

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090319\
 Data File : BG042696.D
 Acq On : 3 Sep 2019 19:46
 Operator : HP/JU
 Sample : K4602-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PAR-D1-D4-(0-3.11)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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	3.116	3	5	18	rVB	100841	130835	9.54%	0.961%
2	5.555	413	420	432	rBV	276627	449773	32.81%	3.302%
3	7.159	686	693	707	rBV	283763	532730	38.86%	3.912%
4	7.529	749	756	766	rBV	311938	545972	39.83%	4.009%
5	7.993	828	835	846	rBV	102756	175526	12.80%	1.289%
6	8.322	884	891	901	rBV	242241	422134	30.79%	3.100%
7	9.162	1026	1034	1051	rBV	162779	322909	23.56%	2.371%
8	10.819	1307	1316	1326	rBV	126952	248449	18.12%	1.824%
9	13.275	1727	1734	1754	rBV	506950	843819	61.56%	6.196%
10	14.109	1869	1876	1890	rBV	39705	75240	5.49%	0.552%
11	14.656	1962	1969	1979	rBV	252147	413745	30.18%	3.038%
12	16.148	2216	2223	2239	rBV	475760	829096	60.48%	6.088%
13	17.405	2431	2437	2442	rBV2	347313	536397	39.13%	3.938%
