

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
 Data File : BF085953.D
 Acq On : 1 Apr 2016 3:33
 Operator : UM/SJ
 Sample : H2046-04
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AMBOY-SB-34(0.5-15.0COMP)

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-BF032416.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	2.435	11	13	16	rBV	101356	222650	6.28%	0.713%
2	2.492	16	18	19	rVV2	127154	187657	5.30%	0.601%
3	2.527	19	21	22	rVV2	191269	236001	6.66%	0.756%
4	2.561	22	24	27	rVB2	260589	372333	10.51%	1.192%
5	3.007	60	63	68	rVB4	36170	53554	1.51%	0.172%
6	3.167	76	77	80	rVB	43775	41038	1.16%	0.131%
7	3.258	82	85	88	rVV	27779	43179	1.22%	0.138%
8	3.315	88	90	92	rVB	33498	51257	1.45%	0.164%
9	3.441	99	101	103	rBV2	71373	54179	1.53%	0.174%
10	3.830	133	135	139	rBV2	80823	149243	4.21%	0.478%
11	4.390	181	184	185	rBV2	257520	493172	13.92%	1.579%
12	4.413	185	186	189	rVV2	746973	665778	18.79%	2.132%
13	4.470	189	191	193	rVV	30375	44583	1.26%	0.143%
14	4.516	193	195	196	rVV	38780	36929	1.04%	0.118%
15	4.653	203	207	209	rVV	56203	87967	2.48%	0.282%
16	4.756	213	216	217	rVV	25749	42708	1.21%	0.137%
17	4.778	217	218	221	rVV2	76662	90474	2.55%	0.290%
18	4.847	222	224	225	rVV	47591	50014	1.41%	0.160%
19	4.881	225	227	229	rVV	104971	164442	4.64%	0.527%
20	4.916	229	230	233	rVB	65371	70338	1.98%	0.225%
21	4.973	233	235	245	rBV	103185	207347	5.85%	0.664%
22	5.384	268	271	274	rBV	2126494	3253489	91.82%	10.419%
23	5.464	276	278	281	rVB	27698	43524	1.23%	0.139%
