

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
 Data File : BG026371.D
 Acq On : 22 Mar 2017 10:43
 Operator : SJ/MA
 Sample : I2304-11
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SPA-B6(0-5)

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_G\METHODS\8270-BG032017.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	5.150	345	351	361	rBV	472864	719414	8.16%	1.150%
2	5.620	424	431	447	rBV	2690364	4381190	49.71%	7.005%
3	7.218	694	703	719	rBV	2639023	4896450	55.56%	7.829%
4	7.588	756	766	776	rBV	2823553	4976863	56.47%	7.958%
5	8.052	837	845	853	rBV	527730	900144	10.21%	1.439%
6	8.375	892	900	909	rBV	2171305	3725941	42.28%	5.957%
7	9.210	1035	1042	1050	rVB	1652509	2906399	32.98%	4.647%
8	10.849	1311	1321	1328	rBV	804647	1560240	17.70%	2.495%
9	12.253	1555	1560	1565	rBV	87184	119964	1.36%	0.192%
10	12.500	1591	1602	1612	rVB3	36013	105305	1.19%	0.168%
11	13.199	1716	1721	1727	rVB3	75474	112418	1.28%	0.180%
12	13.287	1728	1736	1743	rBV	4717963	7662454	86.94%	12.252%
13	13.481	1761	1769	1777	rBV	170193	279118	3.17%	0.446%
14	13.822	1820	1827	1829	rBV4	48223	90682	1.03%	0.145%
15	13.980	1849	1854	1859	rBV2	66625	121810	1.38%	0.195%
16	14.033	1859	1863	1868	rVB5	51680	94035	1.07%	0.150%
17	14.098	1868	1874	1878	rBV	435593	689523	7.82%	1.102%
18	14.133	1878	1880	1884	rVB2	111764	128645	1.46%	0.206%
19	14.544	1946	1950	1956	rBV	254837	323995	3.68%	0.518%
20	14.656	1959	1969	1976	rBV2	1264140	2112604	23.97%	3.378%
21	14.862	2000	2004	2012	rVB3	49509	123846	1.41%	0.198%
22	15.044	2031	2035	2041	rVB2	75894	112862	1.28%	0.180%
23	15.161	2052	2055	2062	rVB7	55824	91809	1.04%	0.147%
24	15.490	2106	2111	2115	rVB	327538	413168	4.69%	0.661%
