

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
 Data File : BM010182.D
 Acq On : 24 May 2017 16:03
 Operator : SJ/MA
 Sample : I3305-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DSK-SB3(5-10)

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_M\METHODS\8270-BM051917.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	5.069	333	337	344	rBV	137078	201182	3.14%	0.500%
2	5.534	410	416	423	rBV	1835536	2714540	42.35%	6.747%
3	7.140	682	689	702	rBV	1663714	2660080	41.50%	6.612%
4	7.492	741	749	760	rBV	1805348	2896415	45.19%	7.200%
5	7.951	818	827	843	rBV	566254	893653	13.94%	2.221%
6	8.269	875	881	889	rBV	1384274	2196560	34.27%	5.460%
7	9.133	1021	1028	1038	rBV	948367	1596558	24.91%	3.969%
8	10.757	1298	1304	1311	rBV	627622	1047240	16.34%	2.603%
9	11.969	1503	1510	1515	rBV5	45499	90498	1.41%	0.225%
10	12.322	1565	1570	1579	rVB5	28053	67427	1.05%	0.168%
11	12.439	1582	1590	1599	rBV10	37943	111961	1.75%	0.278%
12	12.745	1635	1642	1647	rBV10	21807	65125	1.02%	0.162%
13	12.986	1679	1683	1687	rVB4	62639	86409	1.35%	0.215%
14	13.204	1714	1720	1726	rVB	2446731	3542837	55.27%	8.806%
15	13.321	1734	1740	1750	rBV6	114155	273872	4.27%	0.681%
16	13.421	1753	1757	1761	rBV7	41368	79036	1.23%	0.196%
17	13.963	1844	1849	1857	rVB	484221	695068	10.84%	1.728%
18	14.045	1858	1863	1866	rBV	303147	449605	7.01%	1.118%
19	14.286	1898	1904	1908	rBV2	179026	314711	4.91%	0.782%
20	14.374	1914	1919	1924	rVB	337639	479677	7.48%	1.192%
21	14.445	1928	1931	1936	rVB6	61795	78345	1.22%	0.195%
22	14.515	1936	1943	1949	rBV6	99396	240991	3.76%	0.599%
23	14.586	1949	1955	1963	rBV2	876349	1432427	22.35%	3.561%
24	15.192	2056	2058	2064	rVB5	71043	103963	1.62%	0.258%
25	15.327	2077	2081	2085	rBV3	127753	185126	2.89%	0.460%
26	16.074	2202	2208	2213	rBV	2282092	3131547	48.85%	7.784%
27	17.327	2416	2421	2429	rVB	1299865	1808772	28.22%	4.496%
28	17.709	2483	2486	2490	rBV6	44297	77501	1.21%	0.193%
29	18.174	2561	2565	2570	rBV2	212894	299352	4.67%	0.744%
30	19.445	2777	2781	2785	rBV3	114227	146035	2.28%	0.363%
31	19.927	2858	2863	2870	rBV	5048555	6410069	100.00%	15.933%
32	21.486	3123	3128	3136	rBV	2190144	2799641	43.68%	6.959%
33	23.850	3523	3530	3539	rVB	1470724	3054447	47.65%	7.592%

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Instrument :
BNA_M
ClientSampleId :
DSK-SB3(5-10)

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_M\METHODS\8270-BM051917.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

