

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
 Data File : BM016255.D
 Acq On : 08 Aug 2018 18:18
 Operator : SJ/JU
 Sample : J4313-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C-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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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	5.187	316	323	334	rBV	144396	213243	11.79%	1.131%
2	5.664	398	404	422	rBV	797976	1207243	66.76%	6.401%
3	7.305	677	683	698	rBV	776671	1248637	69.05%	6.621%
4	7.663	737	744	755	rBV	850347	1371918	75.87%	7.275%
5	8.134	819	824	836	rBB	203757	336685	18.62%	1.785%
6	8.458	872	879	891	rBB	656345	1049191	58.02%	5.563%
7	9.322	1019	1026	1043	rBV	458773	770344	42.60%	4.085%
8	10.951	1296	1303	1310	rBV	234568	385886	21.34%	2.046%
9	13.392	1711	1718	1724	rBV	1013338	1424488	78.78%	7.553%
10	13.634	1752	1759	1765	rBB2	28826	42053	2.33%	0.223%
11	14.222	1853	1859	1867	rBB	44073	63045	3.49%	0.334%
12	14.769	1945	1952	1959	rBV2	253562	399185	22.08%	2.117%
13	14.834	1959	1963	1968	rVB2	20471	28499	1.58%	0.151%
14	15.816	2123	2130	2134	rBV	17049	25474	1.41%	0.135%
15	16.257	2199	2205	2215	rBV	772501	1053329	58.25%	5.585%
16	17.175	2357	2361	2365	rBV	17178	23297	1.29%	0.124%
17	17.328	2382	2387	2391	rBV2	12925	18237	1.01%	0.097%
18	17.504	2412	2417	2421	rBV	313262	441724	24.43%	2.342%
19	17.551	2421	2425	2431	rVB	377412	521580	28.84%	2.766%
20	17.639	2434	2440	2445	rBV	74015	100039	5.53%	0.530%
21	17.922	2479	2488	2494	rBV2	35110	61581	3.41%	0.327%
22	18.239	2533	2542	2546	rBV6	9130	22080	1.22%	0.117%
23	18.357	2557	2562	2569	rBV3	138018	239519	13.25%	1.270%