25	15.896	2171	2180	2190	rBV	174408	369553	4.19%	0.591%
26	16.137	2213	2221	2229	rBV	3368792	5294384	60.07%	8.465%
27	16.348	2252	2257	2259	rBV	365235	542773	6.16%	0.868%
28	16.372	2259	2261	2267	rVB	379902	449618	5.10%	0.719%
29	16.848	2339	2342	2345	rVB2	72328	90801	1.03%	0.145%
30	17.136	2387	2391	2395	rBV	319682	368783	4.18%	0.590%
31	17.188	2396	2400	2404	rVV	242206	330733	3.75%	0.529%
32	17.388	2428	2434	2439	rBV2	1434838	2215186	25.13%	3.542%
33	17.788	2499	2502	2506	rBV2	106534	149994	1.70%	0.240%
34	17.870	2512	2516	2521	rVB	339596	420149	4.77%	0.672%

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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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35	18.264	2579	2583	2588	rBV	331743	469738	5.33%	0.751%
36	18.557	2629	2633	2637	rBV	227627	278548	3.16%	0.445%
37	19.180	2736	2739	2743	rVB2	171523	202611	2.30%	0.324%
38	19.527	2795	2798	2801	rBV4	126369	165830	1.88%	0.265%
39	19.985	2871	2876	2881	rVB	6724542	8813480	100.00%	14.092%
40	21.630	3151	3156	3164	rVB	1466447	2503843	28.41%	4.003%
41	24.815	3690	3698	3708	rVB2	893173	2500728	28.37%	3.998%
42	27.653	4176	4181	4195	rVB5	198802	726630	8.24%	1.162%

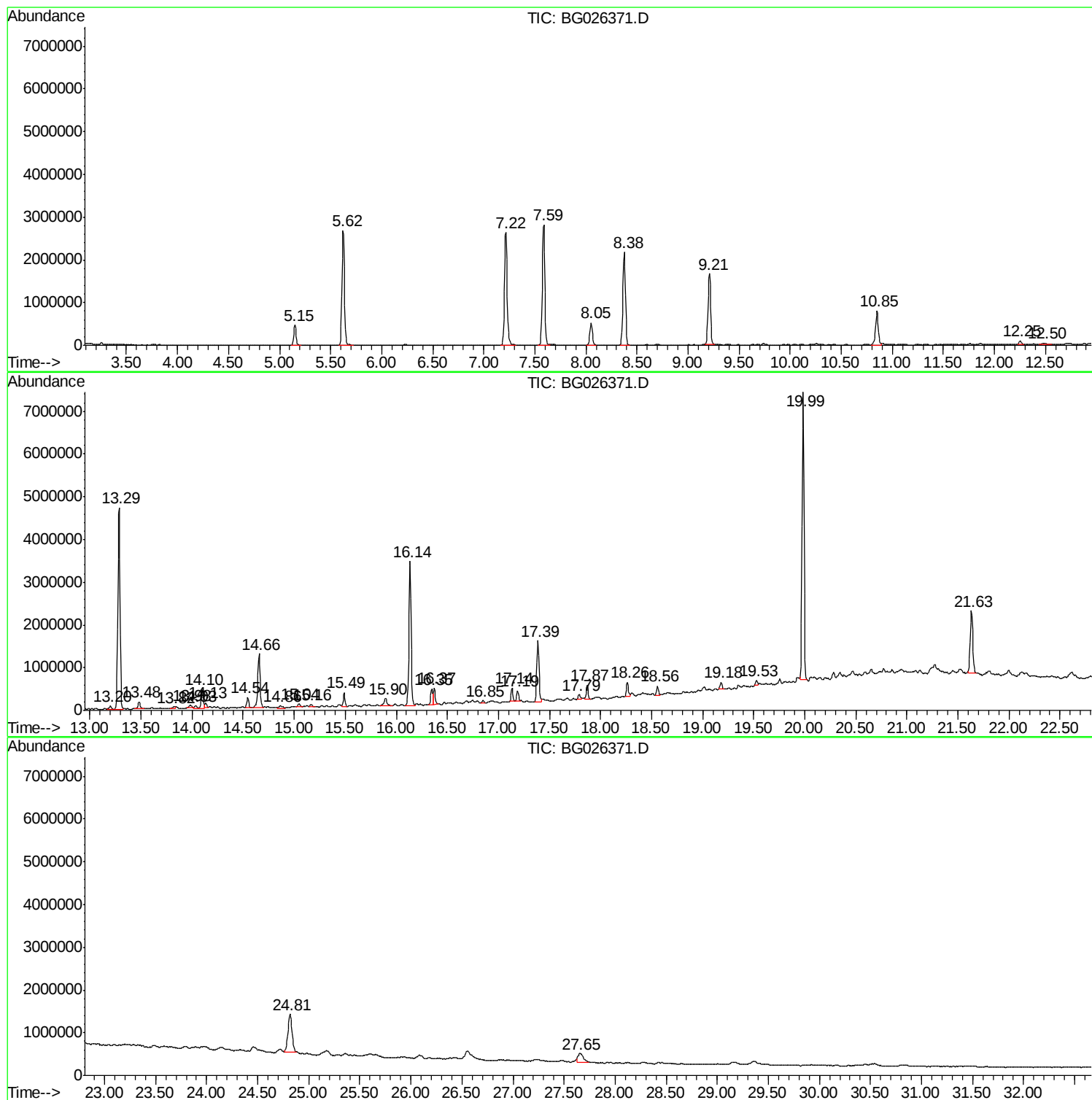
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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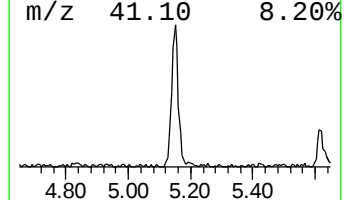
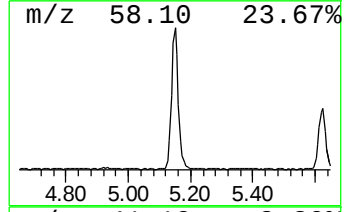
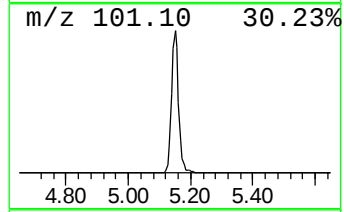
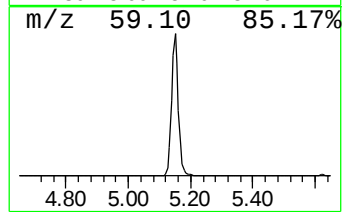
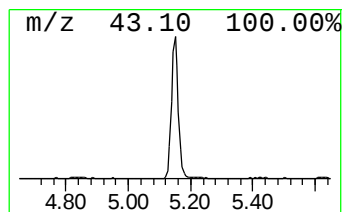
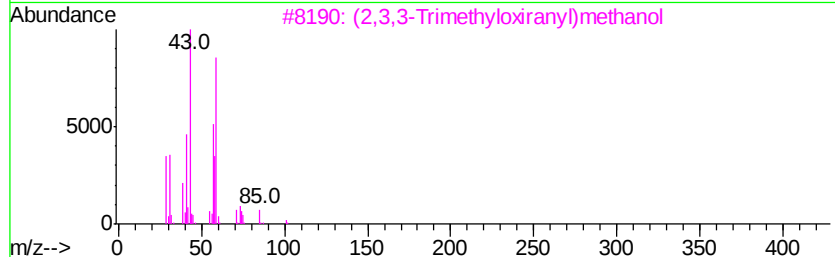
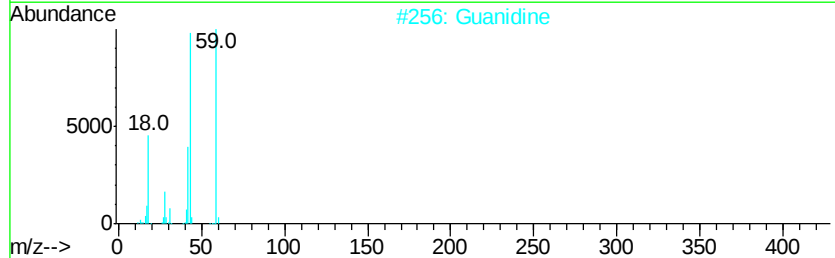
