

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
 Data File : BF094688.D
 Acq On : 28 Apr 2017 17:23
 Operator : SJ/MA
 Sample : I2895-12
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-12-2.0-3.0

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-BF041717.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	3.943	337	341	349	rBV	441462	536916	17.41%	2.217%
2	4.331	403	407	420	rBV	3019648	2992588	97.04%	12.354%
3	4.713	468	472	478	rVB	37648	38872	1.26%	0.160%
4	5.401	584	589	592	rBV	2752662	2964511	96.13%	12.238%
5	5.525	605	610	613	rBV	3163980	3083839	100.00%	12.731%
6	5.772	648	652	656	rBV	517264	490998	15.92%	2.027%
7	5.948	677	682	685	rBV	2396815	2179801	70.68%	8.999%
8	6.419	757	762	765	rBV	1743067	1865539	60.49%	7.701%
9	6.589	787	791	798	rVB	30492	31036	1.01%	0.128%
10	7.260	901	905	911	rBV	764687	657352	21.32%	2.714%
11	8.583	1125	1130	1133	rBV	2781293	2610118	84.64%	10.775%
12	8.989	1193	1199	1201	rBV	55084	59422	1.93%	0.245%
13	9.083	1212	1215	1219	rBV	285802	258089	8.37%	1.065%
14	9.395	1257	1268	1273	rBV	726033	709688	23.01%	2.930%
15	9.613	1302	1305	1310	rVB	53311	54647	1.77%	0.226%
16	9.995	1366	1370	1375	rBV2	57163	71951	2.33%	0.297%
