

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
 Data File : BM050001.D
 Acq On : 22 Apr 2025 18:26
 Operator : RC/JU
 Sample : Q1841-02 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VNJ-231

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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050001.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	318	323	332	rVB	373741	524644	6.56%	0.595%
2	5.357	396	403	417	rBV	1590168	2431233	30.42%	2.758%
3	5.963	501	506	513	rVB	59845	90819	1.14%	0.103%
4	6.951	667	674	687	rBV	1487064	2637888	33.00%	2.992%
5	7.763	805	812	821	rBV	934953	1467794	18.36%	1.665%
6	8.922	1003	1009	1023	rBV	901741	1584515	19.82%	1.797%
7	10.557	1279	1287	1295	rBV	1027627	1828894	22.88%	2.075%
8	13.027	1700	1707	1726	rBV	2746764	4168957	52.16%	4.729%
9	14.133	1888	1895	1905	rBV	189014	313467	3.92%	0.356%
10	14.410	1934	1942	1949	rBV	1643549	2505854	31.35%	2.843%
11	14.474	1949	1953	1961	rVB	64580	111605	1.40%	0.127%
12	15.462	2115	2121	2130	rBV2	89553	164461	2.06%	0.187%
13	15.768	2167	2173	2187	rVB	701227	1010862	12.65%	1.147%
14	15.904	2190	2196	2216	rVB	2331075	3541045	44.30%	4.017%
15	16.139	2231	2236	2243	rVB3	85762	156456	1.96%	0.177%
16	16.333	2265	2269	2278	rVB	117756	169959	2.13%	0.193%
17	16.821	2347	2352	2359	rBV2	124929	205160	2.57%	0.233%
18	16.974	2374	2378	2388	rVB	76530	137034	1.71%	0.155%
19	17.156	2403	2409	2413	rBV	2139918	2902694	36.32%	3.293%
20	17.198	2413	2416	2423	rVV	1196186	1638744	20.50%	1.859%
21	17.292	2427	2432	2438	rVV	506240	739256	9.25%	0.839%
22	17.356	2438	2443	2449	rVV2	56642	114186	1.43%	0.130%
23	17.562	2473	2478	2489	rBV	134192	270123	3.38%	0.306%
24	18.056	2553	2562	2565	rBV2	598426	1213447	15.18%	1.377%
25	18.162	2576	2580	2586	rVB	192255	262197	3.28%	0.297%
26	18.233	2586	2592	2596	rBV3	376029	705021	8.82%	0.800%
27	18.533	2639	2643	2647	rBV	166898	226419	2.83%	0.257%
28	18.580	2647	2651	2658	rVB2	156355	228066	2.85%	0.259%
29	18.780	2682	2685	2689	rVB	72216	86469	1.08%	0.098%
30	18.950	2710	2714	2718	rBV2	147100	239059	2.99%	0.271%
31	19.097	2734	2739	2747	rBV2	328511	525637	6.58%	0.596%
32	19.215	2754	2759	2766	rBV	4864291	6381231	79.84%	7.239%
33	19.333	2773	2779	2781	rBV2	217383	401221	5.02%	0.455%
34	19.362	2781	2784	2789	rVB2	266625	392512	4.91%	0.445%
35	19.550	2808	2816	2817	rBV	828465	1122513	14.04%	1.273%
36	19.580	2817	2821	2829	rVV	4200710	5665136	70.88%	6.427%

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37	19.656	2830	2834	2839	rVB2	182772	283404	3.55%	0.321%
38	19.780	2848	2855	2860	rBV	5043338	6041636	75.59%	6.854%
39	19.903	2871	2876	2883	rBV3	332033	818391	10.24%	0.928%
40	20.074	2895	2905	2910	rBV	831322	1700559	21.28%	1.929%
41	20.174	2918	2922	2926	rBV	641063	842894	10.55%	0.956%
42	20.239	2927	2933	2936	rVV2	410838	699574	8.75%	0.794%
43	20.374	2953	2956	2960	rBV	302815	356111	4.46%	0.404%
44	20.421	2960	2964	2968	rVV2	297703	424620	5.31%	0.482%
45	20.827	3030	3033	3040	rVB	374003	535298	6.70%	0.607%
46	21.003	3059	3063	3066	rBV	373258	484773	6.07%	0.550%
47	21.039	3066	3069	3072	rVV	324846	360430	4.51%	0.409%
48	21.086	3073	3077	3082	rVB2	381592	727188	9.10%	0.825%
49	21.391	3122	3129	3134	rBV3	3387159	7992841	100.00%	9.067%
50	21.444	3134	3138	3150	rVB	2370980	3896923	48.76%	4.421%
51	21.586	3159	3162	3170	rVB	326628	488594	6.11%	0.554%
52	23.456	3473	3480	3487	rBV	2244267	6277690	78.54%	7.122%
53	24.127	3588	3594	3606	rVB	1275586	3103172	38.82%	3.520%
54	24.262	3610	3617	3629	rVB	1640710	3934939	49.23%	4.464%
55	24.403	3634	3641	3648	rBV	1242012	3017593	37.75%	3.423%

