

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
 Data File : BF081599.D
 Acq On : 12 Sep 2015 00:14
 Operator : UM/IZ
 Sample : G3526-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13(0-0.16)

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-BF090115.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	1.462	10	11	17	rBV	29806	70031	4.57%	0.441%
2	1.554	17	19	42	rVB	173174	535857	34.96%	3.378%
3	4.560	277	282	292	rBV	313462	884429	57.70%	5.575%
4	5.417	354	357	372	rBV	782969	1397992	91.21%	8.812%
5	7.669	550	554	557	rBV	786537	1488121	97.09%	9.380%
6	7.760	559	562	572	rVB	797320	1516869	98.96%	9.562%
7	8.252	601	605	610	rVB	216502	378469	24.69%	2.386%
8	8.572	629	633	636	rBV	653351	1102568	71.93%	6.950%
9	9.543	714	718	721	rBV	526396	993526	64.82%	6.263%
10	11.143	854	858	862	rBV	300162	488962	31.90%	3.082%
11	13.795	1085	1090	1093	rBV	913665	1532798	100.00%	9.662%
12	13.852	1093	1095	1103	rVB	9548	16581	1.08%	0.105%
13	14.847	1178	1182	1185	rBV	144993	218463	14.25%	1.377%
14	14.927	1186	1189	1194	rVB	25481	40816	2.66%	0.257%
15	15.281	1216	1220	1225	rBV	301062	493866	32.22%	3.113%
16	17.178	1382	1386	1393	rBV	463974	778172	50.77%	4.905%
17	17.601	1420	1423	1428	rBV	56537	88043	5.74%	0.555%
18	17.818	1439	1442	1449	rBV	12548	28983	1.89%	0.183%
19	18.790	1523	1527	1529	rBV	263550	452405	29.51%	2.852%
20	18.836	1529	1531	1534	rVV	49810	73353	4.79%	0.462%
21	18.904	1534	1537	1540	rVV2	11984	21965	1.43%	0.138%
22	18.961	1540	1542	1549	rVB	17618	31702	2.07%	0.200%
23	20.527	1676	1679	1686	rVB	17852	37271	2.43%	0.235%
24	20.767	1696	1700	1703	rBV2	12500	18961	1.24%	0.120%
25	21.442	1756	1759	1762	rBV	87771	121408	7.92%	0.765%
26	21.796	1787	1790	1794	rBV	96814	126184	8.23%	0.795%
27	22.127	1816	1819	1821	rBV	901691	995925	64.97%	6.278%
