

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090117\
 Data File : BF098233.D
 Acq On : 1 Sep 2017 18:13
 Operator : SJ/JU
 Sample : I5050-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT4651-1540

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-BF081517.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	3.093	169	171	184	rBV2	54317	110878	3.46%	0.381%
2	4.263	366	370	379	rBV	102269	144676	4.51%	0.498%
3	4.916	478	481	497	rVB	184822	283710	8.84%	0.976%
4	5.334	547	552	556	rBV	2735946	3067084	95.57%	10.549%
5	6.369	722	728	731	rBV	2853967	3209197	100.00%	11.038%
6	6.492	744	749	752	rBV	3008027	2998462	93.43%	10.313%
7	6.716	784	787	791	rBV	836856	750352	23.38%	2.581%
8	6.875	810	814	818	rBV	2492405	2336365	72.80%	8.036%
9	7.287	879	884	887	rBV	1919546	1927724	60.07%	6.630%
10	7.392	895	902	909	rBV	37948	47693	1.49%	0.164%
11	8.004	1002	1006	1012	rBV	1033014	939797	29.28%	3.232%
12	9.081	1184	1189	1192	rBV	3249470	2979225	92.83%	10.247%
13	9.475	1251	1256	1259	rBV	467369	440868	13.74%	1.516%
14	9.516	1261	1263	1267	rVB3	29174	41879	1.30%	0.144%
15	9.622	1277	1281	1283	rBV2	102222	131007	4.08%	0.451%
16	9.663	1285	1288	1291	rVB	169839	138782	4.32%	0.477%
17	9.704	1291	1295	1297	rBV5	54021	83477	2.60%	0.287%
18	9.751	1300	1303	1307	rVB	903993	855752	26.67%	2.943%
19	9.786	1307	1309	1312	rBV3	74256	91695	2.86%	0.315%
20	10.086	1358	1360	1363	rVB2	105973	94547	2.95%	0.325%
21	10.122	1363	1366	1369	rBV3	93059	131222	4.09%	0.451%
22	10.157	1369	1372	1375	rBV2	272468	249915	7.79%	0.860%
23	10.545	1434	1438	1441	rBV	1222665	1193204	37.18%	4.104%
24	11.239	1553	1556	1558	rBV	764809	682423	21.26%	2.347%
25	11.263	1558	1560	1566	rVB	372654	312167	9.73%	1.074%
26	12.445	1759	1761	1766	rVB	504586	460812	14.36%	1.585%
27	12.674	1798	1800	1803	rVB	427435	330332	10.29%	1.136%
28	12.822	1821	1825	1831	rVB	1981166	1911060	59.55%	6.573%
29	13.716	1975	1977	1984	rVB2	124076	171362	5.34%	0.589%
30	13.868	1998	2003	2006	rBV2	878647	1085755	33.83%	3.734%
31	13.892	2006	2007	2014	rVB	264389	224677	7.00%	0.773%
32	14.498	2108	2110	2113	rBV2	38005	33350	1.04%	0.115%
33	14.880	2171	2175	2184	rBV	210609	378226	11.79%	1.301%
34	15.163	2220	2223	2229	rVB	101311	137880	4.30%	0.474%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.221	2229	2233	2238	rBV	146122	180033	5.61%	0.619%
36	15.286	2239	2244	2247	rBV	428894	540098	16.83%	1.858%
37	15.715	2314	2317	2323	rVB2	51725	80387	2.50%	0.276%
38	16.186	2393	2397	2402	rVB2	38965	61717	1.92%	0.212%
39	16.651	2472	2476	2485	rVB2	49471	90932	2.83%	0.313%
40	16.733	2486	2490	2496	rVB3	39668	74391	2.32%	0.256%
41	17.062	2541	2546	2552	rVB	34877	71312	2.22%	0.245%

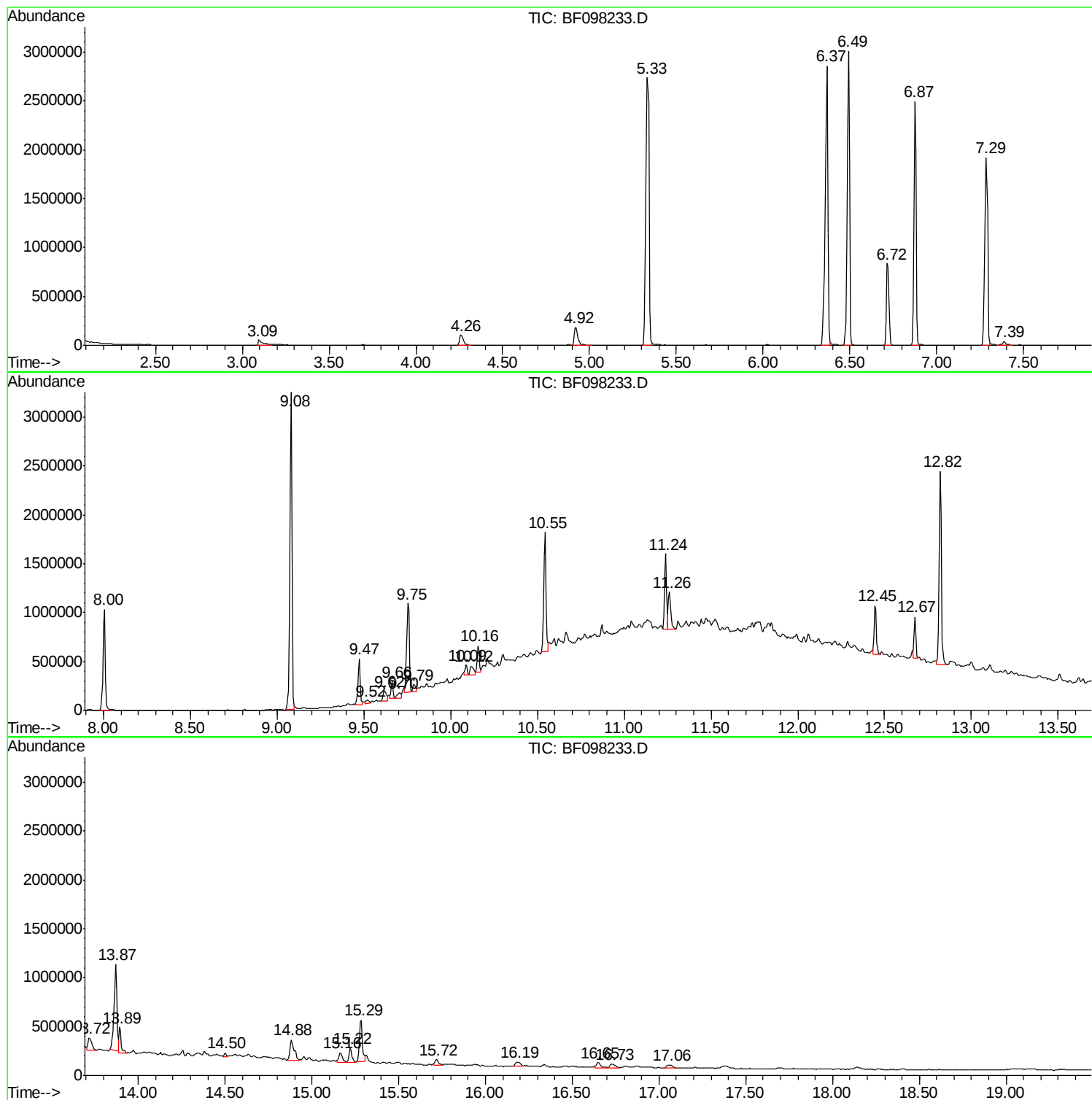
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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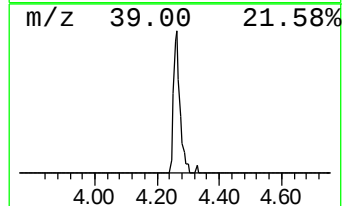
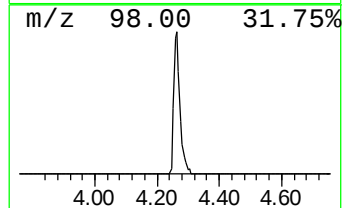
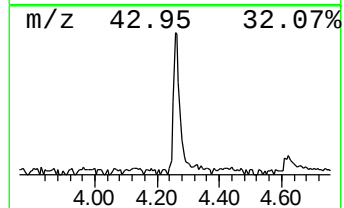
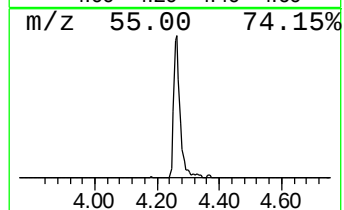
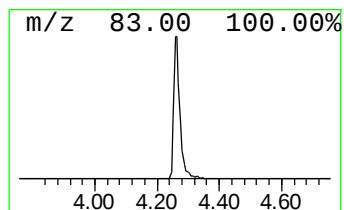
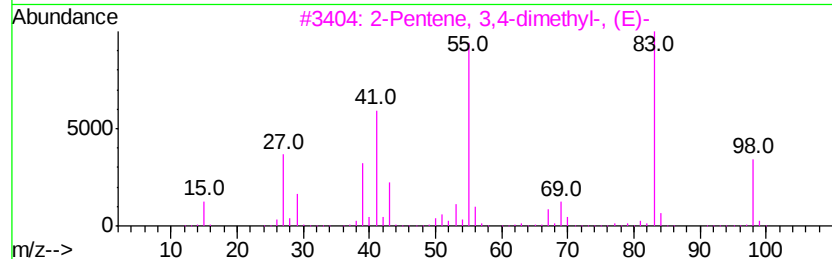
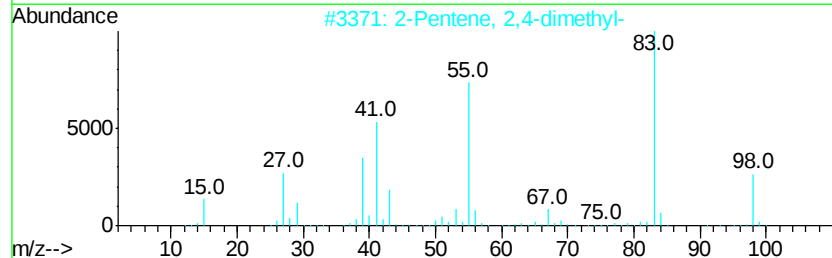
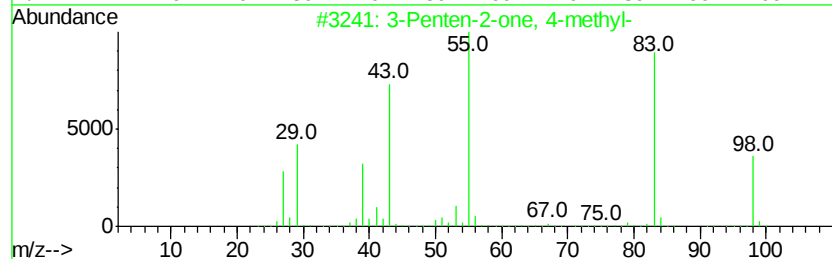
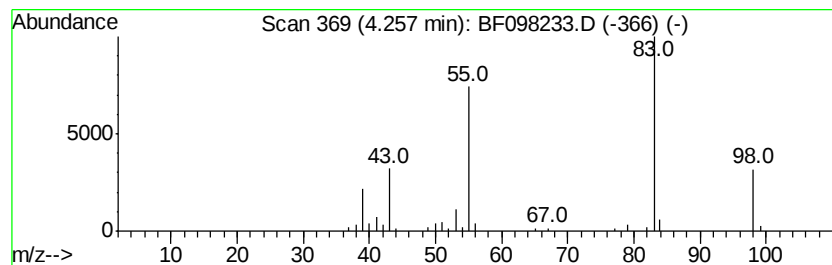
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	3.86 ng	144676	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			3-Hexen-2-one	98	C6H10O	000763-93-9	90
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90