24	18.422	2569	2573	2579	rVB2	64967	93425	5.17%	0.495%
25	18.504	2582	2587	2592	rBV	16207	24535	1.36%	0.130%
26	18.569	2592	2598	2602	rBV4	52612	104763	5.79%	0.555%
27	18.604	2602	2604	2608	rVB	26888	26745	1.48%	0.142%
28	18.863	2643	2648	2653	rBV	31889	42503	2.35%	0.225%
29	18.927	2653	2659	2664	rVB2	38852	53754	2.97%	0.285%
30	19.274	2712	2718	2721	rBV2	25289	38208	2.11%	0.203%
31	19.433	2737	2745	2749	rBV2	28633	49904	2.76%	0.265%
32	19.539	2753	2763	2770	rVV	618347	879267	48.63%	4.662%
33	19.616	2772	2776	2785	rVB7	46383	81546	4.51%	0.432%
34	19.863	2814	2818	2821	rBV2	91628	139308	7.70%	0.739%

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35	19.904	2821	2825	2832	rVV	506909	651911	36.05%	3.457%
36	19.969	2832	2836	2841	rVB	31910	39509	2.18%	0.209%
37	20.086	2850	2856	2861	rBV	1584696	1808235	100.00%	9.588%
38	20.151	2863	2867	2871	rVB2	26616	40056	2.22%	0.212%
39	20.216	2871	2878	2885	rBV7	41119	105375	5.83%	0.559%
40	20.357	2895	2902	2904	rBV7	43750	82964	4.59%	0.440%
41	20.386	2904	2907	2913	rVB	60586	87026	4.81%	0.461%
42	20.486	2920	2924	2927	rBV2	36075	51102	2.83%	0.271%
43	20.545	2928	2934	2937	rVV2	45169	75251	4.16%	0.399%
44	20.686	2954	2958	2961	rBV3	28438	38771	2.14%	0.206%
45	20.727	2962	2965	2967	rVV2	27267	27194	1.50%	0.144%
46	21.133	3030	3034	3038	rBV	76989	106816	5.91%	0.566%
47	21.286	3057	3060	3061	rBV2	63781	68949	3.81%	0.366%
48	21.368	3071	3074	3078	rBV3	47009	73757	4.08%	0.391%
49	21.427	3081	3084	3087	rVB	78927	93418	5.17%	0.495%
50	21.633	3113	3119	3123	rBV2	530511	1019878	56.40%	5.408%
51	21.674	3123	3126	3131	rVB	281367	353448	19.55%	1.874%
