

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
 Data File : BG060691.D
 Acq On : 20 Mar 2024 14:35
 Operator : MA/JU
 Sample : P1803-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TRENCH-PIT

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_G\Methods\8270-BG031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.785	400	408	416	rBV	1256813	1975037	40.70%	5.336%
2	7.412	677	685	694	rBV	1399001	2416515	49.79%	6.529%
3	8.293	827	835	845	rBV	293993	503341	10.37%	1.360%
4	9.492	1030	1039	1051	rBV	857847	1563569	32.22%	4.224%
5	11.137	1308	1319	1325	rBV	385314	704043	14.51%	1.902%
6	13.546	1722	1729	1738	rVB	1923294	2945383	60.69%	7.958%
7	14.921	1956	1963	1970	rBV	655635	1008073	20.77%	2.724%
8	14.986	1970	1974	1979	rVB	39218	59122	1.22%	0.160%
9	15.185	2001	2008	2018	rBV	131270	237022	4.88%	0.640%
10	15.315	2025	2030	2036	rVB2	32226	55178	1.14%	0.149%
11	15.967	2135	2141	2149	rVB3	41874	72919	1.50%	0.197%
12	16.407	2209	2216	2227	rBV	1938331	2968731	61.17%	8.021%
13	17.324	2368	2372	2377	rVB	62486	95170	1.96%	0.257%
14	17.489	2392	2400	2408	rVB2	43277	78025	1.61%	0.211%
15	17.671	2424	2431	2435	rBV	857680	1378756	28.41%	3.725%
16	17.718	2435	2439	2444	rVB	820945	1192320	24.57%	3.221%
17	17.806	2449	2454	2459	rVB	118137	181567	3.74%	0.491%
18	18.082	2492	2501	2507	rBV2	103735	195401	4.03%	0.528%
19	18.493	2566	2571	2576	rBV	484972	653410	13.46%	1.765%
20	18.540	2576	2579	2583	rVV	106861	163631	3.37%	0.442%
21	18.587	2583	2587	2593	rVB2	141448	216595	4.46%	0.585%
22	18.664	2595	2600	2605	rVB	36376	54777	1.13%	0.148%
23	18.740	2605	2613	2616	rBV3	108416	213973	4.41%	0.578%
24	18.769	2616	2618	2624	rVB	59751	70951	1.46%	0.192%
25	19.028	2657	2662	2667	rBV2	77400	116132	2.39%	0.314%
26	19.081	2667	2671	2677	rVB	132521	188669	3.89%	0.510%
27	19.433	2727	2731	2734	rBV2	32669	54859	1.13%	0.148%
28	19.586	2751	2757	2763	rBV3	66790	132542	2.73%	0.358%
29	19.709	2772	2778	2783	rBV	1279456	1831352	37.73%	4.948%
30	19.751	2783	2785	2790	rVB2	133267	157575	3.25%	0.426%
31	19.956	2817	2820	2827	rVB2	47821	73815	1.52%	0.199%
32	20.027	2827	2832	2835	rBV2	167314	275671	5.68%	0.745%
33	20.074	2835	2840	2845	rVV	1070639	1505899	31.03%	4.069%
34	20.127	2846	2849	2854	rVB	61729	86901	1.79%	0.235%
35	20.256	2864	2871	2877	rBV	3433118	4853248	100.00%	13.112%
36	20.315	2878	2881	2886	rVB2	48119	66590	1.37%	0.180%

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

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37	20.385	2888	2893	2900	rVB4	68649	165295	3.41%	0.447%
38	20.450	2900	2904	2908	rBV	36224	65462	1.35%	0.177%
39	20.509	2908	2914	2915	rBV4	55599	88349	1.82%	0.239%
40	20.708	2946	2948	2952	rVB2	62633	71893	1.48%	0.194%
41	20.849	2969	2972	2977	rBV	54508	94043	1.94%	0.254%
42	21.343	3052	3056	3062	rVB	126832	192836	3.97%	0.521%
43	21.537	3084	3089	3094	rBV4	249346	395434	8.15%	1.068%
44	21.631	3102	3105	3111	rVV2	73124	132880	2.74%	0.359%
45	21.701	3112	3117	3122	rVB	114921	203764	4.20%	0.551%
46	21.807	3131	3135	3138	rBV3	96014	129449	2.67%	0.350%
47	21.989	3157	3166	3171	rBV3	958224	2401569	49.48%	6.488%
48	22.042	3171	3175	3181	rVB	433175	727548	14.99%	1.966%
49	22.765	3294	3298	3303	rBV3	82975	143617	2.96%	0.388%
50	24.386	3566	3574	3583	rBV	325876	1145466	23.60%	3.095%
51	25.185	3704	3710	3723	rVB2	182197	549402	11.32%	1.484%
52	25.356	3731	3739	3750	rVB2	232706	687075	14.16%	1.856%
53	25.532	3759	3769	3777	rBV2	488731	1472535	30.34%	3.978%