28	22.276	1828	1832	1834	rBV2	7293	16470	1.07%	0.104%
29	22.550	1852	1856	1858	rBV2	12535	24974	1.63%	0.157%
30	22.973	1889	1893	1895	rBV2	23544	32459	2.12%	0.205%
31	23.099	1901	1904	1906	rBV2	12148	18652	1.22%	0.118%
32	23.145	1906	1908	1910	rVB2	12473	19786	1.29%	0.125%
33	23.225	1913	1915	1918	rBV	16318	18537	1.21%	0.117%
34	23.396	1925	1930	1932	rBV	361025	577931	37.70%	3.643%

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Instrument :
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ClientSampleId :
SB-13(0-0.16)

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.510	1938	1940	1941	rBV	15205	17406	1.14%	0.110%
36	23.568	1941	1945	1947	rBV2	22167	28972	1.89%	0.183%
37	23.682	1953	1955	1957	rBV2	13067	21753	1.42%	0.137%
38	23.728	1957	1959	1961	rVV2	11560	19653	1.28%	0.124%
39	23.842	1964	1969	1971	rBV	23589	45950	3.00%	0.290%
40	24.059	1985	1988	1991	rVB	43629	60477	3.95%	0.381%
41	24.356	2012	2014	2018	rVB4	13337	22213	1.45%	0.140%
42	24.413	2018	2019	2022	rBV2	14127	16632	1.09%	0.105%
43	24.493	2024	2026	2031	rVB	103618	165341	10.79%	1.042%
44	24.585	2031	2034	2036	rBV	26841	37589	2.45%	0.237%
45	24.653	2038	2040	2044	rBV2	21093	53064	3.46%	0.334%
46	24.733	2045	2047	2049	rBV	64983	58872	3.84%	0.371%
47	24.779	2049	2051	2053	rVB	72799	79581	5.19%	0.502%
48	24.836	2053	2056	2058	rBV	220622	300302	19.59%	1.893%
49	25.076	2075	2077	2082	rVB3	17500	36763	2.40%	0.232%
50	25.236	2089	2091	2093	rVB	30472	38733	2.53%	0.244%
51	25.282	2093	2095	2098	rBV4	9607	18528	1.21%	0.117%
52	25.625	2124	2125	2128	rBV3	8441	15907	1.04%	0.100%
53	25.785	2137	2139	2142	rVB2	12567	22102	1.44%	0.139%
54	25.888	2145	2148	2151	rVB2	27555	51841	3.38%	0.327%
55	25.991	2155	2157	2160	rBV3	9856	24844	1.62%	0.157%
56	26.185	2172	2174	2178	rVV	20929	32944	2.15%	0.208%
