

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061316\
 Data File : BG022331.D
 Acq On : 13 Jun 2016 19:37
 Operator : UM/SJ
 Sample : H3474-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S6-B3(0-7)C

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-BG060616.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.939	11	17	38	rVB	808278	1453810	100.00%	11.034%
2	5.154	387	394	405	rVB	30148	60704	4.18%	0.461%
3	5.636	469	476	491	rBV	365501	735618	50.60%	5.583%
4	7.258	743	752	770	rBV	410504	835207	57.45%	6.339%
5	7.622	806	814	824	rBV	457087	895624	61.61%	6.797%
6	8.092	887	894	901	rBV	115768	224043	15.41%	1.700%
7	8.415	939	949	958	rBV	362393	714482	49.15%	5.423%
8	9.261	1086	1093	1104	rBV	242712	501121	34.47%	3.803%
9	10.912	1366	1374	1389	rVB	178487	368037	25.32%	2.793%
10	13.345	1779	1788	1803	rBV	819808	1397477	96.13%	10.606%
11	13.521	1812	1818	1824	rBV3	9061	17983	1.24%	0.136%
12	14.050	1902	1908	1912	rBV4	8574	15915	1.09%	0.121%
13	14.167	1919	1928	1935	rBV	88948	158982	10.94%	1.207%
14	14.590	1996	2000	2008	rVB	23964	36241	2.49%	0.275%
15	14.726	2016	2023	2030	rBV2	277761	484180	33.30%	3.675%
16	14.790	2030	2034	2042	rVB	18772	32100	2.21%	0.244%
17	15.125	2084	2091	2099	rVB3	10086	24784	1.70%	0.188%
18	15.201	2099	2104	2110	rBV8	9013	18111	1.25%	0.137%
19	15.542	2157	2162	2166	rVB	36102	53179	3.66%	0.404%