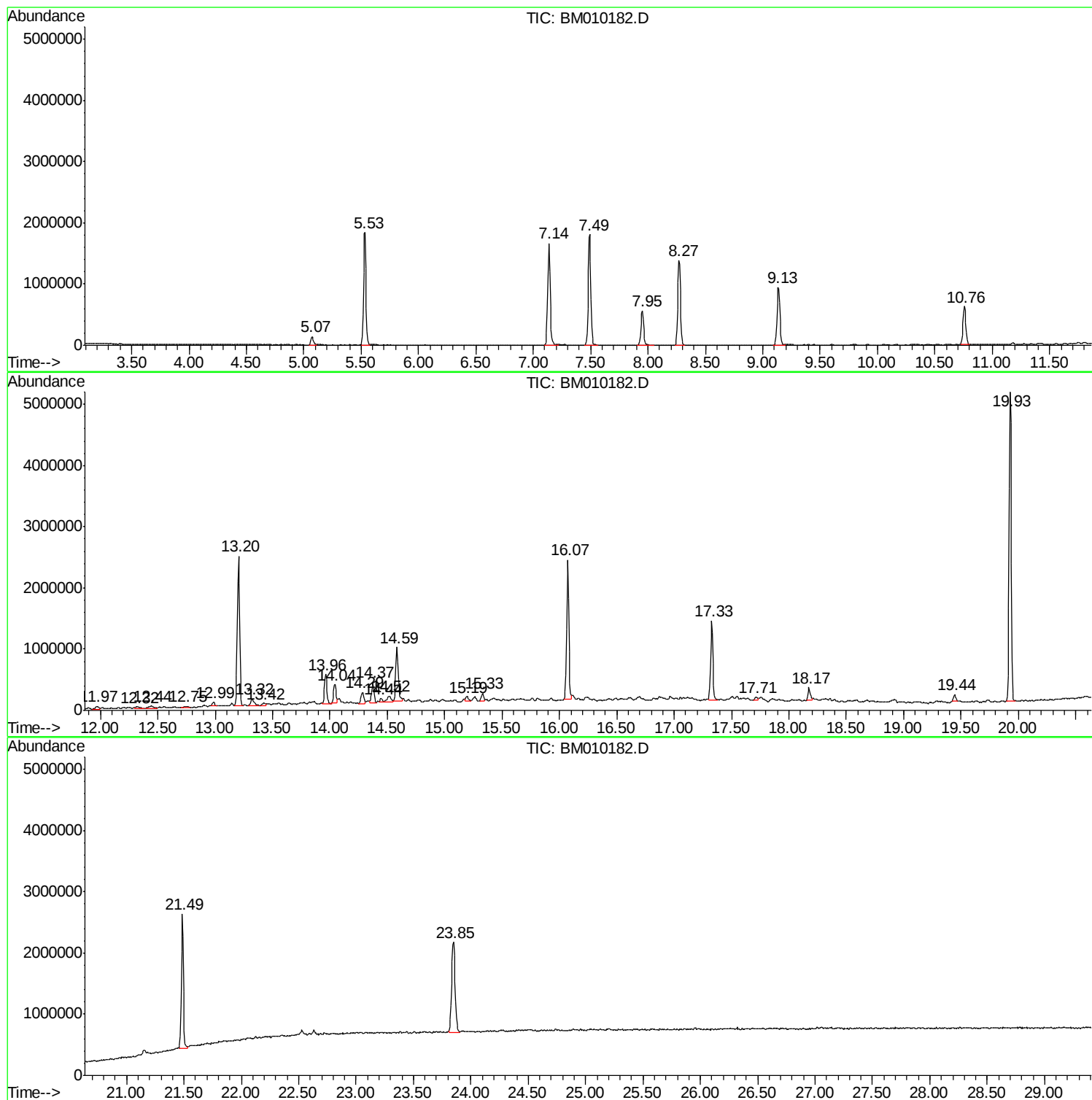
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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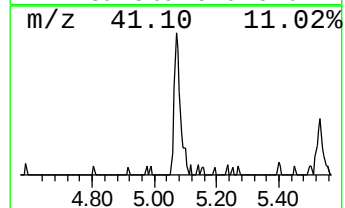
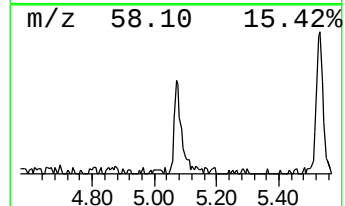
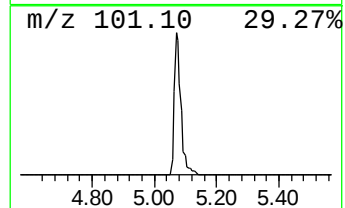
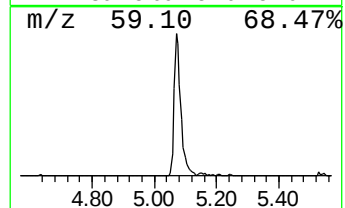
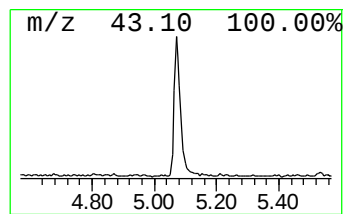
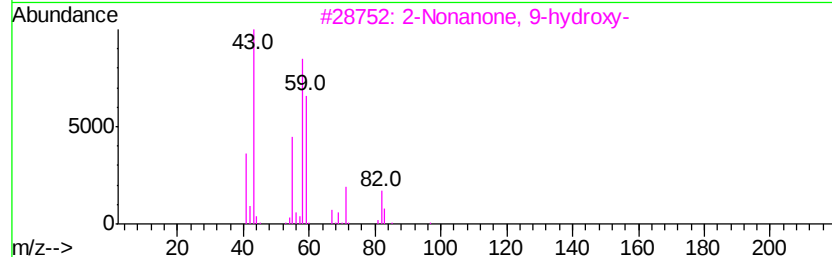
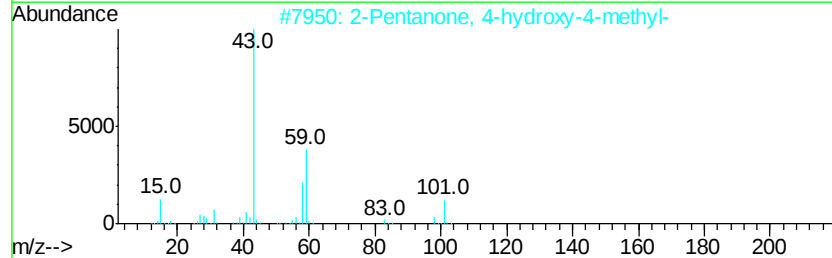
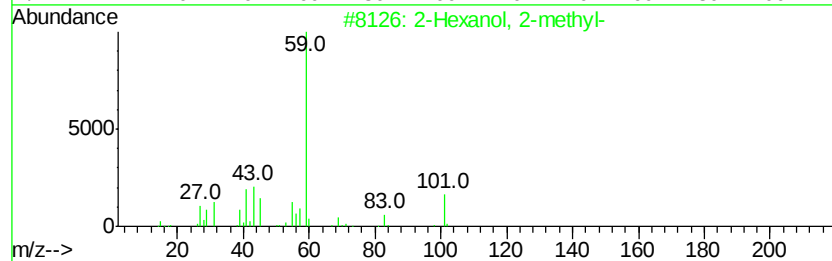
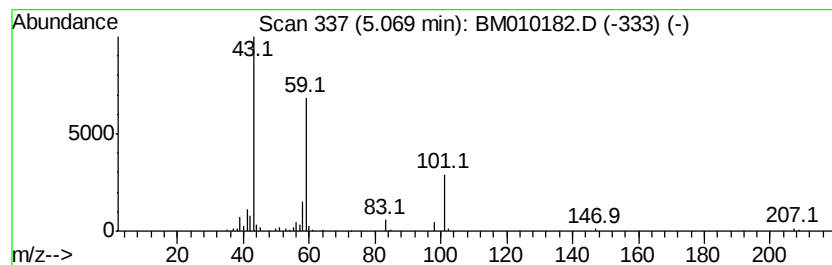
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Hexanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	4.50 ng	201182	1,4-Dichlorobenzene-d4	7.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4			Dimethadione	129	C5H7N03	000695-53-4	28
5			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25