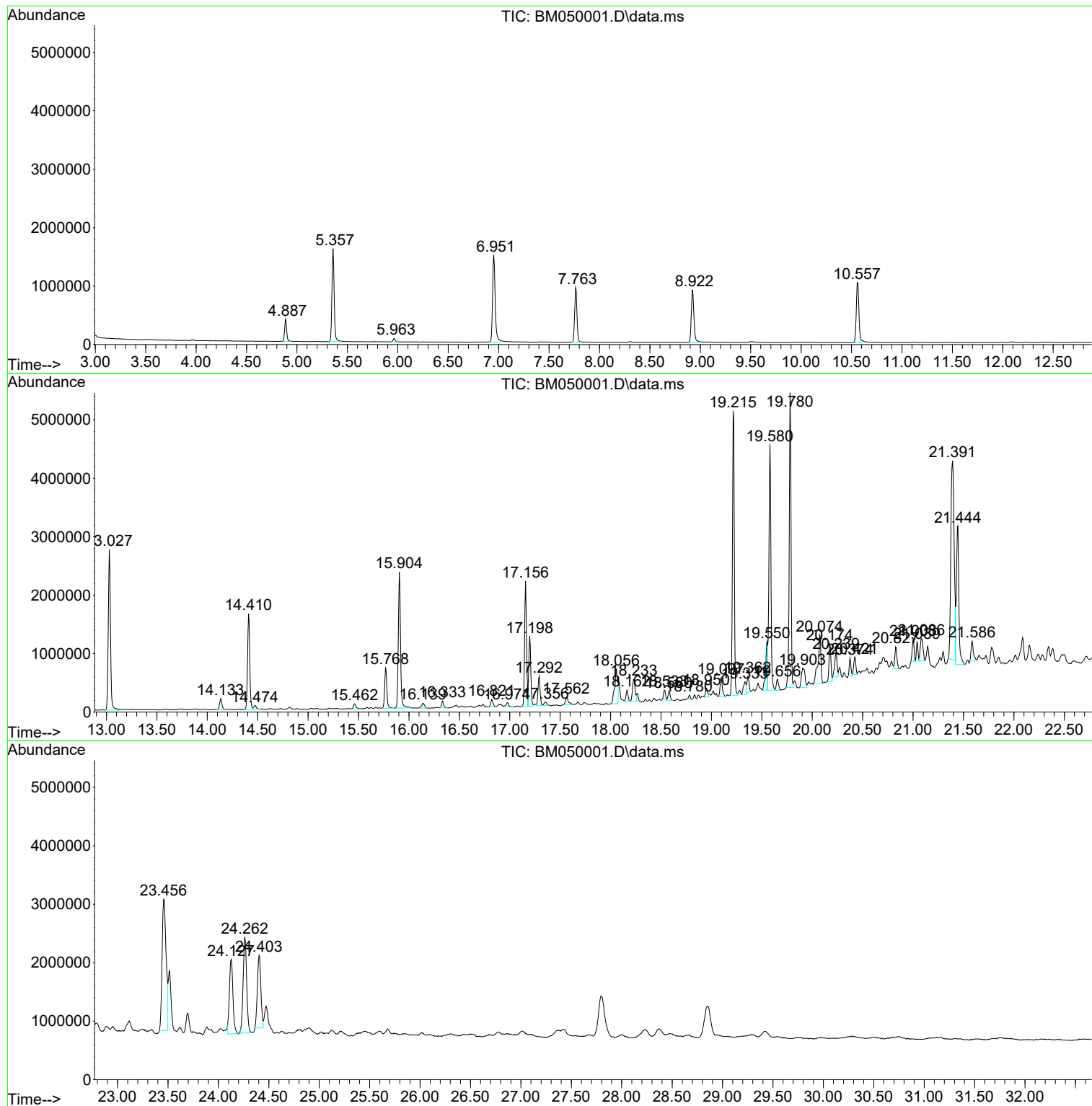
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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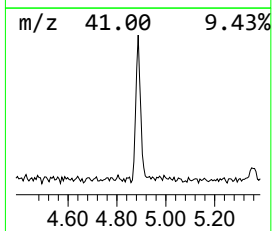
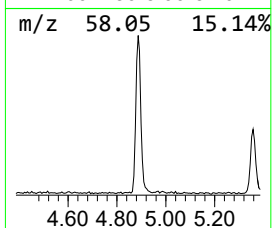
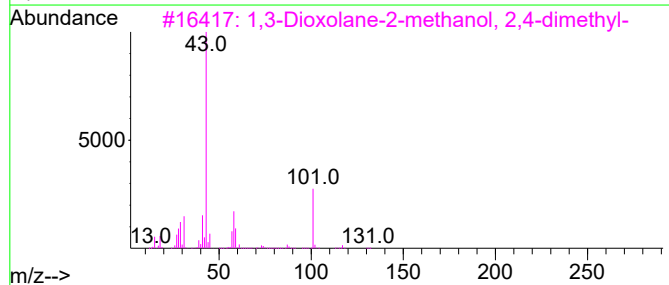
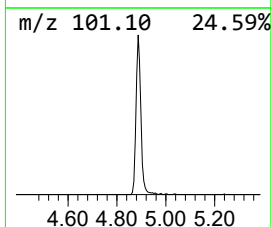
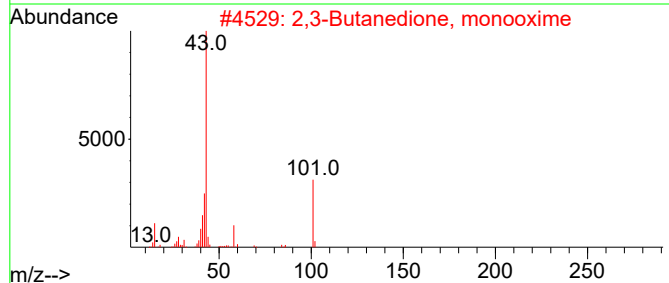
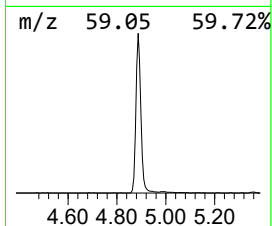
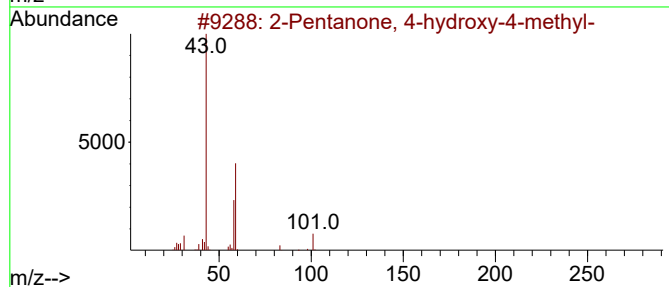
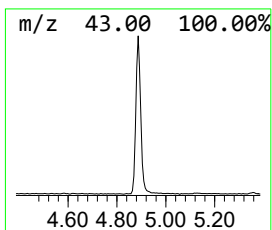
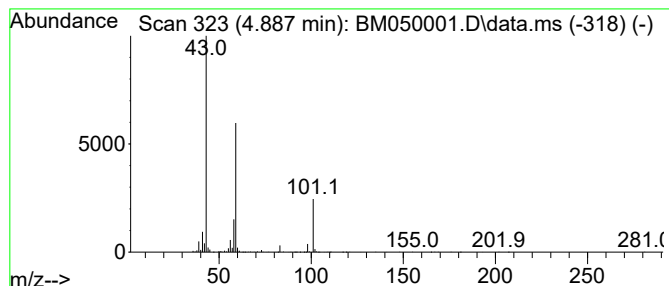
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	7.15 ng	524644	1,4-Dichlorobenzene-d4	7.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25	
4	Tetraglyme	222	C10H22O5	000143-24-8	23	
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17	