20	15.771	2195	2201	2210	rVB2	18372	37041	2.55%	0.281%
21	15.942	2223	2230	2235	rBV3	14468	29081	2.00%	0.221%
22	16.212	2270	2276	2285	rVV	383504	664179	45.69%	5.041%
23	16.400	2303	2308	2318	rBV3	42209	107273	7.38%	0.814%
24	17.193	2438	2443	2447	rBV	32755	49445	3.40%	0.375%
25	17.240	2448	2451	2456	rVB4	14237	22718	1.56%	0.172%
26	17.469	2483	2490	2494	rBV2	290383	510154	35.09%	3.872%
27	17.511	2494	2497	2504	rVV	201235	324976	22.35%	2.466%
28	17.605	2508	2513	2518	rVB	42762	74760	5.14%	0.567%
29	17.928	2565	2568	2573	rVB2	23961	31785	2.19%	0.241%
30	18.057	2586	2590	2593	rBV6	9300	15239	1.05%	0.116%
31	18.345	2634	2639	2642	rBV3	24217	42517	2.92%	0.323%
32	18.392	2644	2647	2652	rVB3	33106	49670	3.42%	0.377%
33	18.539	2667	2672	2676	rBV2	37615	75544	5.20%	0.573%
34	18.615	2682	2685	2688	rBV	19259	21521	1.48%	0.163%

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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

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.244	2788	2792	2798	rBV2	47345	82314	5.66%	0.625%
36	19.514	2833	2838	2846	rBV	285918	451769	31.07%	3.429%
37	19.737	2872	2876	2882	rBV2	92562	134048	9.22%	1.017%
38	19.878	2896	2900	2906	rVB	231279	364984	25.11%	2.770%
39	20.066	2926	2932	2938	rBV	1021603	1406150	96.72%	10.672%
40	20.348	2977	2980	2987	rVB3	52356	93173	6.41%	0.707%
41	20.771	3050	3052	3056	rBV2	41235	48399	3.33%	0.367%