52	23.274	3393	3398	3403	rBV	184701	374208	20.69%	1.984%
53	23.774	3479	3483	3493	rVB	163099	317034	17.53%	1.681%
54	23.874	3496	3500	3509	rVB	204742	382161	21.13%	2.026%
55	23.974	3512	3517	3523	rBV	266258	480974	26.60%	2.550%

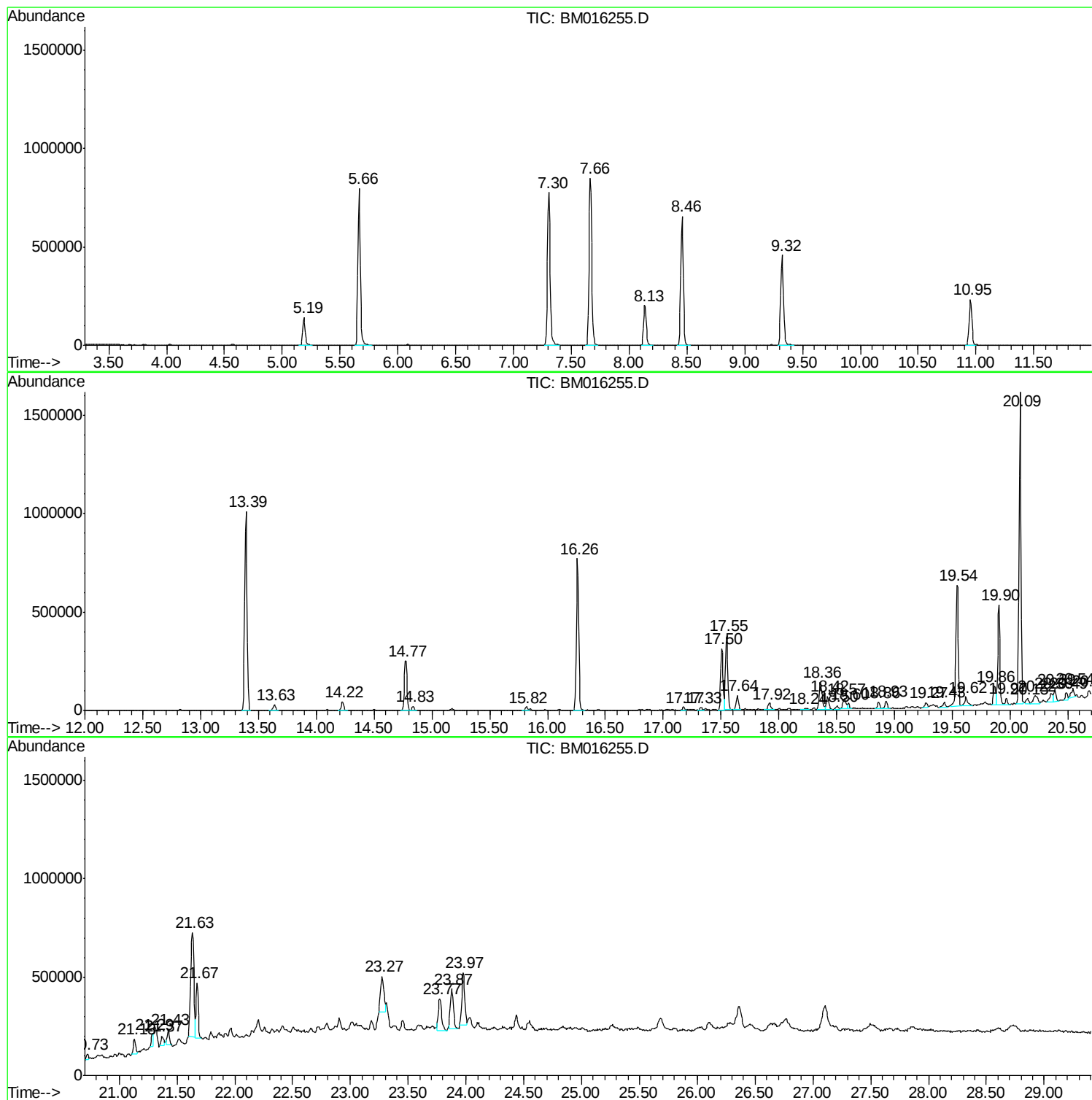
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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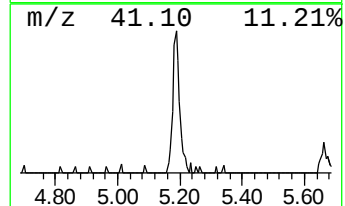
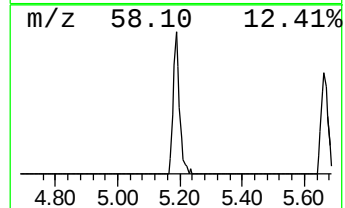
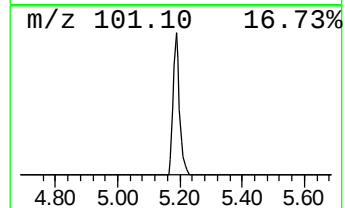
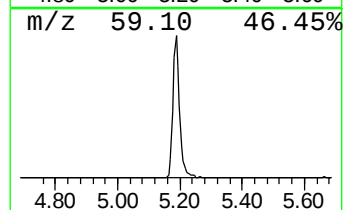
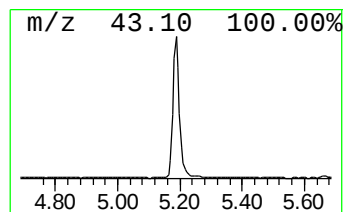
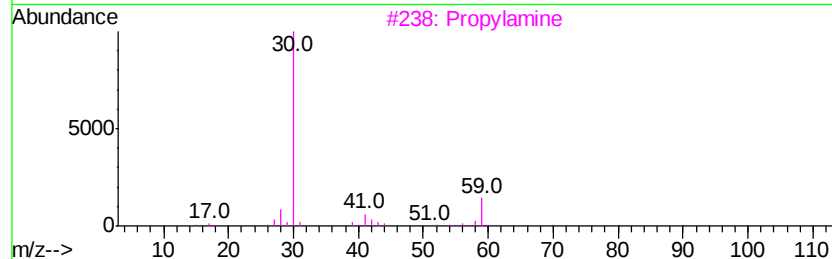
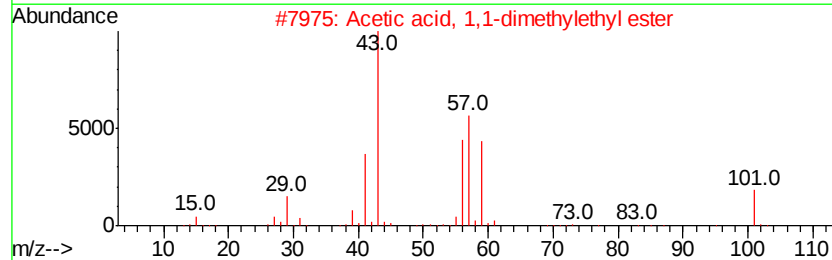
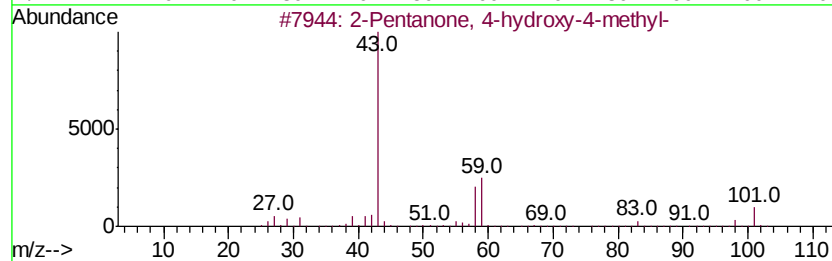
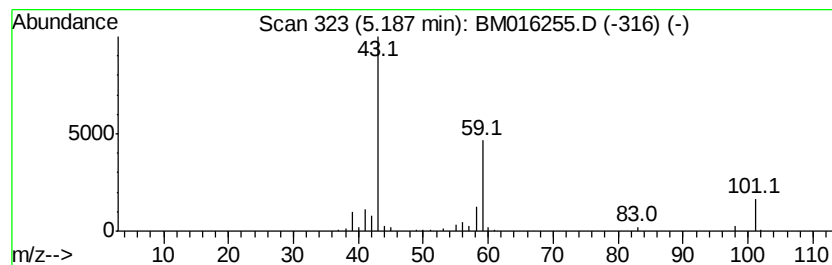
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	12.67 ng	213243	1,4-Dichlorobenzene-d4	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		Propylamine	59	C3H9N	000107-10-8	40
4		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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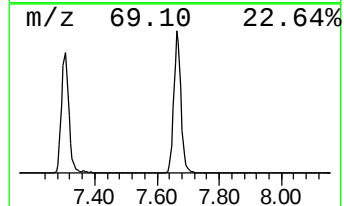
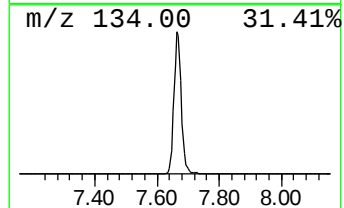
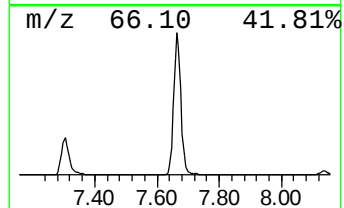
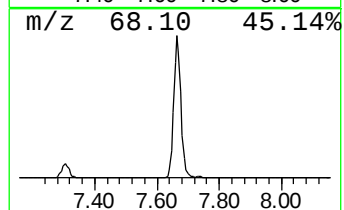
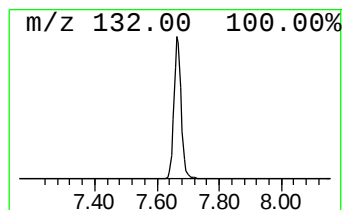
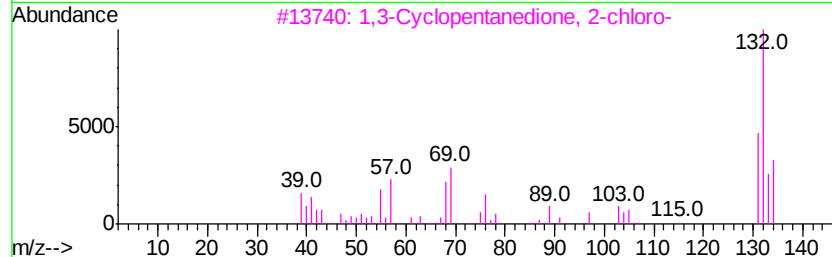
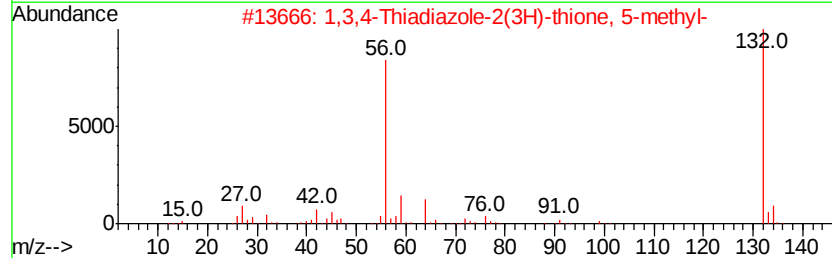
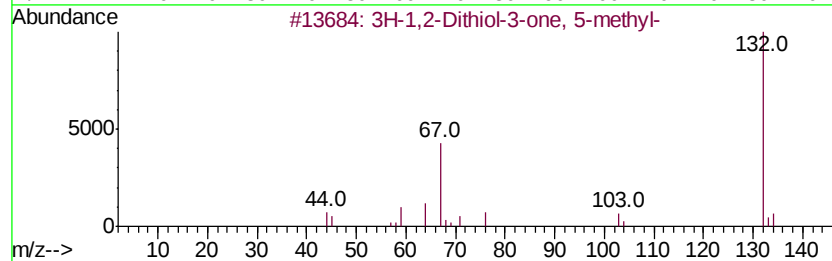
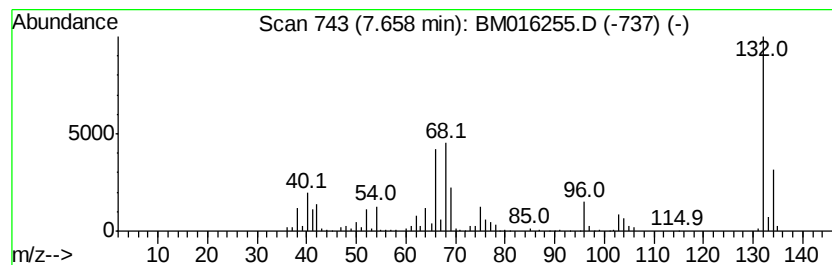
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	81.50 ng	1371920	1,4-Dichlorobenzene-d4	8.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14		