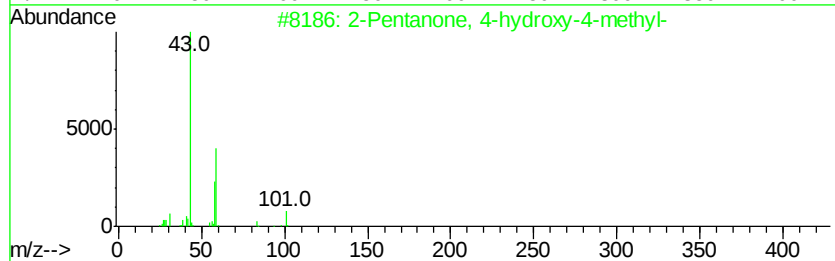
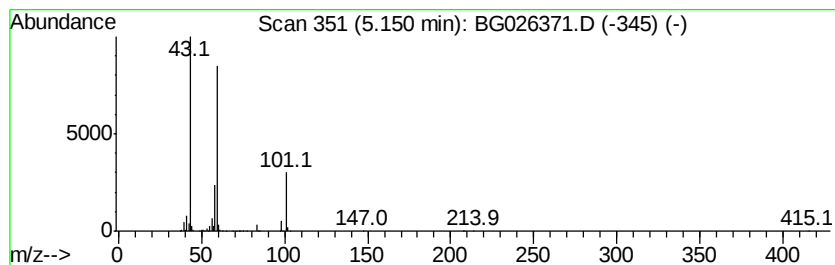
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.98 ng	719414	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Guanidine	59	CH5N3	000113-00-8	47
3			(2,3,3-Trimethyloxiran-yl)methanol	116	C6H12O2	1000306-64-7	38
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	27
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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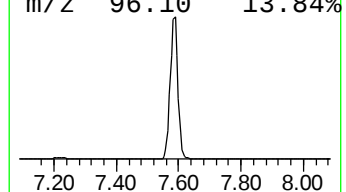
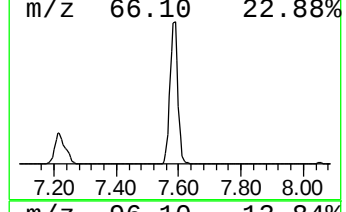
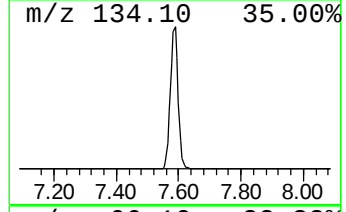
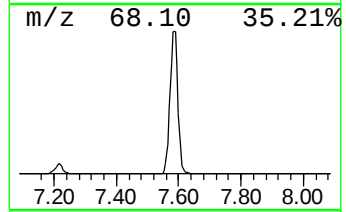
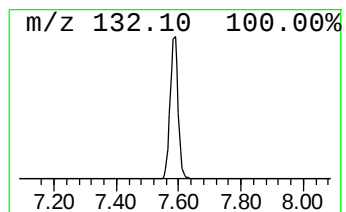
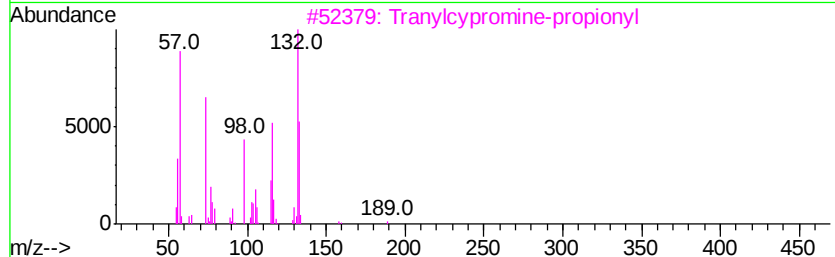
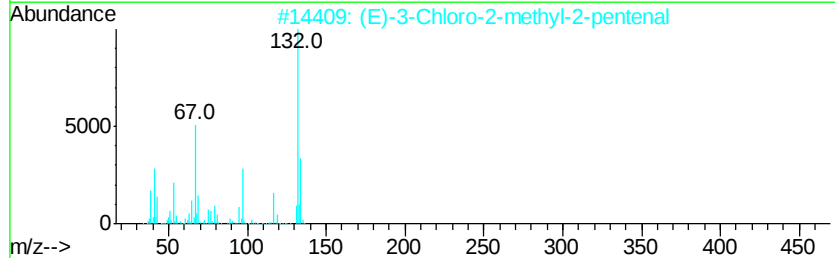
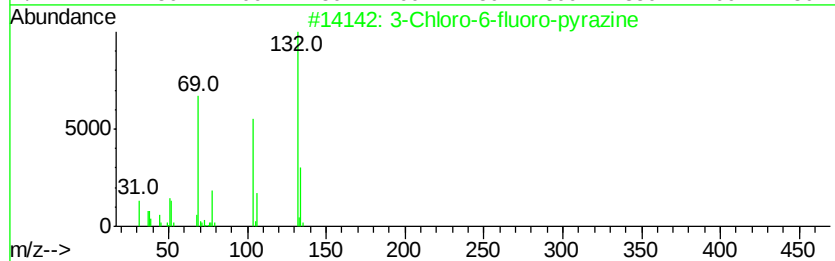
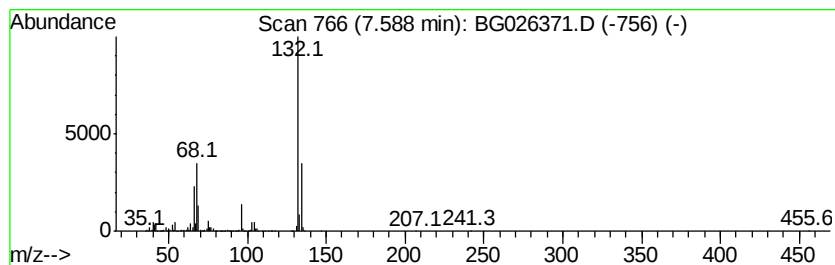
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	110.58 ng	4976860	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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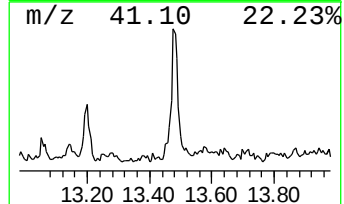
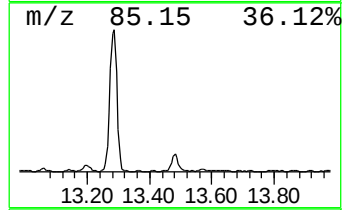
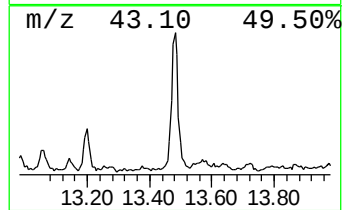
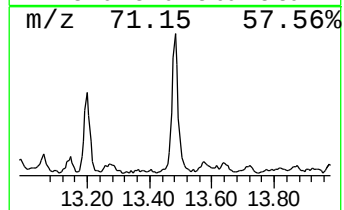
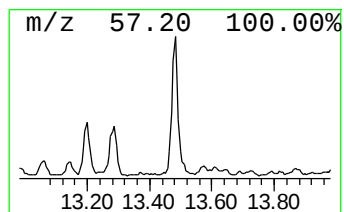
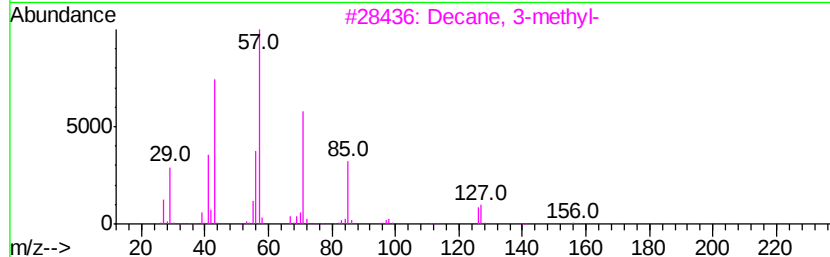
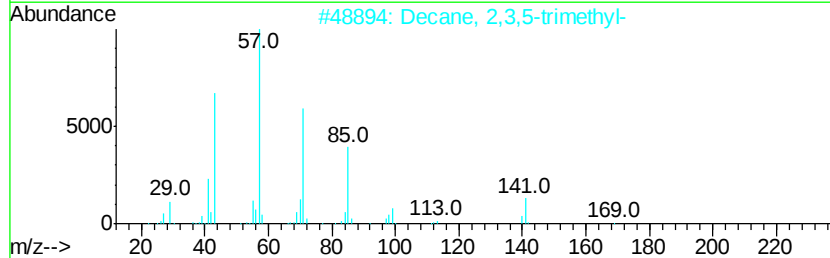
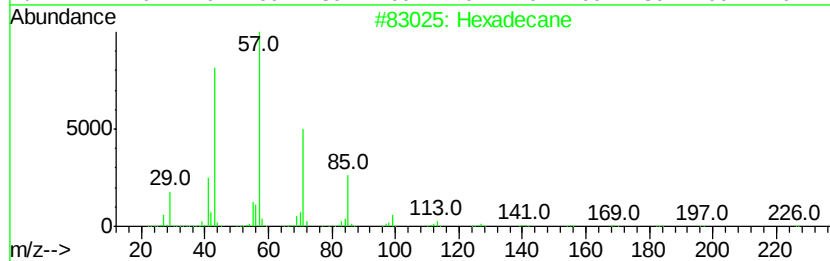
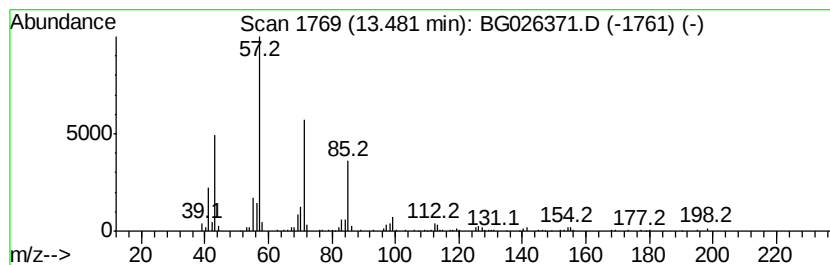
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.64 ng	279118	Acenaphthene-d10	14.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
3			Decane, 3-methyl-	156	C11H24	013151-34-3	64
4			Bacchotricuneatin c	342	C20H22O5	066563-30-2	58
5			Tetradecane	198	C14H30	000629-59-4	58



