

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022417\
 Data File : BG025948.D
 Acq On : 25 Feb 2017 1:40
 Operator : SJ/MA
 Sample : I1973-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 E2-Y6E-SW

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-BG021717.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	5.177	306	313	322	rBV	677618	1023387	12.98%	1.906%
2	5.647	386	393	403	rBV	1914313	3046223	38.64%	5.674%
3	7.240	656	664	673	rBV	1938097	3567321	45.25%	6.645%
4	7.616	719	728	737	rBV	1902332	3253544	41.27%	6.060%
5	8.080	799	807	814	rBV	301833	506120	6.42%	0.943%
6	8.403	854	862	871	rBV	1259938	2218336	28.14%	4.132%
7	9.061	965	974	975	rBV3	47798	82101	1.04%	0.153%
8	9.090	976	979	990	rVV3	55370	116480	1.48%	0.217%
9	9.237	990	1004	1013	rVV	1114847	1971356	25.01%	3.672%
10	10.882	1275	1284	1291	rBV	460515	856037	10.86%	1.595%
11	13.315	1690	1698	1707	rVB	3278015	5063717	64.23%	9.432%
12	13.867	1783	1792	1797	rBV2	37528	85511	1.08%	0.159%
13	14.008	1810	1816	1822	rVB	77852	131521	1.67%	0.245%
14	14.126	1831	1836	1842	rVB	880924	1235231	15.67%	2.301%
15	14.684	1919	1931	1938	rBV2	862107	1379392	17.50%	2.569%
16	15.471	2056	2065	2071	rBV3	49385	115053	1.46%	0.214%
17	16.159	2175	2182	2192	rBV	3147364	4956351	62.87%	9.232%