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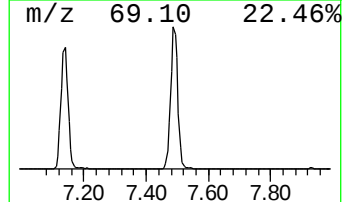
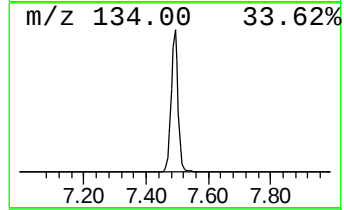
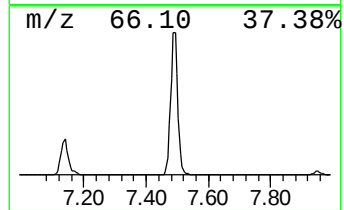
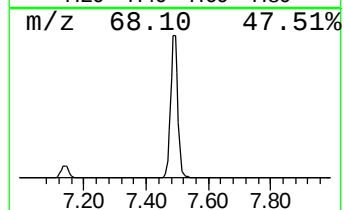
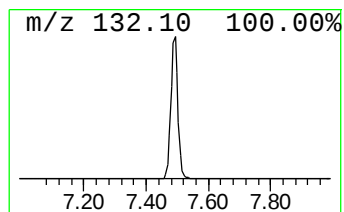
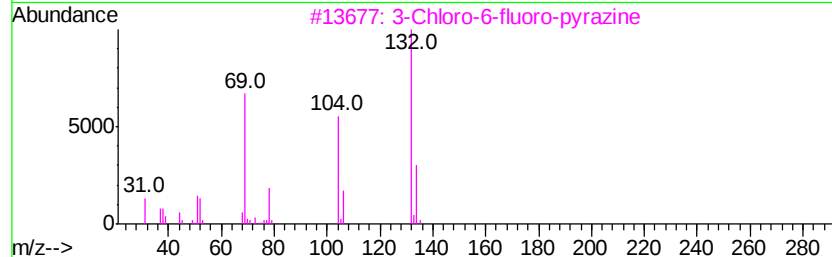
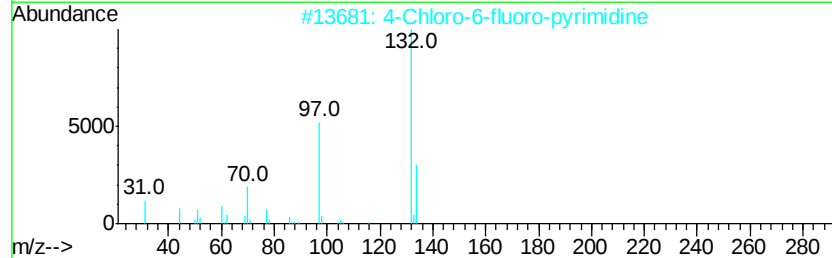
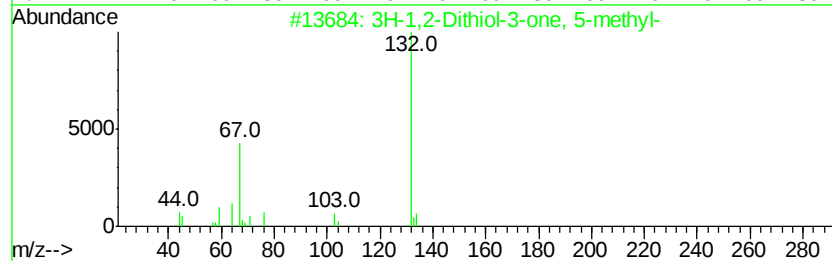
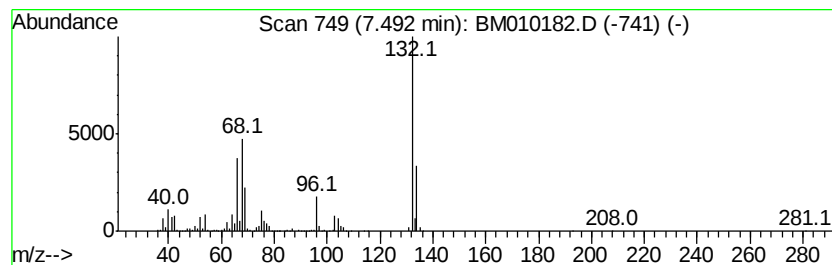
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	64.82 ng	2896420	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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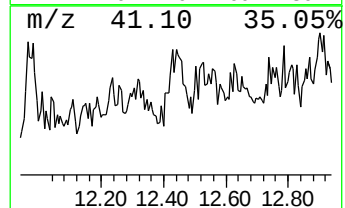
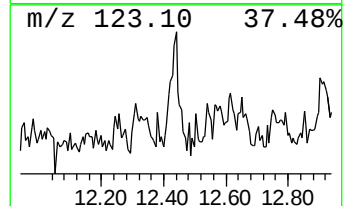
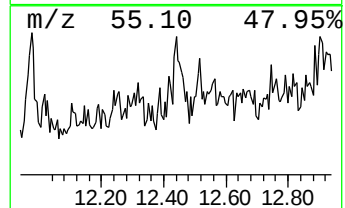
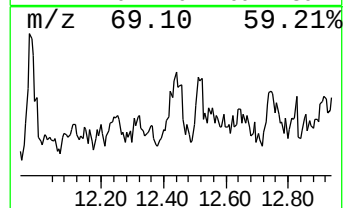
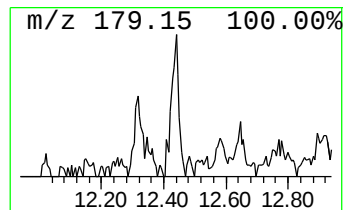
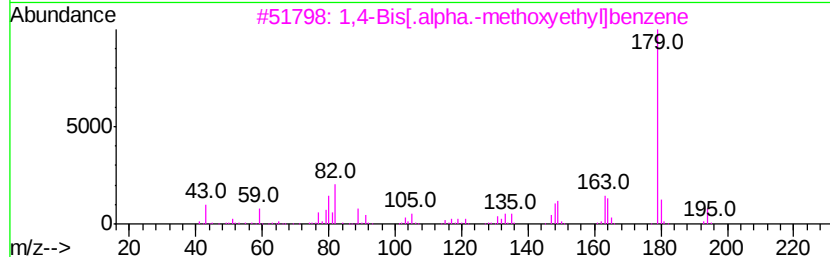
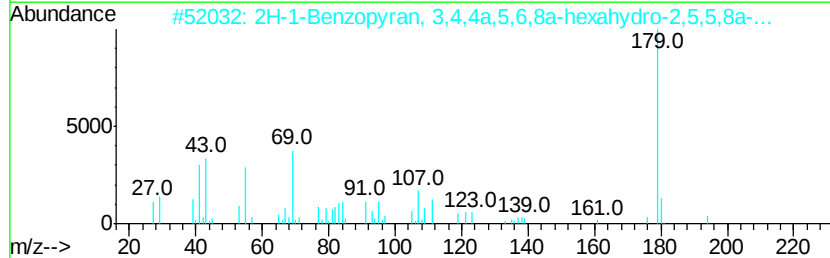
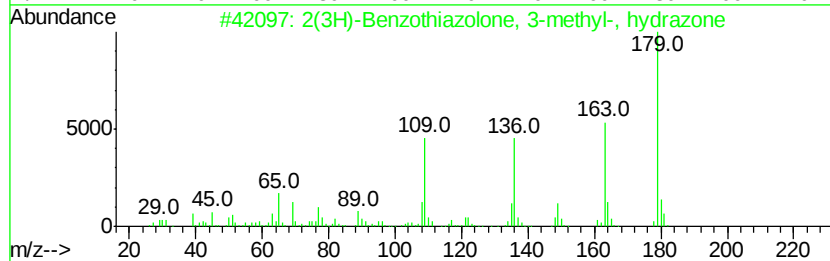
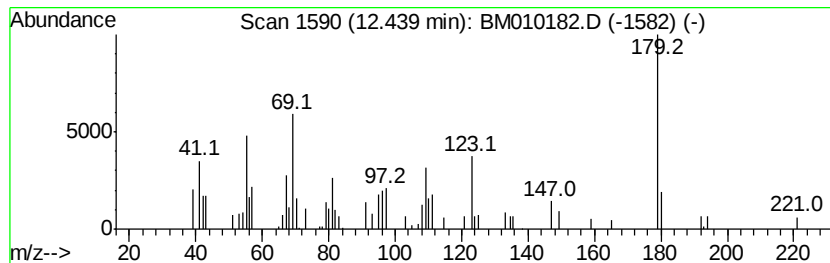
Instrument :
BNA_M
ClientSampleId :
DSK-SB3(5-10)