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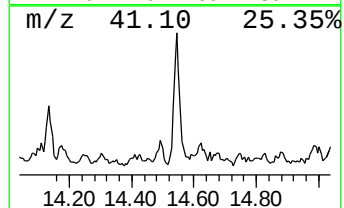
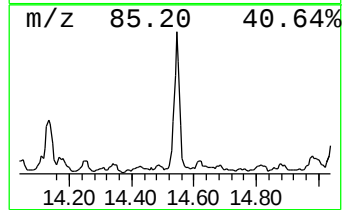
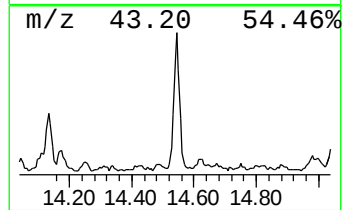
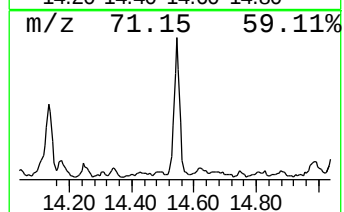
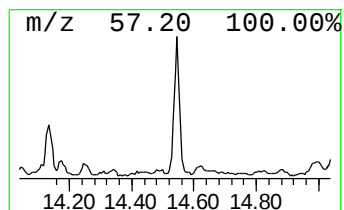
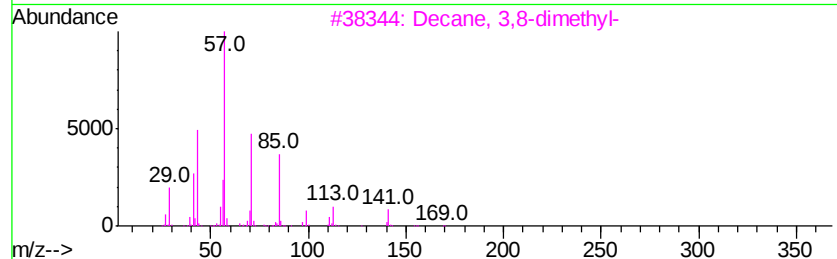
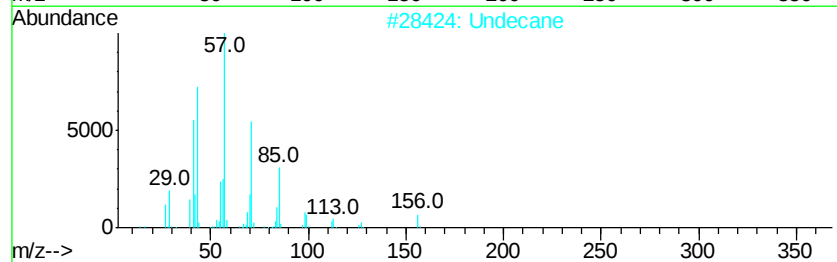
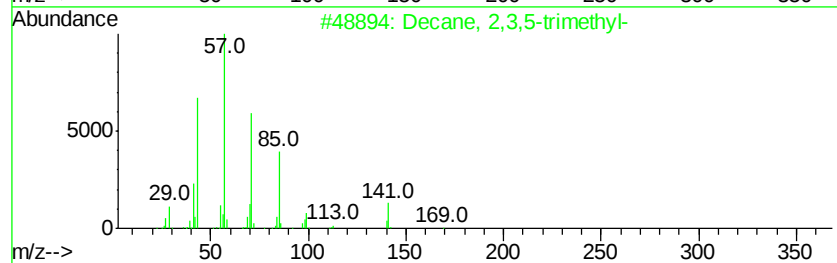
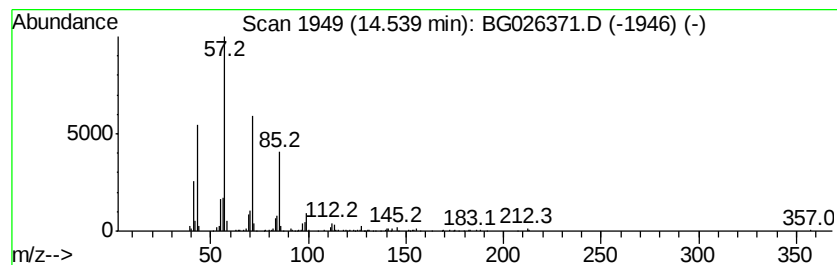
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Decane, 2,3,5-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.54	3.07 ng	323995	Acenaphthene-d10		14.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
2			Undecane	156	C11H24	001120-21-4	72
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
4			Bacchotricuneatin c	342	C20H22O5	066563-30-2	68
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64



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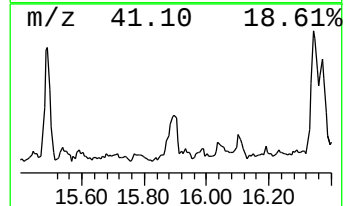
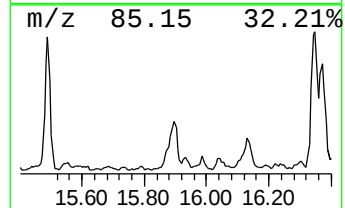
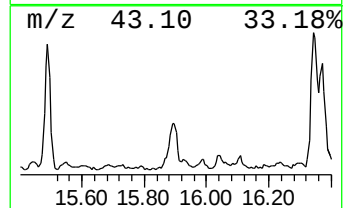
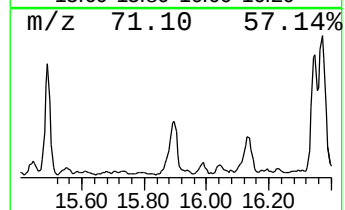
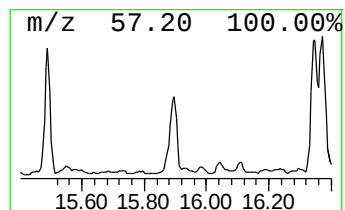
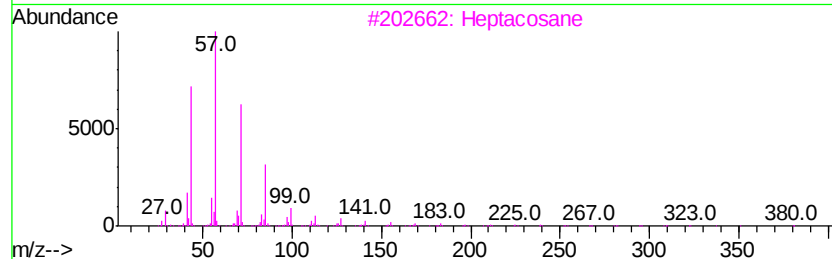
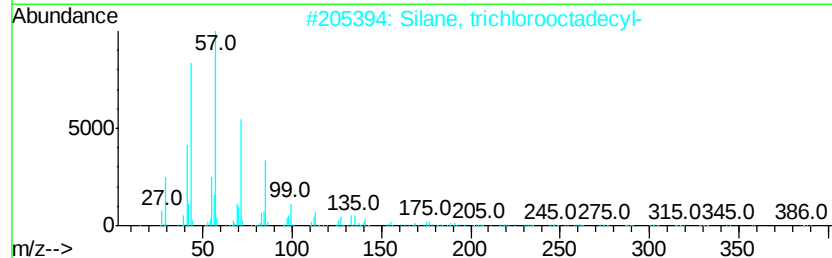
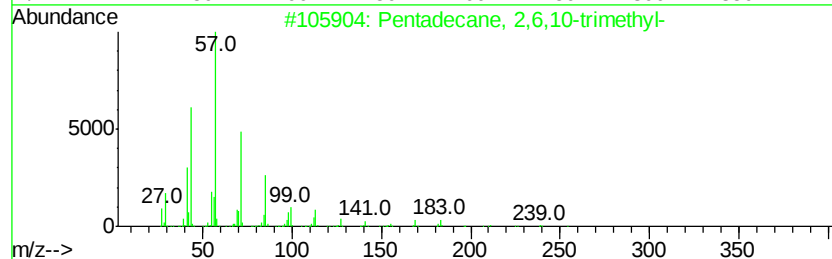
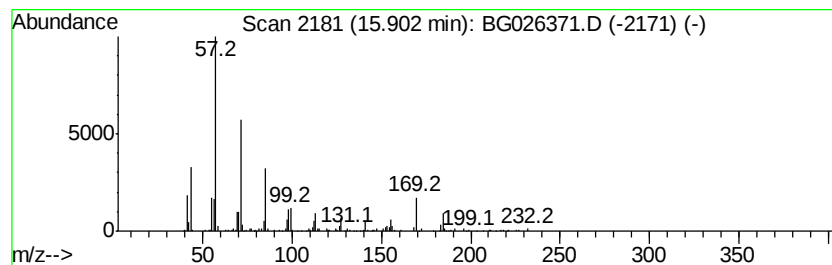
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentadecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.50 ng	369553	Acenaphthene-d10	14.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	87
2		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72
3		Heptacosane	380	C27H56	000593-49-7	64
4		Hexadecane, 7-methyl-	240	C17H36	026730-20-1	64
5		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	59