18	17.228	2360	2364	2373	rVB3	43944	79087	1.00%	0.147%
19	17.410	2389	2395	2401	rBV2	1246303	1942727	24.64%	3.619%
20	17.780	2452	2458	2469	rBV2	341937	516771	6.56%	0.963%
21	18.291	2540	2545	2555	rBV	181766	297532	3.77%	0.554%
22	18.879	2641	2645	2648	rBV3	63413	89622	1.14%	0.167%
23	19.020	2665	2669	2676	rVB2	83726	111299	1.41%	0.207%
24	19.137	2685	2689	2698	rBV	880611	1178970	14.96%	2.196%
25	19.214	2699	2702	2709	rVB2	55667	89559	1.14%	0.167%
26	19.455	2736	2743	2747	rBV	100737	169984	2.16%	0.317%
27	19.508	2747	2752	2756	rVB	76397	97408	1.24%	0.181%
28	19.555	2756	2760	2764	rBV4	63420	94706	1.20%	0.176%
29	19.701	2781	2785	2794	rBV5	70837	110058	1.40%	0.205%
30	19.784	2796	2799	2801	rVV2	68663	83150	1.05%	0.155%
31	19.813	2801	2804	2810	rVB	90507	128185	1.63%	0.239%
32	20.007	2831	2837	2848	rVB	5519262	7883206	100.00%	14.684%
33	20.636	2941	2944	2948	rVB	78467	98534	1.25%	0.184%
34	20.689	2949	2953	2957	rVB4	62028	86326	1.10%	0.161%

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ClientSampleId :
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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-BG021717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.300	3053	3057	3065	rBV4	119810	187727	2.38%	0.350%