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

Peak Number 4 unknown12.44 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.44	2.14 ng	111961	Naphthalene-d8	10.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone, 3-methyl-...	179	C8H9N3S	001128-67-2	46
2	2H-1-Benzopyran, 3,4,4a,5,6,8a-h...	194	C13H22O	063335-66-0	43
3	1,4-Bis[.alpha.-methoxvethyl]ben...	194	C12H18O2	129770-42-9	38
4	1,5-Dimethyl-4-allylaminocytosine	179	C9H13N3O	138002-90-1	32
5	1,4-Bis(trimethylsilyl)-1,3-buta...	194	C10H18Si2	004526-07-2	32



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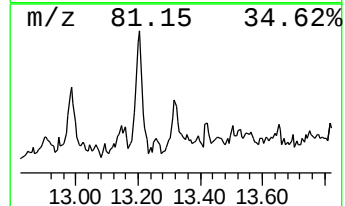
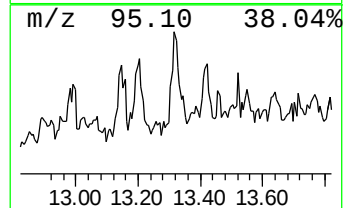
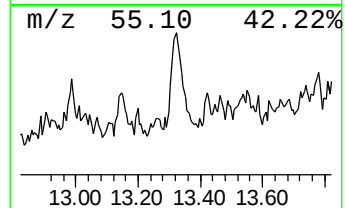
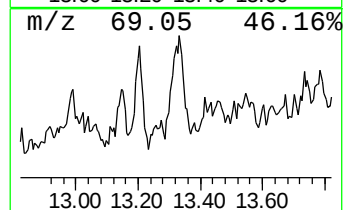
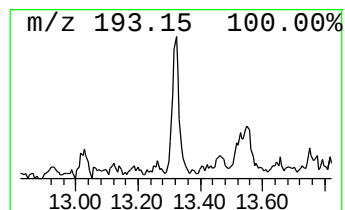
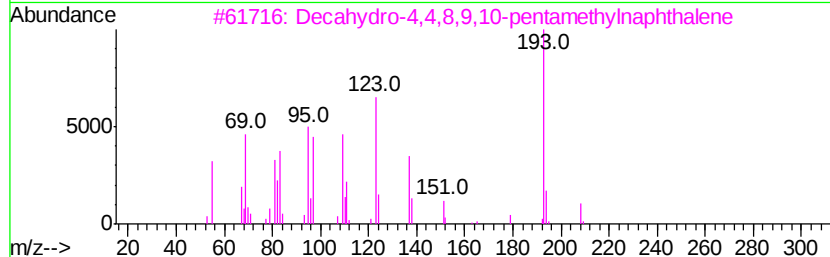
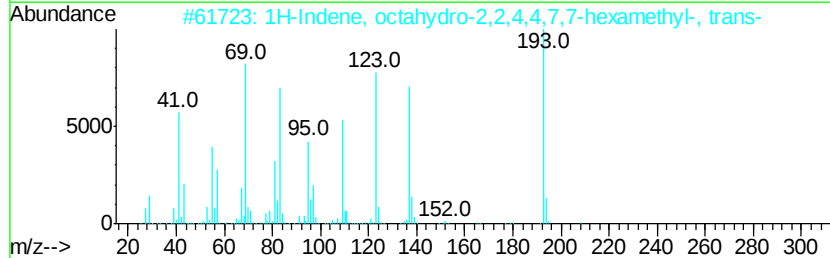
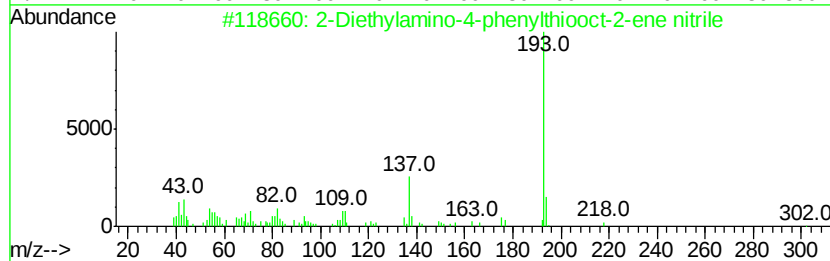
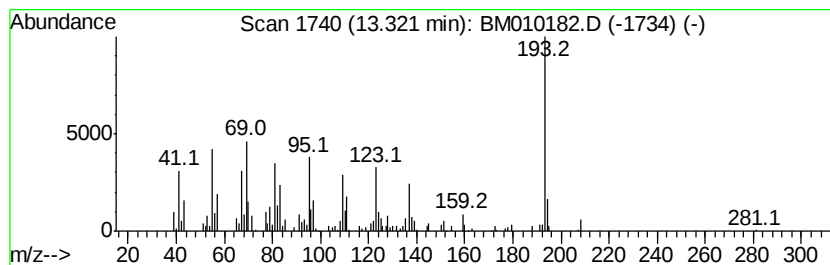
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.32 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.32	3.82 ng	273872	Acenaphthene-d10	14.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	47
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
3	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	43
4	1,5-Hexadien-3-ol, 3-methyl-6-(m...	280	C17H28OS	097369-78-3	42
5	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	42



