

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
 Data File : BM039075.D
 Acq On : 21 Mar 2023 18:58
 Operator : CG/JU
 Sample : 02001-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 IRV-3

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:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039075.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	295	301	309	rBV	2442724	3307349	26.11%	2.748%
2	5.522	373	380	391	rBV	5722790	7973252	62.93%	6.625%
3	7.128	645	653	668	rBV	5400326	8400810	66.31%	6.980%
4	7.969	787	796	803	rBV	1105786	1721865	13.59%	1.431%
5	9.133	985	994	1006	rBV	3157827	5193511	40.99%	4.315%
6	10.780	1266	1274	1281	rBV	1424476	2366548	18.68%	1.966%
7	13.233	1684	1691	1700	rBV	6963450	10034583	79.20%	8.338%
8	14.327	1870	1877	1890	rBV	253172	448505	3.54%	0.373%
9	14.604	1916	1924	1931	rBV	1864947	2834290	22.37%	2.355%
10	14.668	1931	1935	1943	rVB	82734	130972	1.03%	0.109%
11	15.962	2147	2155	2164	rVB	699149	960096	7.58%	0.798%
12	16.092	2169	2177	2187	rBV	5380924	7479245	59.03%	6.215%
13	17.351	2385	2391	2395	rBV	2258288	3134577	24.74%	2.605%
14	17.392	2395	2398	2405	rVV	807089	1059302	8.36%	0.880%
15	17.480	2408	2413	2418	rVV	291726	432206	3.41%	0.359%
16	18.245	2536	2543	2546	rBV2	694793	1161460	9.17%	0.965%
17	18.274	2546	2548	2553	rVB	291679	379701	3.00%	0.316%
18	18.356	2558	2562	2566	rVV	125239	206866	1.63%	0.172%
19	18.421	2567	2573	2577	rVV2	326968	649447	5.13%	0.540%
20	18.456	2577	2579	2585	rVB	194165	239245	1.89%	0.199%
21	18.727	2621	2625	2629	rBV	169958	213781	1.69%	0.178%
22	19.145	2691	2696	2701	rBV	253898	449531	3.55%	0.374%