17	10.266	1409	1416	1422	rBV6	13959	31291	1.01%	0.129%
18	10.372	1430	1434	1438	rBV	1329428	1426306	46.25%	5.888%
19	10.577	1465	1469	1476	rBV	47734	64387	2.09%	0.266%
20	11.130	1559	1563	1566	rBV	38591	36347	1.18%	0.150%
21	11.219	1574	1578	1587	rVB	623936	599230	19.43%	2.474%
22	11.954	1698	1703	1711	rBV2	94526	143056	4.64%	0.591%
23	13.195	1909	1914	1918	rBV	1630808	1690035	54.80%	6.977%
24	14.360	2108	2112	2120	rBV3	118531	202116	6.55%	0.834%
25	14.471	2126	2131	2137	rBV	493756	554200	17.97%	2.288%
26	14.765	2178	2181	2189	rVB9	21756	36487	1.18%	0.151%
27	15.142	2241	2245	2254	rBV3	155755	252598	8.19%	1.043%
28	15.859	2364	2367	2377	rBV3	79861	140386	4.55%	0.580%
29	16.095	2404	2407	2412	rBV	338456	388916	12.61%	1.606%
30	16.471	2468	2471	2478	rBV2	35602	52437	1.70%	0.216%

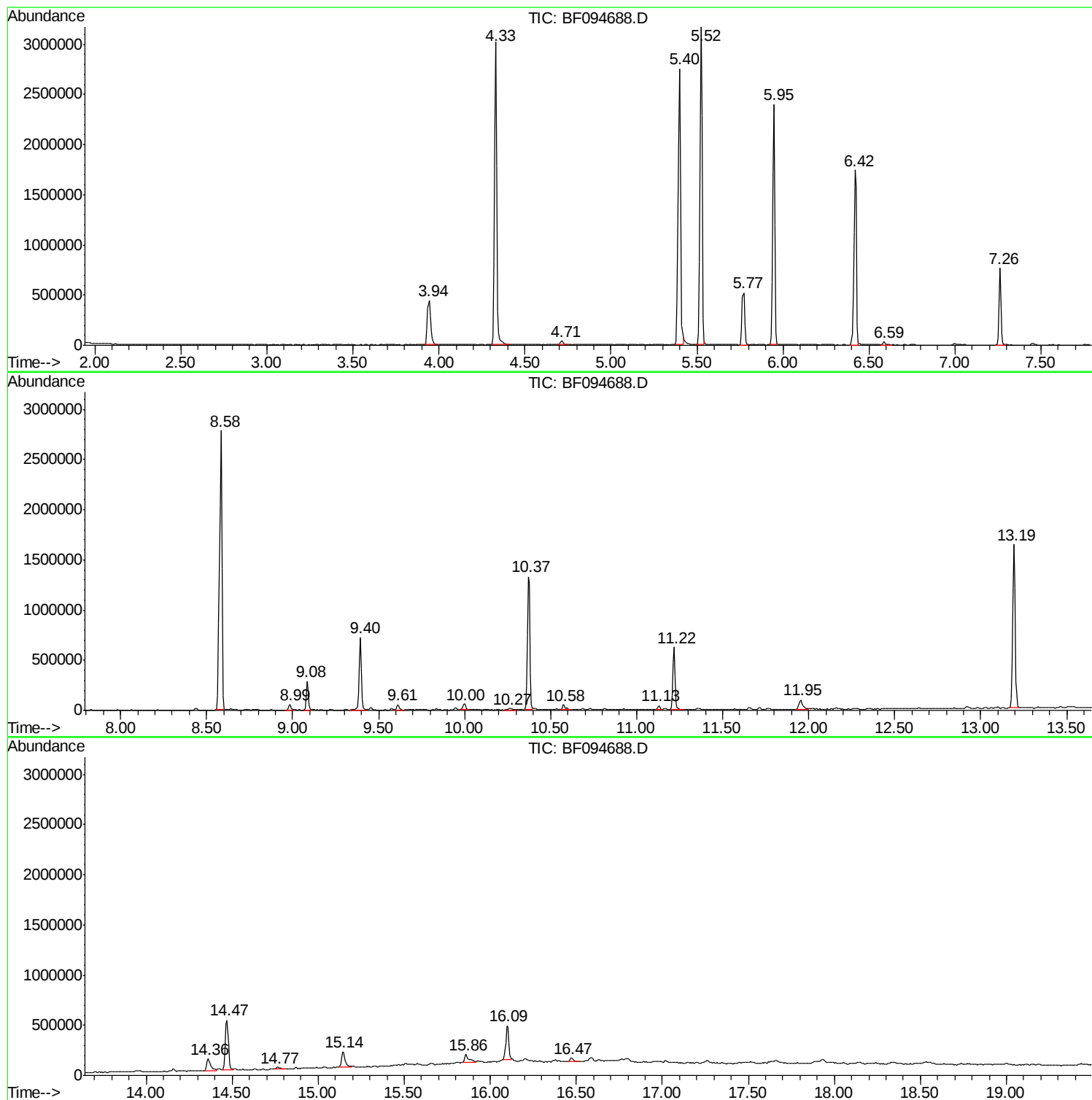
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SB-12-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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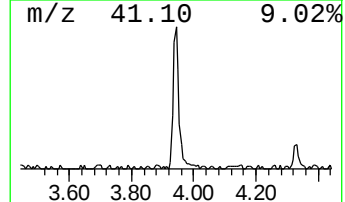
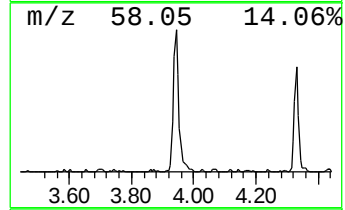
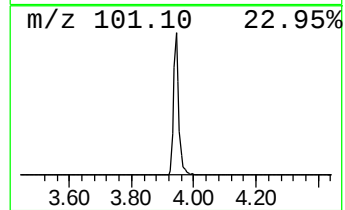
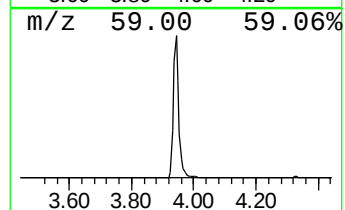
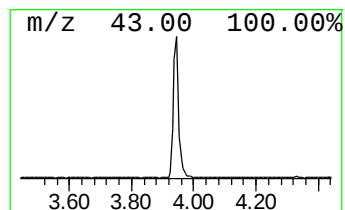
