

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
 Data File : BG033963.D
 Acq On : 24 Apr 2018 20:42
 Operator : SJ/JU
 Sample : J2512-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-2-12

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-BG041918.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	4.992	284	290	295	rBV	77873	116561	2.74%	0.365%
2	5.439	359	366	382	rBV	1379967	2222269	52.28%	6.950%
3	7.002	624	632	646	rBV	1408825	2370195	55.76%	7.412%
4	7.366	686	694	701	rBV	1394796	2348904	55.26%	7.346%
5	7.830	764	773	780	rBV	287298	486277	11.44%	1.521%
6	8.148	818	827	835	rVB	1002702	1710706	40.25%	5.350%
7	8.976	959	968	978	rBV	815331	1418239	33.37%	4.435%
8	10.609	1237	1246	1255	rBV	394098	690050	16.24%	2.158%
9	13.083	1659	1667	1675	rBV	1876603	2901314	68.26%	9.073%
10	13.917	1804	1809	1815	rBV	182222	264781	6.23%	0.828%
11	14.376	1882	1887	1894	rBV	41271	57392	1.35%	0.179%
12	14.458	1894	1901	1909	rVV2	602801	966046	22.73%	3.021%
13	15.333	2045	2050	2055	rVB	54281	69306	1.63%	0.217%
14	15.950	2148	2155	2166	rBV	1748377	2647136	62.28%	8.278%
15	16.197	2192	2197	2201	rBV2	52398	72238	1.70%	0.226%
16	16.990	2328	2332	2337	rBV	32648	43099	1.01%	0.135%
17	17.131	2351	2356	2363	rBV	95649	123365	2.90%	0.386%
18	17.208	2363	2369	2379	rVV2	833991	1254754	29.52%	3.924%
19	17.595	2430	2435	2440	rBV	34967	45881	1.08%	0.143%
20	17.895	2481	2486	2491	rBV	125517	163660	3.85%	0.512%
21	17.948	2491	2495	2497	rBV	89365	118248	2.78%	0.370%
22	17.971	2497	2499	2504	rVV2	87261	95588	2.25%	0.299%
23	18.018	2504	2507	2515	rVB	100717	137794	3.24%	0.431%
24	18.124	2518	2525	2535	rBV2	230588	413402	9.73%	1.293%