14	17.447	2442	2444	2450	rVB	33877	48597	3.55%	0.357%
15	17.546	2459	2461	2466	rVB	11925	13993	1.02%	0.103%
16	18.298	2586	2589	2592	rBV4	11407	16549	1.21%	0.122%
17	18.481	2617	2620	2625	rVB4	16933	22945	1.67%	0.168%
18	19.197	2739	2742	2747	rBV	16342	25971	1.89%	0.191%
19	19.462	2782	2787	2794	rBV	262649	370593	27.03%	2.721%
20	19.797	2839	2844	2845	rBV2	64712	89741	6.55%	0.659%
21	19.826	2845	2849	2857	rVV	246219	389440	28.41%	2.859%
22	19.897	2858	2861	2866	rVB3	26753	38758	2.83%	0.285%
23	20.020	2876	2882	2888	rBV	1032656	1370803	100.00%	10.065%
24	20.143	2899	2903	2912	rVB5	22319	57509	4.20%	0.422%
25	20.314	2929	2932	2937	rVB	64703	95147	6.94%	0.699%
26	20.420	2945	2950	2953	rBV	46224	66305	4.84%	0.487%
27	20.472	2955	2959	2963	rVB2	27826	48474	3.54%	0.356%
28	20.613	2980	2983	2987	rBV	28483	40279	2.94%	0.296%
29	21.036	3052	3055	3058	rBV5	14905	24112	1.76%	0.177%
30	21.078	3059	3062	3069	rVB	39787	62707	4.57%	0.460%
31	21.266	3086	3094	3098	rBV3	37461	93492	6.82%	0.686%