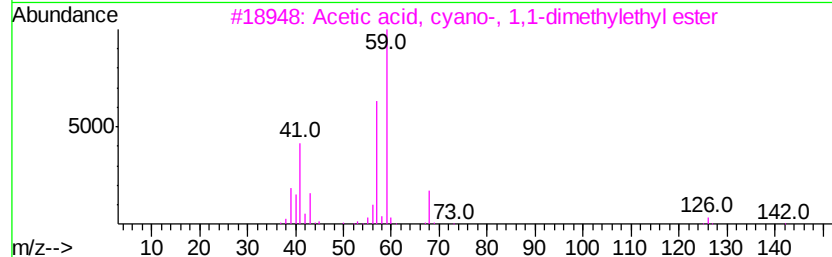
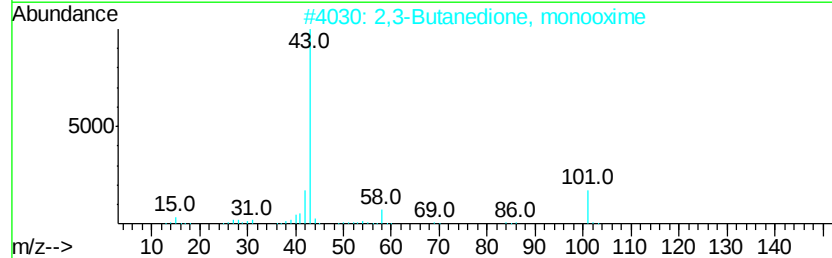
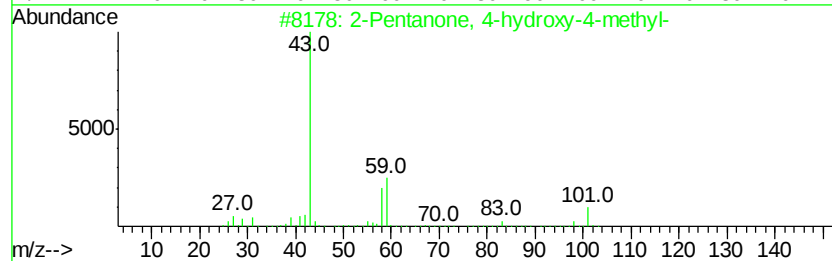
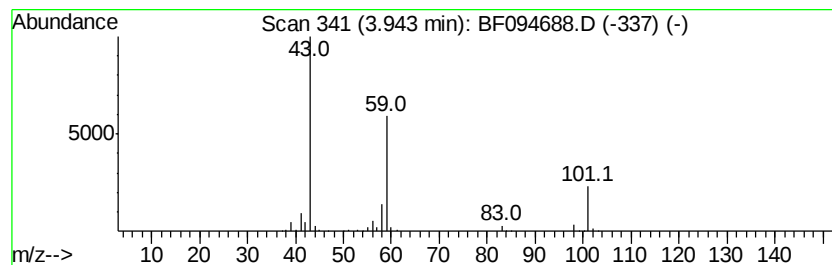
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
3.94	21.87 ng	536916	1,4-Dichlorobenzene-d4	5.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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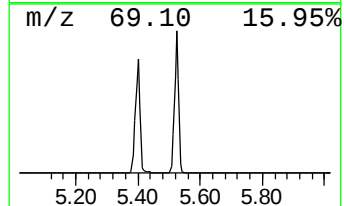
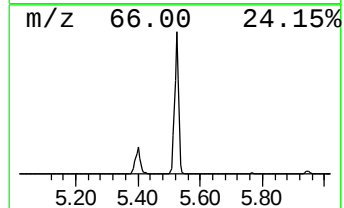
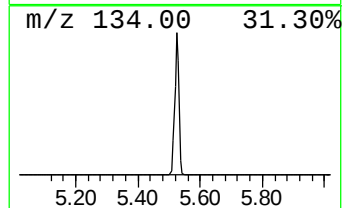
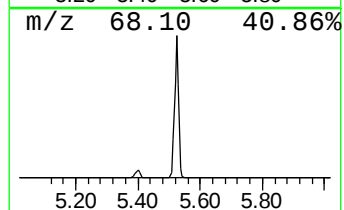
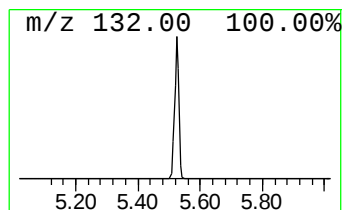
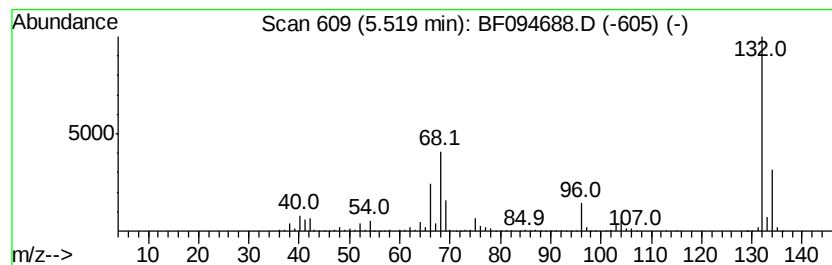
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	125.62 ng	3083840	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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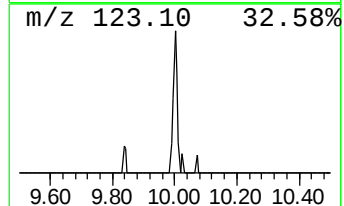
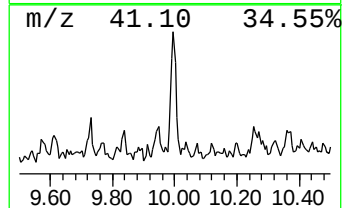
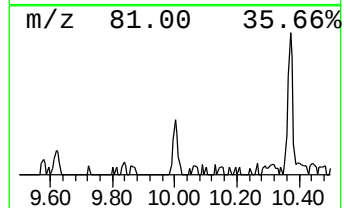
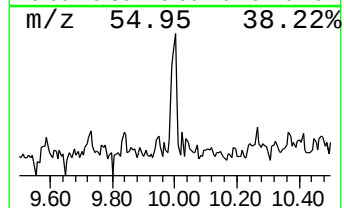
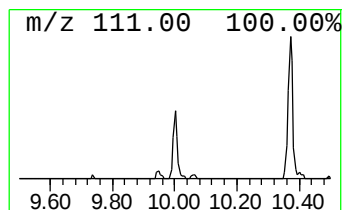
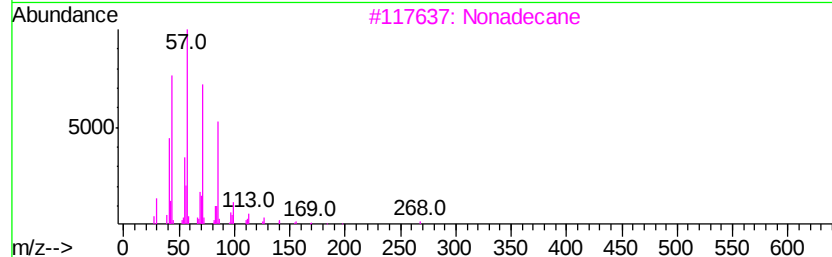
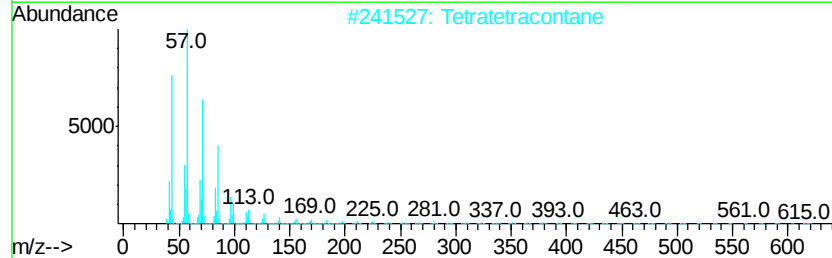
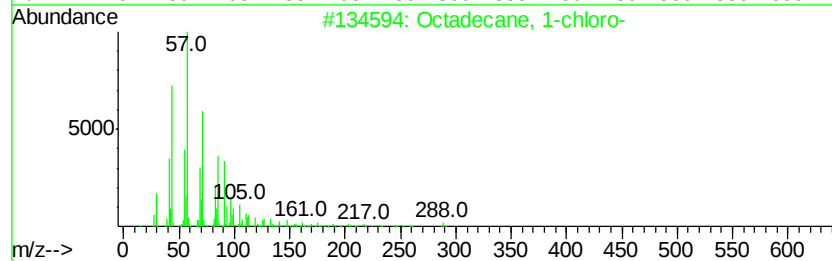
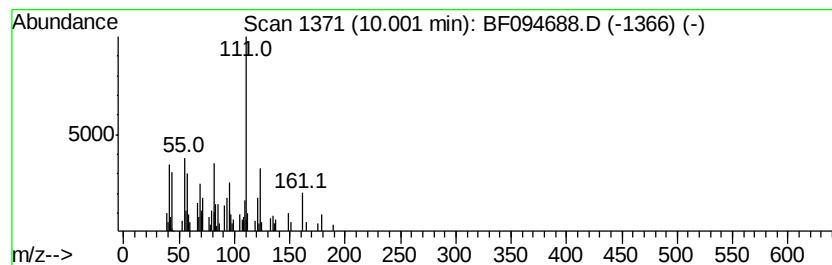