25	18.324	2554	2559	2564	rBV	197545	248619	5.85%	0.778%
26	18.606	2602	2607	2613	rBV	542943	677185	15.93%	2.118%
27	19.405	2739	2743	2749	rBV3	44879	67858	1.60%	0.212%
28	19.675	2786	2789	2798	rVB4	39157	57419	1.35%	0.180%
29	19.846	2812	2818	2825	rBV	3325756	4250380	100.00%	13.292%
30	20.545	2930	2937	2943	rBV	200811	290690	6.84%	0.909%
31	20.698	2960	2963	2967	rBV5	23816	43172	1.02%	0.135%
32	20.921	2998	3001	3005	rBV4	36215	49279	1.16%	0.154%
33	21.103	3026	3032	3036	rBV8	23101	45978	1.08%	0.144%
34	21.156	3036	3041	3045	rBV2	155498	235061	5.53%	0.735%

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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-BG041918.M
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35	21.303	3063	3066	3070	rVB6	43056	51708	1.22%	0.162%
36	21.461	3087	3093	3104	rVB2	974597	1717158	40.40%	5.370%
37	21.597	3110	3116	3119	rBV6	44331	100853	2.37%	0.315%
38	21.720	3132	3137	3145	rVB4	71343	150665	3.54%	0.471%
39	21.820	3148	3154	3158	rBV4	72920	146168	3.44%	0.457%
40	22.037	3187	3191	3201	rVB6	86228	194730	4.58%	0.609%
41	22.143	3205	3209	3213	rBV6	57798	107770	2.54%	0.337%
42	22.231	3222	3224	3228	rVB5	40430	49528	1.17%	0.155%
43	22.302	3229	3236	3244	rVB5	67085	180918	4.26%	0.566%
44	22.401	3247	3253	3258	rBV5	74059	153008	3.60%	0.479%
45	22.560	3276	3280	3285	rBV5	36504	72680	1.71%	0.227%
46	22.613	3286	3289	3292	rVV4	48607	73647	1.73%	0.230%
47	22.660	3294	3297	3306	rVB4	65283	103696	2.44%	0.324%
48	22.789	3313	3319	3327	rBV3	72468	171033	4.02%	0.535%
49	22.948	3343	3346	3353	rVB5	32670	61494	1.45%	0.192%
