

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
 Data File : BF099927.D
 Acq On : 28 Oct 2017 19:50
 Operator : SJ/JU
 Sample : I6166-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72-11966

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	4.998	493	495	510	rBV	140516	212587	1.36%	0.587%
2	5.410	561	565	592	rBV	1097260	1353172	8.64%	3.737%
3	6.428	735	738	757	rBV	1234034	1374966	8.78%	3.797%
4	6.557	757	760	767	rVB	1556550	1453120	9.28%	4.013%
5	6.787	795	799	808	rBV	645876	590639	3.77%	1.631%
6	6.939	821	825	838	rBV	1365167	1198014	7.65%	3.309%
7	7.357	892	896	907	rBV	889284	865759	5.53%	2.391%
8	8.069	1013	1017	1028	rVB	900106	810578	5.18%	2.239%
9	9.139	1195	1199	1203	rBV	2061203	1771326	11.31%	4.892%
10	9.539	1264	1267	1270	rVB	239574	188226	1.20%	0.520%
11	9.822	1311	1315	1319	rBV2	928640	791971	5.06%	2.187%
12	10.616	1446	1450	1458	rBV	820124	764731	4.88%	2.112%
13	11.316	1565	1569	1571	rBV	715709	674635	4.31%	1.863%
14	11.339	1571	1573	1577	rVB	208302	181300	1.16%	0.501%
15	11.845	1653	1659	1671	rBV2	1081873	1446067	9.24%	3.994%
16	12.398	1749	1753	1757	rBV2	271618	262917	1.68%	0.726%
17	12.616	1771	1790	1795	rBV4	3976968	15656704	100.00%	43.239%
18	12.657	1795	1797	1808	rVV	1099471	1516968	9.69%	4.189%