24	5.624	289	292	294	rVB3	32176	50284	1.42%	0.161%
25	6.436	360	363	365	rBV	2642115	2966468	83.72%	9.500%
26	6.561	371	374	376	rBV	2905871	3171938	89.51%	10.158%
27	6.790	391	394	396	rBV	678832	649458	18.33%	2.080%
28	6.939	405	407	410	rBV	1882999	2378501	67.12%	7.617%
29	7.362	441	444	446	rBV	1801394	2139540	60.38%	6.852%
30	7.464	451	453	459	rVB	43182	66679	1.88%	0.214%
31	8.070	504	506	509	rBV	890202	844584	23.83%	2.705%
32	9.156	598	601	603	rBV	3314304	3543509	100.00%	11.348%
33	9.545	633	635	638	rBV	459194	497243	14.03%	1.592%
34	9.762	652	654	655	rBV	72627	58703	1.66%	0.188%

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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	9.830	658	660	662 rVB	859309	875930	24.72%	2.805%
36	10.265	694	698	699 rBV	71983	98556	2.78%	0.316%
37	10.482	714	717	718 rBV	29872	44036	1.24%	0.141%
38	10.619	726	729	731 rBV	2035792	1958918	55.28%	6.273%
39	10.733	737	739	746 rVB	102111	115014	3.25%	0.368%
40	11.179	776	778	779 rBV	61309	50837	1.43%	0.163%
41	11.305	787	789	792 rBV2	623613	791862	22.35%	2.536%
42	11.842	834	836	840 rBV	45055	53376	1.51%	0.171%
43	12.173	862	865	868 rVB3	27785	41613	1.17%	0.133%
44	12.253	868	872	874 rBV3	28051	41320	1.17%	0.132%
45	12.894	925	928	930 rBV	2701881	2432511	68.65%	7.790%
46	12.928	930	931	933 rVV2	111218	147003	4.15%	0.471%
47	12.962	933	934	939 rVB2	36348	77963	2.20%	0.250%
48	13.374	964	970	972 rBV4	10299	35834	1.01%	0.115%
49	13.465	976	978	981 rVB	41367	39891	1.13%	0.128%