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14		
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12		
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10		
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9		



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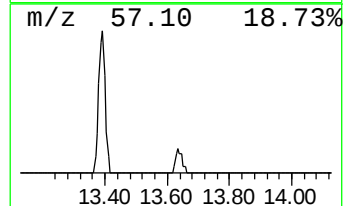
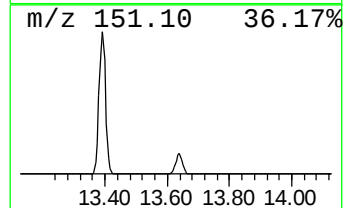
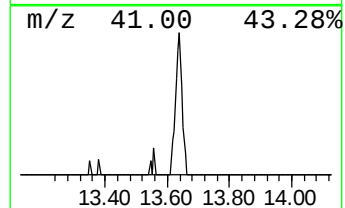
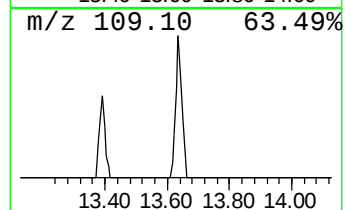
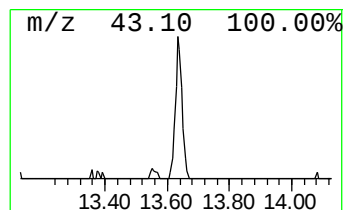
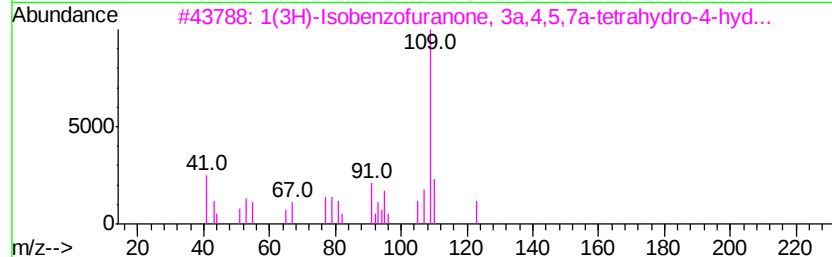
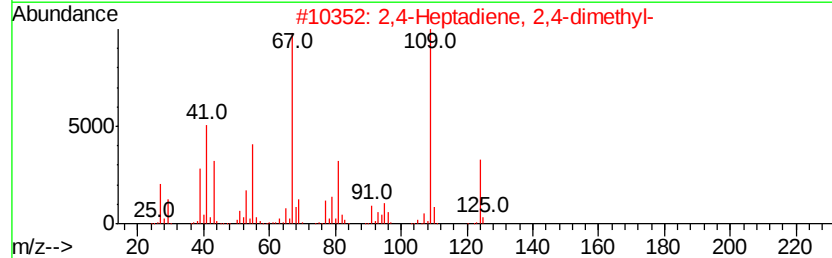
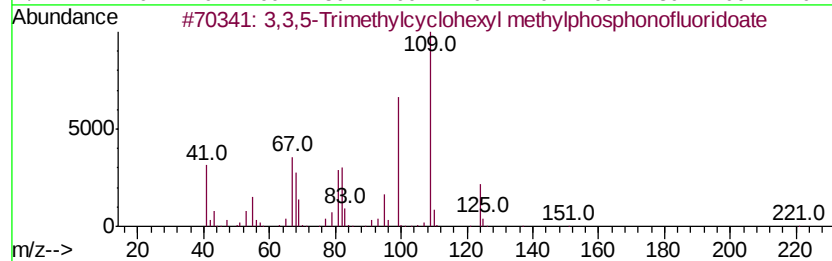
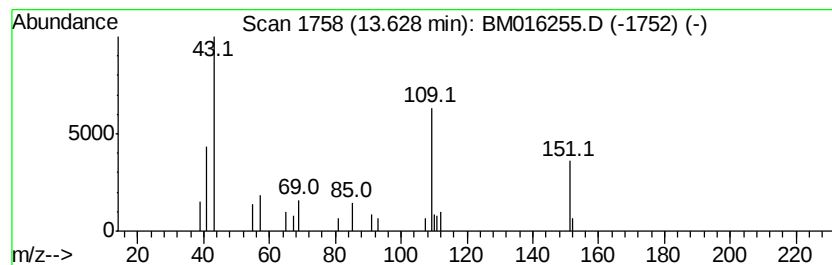
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 3,3,5-Trimethylcyclohexyl m... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.11 ng	42053	Acenaphthene-d10	14.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3,5-Trimethylcyclohexyl methyl...	222	C10H20F02P	1000298-38-1	25
2			2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	074421-05-9	25
3			1(3H)-Isobenzofuranone, 3a,4,5,7...	182	C10H14O3	054346-06-4	17
4			3,3,5,5-Tetramethylcyclopentene	124	C9H16	038667-10-6	12
5			2-Hydrazinopyridine	109	C5H7N3	004930-98-7	12



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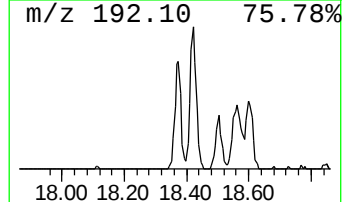
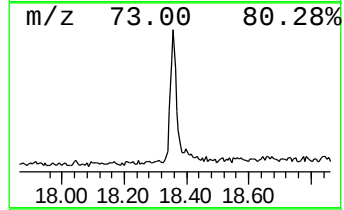
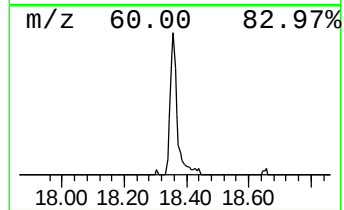
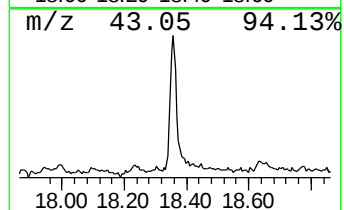
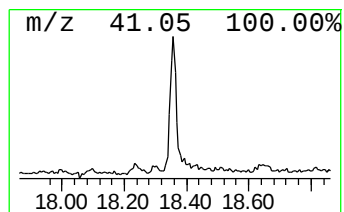
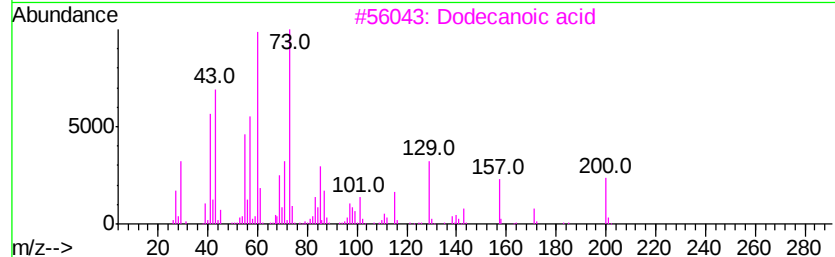
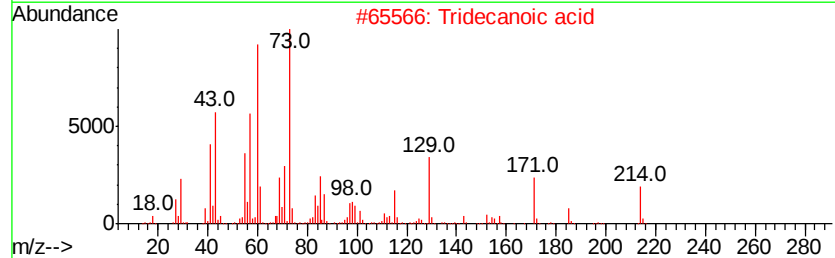
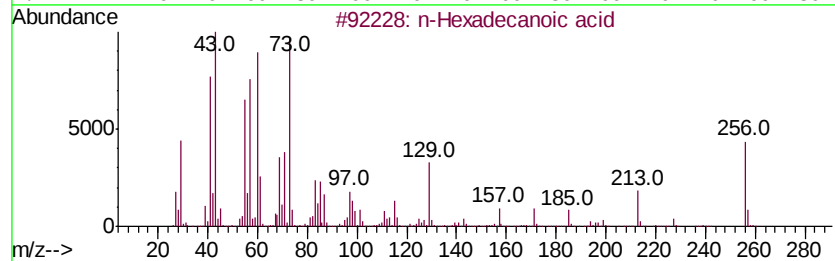
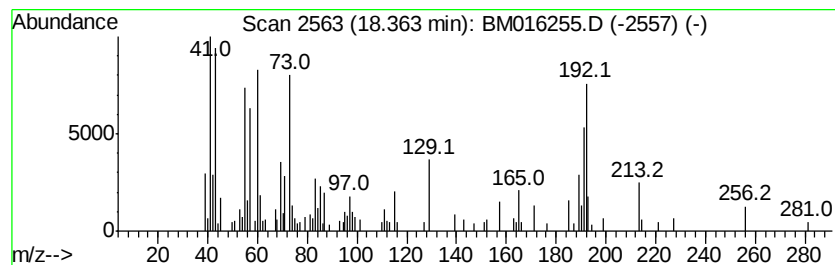