19	12.763	1812	1815	1822	rVB	270720	342059	2.18%	0.945%
20	12.898	1834	1838	1842	rVB	1242836	1088963	6.96%	3.007%
21	13.921	2009	2012	2015	rVB	193110	159977	1.02%	0.442%
22	13.963	2016	2019	2022	rBV2	538089	577389	3.69%	1.595%
23	14.433	2096	2099	2104	rVB	740364	750838	4.80%	2.074%
24	15.027	2194	2200	2203	rBV2	199149	352206	2.25%	0.973%
25	15.427	2265	2268	2273	rVV	384102	463134	2.96%	1.279%
26	15.810	2331	2333	2339	rVB	146663	190701	1.22%	0.527%
27	16.580	2461	2464	2476	rVB	132128	230585	1.47%	0.637%
28	17.368	2592	2598	2608	rBV6	150391	403688	2.58%	1.115%
29	18.639	2805	2814	2824	rBV4	162304	536110	3.42%	1.481%

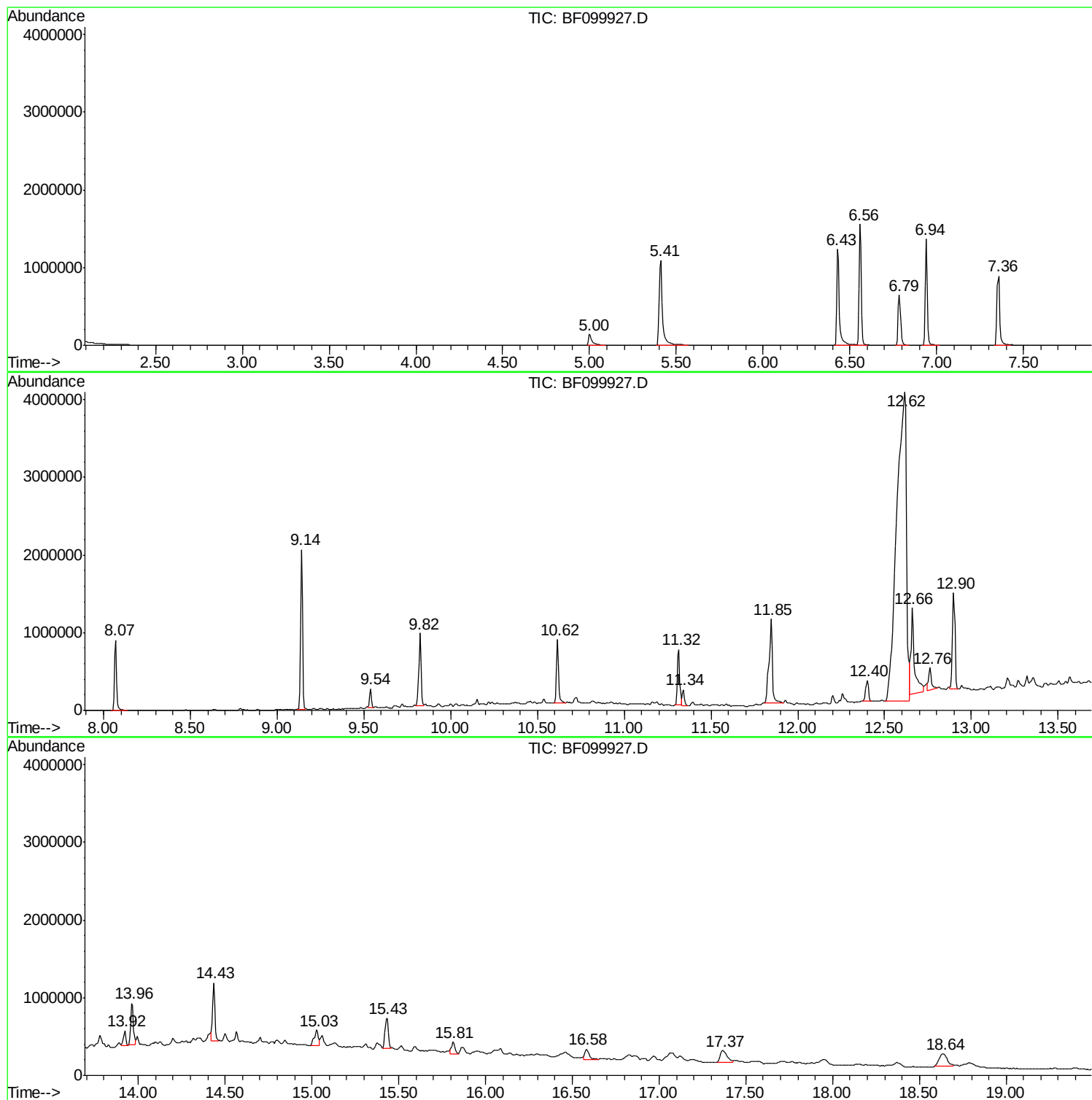
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampled :
RO-72-11966

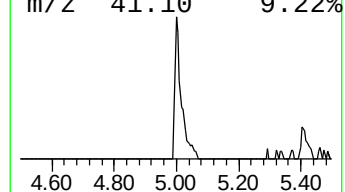
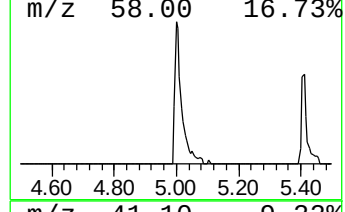
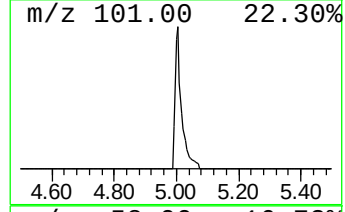
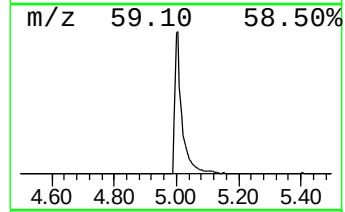
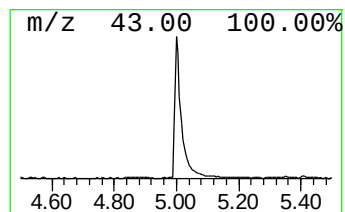
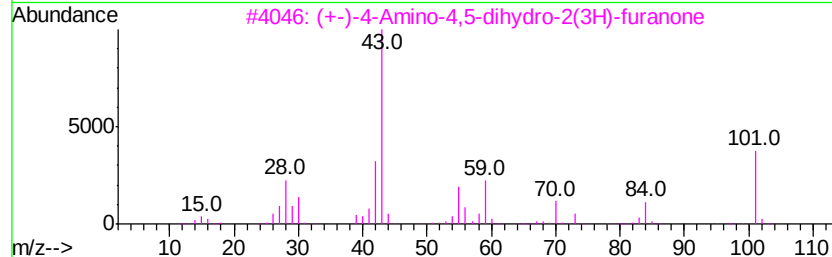
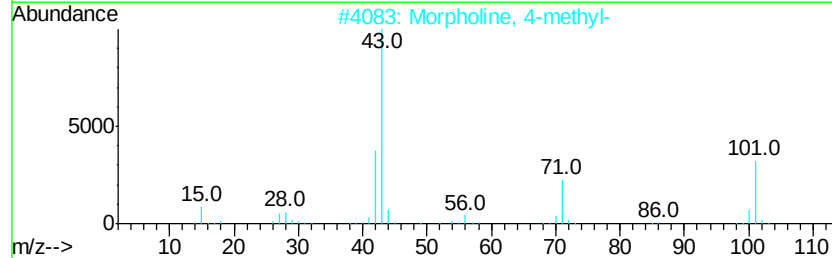
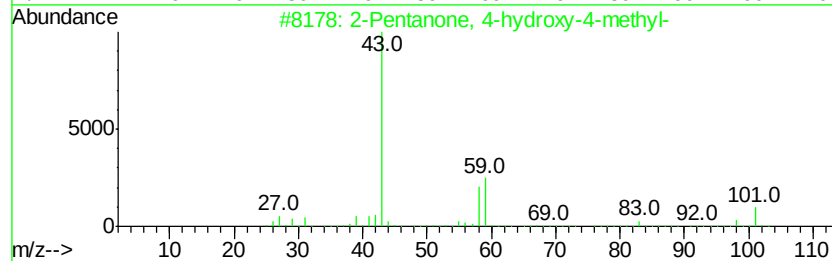
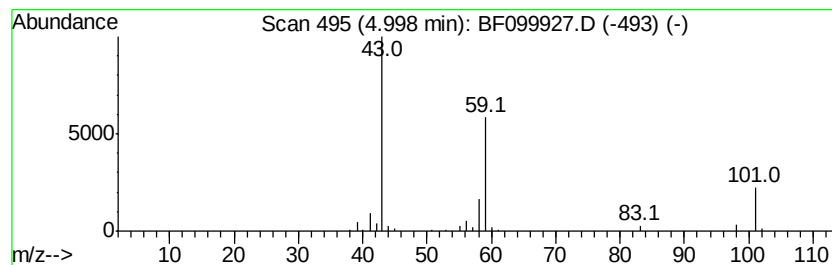
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	7.20 ng	212587	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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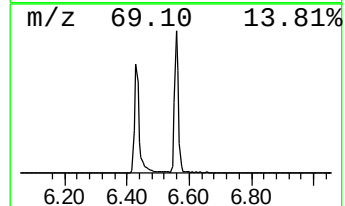