50	13.796	1004	1007	1012 rBV	72029	116135	3.28%	0.372%
51	13.945	1018	1020	1023 rVB	605468	541139	15.27%	1.733%
52	14.197	1041	1042	1043 rBV	70978	49121	1.39%	0.157%
53	15.362	1141	1144	1148 rBV	401909	541322	15.28%	1.734%
54	17.294	1311	1313	1314 rBV	103435	77309	2.18%	0.248%
55	17.568	1336	1337	1341 rVB3	56359	67629	1.91%	0.217%

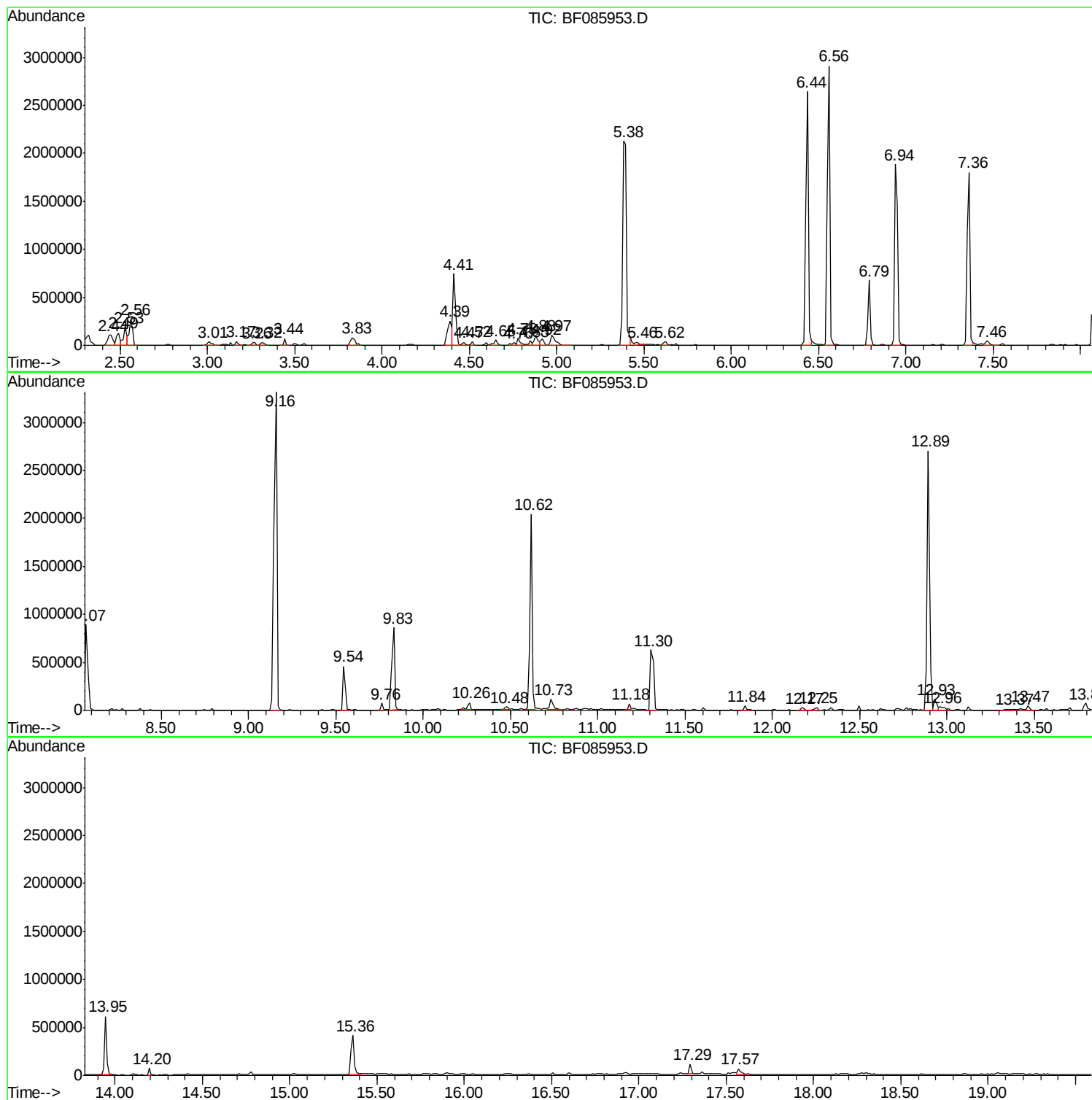
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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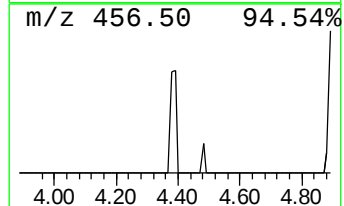
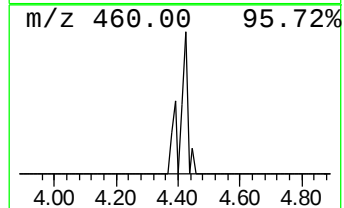
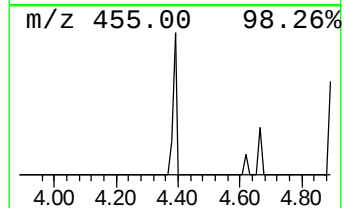
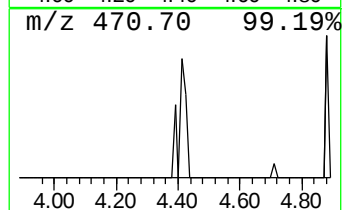
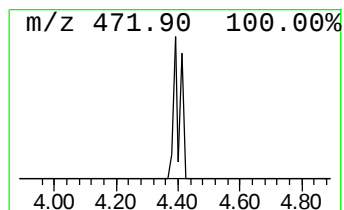
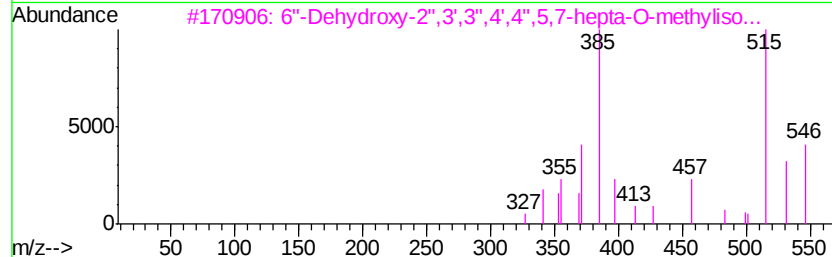
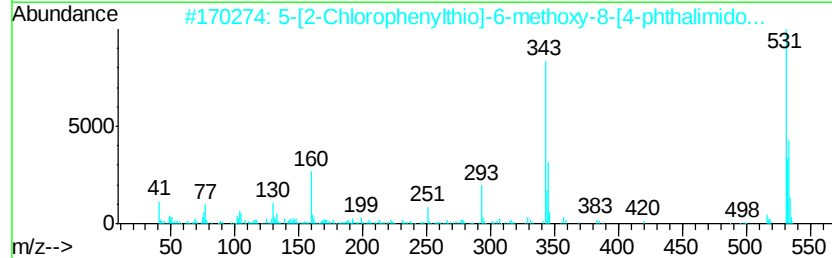
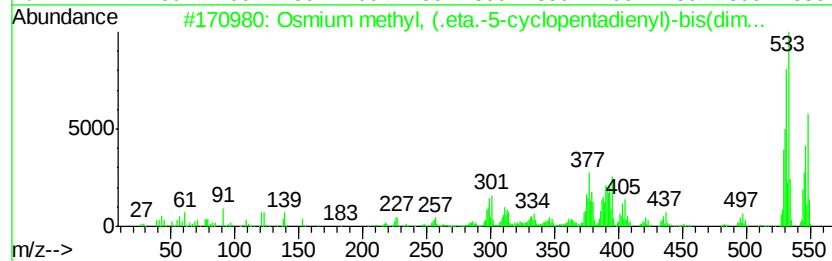
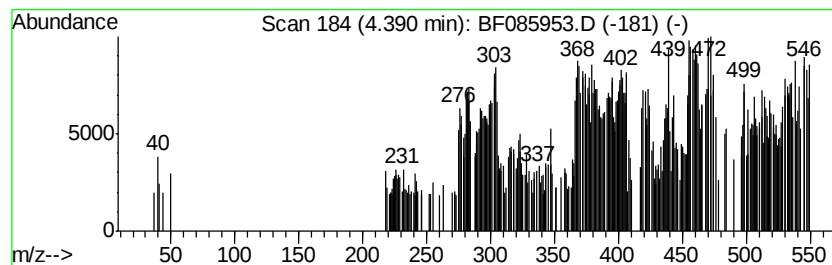
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown4.39 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	15.19 ng	493172	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Osmium methyl, (.eta.-5-cyclopentadienyl)-bis(dimethylamino)phosphine oxide	548	C22H30O5P2	1000158-92-4	20
2		5-[2-Chlorophenylthio]-6-methoxy-2-methyl-2H-pyran	531	C29H26ClN3O3S	064895-64-3	9
3		6"-Dehydroxy-2",3',3",4',4",5,7-hepta-O-methylisovanillin	546	C28H34O11	1000064-97-6	9
4		Iron, [1,2-ethanedithiolbis(diphenylthio)]	534	C32H32FeP2	115161-07-4	9
5		1,3,7,9,2,8-Parazabol, 4,6,10,12-tetramethyl-1,3,7,9-tetraazabicyclo[3.3.1]non-2-ene	563	C33H60B2N6	1000162-58-7	9