42	21.741	3211	3217	3223	rBV3	234706	511557	35.19%	3.883%

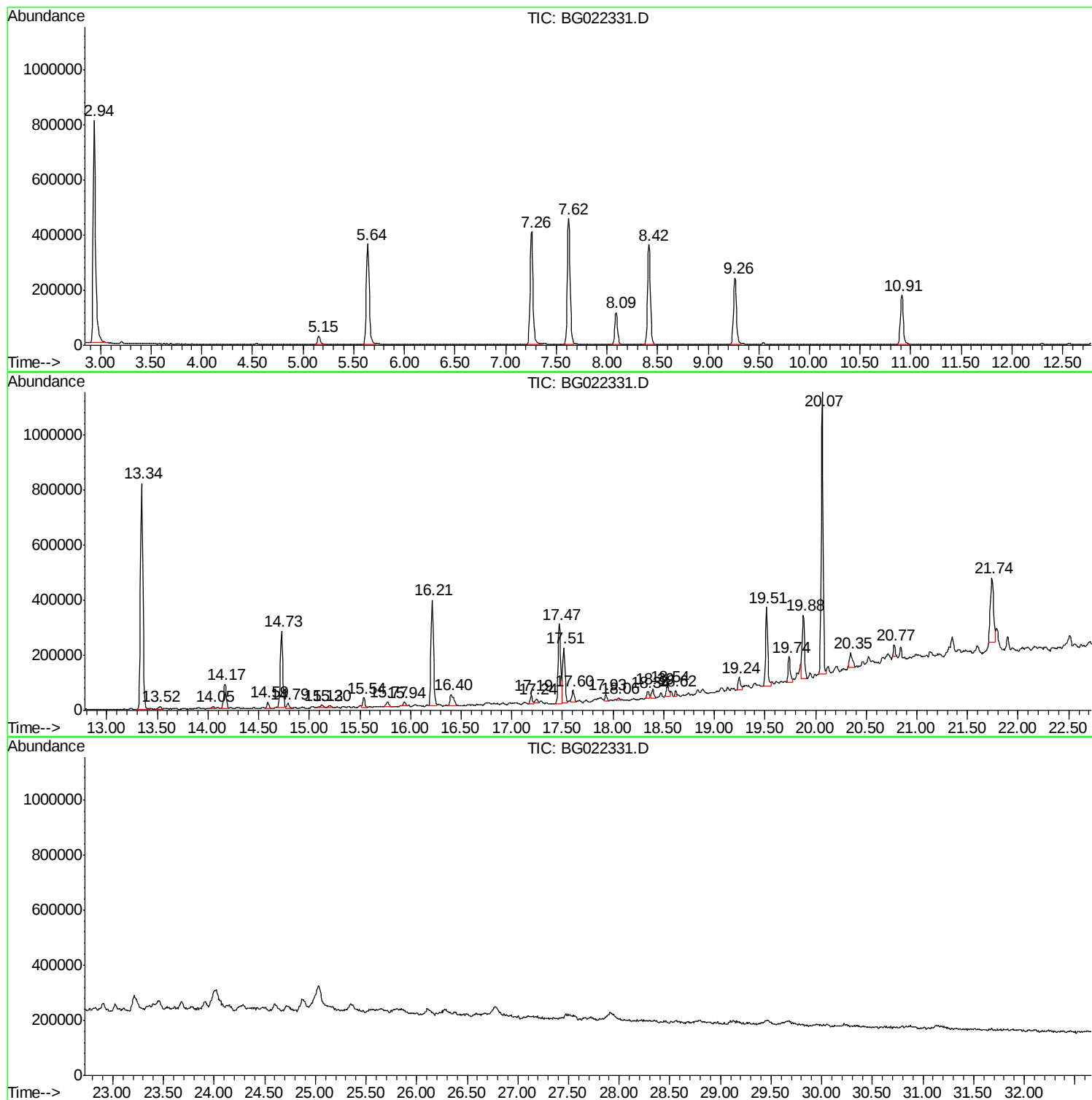
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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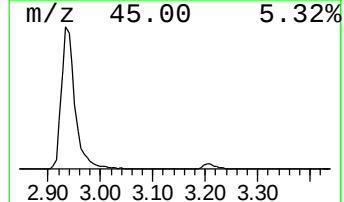
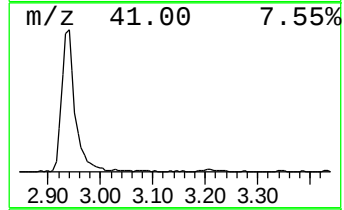
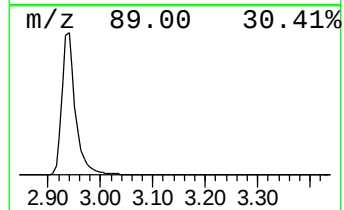
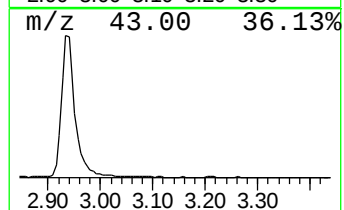
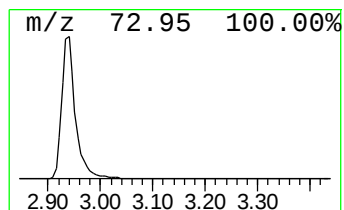
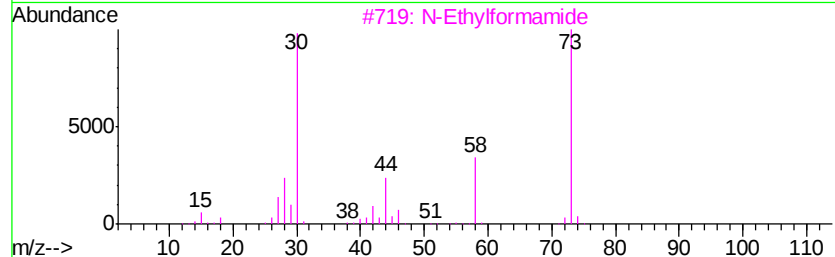
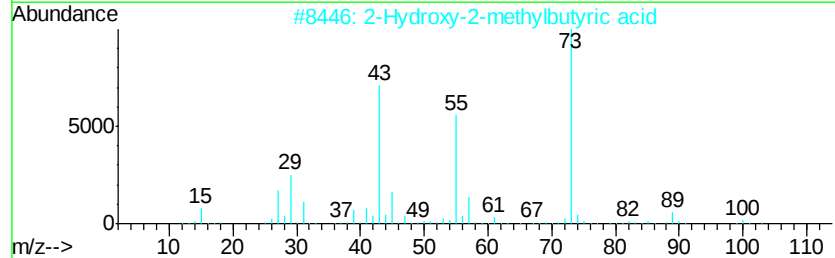
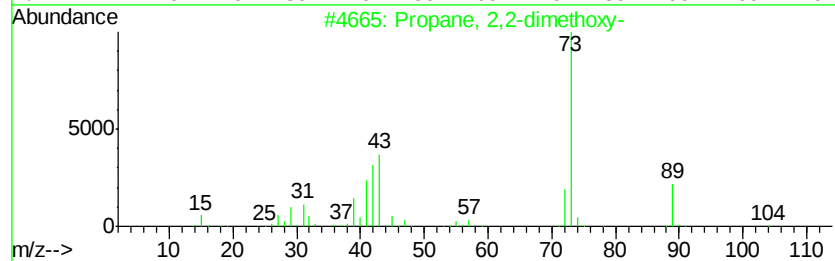
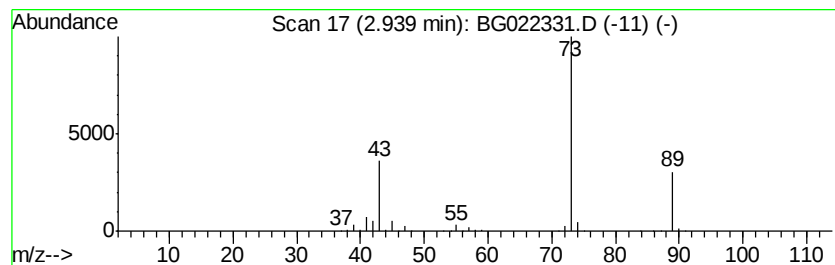
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	129.78 ng	1453810	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	7
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
5		1,3,5-Trioxane	90	C3H6O3	000110-88-3	4



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Instrument :
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ClientSampleId :
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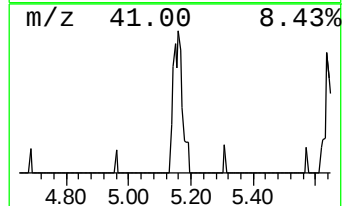
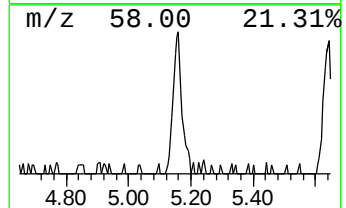
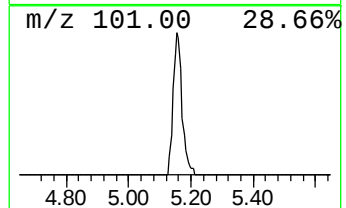
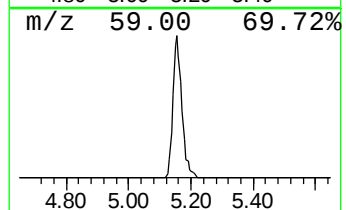
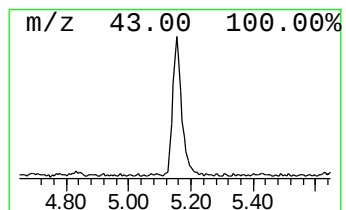
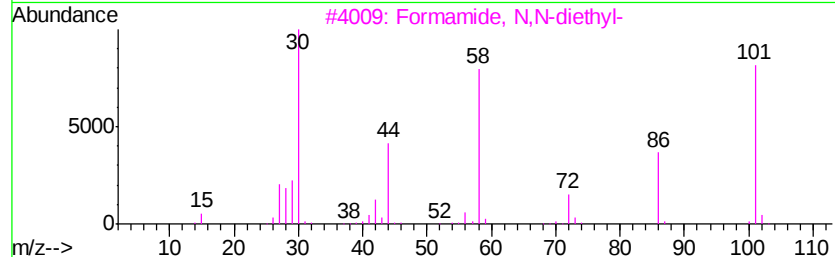
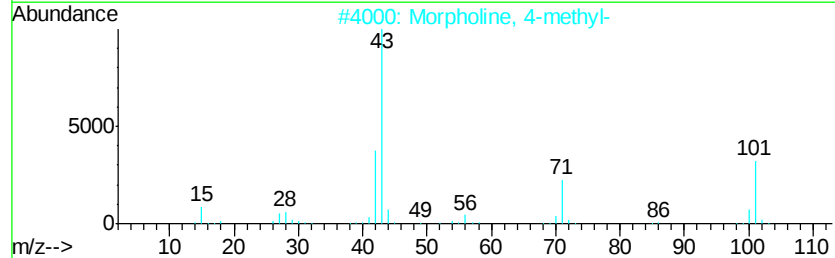
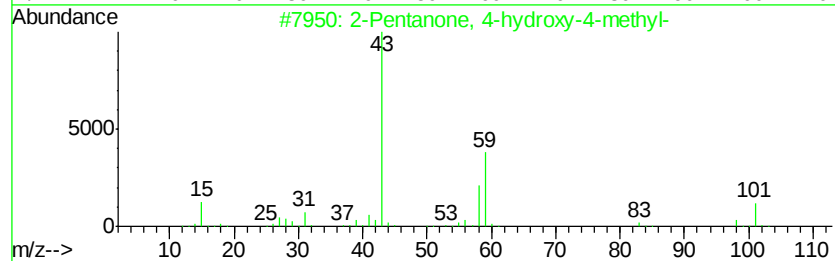
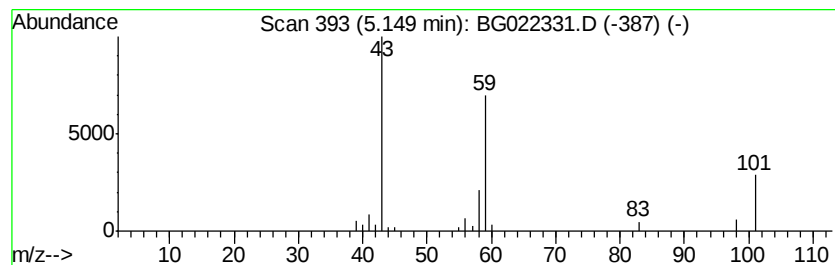