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
Data File : BG026371.D
Acq On : 22 Mar 2017 10:43
Operator : SJ/MA
Sample : I2304-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SPA-B6(0-5)

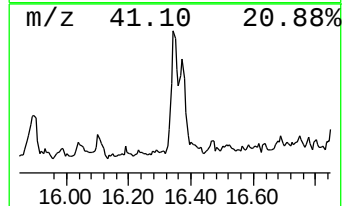
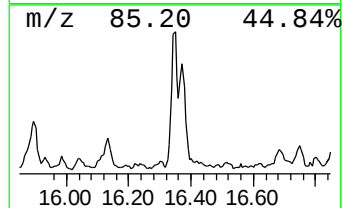
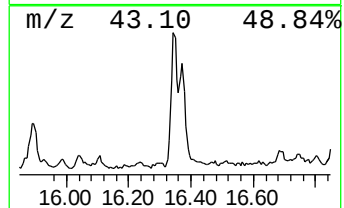
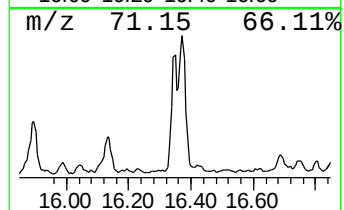
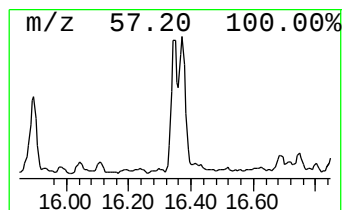
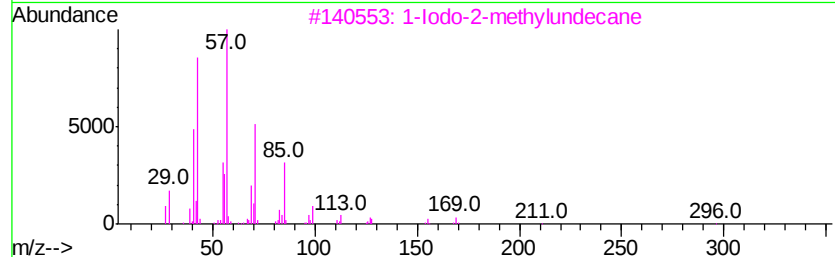
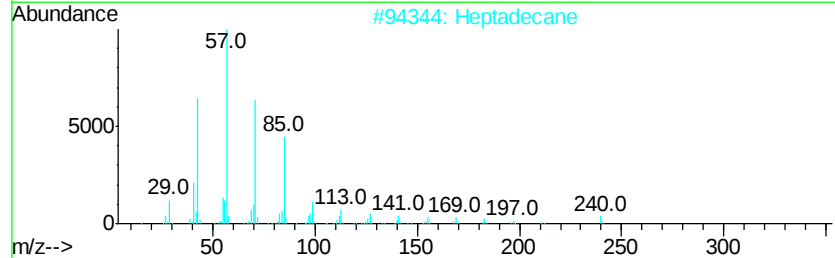
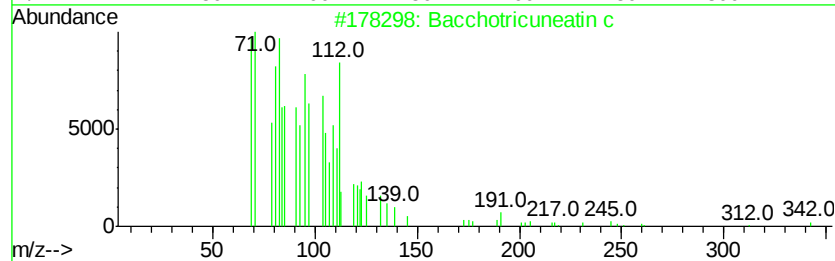
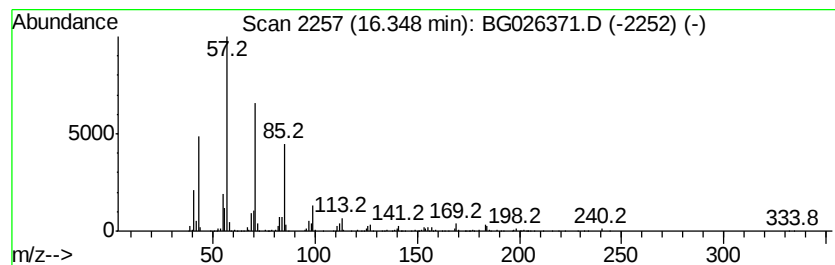
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	4.90 ng	542773	Phenanthrene-d10	17.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bacchotricuneatin c	342	C20H22O5	066563-30-2	99
2		Heptadecane	240	C17H36	000629-78-7	96
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
4		Pentadecane	212	C15H32	000629-62-9	87
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
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Acq On : 22 Mar 2017 10:43
Operator : SJ/MA
Sample : I2304-11
Misc :
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Instrument :
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ClientSampleId :
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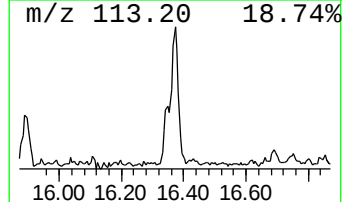
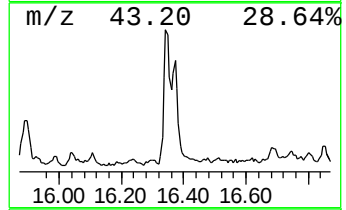
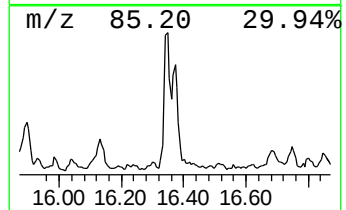
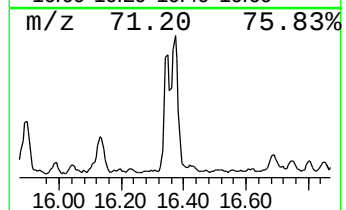
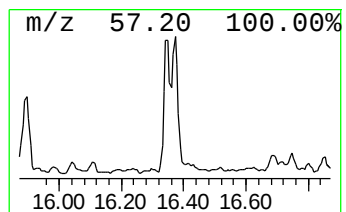
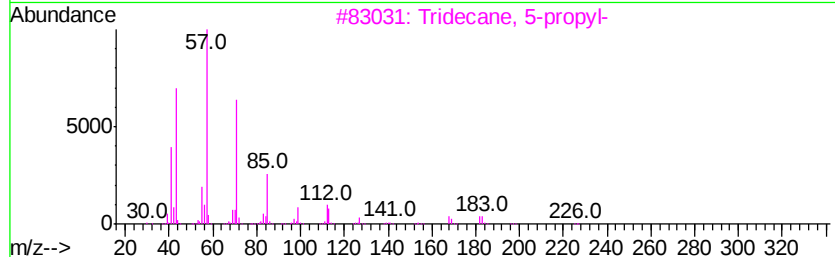
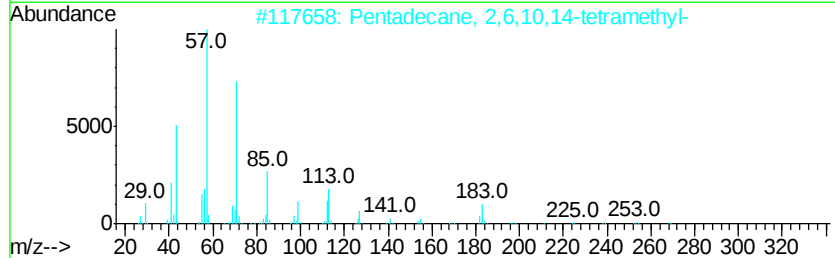
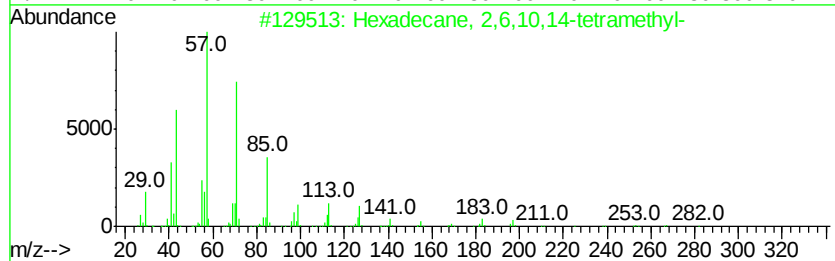
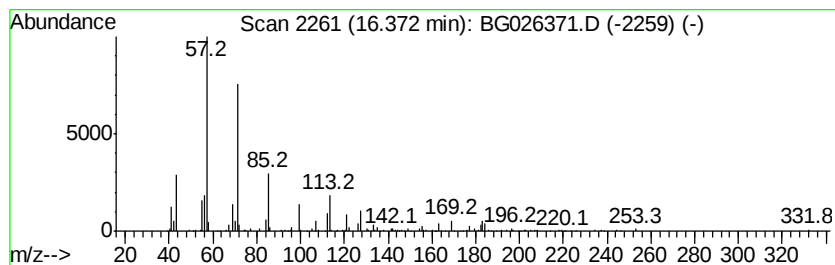