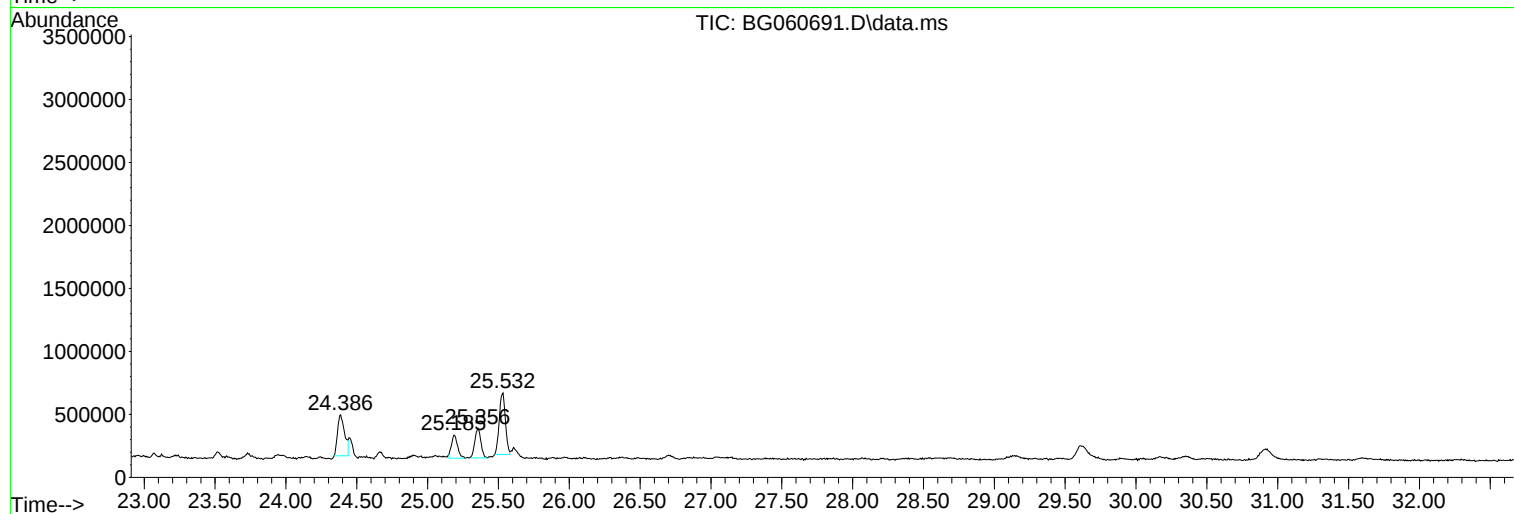
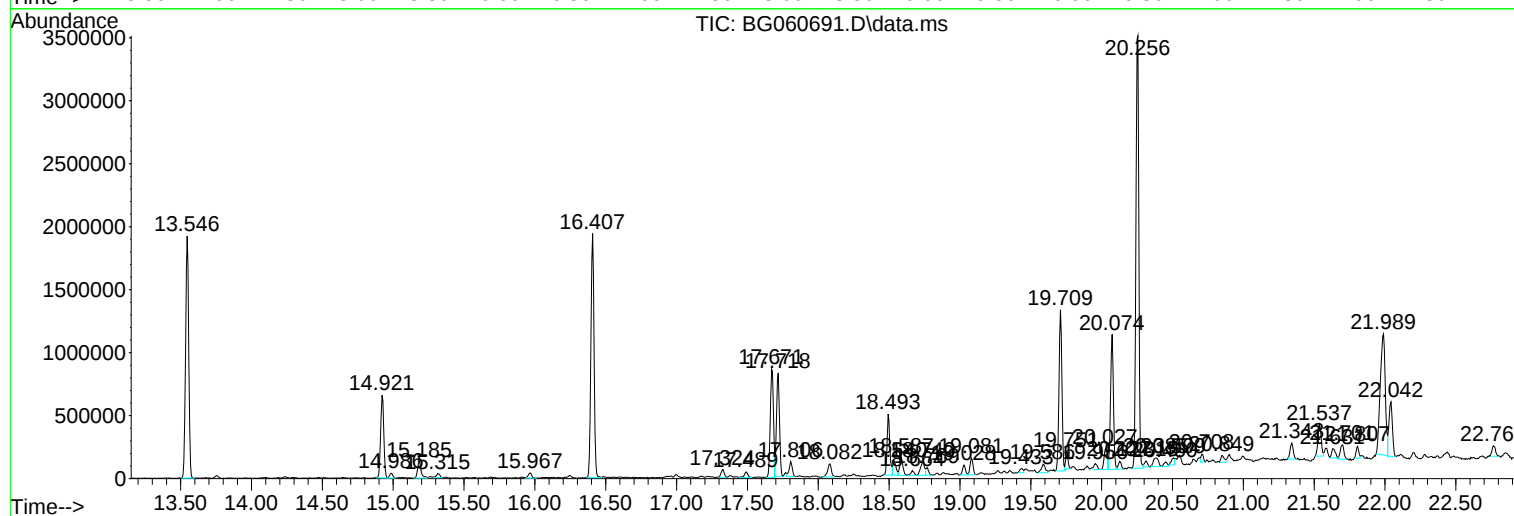
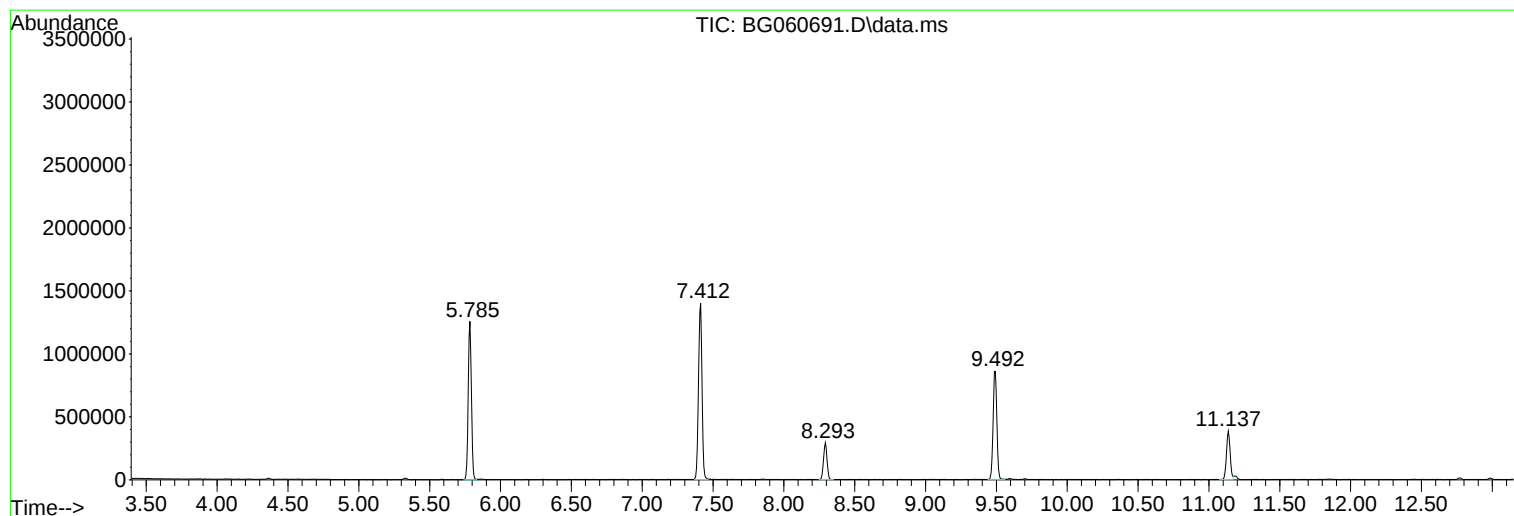
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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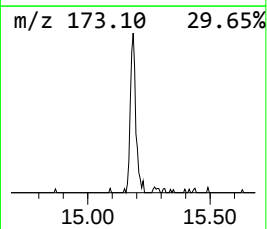
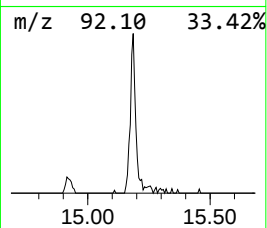
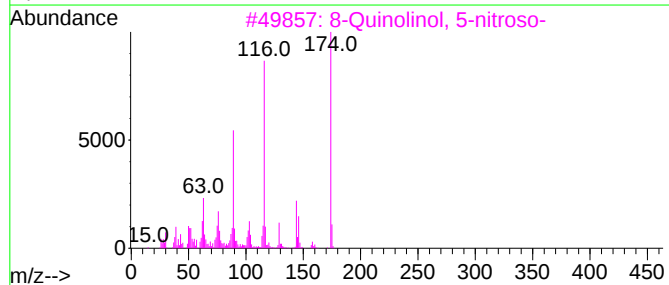
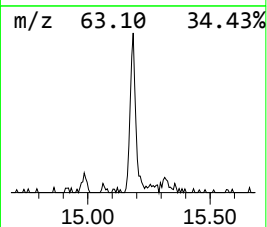