32	21.318	3098	3103	3107	rBV2	59953	102593	7.48%	0.753%
33	21.683	3156	3165	3170	rBV3	453788	1090434	79.55%	8.006%
34	21.730	3170	3173	3185	rVB	199290	334348	24.39%	2.455%

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35	21.830	3186	3190	3193	rVB4	18535	26614	1.94%	0.195%
36	21.883	3194	3199	3208	rVB3	60834	111363	8.12%	0.818%
37	21.971	3209	3214	3218	rBV7	13922	27984	2.04%	0.205%
38	22.094	3231	3235	3243	rVB4	25188	57795	4.22%	0.424%
39	22.347	3273	3278	3281	rBV5	15879	30204	2.20%	0.222%
40	22.423	3282	3291	3296	rVV2	42084	105891	7.72%	0.778%
41	22.488	3297	3302	3311	rVB3	36322	72890	5.32%	0.535%
42	22.635	3323	3327	3330	rBV4	8428	14008	1.02%	0.103%
43	22.693	3330	3337	3343	rBV	260756	492266	35.91%	3.614%
44	22.828	3356	3360	3370	rVB4	19125	47671	3.48%	0.350%
45	23.110	3399	3408	3409	rBV5	13716	34292	2.50%	0.252%
46	23.281	3433	3437	3445	rBV4	8236	23340	1.70%	0.171%
47	23.357	3445	3450	3459	rVB6	17747	49165	3.59%	0.361%
48	23.898	3532	3542	3550	rBV2	176684	600155	43.78%	4.407%