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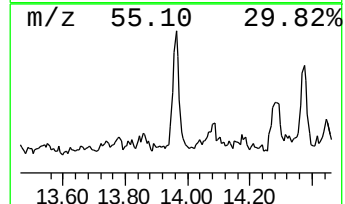
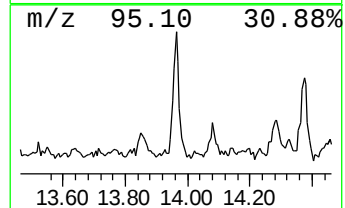
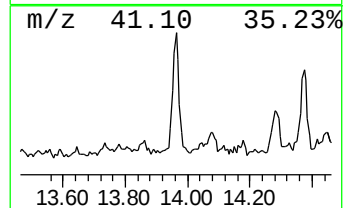
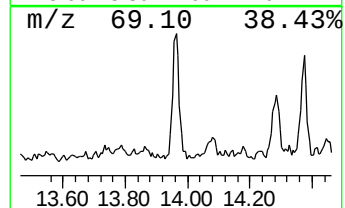
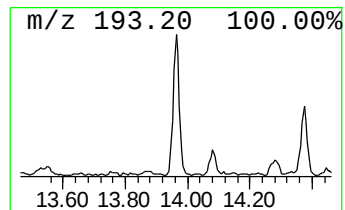
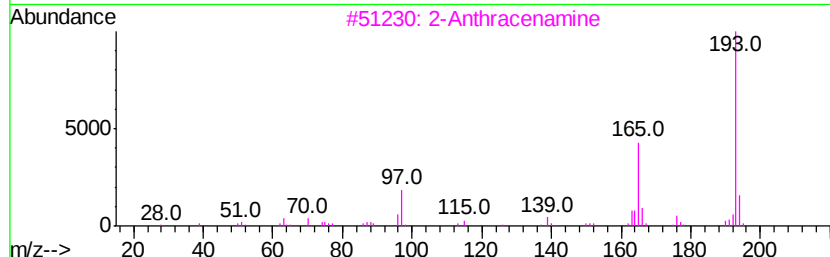
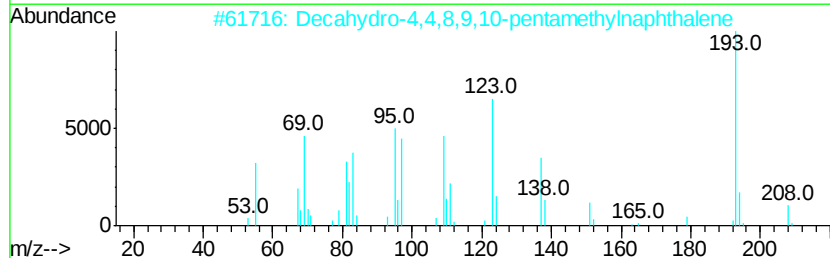
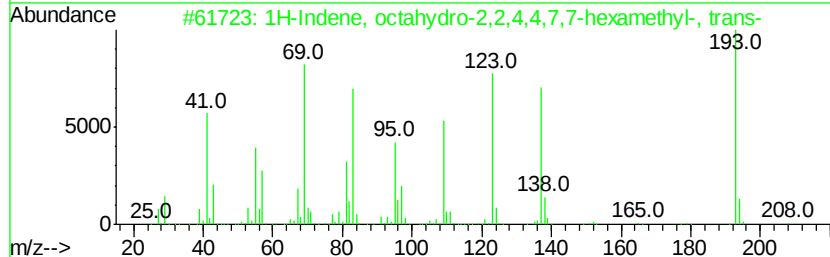
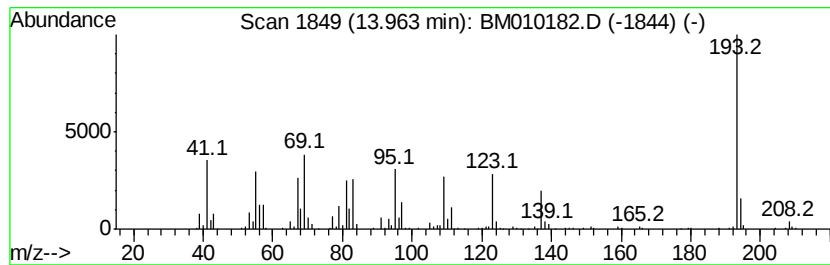
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.96 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.96	9.70 ng	695068	Acenaphthene-d10	14.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	47
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
3	2-Anthracenamine	193	C14H11N	000613-13-8	35
4	Iminostilbene	193	C14H11N	000256-96-2	35
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	35



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

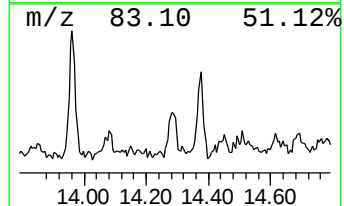
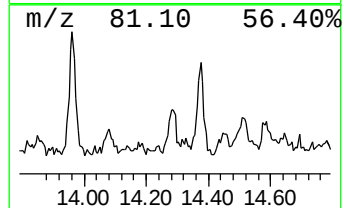
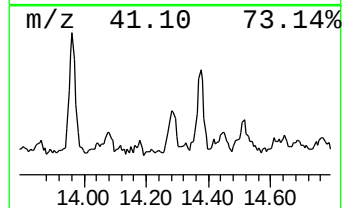
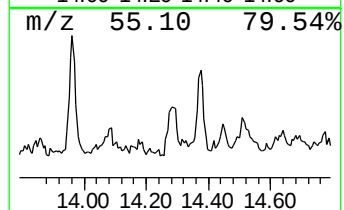
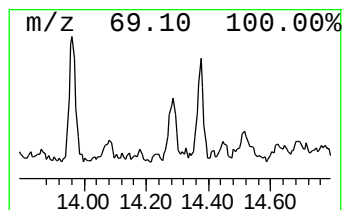
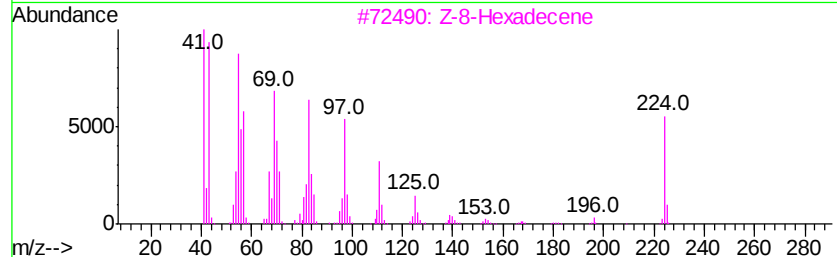
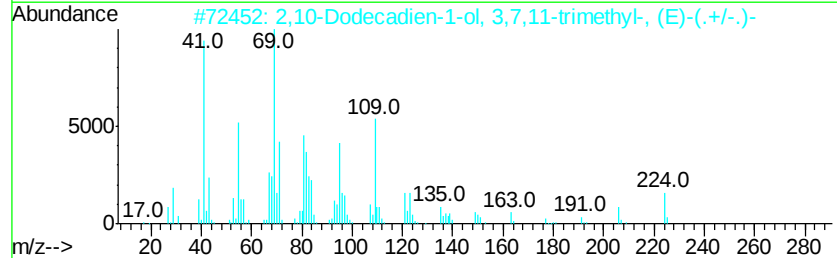
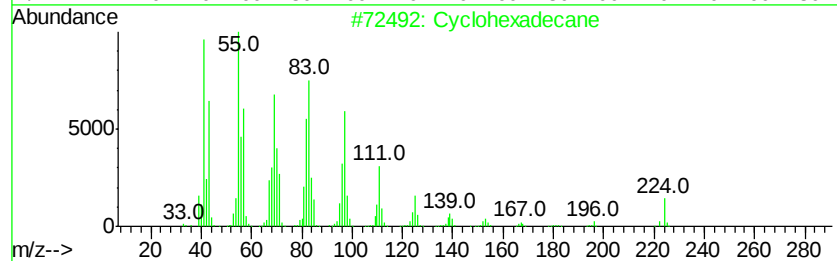
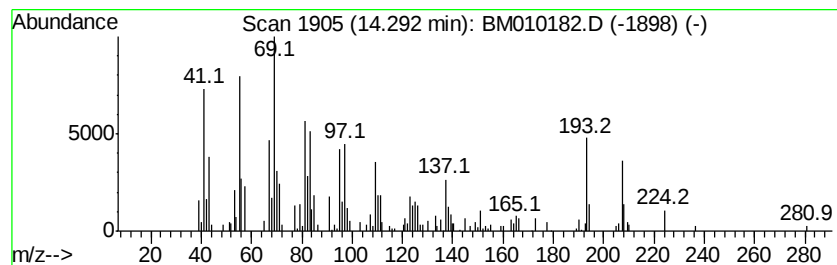
Instrument :
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ClientSampleId :
DSK-SB3(5-10)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.29 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.29	4.39 ng	314711	Acenaphthene-d10	14.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	42
2	2,10-Dodecadien-1-ol, 3,7,11-tri...	224	C15H28O	020576-59-4	42
3	Z-8-Hexadecene	224	C16H32	1000130-87-5	40
4	Spiro[2.3]hexan-4-one, 5,5-dieth...	166	C11H18O	1000152-25-2	30
5	Neopentylidenecyclohexane	152	C11H20	039546-80-0	30