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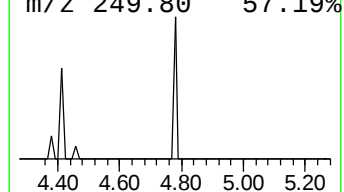
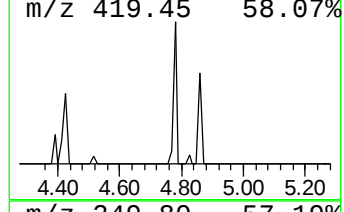
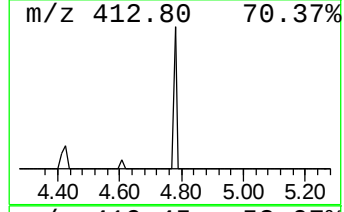
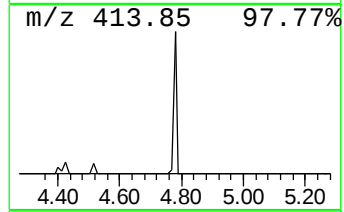
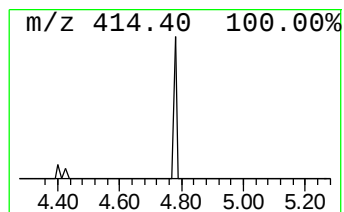
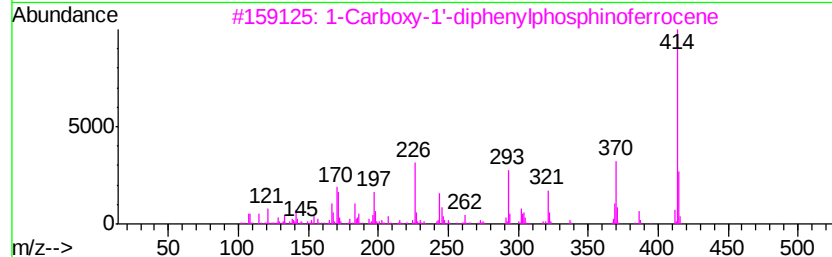
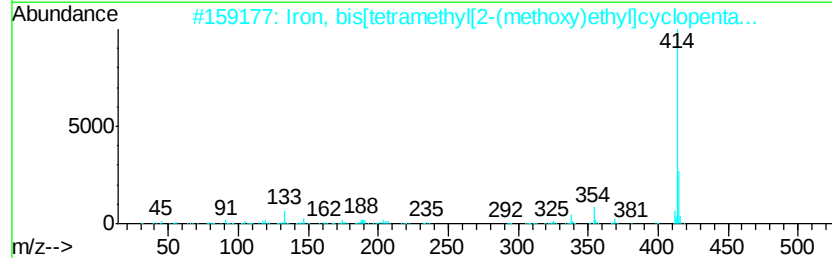
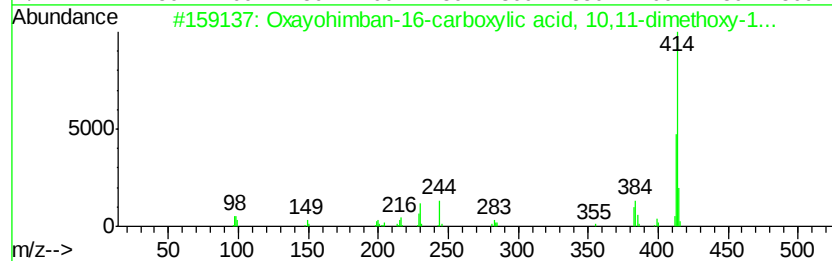
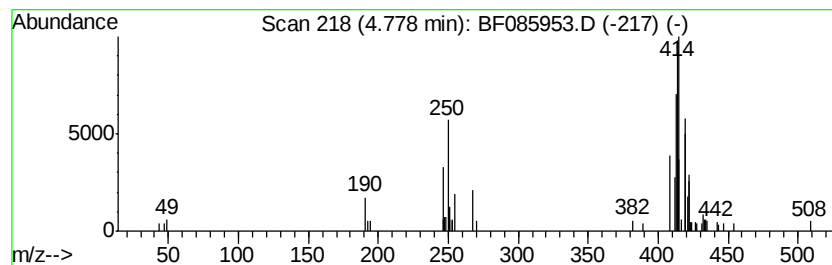
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown4.78 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	2.79 ng	90474	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxayohimban-16-carboxylic acid, ...	414	C23H30N2O5	005308-79-2	22
2		Iron, bis[tetramethyl[2-(methoxy...	414	C24H38FeO2	1000160-98-8	10
3		1-Carboxy-1'-diphenylphosphinofer...	414	C23H19FeO2P	1000281-03-1	10
4		9,12,15,18,21,24-Hexaoxa(2,16)[3...	414	C24H30O6	1000164-73-4	9
5		Stigmast-8(14)-en-3.beta.-ol	414	C29H50O	018069-99-3	9



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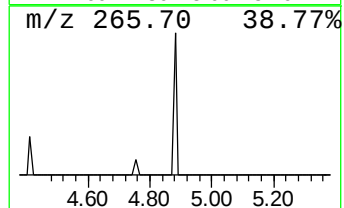
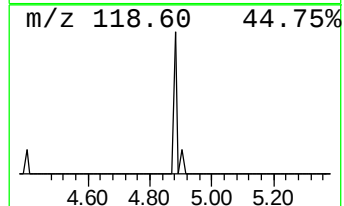
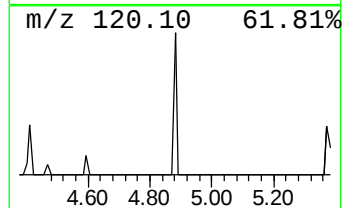
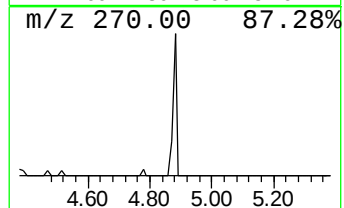
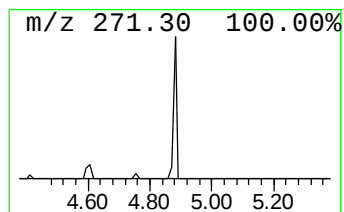
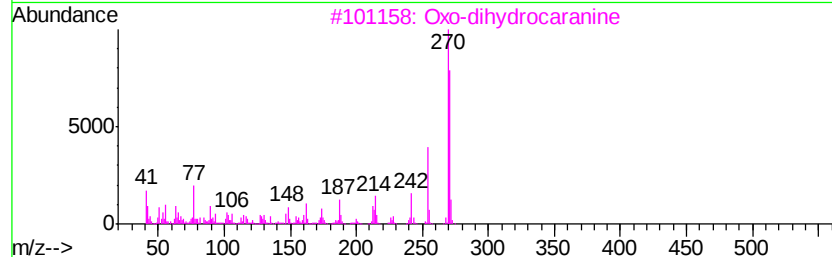
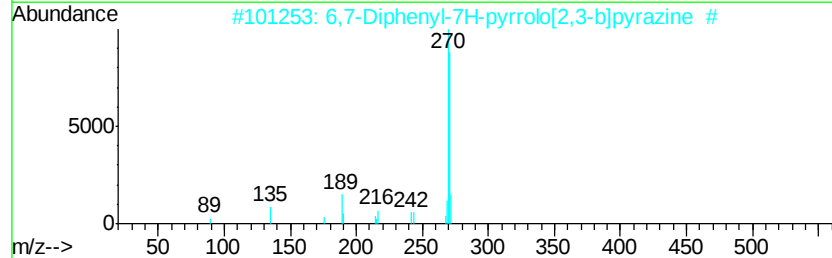
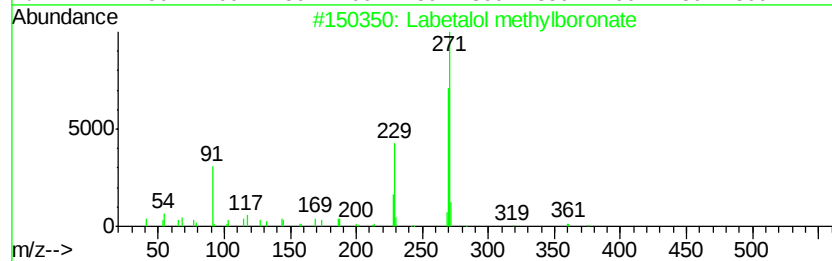
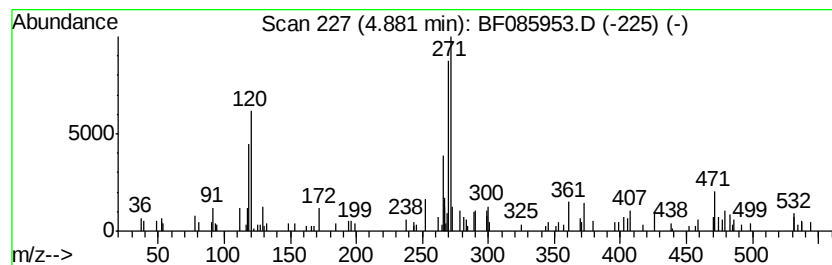