23	19.203	2701	2706	2709	rVV3	141050	285858	2.26%	0.238%
24	19.233	2709	2711	2715	rVB	116047	129875	1.03%	0.108%
25	19.280	2715	2719	2730	rBV2	160359	321863	2.54%	0.267%
26	19.403	2735	2740	2747	rVB	3333962	4331340	34.19%	3.599%
27	19.515	2754	2759	2763	rBV2	339255	530539	4.19%	0.441%
28	19.556	2763	2766	2770	rVB	116409	155250	1.23%	0.129%
29	19.739	2792	2797	2798	rBV	543539	734676	5.80%	0.610%
30	19.768	2798	2802	2810	rVV	3295486	4447036	35.10%	3.695%
31	19.839	2810	2814	2821	rVB2	174835	297381	2.35%	0.247%
32	19.974	2829	2837	2842	rBV	9865260	12669404	100.00%	10.527%
33	20.097	2852	2858	2864	rBV2	297312	744732	5.88%	0.619%
34	20.233	2875	2881	2882	rBV3	242343	433240	3.42%	0.360%
35	20.262	2882	2886	2892	rVB3	557832	978419	7.72%	0.813%
36	20.362	2899	2903	2907	rBV	320024	426725	3.37%	0.355%

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Min Area: 3 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	20.421	2907	2913	2917	rVV2	472493	756651	5.97%	0.629%
38	20.562	2933	2937	2940	rBV	287576	355416	2.81%	0.295%
39	20.609	2941	2945	2948	rVV	272963	367486	2.90%	0.305%
40	20.662	2951	2954	2958	rVB	287384	330657	2.61%	0.275%
41	20.774	2970	2973	2976	rVB	292212	300294	2.37%	0.250%
42	21.009	3009	3013	3019	rVB	325534	442277	3.49%	0.368%
43	21.174	3039	3041	3044	rVB	252448	269529	2.13%	0.224%
44	21.233	3045	3051	3059	rVV5	1436033	2759324	21.78%	2.293%
45	21.303	3060	3063	3071	rVB2	395535	578958	4.57%	0.481%
46	21.527	3094	3101	3105	rBV2	3798675	8093976	63.89%	6.726%
47	21.568	3105	3108	3118	rVB	2531344	3264546	25.77%	2.713%
48	21.686	3125	3128	3135	rVB2	652897	855534	6.75%	0.711%