50	23.071	3361	3367	3372	rBV5	59372	118652	2.79%	0.371%
51	23.130	3373	3377	3386	rVB2	65650	127964	3.01%	0.400%
52	23.524	3439	3444	3455	rVB4	44405	102206	2.40%	0.320%
53	24.523	3603	3614	3625	rBV2	572542	1527808	35.95%	4.778%
54	29.587	4468	4476	4477	rBV7	30946	61792	1.45%	0.193%

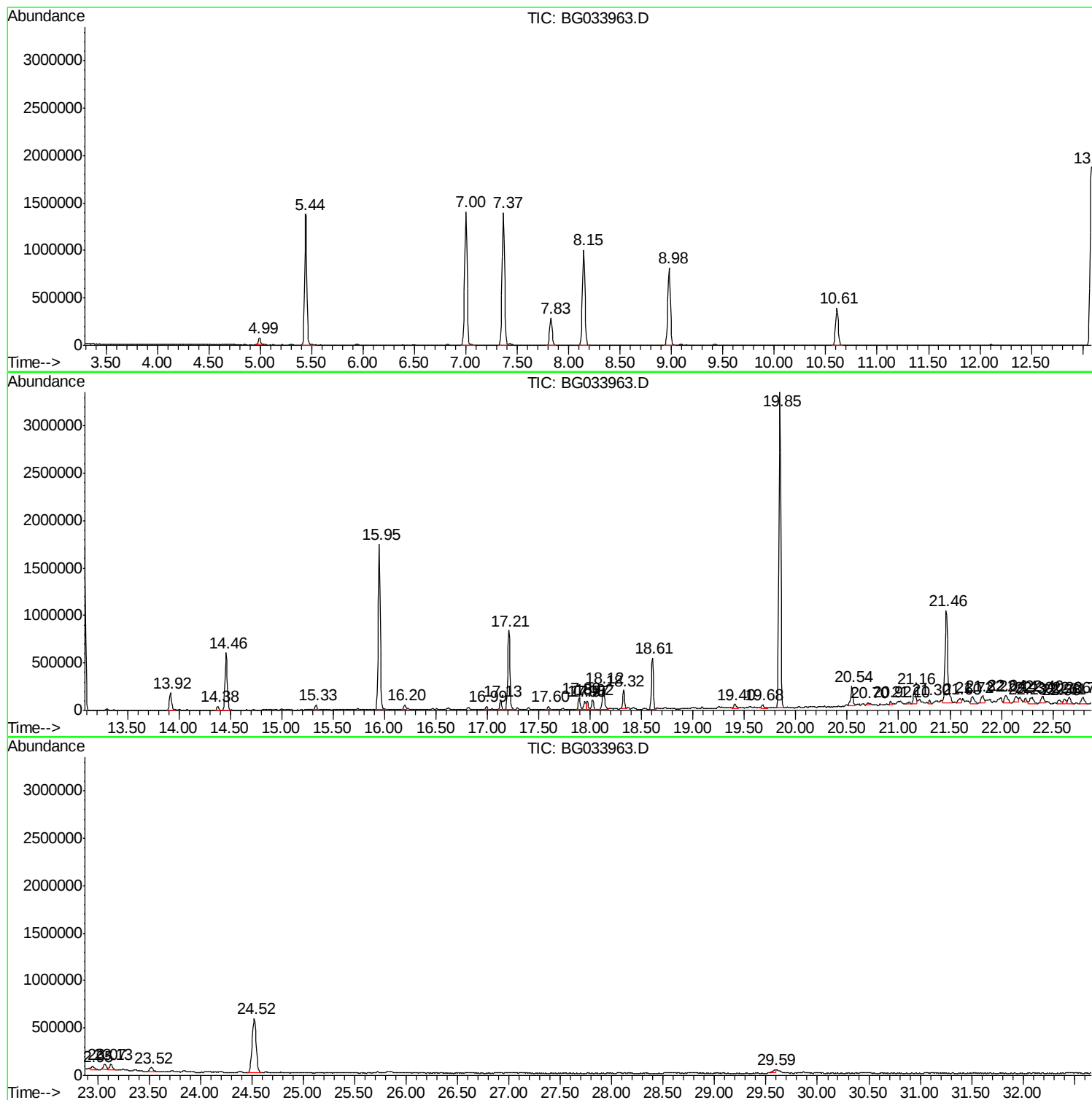
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BNA_G
ClientSampled :
TP-2-12

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041918.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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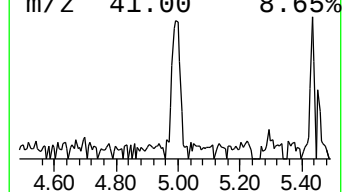
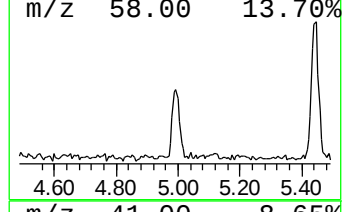
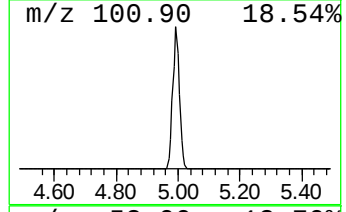
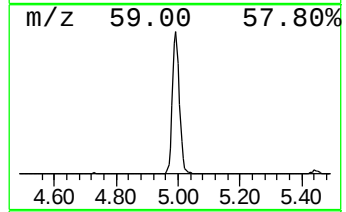
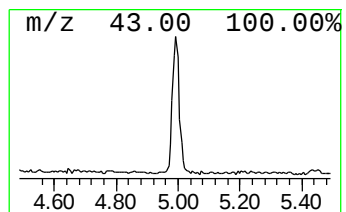
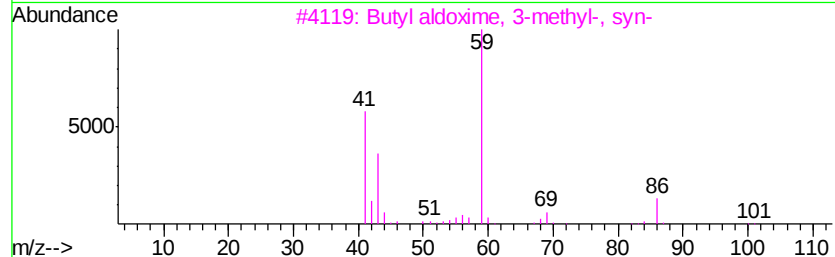
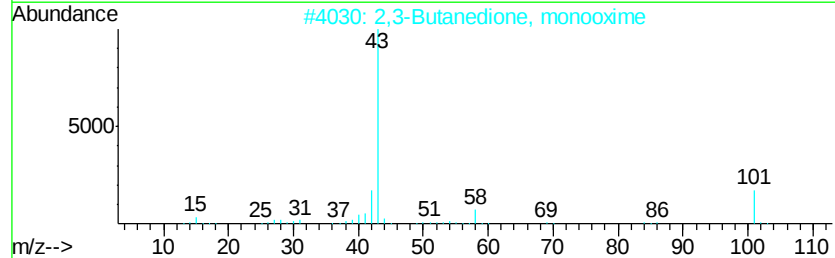
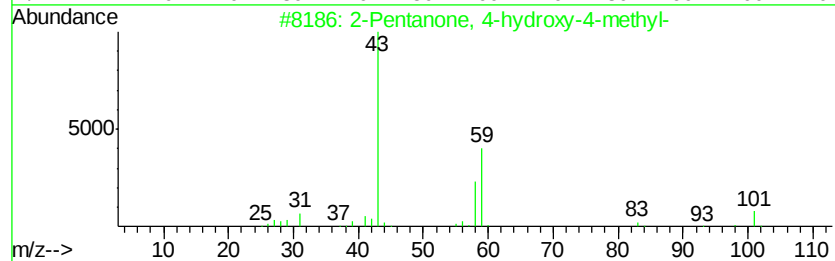
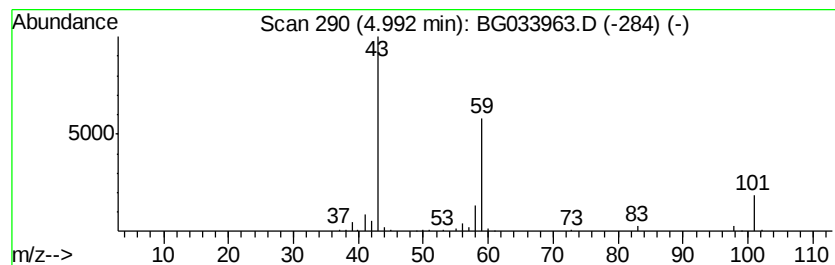
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.79 ng	116561	1,4-Dichlorobenzene-d4	7.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23	
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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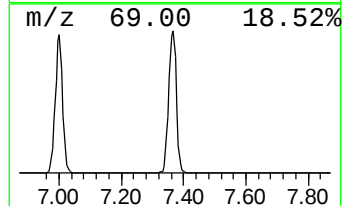
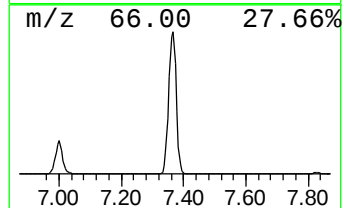
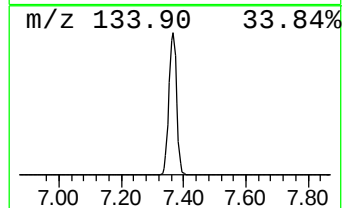
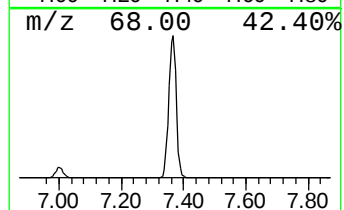
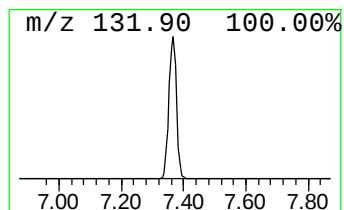
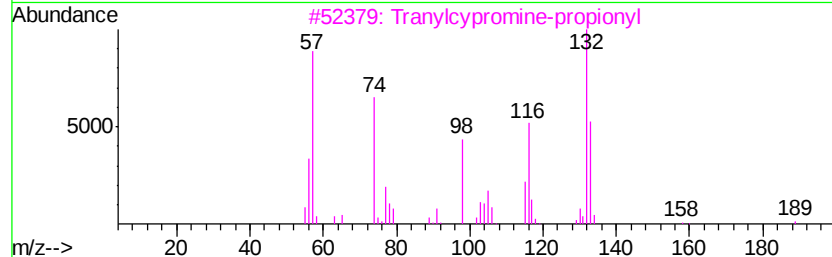
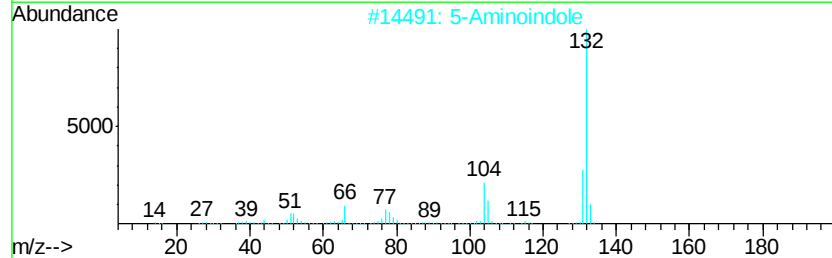
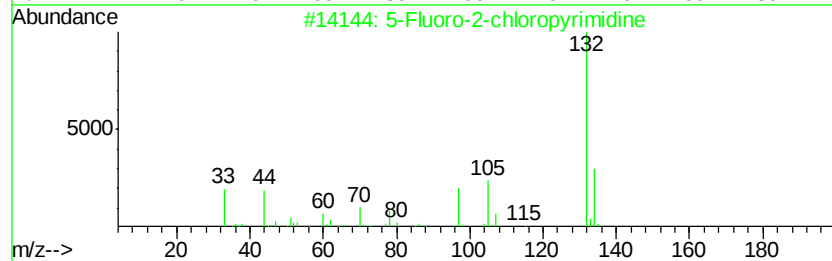
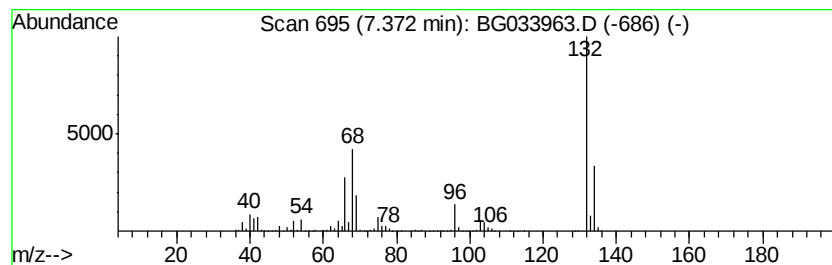