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	4.06 ng	449618	Phenanthrene-d10	17.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
3		Tridecane, 5-propyl-	226	C16H34	055045-11-9	72
4		Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	72
5		Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
Data File : BG026371.D
Acq On : 22 Mar 2017 10:43
Operator : SJ/MA
Sample : I2304-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

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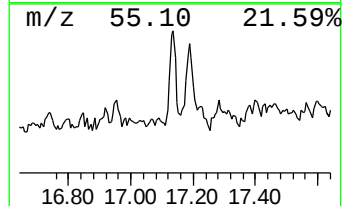
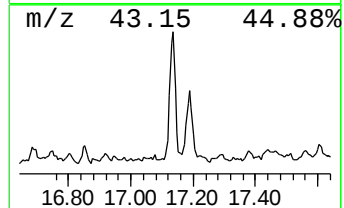
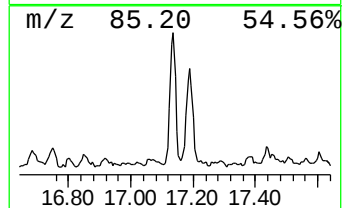
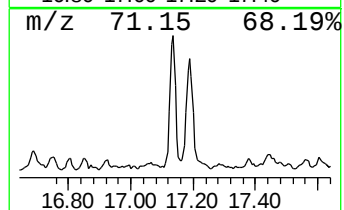
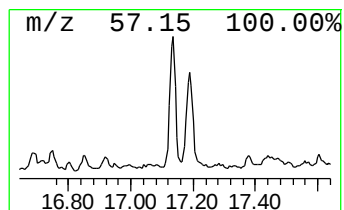
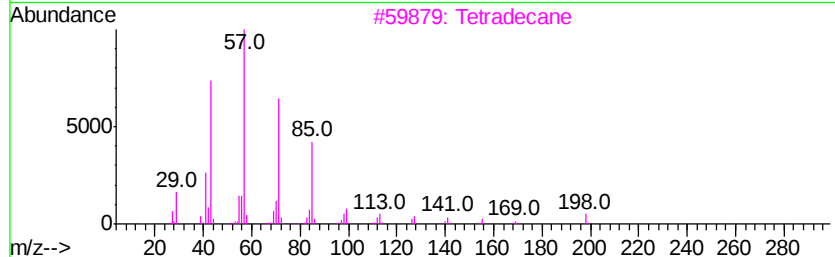
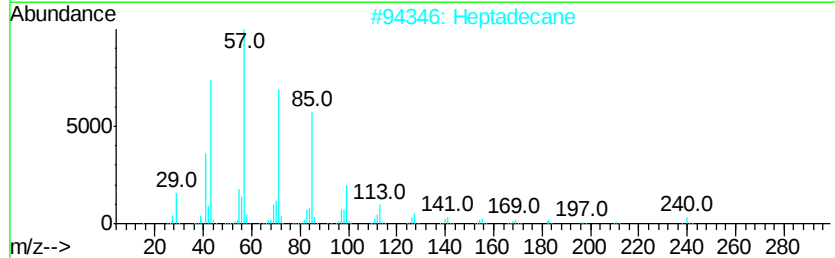
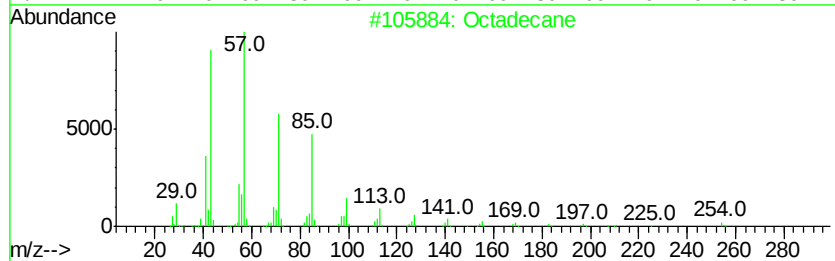
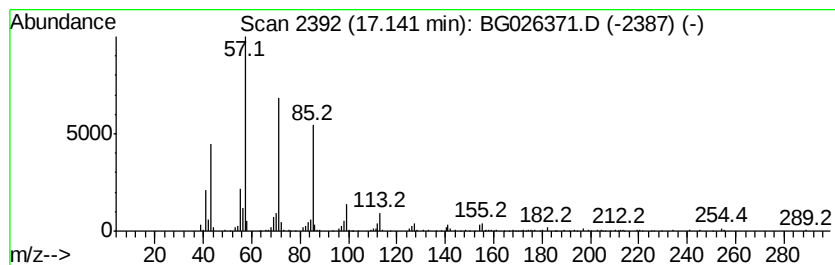
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	3.33 ng	368783	Phenanthrene-d10	17.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			Tetradecane	198	C14H30	000629-59-4	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Hexadecane	226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
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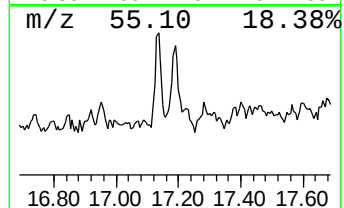
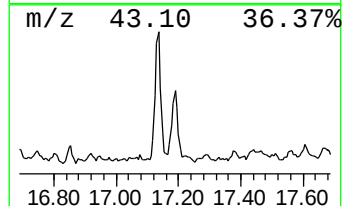
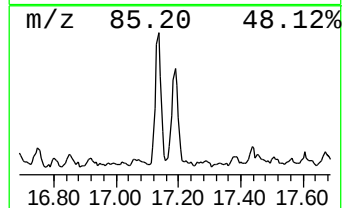
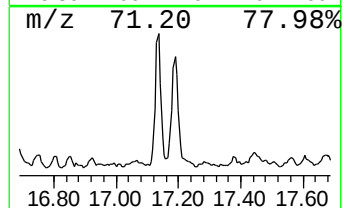
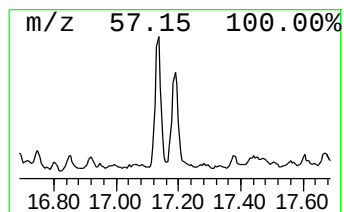
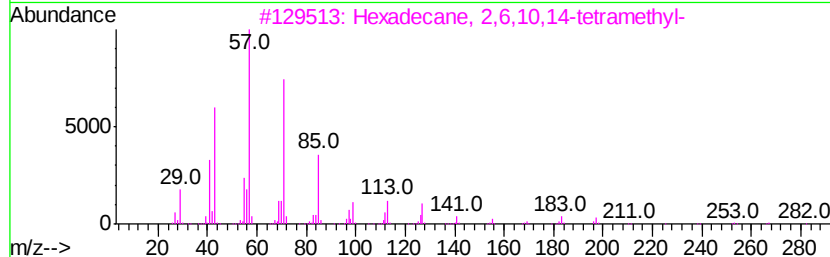
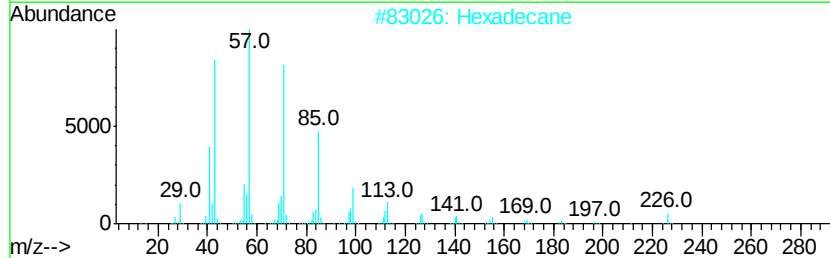
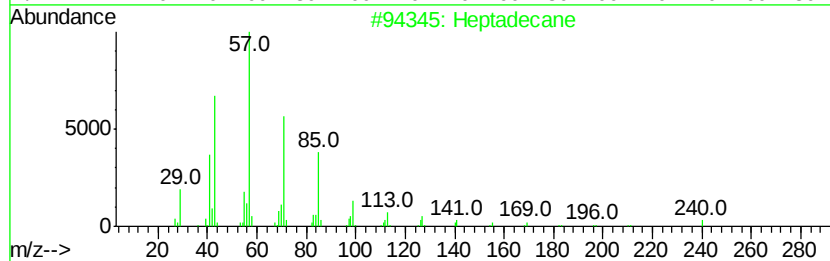
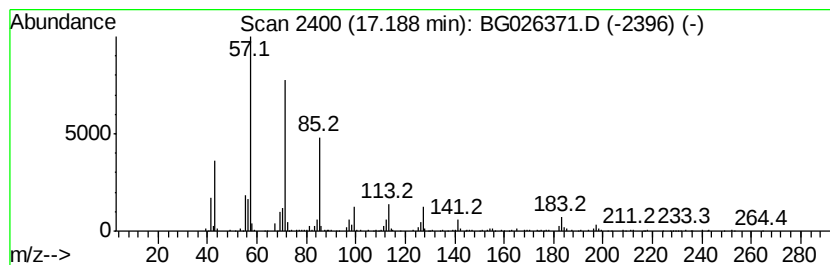
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.			