36	21.658	3112	3118	3126	rBV	1308293	2211008	28.05%	4.118%
37	22.345	3200	3235	3236	rBV3	862031	6413935	81.36%	11.947%
38	24.866	3654	3664	3676	rVB2	784412	2209184	28.02%	4.115%

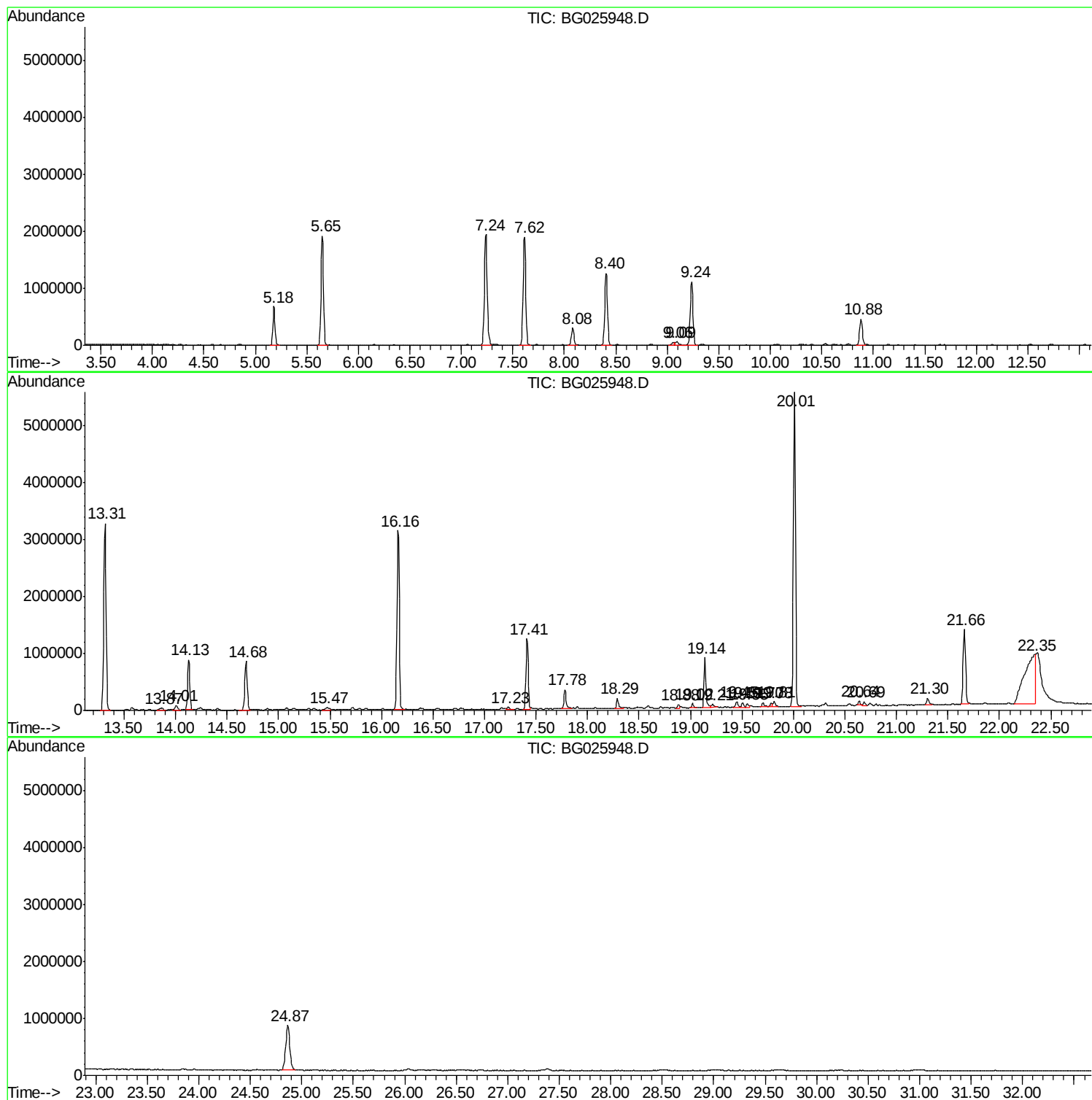
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : SJ/MA
Sample : I1973-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
E2-Y6E-SW

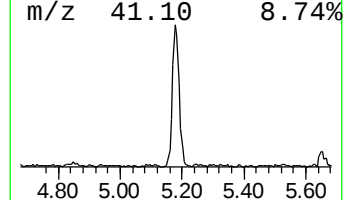
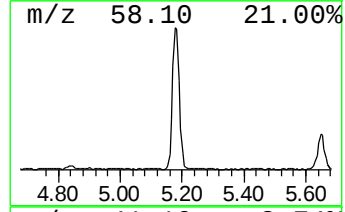
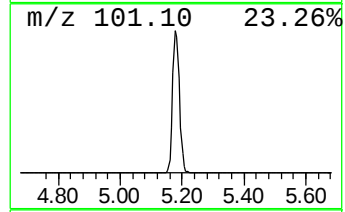
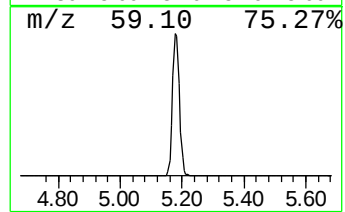
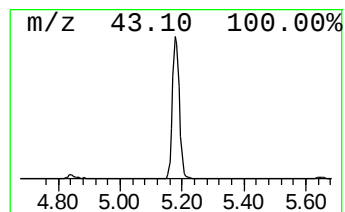
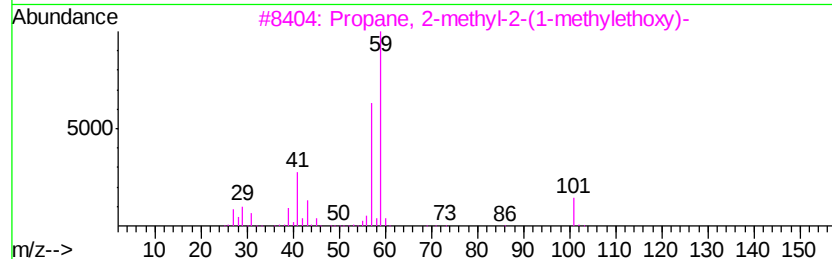
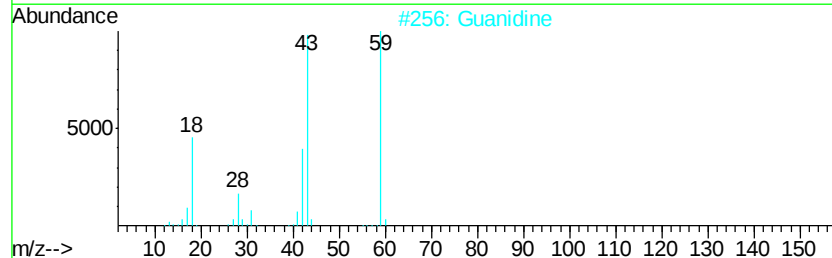
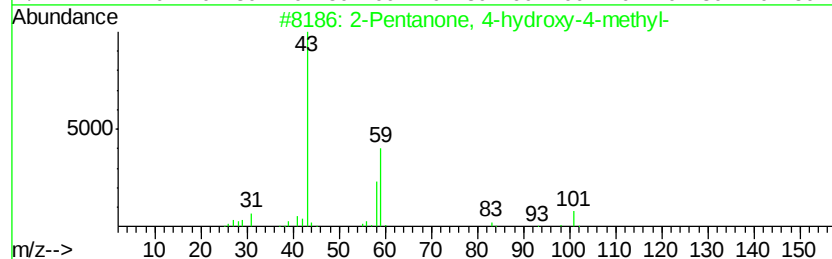
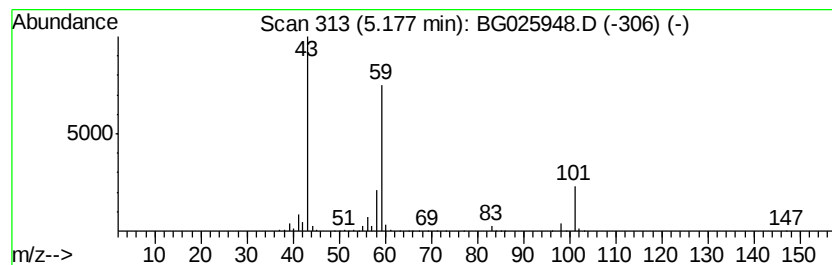
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	40.44 ng	1023390	1,4-Dichlorobenzene-d4	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	47
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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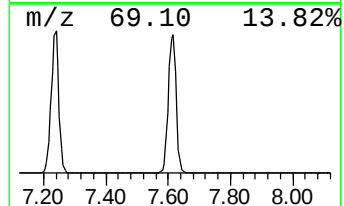
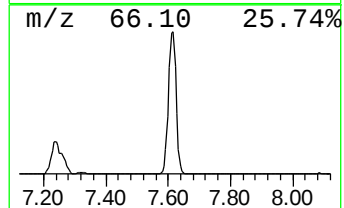
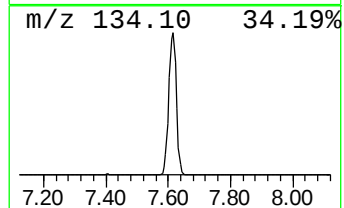
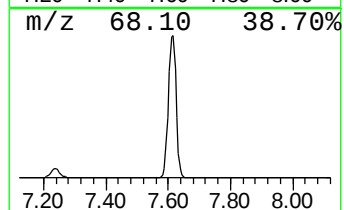
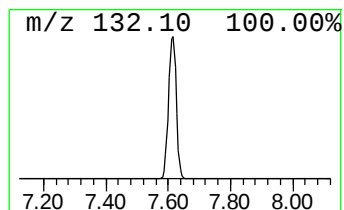
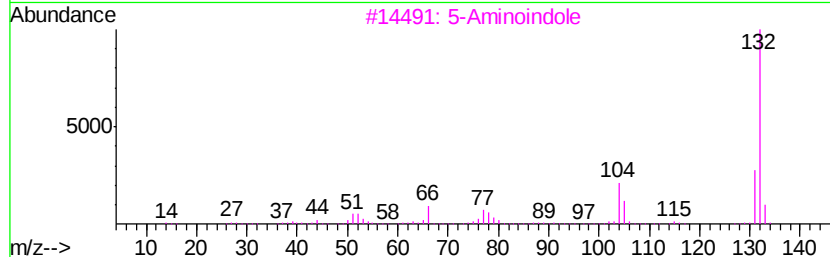