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

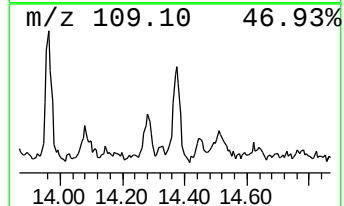
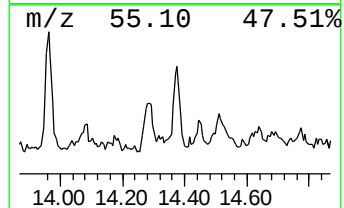
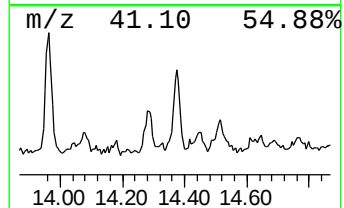
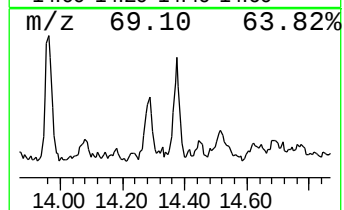
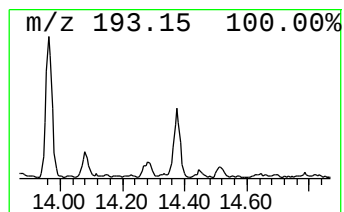
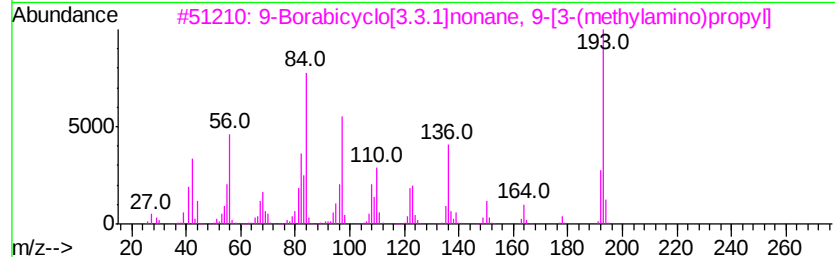
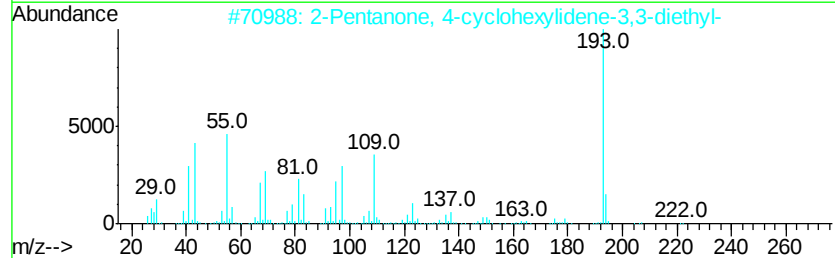
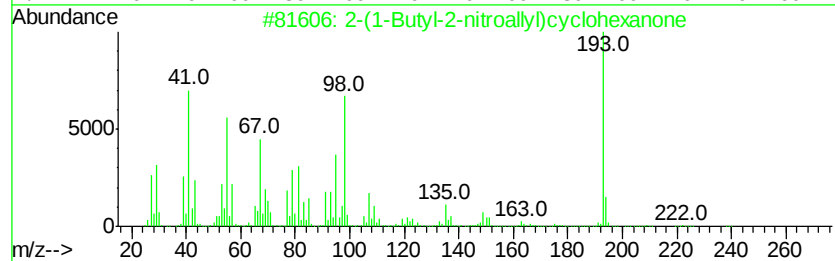
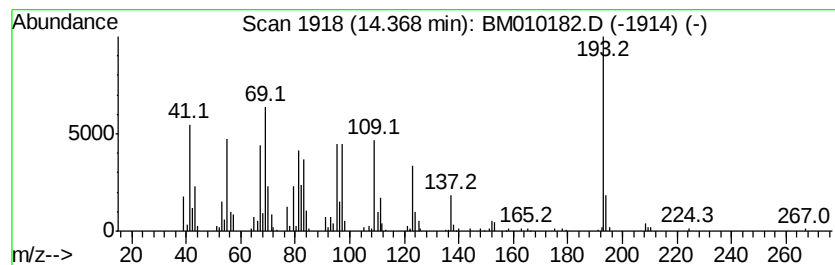
Instrument :
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ClientSampleId :
DSK-SB3(5-10)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.37	6.70 ng	479677	Acenaphthene-d10	14.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Butyl-2-nitroallyl)cyclohex...	239	C13H21NO3	1000192-05-9	40
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
3	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1000162-56-0	37
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	37
5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	35