17.19	2.99 ng	330733	Phenanthrene-d10	17.39			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	86
2			Hexadecane	226	C16H34	000544-76-3	86
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4			Tetradecane	198	C14H30	000629-59-4	80
5			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	80



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
Data File : BG026371.D
Acq On : 22 Mar 2017 10:43
Operator : SJ/MA
Sample : I2304-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

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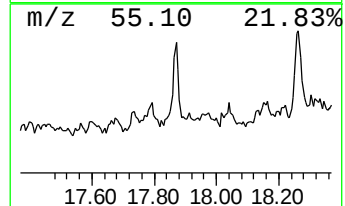
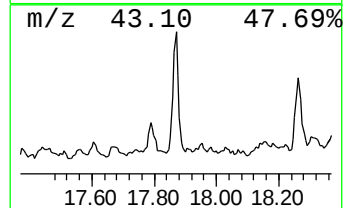
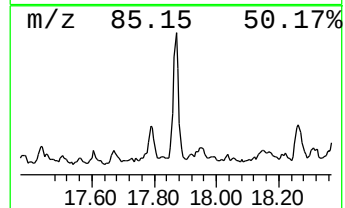
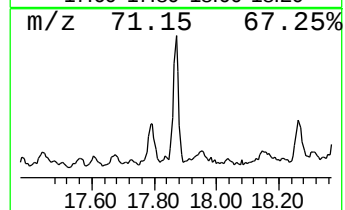
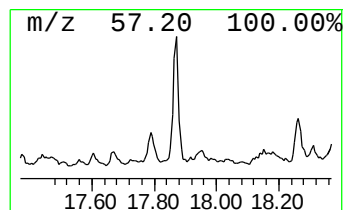
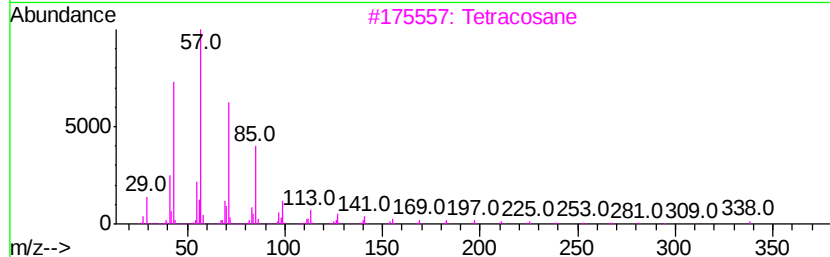
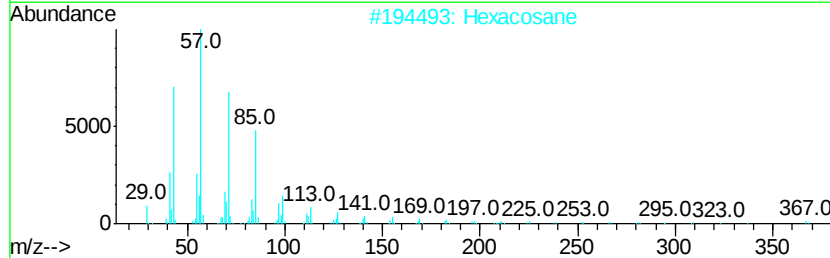
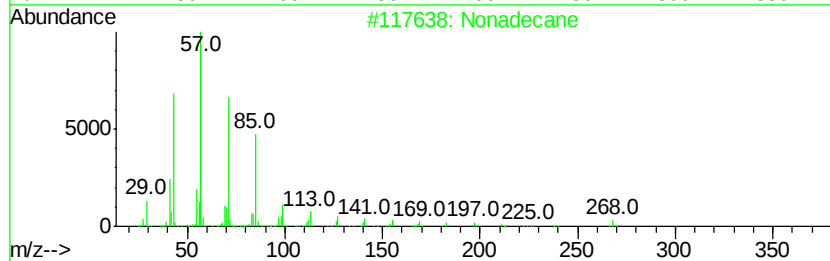
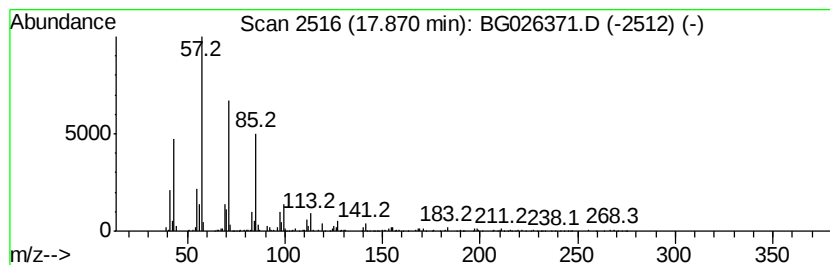
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	3.79 ng	420149	Phenanthrene-d10	17.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
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Sample : I2304-11
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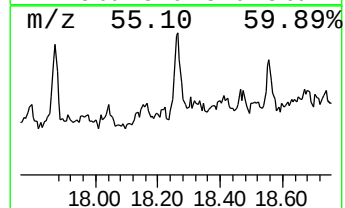
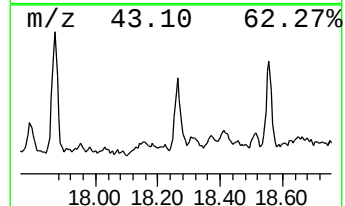
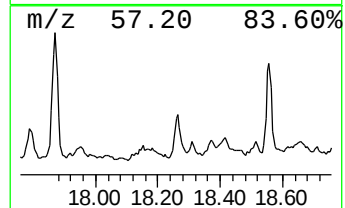
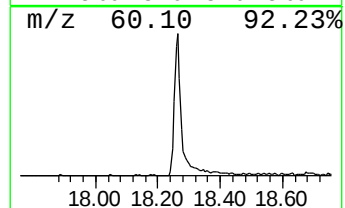
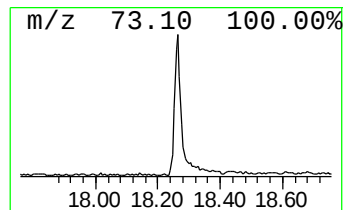
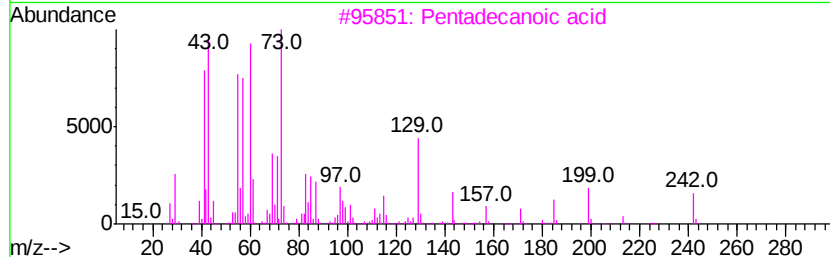
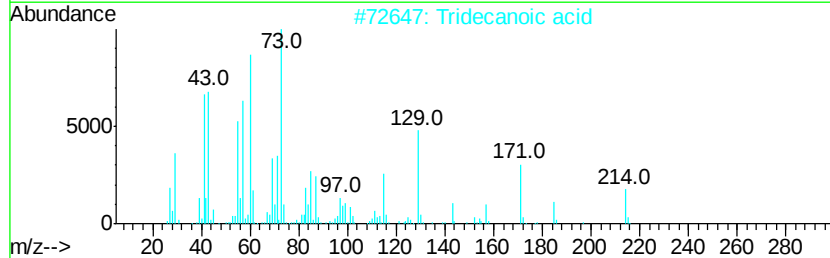
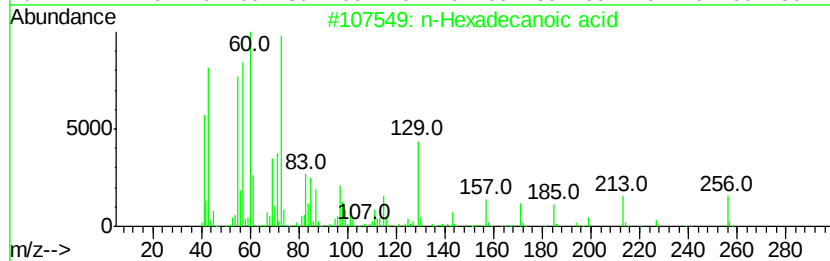
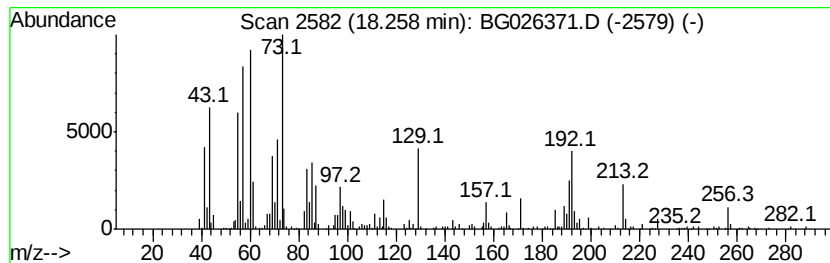
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.26	4.24 ng	469738	Phenanthrene-d10	17.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032217\
Data File : BG026371.D
Acq On : 22 Mar 2017 10:43
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Sample : I2304-11
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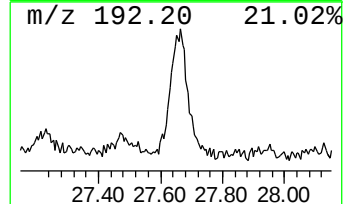