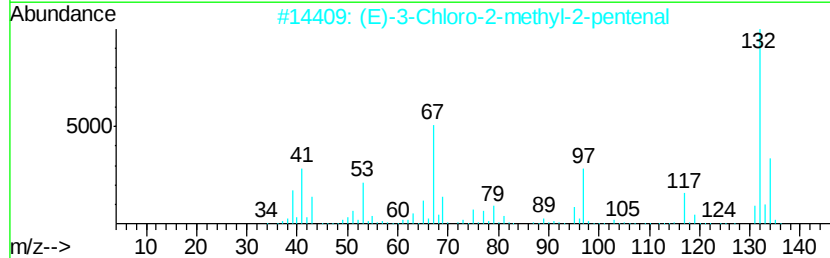
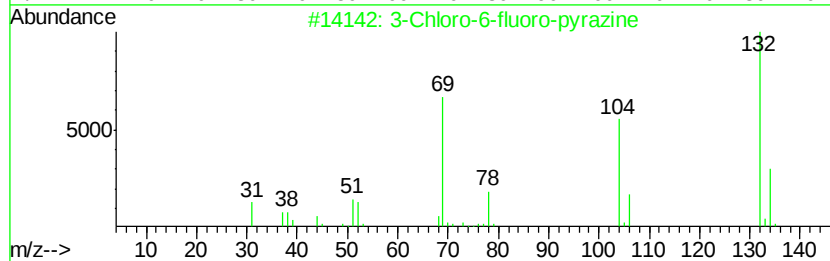
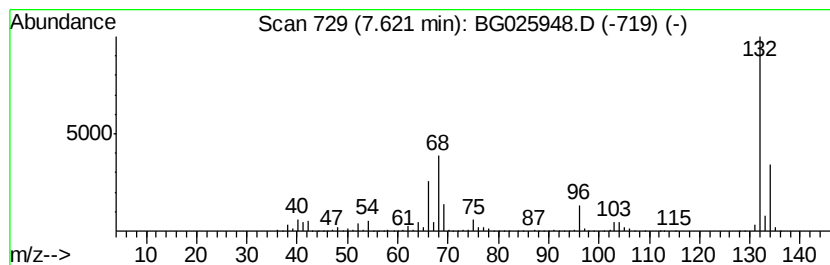
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	128.57 ng	3253540	1,4-Dichlorobenzene-d4	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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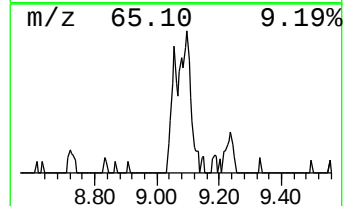
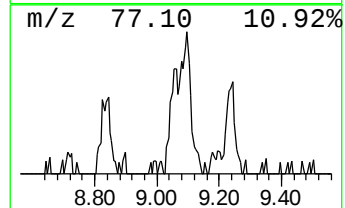
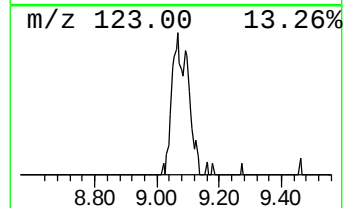
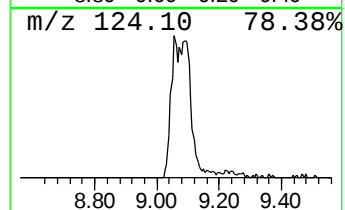
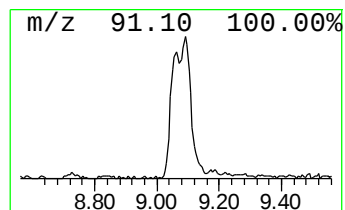
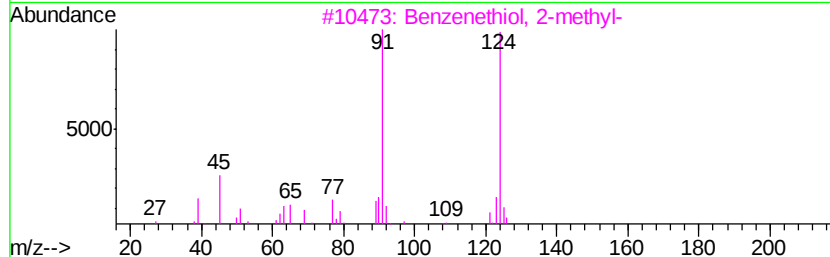
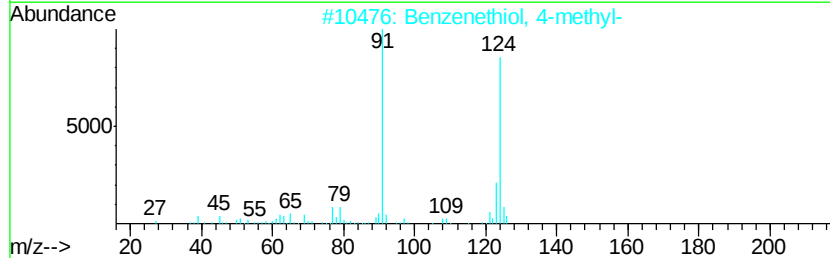
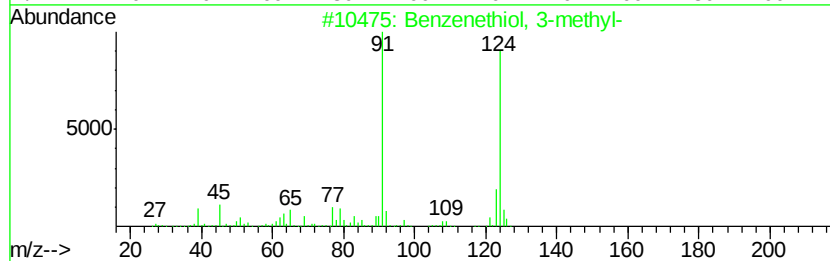
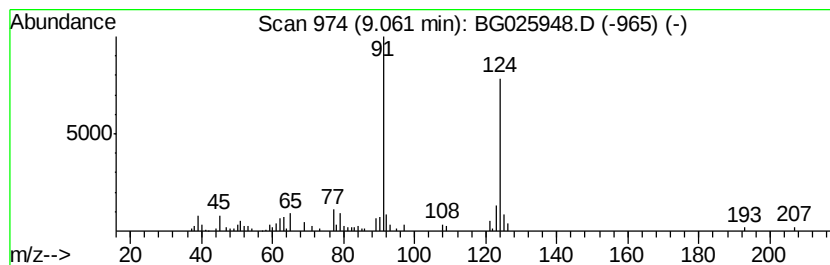
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzenethiol, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	3.24 ng	82101	1,4-Dichlorobenzene-d4	8.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenethiol, 3-methyl-	124	C7H8S	000108-40-7	96
2			Benzenethiol, 4-methyl-	124	C7H8S	000106-45-6	93
3			Benzenethiol, 2-methyl-	124	C7H8S	000137-06-4	90
4			Benzenemethanethiol	124	C7H8S	000100-53-8	83
5			Benzene, 1-methyl-2-[(1-methylet...	166	C10H14S	015560-98-2	72



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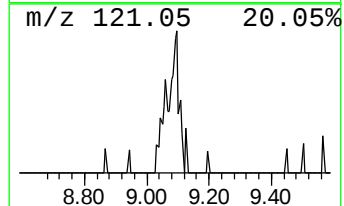