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	96.61 ng	2348900	1,4-Dichlorobenzene-d4	7.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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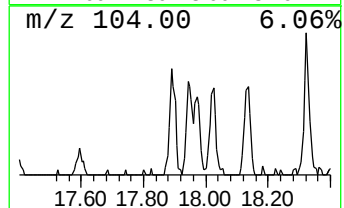
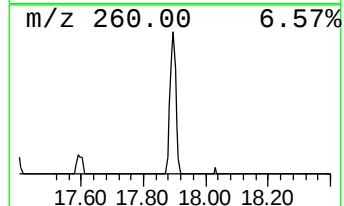
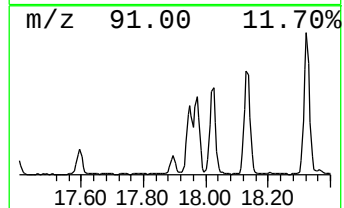
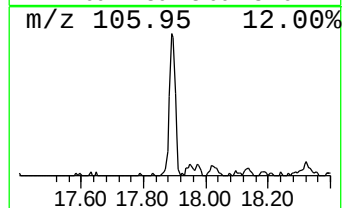
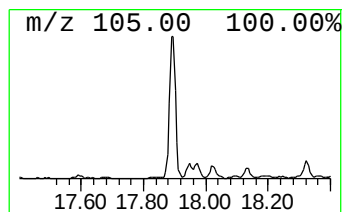
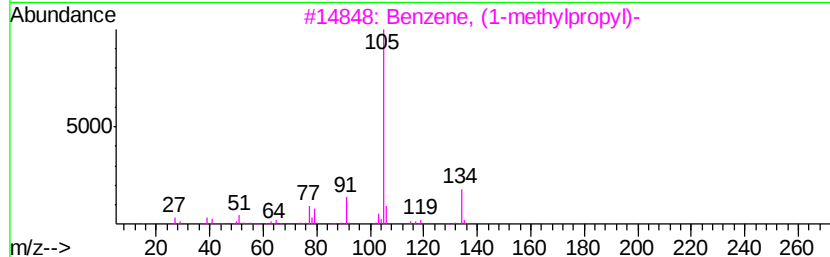
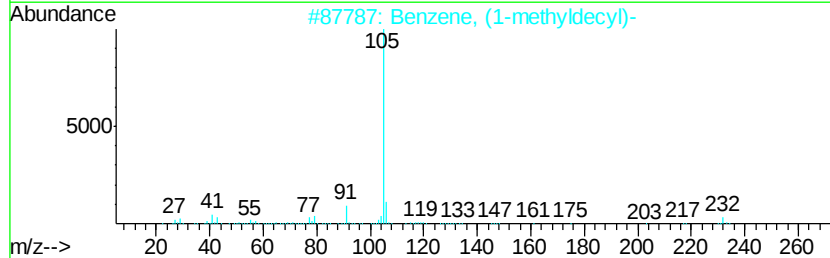
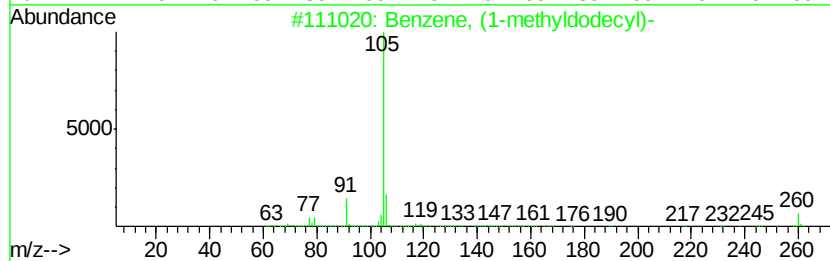
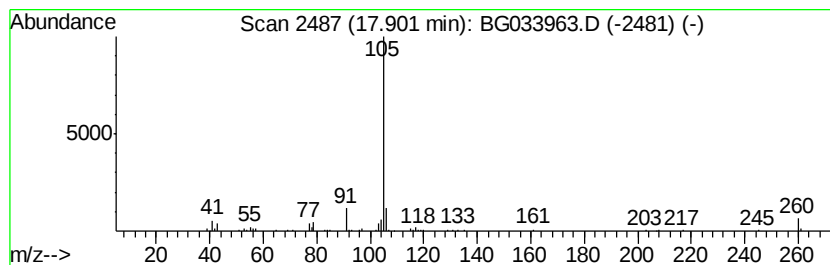
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, (1-methyldodecyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	2.61 ng	163660	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	93
2		Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	59
3		Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	59
4		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53
5		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	53



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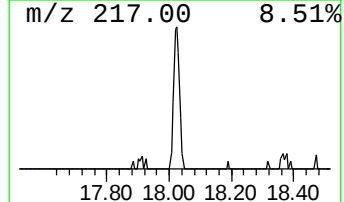
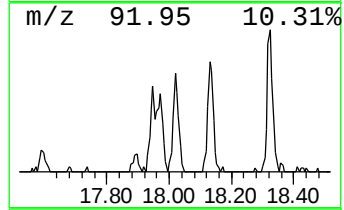
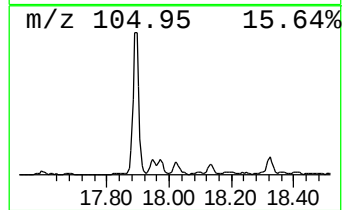
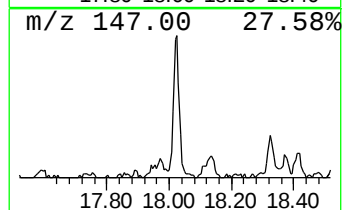
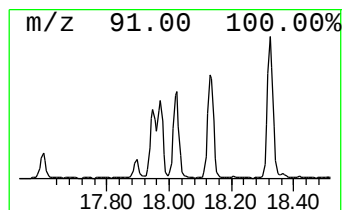
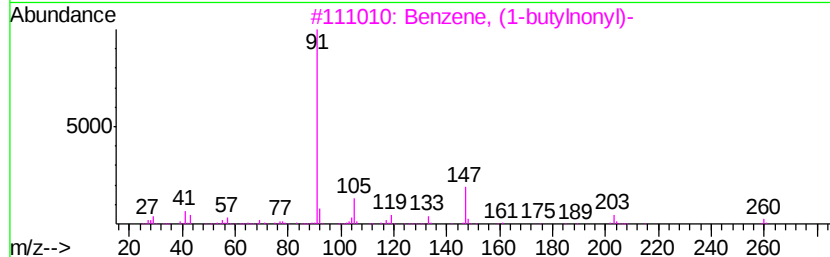
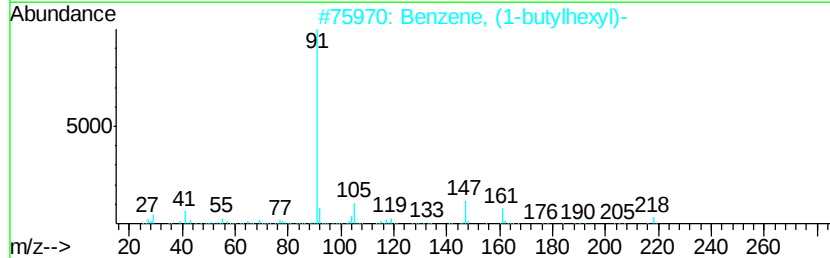
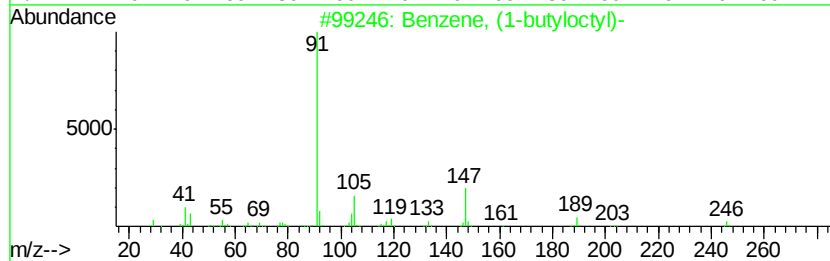
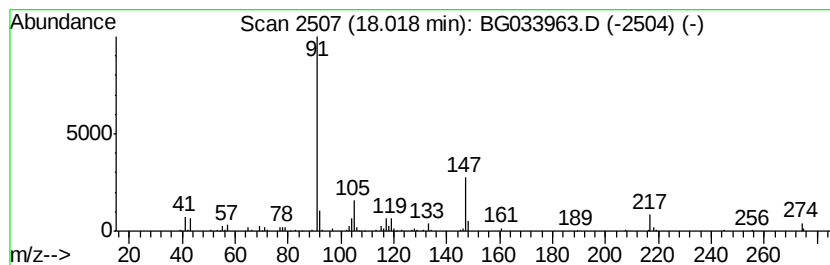
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, (1-butyloctyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	2.20 ng	137794	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-butyloctyl)-	246	C18H30	002719-63-3	64
2		Benzene, (1-butylohexyl)-	218	C16H26	004537-11-5	59