49	24.156	3579	3586	3594	rVB2	28828	71268	5.20%	0.523%
50	24.362	3615	3621	3627	rBV6	15428	40795	2.98%	0.300%
51	24.626	3657	3666	3677	rVB	98851	279989	20.43%	2.056%
52	24.773	3681	3691	3705	rVB	129550	378396	27.60%	2.778%
53	24.926	3705	3717	3726	rBV2	248395	799654	58.33%	5.871%
54	26.095	3911	3916	3925	rVB10	10362	27223	1.99%	0.200%
55	28.628	4332	4347	4368	rVB4	40492	219293	16.00%	1.610%
56	29.109	4425	4429	4441	rVB9	9039	28928	2.11%	0.212%
57	29.791	4530	4545	4560	rBV4	30714	150797	11.00%	1.107%

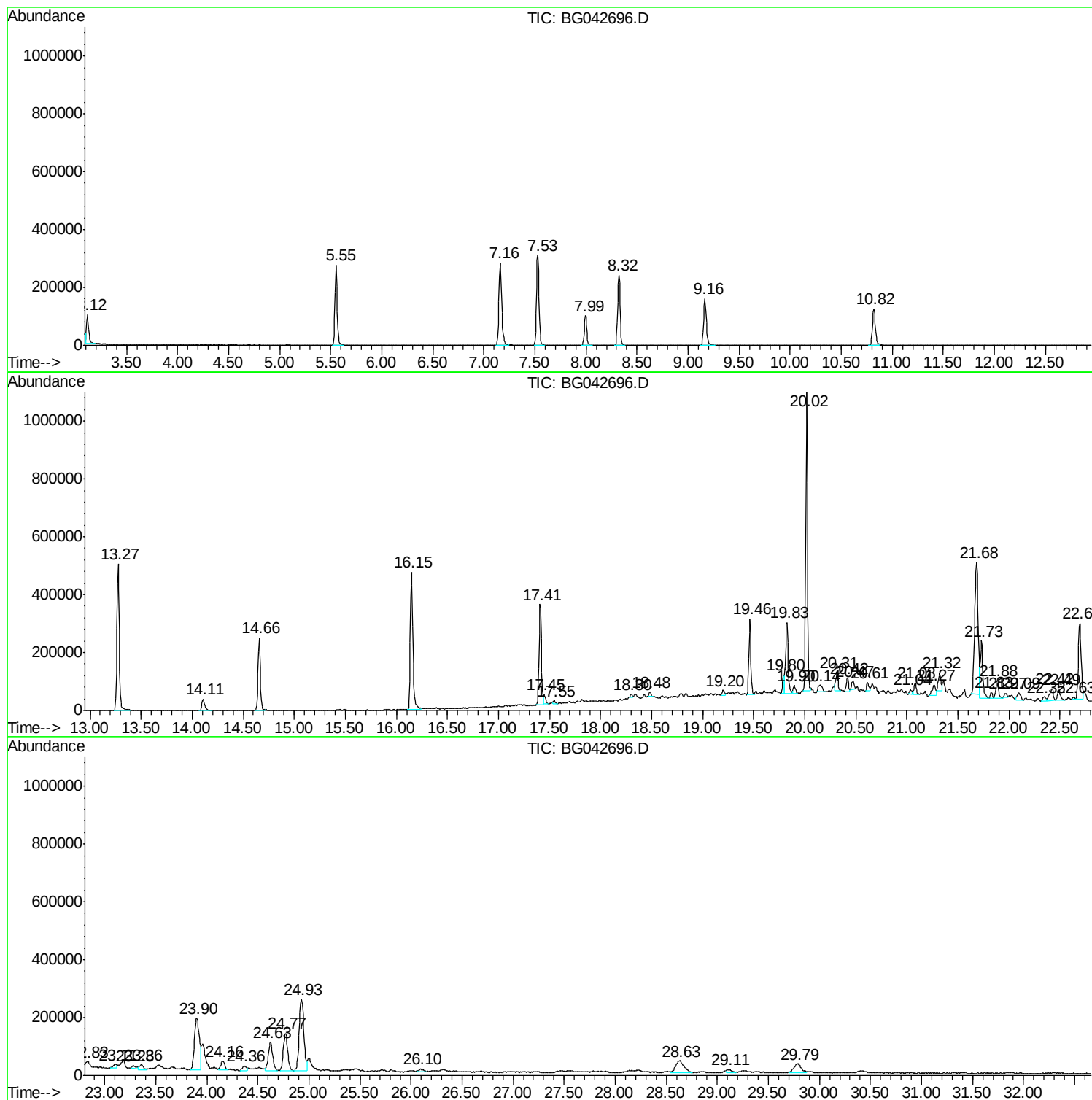
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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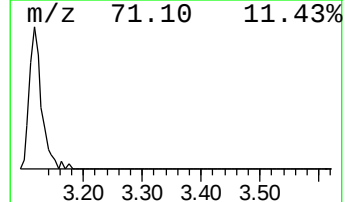
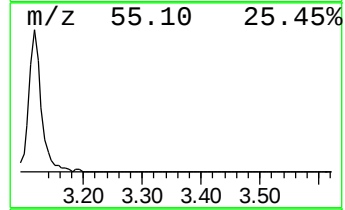
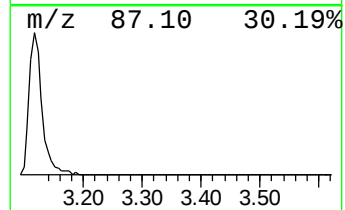
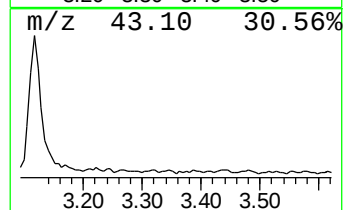
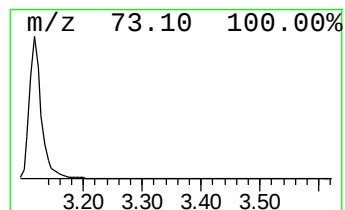
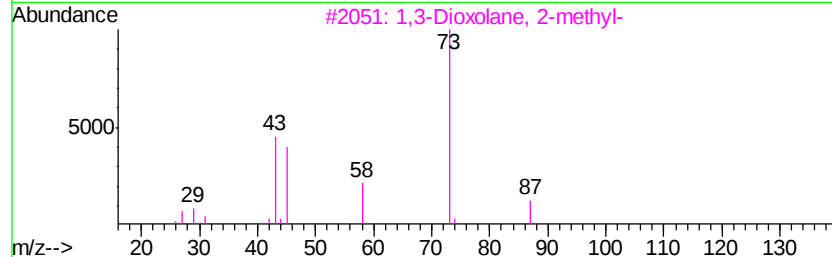
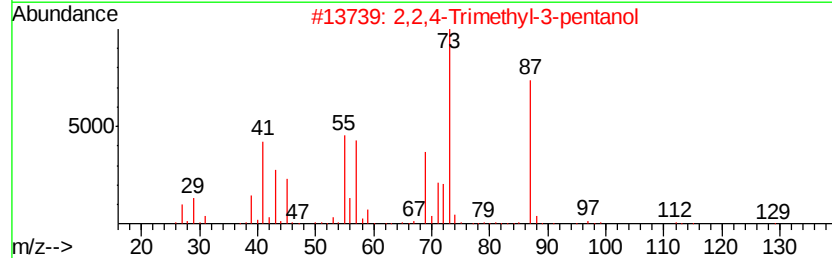
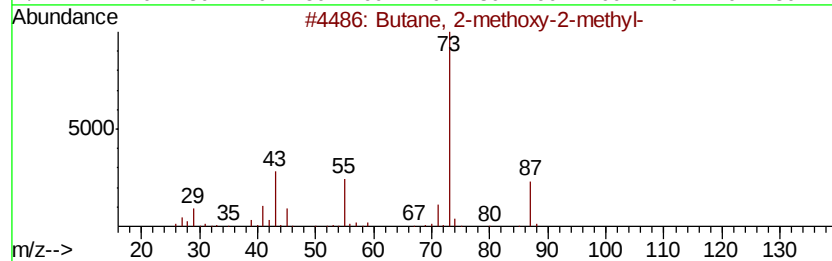