49	22.115	3198	3201	3204	rVB	368817	431701	3.41%	0.359%
50	22.150	3204	3207	3208	rBV	341952	355310	2.80%	0.295%
51	22.656	3290	3293	3305	rVB3	346202	721056	5.69%	0.599%
52	23.221	3383	3389	3395	rBV	1999002	5100118	40.26%	4.238%
53	23.750	3473	3479	3489	rVB	1174655	2386935	18.84%	1.983%
54	23.856	3491	3497	3506	rVB	1934588	3718849	29.35%	3.090%
55	23.962	3509	3515	3521	rBV	1992604	3995111	31.53%	3.320%

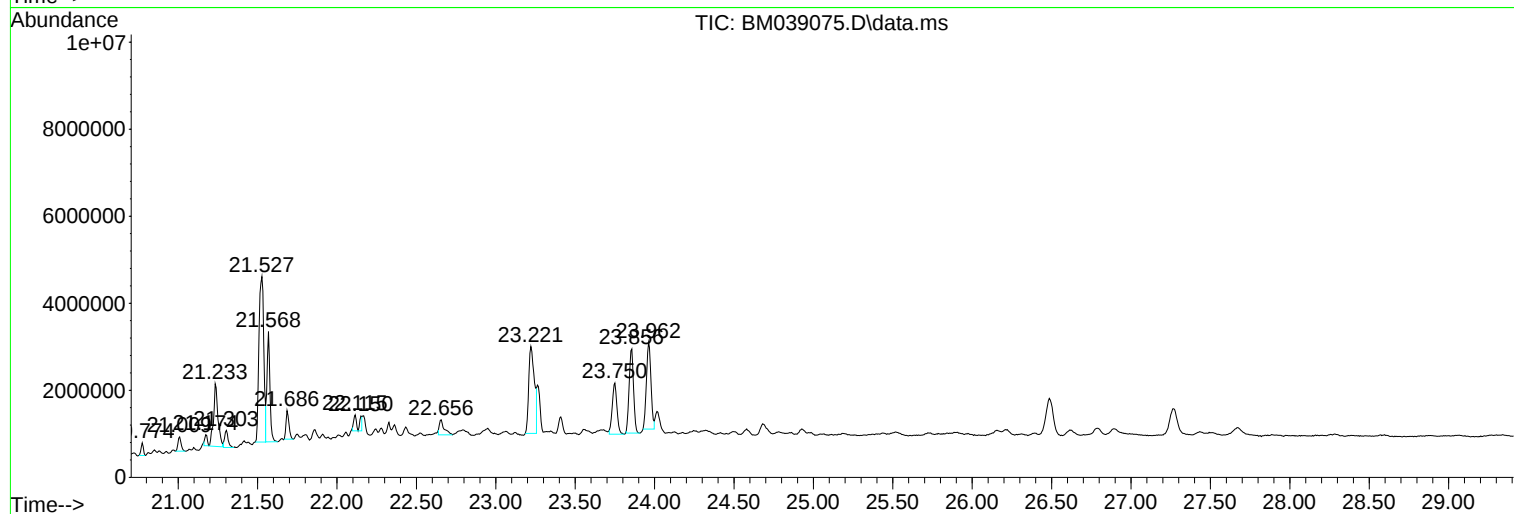
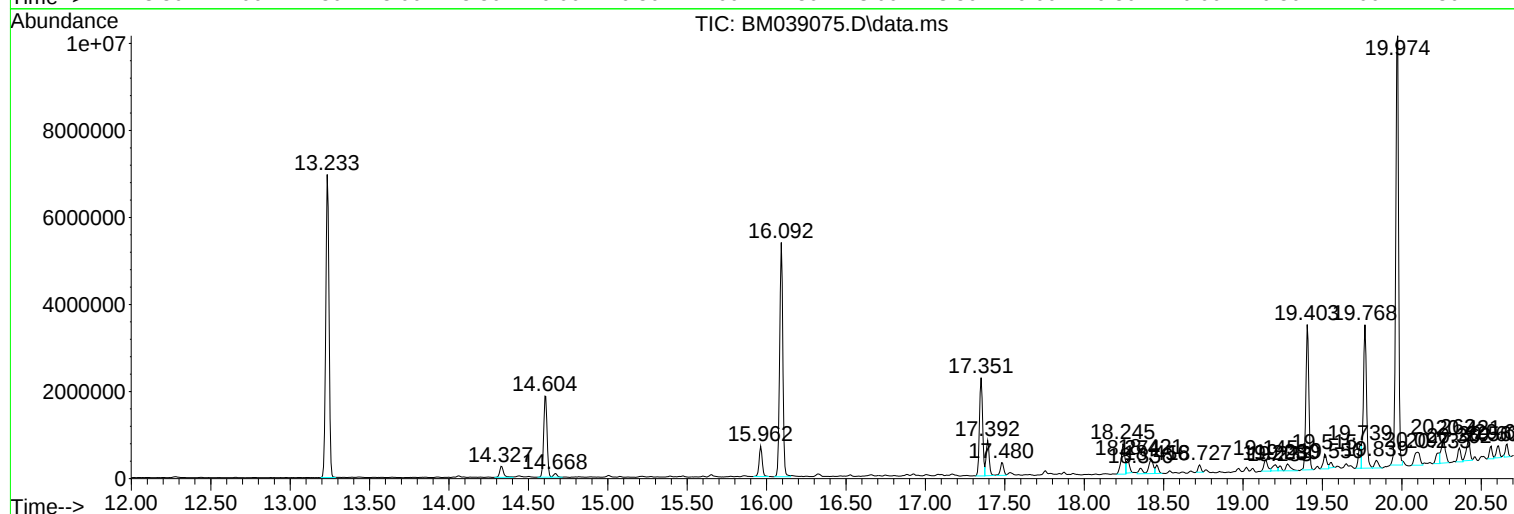
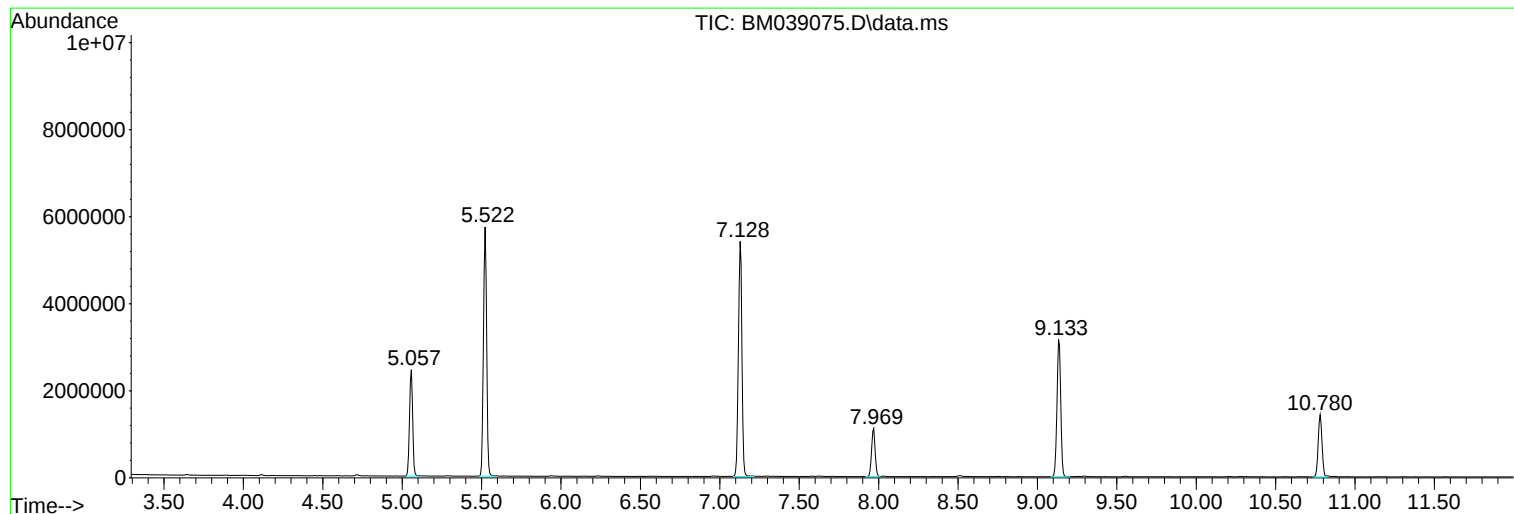
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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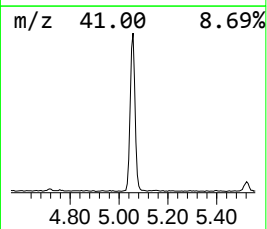
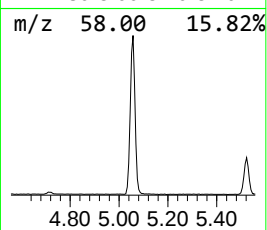
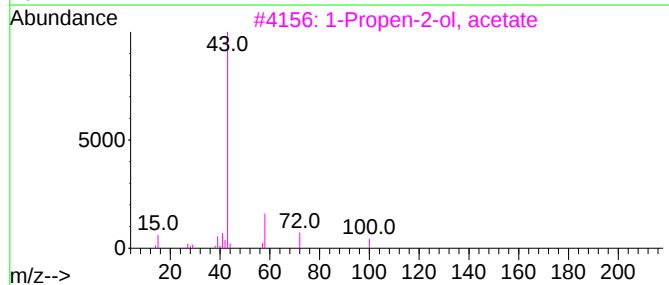
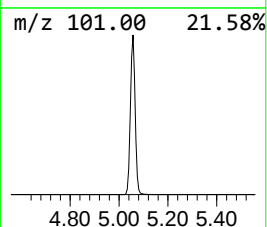
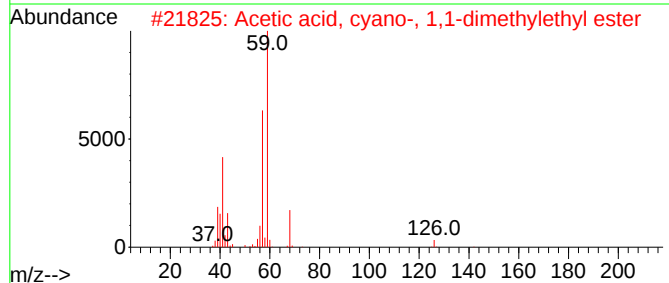
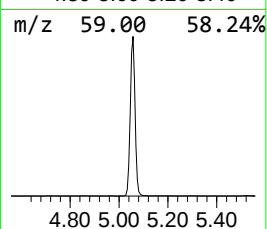
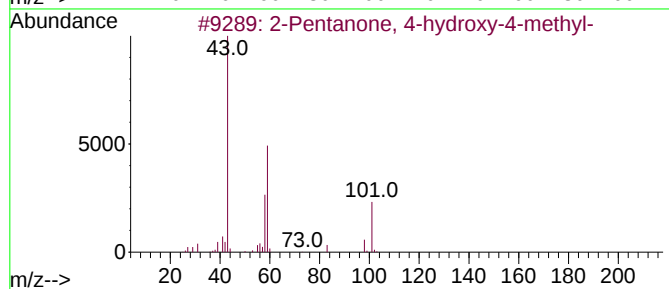
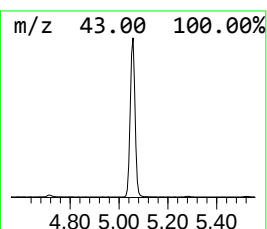
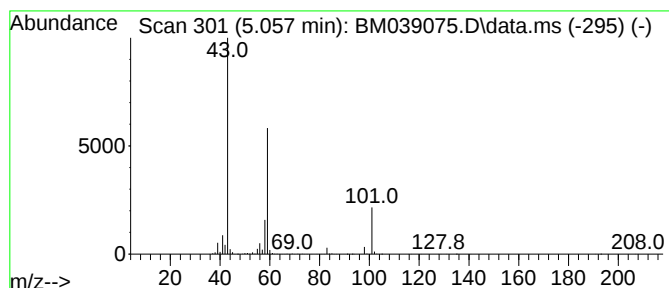
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	38.42 ng	3307350	1,4-Dichlorobenzene-d4	7.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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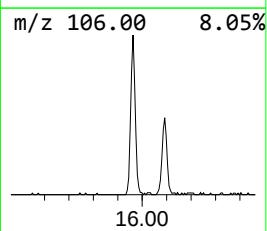
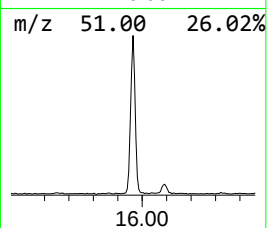
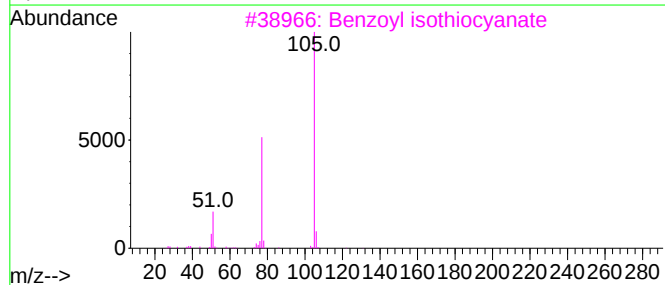
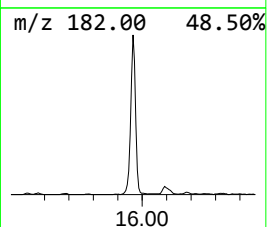
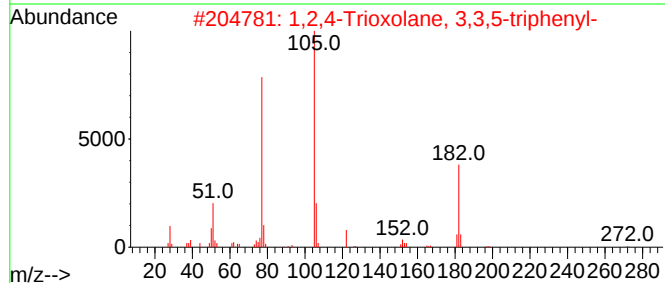
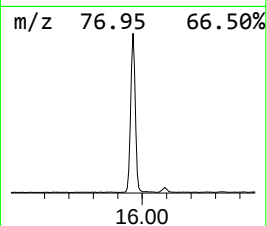
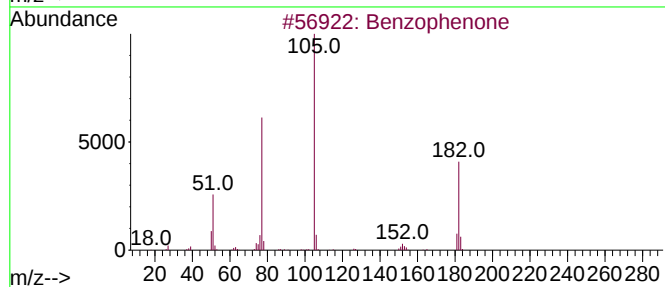
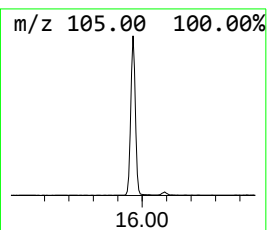
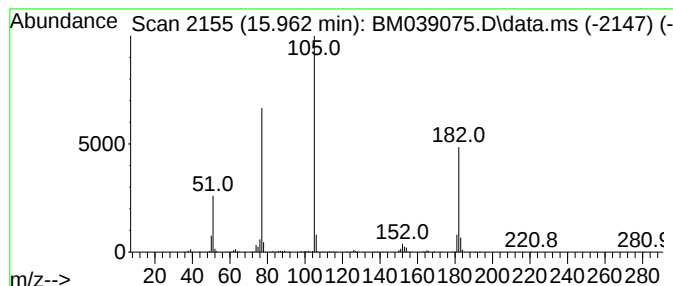