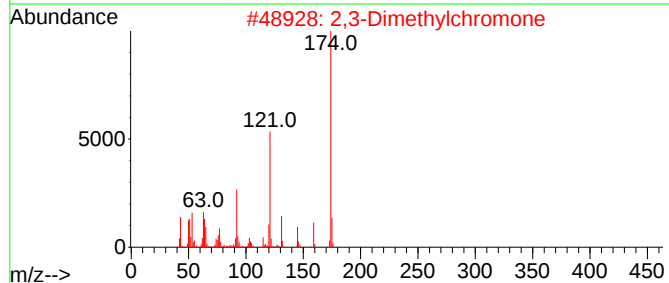
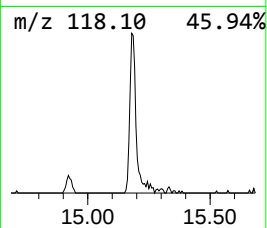
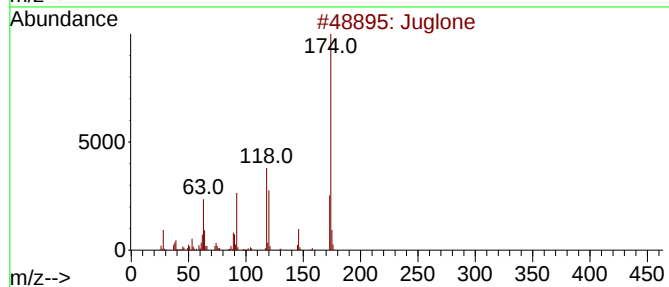
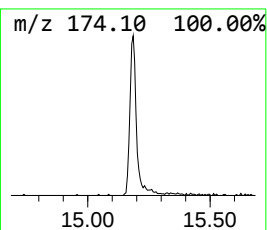
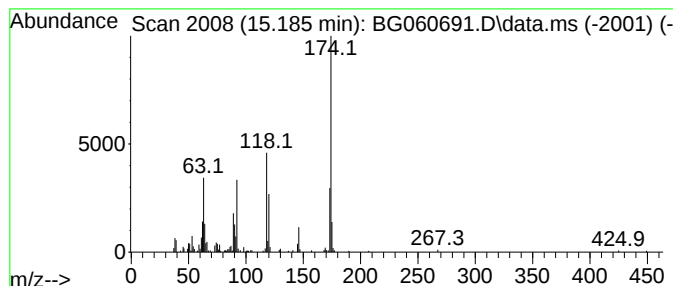
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Juglone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.185	4.70 ng	237022	Acenaphthene-d10	14.921