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.42 ng	60704	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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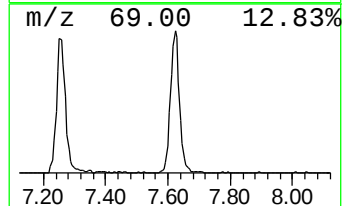
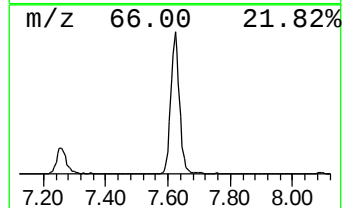
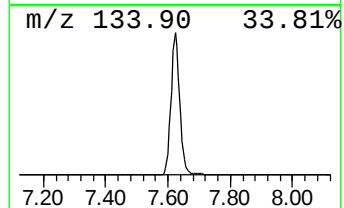
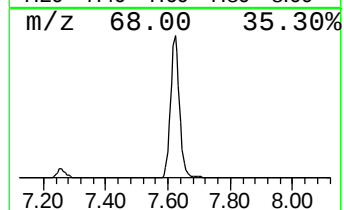
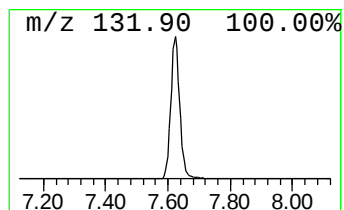
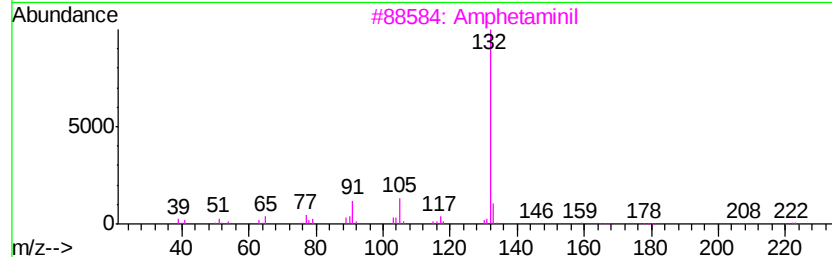
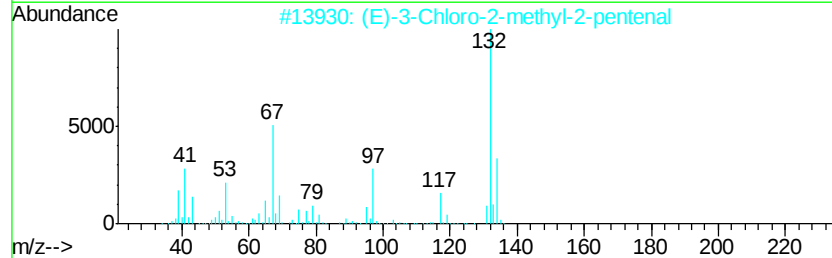
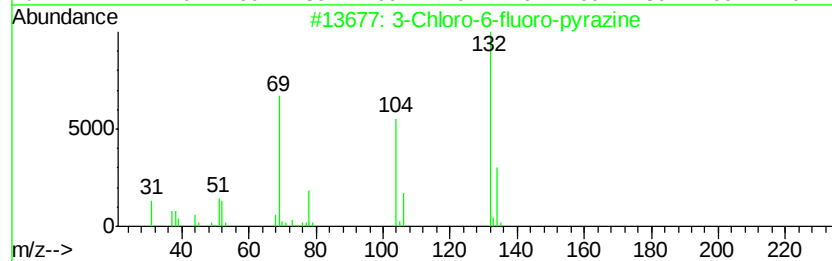
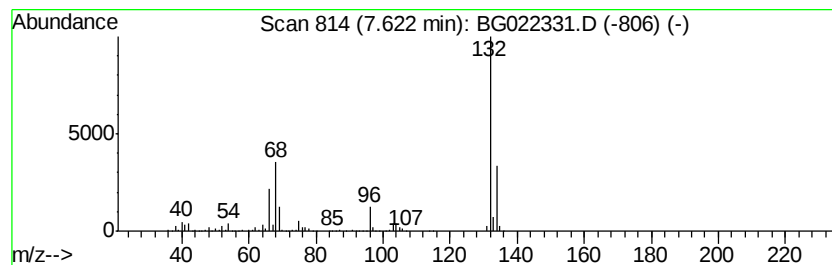
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	79.95 ng	895624	1,4-Dichlorobenzene-d4	8.09

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	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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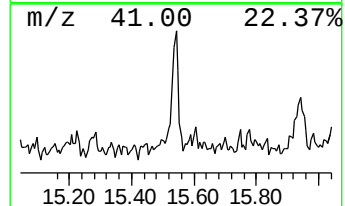
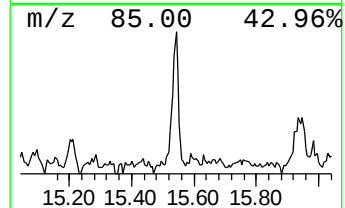
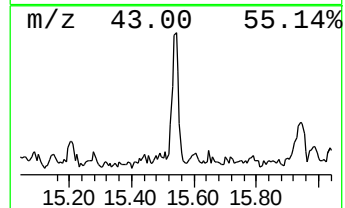
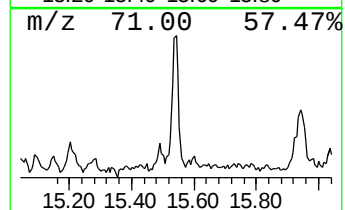
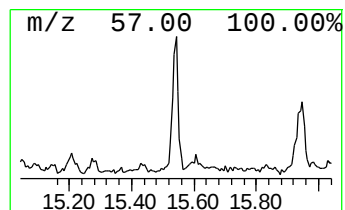
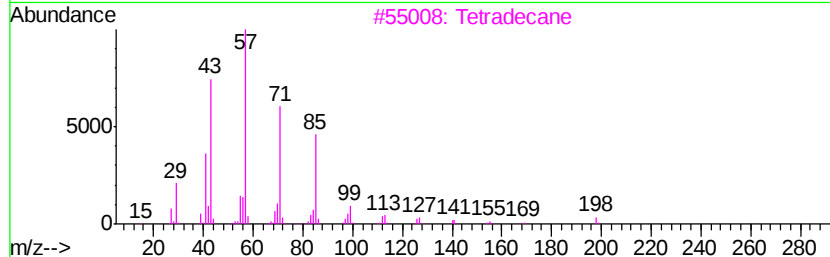
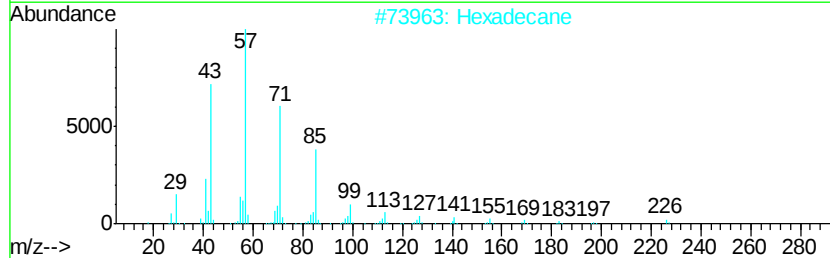
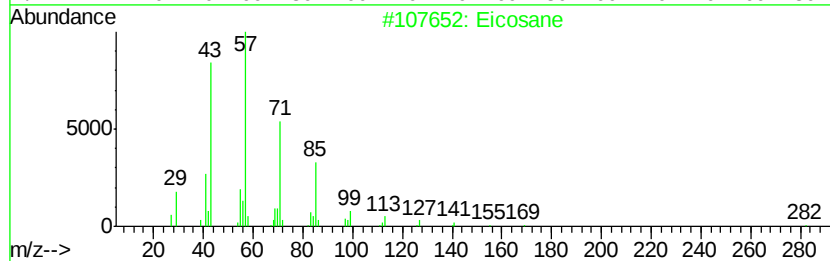
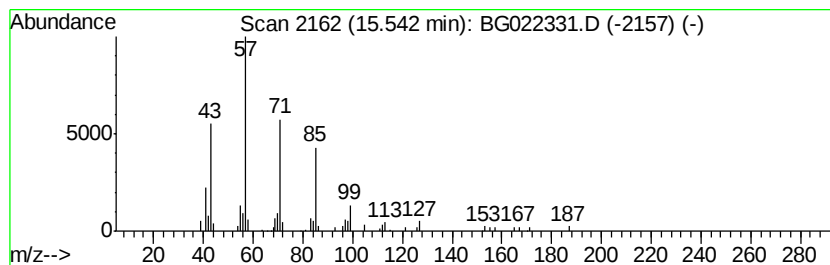
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.20 ng	53179	Acenaphthene-d10	14.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hexadecane		226	C16H34	000544-76-3	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Heneicosane		296	C21H44	000629-94-7	80