3		Benzene, (1-butylnonyl)-	260	C19H32	004534-50-3	53
4		Benzene, (1-butyloheptyl)-	232	C17H28	004537-15-9	47
5		Benzene, (1,1-diethylpropyl)-	176	C13H20	004170-84-7	45



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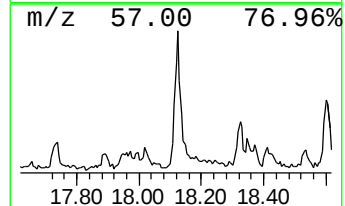
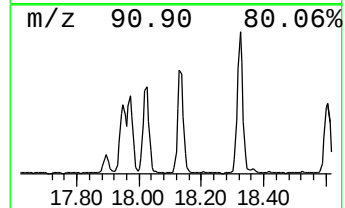
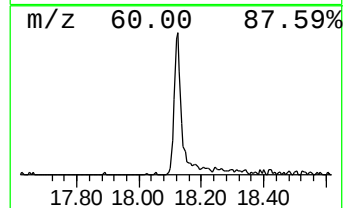
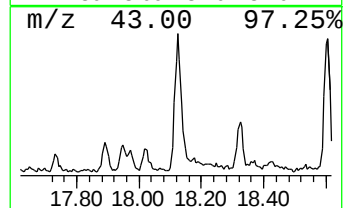
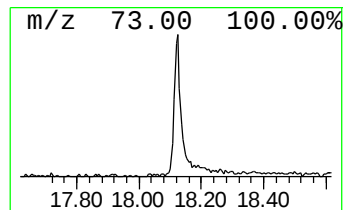
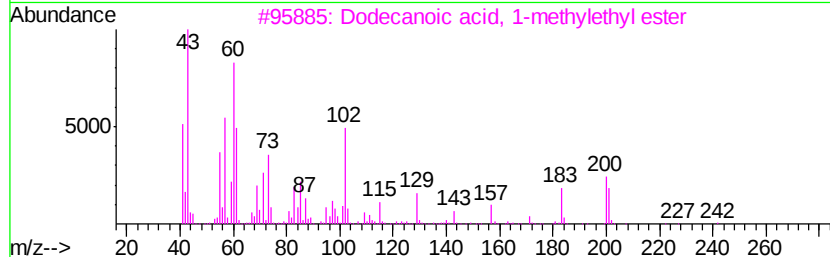
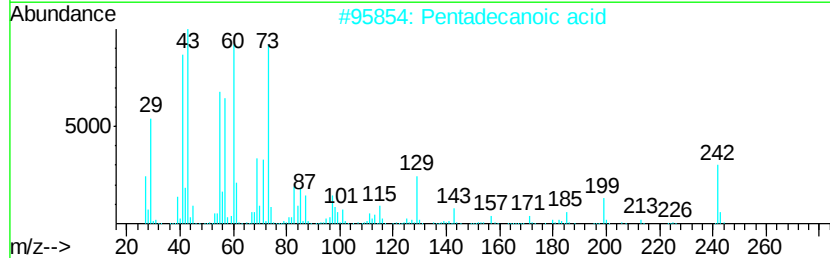
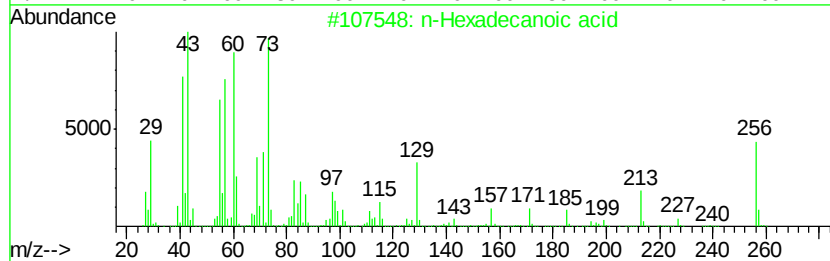
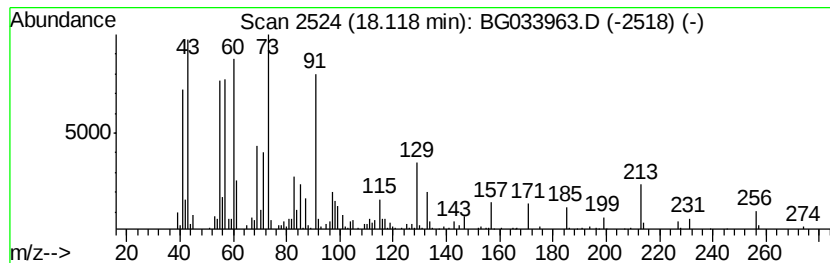
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	6.59 ng	413402	Phenanthrene-d10	17.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	32
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	22
5	Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	14



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
Operator : SJ/JU
Sample : J2512-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2-12

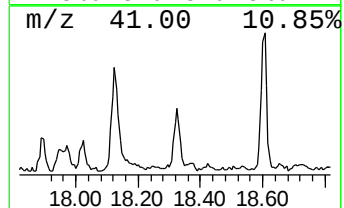
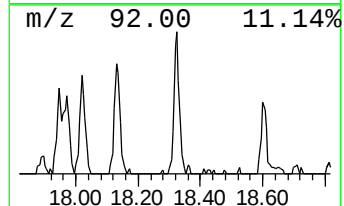
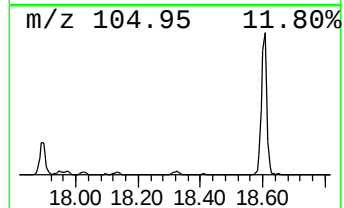
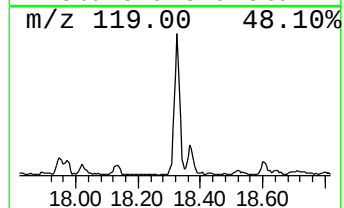
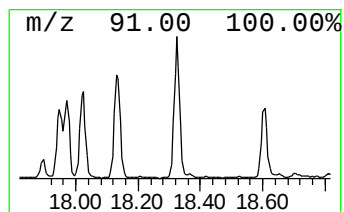
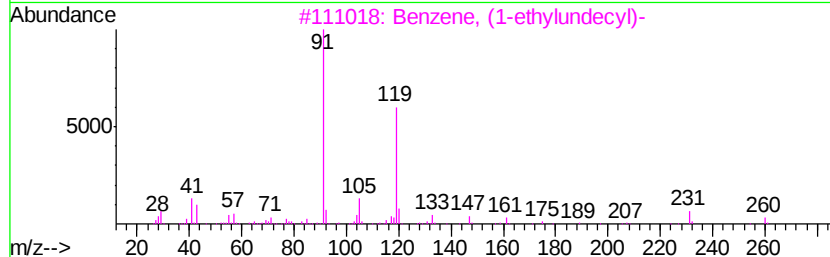
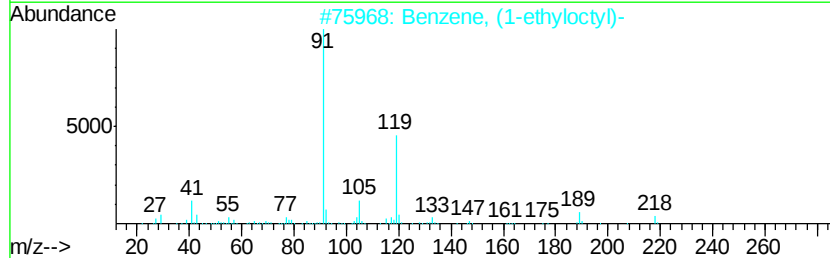
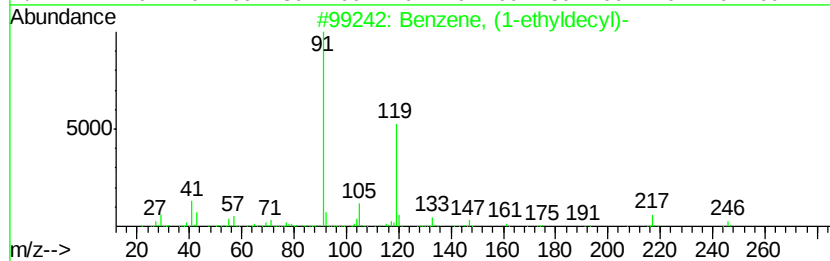
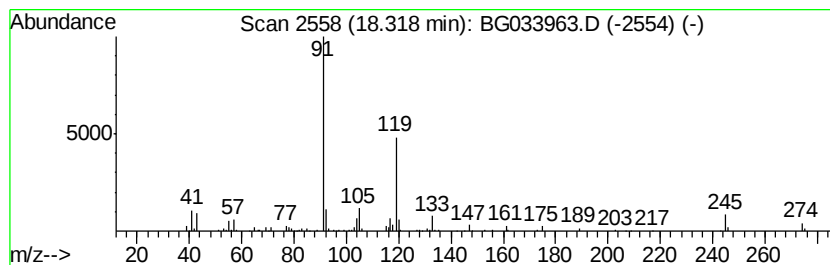
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, (1-ethyldecyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	3.96 ng	248619	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	59
2		Benzene, (1-ethyloctyl)-	218	C16H26	004621-36-7	58