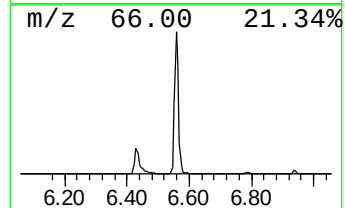
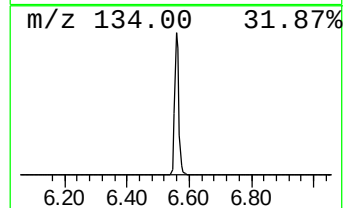
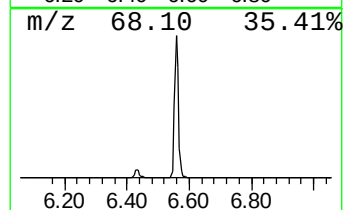
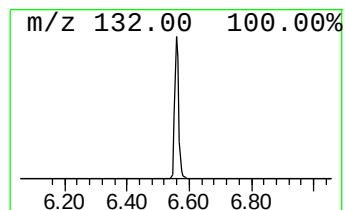
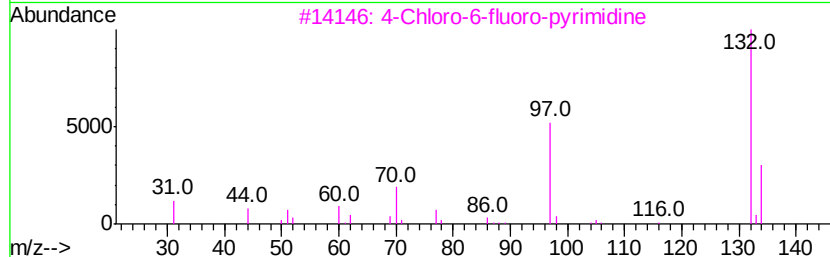
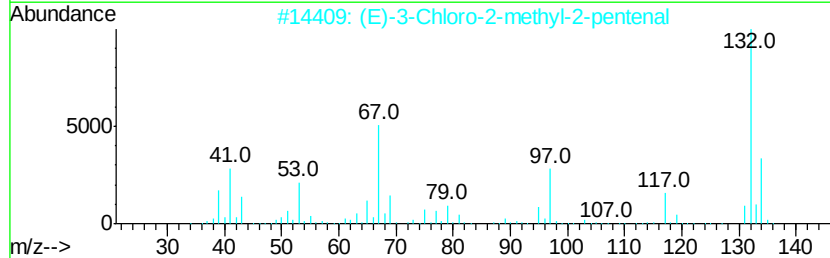
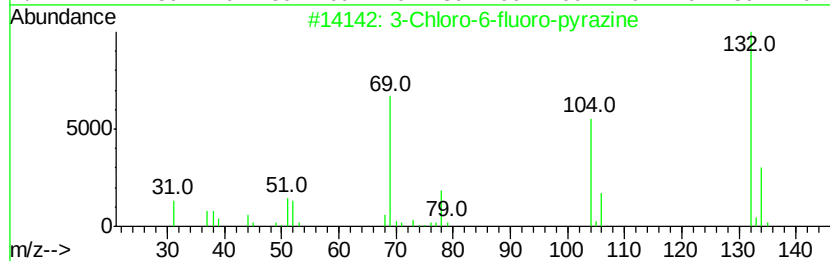
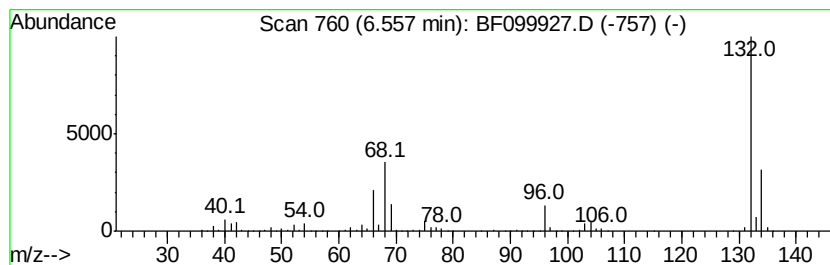
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Peak Number 2 unknown6.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	49.21 ng	1453120	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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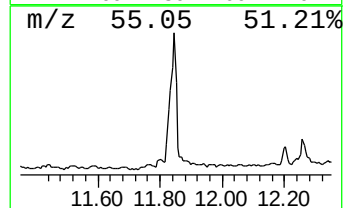
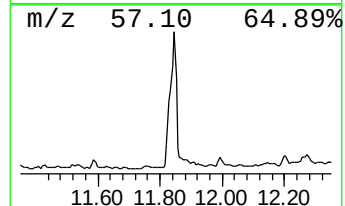
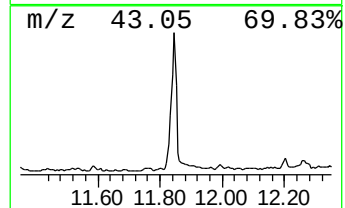
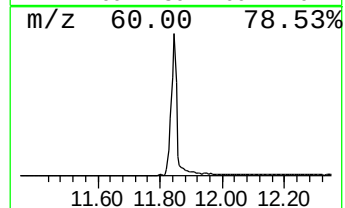
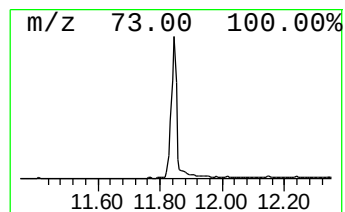
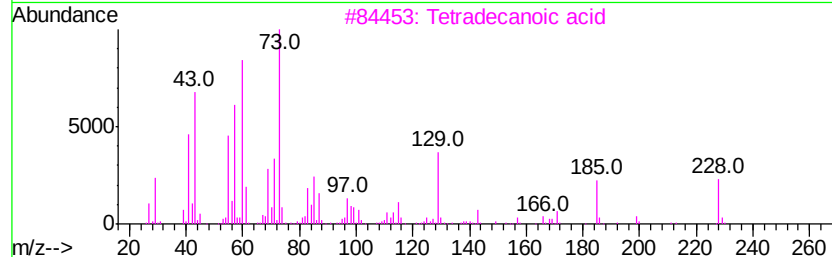
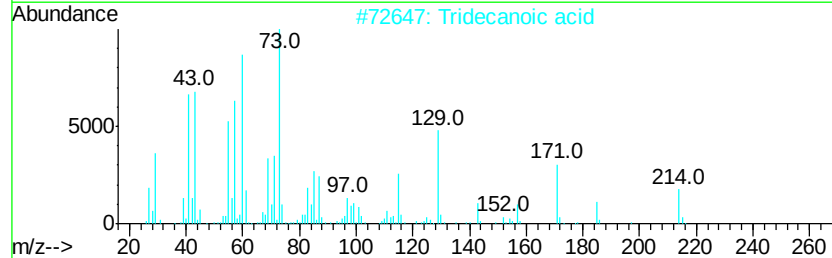
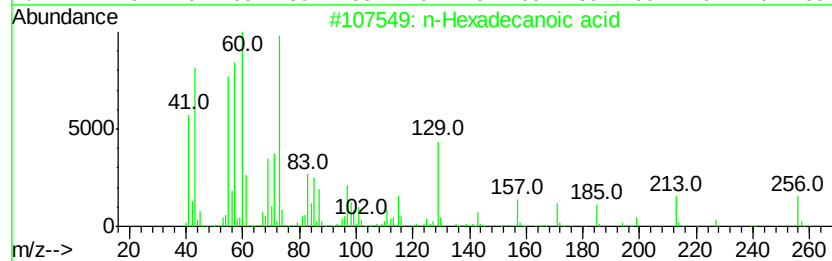
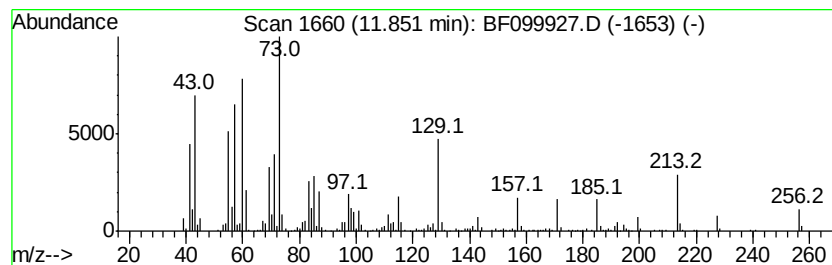
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	42.87 ng	1446070	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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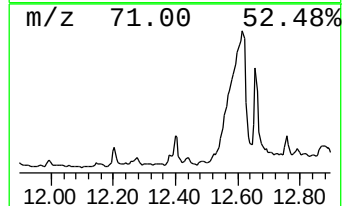
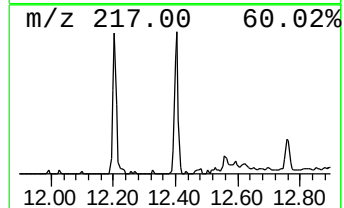
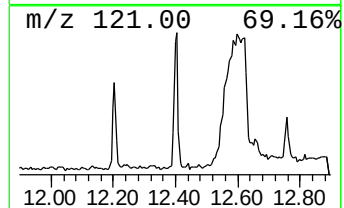