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.962	6.77 ng	960096	Acenaphthene-d10	14.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4		Vinyl benzoate	148	C9H8O2	000769-78-8	47
5		1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47



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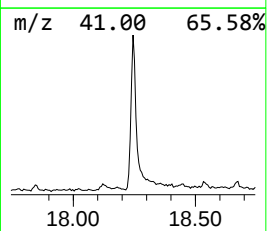
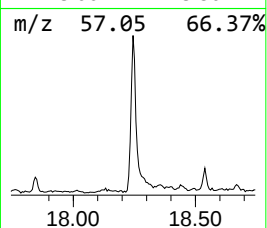
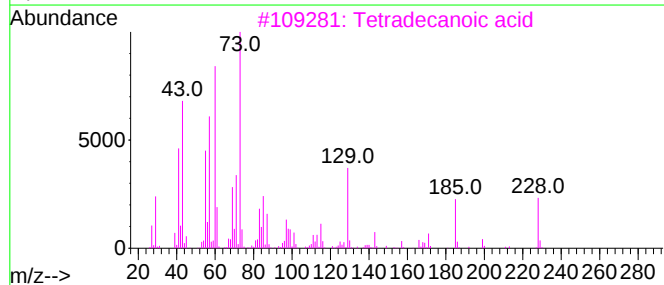
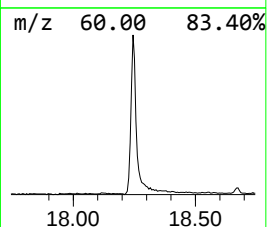
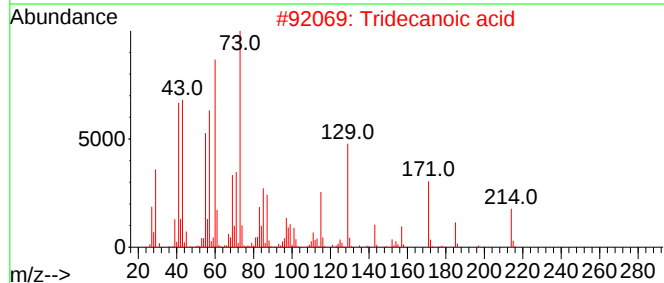
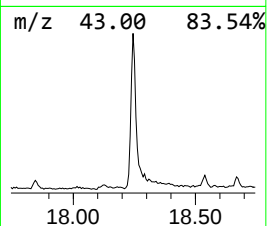
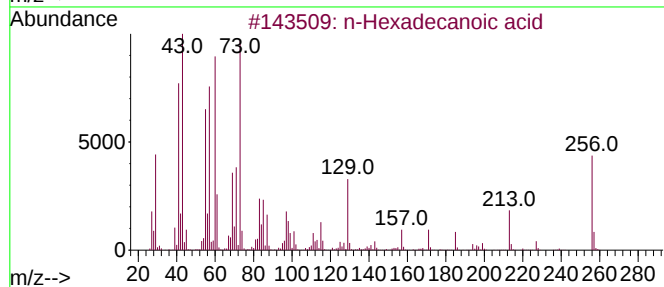
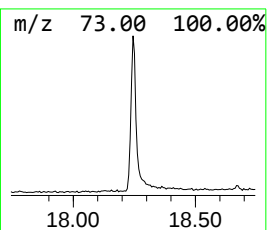
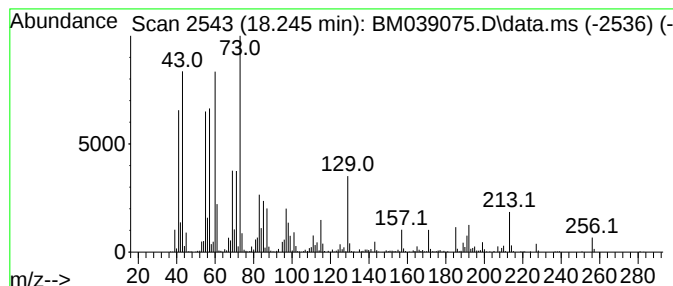
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.245	7.41 ng	1161460	Phenanthrene-d10	17.351	
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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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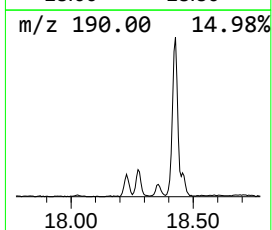
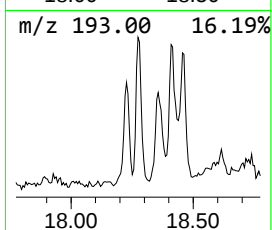
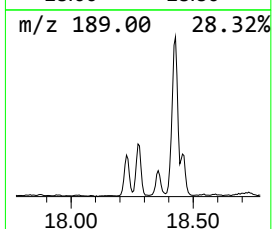
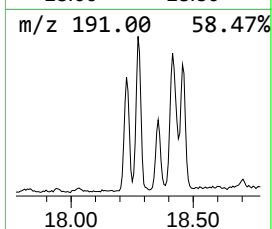
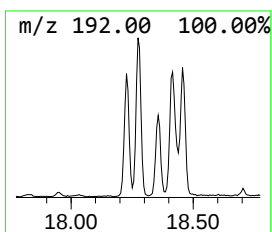
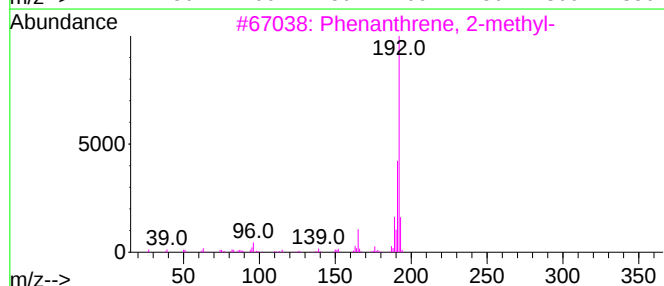
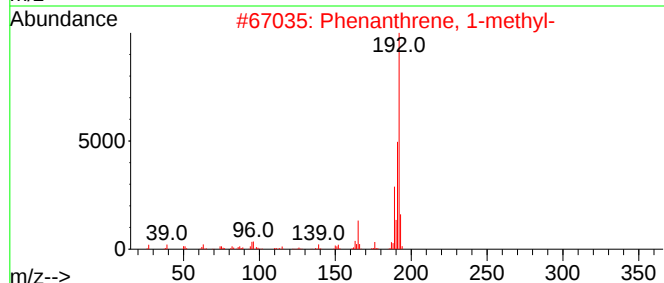
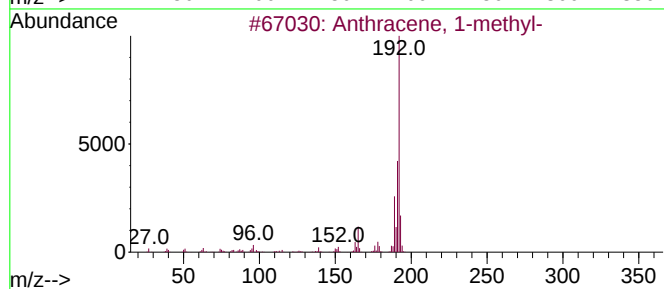
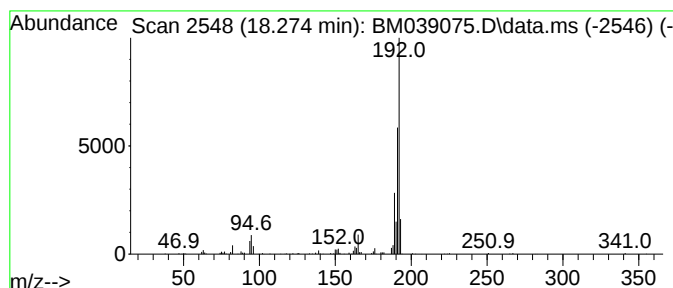
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	2.42 ng	379701	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	89
4			Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81



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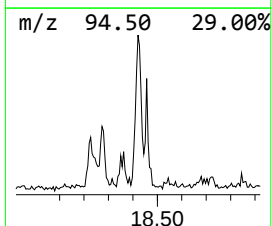
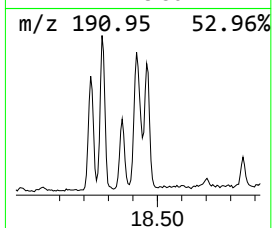
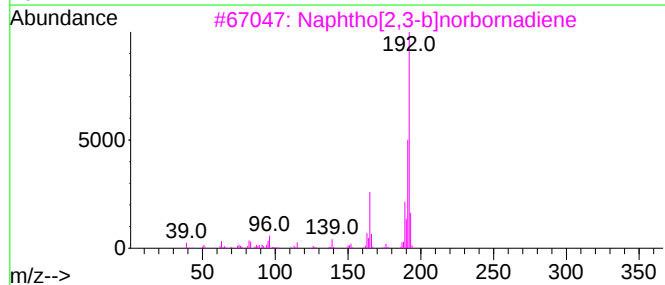