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown4.88 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	5.06 ng	164442	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Labetalol methylboronate	376	C21H26B2N2O3	127202-00-0	47
2			6,7-Diphenyl-7H-pyrrolo[2,3-b]py...	271	C18H13N3	1000148-45-1	47
3			Oxo-dihydrocaranine	271	C16H17N03	112529-25-6	38
4			6-Phenoxyphenanthridine	271	C19H13N0	003340-87-2	38
5			Pyrazolo[1,5-a]pyrimidine, 2,5-d...	271	C18H13N3	130159-66-9	28



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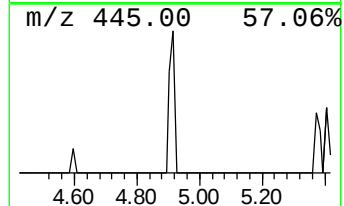
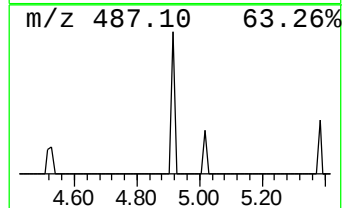
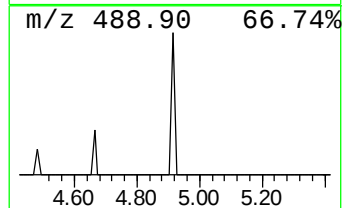
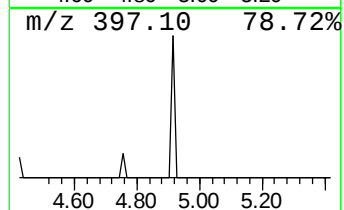
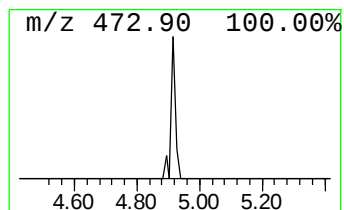
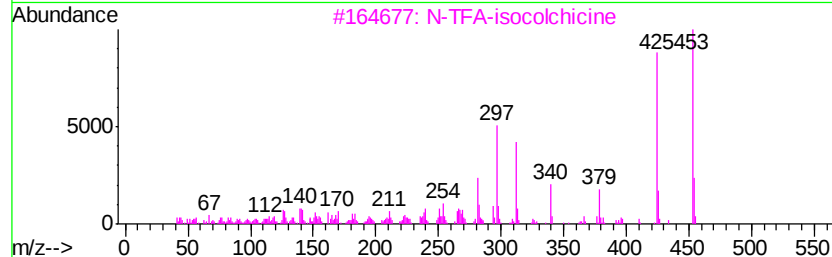
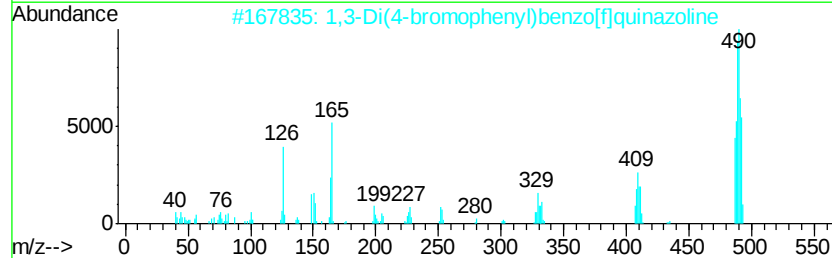
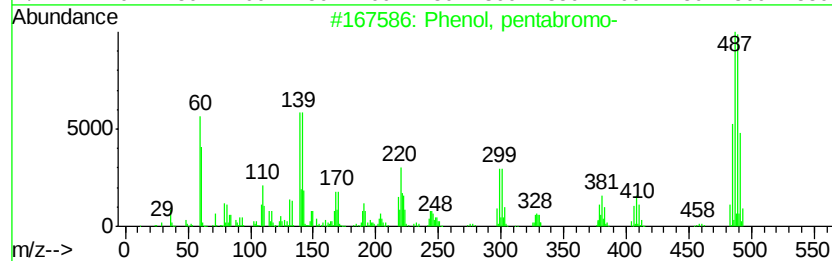
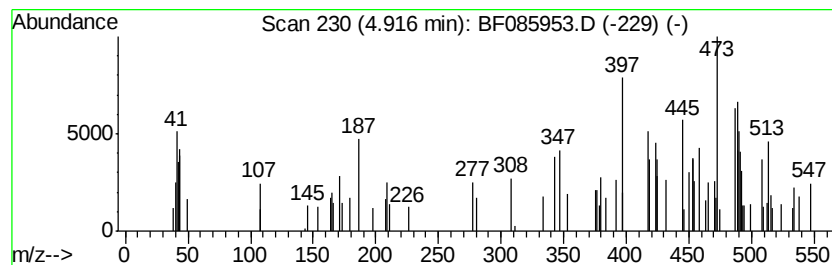
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Peak Number 11 Phenol, pentabromo- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.17 ng	70338	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, pentabromo-	484	C6HBr5O	000608-71-9	59
2		1,3-Di(4-bromophenyl)benzo[f]qui...	488	C24H14Br2N2	065958-13-6	14
3		N-TFA-isocolchicine	453	C22H22F3N06	1000127-10-6	10
4		1'H-Cholest-2-eno[3,2-b]indole, ...	473	C34H51N	055493-67-9	9
5		Iridium, tris(2,4-pentanedionato...	490	C15H21IrO6	015635-87-7	7



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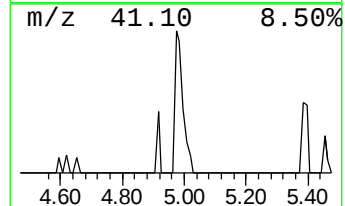
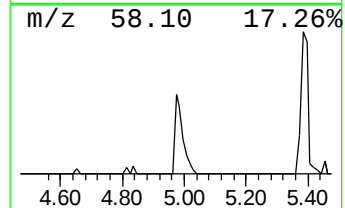
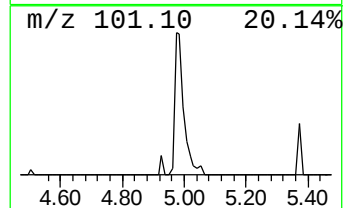