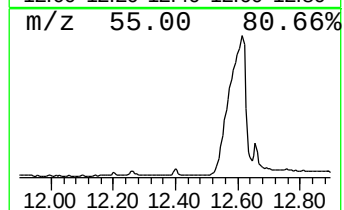
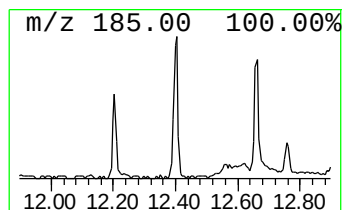
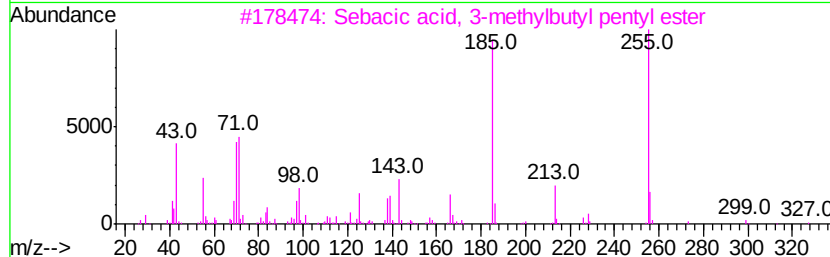
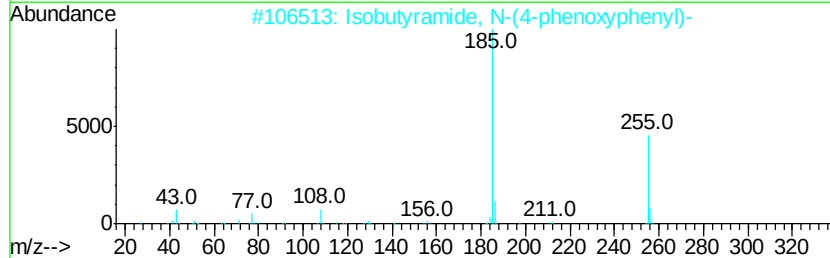
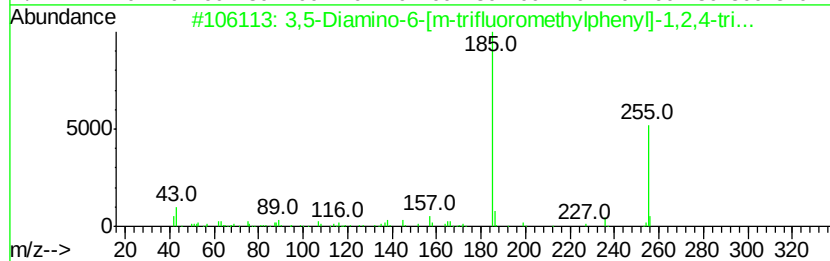
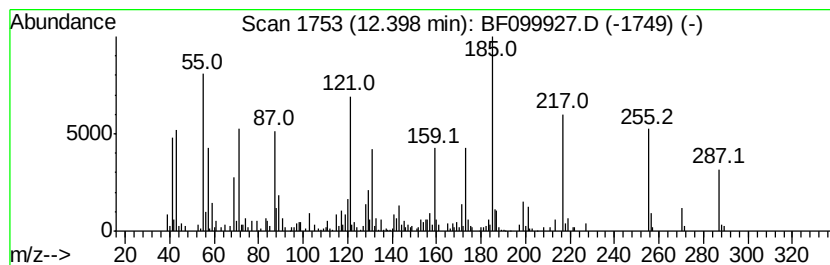
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Peak Number 5 unknown12.40 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.40	7.79 ng	262917	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Diamino-6-[m-trifluoromethyl...	255	C10H8F3N5	035857-40-0	38
2	Isobutyramide, N-(4-phenoxyphenyl)-	255	C16H17N02	1000339-96-7	25
3	Sebacic acid, 3-methylbutyl pent...	342	C20H38O4	1000355-36-8	22
4	Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	14
5	Sebacic acid, 2,4-dimethylpent-3...	370	C22H42O4	1000355-42-7	12



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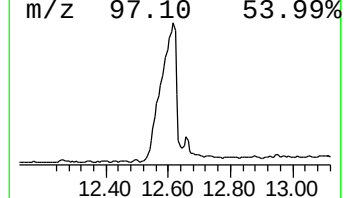
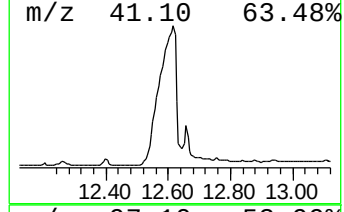
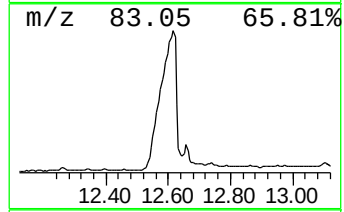
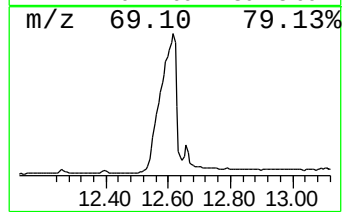
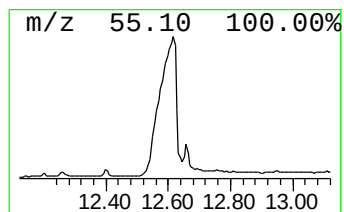
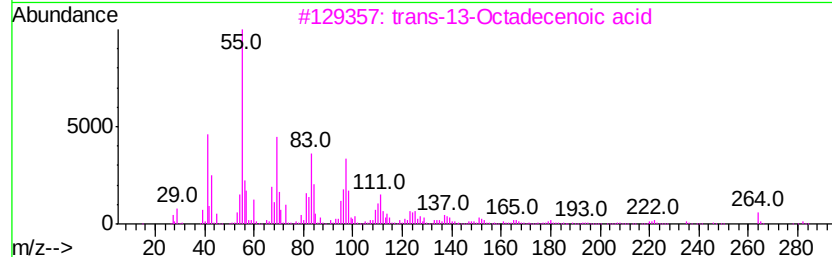
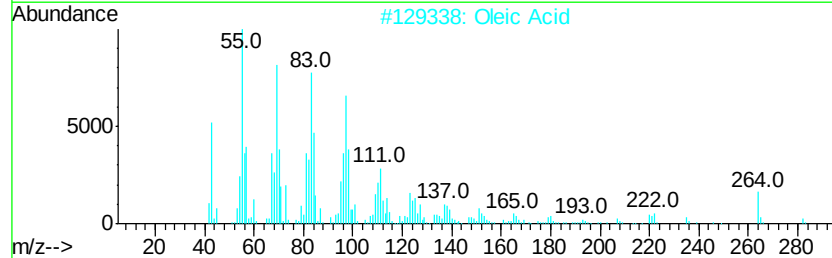
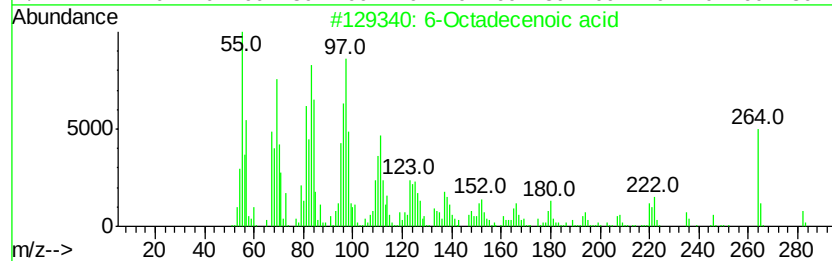
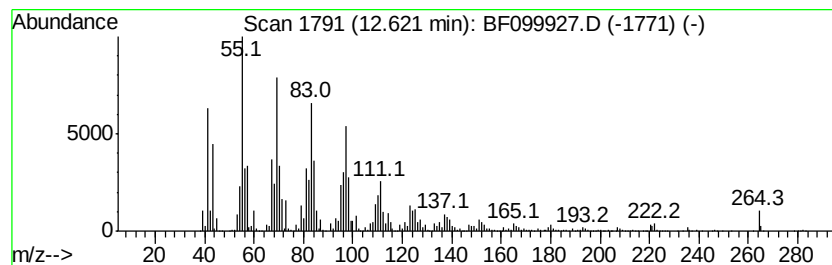