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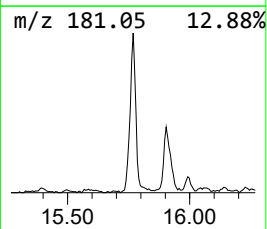
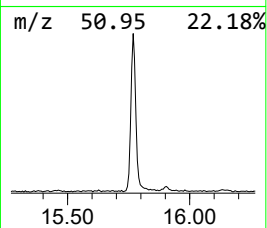
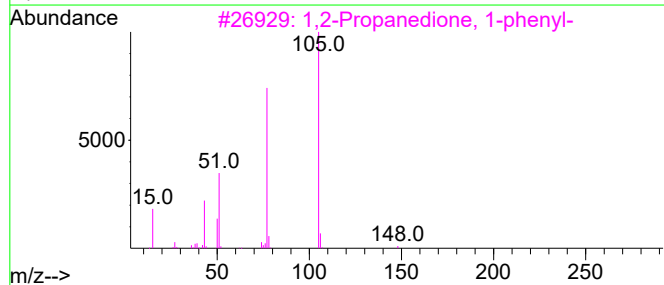
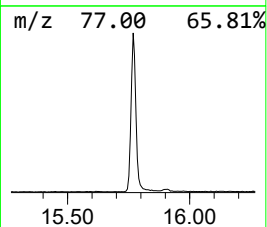
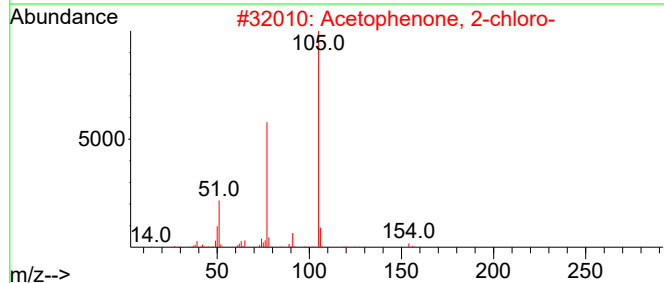
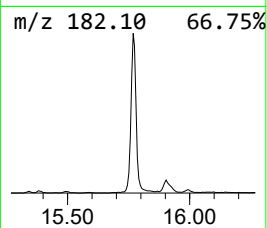
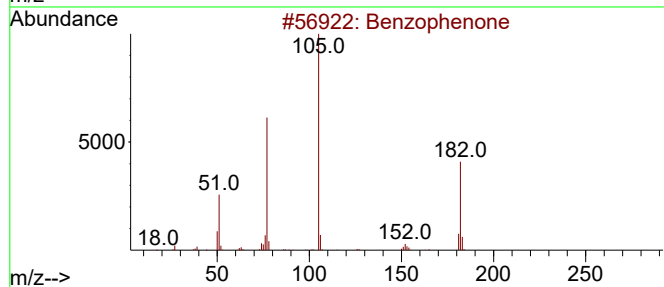
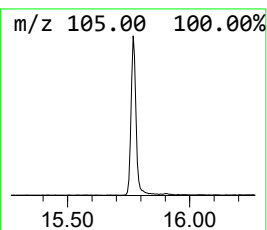
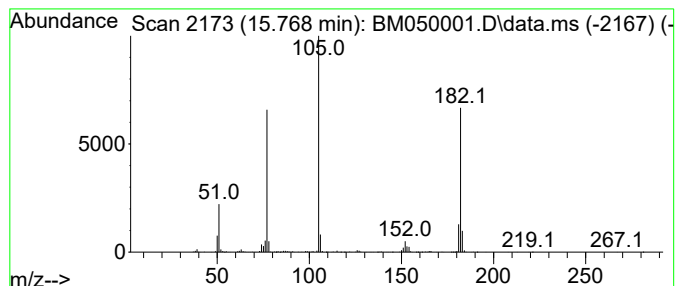
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	8.07 ng	1010860	Acenaphthene-d10	14.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
3		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
4		N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
5		Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43