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Peak Number 4 unknown10.00 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.00	2.03 ng	71951	Acenaphthene-d10		9.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	43
2	Tetratetracontane	619	C44H90	007098-22-8	43
3	Nonadecane	268	C19H40	000629-92-5	38
4	2-methyltetracosane	352	C25H52	1000376-72-6	38
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	38



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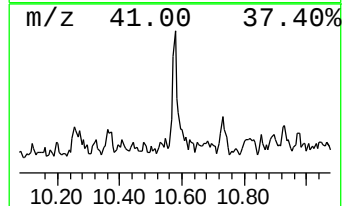
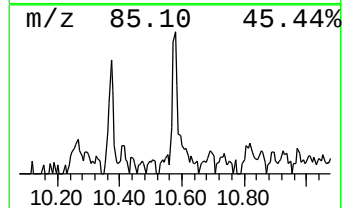
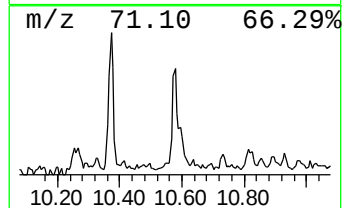
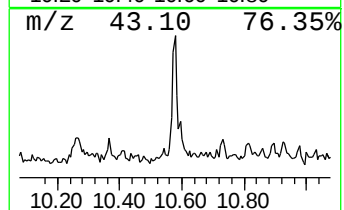
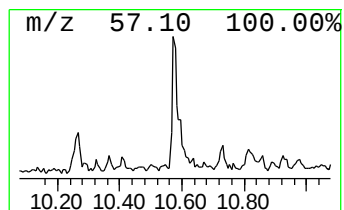
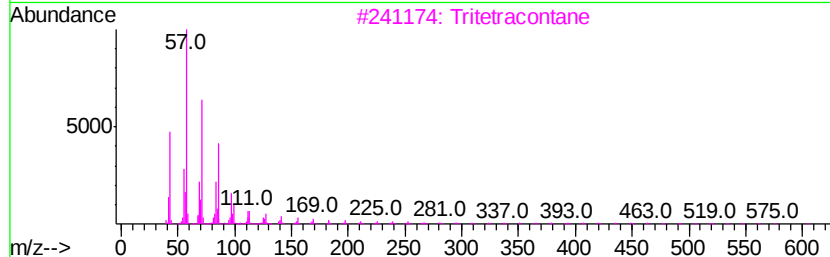
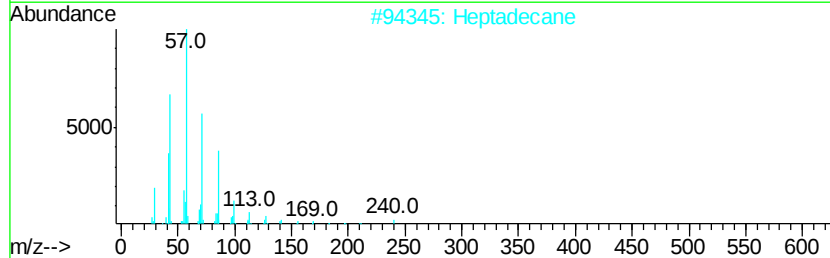
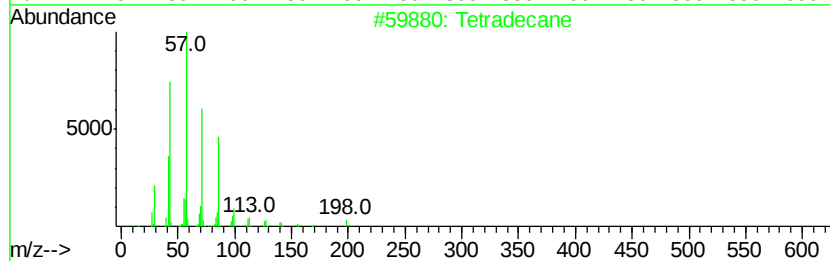
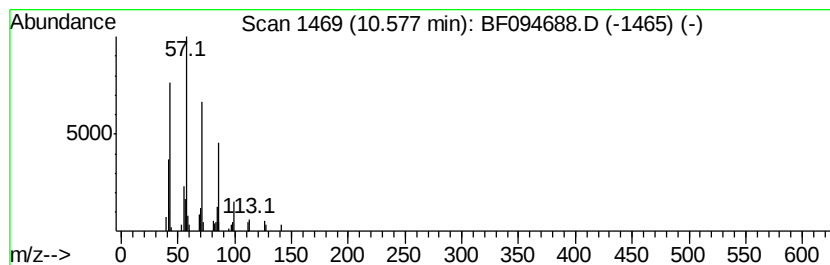
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Peak Number 5 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	2.15 ng	64387	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Tritetracontane	605	C43H88	007098-21-7	86
4	Pentadecane	212	C15H32	000629-62-9	83
5	Hexadecane	226	C16H34	000544-76-3	74