57	26.276	2180	2182	2187	rVB4	12024	28331	1.85%	0.179%
58	27.659	2300	2303	2308	rVB4	10818	24010	1.57%	0.151%

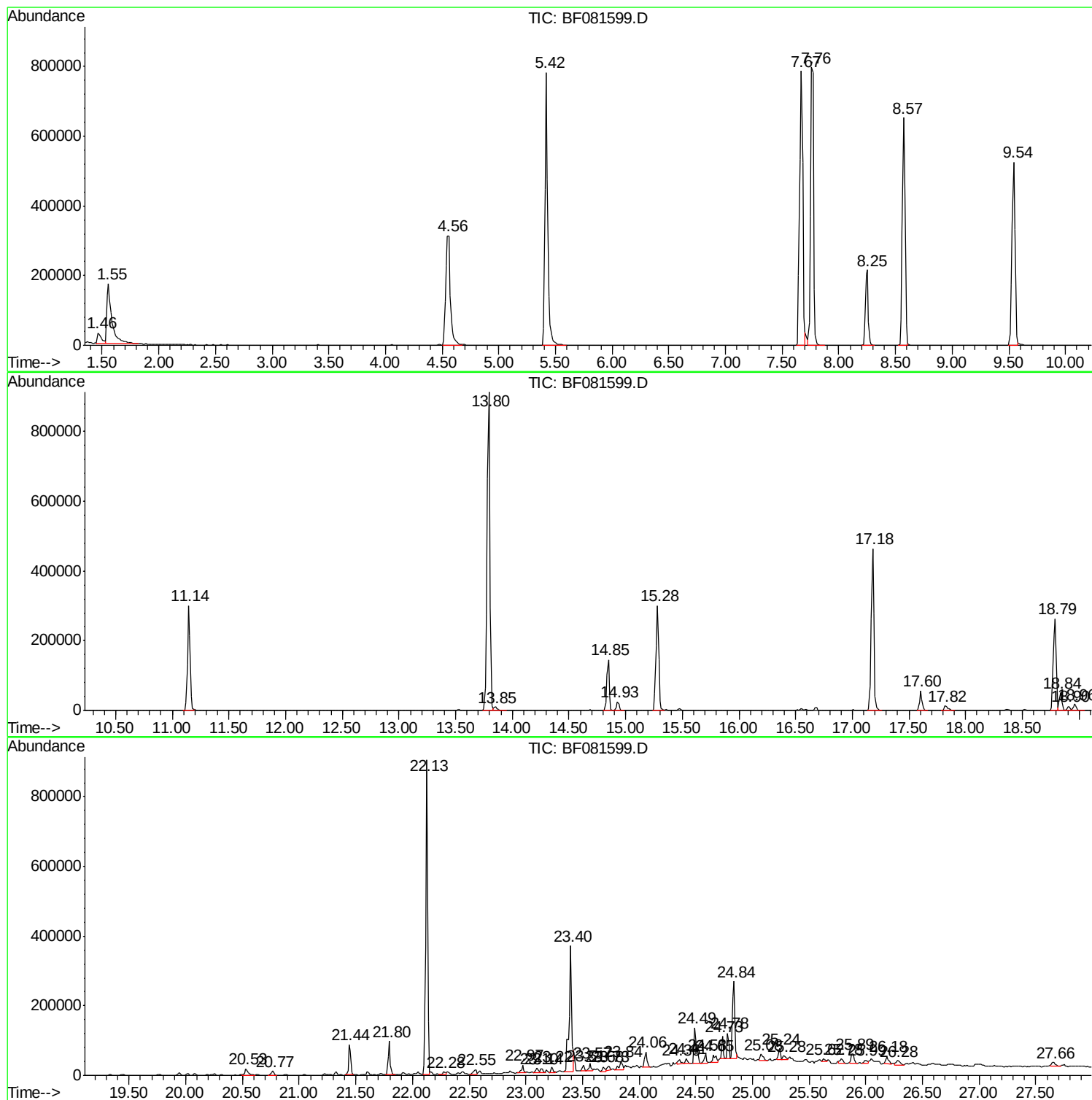
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : G3526-09
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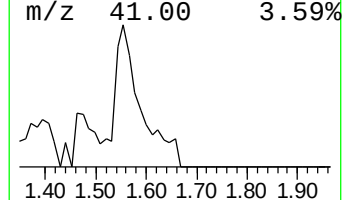
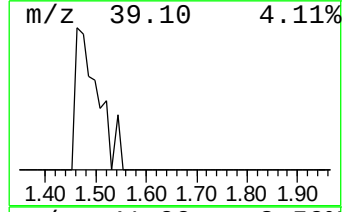
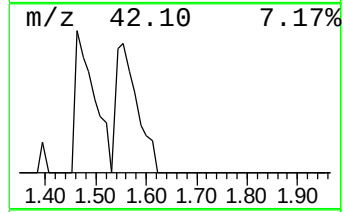
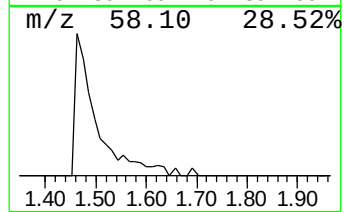
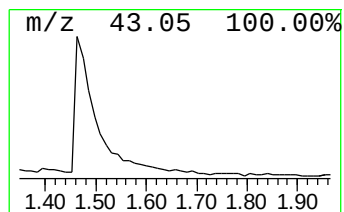
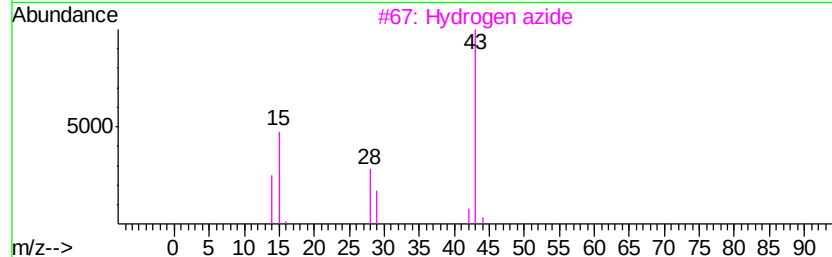
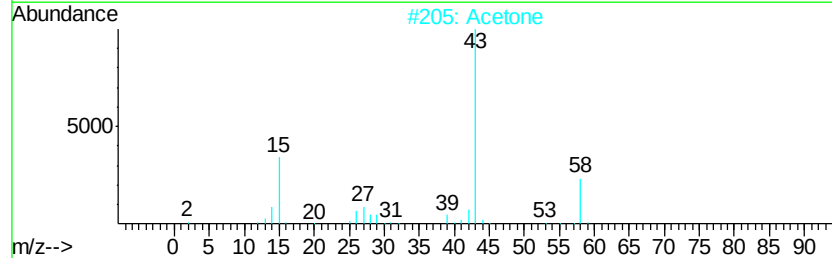
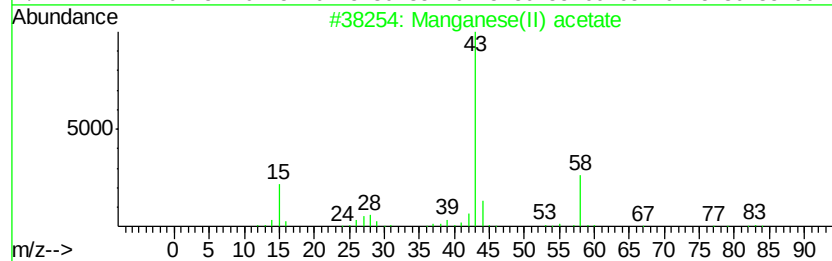
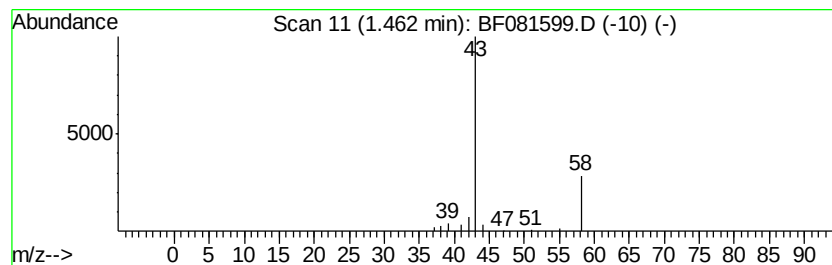
Instrument :
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ClientSampleId :
SB-13(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Manganese(II) acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.46	3.70 ng	70031	1,4-Dichlorobenzene-d4	8.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	64
2	Acetone	58	C3H6O	000067-64-1	64
3	Hydrogen azide	43	HN3	007782-79-8	4
4	Ethene, methoxy-	58	C3H6O	000107-25-5	3
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3



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Instrument :
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ClientSampleId :
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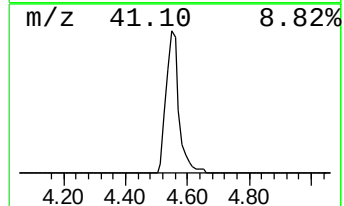
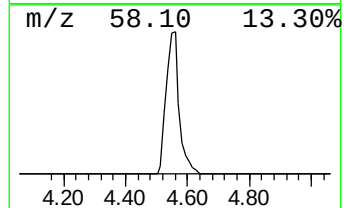
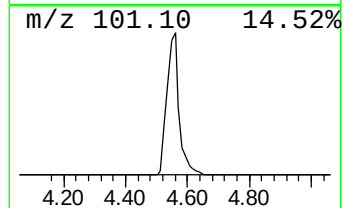
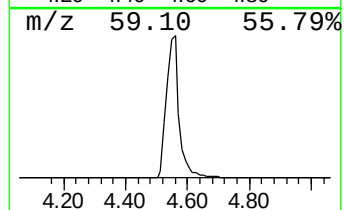
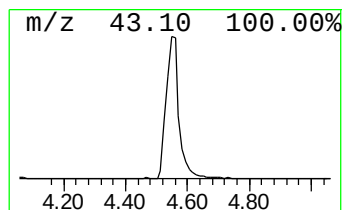
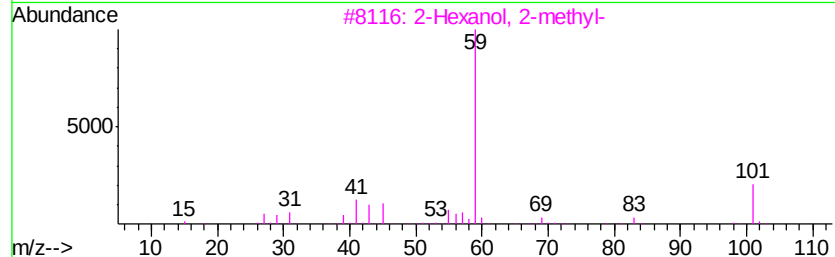
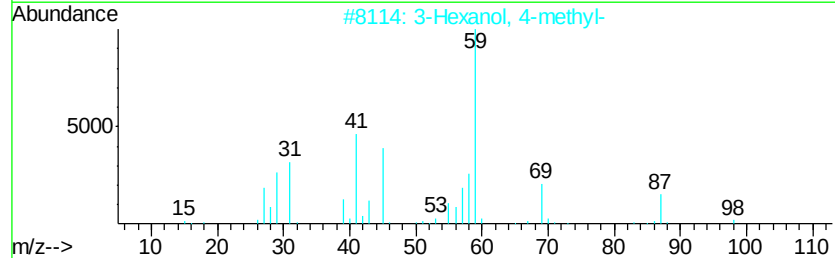
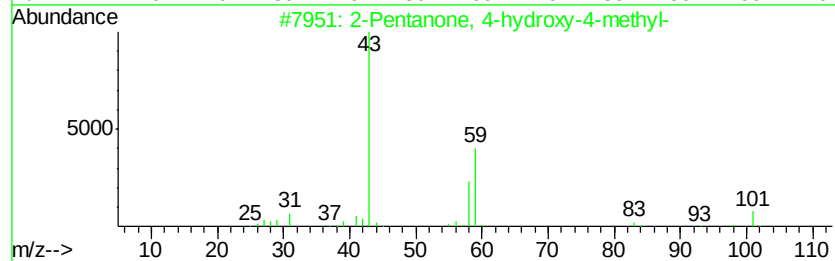
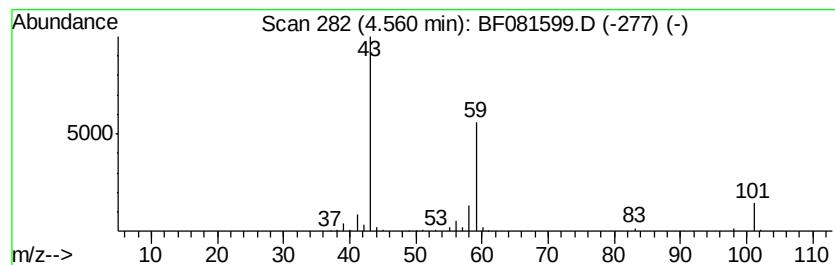
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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.