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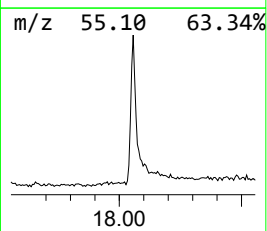
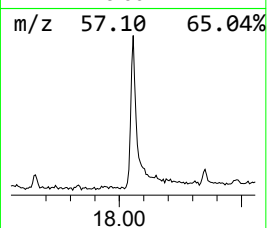
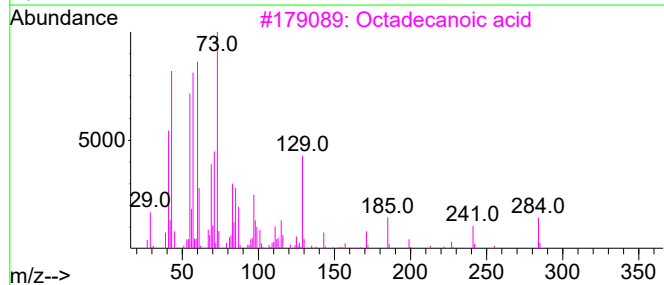
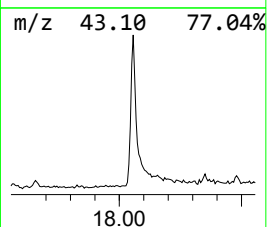
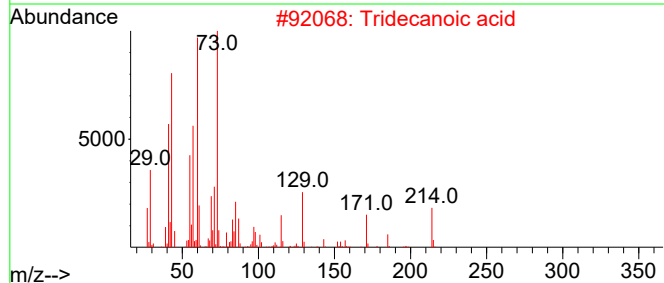
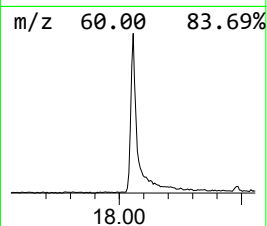
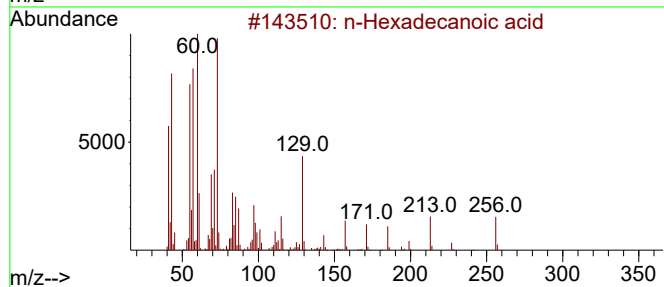
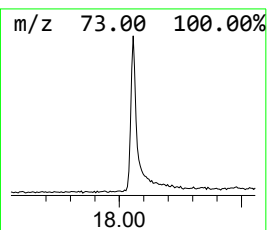
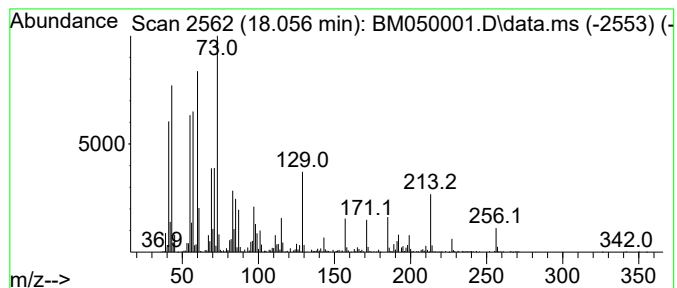
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	8.36 ng	1213450	Phenanthrene-d10	17.156

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	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tetradecane	198	C14H30	000629-59-4	53



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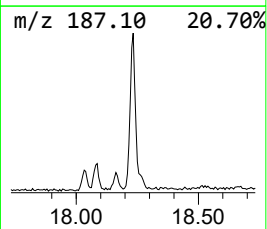
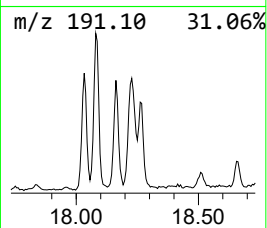
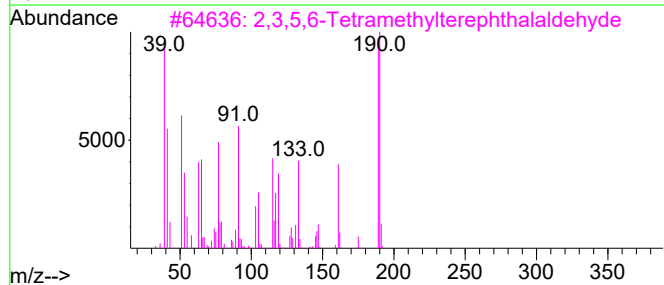
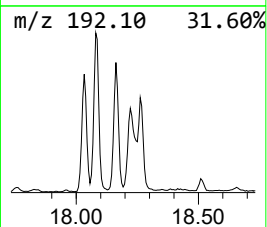
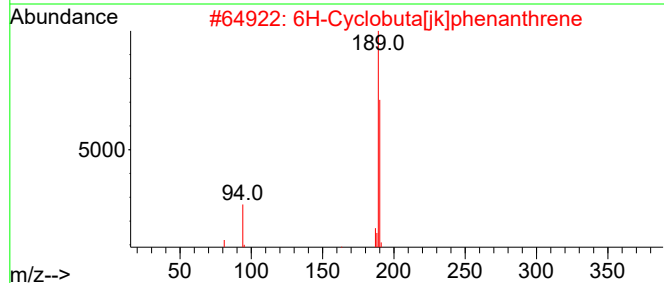
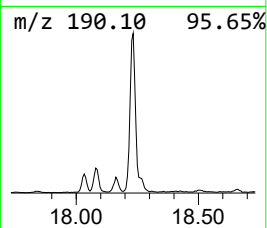
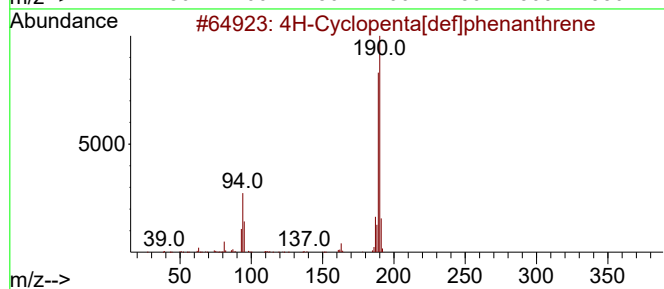
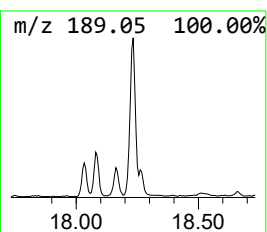
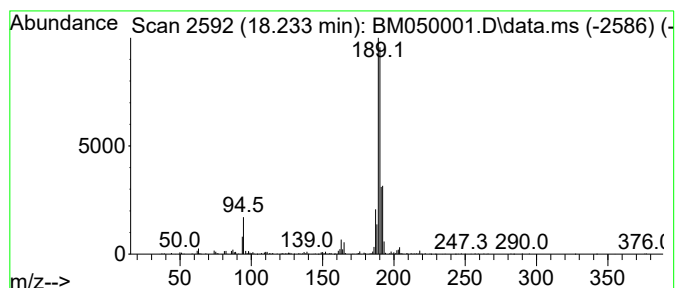
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Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	4.86 ng	705021	Phenanthrene-d10	17.156