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Peak Number 6 6-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.62	464.15 ng	15656700	Phenanthrene-d10	11.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	96	
2	Oleic Acid	282	C18H34O2	000112-80-1	91	
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	87	
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	86	
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	86	



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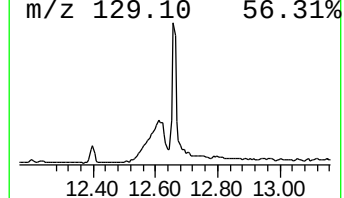
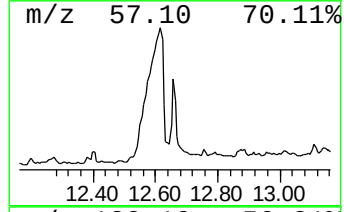
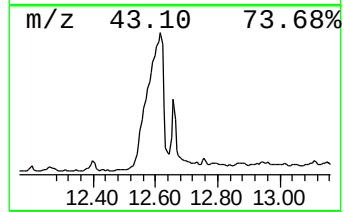
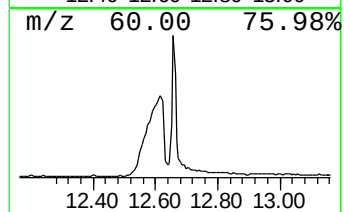
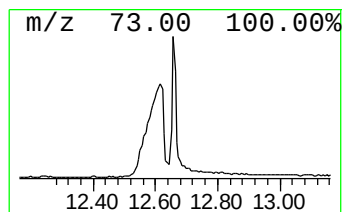
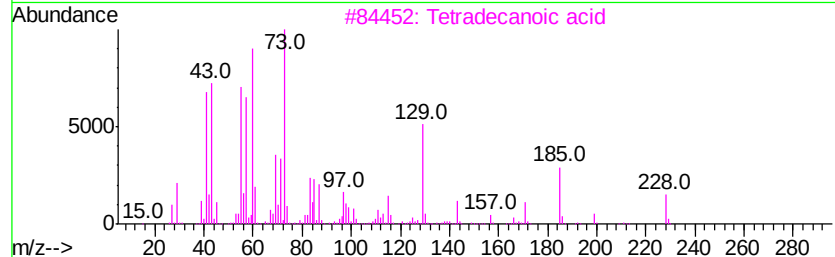
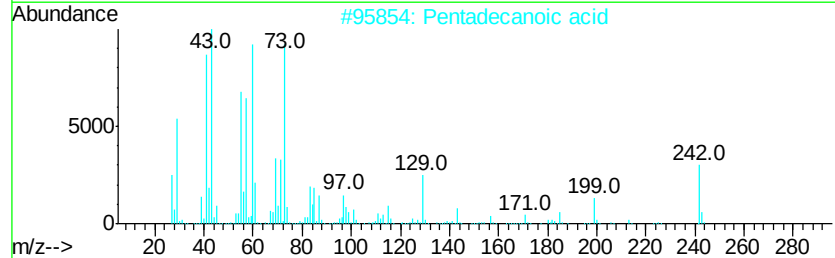
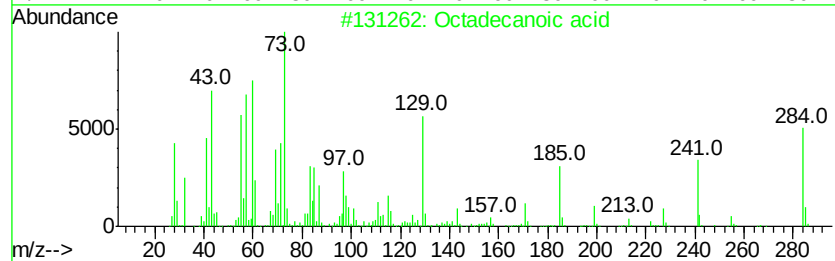
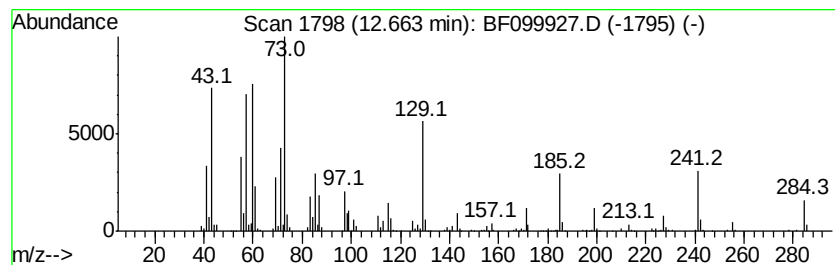
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.66	52.55 ng	1516970	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099927.D
Acq On : 28 Oct 2017 19:50
Operator : SJ/JU
Sample : I6166-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11966

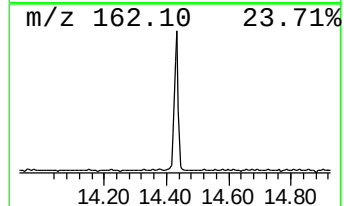
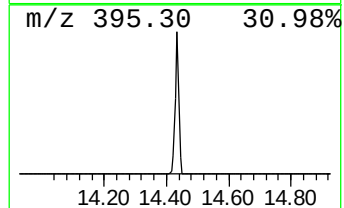
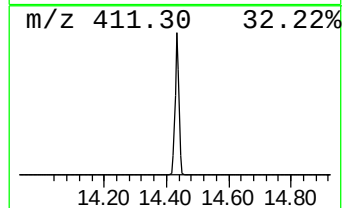
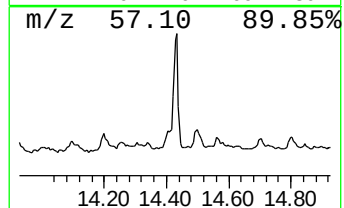
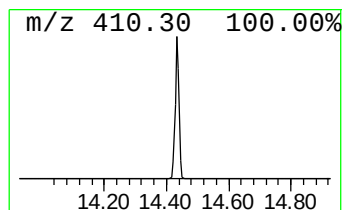
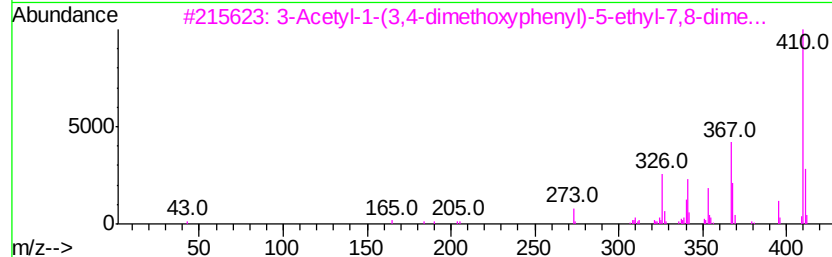