3		Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	53
4		2-phenylbutyric acid, 2,2,2-trif...	246	C12H13F3O2	1000376-55-3	53
5		Aziridine, 1-phenyl-	119	C8H9N	000696-18-4	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
Operator : SJ/JU
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ALS Vial : 14 Sample Multiplier: 1

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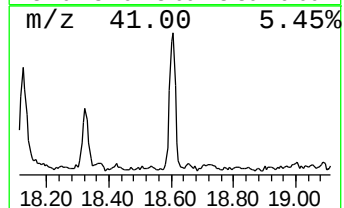
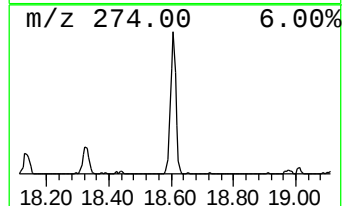
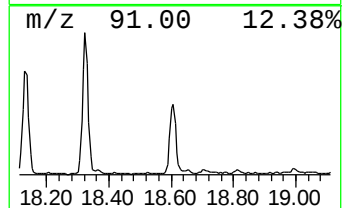
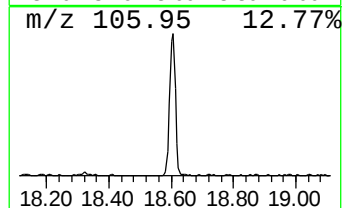
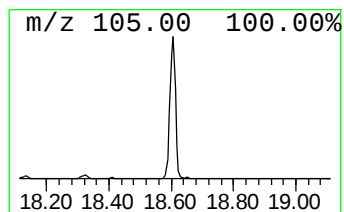
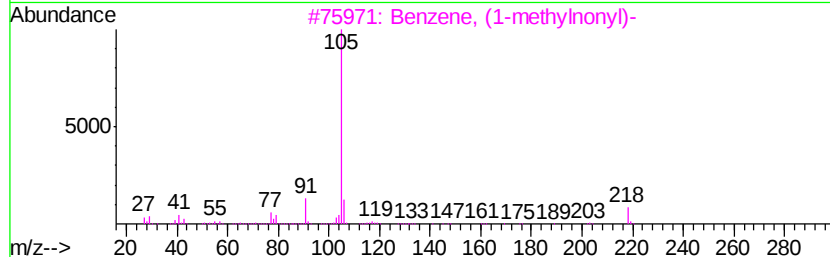
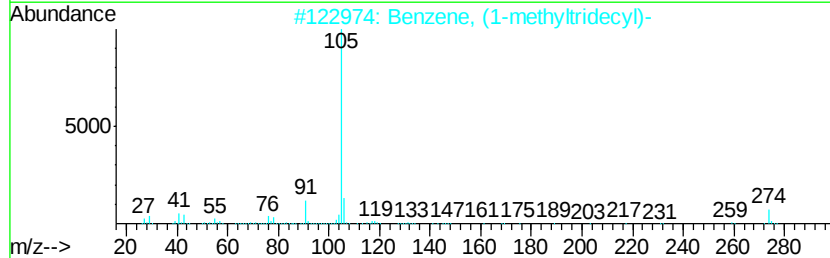
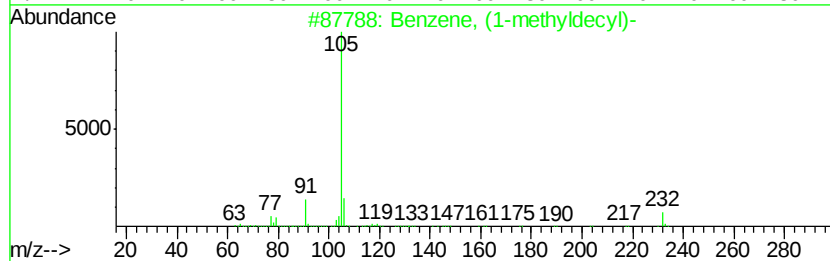
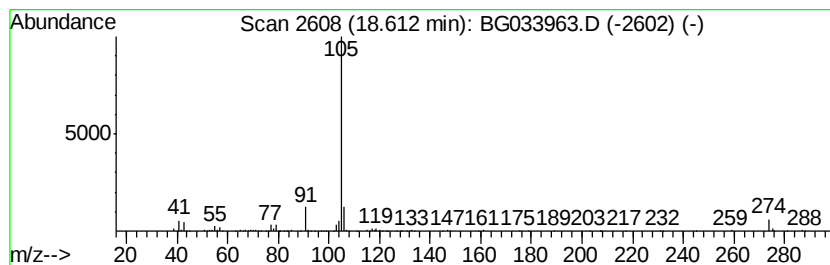
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, (1-methyldecyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.61	10.79 ng	677185	Phenanthrene-d10	17.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	87
2		Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	76
3		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	72
4		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
5		Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
Operator : SJ/JU
Sample : J2512-02
Misc :
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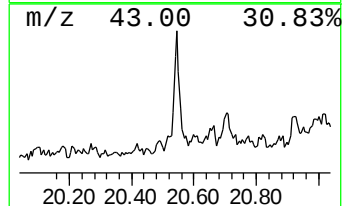
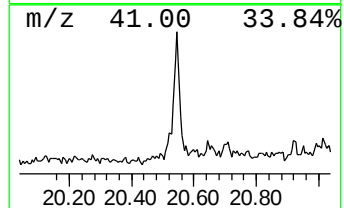
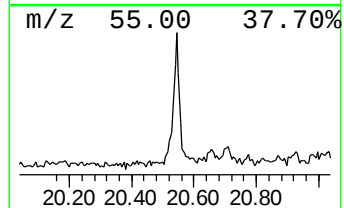
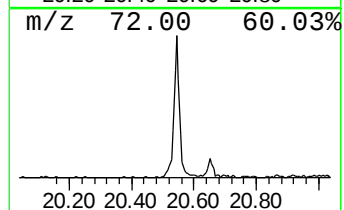
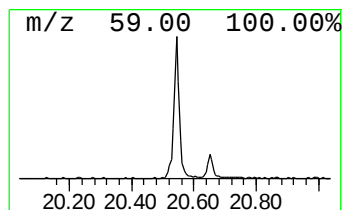
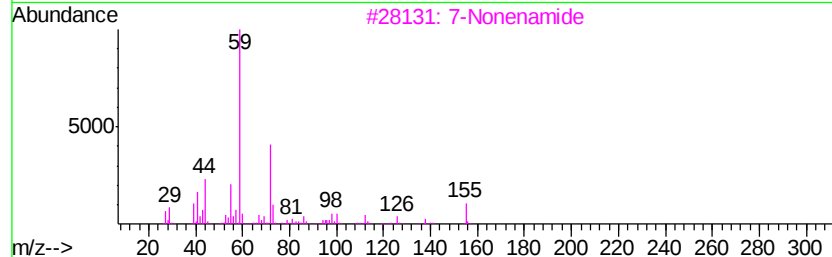
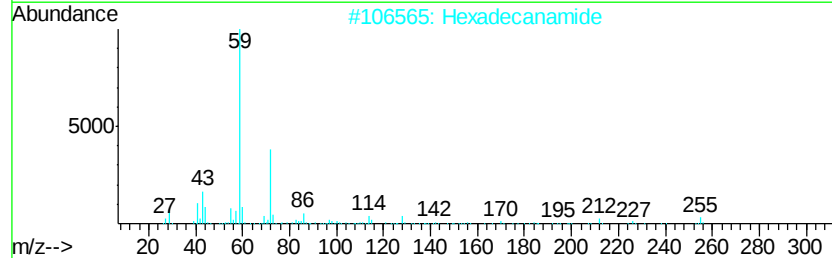