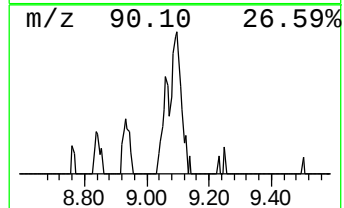
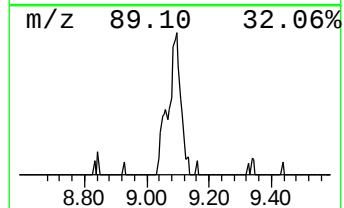
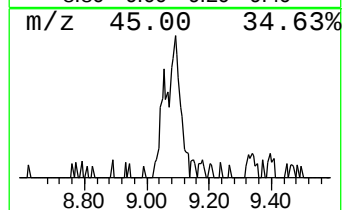
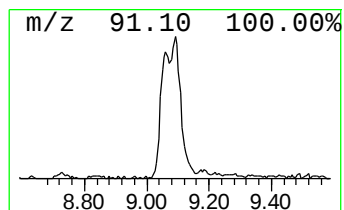
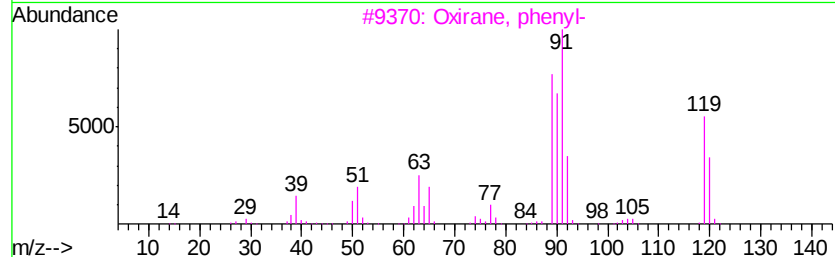
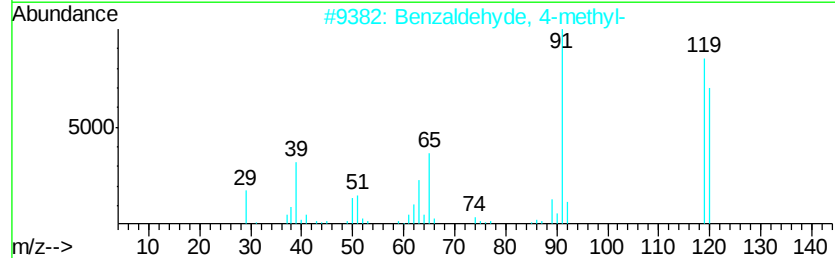
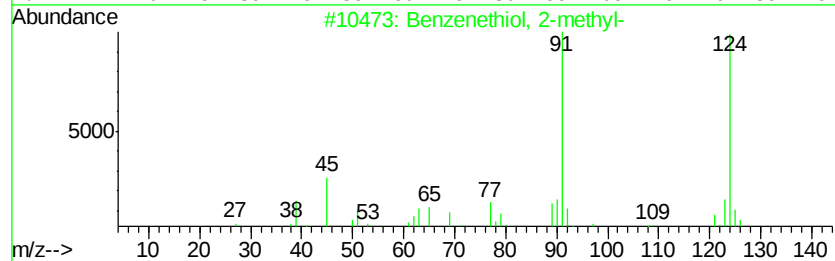
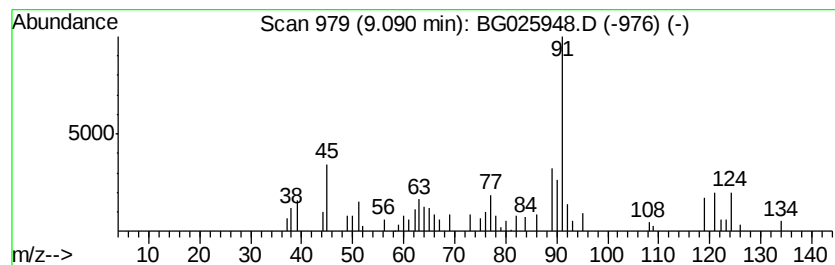
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzenethiol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	4.60 ng	116480	1,4-Dichlorobenzene-d4	8.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenethiol, 2-methyl-	124	C7H8S	000137-06-4	52
2		Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	37
3		Oxirane, phenyl-	120	C8H8O	000096-09-3	35
4		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	27
5		1,5-Hexadien-3-yne, 2-methyl-	92	C7H8	000820-54-2	25



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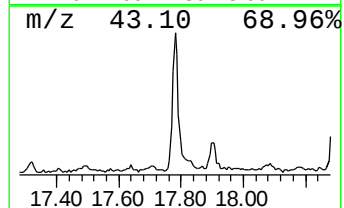
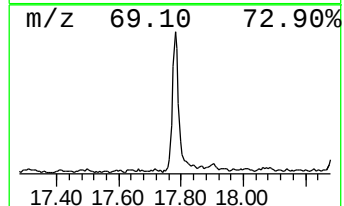
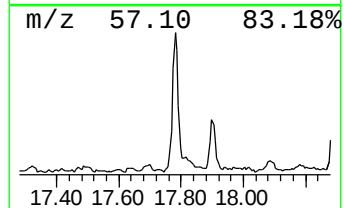
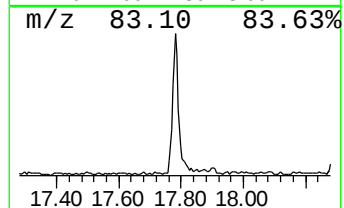
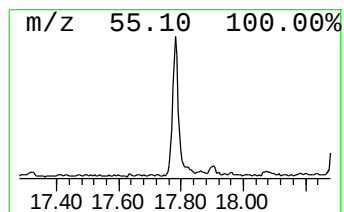
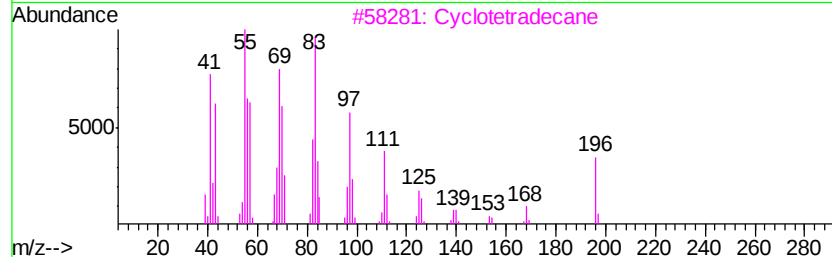
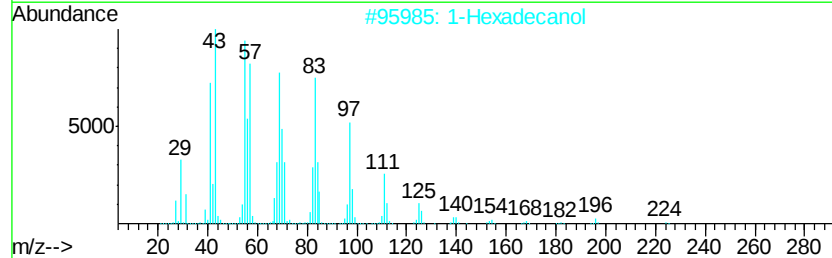
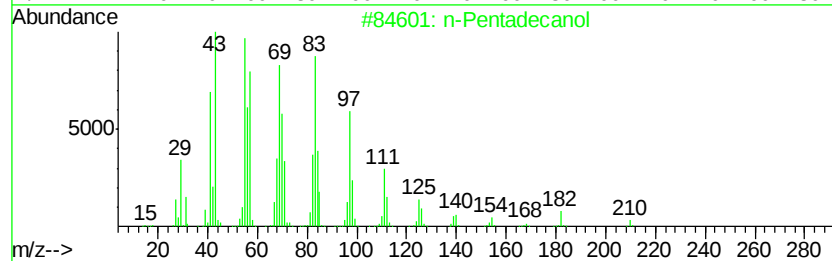
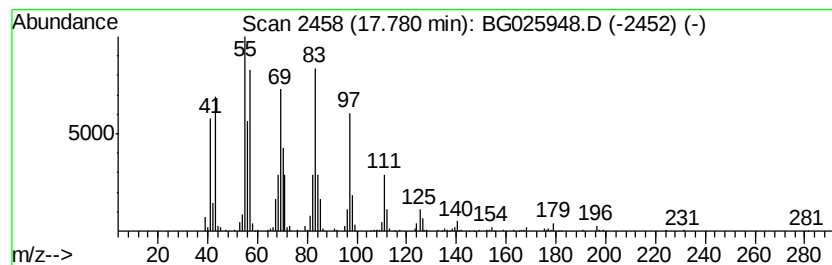