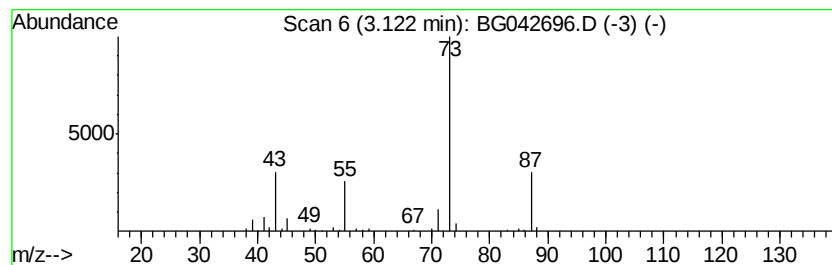
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	14.91 ng	130835	1,4-Dichlorobenzene-d4	8.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	7
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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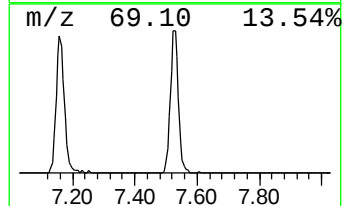
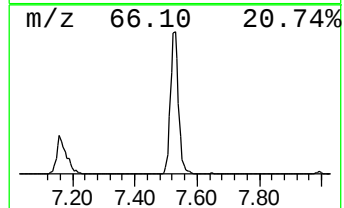
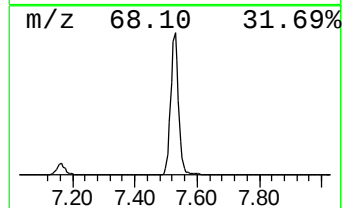
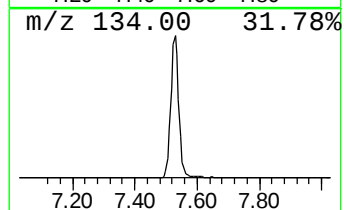
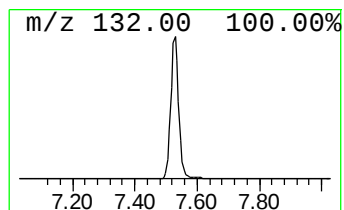
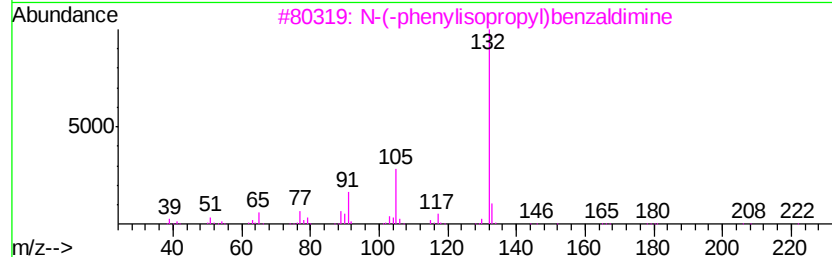
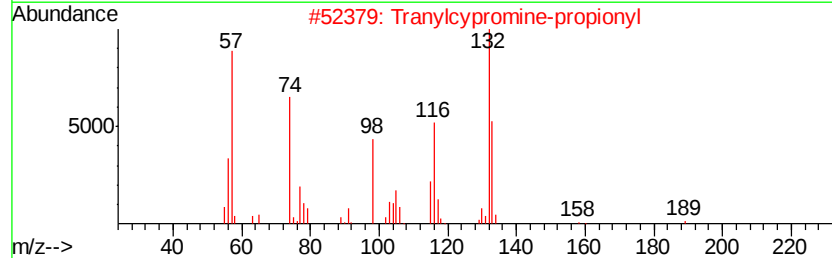
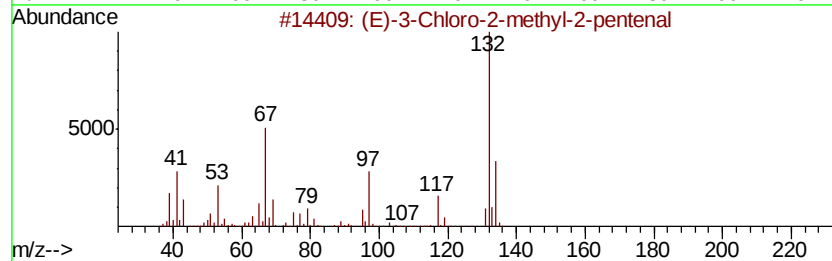
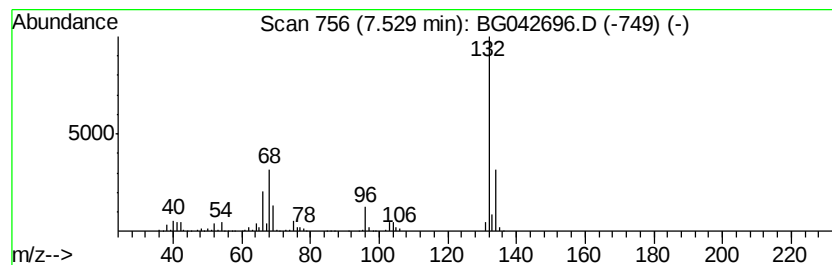
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	62.21 ng	545972	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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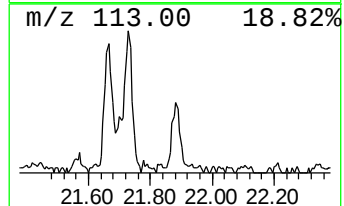
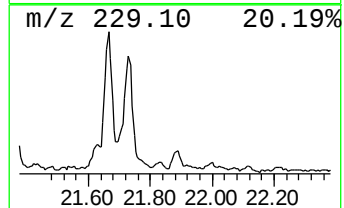
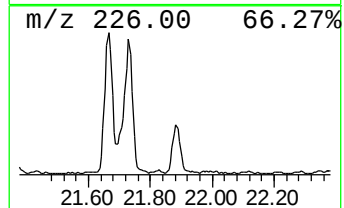
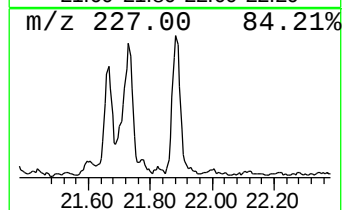