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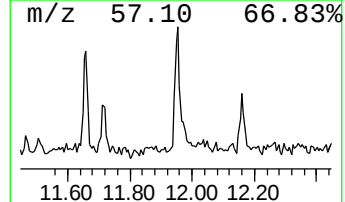
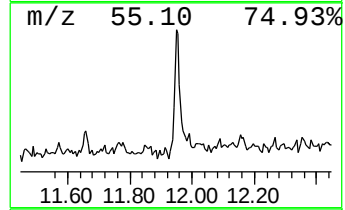
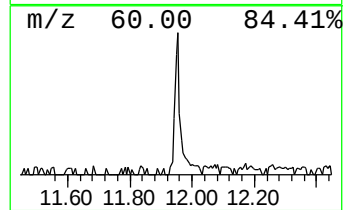
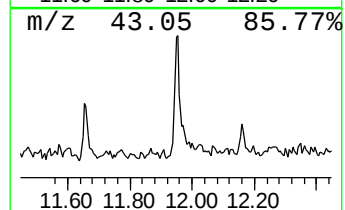
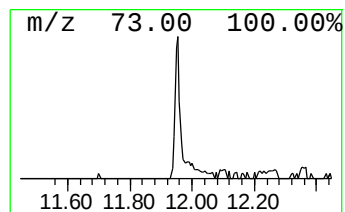
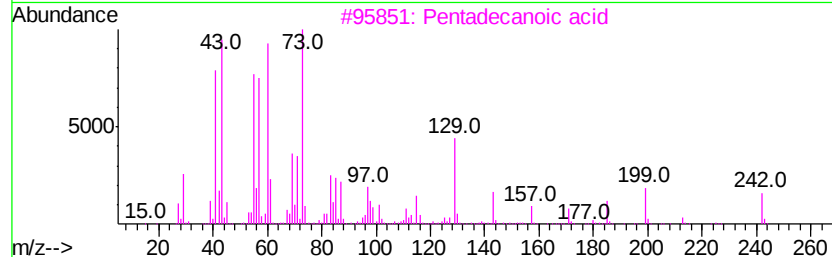
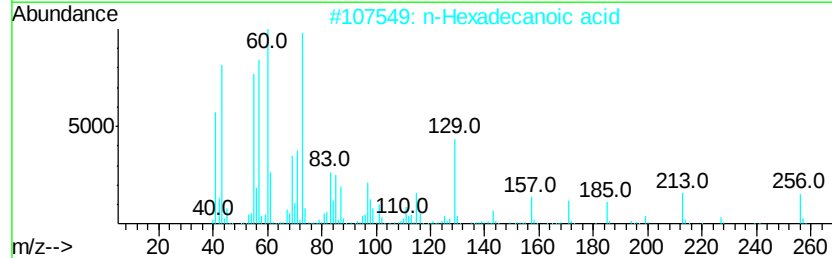
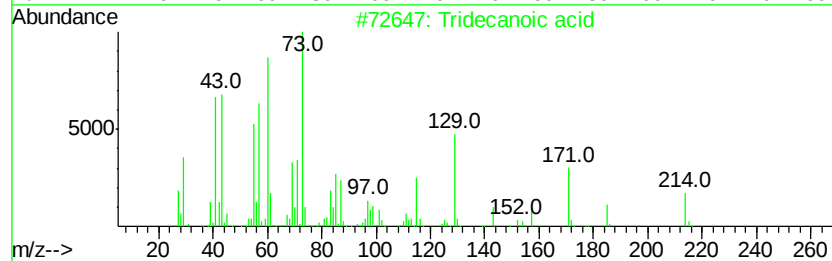
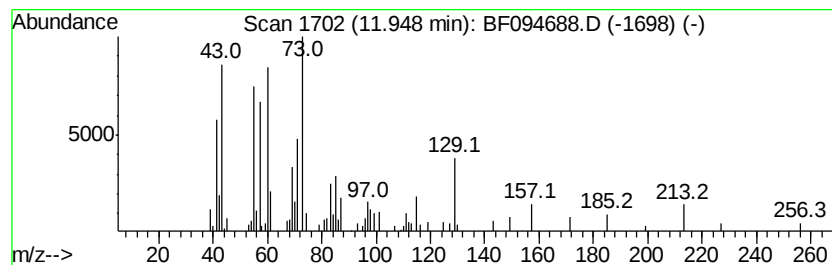
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Peak Number 6 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.95	4.77 ng	143056	Phenanthrene-d10		11.22
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	18



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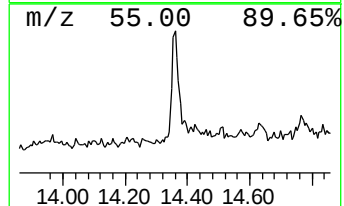
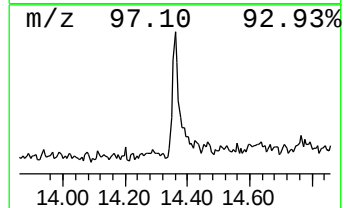
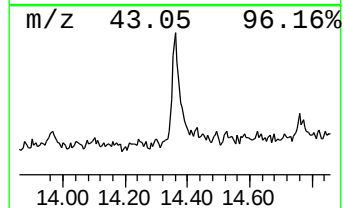
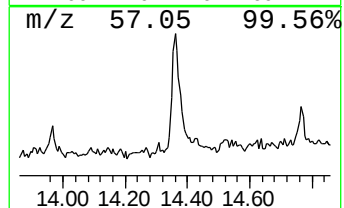
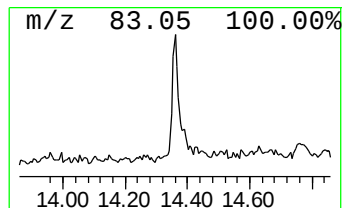
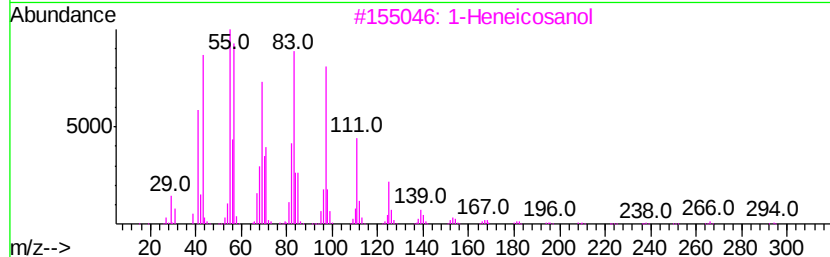
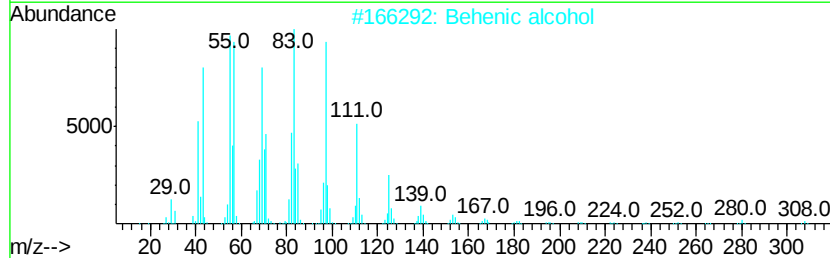
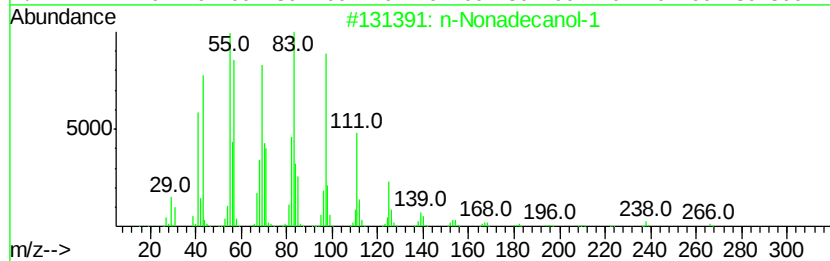
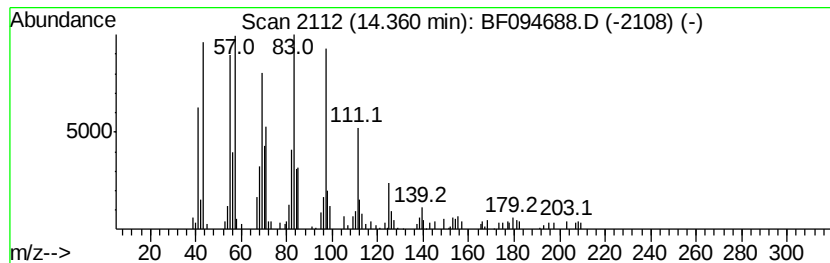
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	7.29 ng	202116	Chrysene-d12	14.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5		1-Nonadecene	266	C19H38	018435-45-5	95