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Pentadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.78	5.32 ng	516771	Phenanthrene-d10		17.41
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Pentadecanol	228	C15H32O	000629-76-5	94
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	Cyclotetradecane	196	C14H28	000295-17-0	93
4	1-Tetradecene	196	C14H28	001120-36-1	92
5	Cyclohexadecane	224	C16H32	000295-65-8	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022417\
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Acq On : 25 Feb 2017 1:40
Operator : SJ/MA
Sample : I1973-08
Misc :
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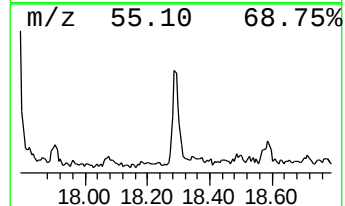
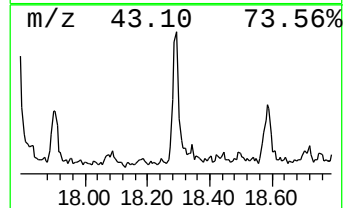
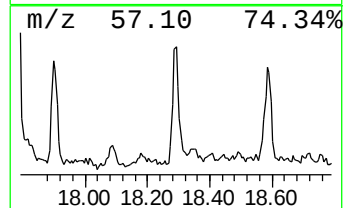
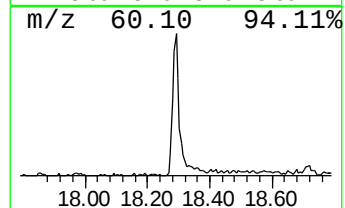
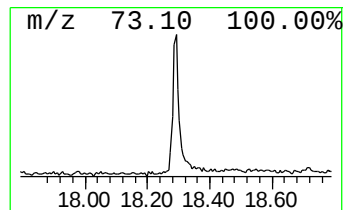
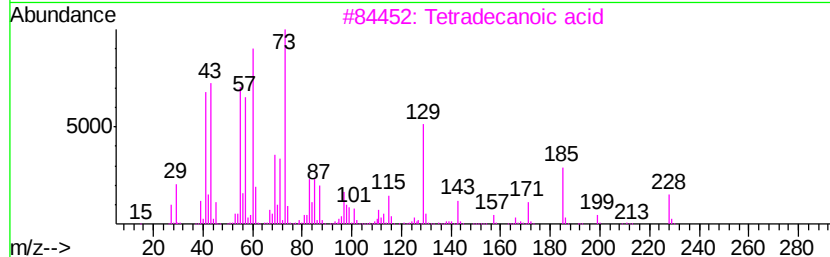
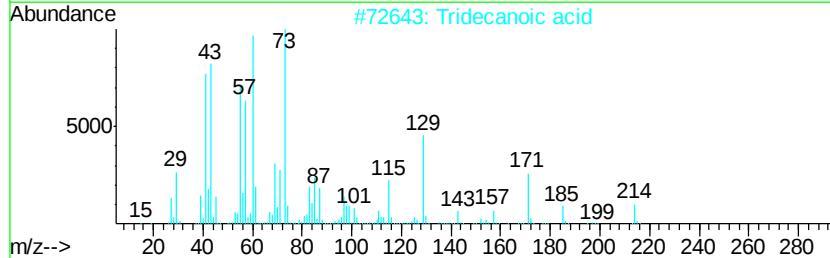
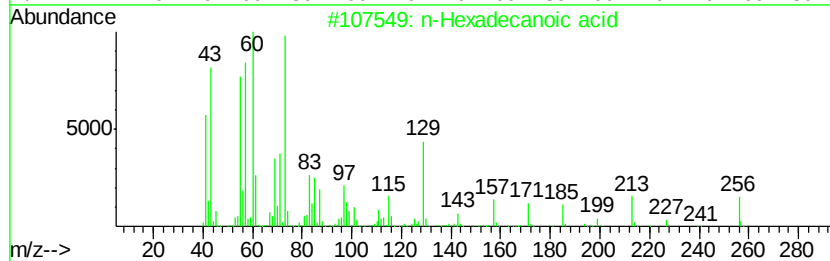
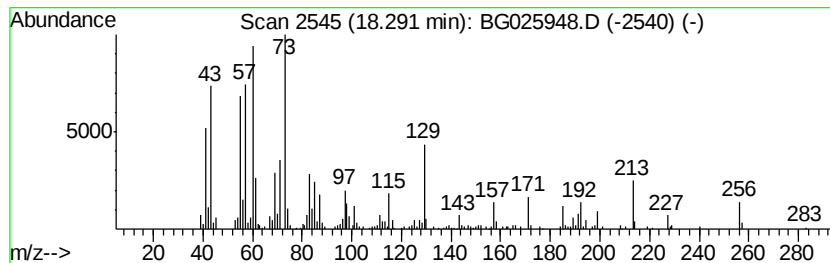
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.29	3.06 ng	297532	Phenanthrene-d10	17.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022417\
Data File : BG025948.D
Acq On : 25 Feb 2017 1:40
Operator : SJ/MA