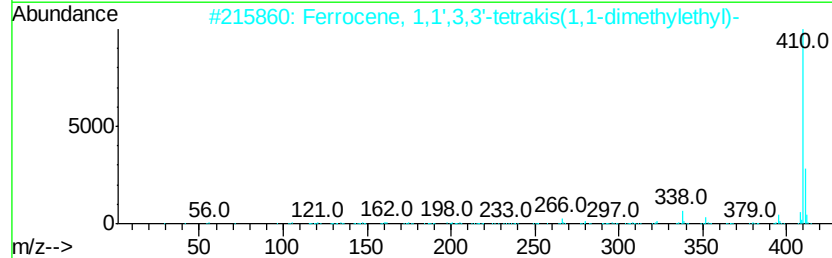
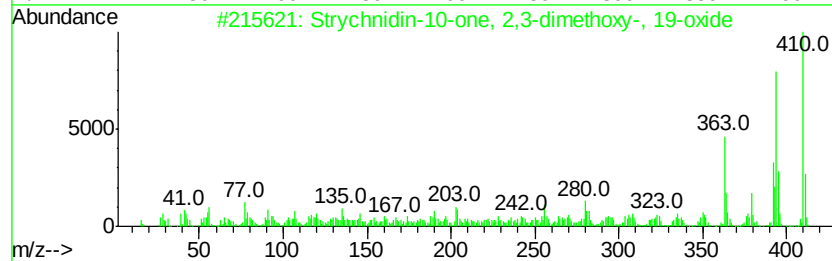
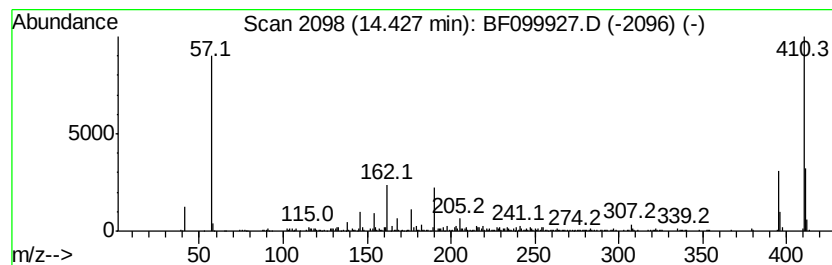
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Strychnidin-10-one, 2,3-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	26.01 ng	750838	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Strychnidin-10-one, 2,3-dimethox...	410	C23H26N2O5	017301-81-4	72
2		Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	70
3		3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	59
4		Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	40
5		6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	40



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
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Sample : I6166-01
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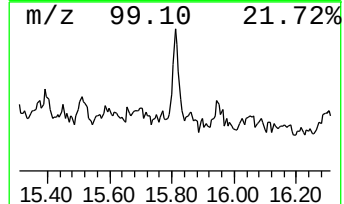
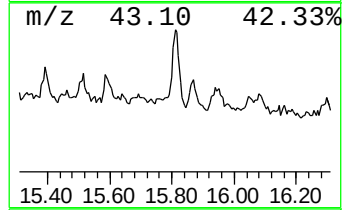
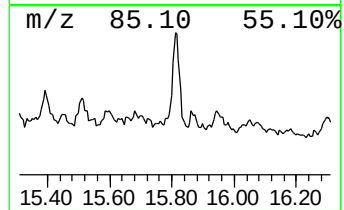
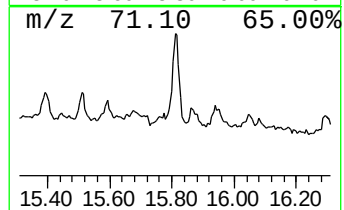
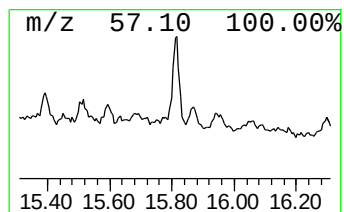
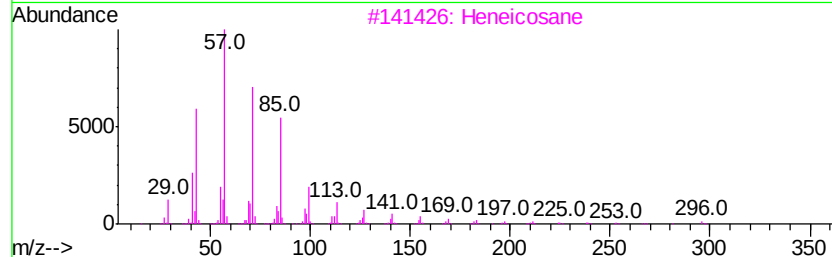
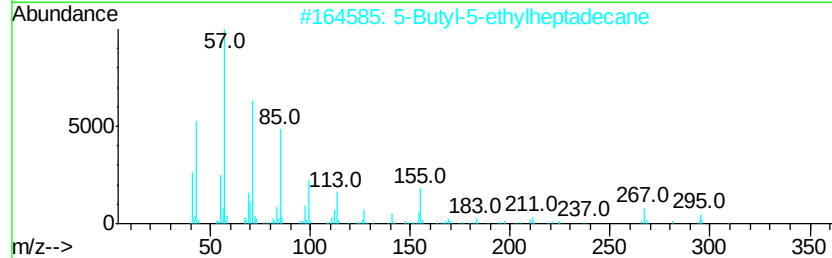
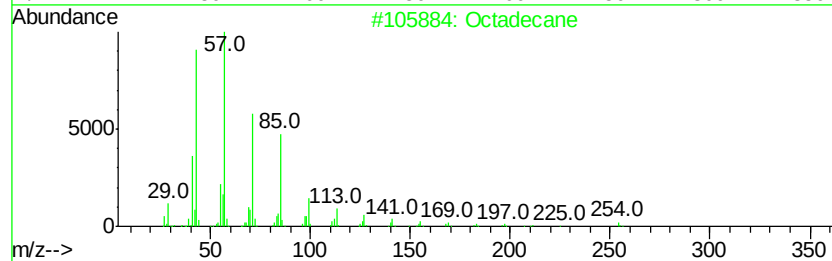
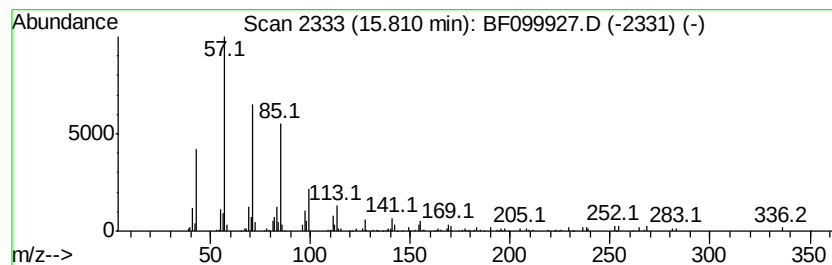
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	8.24 ng	190701	Perylene-d12	15.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	90