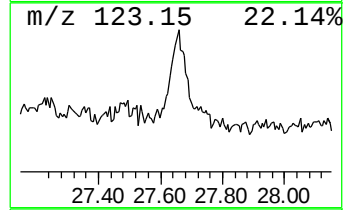
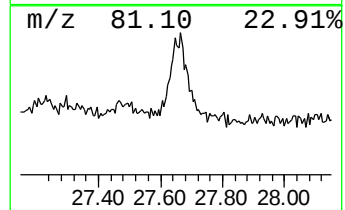
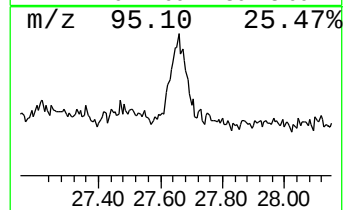
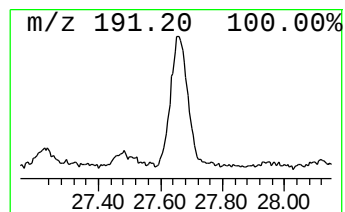
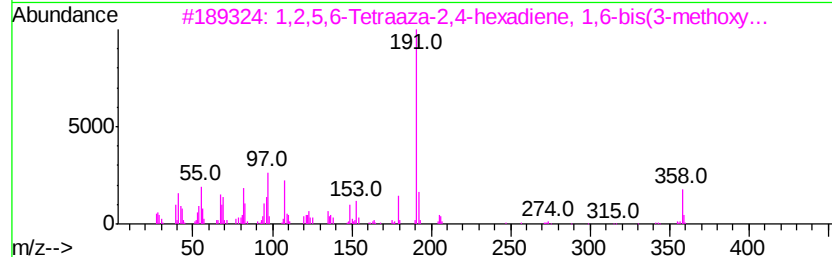
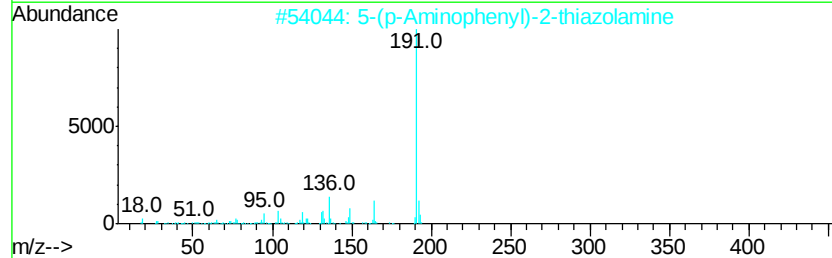
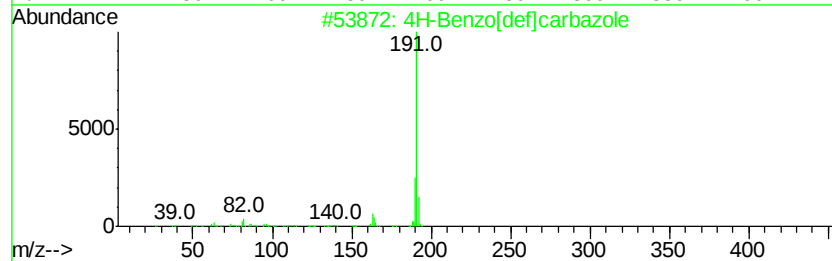
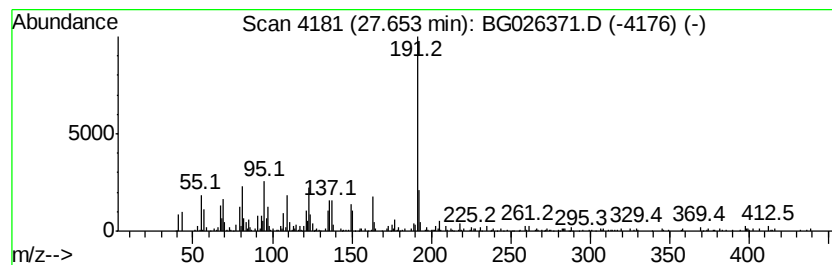
Instrument :
BNA_G
ClientSampleId :
SPA-B6(0-5)

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 4H-Benzo[def]carbazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
27.65	5.81 ng	726630	Perylene-d12	24.81		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Benzo[def]carbazole	191	C14H9N	000203-65-6	50
2		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	47
3		1,2,5,6-Tetraaza-2,4-hexadiene, ...	358	C20H30N4O2	1000188-27-0	47
4		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	45
5		4-Fluoro-3-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-68-8	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032217\
Data File : BG026371.D
Acq On : 22 Mar 2017 10:43
Operator : SJ/MA
Sample : I2304-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SPA-B6(0-5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	16.0	ng	719414	1	8.05	900144	20.0
unknown7.59	7.59	110.6	ng	4976860	1	8.05	900144	20.0
Hexadecane	13.48	2.6	ng	279118	3	14.66	2112600	20.0
Decane, 2,3,5-tri...	14.54	3.1	ng	323995	3	14.66	2112600	20.0
Pentadecane, 2,6,...	15.90	3.5	ng	369553	3	14.66	2112600	20.0
Bacchotricuneatin c	16.35	4.9	ng	542773	4	17.39	2215190	20.0
Hexadecane, 2,6,1...	16.37	4.1	ng	449618	4	17.39	2215190	20.0
Octadecane	17.14	3.3	ng	368783	4	17.39	2215190	20.0
Heptadecane	17.19	3.0	ng	330733	4	17.39	2215190	20.0
Nonadecane	17.87	3.8	ng	420149	4	17.39	2215190	20.0
n-Hexadecanoic acid	18.26	4.2	ng	469738	4	17.39	2215190	20.0
4H-Benzo[def]carb...	27.65	5.8	ng	726630	6	24.81	2500730	20.0