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	10.84 ng	239519	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	50



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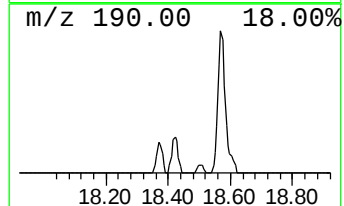
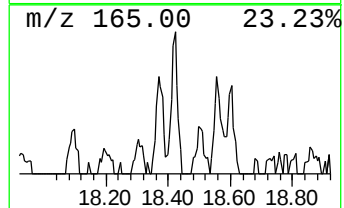
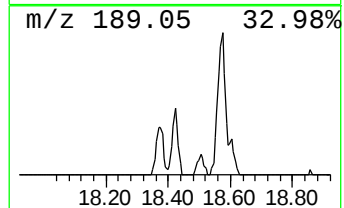
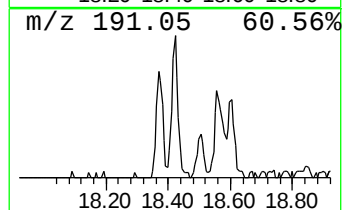
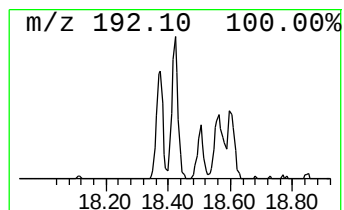
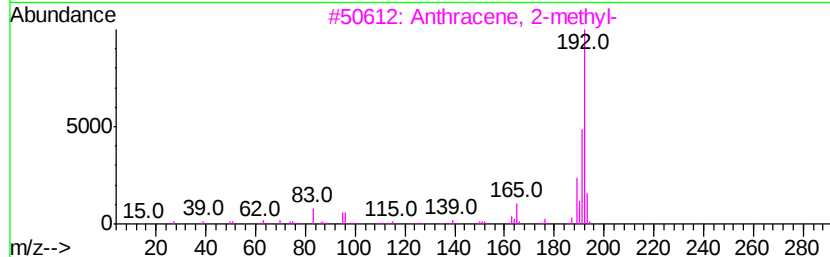
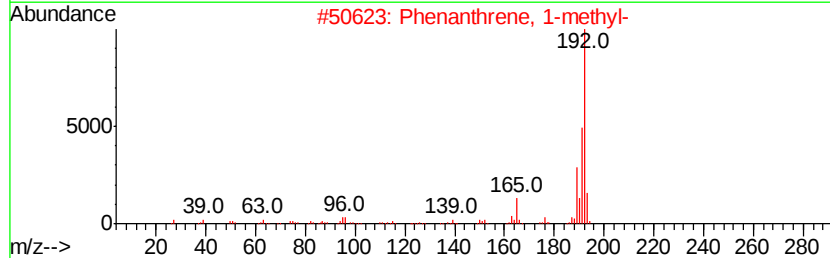
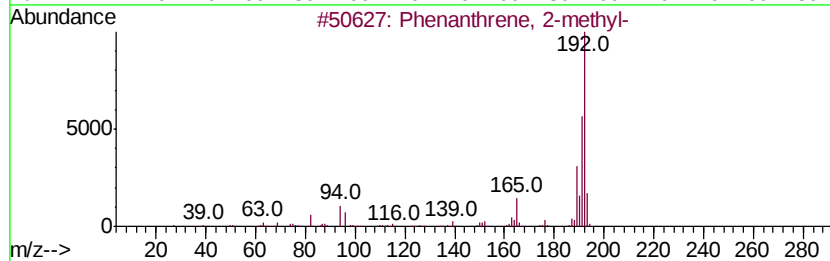
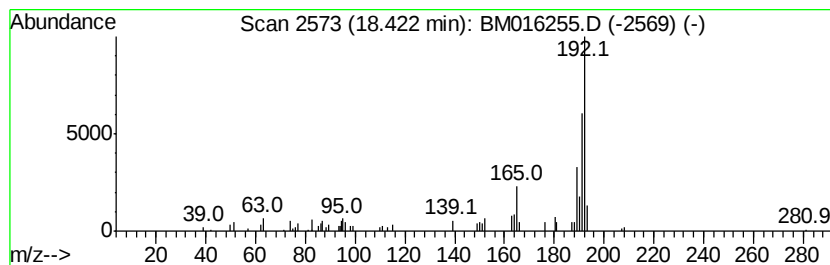
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.42	4.23 ng	93425	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016255.D
Acq On : 08 Aug 2018 18:18
Operator : SJ/JU
Sample : J4313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C-12

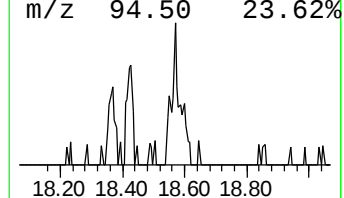
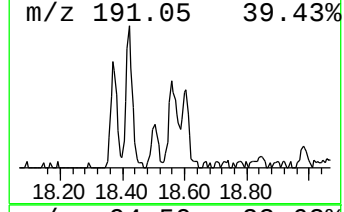
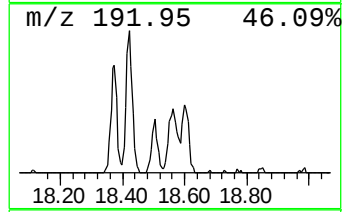
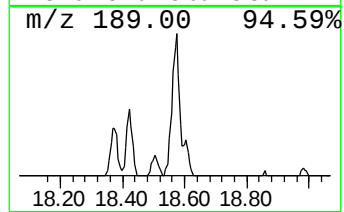
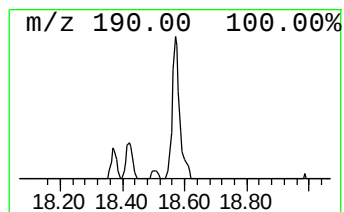
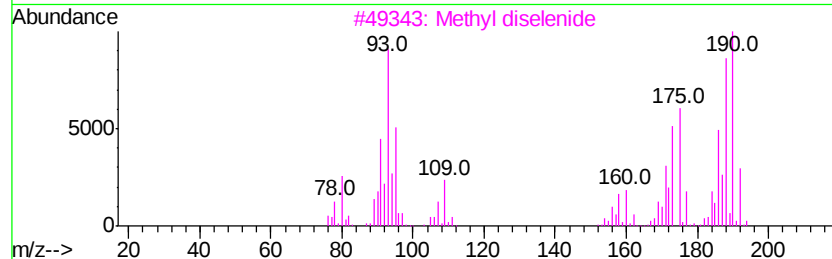
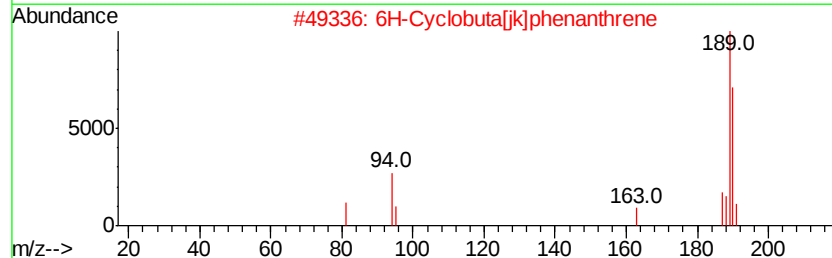
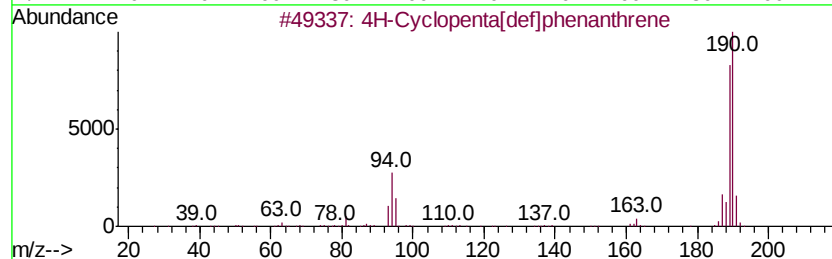
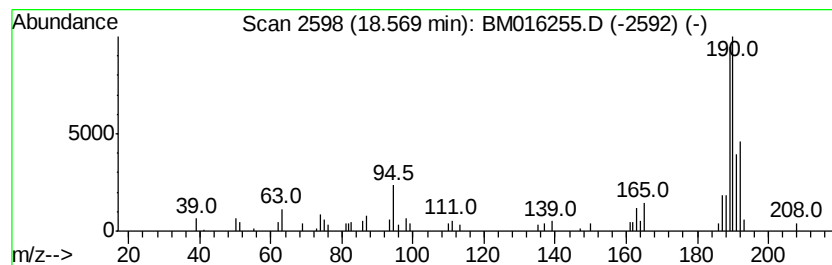
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	4.74 ng	104763	Phenanthrene-d10	17.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2		6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	52
3		Methyl diselenide	190	C2H6Se2	007101-31-7	41
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
5		4,4'-Difluorobiphenyl	190	C12H8F2	000398-23-2	23



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016255.D