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Juglone	174	C10H6O3	000481-39-0	97
2			2,3-Dimethylchromone	174	C11H10O2	017584-90-6	43
3			8-Quinololinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43
4			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	35
5			4-(4-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-19-4	35



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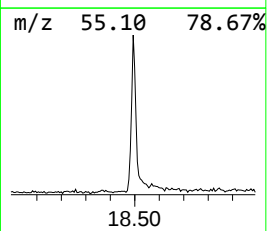
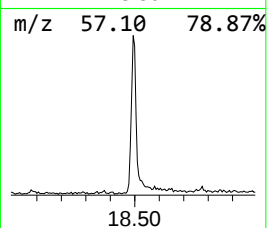
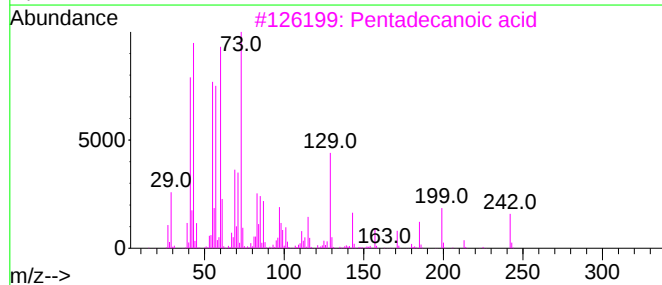
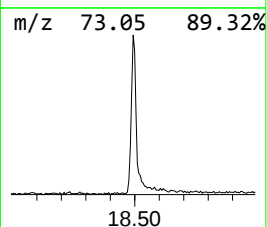
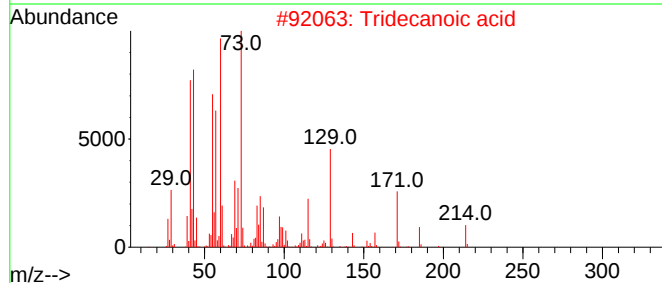
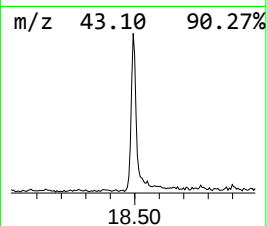
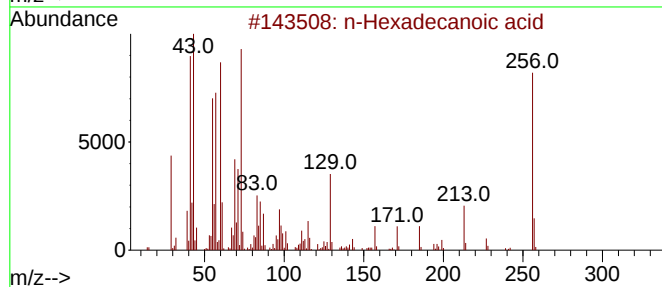
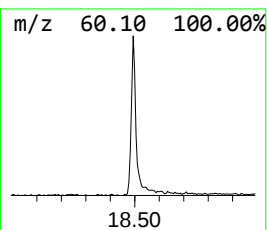
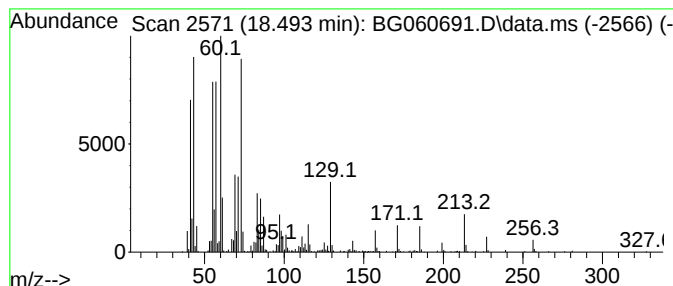
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.493	9.48 ng	653410	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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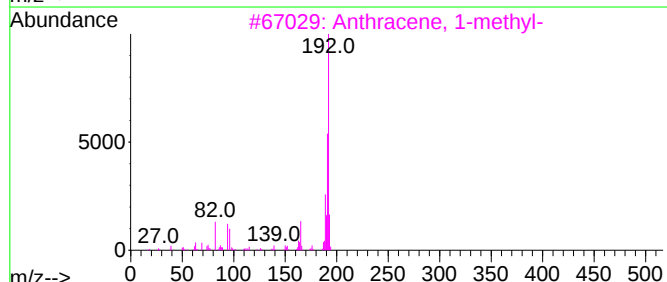
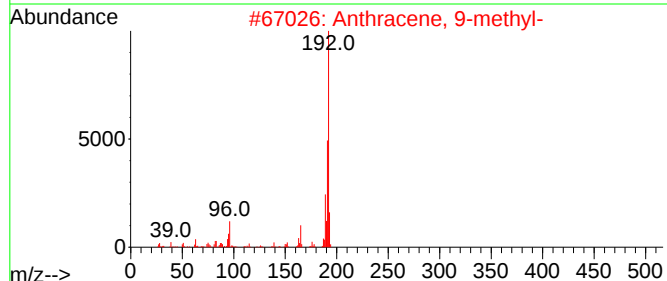
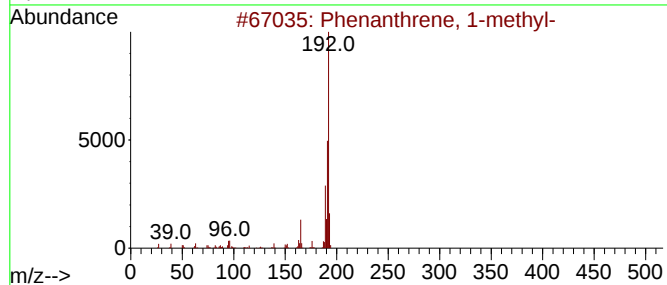
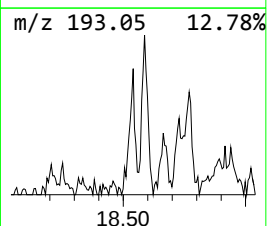
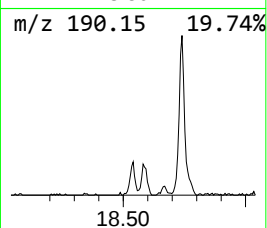
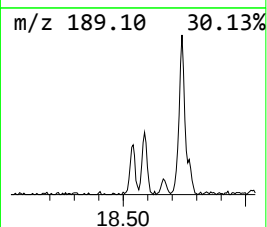
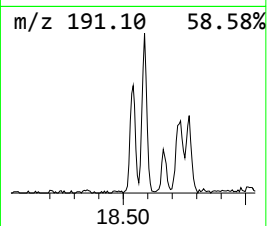
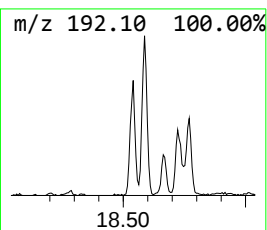
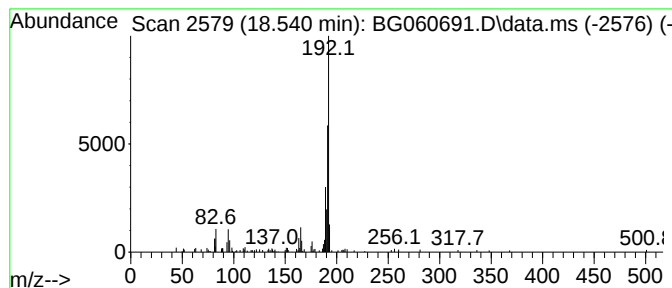
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.540	2.37 ng	163631	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	68
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	62
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	58