2	5-Butyl-5-ethylheptadecane	324 C23H48	1000360-43-0	90
3	Heneicosane	296 C21H44	000629-94-7	87
4	Nonadecane	268 C19H40	000629-92-5	87
5	6,6-Diethyloctadecane	310 C22H46	1000360-41-8	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099927.D
Acq On : 28 Oct 2017 19:50
Operator : SJ/JU
Sample : I6166-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RO-72-11966

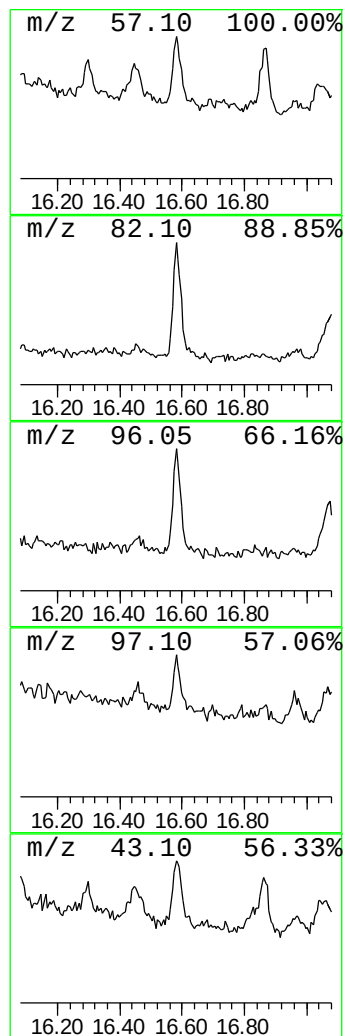
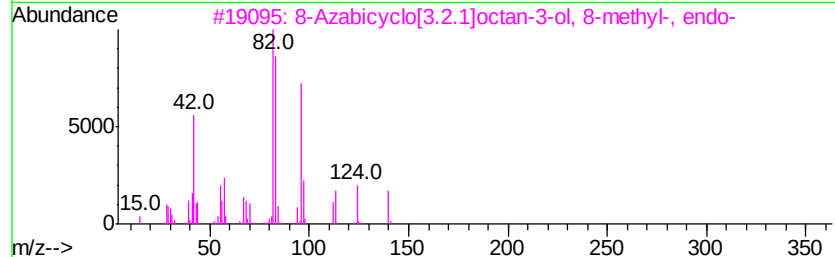
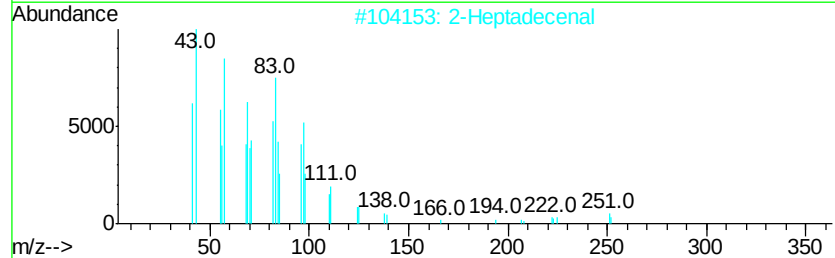
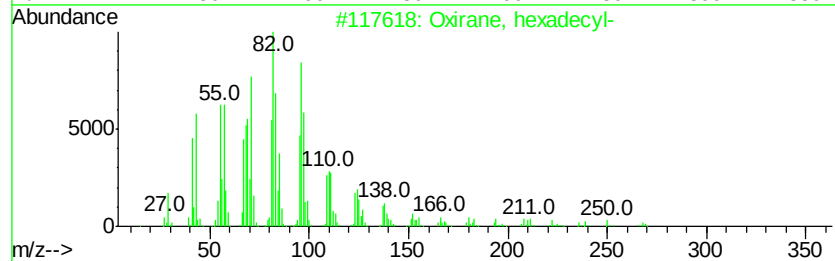
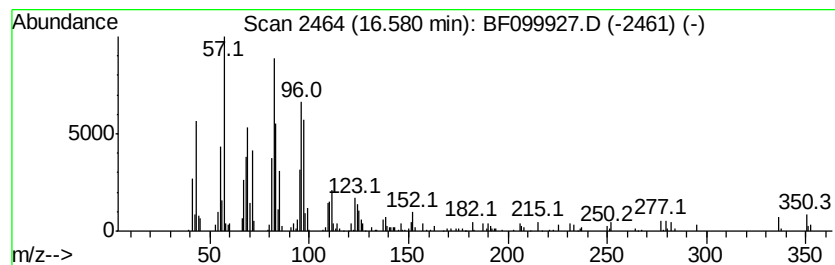
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	9.96 ng	230585	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	76
2		2-Heptadecenal	252	C17H32O	1000143-48-6	70
3		8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	49
4		Cyclododecanol	184	C12H24O	001724-39-6	47
5		Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	46



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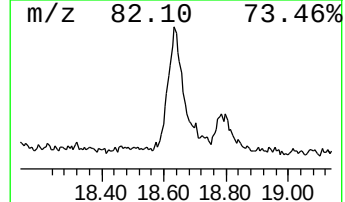
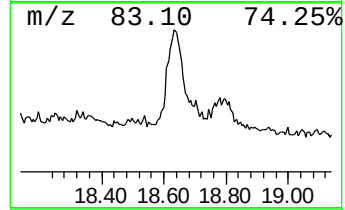
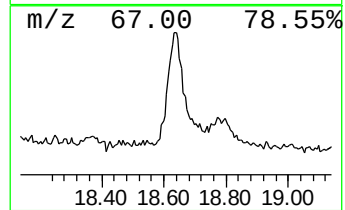
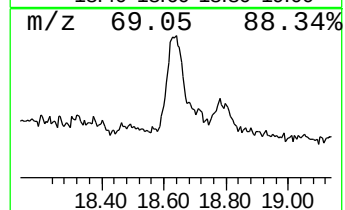
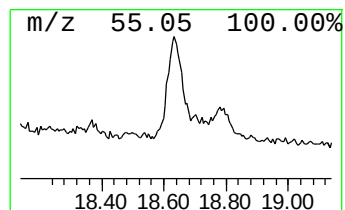
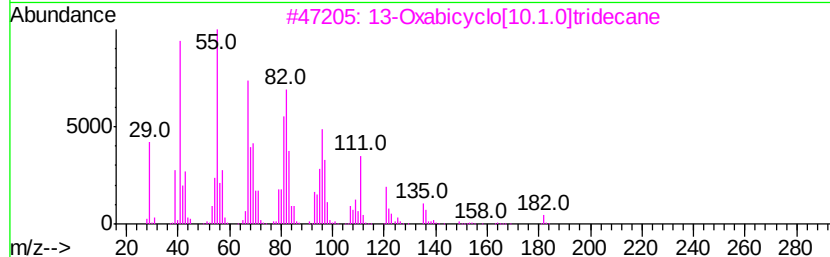