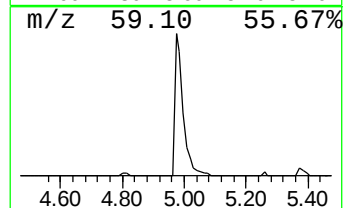
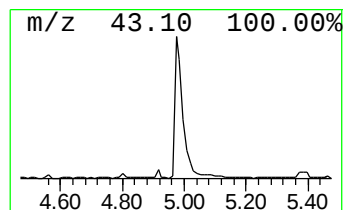
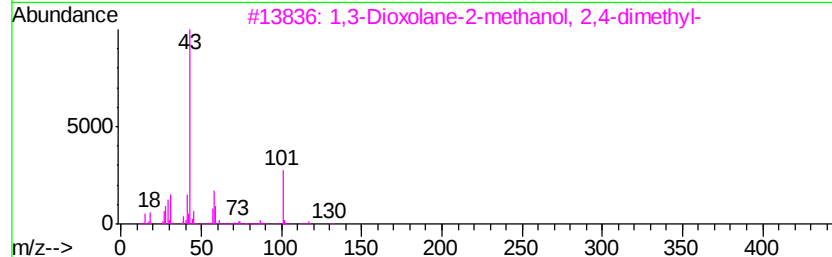
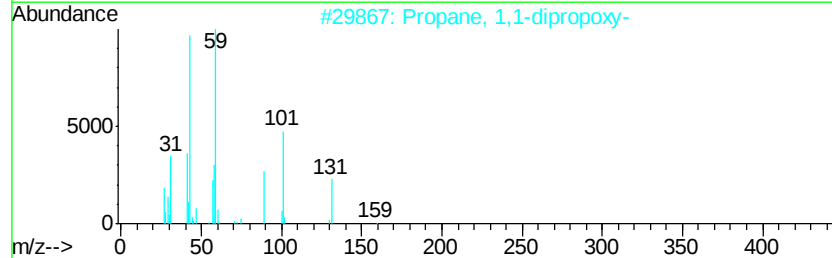
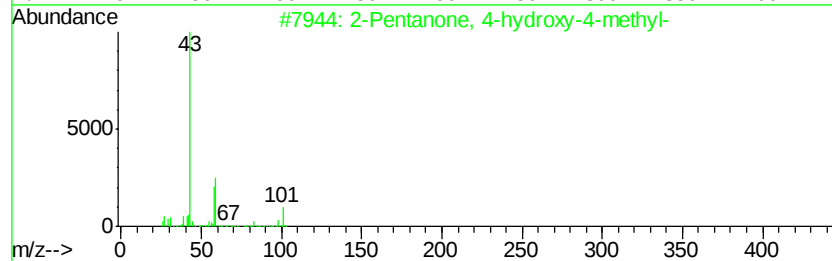
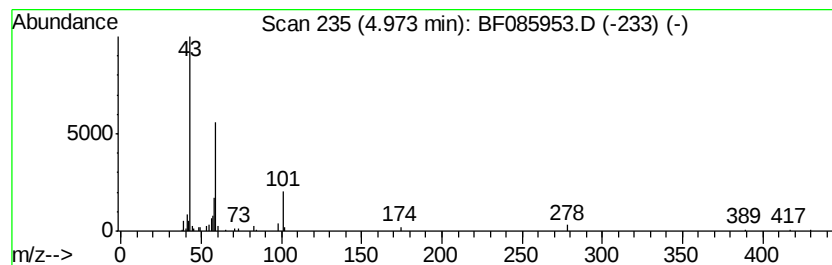
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	6.39 ng	207347	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	53
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36
3			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	32
4			2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	23
5			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	23



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085953.D
Acq On : 1 Apr 2016 3:33
Operator : UM/SJ
Sample : H2046-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

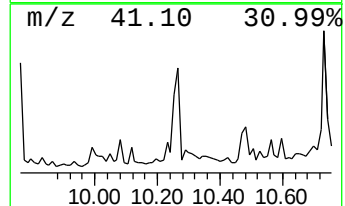
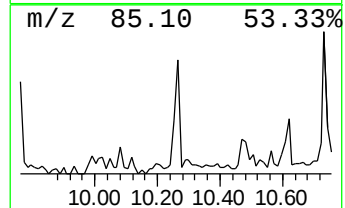
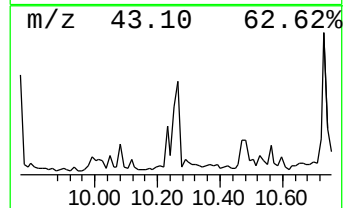
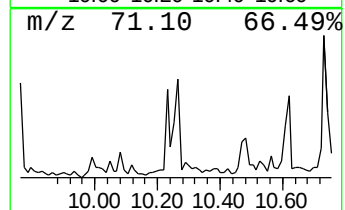
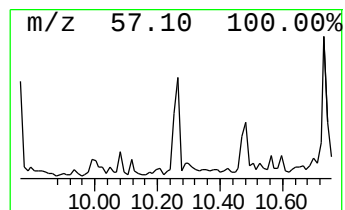
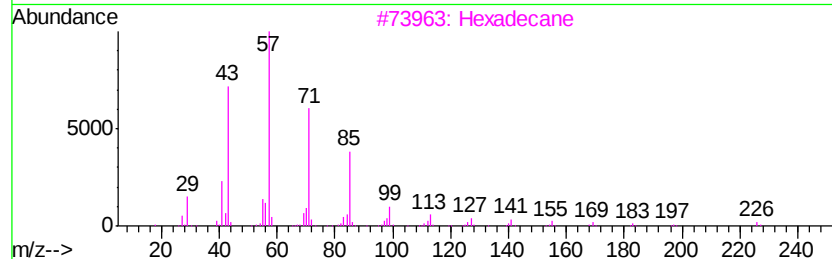
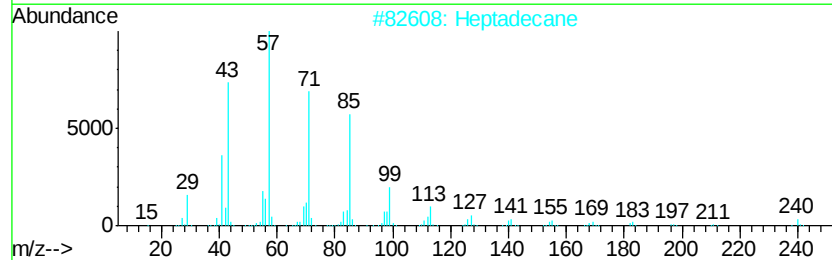
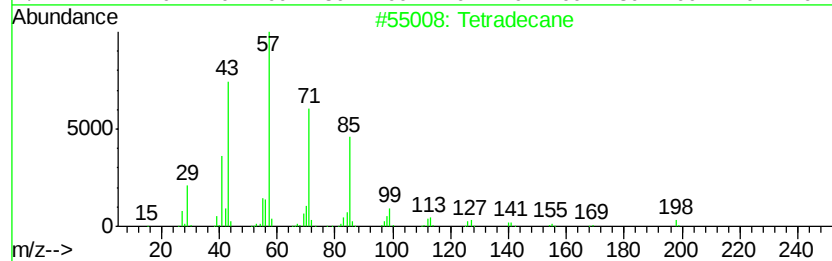
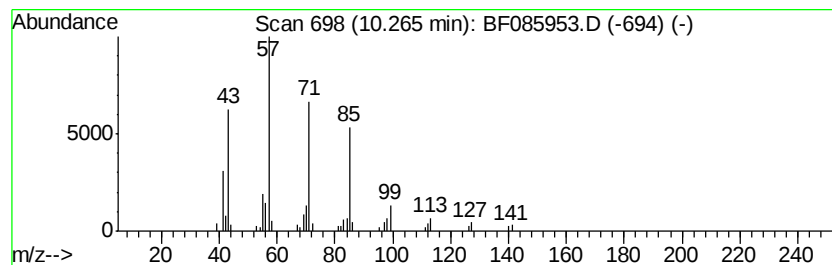
Instrument :
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ClientSampleId :
AMBOY-SB-34(0.5-15.0COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Tetradecane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.26	2.25 ng	98556	Acenaphthene-d10		9.83	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	87