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	78



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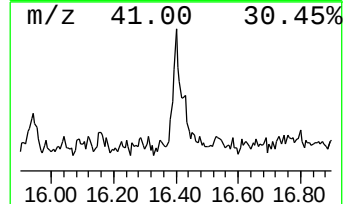
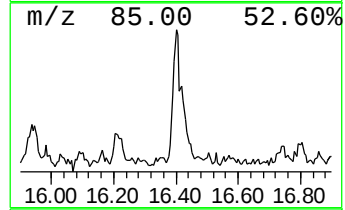
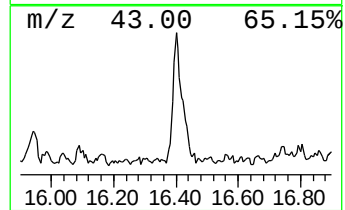
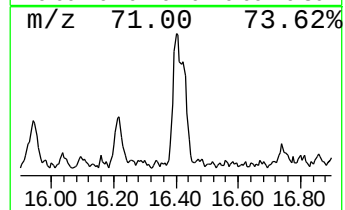
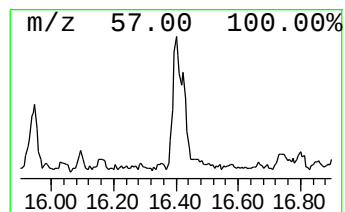
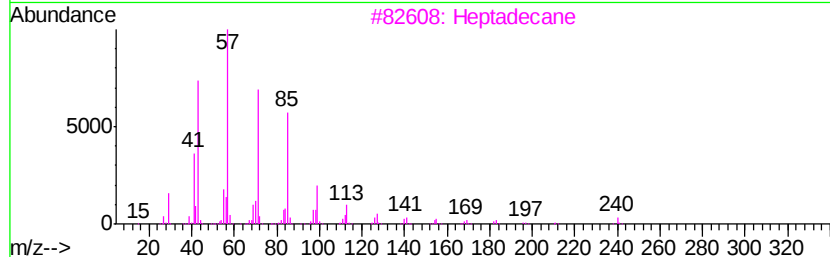
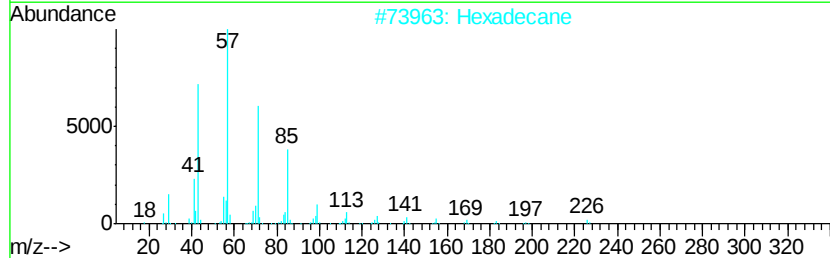
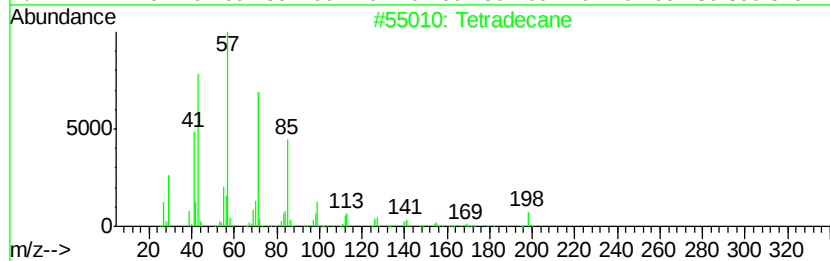
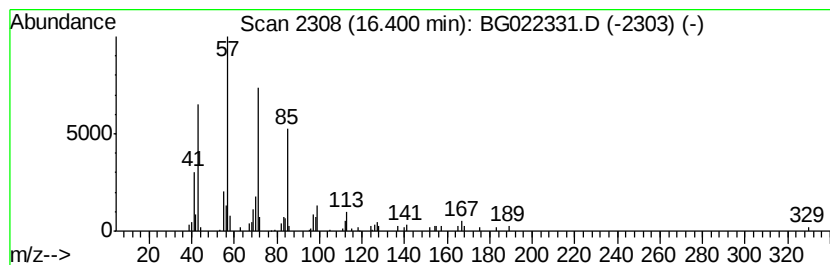
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	4.21 ng	107273	Phenanthrene-d10	17.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	91
2		Hexadecane	226	C16H34	000544-76-3	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		Pentadecane	212	C15H32	000629-62-9	90
5		Nonadecane	268	C19H40	000629-92-5	90



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061316\
Data File : BG022331.D
Acq On : 13 Jun 2016 19:37
Operator : UM/SJ
Sample : H3474-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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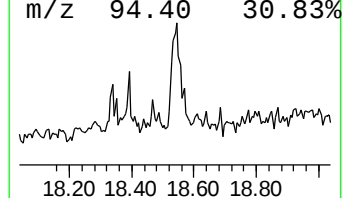
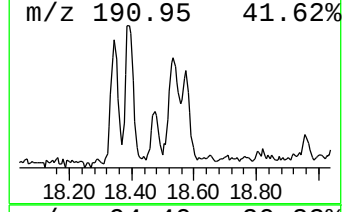
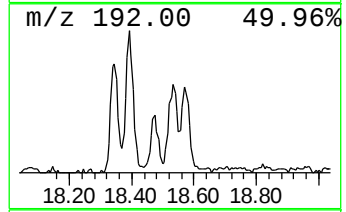
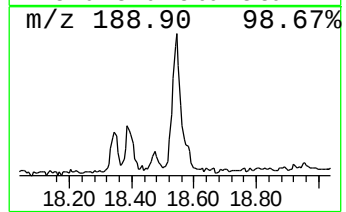
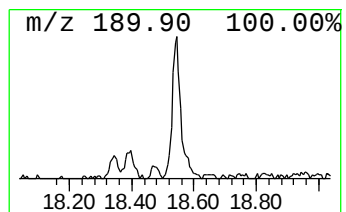
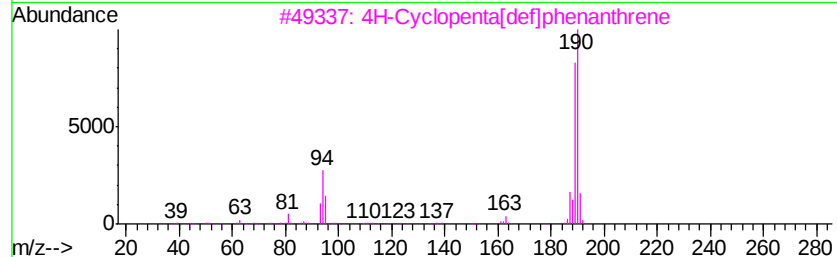
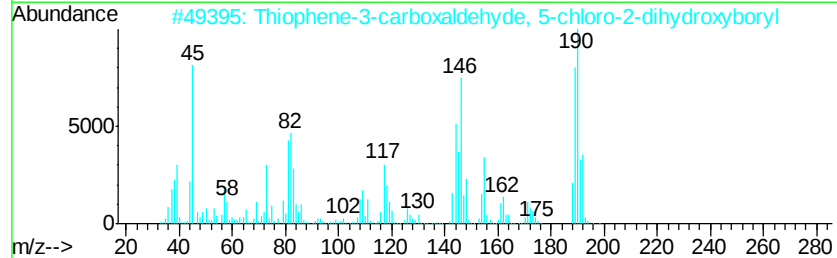