4.56	46.74 ng	884429	1,4-Dichlorobenzene-d4	8.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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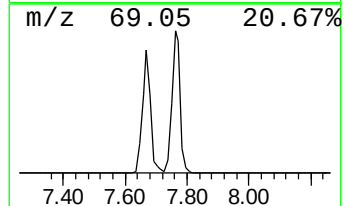
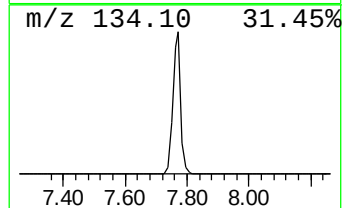
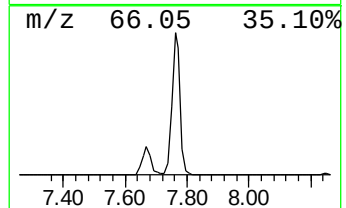
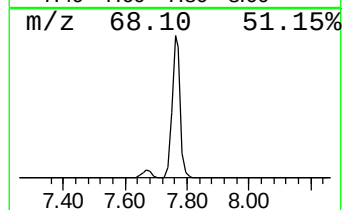
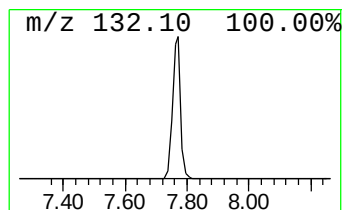
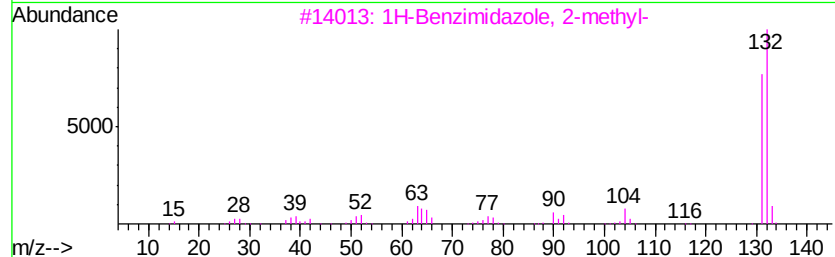
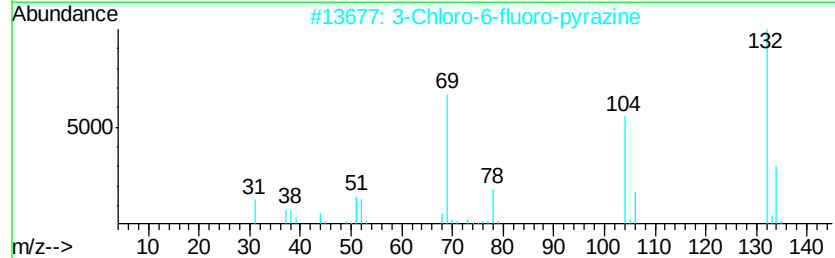
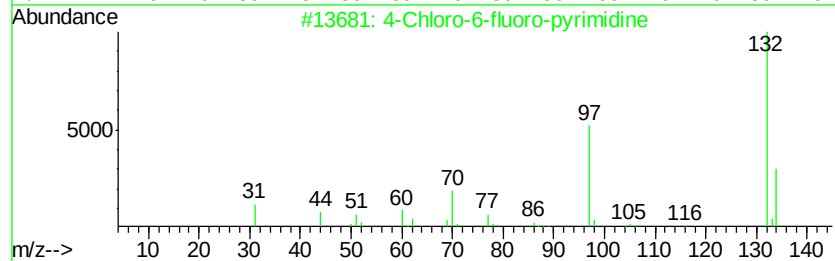
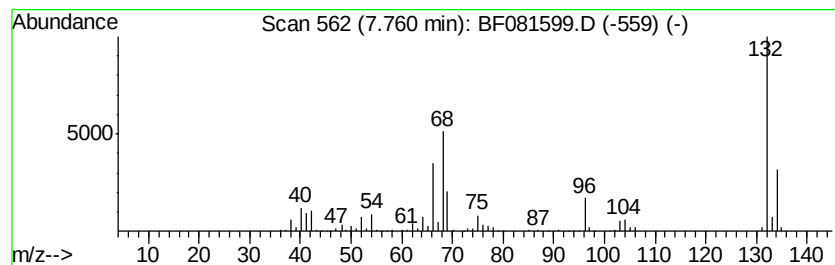
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	80.16 ng	1516870	1,4-Dichlorobenzene-d4	8.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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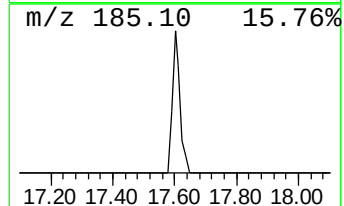
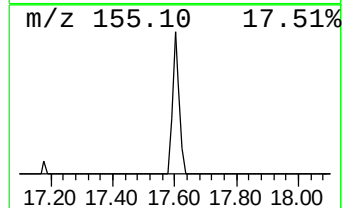
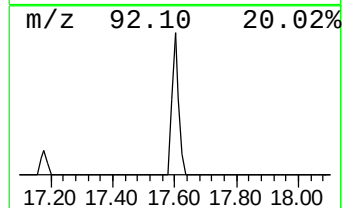
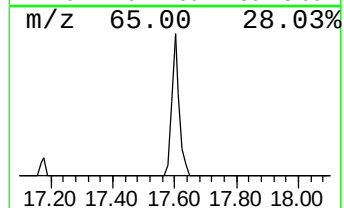
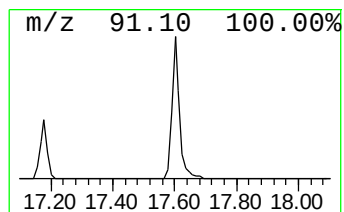
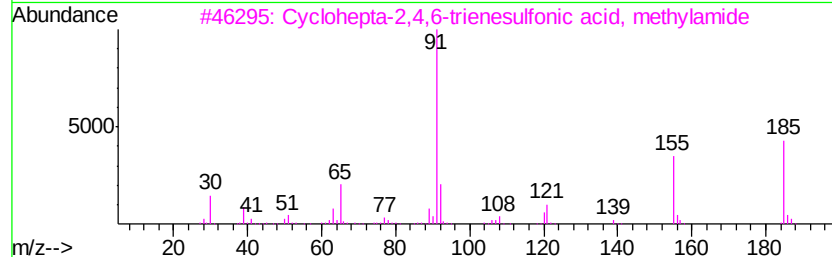
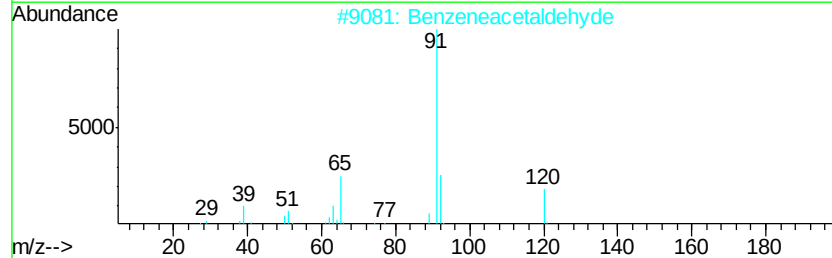
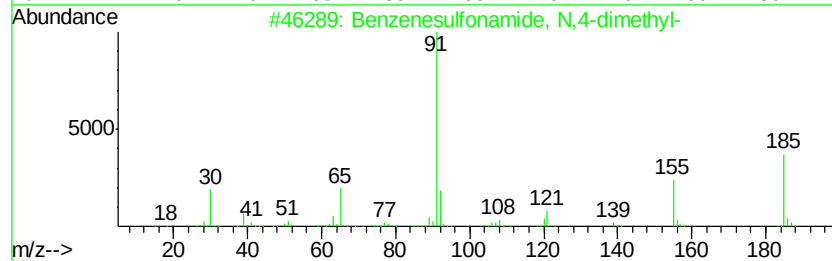
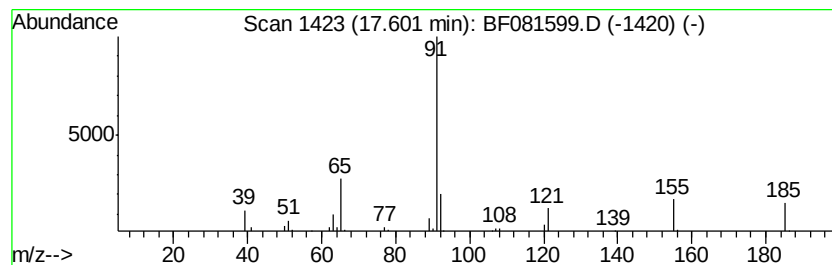