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

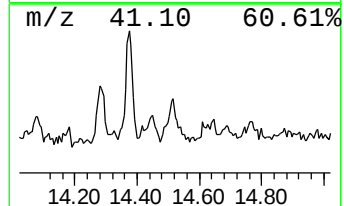
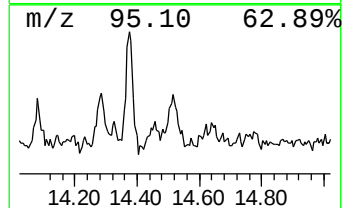
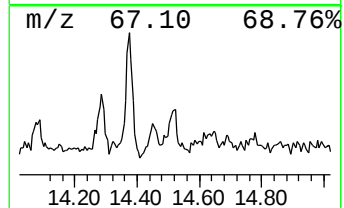
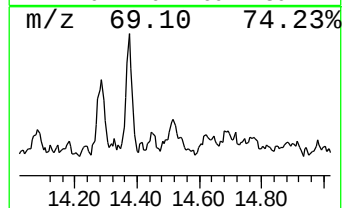
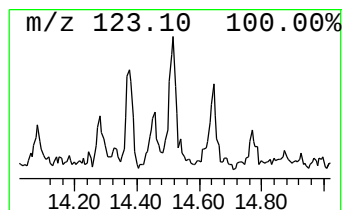
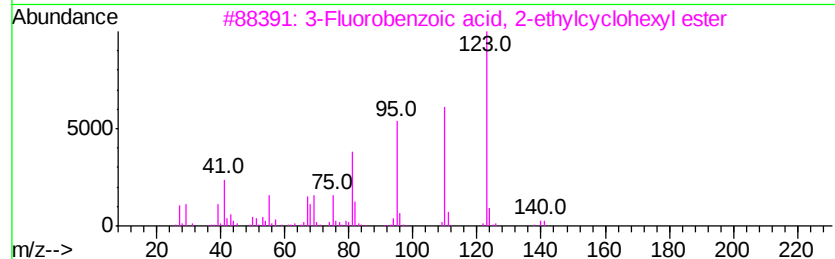
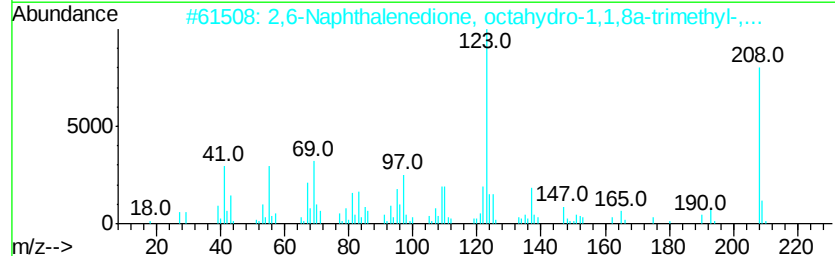
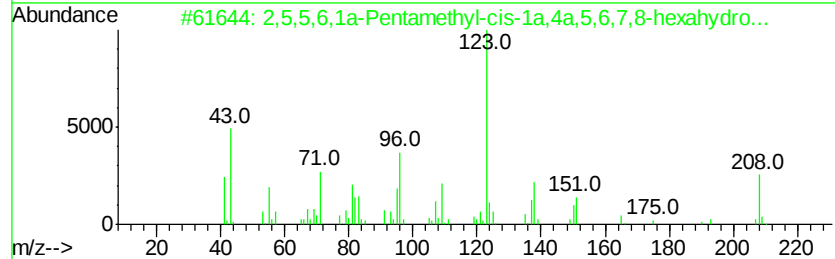
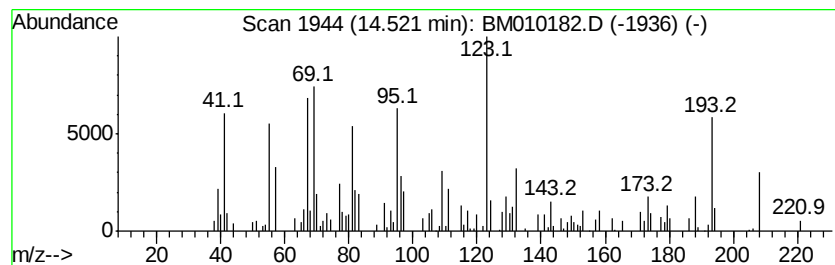
Instrument :
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ClientSampleId :
DSK-SB3(5-10)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.52 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.52	3.36 ng	240991	Acenaphthene-d10	14.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1000215-77-9	49
2	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	49
3	3-Fluorobenzoic acid, 2-ethylcvc...	250	C15H19FO2	1000279-04-9	43
4	4,4-Dimethoxy-2,5-cyclohexadien-...	154	C8H10O3	000935-50-2	43
5	Acetic acid, (4-methoxyphenoxy)-	182	C9H10O4	001877-75-4	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DSK-SB3(5-10)

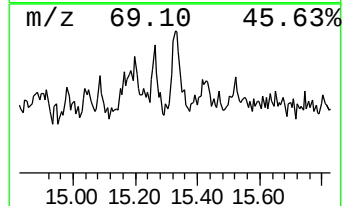
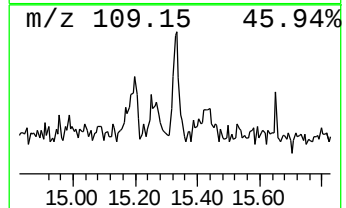
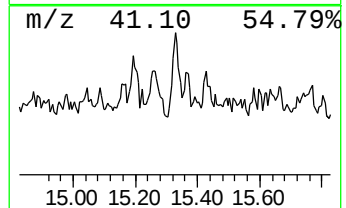
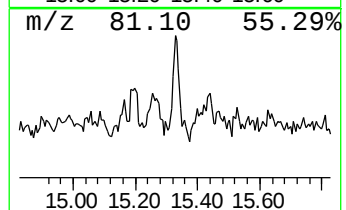
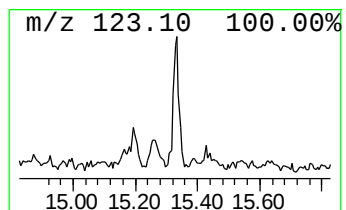
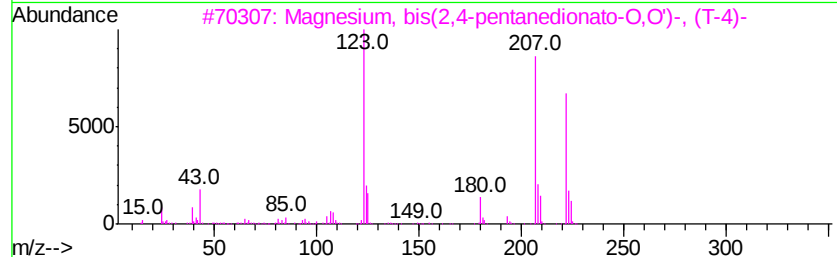
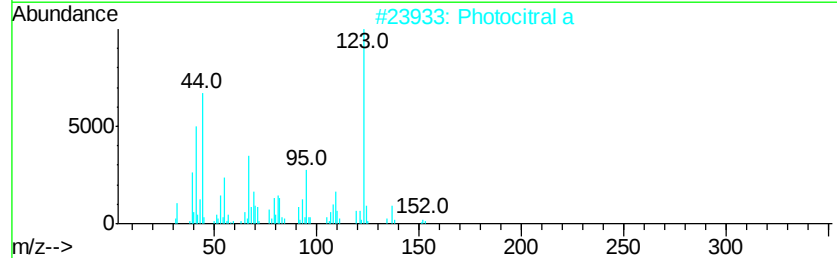
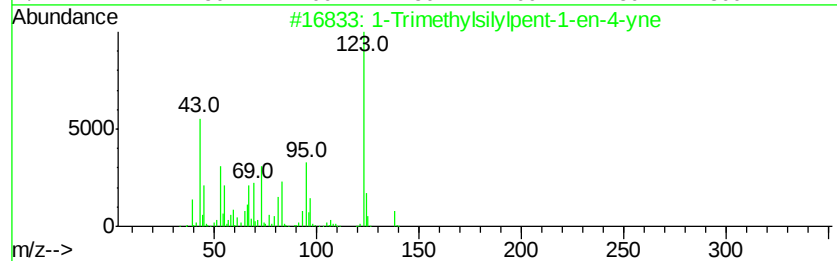
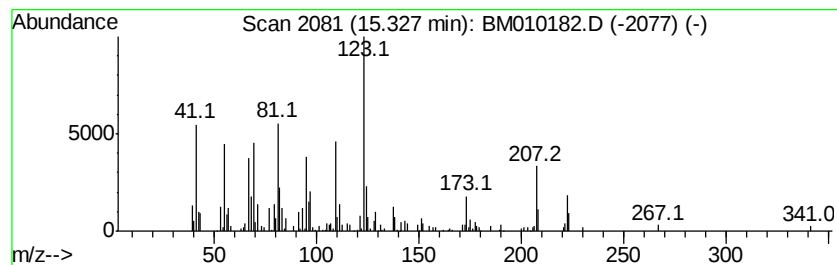
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.33 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.58 ng	185126	Acenaphthene-d10	14.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	49
2			Photocitral a	152	C10H16O	1000292-85-0	46
3			Magnesium, bis(2,4-pentanedionat...	222	C10H14MgO4	014024-56-7	43
4			2(1H)-Naphthalenone, octahydro-4...	222	C15H26O	055332-04-2	38
5			3-Fluorobenzoic acid, undec-2-en...	292	C18H25FO2	1000292-60-8	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DSK-SB3(5-10)