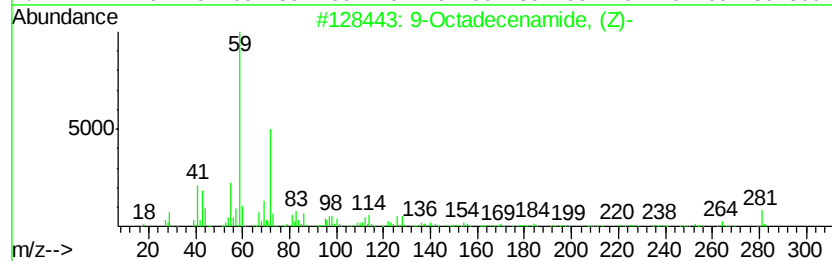
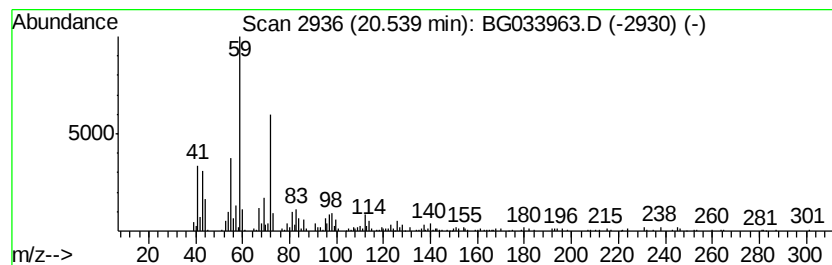
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.54	3.39 ng	290690	Chrysene-d12		21.46	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Hexadecanamide	255	C16H33NO	000629-54-9	59
3		7-Nonenamide	155	C9H17NO	090949-53-4	53
4		Octadecanamide	283	C18H37NO	000124-26-5	50
5		Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	38



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
Operator : SJ/JU
Sample : J2512-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

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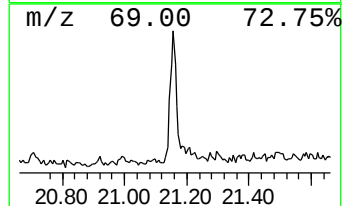
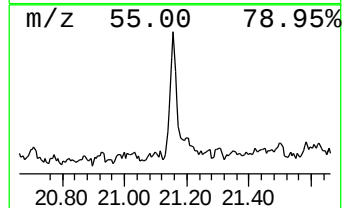
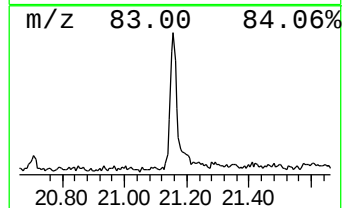
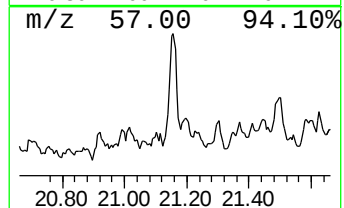
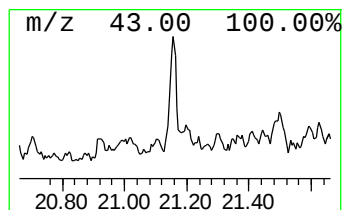
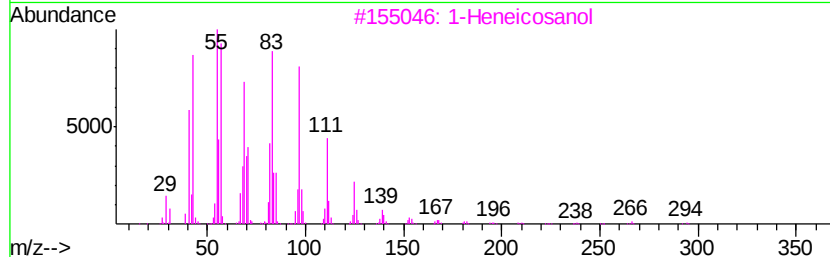
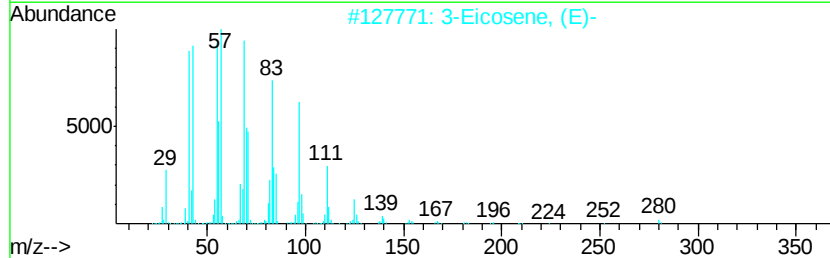
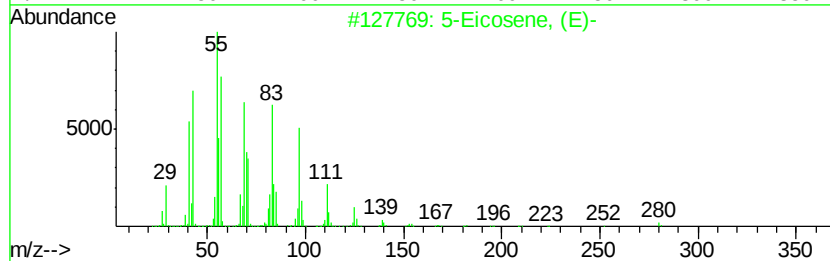
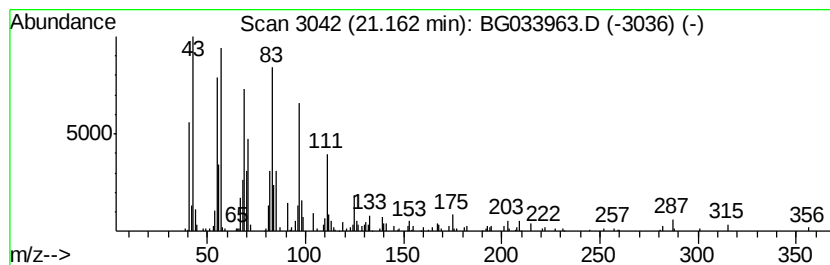
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.16	2.74 ng	235061	Chrysene-d12	21.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	98
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		1-Eicosene	280	C20H40	003452-07-1	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
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ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
TP-2-12

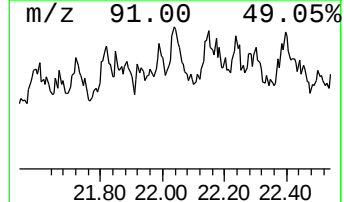
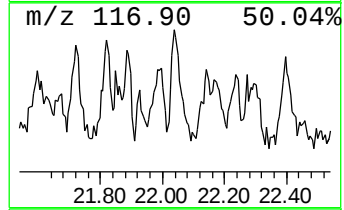
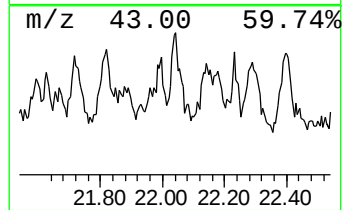
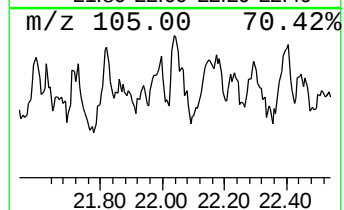
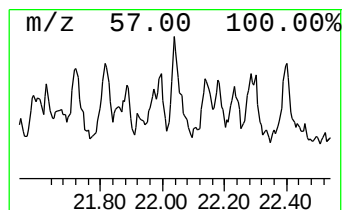
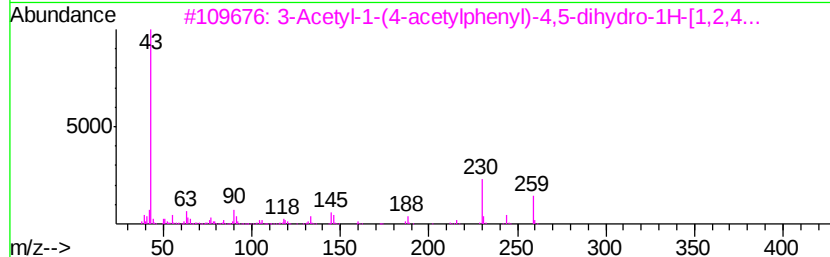