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	3.89 ng	88043	Phenanthrene-d10	18.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11N02S	000640-61-9	90
2		Benzeneacetaldehyde	120	C8H8O	000122-78-1	58
3		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11N02S	1000187-28-7	53
4		Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
5		Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	47



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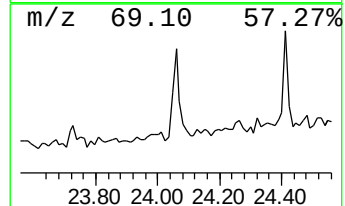
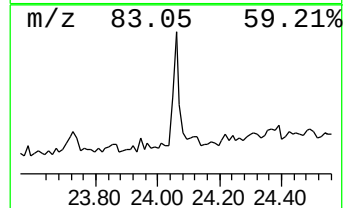
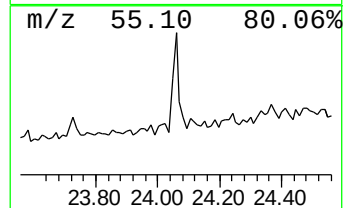
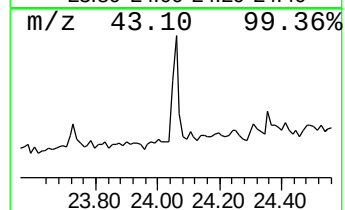
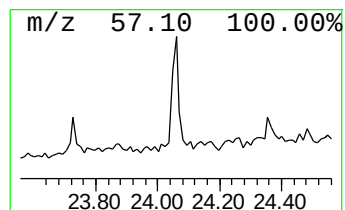
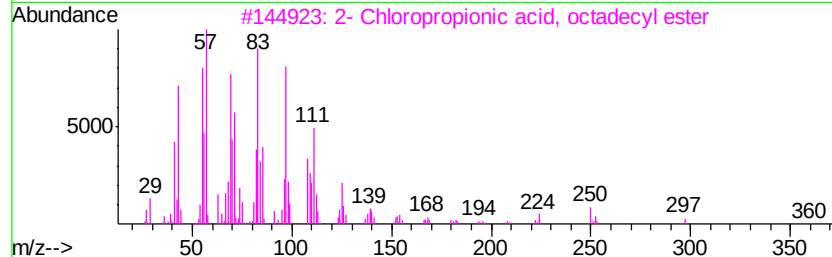
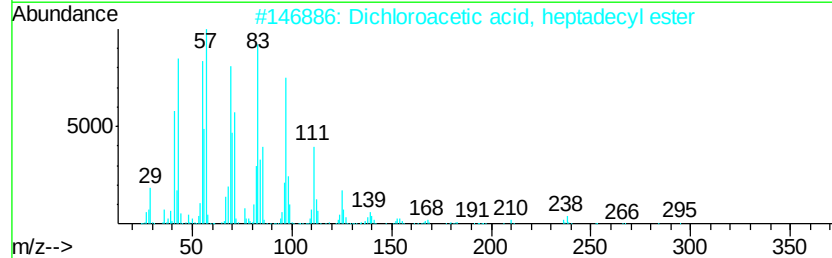
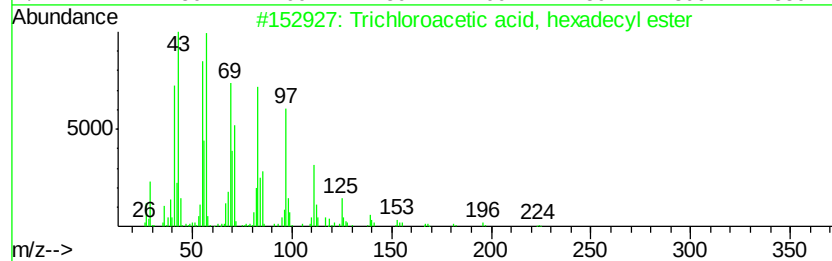
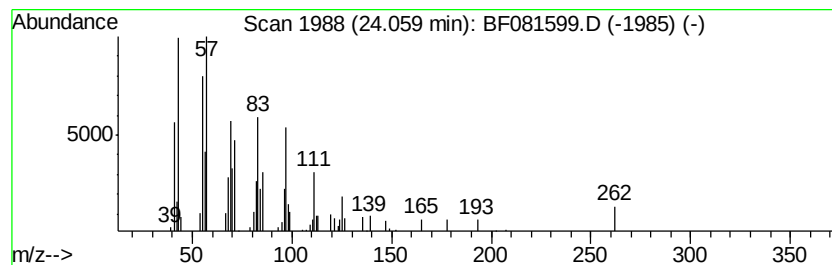
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.06	2.09 ng	60477	Chrysene-d12	23.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
5		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081599.D
Acq On : 12 Sep 2015 00:14
Operator : UM/IZ
Sample : G3526-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

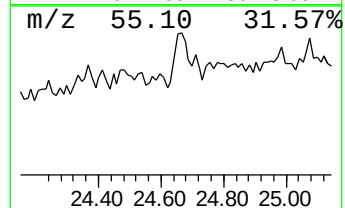