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094688.D
Acq On : 28 Apr 2017 17:23
Operator : SJ/MA
Sample : I2895-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

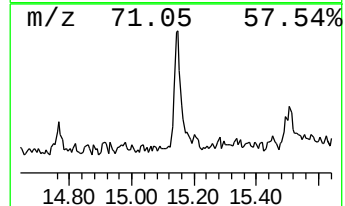
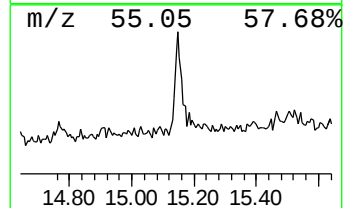
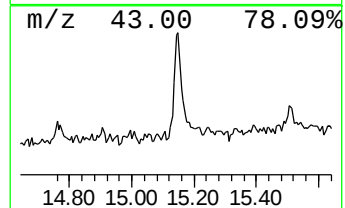
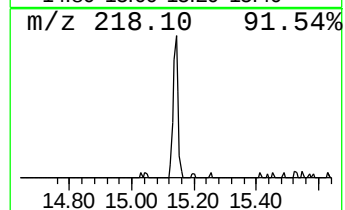
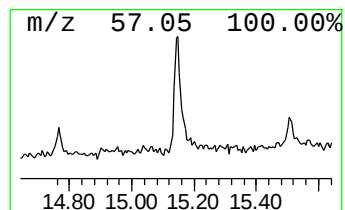
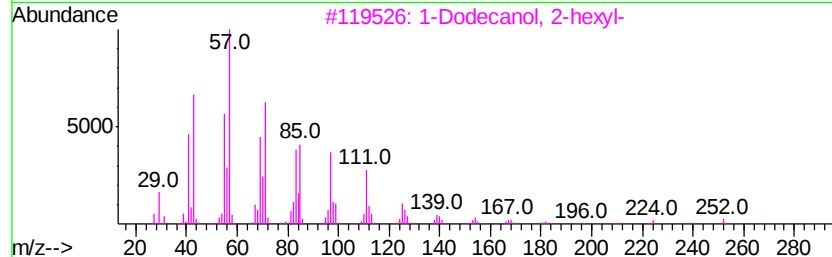
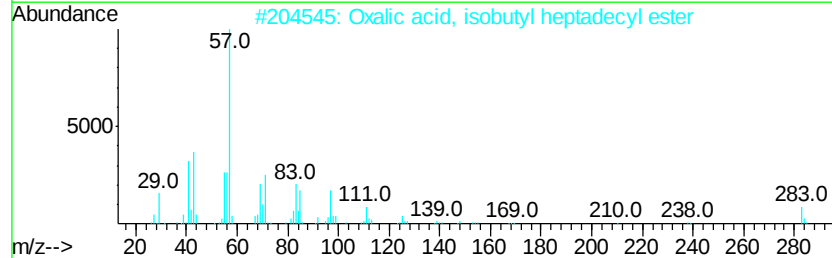
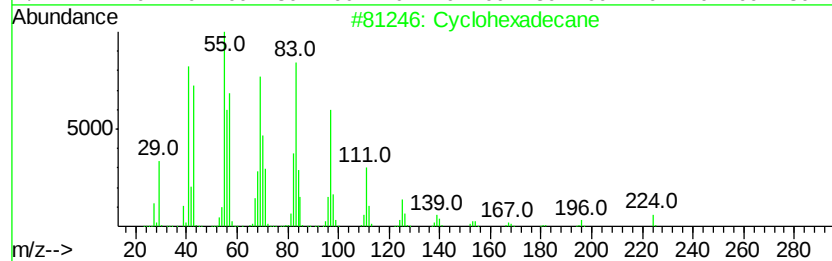
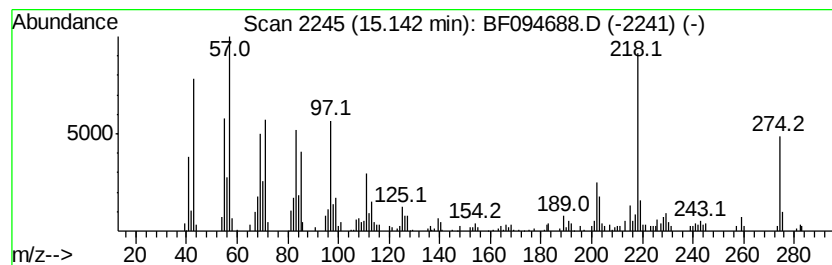
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ClientSampleId :
SB-12-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	9.12 ng	252598	Chrysene-d12	14.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 90
2		Oxalic acid, isobutyl heptadecyl...	384 C23H44O4	1000309-38-2 46
3		1-Dodecanol, 2-hexyl-	270 C18H38O	110225-00-8 46
4		Oxalic acid, isobutyl hexadecyl ...	370 C22H42O4	1000309-38-1 45
5		Heptadecyl heptafluorobutyrate	452 C21H35F7O2	959085-66-6 42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042817\
Data File : BF094688.D
Acq On : 28 Apr 2017 17:23
Operator : SJ/MA
