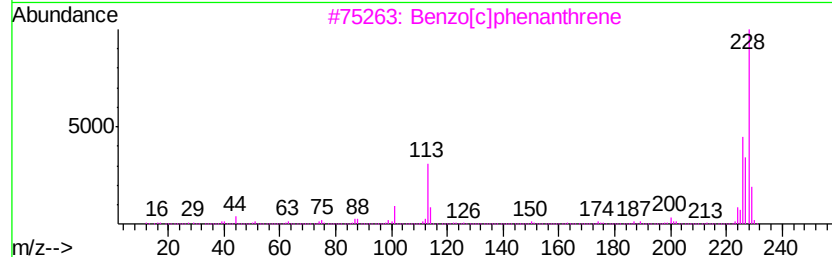
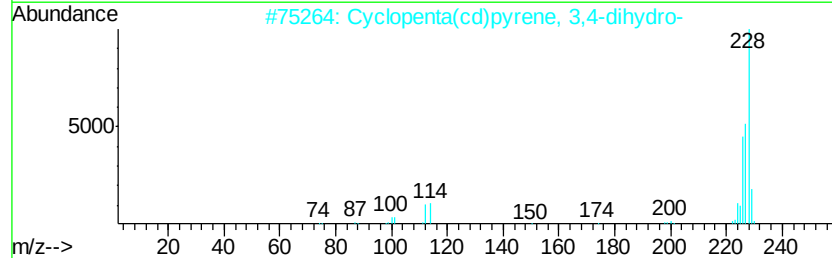
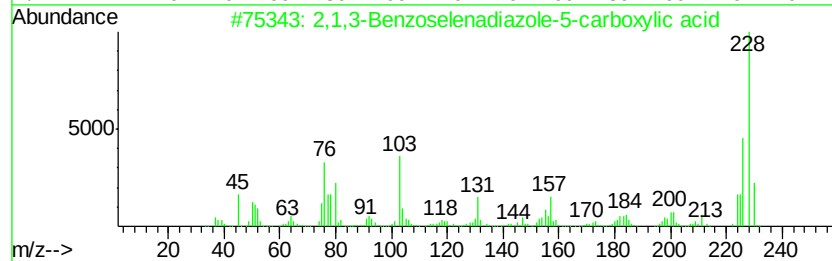
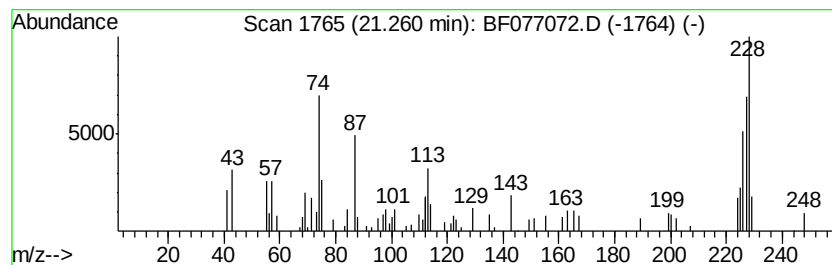
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown21.26 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	2.46 ng	70843	Chrysene-d12	21.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,1,3-Benzoselenadiazole-5-carbo...	228	C7H4N2O2Se	140669-75-6	43		
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	38		
3	Benzo[c]phenanthrene	228	C18H12	000195-19-7	35		
4	Benz[a]anthracene	228	C18H12	000056-55-3	30		
5	Chrysene	228	C18H12	000218-01-9	30		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
 Data File : BF077072.D
 Acq On : 27 Jan 2015 4:14
 Operator : TP/IZ
 Sample : G1159-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-84(17-19)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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...	3.83	16.6	ng	109374	1	7.77	131484	20.0
unknown7.26	7.26	110.5	ng	726602	1	7.77	131484	20.0
Hexadecanoic acid...	18.46	92.6	ng	949787	4	17.64	205167	20.0
Undecanoic acid	18.64	4.5	ng	45712	4	17.64	205167	20.0
9-Octadecenoic ac...	19.39	160.6	ng	1647900	4	17.64	205167	20.0
Octadecanoic acid...	19.50	14.1	ng	405837	5	21.15	575772	20.0
Undecanoic acid, ...	20.43	3.4	ng	96543	5	21.15	575772	20.0
unknown20.49	20.49	2.4	ng	68126	5	21.15	575772	20.0
unknown20.68	20.68	3.4	ng	98956	5	21.15	575772	20.0
unknown20.95	20.95	3.6	ng	104604	5	21.15	575772	20.0
unknown21.26	21.26	2.5	ng	70843	5	21.15	575772	20.0