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Instrument :
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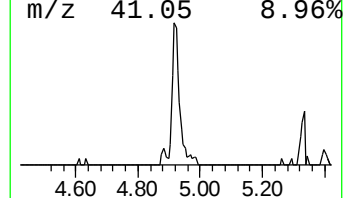
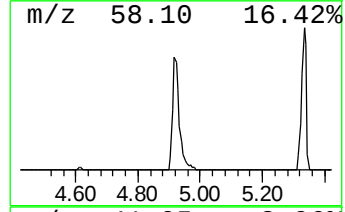
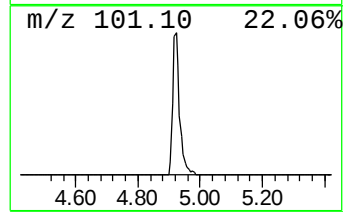
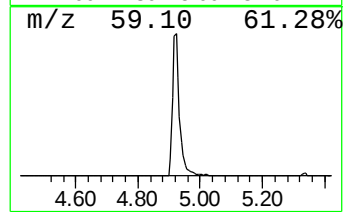
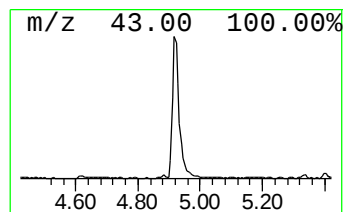
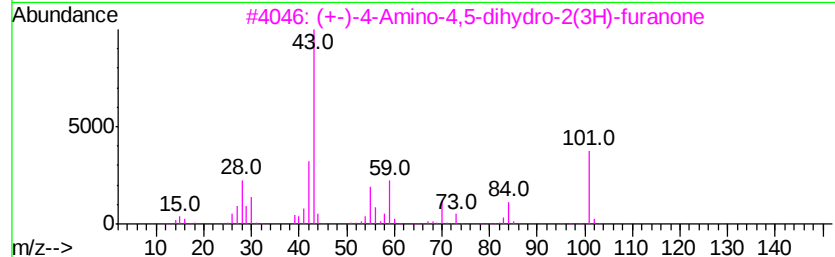
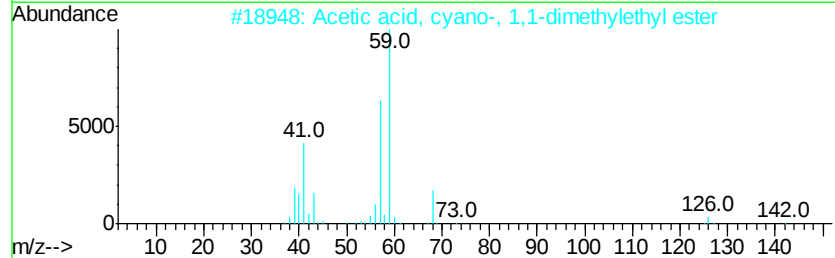
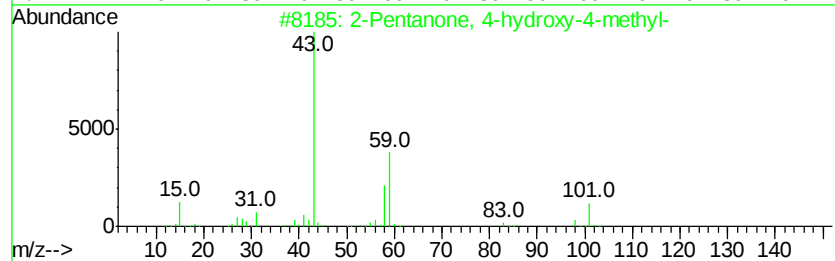
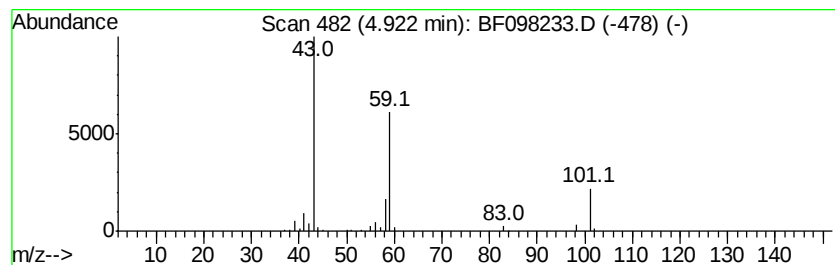
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	7.56 ng	283710	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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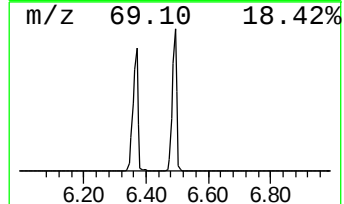
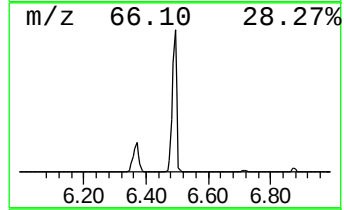
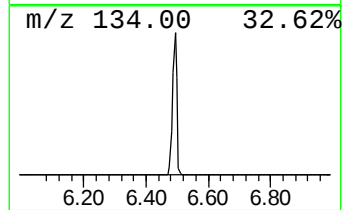
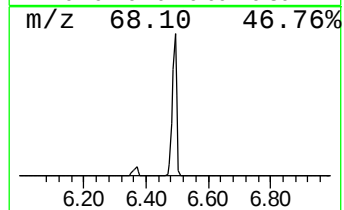
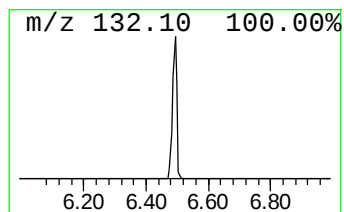
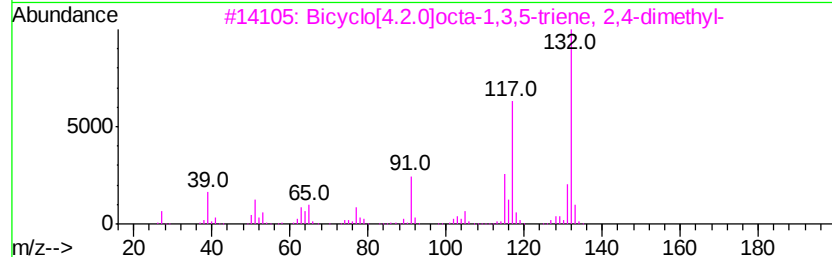
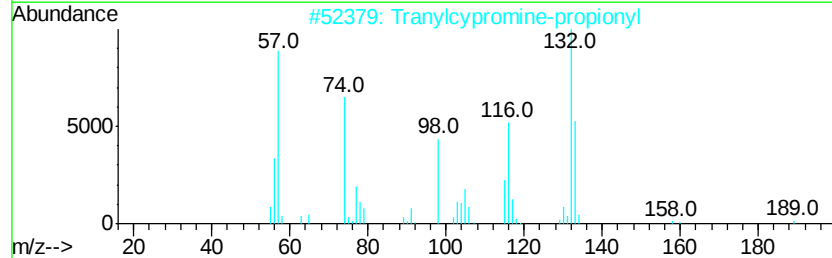
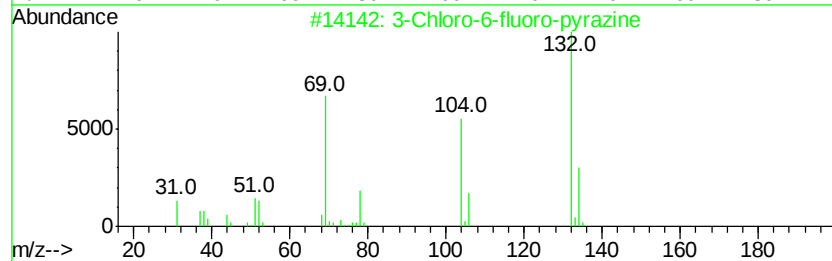
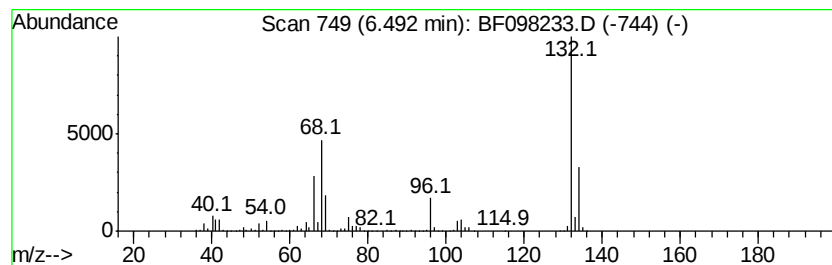
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	79.92 ng	2998460	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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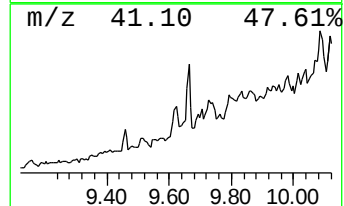
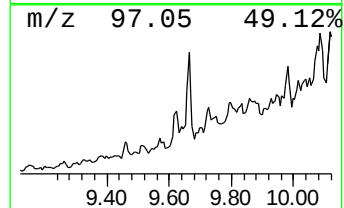
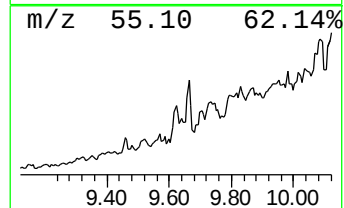
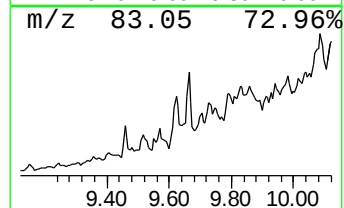
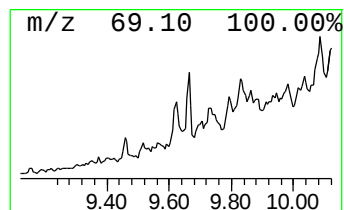
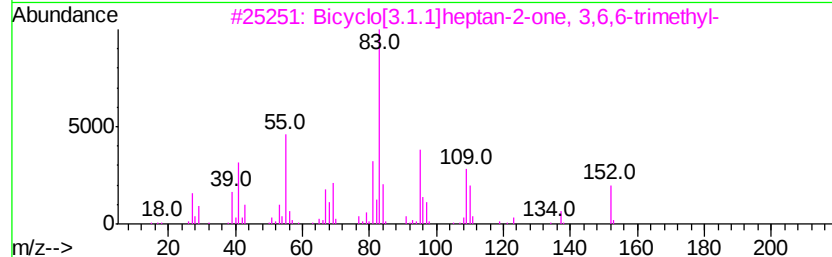
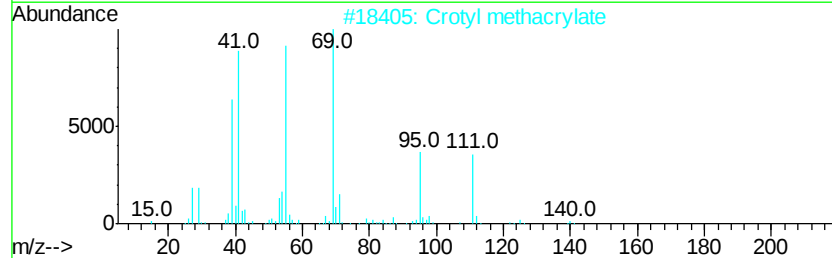
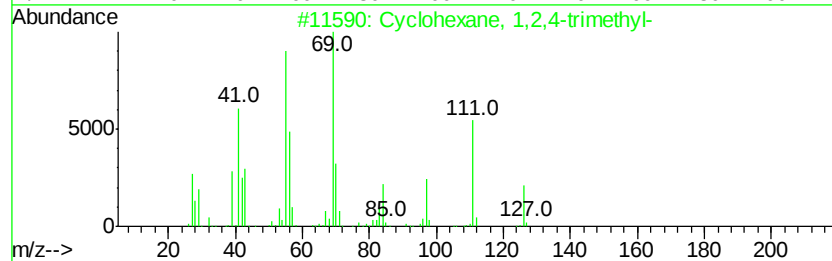
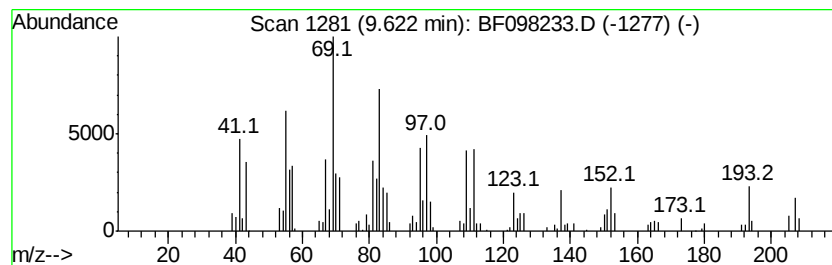
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 unknown9.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	3.06 ng	131007	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
2		Crotyl methacrylate	140	C8H12O2	007376-45-6	35
3		Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	25
4		Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	25
5		Cyclopentane, 1-butyl-2-ethyl-	154	C11H22	072993-32-9	22