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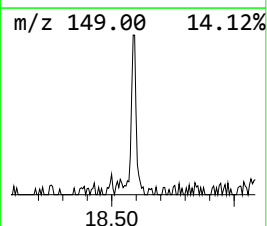
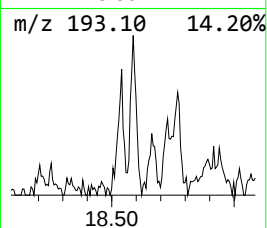
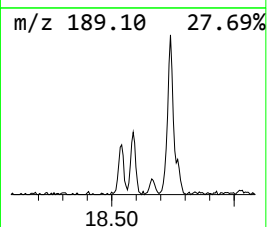
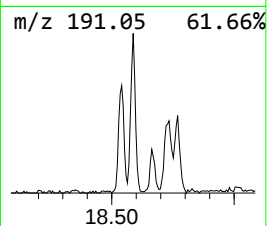
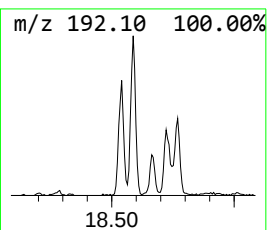
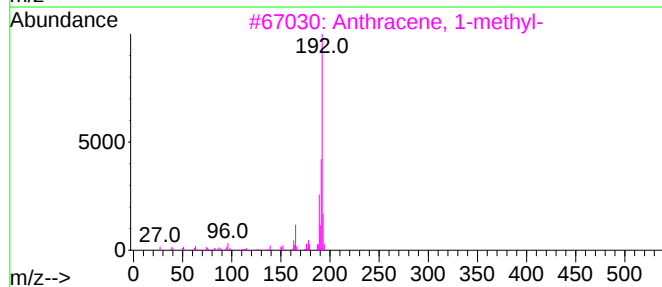
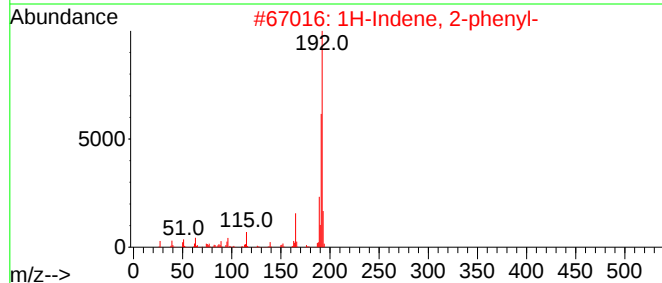
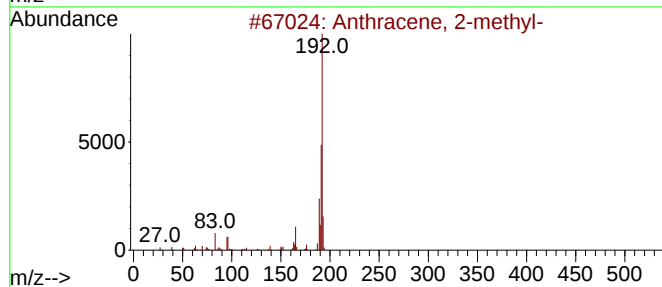
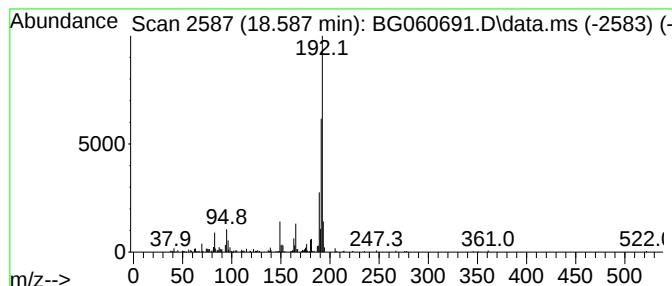
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.587	3.14 ng	216595	Phenanthrene-d10	17.671