Sample : I1973-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E2-Y6E-SW

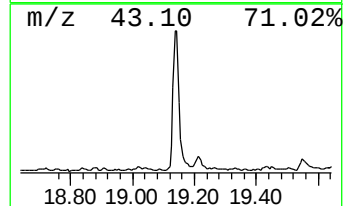
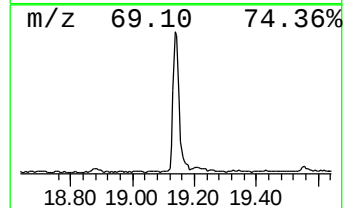
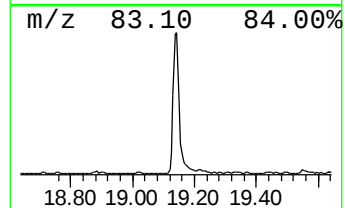
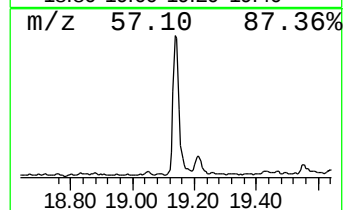
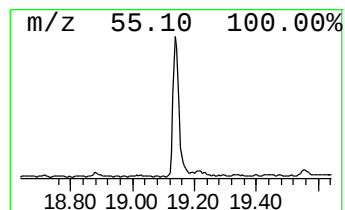
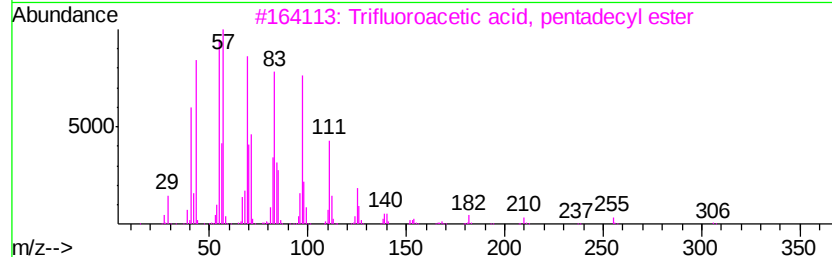
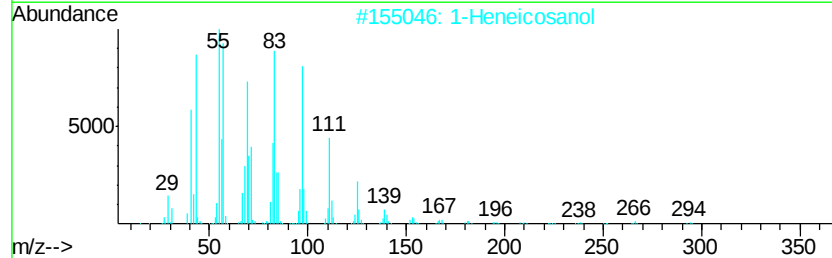
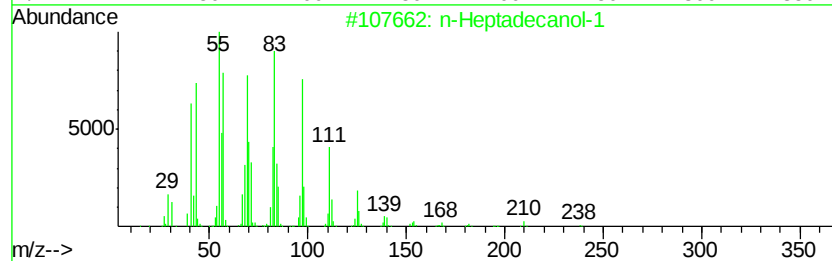
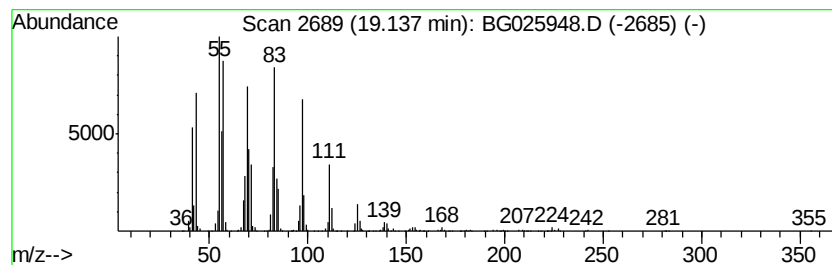
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Heptadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	12.14 ng	1178970	Phenanthrene-d10	17.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4		3-Octadecene, (E)-	252	C18H36	007206-19-1	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022417\
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Acq On : 25 Feb 2017 1:40
Operator : SJ/MA
Sample : I1973-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E2-Y6E-SW

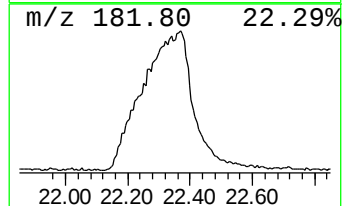
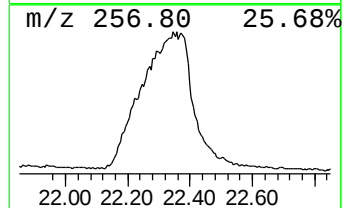
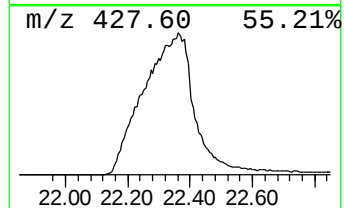
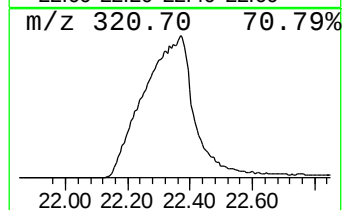
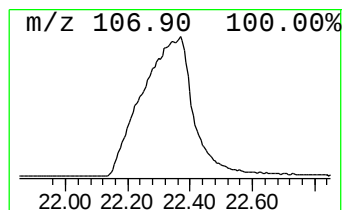
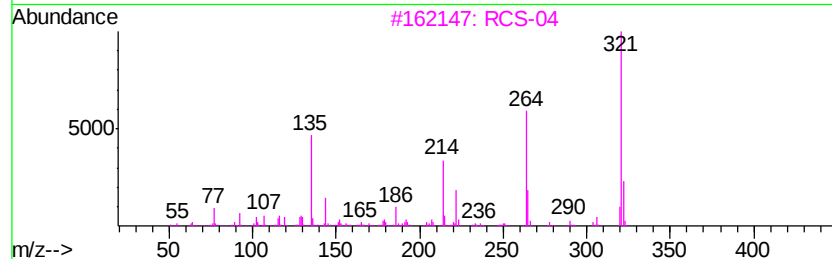
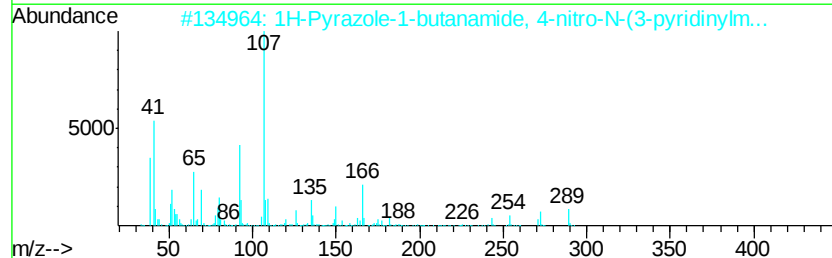
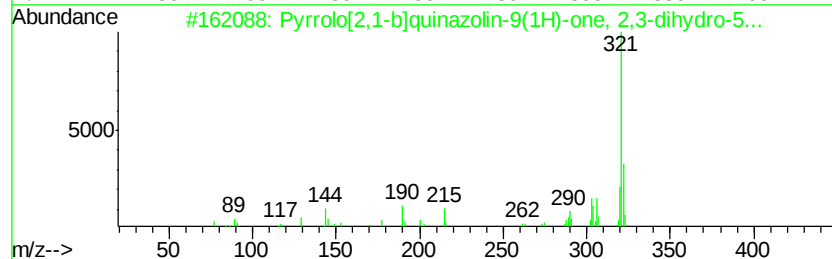