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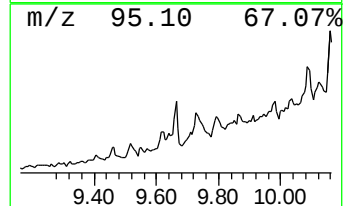
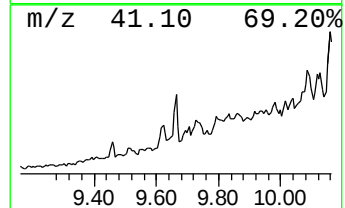
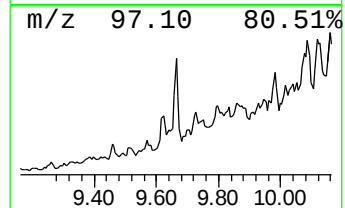
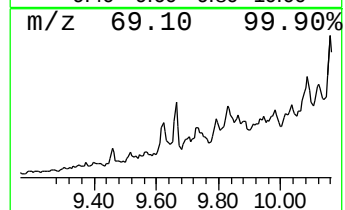
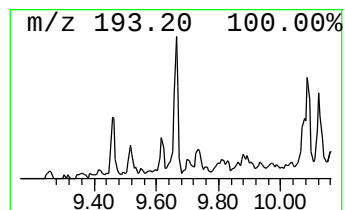
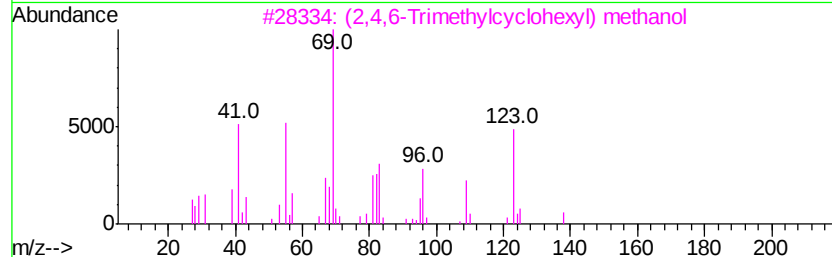
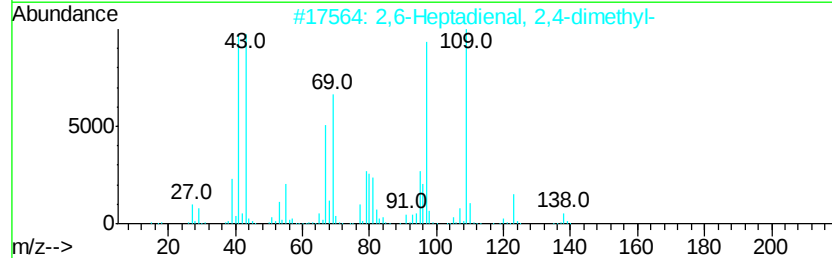
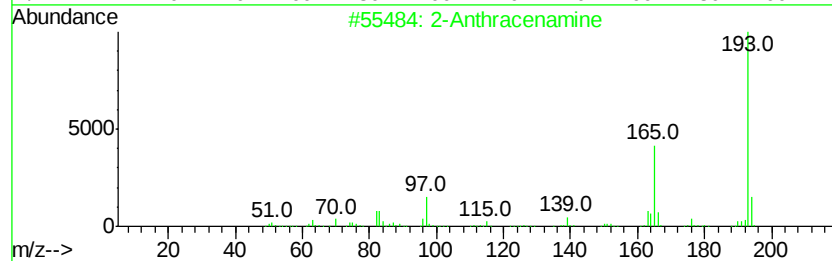
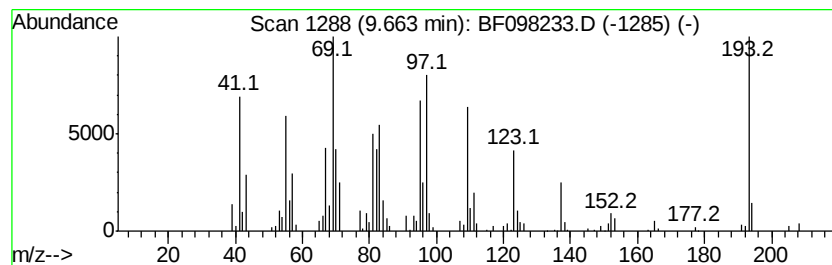
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.66 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	3.24 ng	138782	Acenaphthene-d10	9.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Anthracenamine			193	C14H11N	000613-13-8	46
2	2,6-Heptadienal, 2,4-dimethyl-			138	C9H14O	085136-08-9	38
3	(2,4,6-Trimethylcyclohexyl) meth...			156	C10H20O	013702-56-2	22
4	1,6-Heptadiene, 2,5,5-trimethyl-			138	C10H18	062238-28-2	20
5	Cyclohexane, 1-(cyclohexylmethyl)...			194	C14H26	054824-04-3	18