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	90



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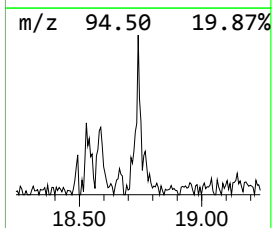
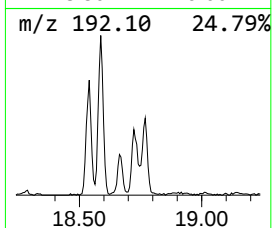
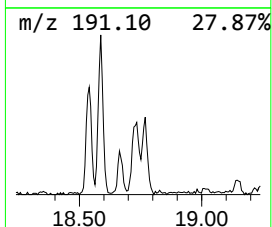
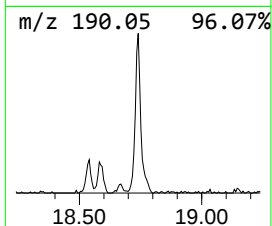
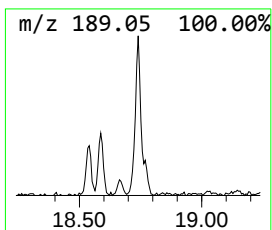
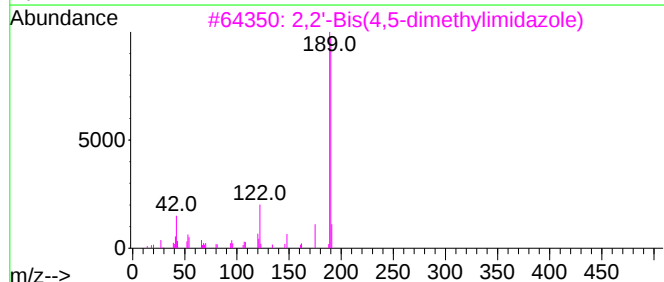
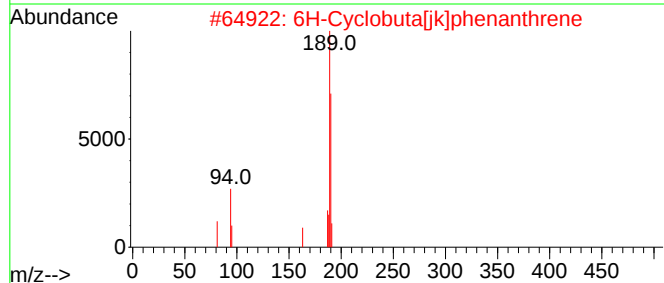
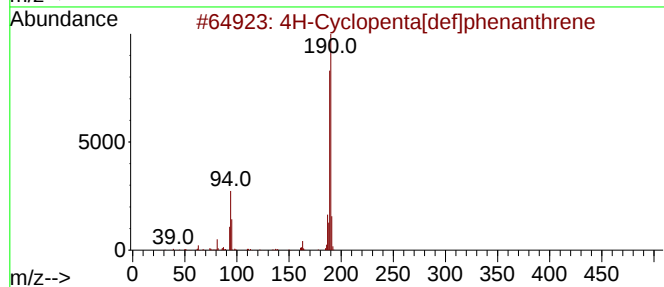
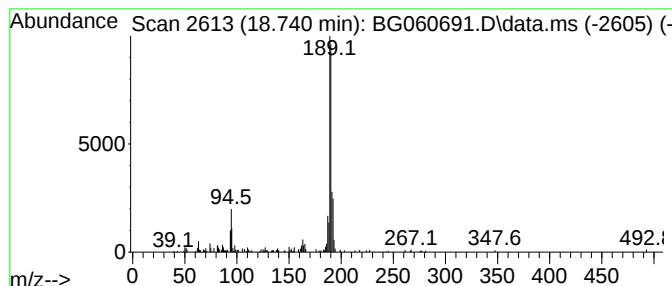
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.740	3.10 ng	213973	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4			Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	27
5			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060691.D
Acq On : 20 Mar 2024 14:35
Operator : MA/JU
Sample : P1803-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TRENCH-PIT