2		Heptadecane	240	C17H36	000629-78-7	87
3		Hexadecane	226	C16H34	000544-76-3	86
4		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
5		Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085953.D
Acq On : 1 Apr 2016 3:33
Operator : UM/SJ
Sample : H2046-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

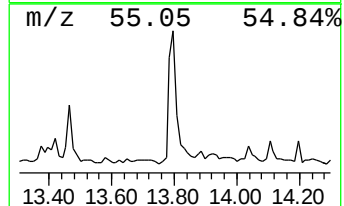
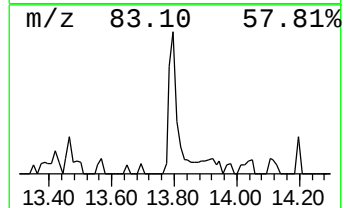
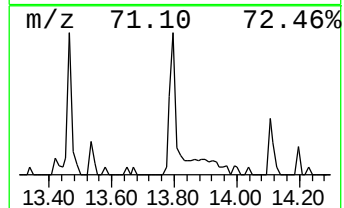
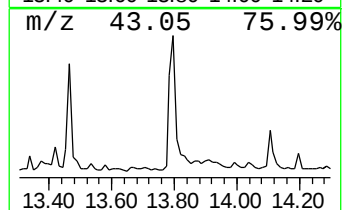
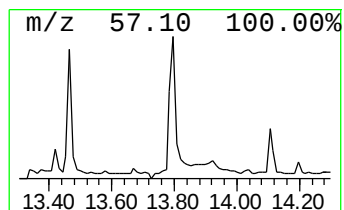
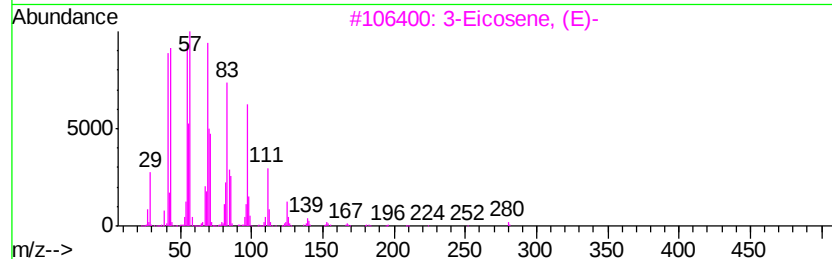
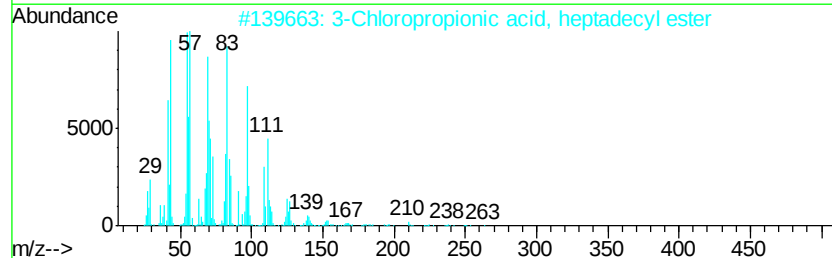
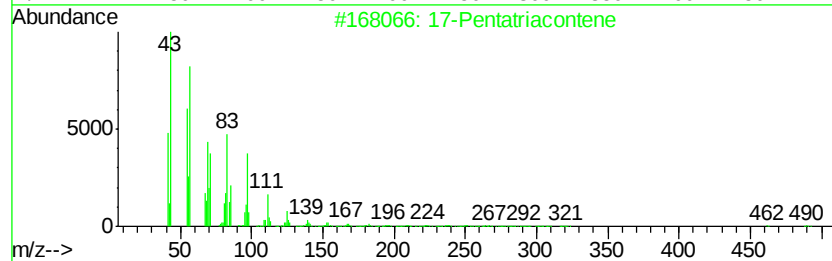
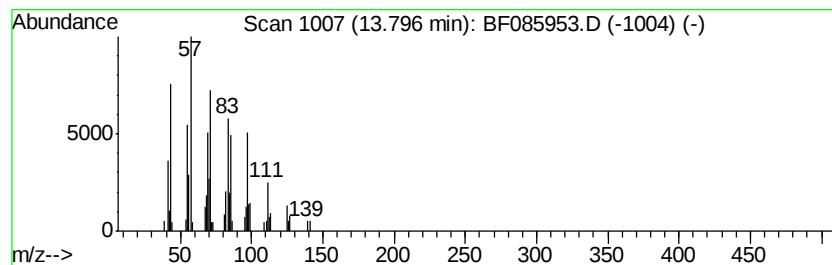
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ClientSampleId :
AMBOY-SB-34(0.5-15.0COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 17-Pentatriacontene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	4.29 ng	116135	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	74
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	68
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	62
4	1-Octadecene	252	C18H36	000112-88-9	62
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085953.D
Acq On : 1 Apr 2016 3:33
Operator : UM/SJ
Sample : H2046-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AMBOY-SB-34(0.5-15.0COMP)

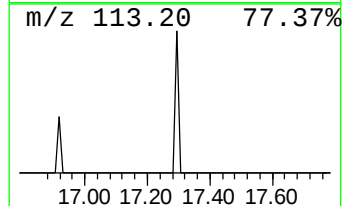
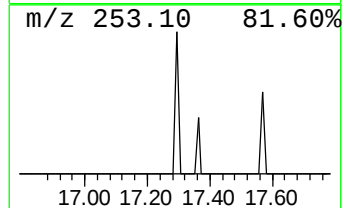
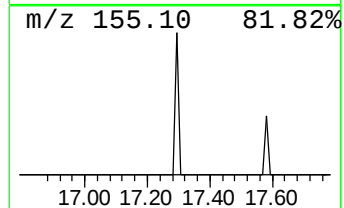
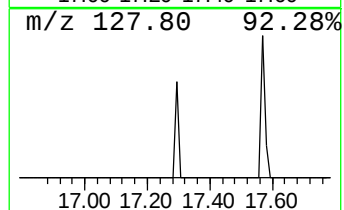