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090117\
Data File : BF098233.D
Acq On : 1 Sep 2017 18:13
Operator : SJ/JU
Sample : I5050-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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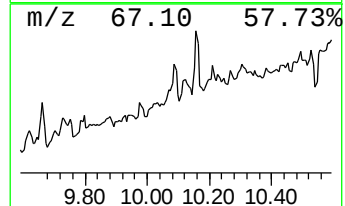
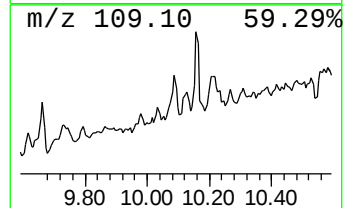
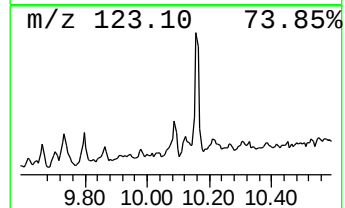
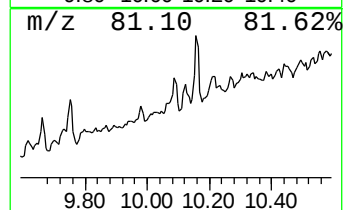
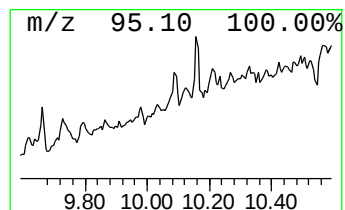
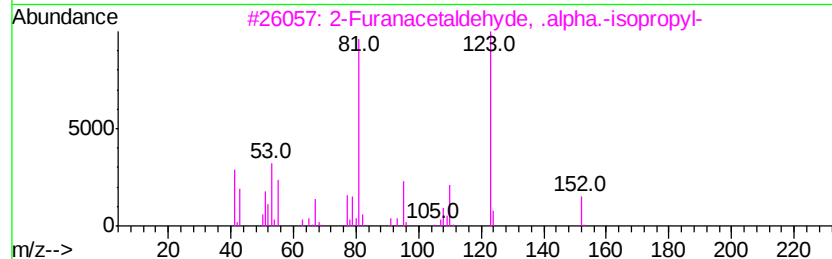
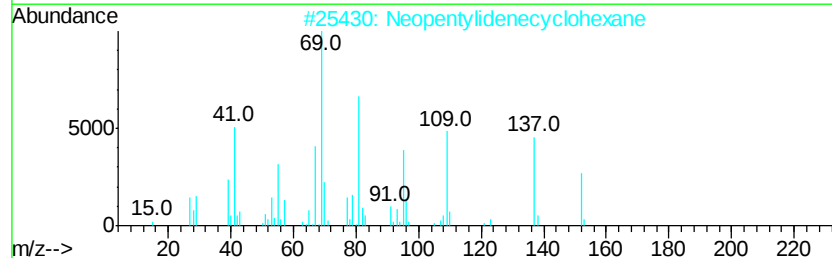
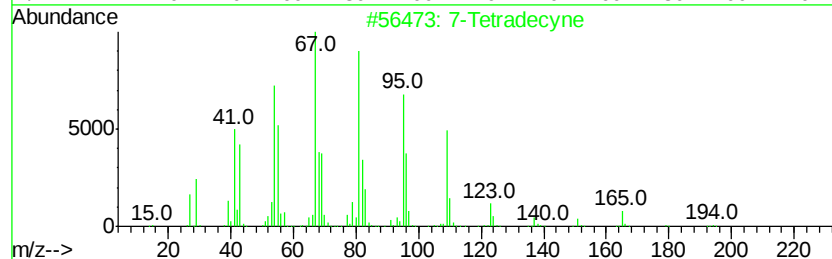
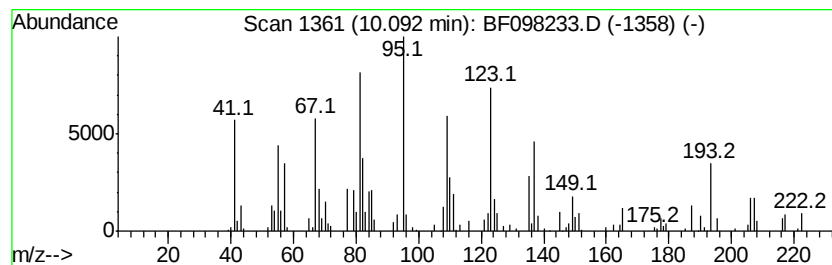
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.09 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.09	2.21 ng	94547	Acenaphthene-d10	9.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Tetradecyne	194	C14H26	035216-11-6	49
2			Neopentylidenecyclohexane	152	C11H20	039546-80-0	35
3			2-Furanacetaldehyde, .alpha.-iso...	152	C9H12O2	031681-30-8	27
4			1-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	001655-03-4	25
5			Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	25