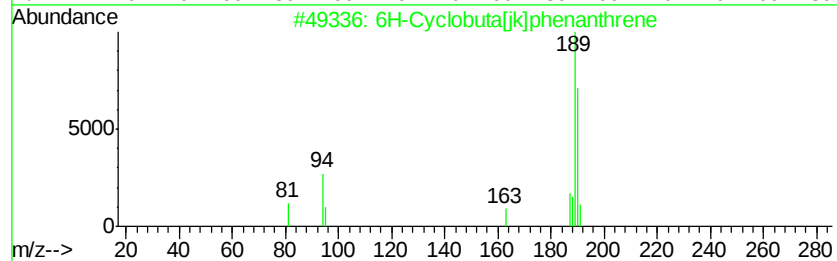
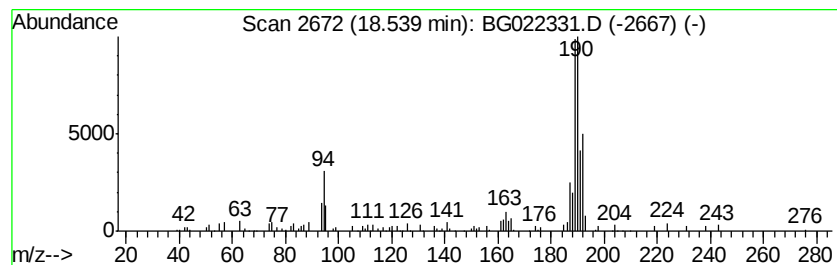
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6H-Cyclobuta[jk]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	2.96 ng	75544	Phenanthrene-d10	17.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	68
2		Thiophene-3-carboxaldehyde, 5-chloro-2-dihydroxyboryl	190	C5H4BClO3S	036155-87-0	64
3		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
4		3H-Indazole-3-carbonitrile, 3-(4-chlorophenyl)-	253	C14H8ClN3	056630-97-8	25
5		5,8-Quinoxalinediol, 2,3-dimethyl-	190	C10H10N2O2	007698-00-2	22



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061316\
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Misc :
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Instrument :
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ClientSampleId :
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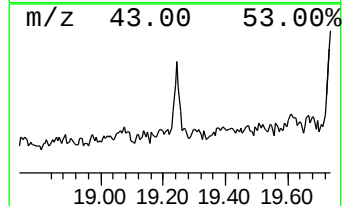
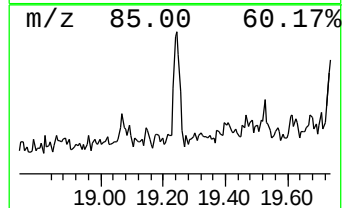
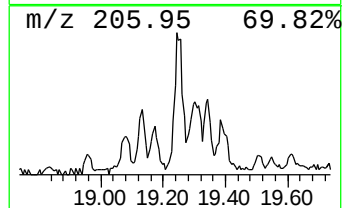
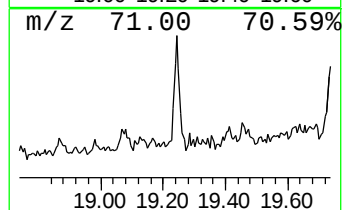
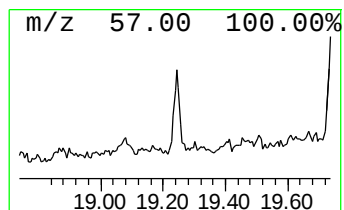
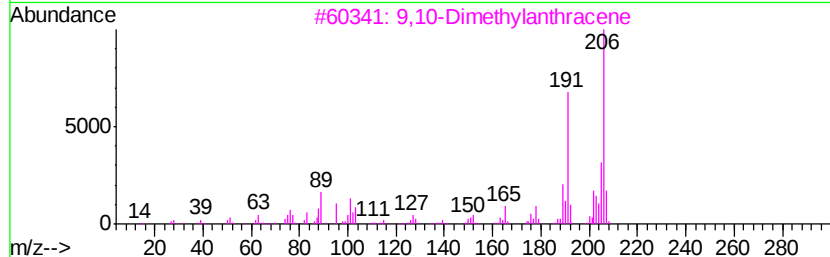
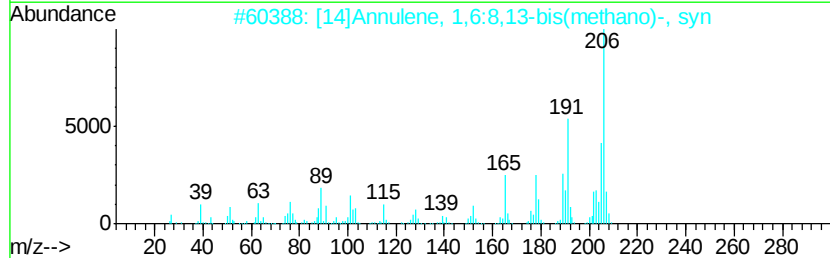
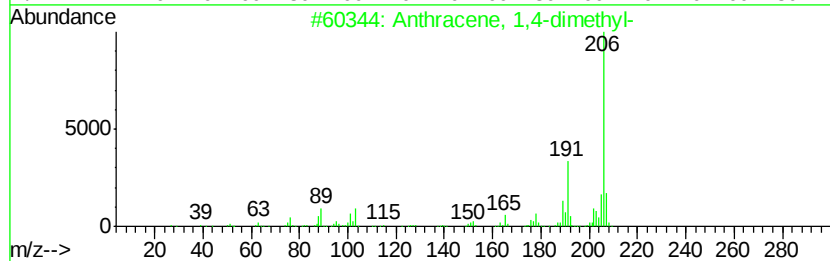
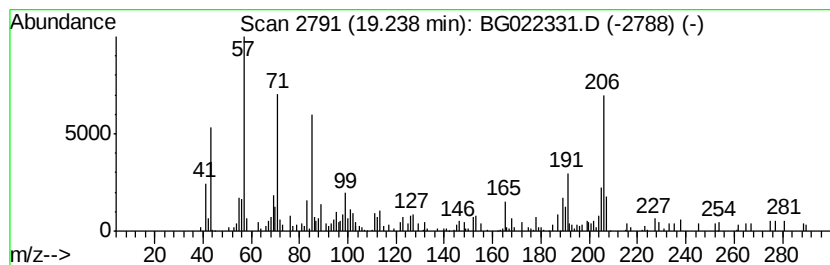
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Anthracene, 1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	3.23 ng	82314	Phenanthrene-d10	17.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	70