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3		2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5		2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



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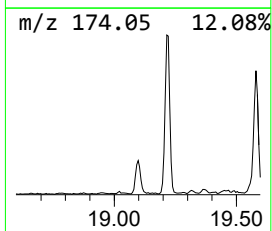
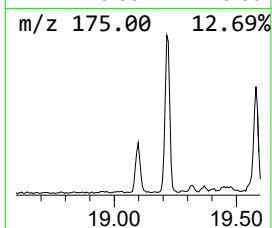
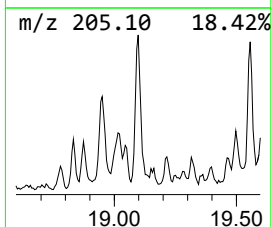
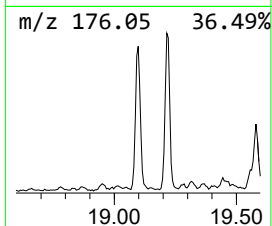
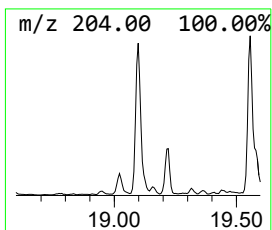
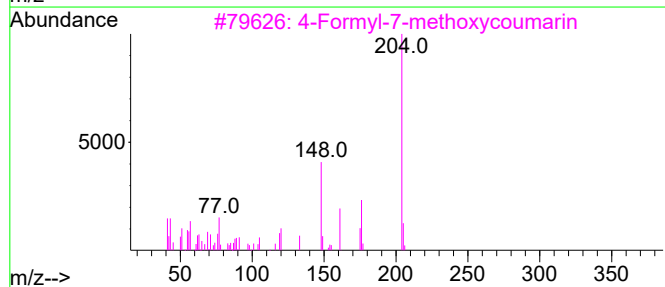
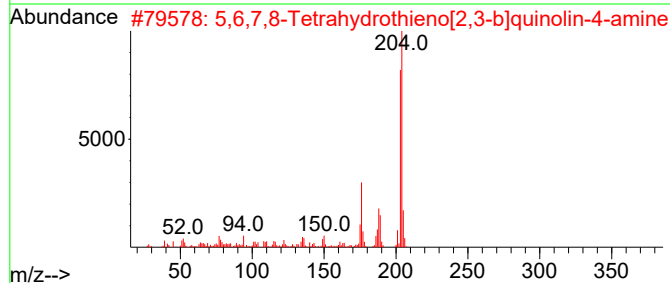
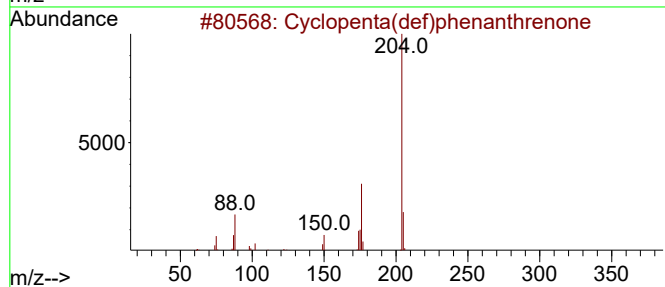
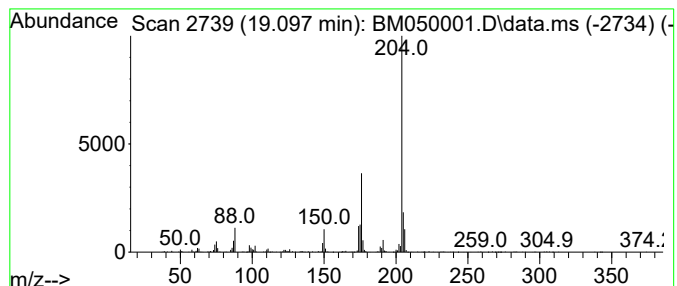
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BNA_M
ClientSampleId :
VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopenta(def)phenanthrenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.098	3.62 ng	525637	Phenanthrene-d10	17.156	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	94
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	64
3	4-Formyl-7-methoxycoumarin	204	C11H8O4	1000429-03-0	59
4	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	50
5	Benzo[1,2-b:4,3-b']dithiophene, ...	204	C11H8S2	013640-86-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
Data File : BM050001.D
Acq On : 22 Apr 2025 18:26
Operator : RC/JU
Sample : Q1841-02 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-231