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Sample : I5050-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

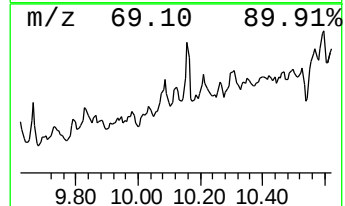
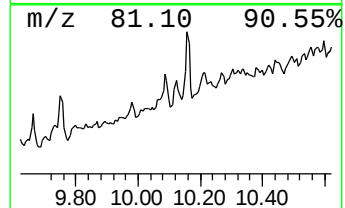
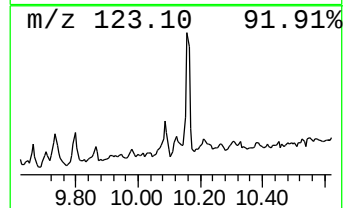
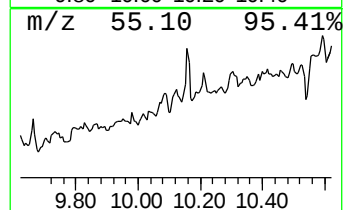
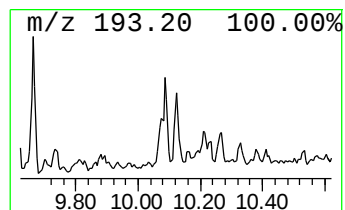
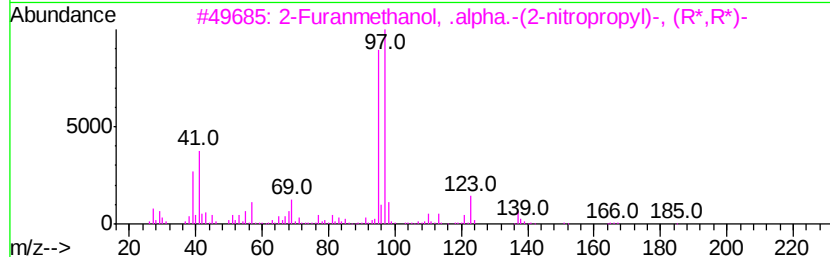
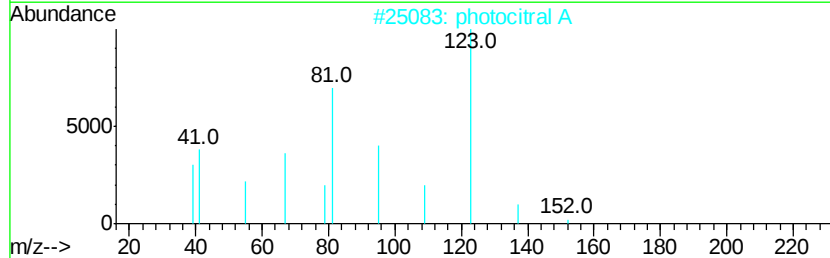
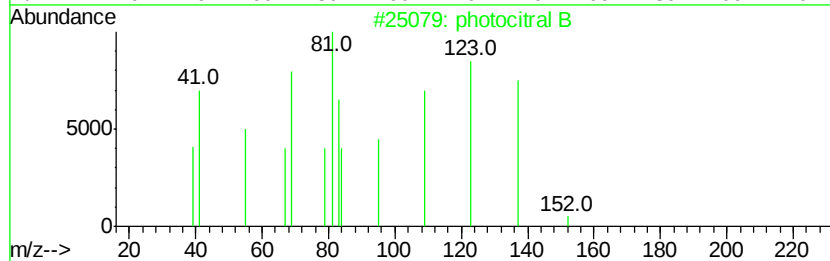
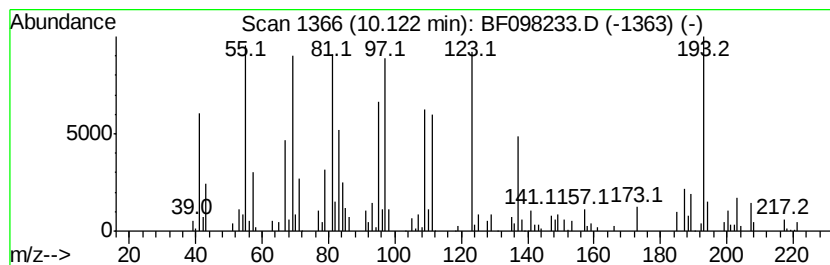
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.12 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.12	3.07 ng	131222	Acenaphthene-d10	9.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	photocitral B	152	C10H16O	006040-45-5	27
2	photocitral A	152	C10H16O	055253-28-6	27
3	2-Furanmethanol, .alpha.-(2-nitr...	185	C8H11NO4	103077-75-4	25
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	22
5	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	22



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090117\
Data File : BF098233.D
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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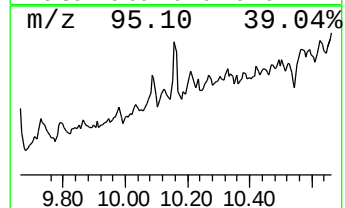
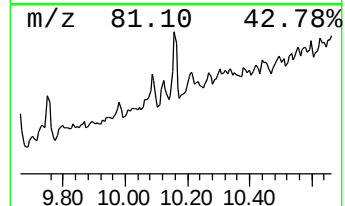
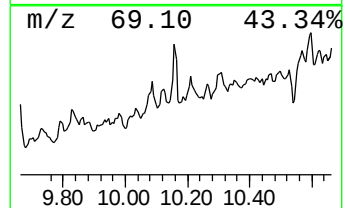
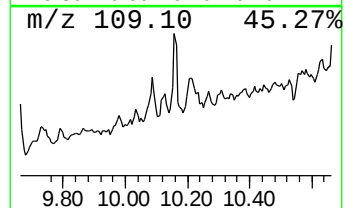
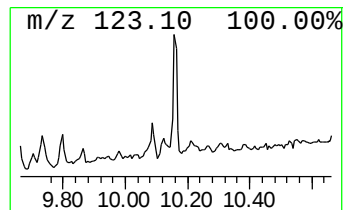
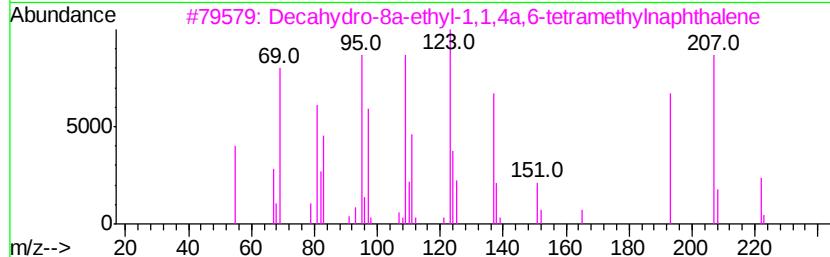
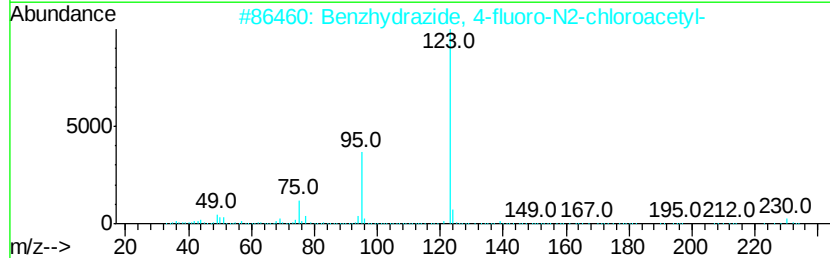
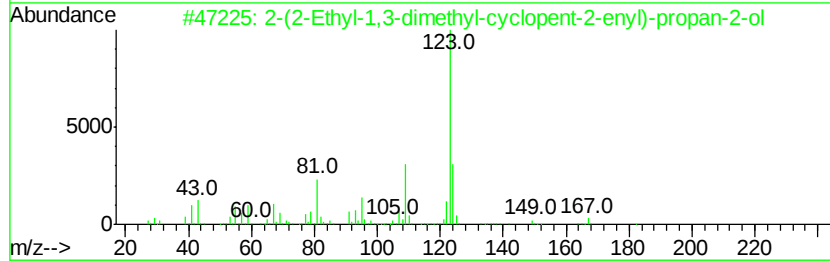
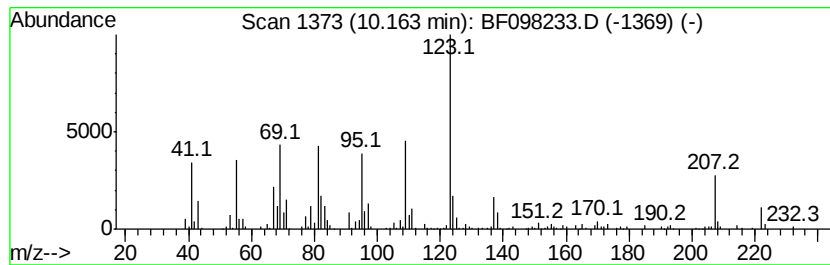
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	5.84 ng	249915	Acenaphthene-d10	9.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(2-Ethyl-1,3-dimethyl-cyclopent-2-enyl)-propan-2-ol	182	C12H22O	1000186-82-4	47
2			Benzhydrazide, 4-fluoro-N2-chloroacetyl-	230	C9H8ClFN2O2	1000266-55-2	38
3			Decahydro-8a-ethyl-1,1,4a,6-tetramethylnaphthalene	222	C16H30	1000100-23-6	38
4			Benzene-1,2,3-triamine	123	C6H9N3	1000316-45-3	38
5			3-Fluorobenzoic acid, undec-10-e-	292	C18H25FO2	1000279-01-2	37