Acq On : 08 Aug 2018 18:18
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Sample : J4313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

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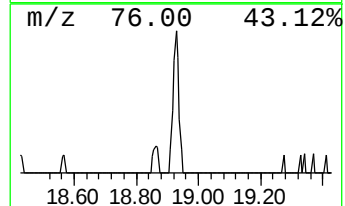
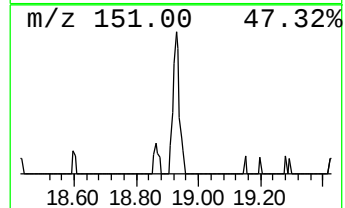
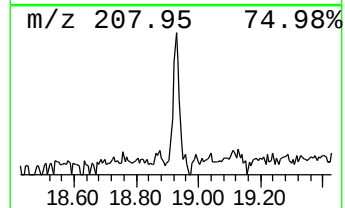
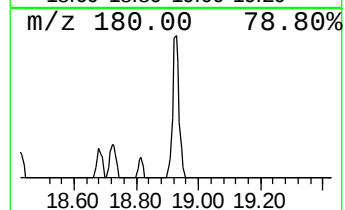
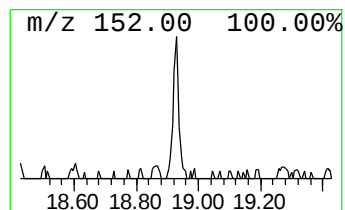
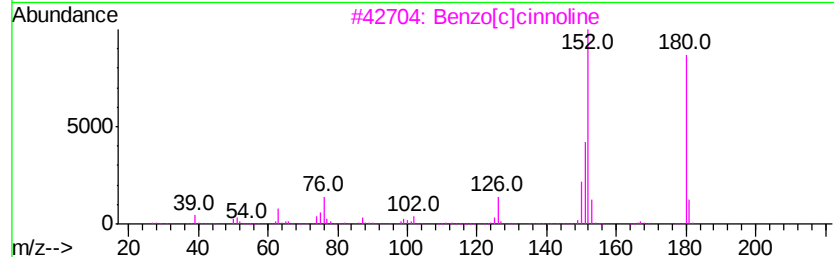
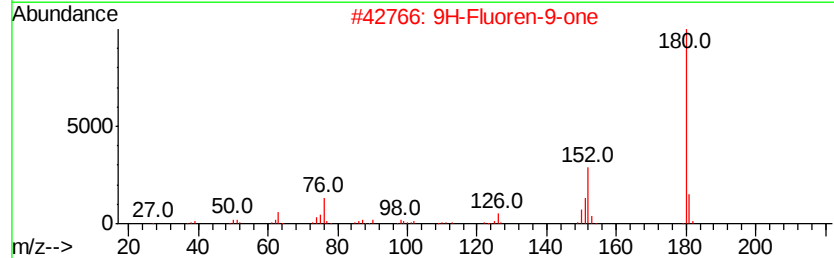
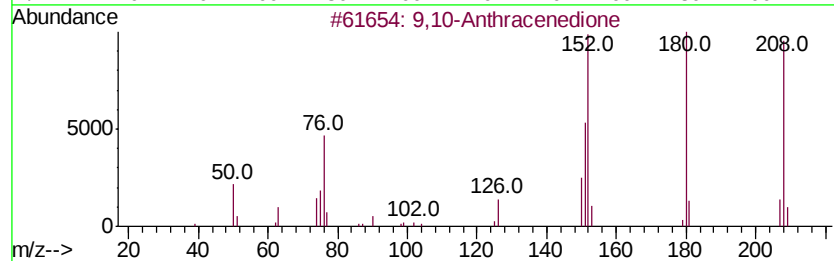
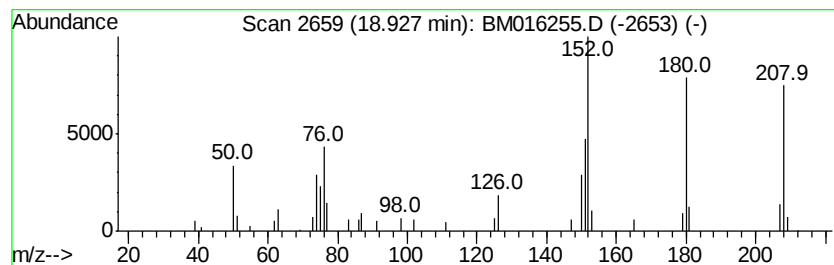
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,10-Anthracenedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.93	2.43 ng	53754	Phenanthrene-d10		17.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	96		
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	96		
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	70		
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	70		
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	52		



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016255.D
Acq On : 08 Aug 2018 18:18
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Sample : J4313-15
Misc :
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Instrument :
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ClientSampleId :
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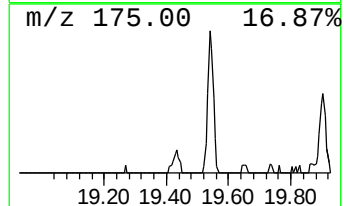
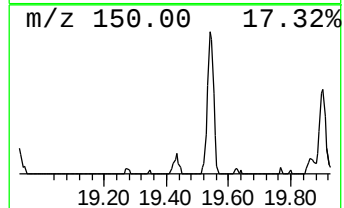
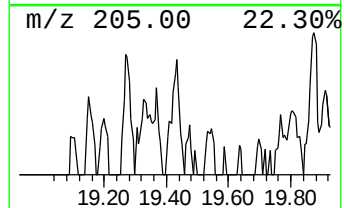
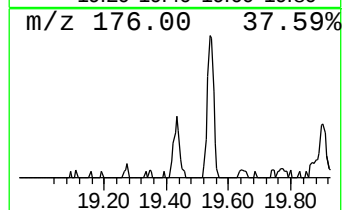
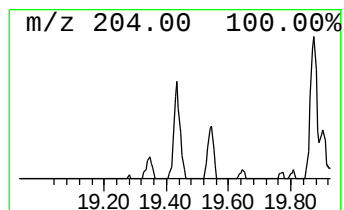