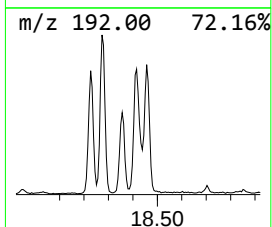
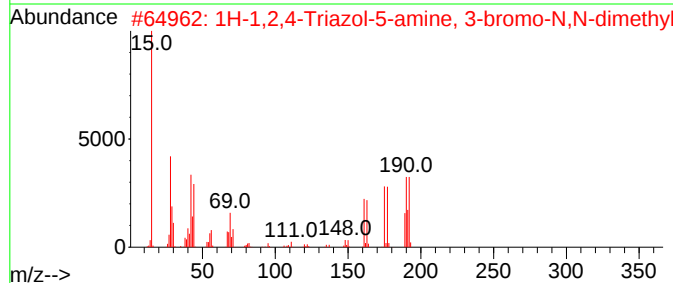
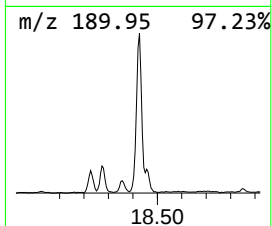
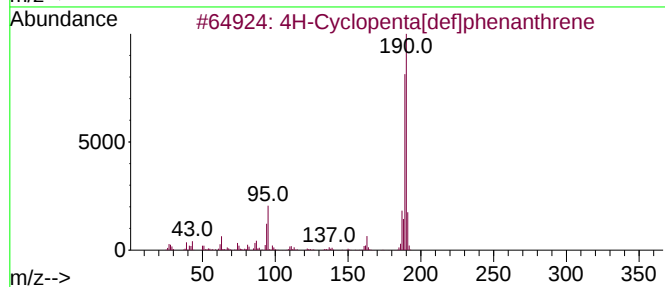
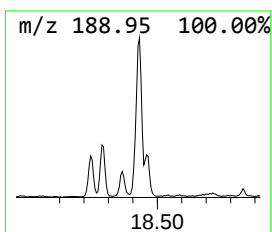
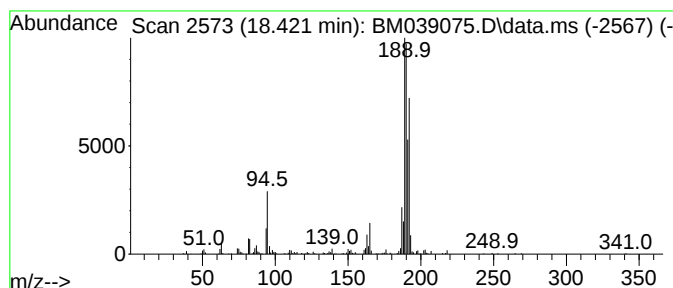
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.421	4.14 ng	649447	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2			1H-1,2,4-Triazol-5-amine, 3-brom...	190	C4H7BrN4	1000460-85-7	43
3			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	25
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	18
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
Data File : BM039075.D
Acq On : 21 Mar 2023 18:58
Operator : CG/JU
Sample : 02001-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

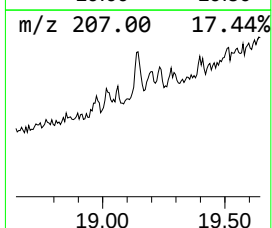
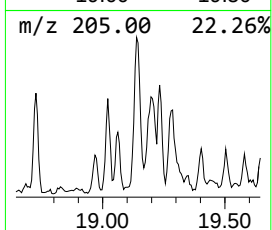
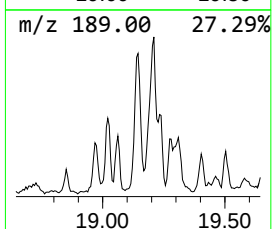
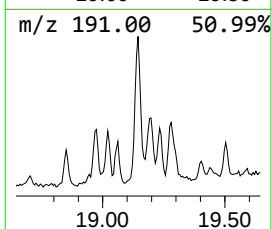
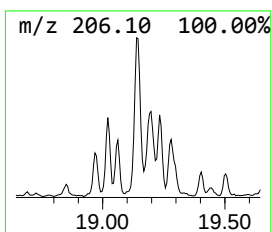
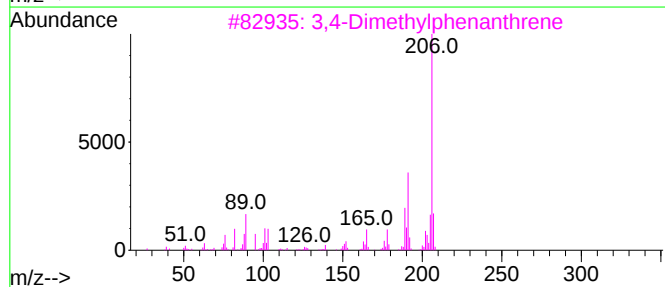
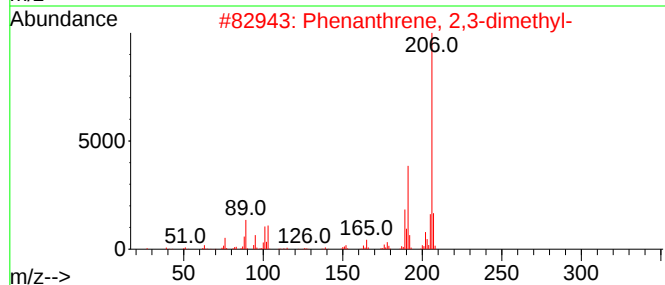
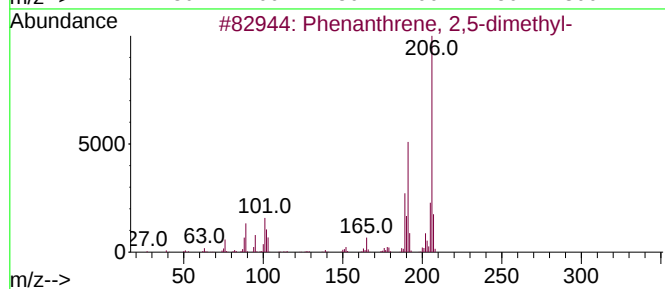
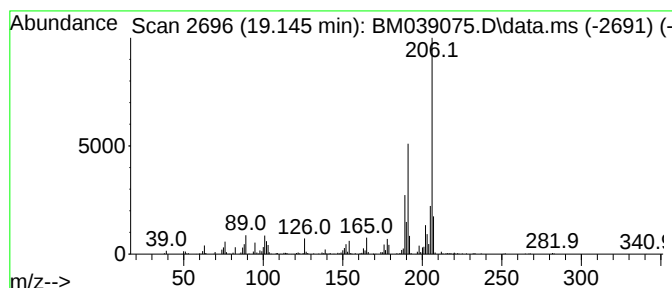
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.145	2.87 ng	449531	Phenanthrene-d10		17.351	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	93
2	Phenanthrene, 2,3-dimethyl-		206	C16H14	003674-65-5	93
3	3,4-Dimethylphenanthrene		206	C16H14	1000452-24-5	93
4	9,10-Dimethylantracene		206	C16H14	000781-43-1	90
5	1H-Indene, 2-methyl-3-phenyl-		206	C16H14	035099-60-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
Data File : BM039075.D
Acq On : 21 Mar 2023 18:58