2		[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	70
3		9,10-Dimethylanthracene	206	C16H14	000781-43-1	70
4		3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	55
5		1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	55



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061316\
Data File : BG022331.D
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Operator : UM/SJ
Sample : H3474-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B3(0-7)C

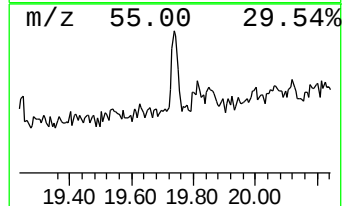
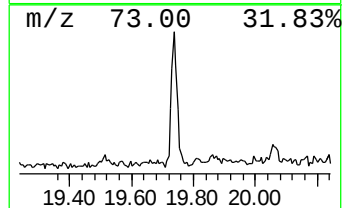
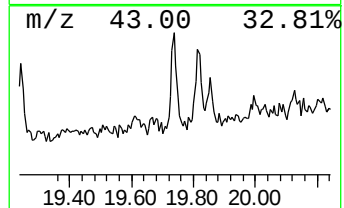
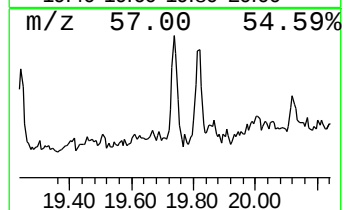
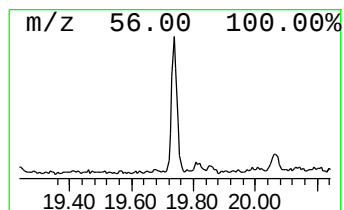
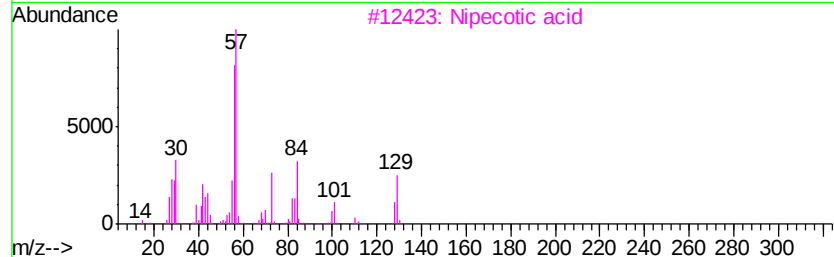
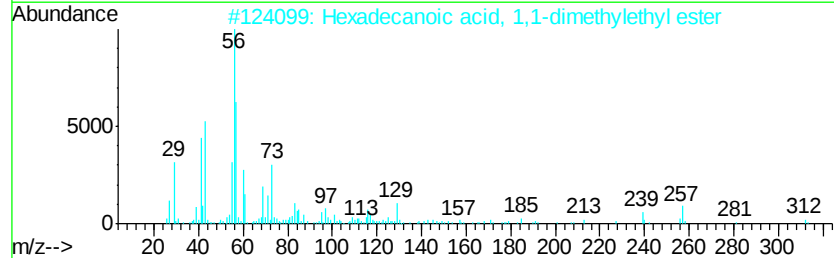
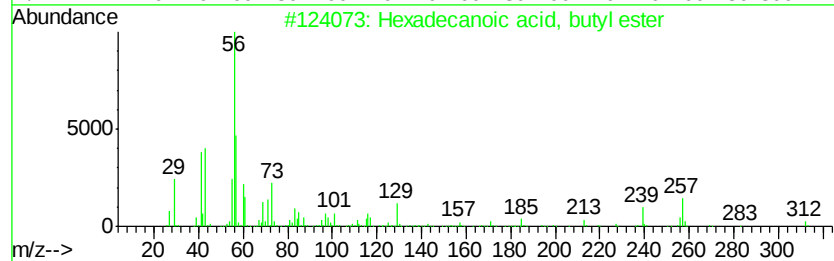
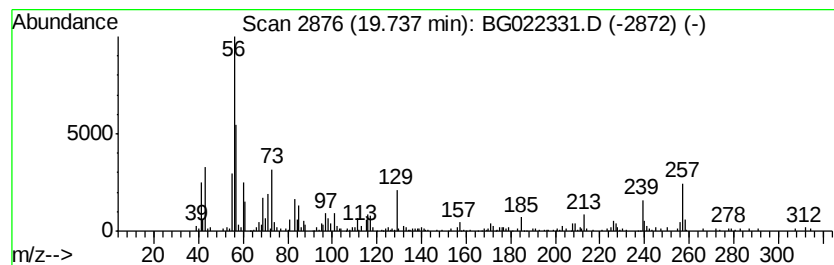
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.74	5.24 ng	134048	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	93
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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Data File : BG022331.D
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Sample : H3474-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B3(0-7)C

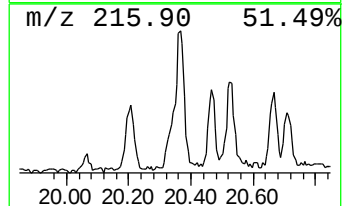