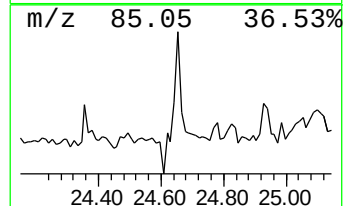
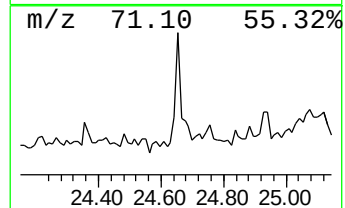
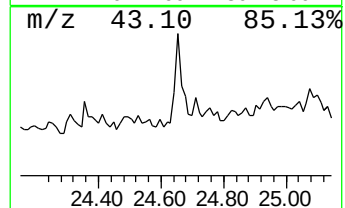
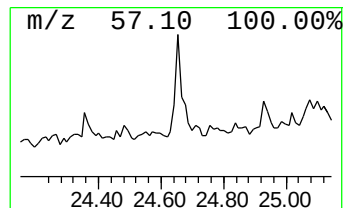
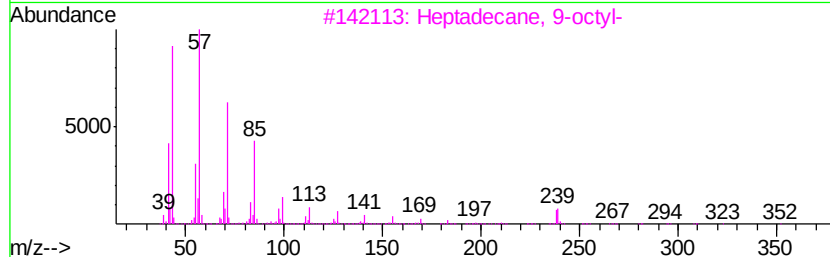
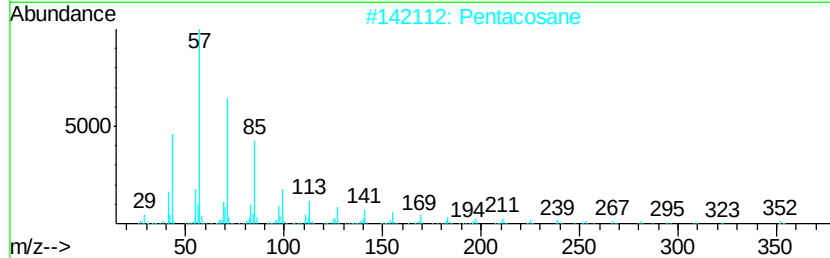
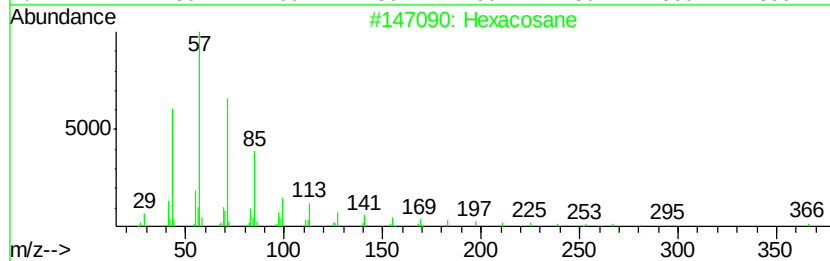
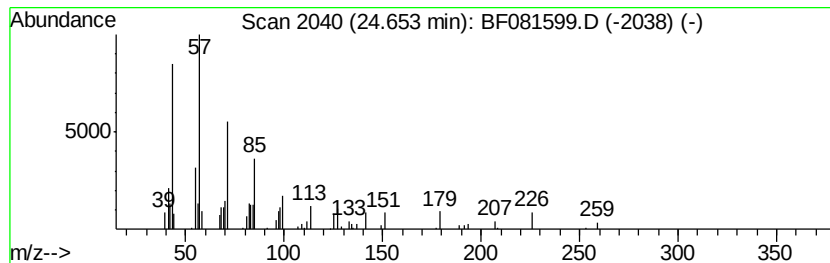
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ClientSampleId :
SB-13(0-0.16)

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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 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.65	3.53 ng	53064	Perylene-d12	24.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	86
2	Pentacosane	352 C25H52	000629-99-2	86
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	80
4	Silane, trichlorooctadecyl-	386 C18H37Cl3Si	000112-04-9	80
5	Hentriacontane	437 C31H64	000630-04-6	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081599.D
Acq On : 12 Sep 2015 00:14
Operator : UM/IZ
Sample : G3526-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13(0-0.16)

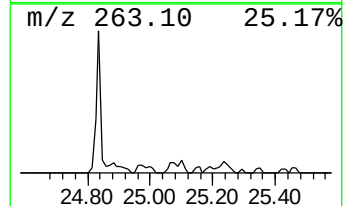
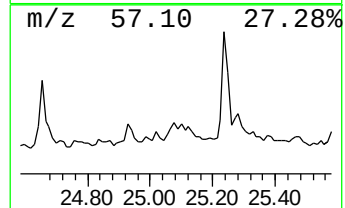