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Misc :
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Instrument :
BNA_M
ClientSampleId :
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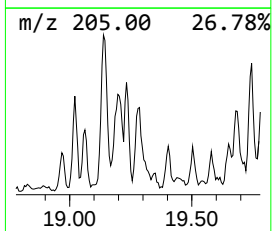
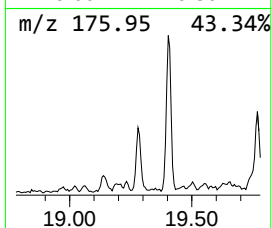
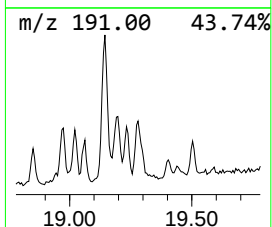
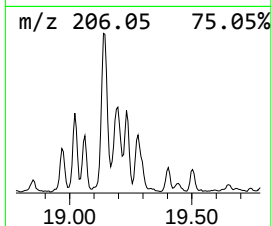
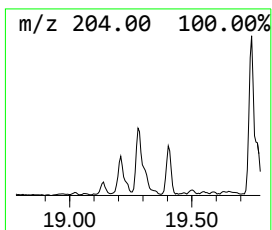
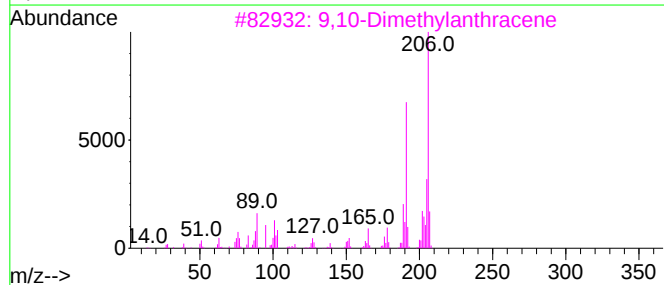
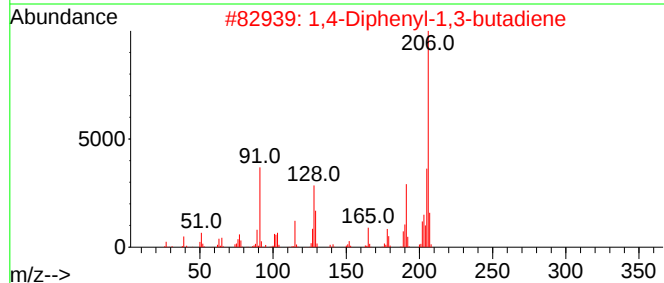
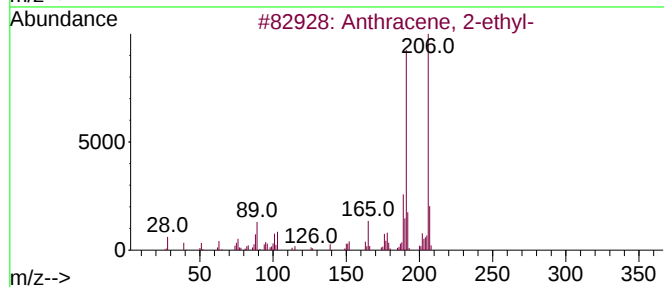
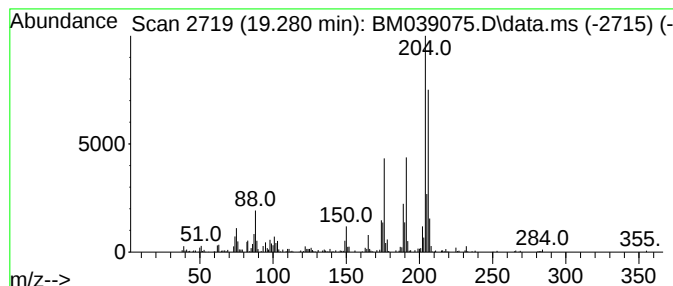
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown19.280 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	2.05 ng	321863	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-ethyl-	206	C16H14	052251-71-5	46
2			1,4-Diphenyl-1,3-butadiene	206	C16H14	000886-65-7	46
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	45
4			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	43
5			1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
Data File : BM039075.D
Acq On : 21 Mar 2023 18:58
Operator : CG/JU
Sample : 02001-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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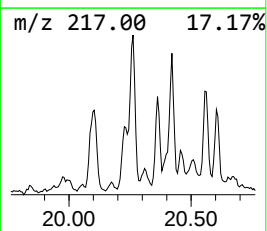
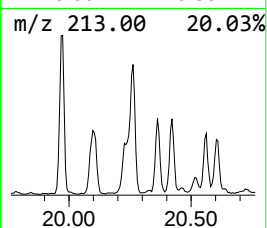
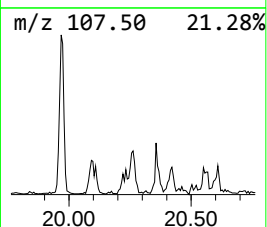
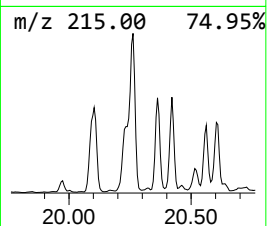
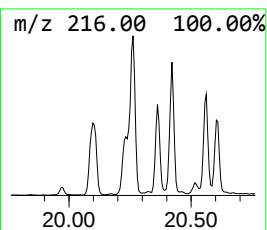
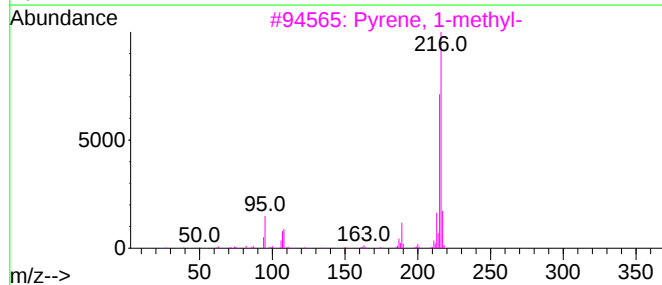
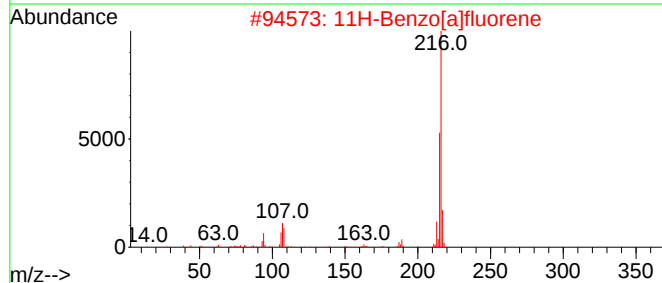
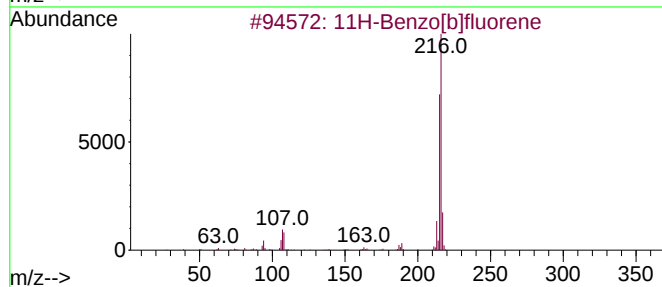
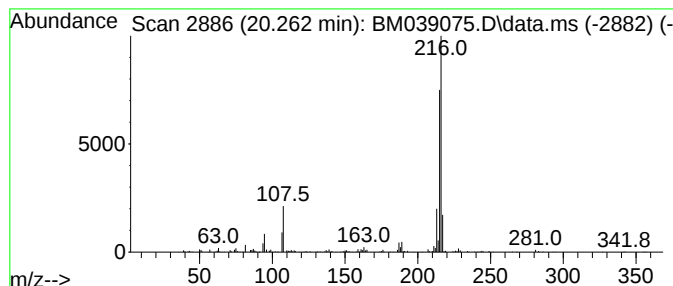