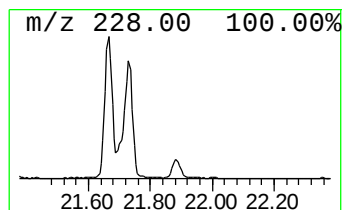
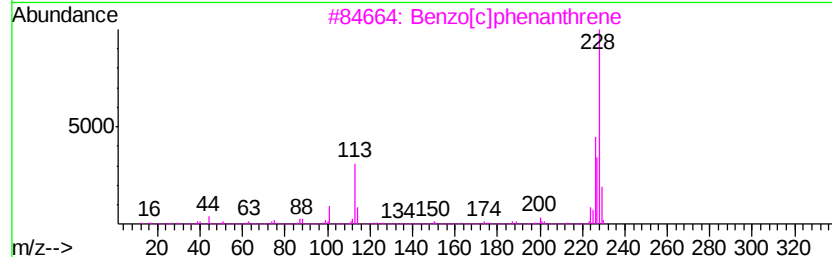
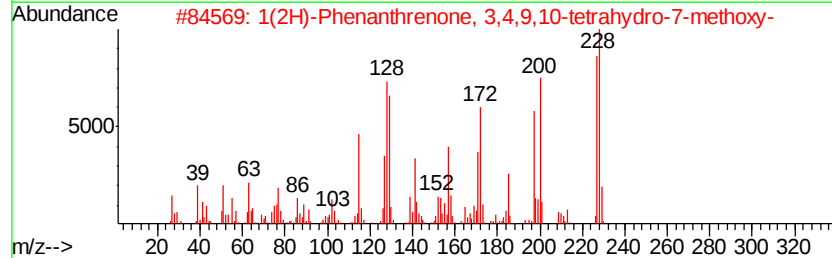
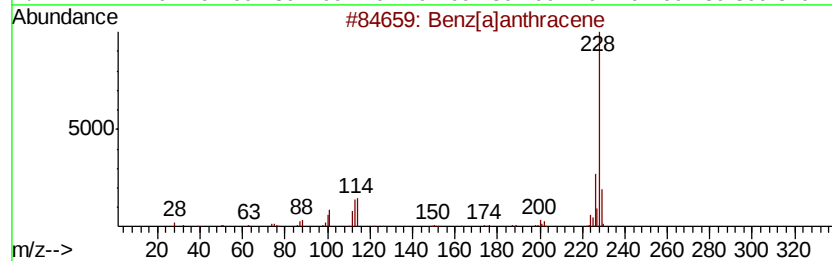
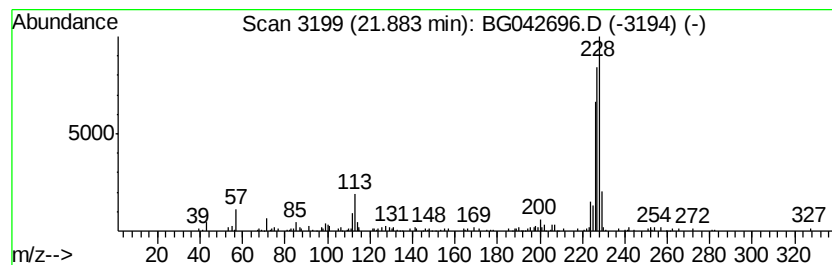
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1(2H)-Phenanthrene, 3,4,9... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	2.04 ng	111363	Chrysene-d12	21.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benz[a]anthracene	228 C18H12	000056-55-3 50
2		1(2H)-Phenanthrene, 3,4,9,10-t...	228 C15H16O2	014427-61-3 50
3		Benzo[c]phenanthrene	228 C18H12	000195-19-7 49
4		Cyclopenta(cd)pyrene, 3,4-dihydro-	228 C18H12	025732-74-5 49
5		Triphenylene	228 C18H12	000217-59-4 45



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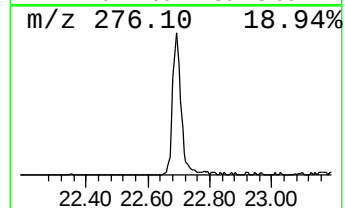
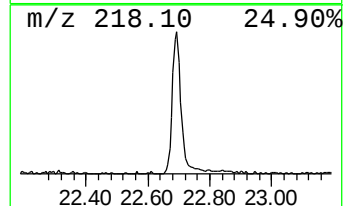
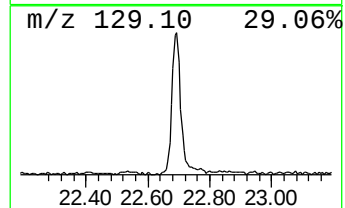
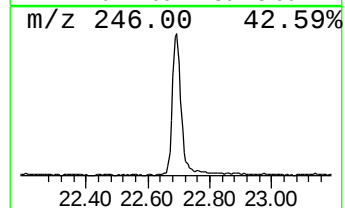
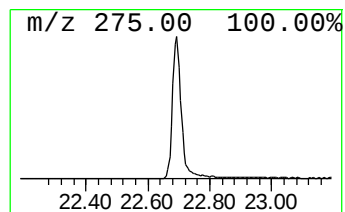
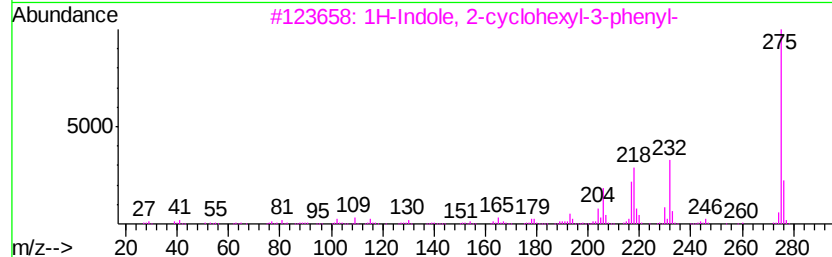
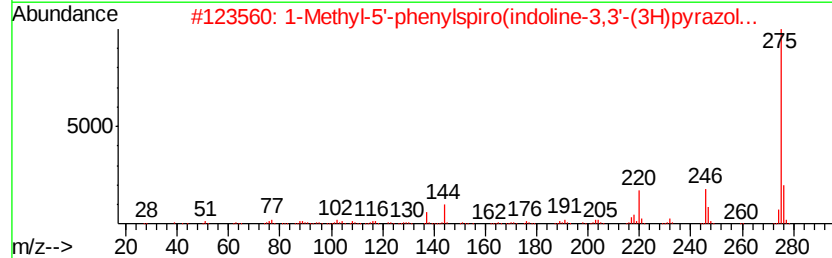