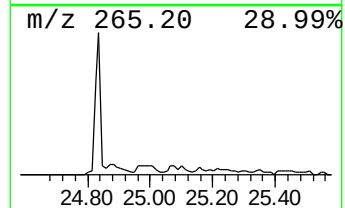
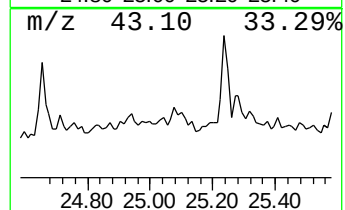
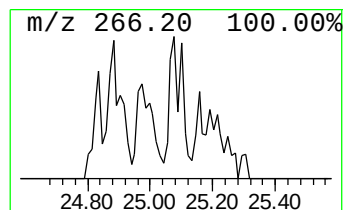
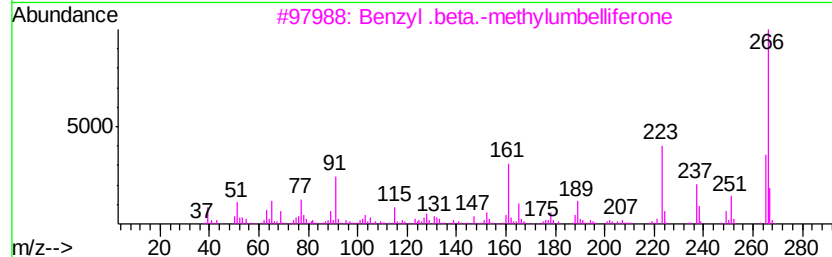
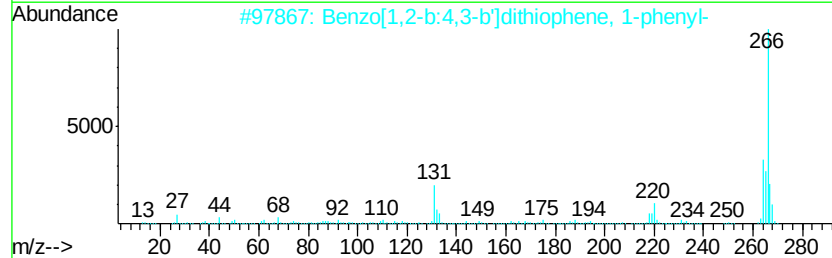
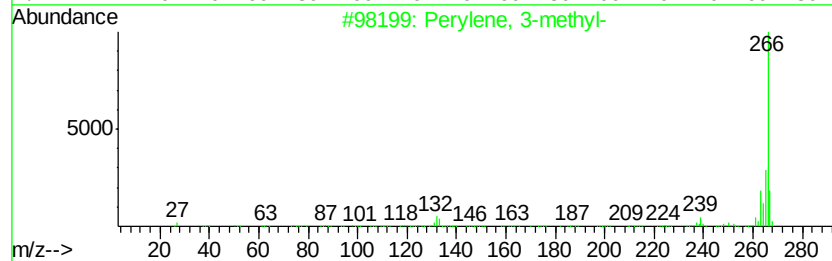
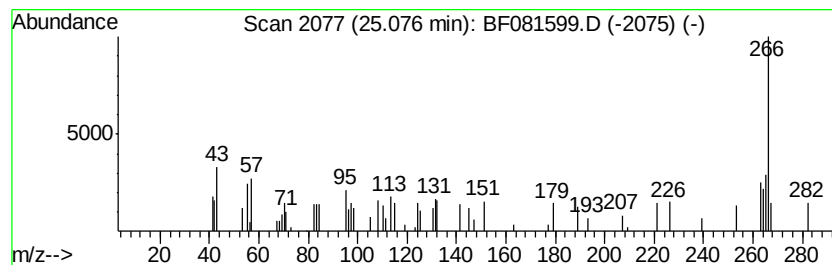
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown25.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.08	2.45 ng	36763	Perylene-d12	24.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene, 3-methyl-	266	C21H14	024471-47-4	43
2		Benzo[1,2-b:4,3-b']dithiophene, ...	266	C16H10S2	016587-58-9	43
3		Benzyl .beta.-methyumbelliferone	266	C17H14O3	000086-44-2	38
4		Benzamide, 3-(4-isopropylbenzyl)-	266	C17H18N2O	304455-80-9	38
5		2,4,8,10-Tetramethylbenzo[1,2-b;...	266	C16H18N4	017377-04-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081599.D
Acq On : 12 Sep 2015 00:14
Operator : UM/IZ
Sample : G3526-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13(0-0.16)

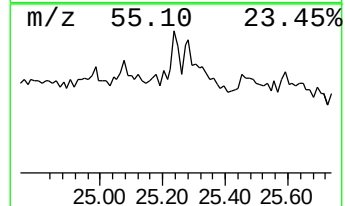
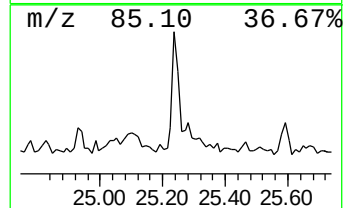
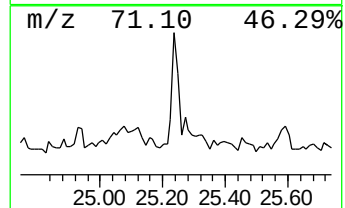
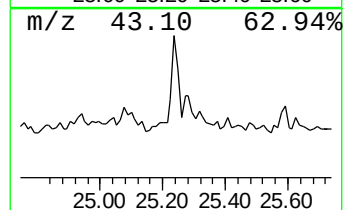
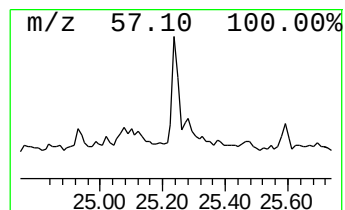