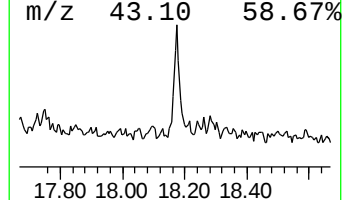
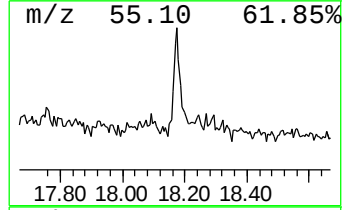
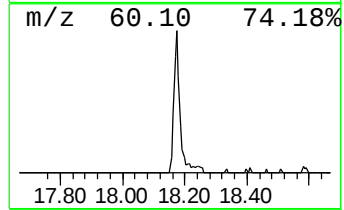
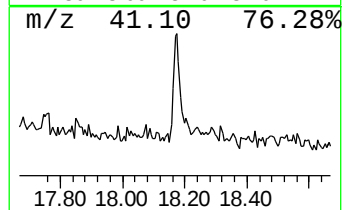
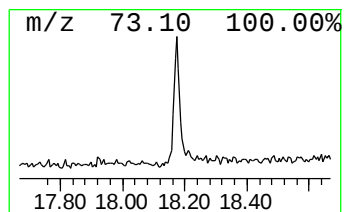
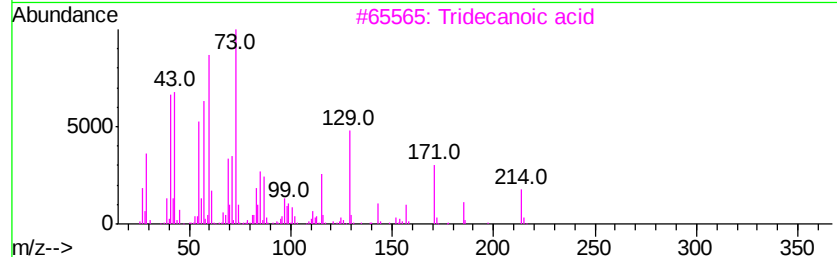
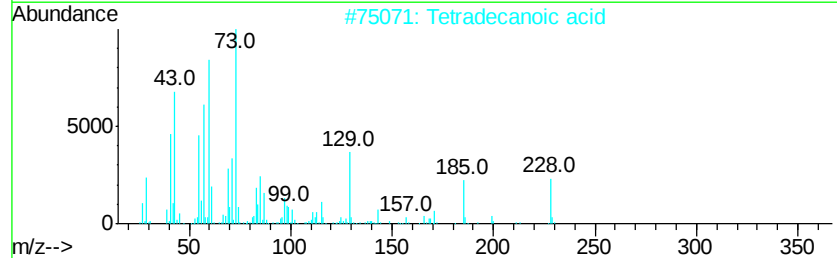
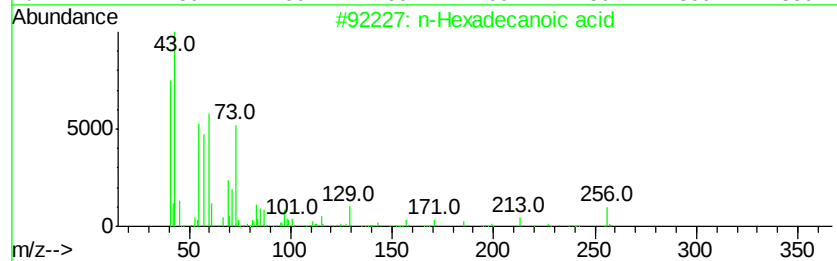
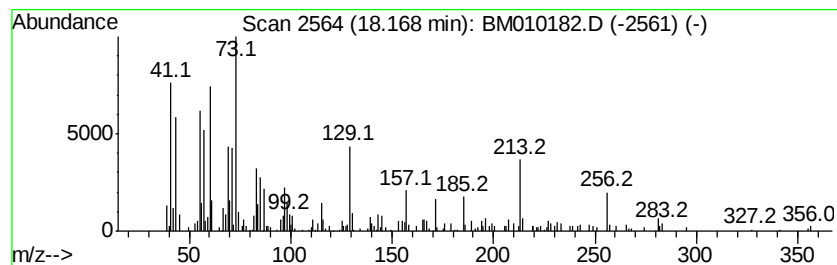
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	3.31 ng	299352	Phenanthrene-d10	17.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	78
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052417\
Data File : BM010182.D
Acq On : 24 May 2017 16:03
Operator : SJ/MA
Sample : I3305-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DSK-SB3(5-10)

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051917.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-Hexanol, 2-methyl-	5.07	4.5 ng		201182	1	7.95	893653	20.0
unknown7.49	7.49	64.8 ng		2896420	1	7.95	893653	20.0
unknown12.44	12.44	2.1 ng		111961	2	10.76	1047240	20.0
unknown13.32	13.32	3.8 ng		273872	3	14.58	1432430	20.0
unknown13.96	13.96	9.7 ng		695068	3	14.58	1432430	20.0
unknown14.29	14.29	4.4 ng		314711	3	14.58	1432430	20.0
unknown14.37	14.37	6.7 ng		479677	3	14.58	1432430	20.0
unknown14.52	14.52	3.4 ng		240991	3	14.58	1432430	20.0
unknown15.33	15.33	2.6 ng		185126	3	14.58	1432430	20.0
n-Hexadecanoic acid	18.17	3.3 ng		299352	4	17.33	1808770	20.0