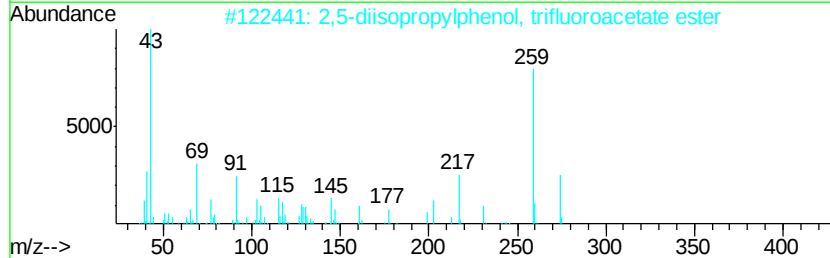
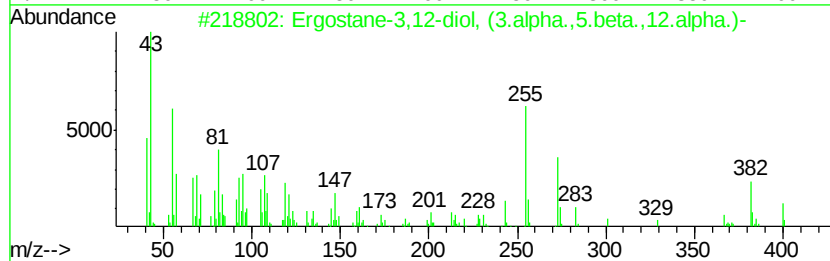
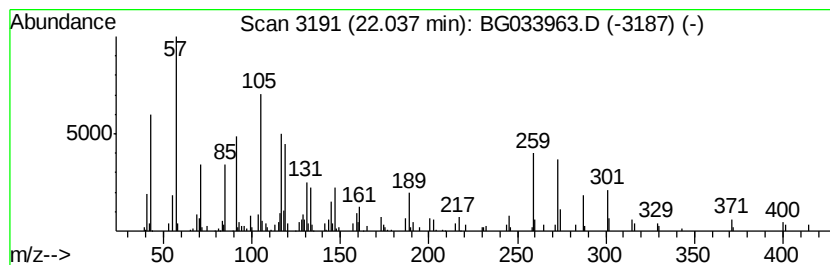
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.04 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.04	2.27 ng	194730	Chrysene-d12	21.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ergostane-3,12-diol, (3.alpha.,5...	418	C28H50O2	056052-70-1	10
2		2,5-diisopropylphenol, trifluoro...	274	C14H17F3O2	1000376-41-2	10
3		3-Acetyl-1-(4-acetylphenyl)-4,5-...	259	C13H13N3O3	139455-69-9	10
4		16-Allopregnen-3.beta.-ol-20-one	316	C21H32O2	000566-61-0	9
5		Benzene, 1-(1-heptyldodecyl)-4-m...	358	C26H46	055191-36-1	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG042418\
Data File : BG033963.D
Acq On : 24 Apr 2018 20:42
Operator : SJ/JU
Sample : J2512-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-2-12

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.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...	4.99	4.8 ng		116561	1	7.83	486277	20.0
unknown7.37	7.37	96.6 ng		2348900	1	7.83	486277	20.0
Benzene, (1-methy...	17.90	2.6 ng		163660	4	17.21	1254750	20.0
Benzene, (1-butyl...	18.02	2.2 ng		137794	4	17.21	1254750	20.0
n-Hexadecanoic acid	18.12	6.6 ng		413402	4	17.21	1254750	20.0
Benzene, (1-ethyl...	18.32	4.0 ng		248619	4	17.21	1254750	20.0
Benzene, (1-methy...	18.61	10.8 ng		677185	4	17.21	1254750	20.0
9-Octadecenamide, ...	20.54	3.4 ng		290690	5	21.46	1717160	20.0
5-Eicosene, (E)-	21.16	2.7 ng		235061	5	21.46	1717160	20.0
unknown22.04	22.04	2.3 ng		194730	5	21.46	1717160	20.0
unknown22.30	22.30	2.1 ng		180918	5	21.46	1717160	20.0