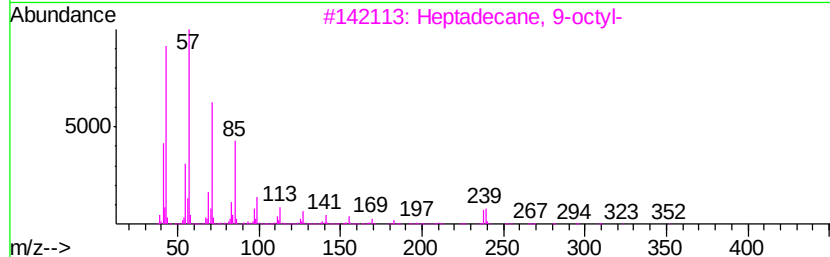
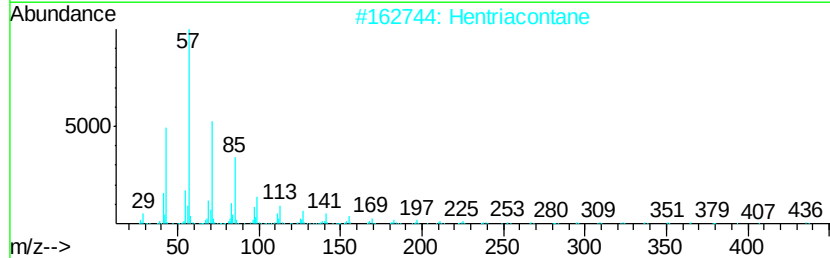
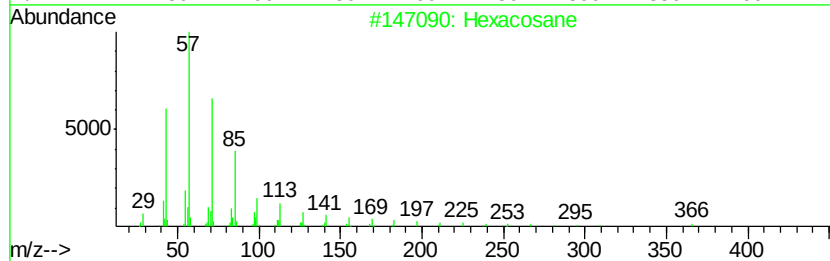
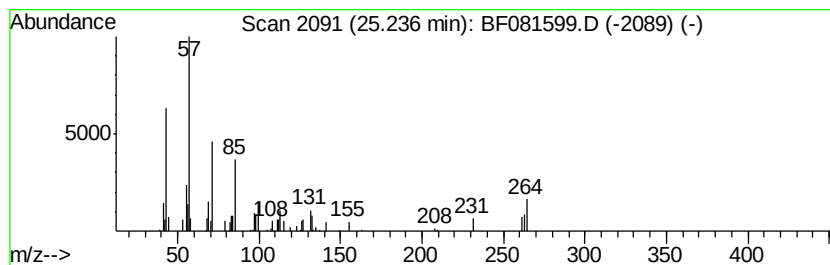
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.24	2.58 ng	38733	Perylene-d12	24.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	68
2		Hentriacontane	437	C31H64	000630-04-6	64
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
4		Octadecane	254	C18H38	000593-45-3	59
5		Docosane	310	C22H46	000629-97-0	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091115\
Data File : BF081599.D
Acq On : 12 Sep 2015 00:14
Operator : UM/IZ
Sample : G3526-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
Manganese(II) ace...	1.46	3.7	ng	70031	1	8.25	378469	20.0
2-Pentanone, 4-hy...	4.56	46.7	ng	884429	1	8.25	378469	20.0
unknown7.76	7.76	80.2	ng	1516870	1	8.25	378469	20.0
Benzenesulfonamid...	17.60	3.9	ng	88043	4	18.79	452405	20.0
Trichloroacetic a...	24.06	2.1	ng	60477	5	23.40	577931	20.0
Hexacosane	24.65	3.5	ng	53064	6	24.84	300302	20.0
unknown25.08	25.08	2.5	ng	36763	6	24.84	300302	20.0
Hentriacontane	25.24	2.6	ng	38733	6	24.84	300302	20.0