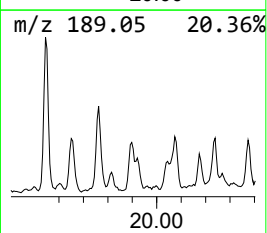
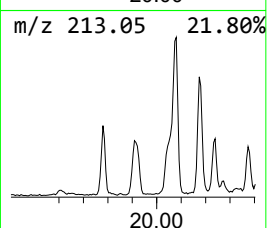
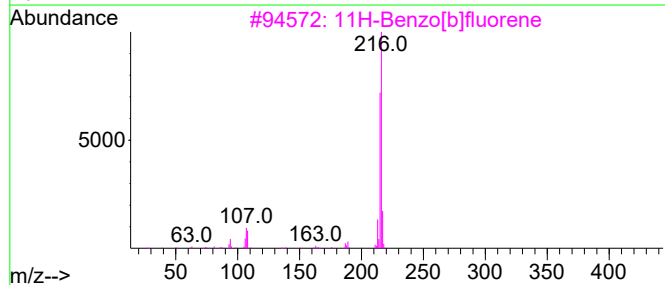
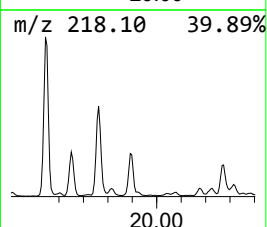
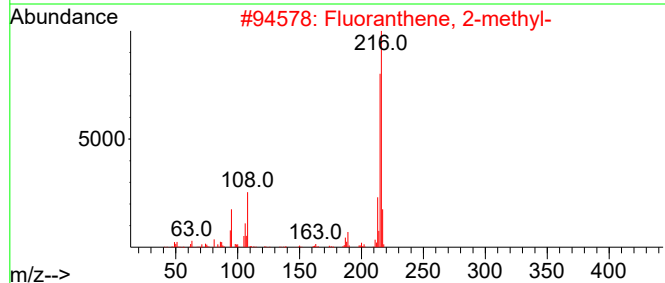
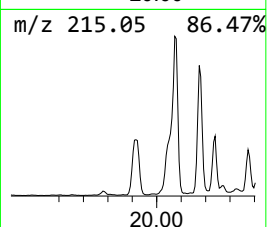
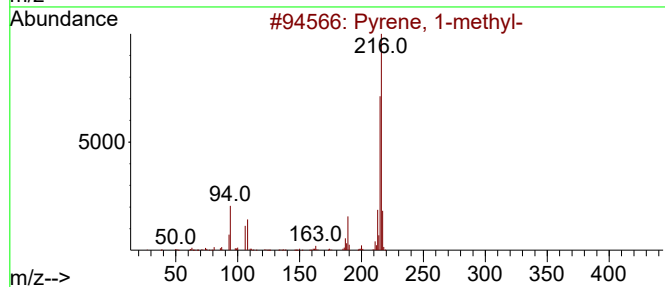
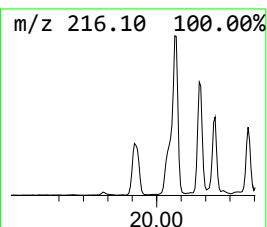
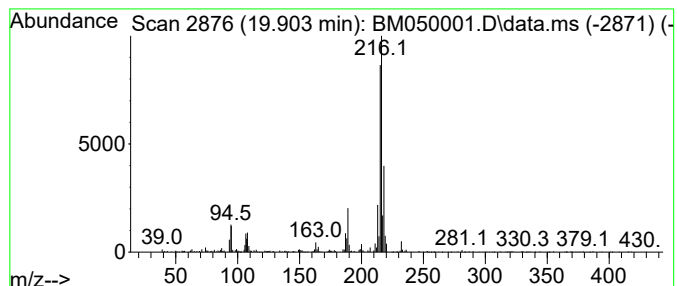
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.903	2.05 ng	818391	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	60
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
Data File : BM050001.D
Acq On : 22 Apr 2025 18:26
Operator : RC/JU
Sample : Q1841-02 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-231