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.262	2.42 ng	978419	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
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Sample : 02001-07
Misc :
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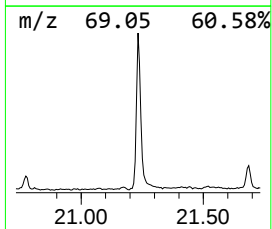
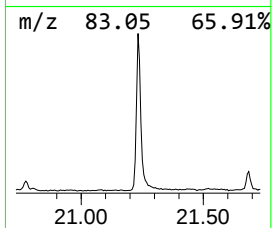
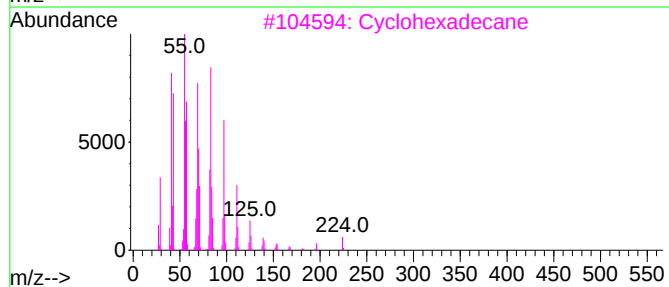
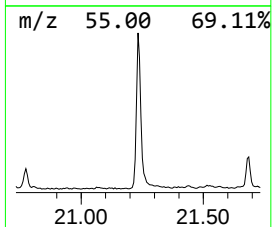
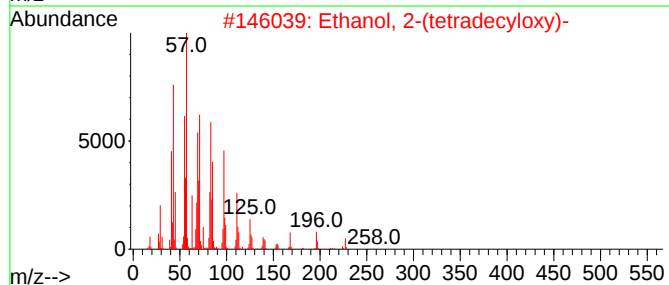
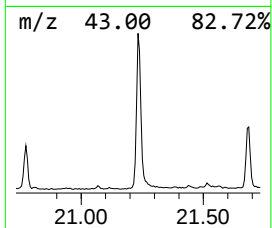
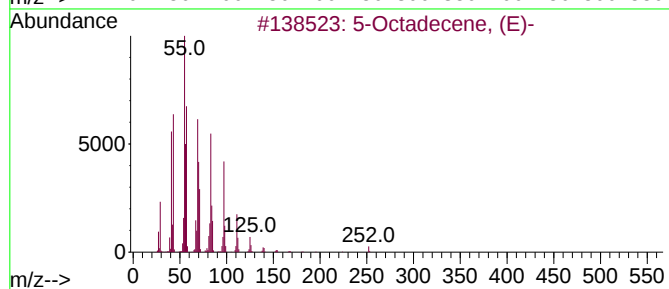
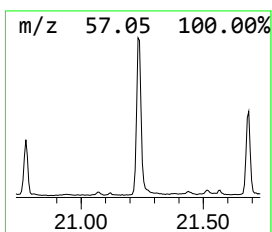
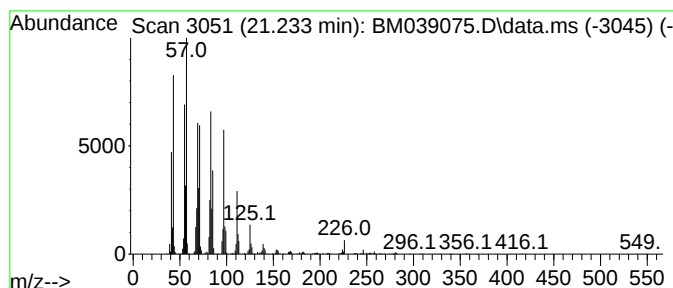
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.233	6.82 ng	2759320	Chrysene-d12	21.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
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Acq On : 21 Mar 2023 18:58
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Misc :
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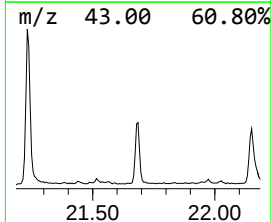
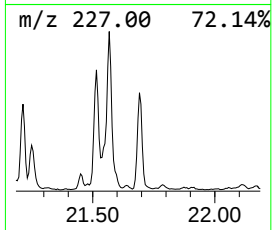
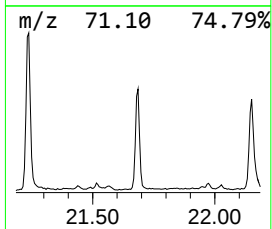
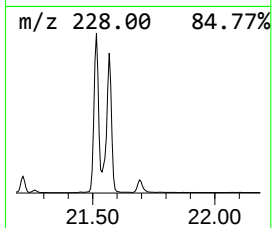
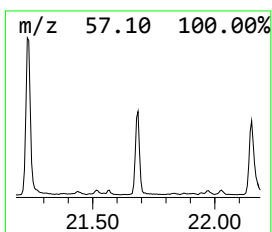
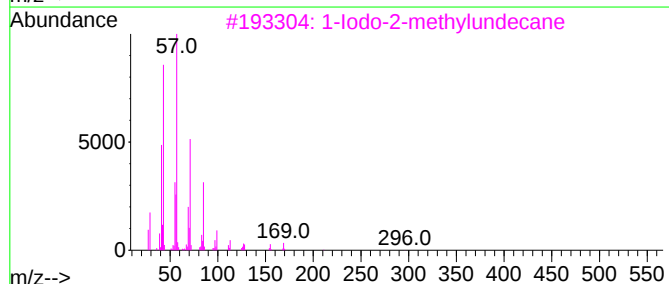
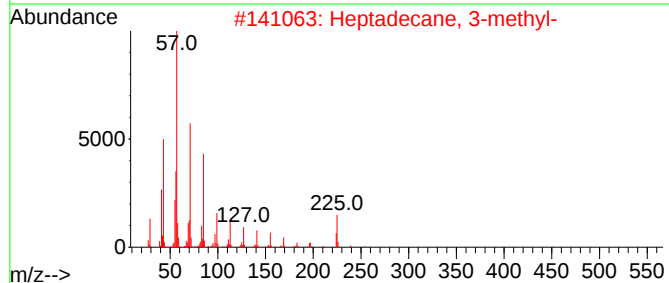
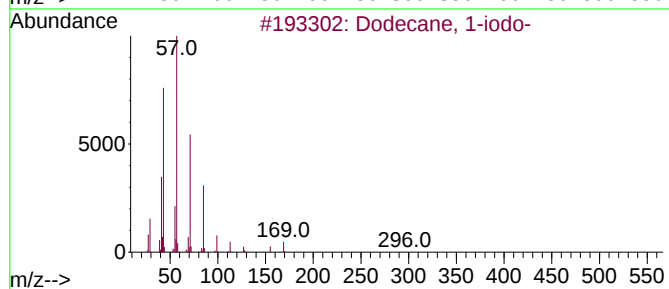
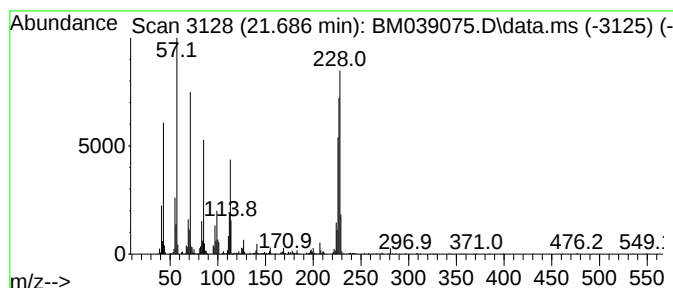
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown21.686 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.686	2.11 ng	855534	Chrysene-d12		21.533	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	42
2	Heptadecane, 3-methyl-		254	C18H38	006418-44-6	41
3	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	38