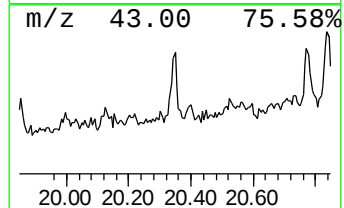
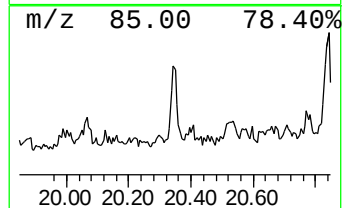
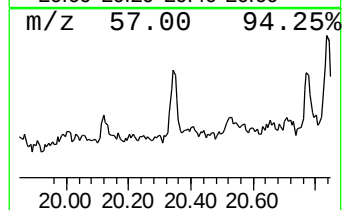
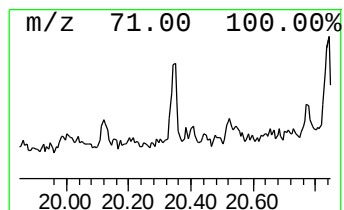
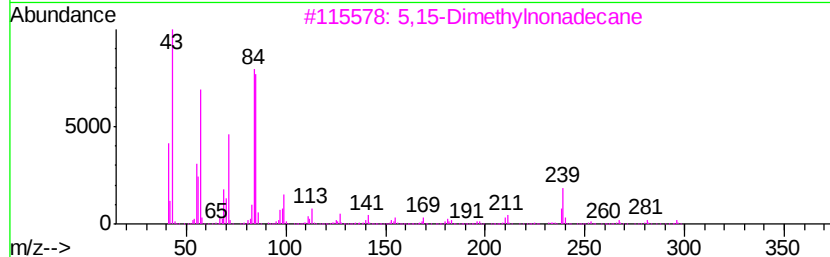
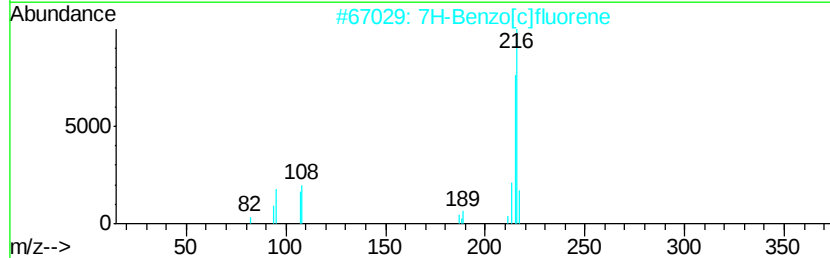
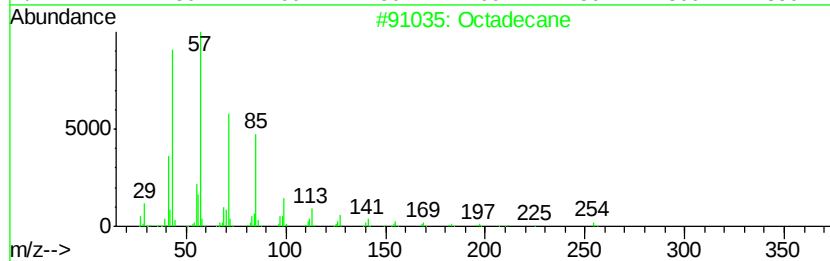
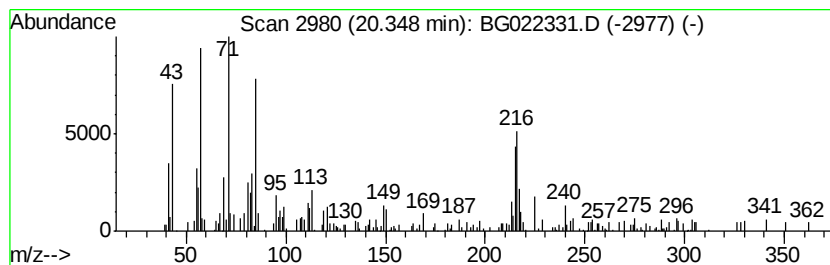
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.35 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.35	3.64 ng	93173	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	41
2		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	22
3		5,15-Dimethylnonadecane	296	C21H44	1000131-09-1	22
4		Phyto1	296	C20H40O	000150-86-7	18
5		Pyrene, 1-methyl-	216	C17H12	002381-21-7	18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061316\
Data File : BG022331.D
Acq On : 13 Jun 2016 19:37
Operator : UM/SJ
Sample : H3474-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S6-B3(0-7)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.15	5.4	ng	60704	1	8.09	224043	20.0
unknown7.62	7.62	80.0	ng	895624	1	8.09	224043	20.0
Eicosane	15.54	2.2	ng	53179	3	14.73	484180	20.0
Tetradecane	16.40	4.2	ng	107273	4	17.47	510154	20.0
6H-Cyclobuta[jk]p...	18.54	3.0	ng	75544	4	17.47	510154	20.0
Anthracene, 1,4-d...	19.24	3.2	ng	82314	4	17.47	510154	20.0
Hexadecanoic acid...	19.74	5.2	ng	134048	5	21.74	511557	20.0
unknown20.35	20.35	3.6	ng	93173	5	21.74	511557	20.0