Sample : I2895-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-2.0-3.0

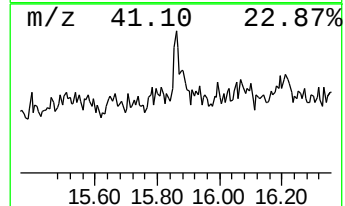
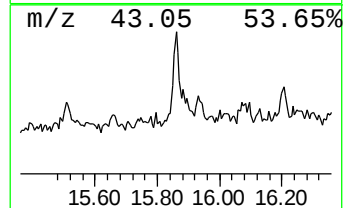
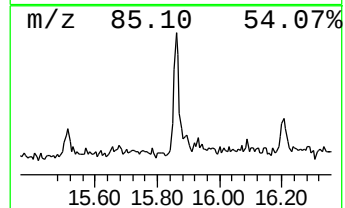
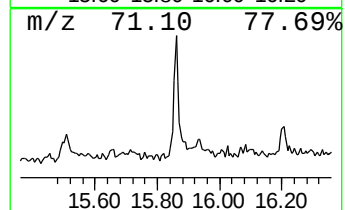
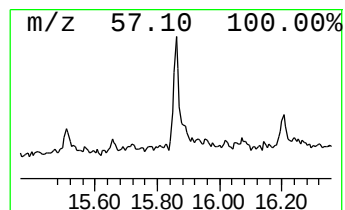
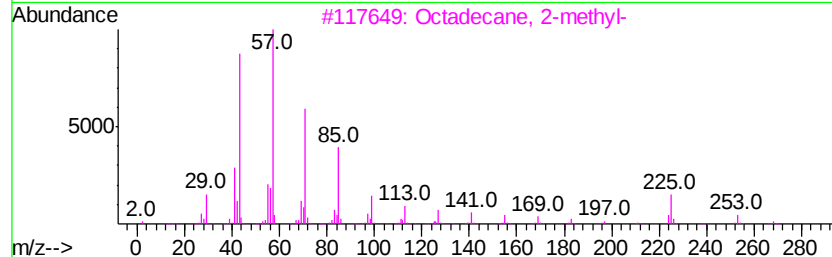
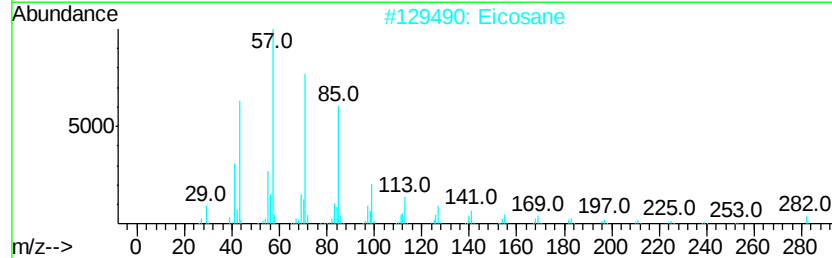
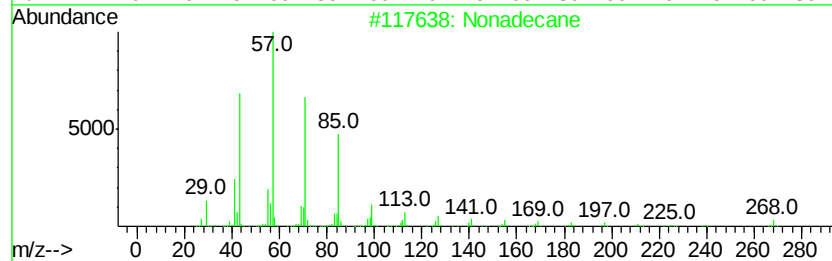
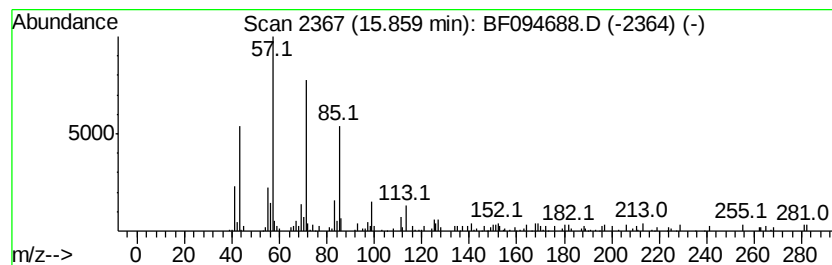
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	7.22 ng	140386	Perylene-d12	16.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Octadecane, 2-methyl-		268	C19H40	001560-88-9	90
4	Eicosane, 9-octyl-		394	C28H58	013475-77-9	90
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094688.D
Acq On : 28 Apr 2017 17:23
Operator : SJ/MA
Sample : I2895-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-2.0-3.0

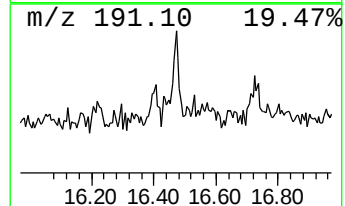
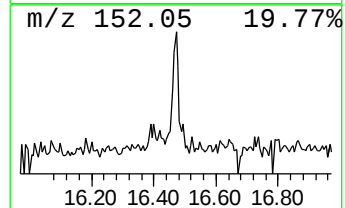
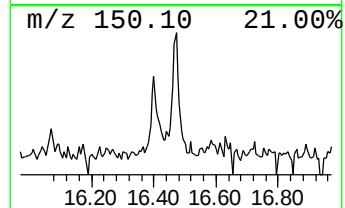
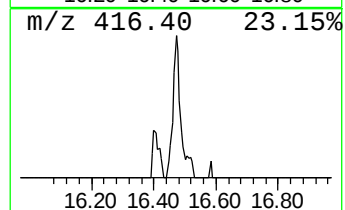
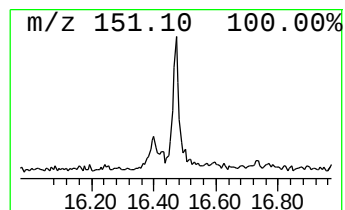
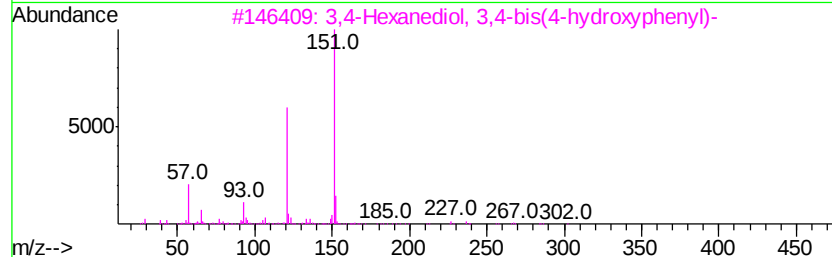
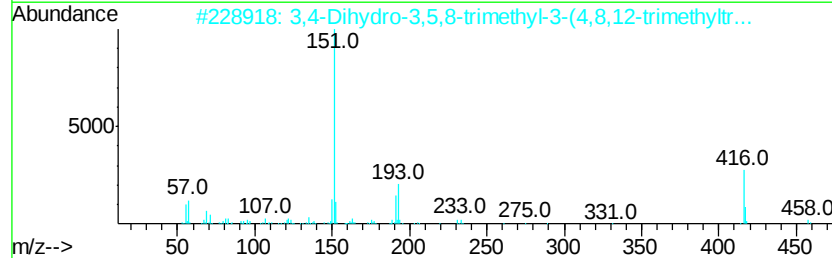
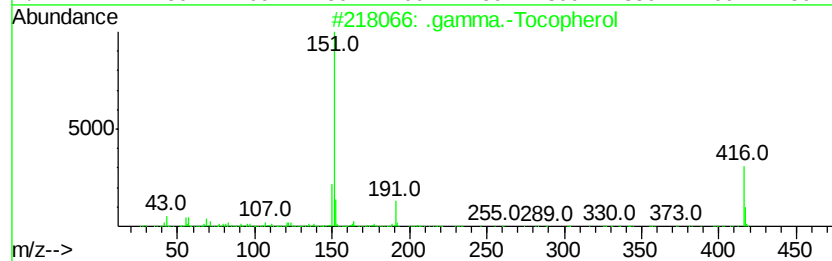