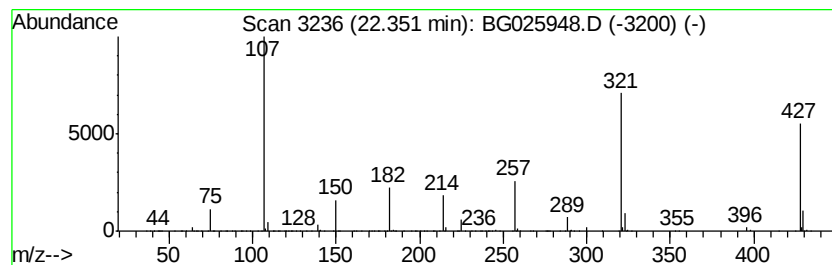
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown22.35 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.35	58.02 ng	6413940	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolo[2,1-b]quinazolin-9(1H)-o...	321	C19H19N3O2	025662-85-5	9
2		1H-Pyrazole-1-butanamide, 4-nitr...	289	C13H15N5O3	1000337-52-9	7
3		RCS-04	321	C21H23N02	1000380-06-4	5
4		1-(4-Hydroxyphenyl)-2-(3-hydroxy...	214	C14H14O2	037116-80-6	5
5		[1,1':3',1''-Terphenyl]-2'-amine...	321	C24H19N	006864-20-6	5



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Acq On : 25 Feb 2017 1:40
Operator : SJ/MA
Sample : I1973-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E2-Y6E-SW

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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...	5.18	40.4	ng	1023390	1	8.08	506120	20.0
unknown7.62	7.62	128.6	ng	3253540	1	8.08	506120	20.0
Benzenethiol, 3-m...	9.06	3.2	ng	82101	1	8.08	506120	20.0
Benzenethiol, 2-m...	9.09	4.6	ng	116480	1	8.08	506120	20.0
n-Pentadecanol	17.78	5.3	ng	516771	4	17.41	1942730	20.0
n-Hexadecanoic acid	18.29	3.1	ng	297532	4	17.41	1942730	20.0
n-Heptadecanol-1	19.14	12.1	ng	1178970	4	17.41	1942730	20.0
unknown22.35	22.35	58.0	ng	6413940	5	21.66	2211010	20.0