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090117\
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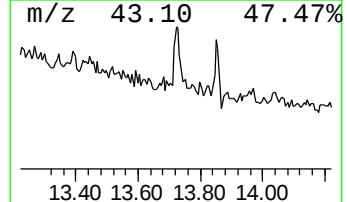
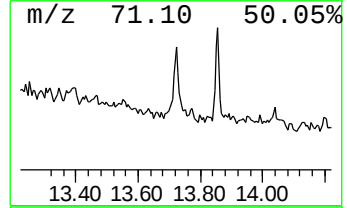
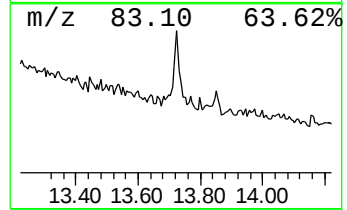
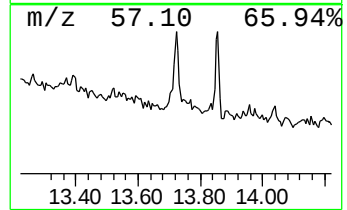
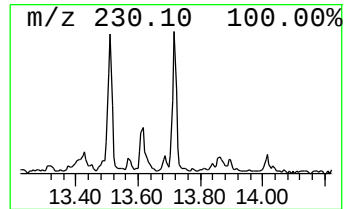
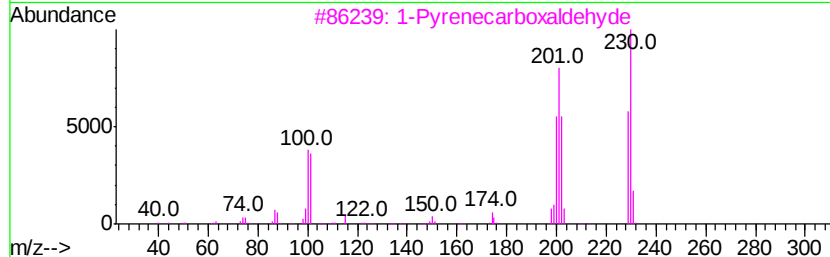
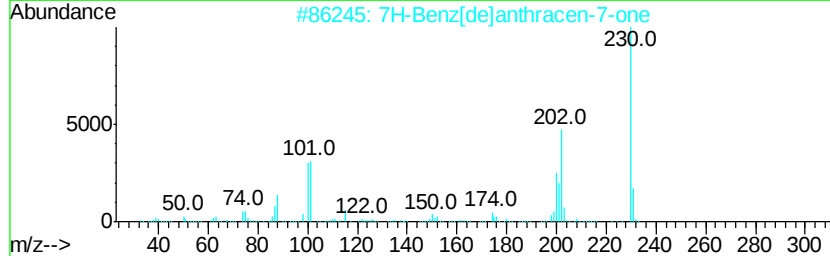
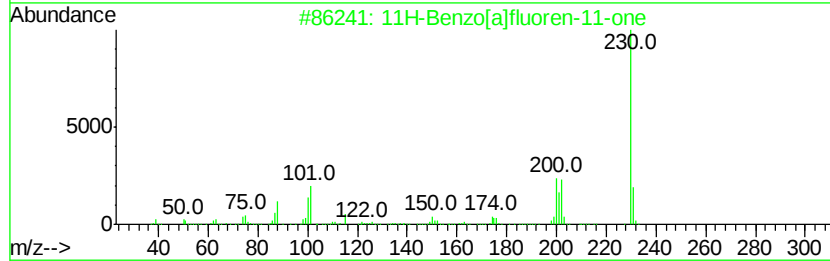
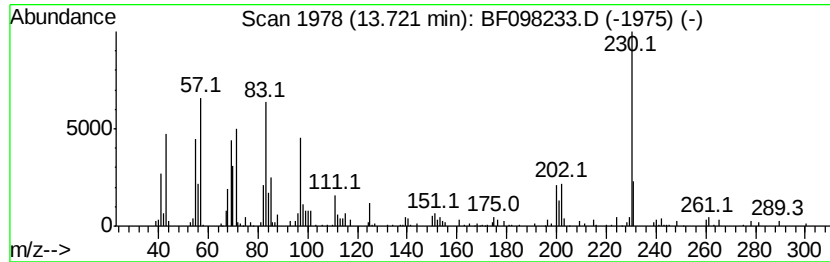
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.72	3.16 ng	171362	Chrysene-d12		13.87		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	93
2			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	74
3			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	72
4			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	53
5			Benzo(b)phenazine	230	C16H10N2	000257-97-6	47