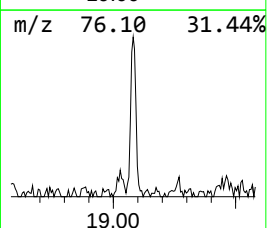
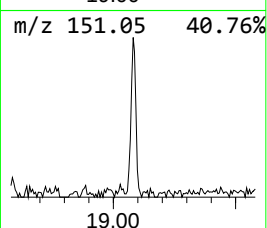
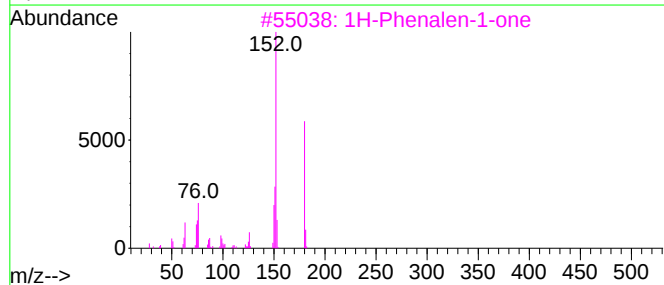
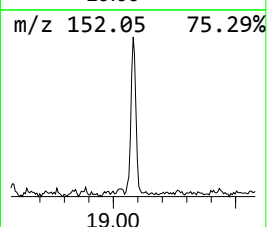
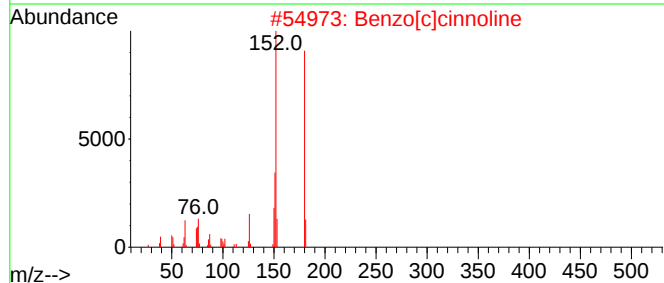
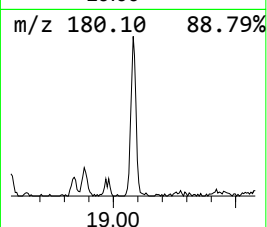
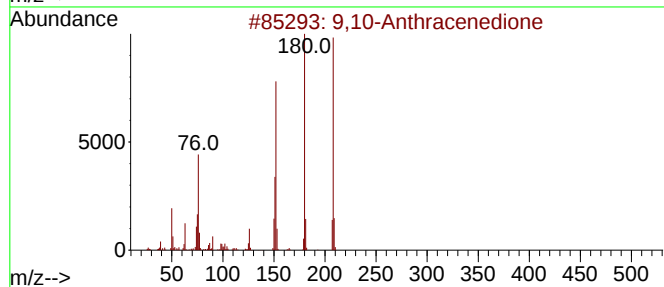
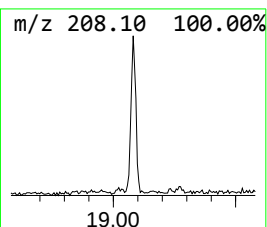
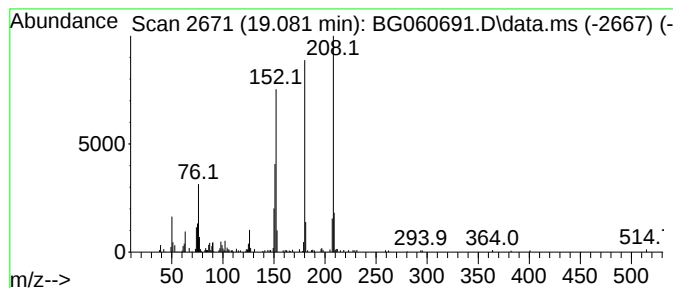
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,10-Anthracenedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.081	2.74 ng	188669	Phenanthrene-d10		17.671

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98	
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	91	
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64	
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	60	
5	9H-Fluoren-9-one	180	C13H8O	000486-25-9	58	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060691.D
Acq On : 20 Mar 2024 14:35
Operator : MA/JU
Sample : P1803-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TRENCH-PIT

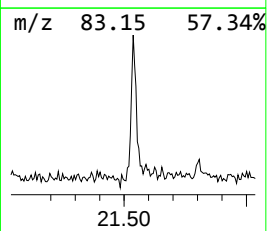
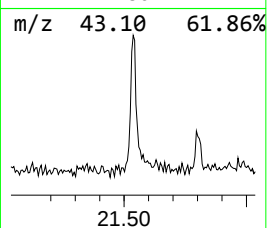
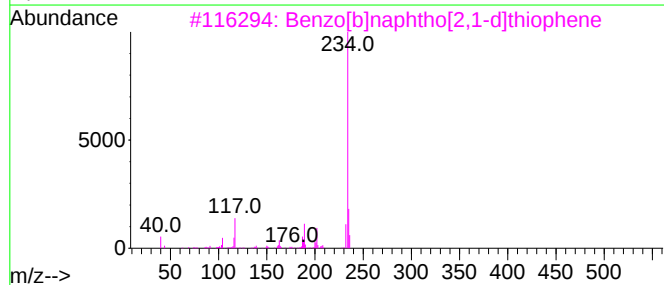
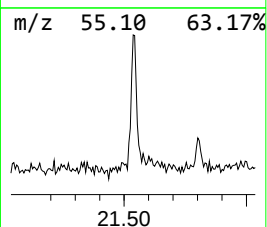
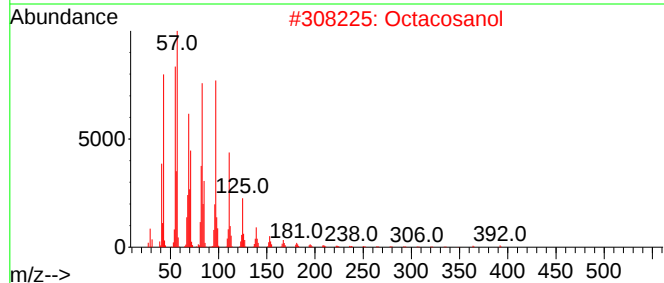
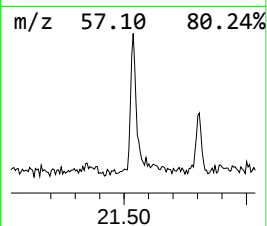
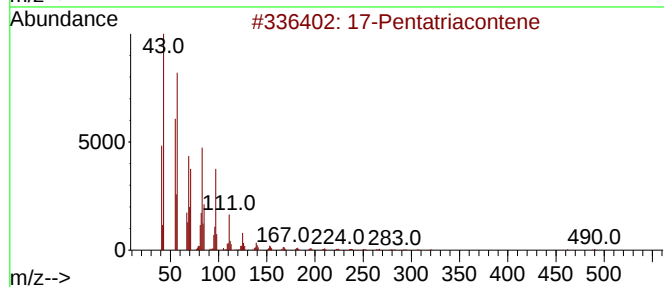
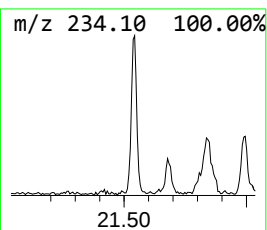
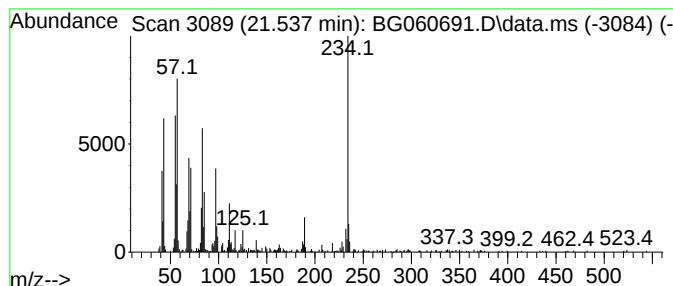
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	3.29 ng	395434	Chrysene-d12	21.989