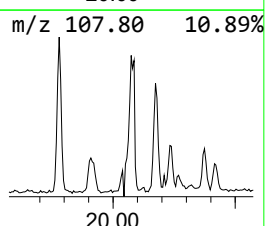
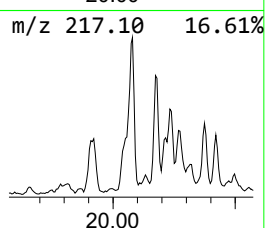
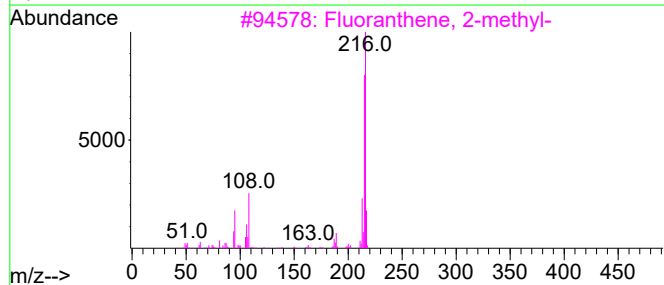
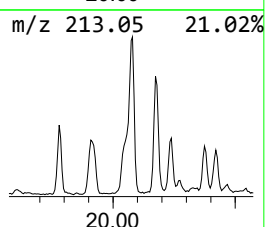
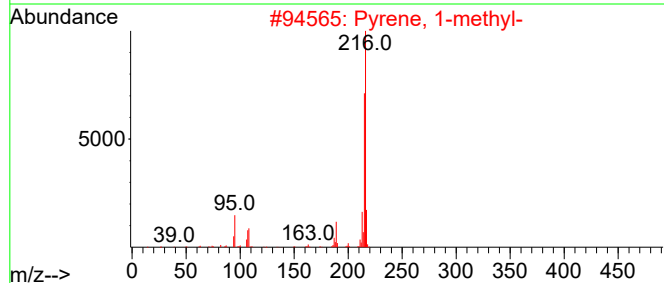
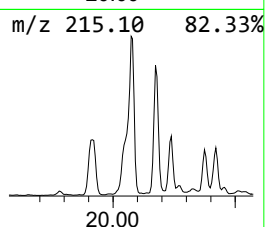
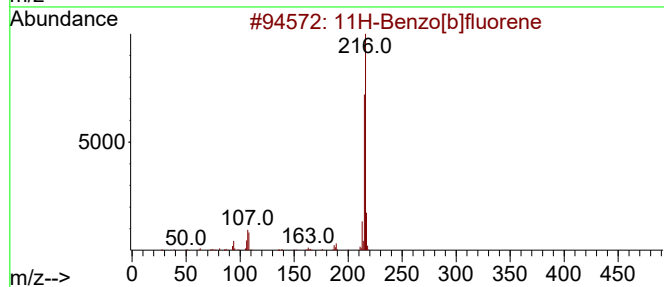
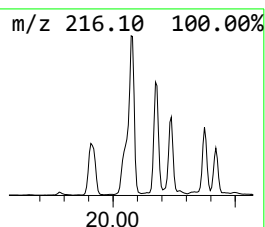
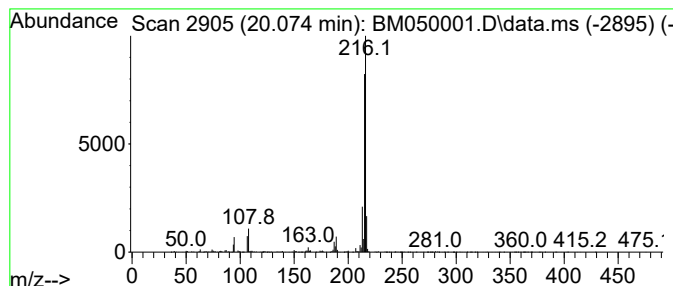
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.074	4.26 ng	1700560	Chrysene-d12	21.397

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
Data File : BM050001.D
Acq On : 22 Apr 2025 18:26
Operator : RC/JU
Sample : Q1841-02 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-231

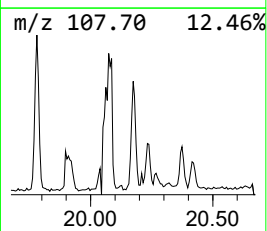
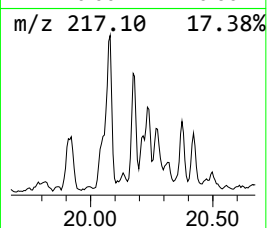
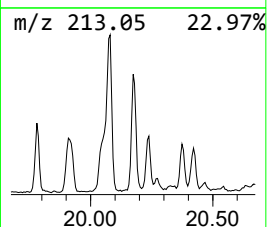
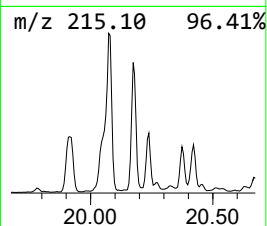
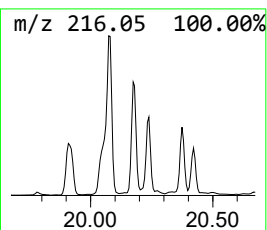
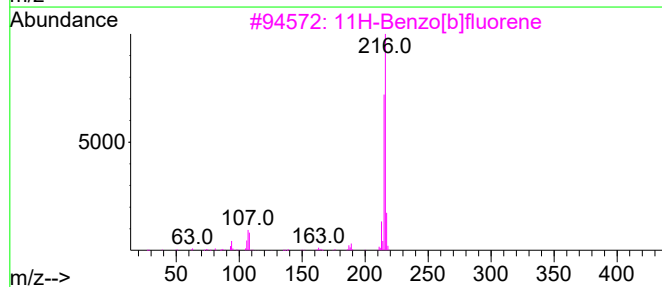
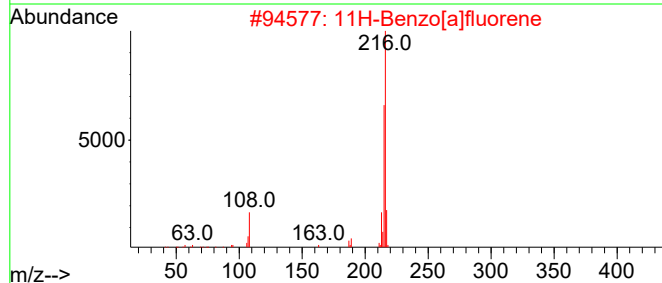
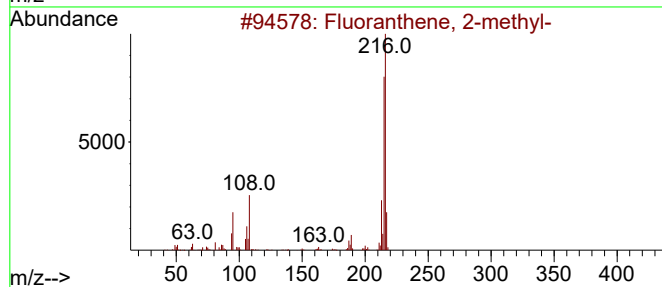
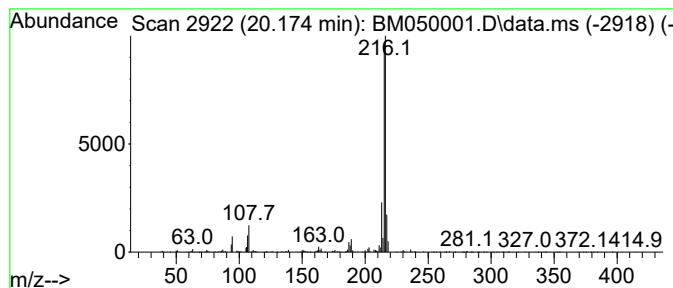
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Fluoranthene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.174	2.11 ng	842894	Chrysene-d12	21.397