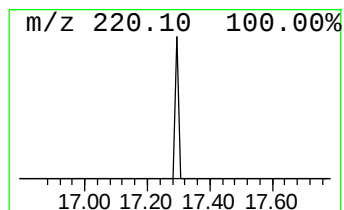
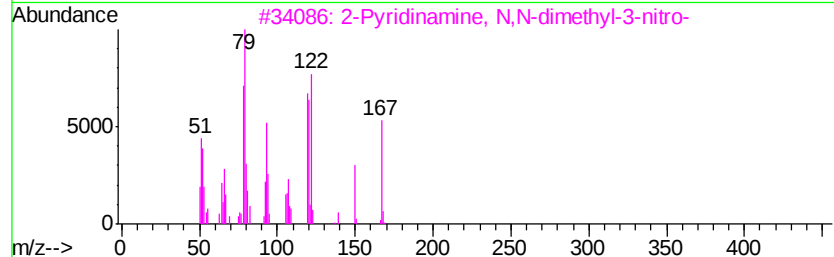
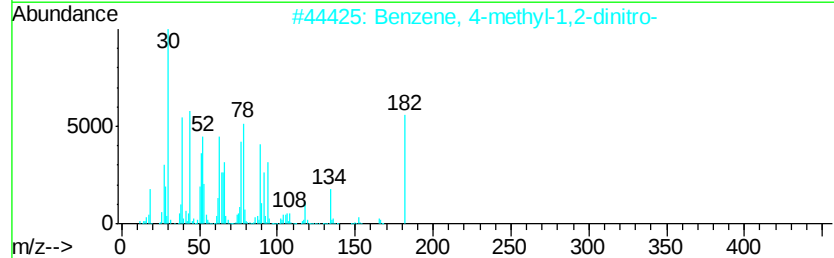
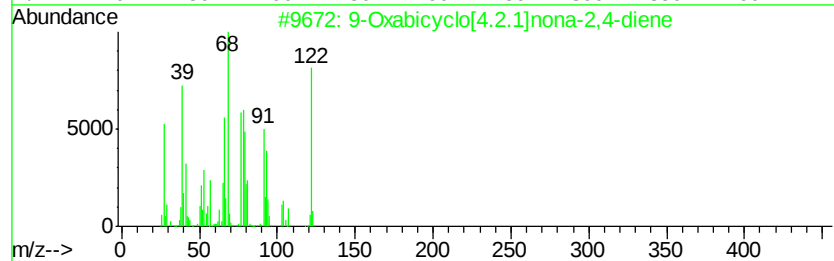
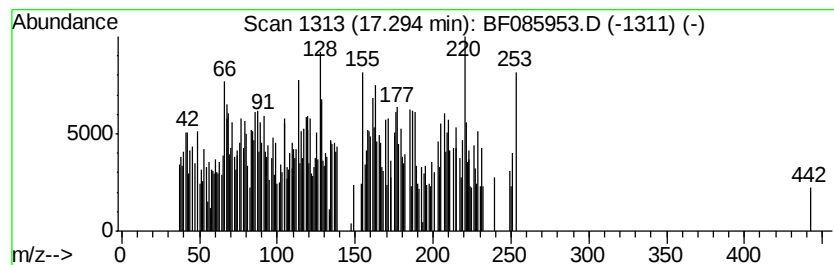
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.29 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.29	2.86 ng	77309	Perylene-d12	15.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Oxabicyclo[4.2.1]nona-2,4-diene	122	C8H10O	019740-75-1	46
2			Benzene, 4-methyl-1,2-dinitro-	182	C7H6N2O4	000610-39-9	35
3			2-Pyridinamine, N,N-dimethyl-3-n...	167	C7H9N3O2	005028-23-9	30
4			2-Amino-3,5-dibromopyrazine	251	C4H3Br2N3	024241-18-7	30
5			4-Oxepincarboxylic acid, 2,3,6,7...	170	C9H14O3	038858-66-1	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033116\
Data File : BF085953.D
Acq On : 1 Apr 2016 3:33
Operator : UM/SJ
Sample : H2046-04
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AMBOY-SB-34(0.5-15.0COMP)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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
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unknown4.78	4.78	2.8	ng	90474	1	6.79	649458	20.0
unknown4.88	4.88	5.1	ng	164442	1	6.79	649458	20.0
Phenol, pentabromo-	4.92	2.2	ng	70338	1	6.79	649458	20.0
2-Pentanone, 4-hy...	4.97	6.4	ng	207347	1	6.79	649458	20.0
Tetradecane	10.26	2.3	ng	98556	3	9.83	875930	20.0
17-Pentatriacontene	13.80	4.3	ng	116135	5	13.95	541139	20.0
unknown17.29	17.29	2.9	ng	77309	6	15.36	541322	20.0