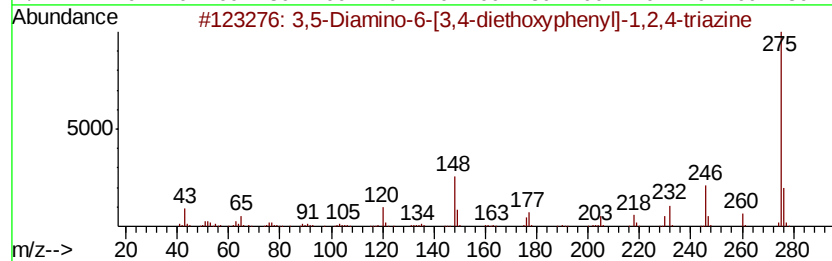
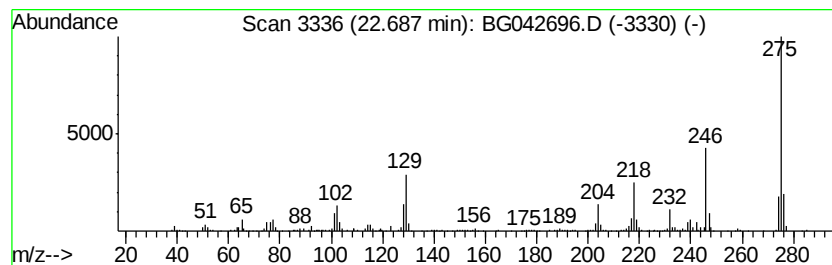
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3,5-Diamino-6-[3,4-diethoxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.69	9.03 ng	492266	Chrysene-d12	21.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Diamino-6-[3,4-diethoxyphenyl]-1H-indole	275	C13H17N5O2	058848-69-4	50
2	1-Methyl-5'-phenylspiro[indoline-3,2'-indole]	275	C17H13N3O	015970-21-5	49
3	1H-Indole, 2-cyclohexyl-3-phenyl-	275	C20H21N	1000163-87-0	49
4	8H-Benzo[<i>a</i>]-1,3-benzodioxolo[6,5- <i>b</i>]indole	275	C17H9NO3	000475-75-2	43
5	4-Pyridinecarboxylic acid, 2,6-dimethyl-	275	C18H13NO2	1000338-16-2	43



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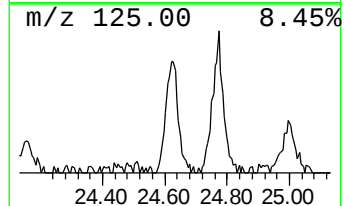
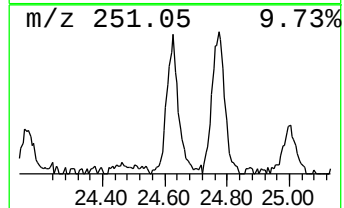
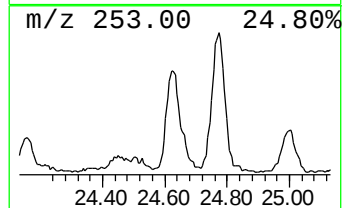
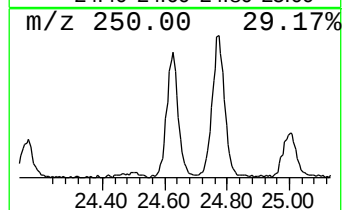
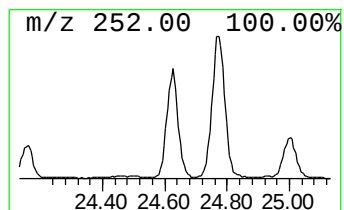
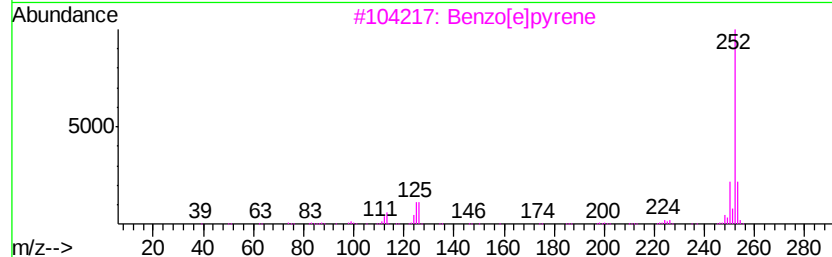