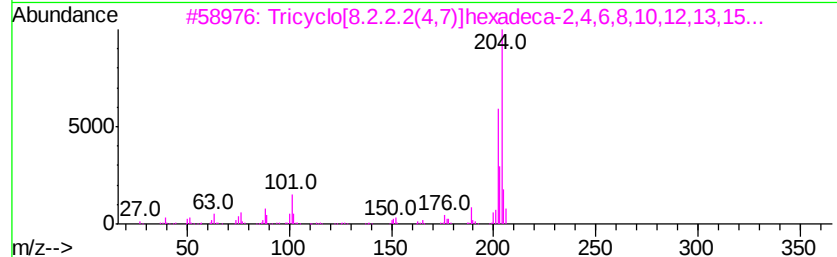
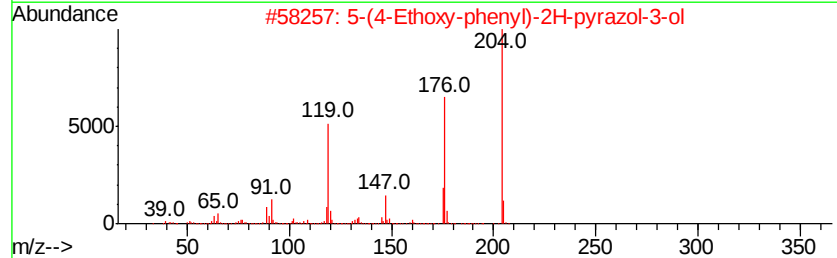
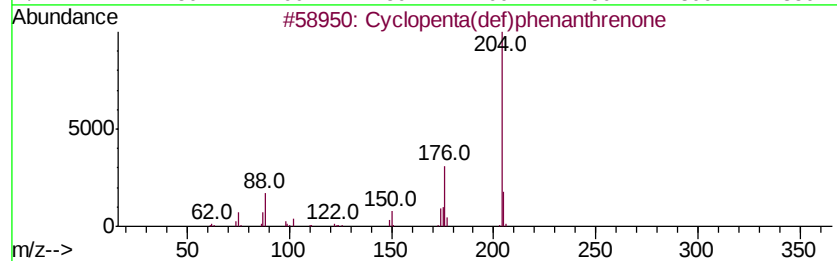
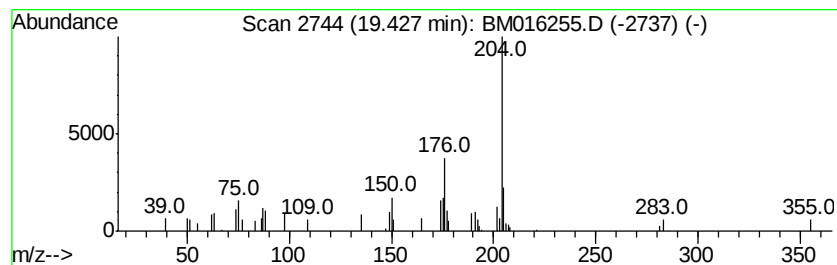
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	2.26 ng	49904	Phenanthrene-d10	17.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	64
2		5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	47
3		Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	43
4		2-Phenylnaphthalene	204	C16H12	035465-71-5	43
5		9-Acridinecarbonitrile	204	C14H8N2	005326-19-2	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016255.D
Acq On : 08 Aug 2018 18:18
Operator : SJ/JU
Sample : J4313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

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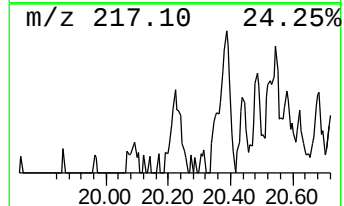
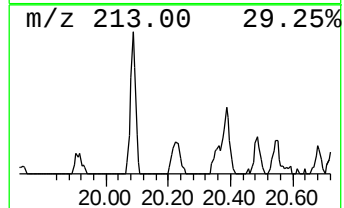
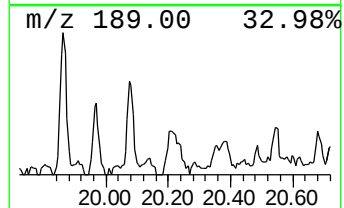
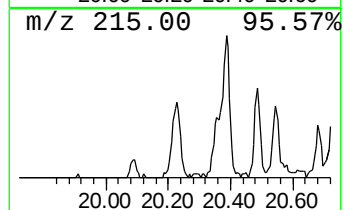
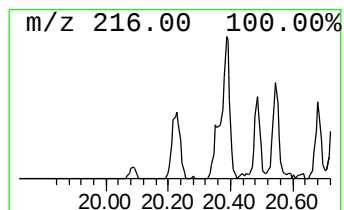
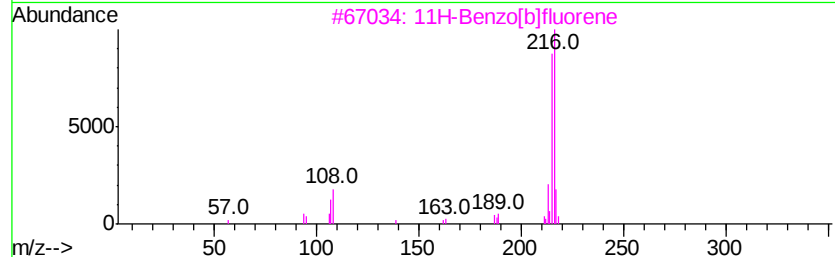
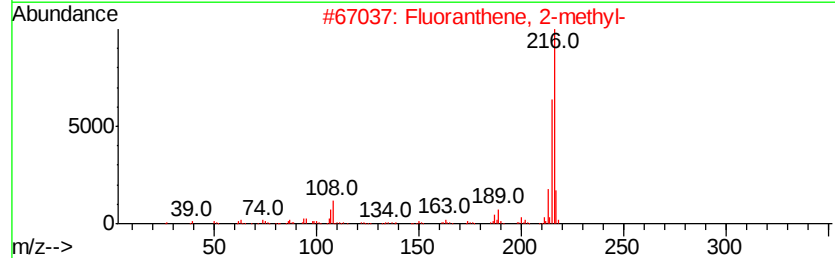
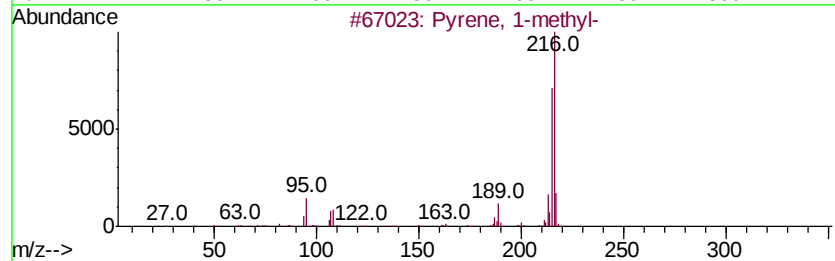
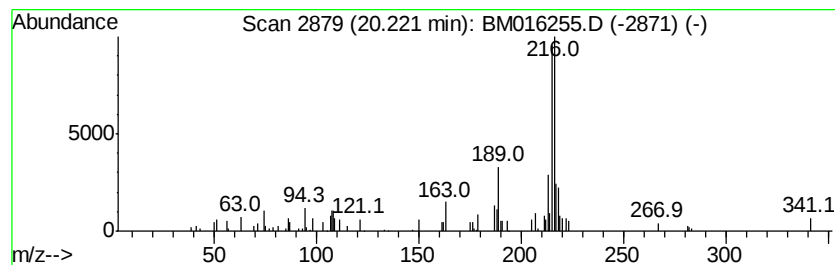
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	2.07 ng	105375	Chrysene-d12	21.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	70
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	62
5			Pyrene, 4-methyl-	216	C17H12	003353-12-6	55



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
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Sample : J4313-15
Misc :
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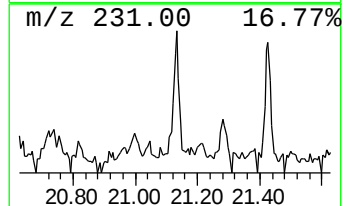