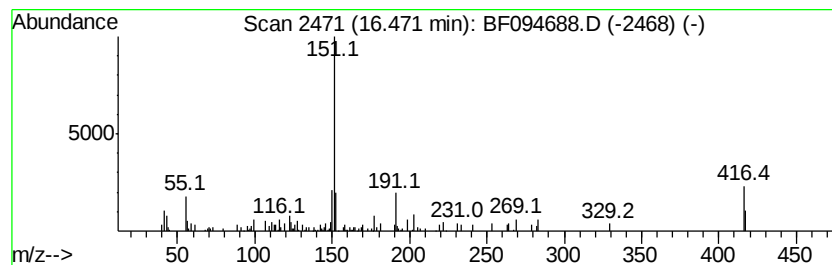
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Tocopherol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.70 ng	52437	Perylene-d12	16.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	68
2		3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	50
3		3,4-Hexanediol, 3,4-bis(4-hydrox...	302	C18H22O4	007507-01-9	43
4		1-Aminoinosine	283	C10H13N5O5	019029-66-4	38
5		[4-(2,4-Dimethoxybenzyl)piperazi...	370	C21H26N2O4	1000311-48-2	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042817\
Data File : BF094688.D
Acq On : 28 Apr 2017 17:23
Operator : SJ/MA
Sample : I2895-12
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
2-Pentanone, 4-hy...	3.94	21.9	ng	536916	1	5.77	490998	20.0
unknown5.52	5.52	125.6	ng	3083840	1	5.77	490998	20.0
unknown10.00	10.00	2.0	ng	71951	3	9.40	709688	20.0
Tetradecane	10.58	2.1	ng	64387	4	11.22	599230	20.0
Tridecanoic acid	11.95	4.8	ng	143056	4	11.22	599230	20.0
n-Nonadecanol-1	14.36	7.3	ng	202116	5	14.47	554200	20.0
Cyclohexadecane	15.14	9.1	ng	252598	5	14.47	554200	20.0
Nonadecane	15.86	7.2	ng	140386	6	16.10	388916	20.0
.gamma.-Tocopherol	16.47	2.7	ng	52437	6	16.10	388916	20.0