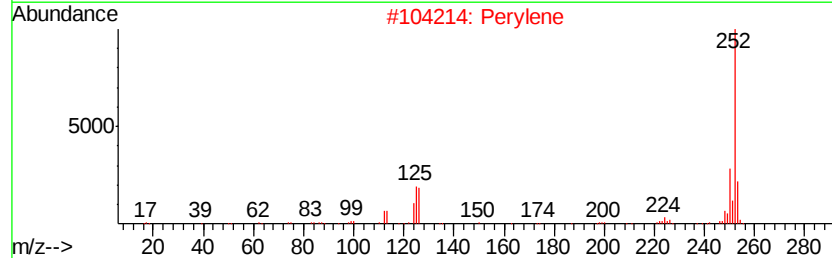
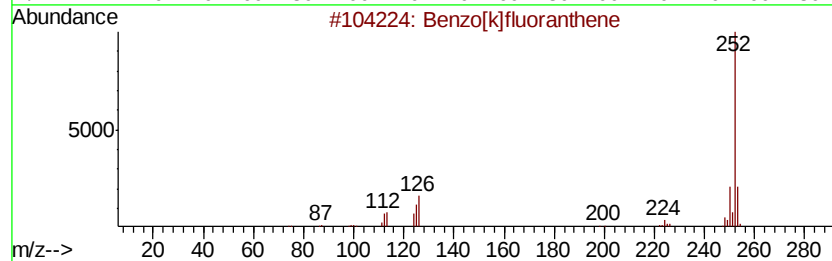
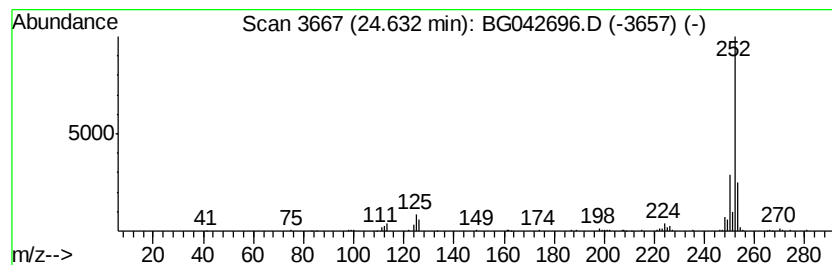
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.63	7.00 ng	279989	Perylene-d12	24.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2		Perylene	252	C20H12	000198-55-0	95
3		Benzo[e]pyrene	252	C20H12	000192-97-2	93
4		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
5		Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG090319\
Data File : BG042696.D
Acq On : 3 Sep 2019 19:46
Operator : HP/JU
Sample : K4602-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PAR-D1-D4-(0-3.11)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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
Butane, 2-methoxy...	3.12	14.9	ng	130835	1	8.00	175526	20.0
unknown7.53	7.53	62.2	ng	545972	1	8.00	175526	20.0
1(2H)-Phenanthren...	21.88	2.0	ng	111363	5	21.68	1090430	20.0
3,5-Diamino-6-[3,...	22.69	9.0	ng	492266	5	21.68	1090430	20.0
Perylene	24.63	7.0	ng	279989	6	24.93	799654	20.0