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090117\
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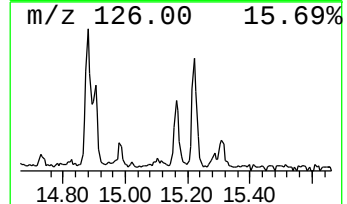
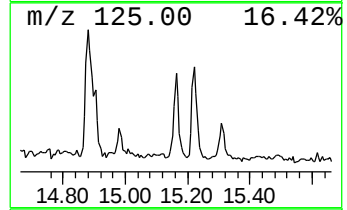
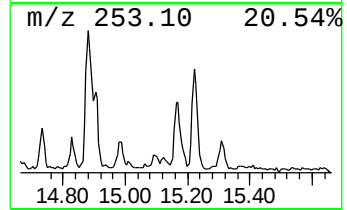
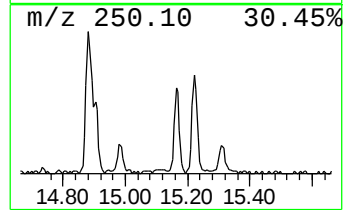
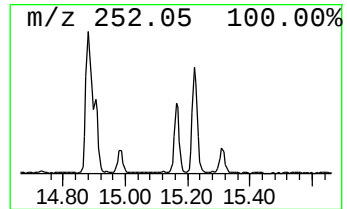
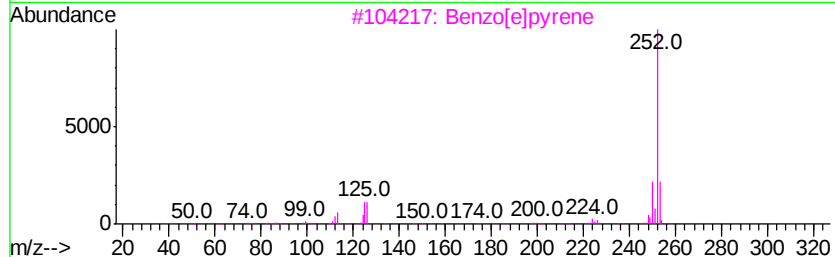
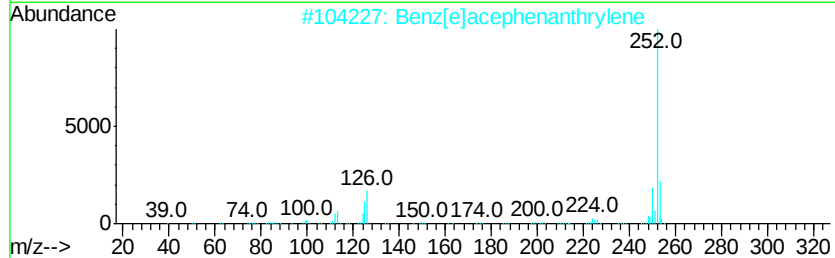
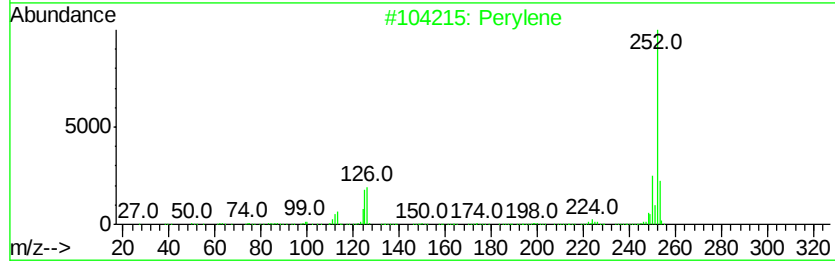
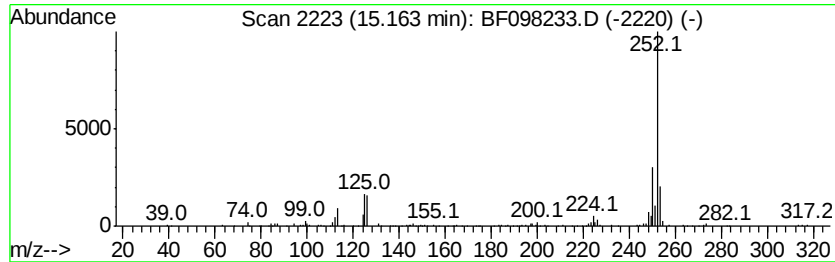
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	5.11 ng	137880	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	96
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3		Benzo[e]pyrene	252	C20H12	000192-97-2	96
4		Benzo[a]pyrene	252	C20H12	000050-32-8	95
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090117\
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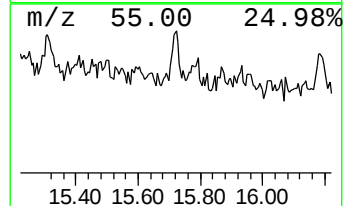
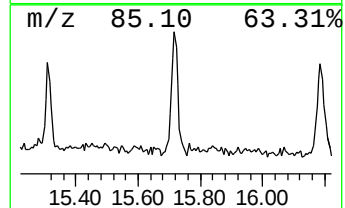
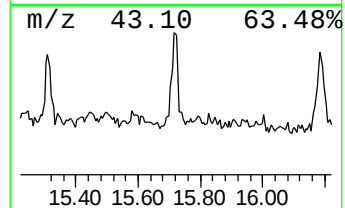
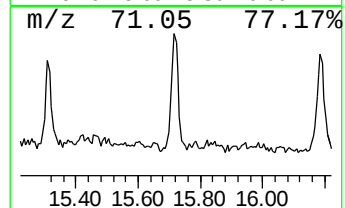
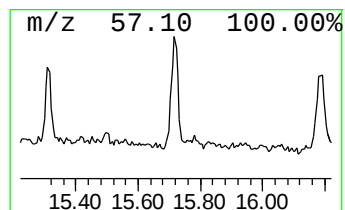
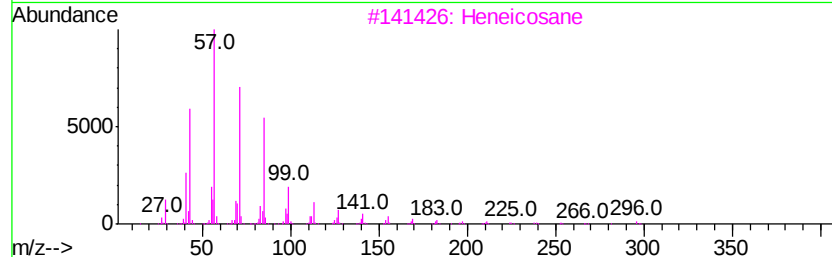
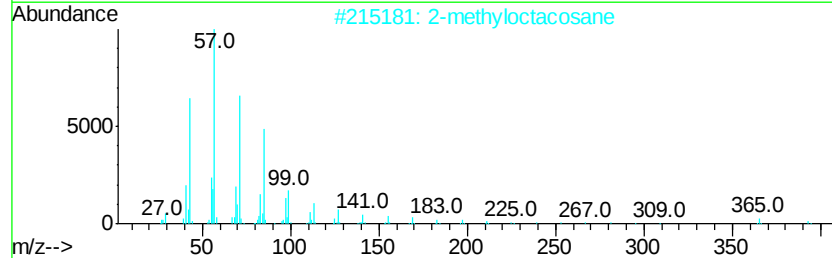
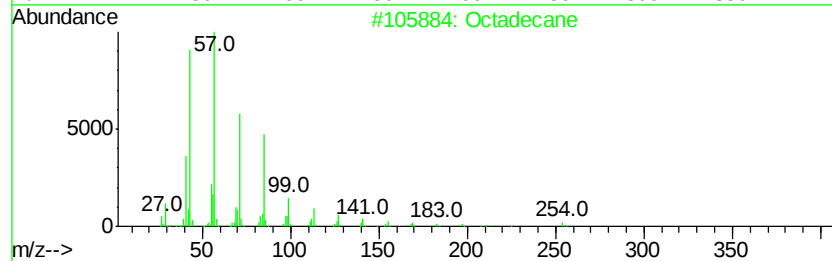
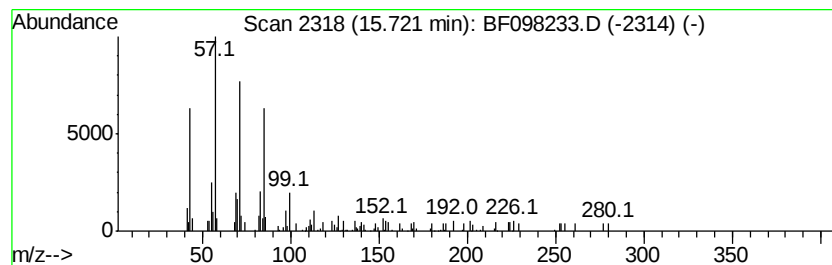
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.98 ng	80387	Perylene-d12	15.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	74
2			2-methyloctacosane	408	C29H60	1000376-72-8	72
3			Heneicosane	296	C21H44	000629-94-7	72
4			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72
5			Hexacosane	366	C26H54	000630-01-3	72