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	60
2			Octacosanol	410	C28H58O	000557-61-9	49
3			Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	47
4			Triacantan-15-ol	438	C30H62O	031849-26-0	46
5			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060691.D
Acq On : 20 Mar 2024 14:35
Operator : MA/JU
Sample : P1803-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TRENCH-PIT

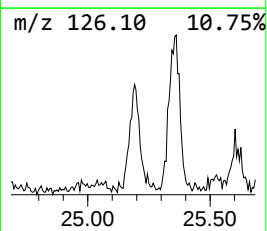
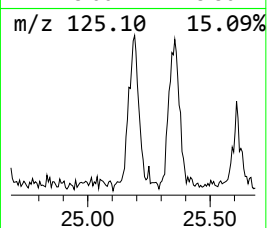
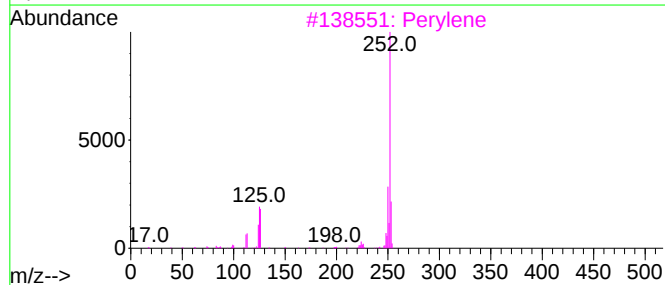
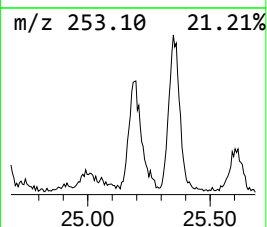
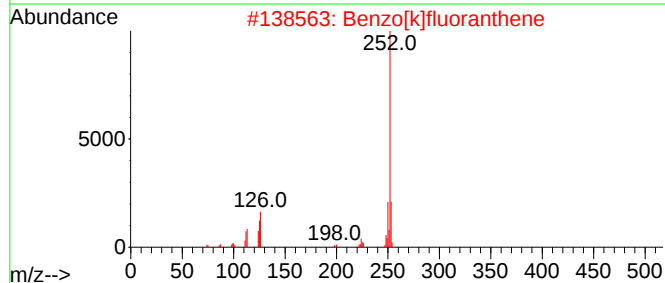
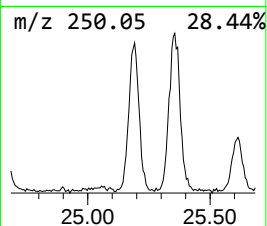
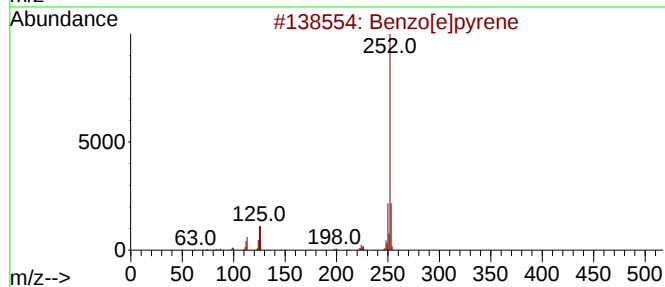
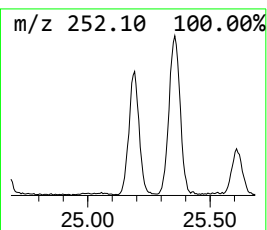
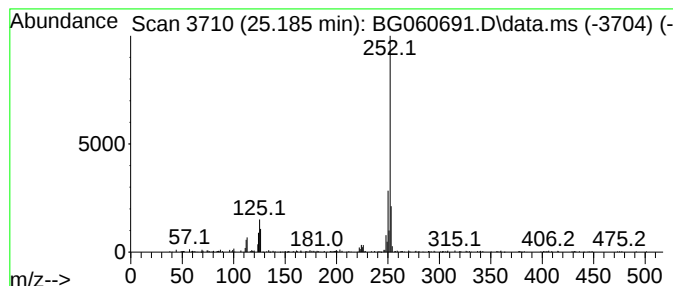
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.185	7.46 ng	549402	Perylene-d12	25.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032024\
Data File : BG060691.D
Acq On : 20 Mar 2024 14:35
Operator : MA/JU
Sample : P1803-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TRENCH-PIT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031324.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
Juglone	15.185	4.7	ng	237022	3	14.921	1008070	20.0
n-Hexadecanoic ...	18.493	9.5	ng	653410	4	17.671	1378760	20.0
Phenanthrene, 1...	18.540	2.4	ng	163631	4	17.671	1378760	20.0
Anthracene, 2-m...	18.587	3.1	ng	216595	4	17.671	1378760	20.0
4H-Cyclopenta[d...	18.740	3.1	ng	213973	4	17.671	1378760	20.0
9,10-Anthracene...	19.081	2.7	ng	188669	4	17.671	1378760	20.0
17-Pentatriacon...	21.537	3.3	ng	395434	5	21.989	2401570	20.0
Benzo[e]pyrene	25.185	7.5	ng	549402	6	25.532	1472540	20.0