4	Heptadecane		240	C17H36	000629-78-7	38
5	Heneicosane		296	C21H44	000629-94-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
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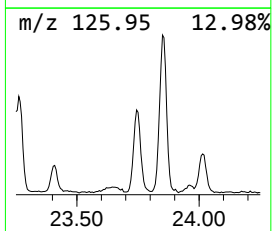
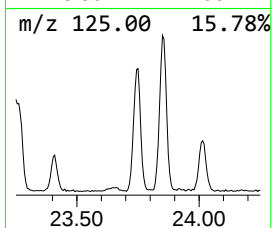
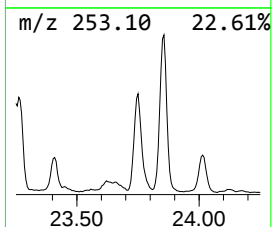
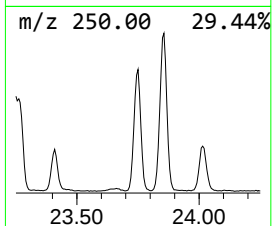
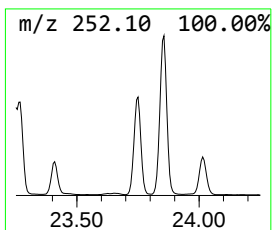
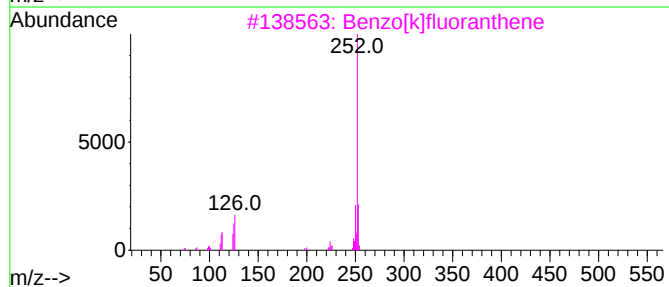
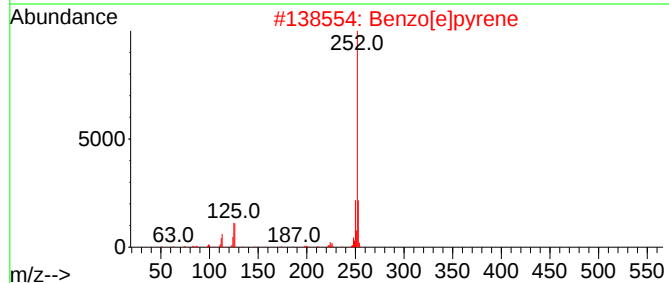
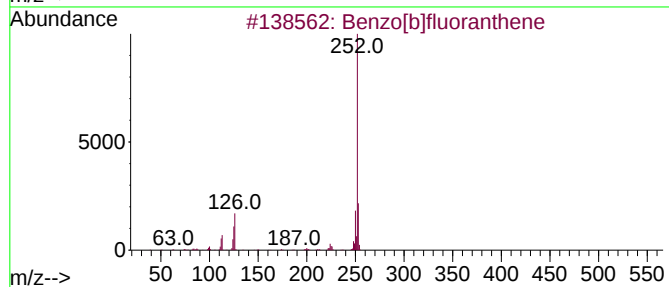
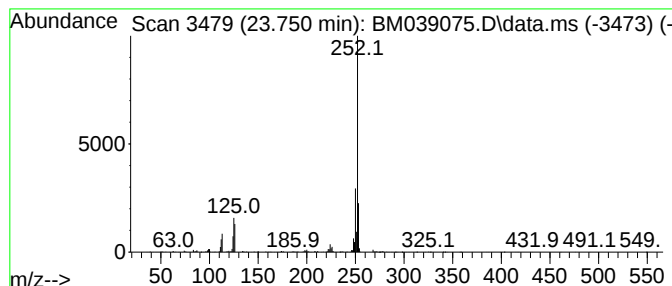
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.750	11.95 ng	2386940	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
4			Perylene	252	C20H12	000198-55-0	95
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
Data File : BM039075.D
Acq On : 21 Mar 2023 18:58
Operator : CG/JU
Sample : 02001-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IRV-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	38.4	ng	3307350	1	7.969	1721870	20.0
Benzophenone	15.962	6.8	ng	960096	3	14.604	2834290	20.0
n-Hexadecanoic ...	18.245	7.4	ng	1161460	4	17.351	3134580	20.0
Anthracene, 1-m...	18.274	2.4	ng	379701	4	17.351	3134580	20.0
4H-Cyclopenta[d...	18.421	4.1	ng	649447	4	17.351	3134580	20.0
Phenanthrene, 2...	19.145	2.9	ng	449531	4	17.351	3134580	20.0
unknown19.280	19.280	2.0	ng	321863	4	17.351	3134580	20.0
11H-Benzo[b]flu...	20.262	2.4	ng	978419	5	21.533	8093980	20.0
5-Octadecene, (E)-	21.233	6.8	ng	2759320	5	21.533	8093980	20.0
unknown21.686	21.686	2.1	ng	855534	5	21.533	8093980	20.0
Benzo[e]pyrene	23.750	11.9	ng	2386940	6	23.962	3995110	20.0