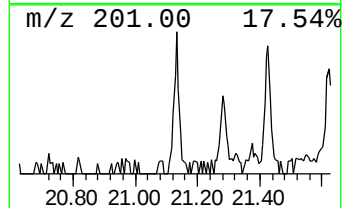
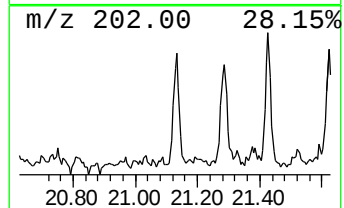
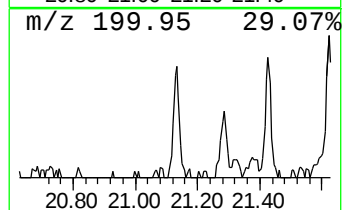
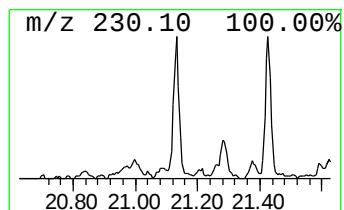
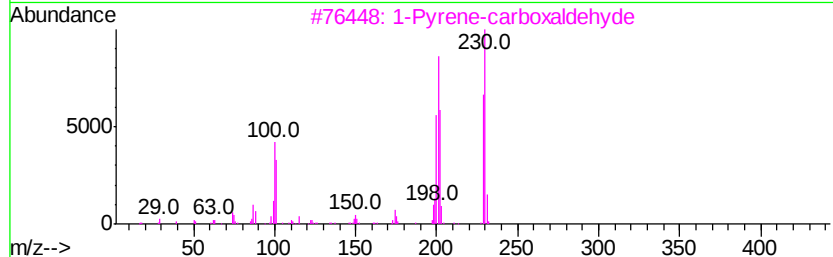
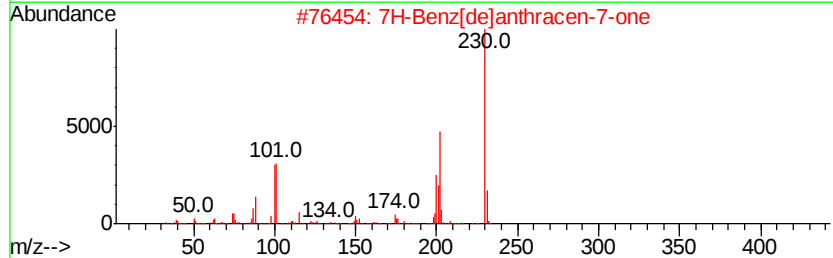
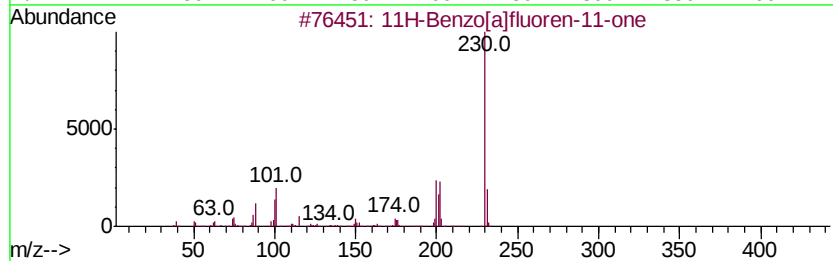
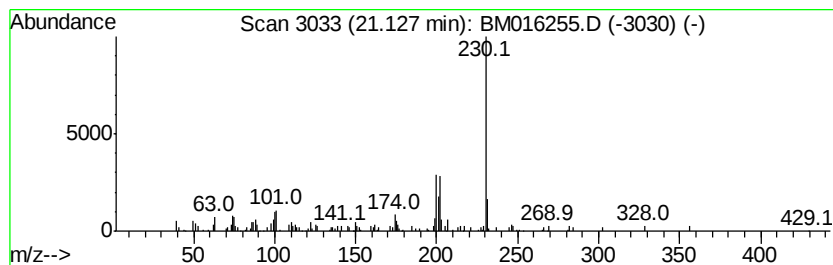
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 11H-Benzo[a]fluoren-11-one Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.13	2.09 ng	106816	Chrysene-d12	21.64		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	95
2		7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	81
3		1-Pyrene-carboxaldehyd	230	C17H10O	003029-19-4	64
4		o-Terphenyl	230	C18H14	000084-15-1	49
5		Benzene, 1-phenyl-4-(2,2-dicyano...	230	C16H10N2	026089-09-8	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080818\
Data File : BM016255.D
Acq On : 08 Aug 2018 18:18
Operator : SJ/JU
Sample : J4313-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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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unknown7.66	7.66	81.5	ng	1371920	1	8.14	336685	20.0
3,3,5-Trimethylcy...	13.63	2.1	ng	42053	3	14.77	399185	20.0
n-Hexadecanoic acid	18.36	10.8	ng	239519	4	17.50	441724	20.0
Phenanthrene, 2-m...	18.42	4.2	ng	93425	4	17.50	441724	20.0
4H-Cyclopenta[def...	18.57	4.7	ng	104763	4	17.50	441724	20.0
9,10-Anthracenedione	18.93	2.4	ng	53754	4	17.50	441724	20.0
Cyclopenta(def)ph...	19.43	2.3	ng	49904	4	17.50	441724	20.0
Pyrene, 1-methyl-	20.22	2.1	ng	105375	5	21.64	1019880	20.0
11H-Benzo[a]fluor...	21.13	2.1	ng	106816	5	21.64	1019880	20.0