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
2		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5		Pyrene, 1-methyl-	216	C17H12	002381-21-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
Data File : BM050001.D
Acq On : 22 Apr 2025 18:26
Operator : RC/JU
Sample : Q1841-02 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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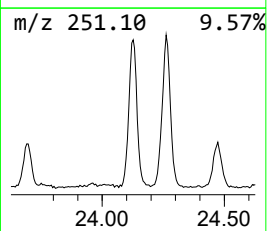
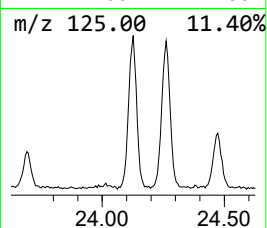
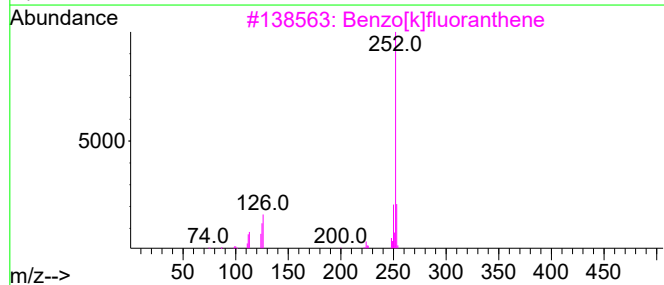
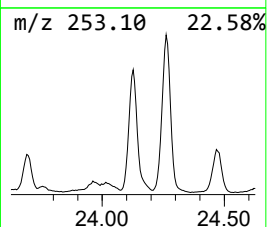
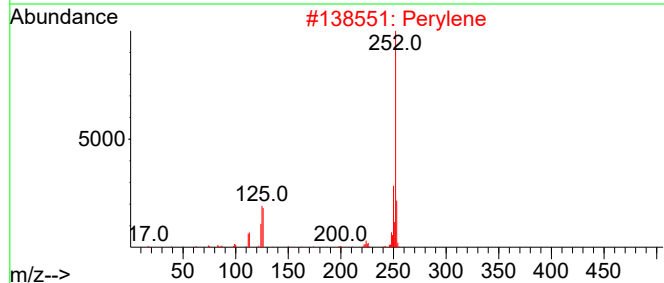
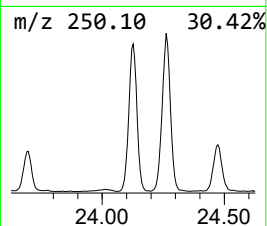
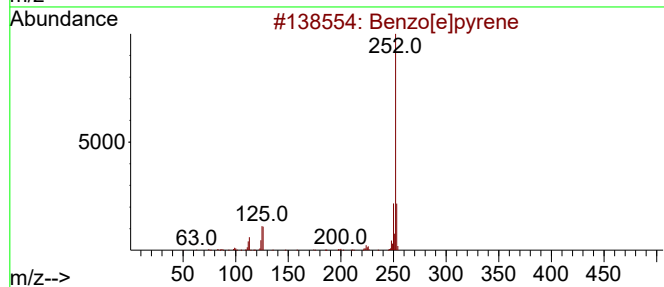
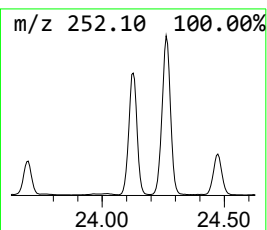
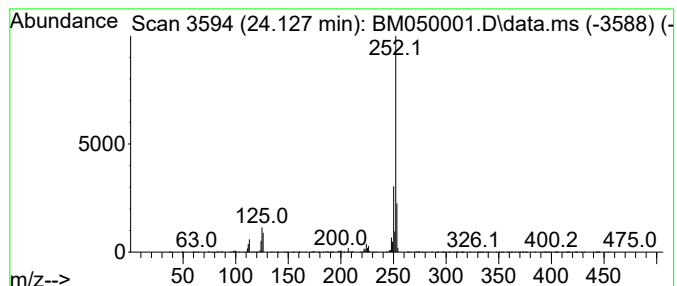
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.127	20.57 ng	3103170	Perylene-d12	24.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Perylene	252	C20H12	000198-55-0	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042225\
Data File : BM050001.D
Acq On : 22 Apr 2025 18:26
Operator : RC/JU
Sample : Q1841-02 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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-...	4.887	7.2	ng	524644	1	7.763	1467790	20.0
Benzophenone	15.768	8.1	ng	1010860	3	14.410	2505850	20.0
n-Hexadecanoic ...	18.056	8.4	ng	1213450	4	17.156	2902690	20.0
4H-Cyclopenta[d]...	18.233	4.9	ng	705021	4	17.156	2902690	20.0
Cyclopenta(def)...	19.098	3.6	ng	525637	4	17.156	2902690	20.0
Pyrene, 1-methyl-	19.903	2.0	ng	818391	5	21.397	7992840	20.0
11H-Benzo[b]flu...	20.074	4.3	ng	1700560	5	21.397	7992840	20.0
Fluoranthene, 2...	20.174	2.1	ng	842894	5	21.397	7992840	20.0
Benzo[e]pyrene	24.127	20.6	ng	3103170	6	24.403	3017590	20.0