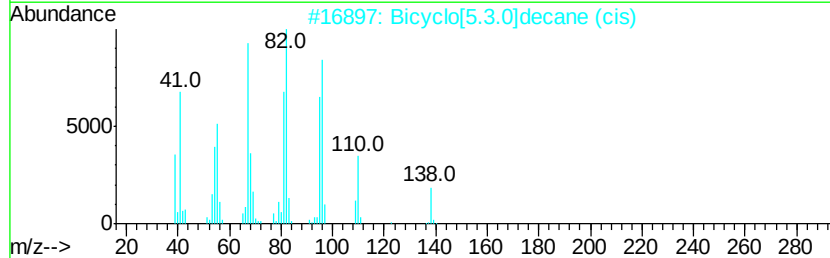
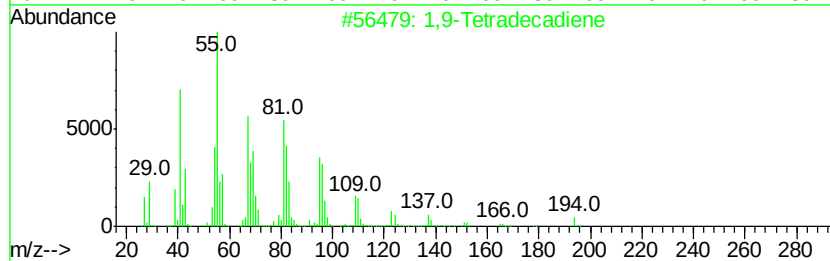
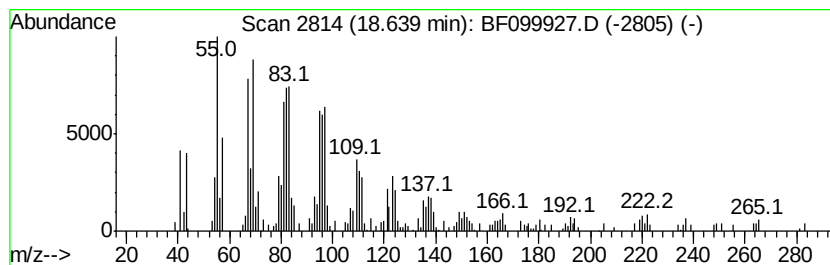
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,9-Tetradecadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.64	23.15 ng	536110	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,9-Tetradecadiene	194	C14H26	112929-06-3	90
2		Bicyclo[5.3.0]decane (cis)	138	C10H18	016189-46-1	86
3		13-Oxabicyclo[10.1.0]tridecane	182	C12H22O	000286-99-7	86
4		7-Methyl-1,6-octadiene	124	C9H16	042152-47-6	55
5		Z-9-Tetradecen-1-ol formate	240	C15H28O2	1000130-78-7	55



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Sample : I6166-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	5.00	7.2	ng	212587	1	6.79	590639	20.0
unknown6.56	6.56	49.2	ng	1453120	1	6.79	590639	20.0
n-Hexadecanoic acid	11.85	42.9	ng	1446070	4	11.32	674635	20.0
unknown12.40	12.40	7.8	ng	262917	4	11.32	674635	20.0
6-Octadecenoic acid	12.62	464.1	ng	15656700	4	11.32	674635	20.0
Octadecanoic acid	12.66	52.5	ng	1516970	5	13.97	577389	20.0
Strychnidin-10-on...	14.43	26.0	ng	750838	5	13.97	577389	20.0
Octadecane	15.81	8.2	ng	190701	6	15.43	463134	20.0
Oxirane, hexadecyl-	16.58	10.0	ng	230585	6	15.43	463134	20.0
1,9-Tetradecadiene	18.64	23.1	ng	536110	6	15.43	463134	20.0