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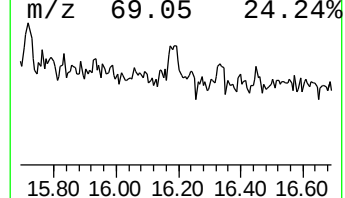
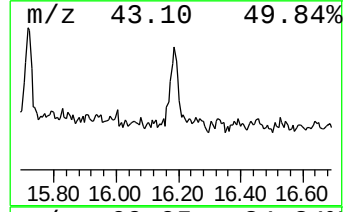
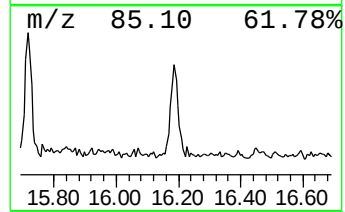
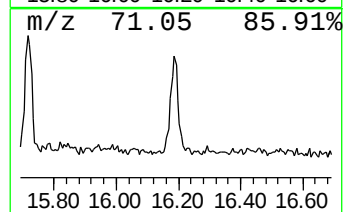
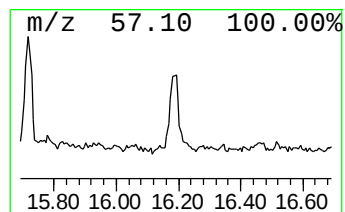
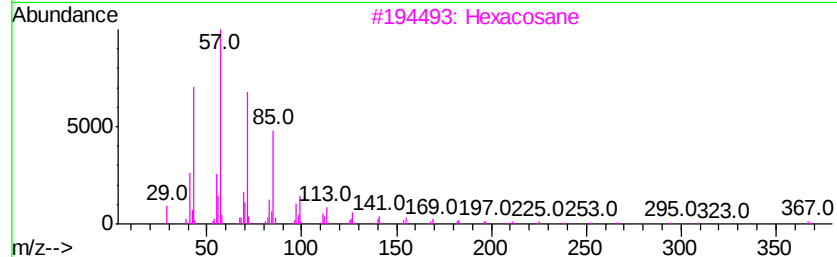
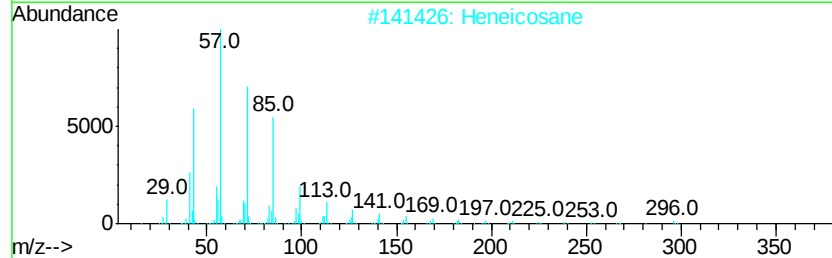
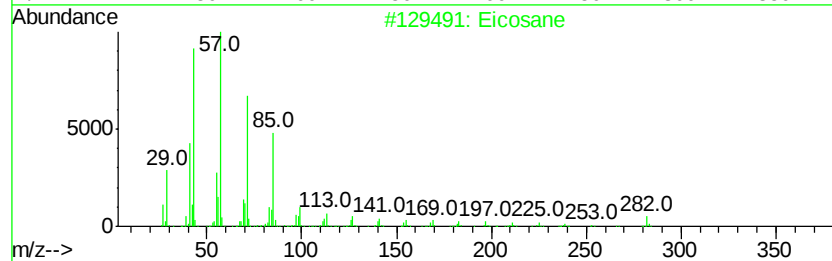
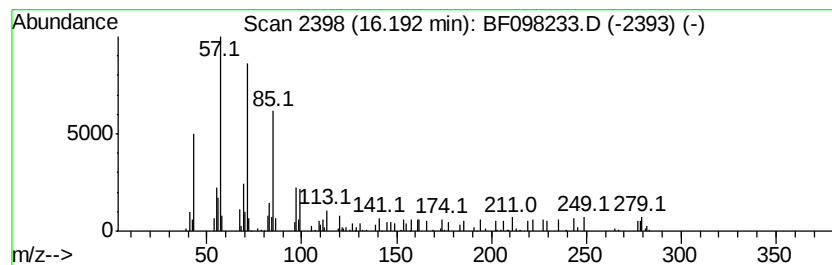
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.29 ng	61717	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	74
2		Heneicosane	296	C21H44	000629-94-7	74
3		Hexacosane	366	C26H54	000630-01-3	74
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
5		Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	72



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF090117\
Data File : BF098233.D
Acq On : 1 Sep 2017 18:13
Operator : SJ/JU
Sample : I5050-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4651-1540

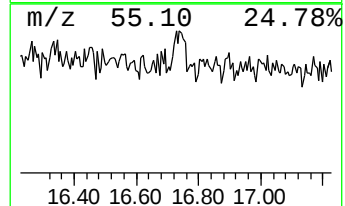
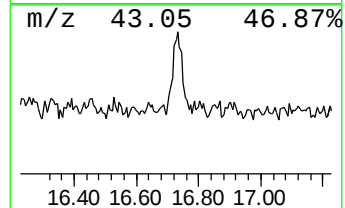
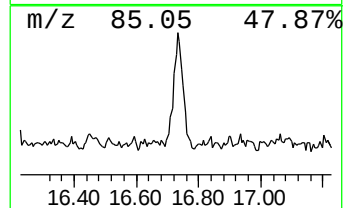
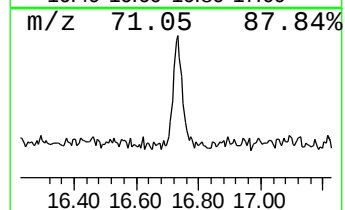
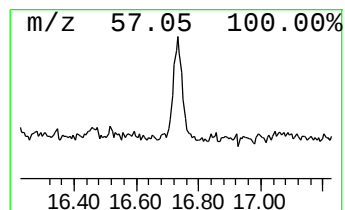
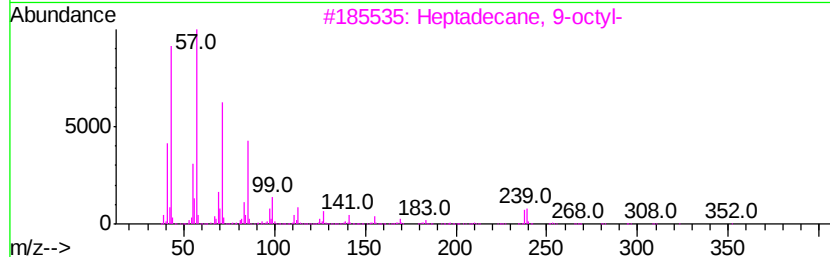
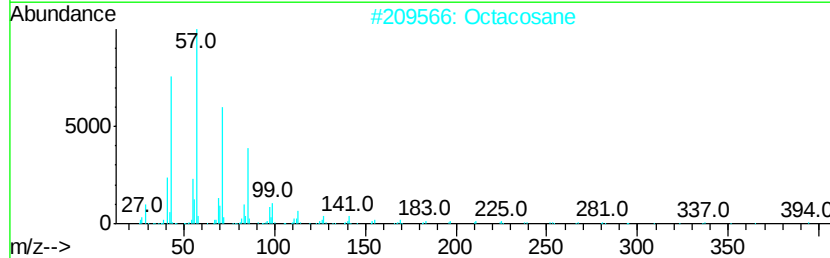
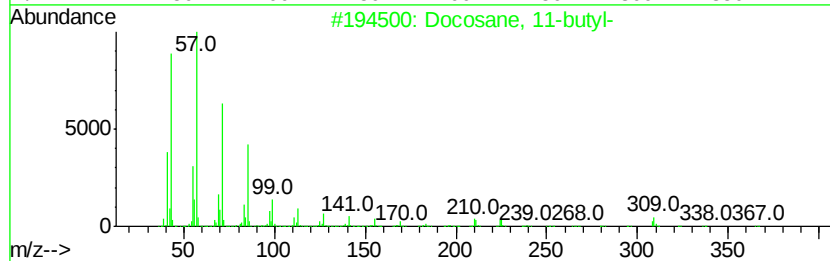
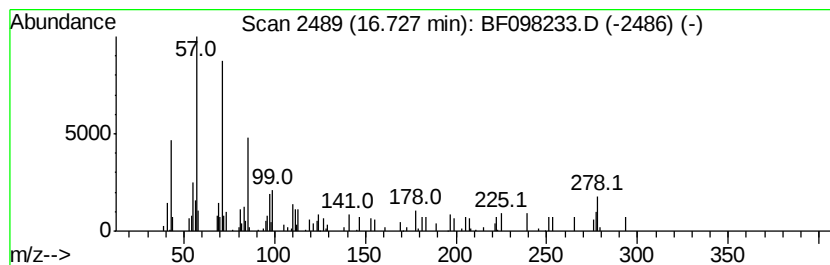
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Docosane, 11-butyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.75 ng	74391	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	62
2		Octacosane	394	C28H58	000630-02-4	62
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	62
4		Hexacosane	366	C26H54	000630-01-3	58
5		Heneicosane	296	C21H44	000629-94-7	58



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090117\
 Data File : BF098233.D
 Acq On : 1 Sep 2017 18:13
 Operator : SJ/JU
 Sample : I5050-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT4651-1540

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
3-Penten-2-one, 4...	4.26	3.9 ng		144676	1	6.72	750352	20.0
2-Pentanone, 4-hy...	4.92	7.6 ng		283710	1	6.72	750352	20.0
unknown6.49	6.49	79.9 ng		2998460	1	6.72	750352	20.0
unknown9.62	9.62	3.1 ng		131007	3	9.75	855752	20.0
unknown9.66	9.66	3.2 ng		138782	3	9.75	855752	20.0
unknown10.09	10.09	2.2 ng		94547	3	9.75	855752	20.0
unknown10.12	10.12	3.1 ng		131222	3	9.75	855752	20.0
unknown10.16	10.16	5.8 ng		249915	3	9.75	855752	20.0
11H-Benzo[a]fluor...	13.72	3.2 ng		171362	5	13.87	1085760	20.0
Perylene	15.16	5.1 ng		137880	6	15.29	540098	20.0
Octadecane	15.72	3.0 ng		80387	6	15.29	540098	20.0
Eicosane	16.19	2.3 ng		61717	6	15.29	540098	20.0
Docosane, 11-butyl-	16.73	2.8 ng		74391	6	15.29	540098	20.0