

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051077.D
 Acq On : 16 Nov 2021 21:59
 Operator : CG/JU
 Sample : M4625-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-03-111021

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-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.763	380	387	402	rVB	496124	818125	51.26%	6.238%
2	7.373	653	661	673	rBV	502596	894720	56.05%	6.822%
3	8.225	800	806	813	rBV	146654	249738	15.65%	1.904%
4	9.400	997	1006	1015	rBV	311259	575548	36.06%	4.388%
5	10.798	1236	1244	1255	rBV	67222	130076	8.15%	0.992%
6	11.057	1280	1288	1295	rBV	199505	371152	23.25%	2.830%
7	13.477	1689	1700	1710	rBV	818186	1311647	82.18%	10.001%
8	14.582	1882	1888	1904	rBV	44788	120732	7.56%	0.921%
9	14.852	1926	1934	1942	rVB	327261	526096	32.96%	4.011%
10	15.722	2076	2082	2092	rBV2	7143	17589	1.10%	0.134%
11	15.898	2108	2112	2122	rVB3	9851	20440	1.28%	0.156%
12	16.344	2181	2188	2200	rVB	571457	931948	58.39%	7.106%
13	16.521	2213	2218	2219	rBV	14253	19015	1.19%	0.145%
14	17.308	2349	2352	2357	rBV2	14180	19257	1.21%	0.147%
15	17.602	2396	2402	2406	rBV	382608	596757	37.39%	4.550%
16	17.643	2406	2409	2415	rVB	81080	120377	7.54%	0.918%
17	17.737	2421	2425	2429	rVB	23913	27285	1.71%	0.208%
18	18.013	2467	2472	2474	rBV6	11137	19992	1.25%	0.152%
19	18.054	2475	2479	2486	rVB3	15980	26844	1.68%	0.205%
20	18.231	2505	2509	2513	rVB	23659	30186	1.89%	0.230%
21	18.448	2543	2546	2548	rBV2	24297	31219	1.96%	0.238%
22	18.524	2555	2559	2564	rVB2	26799	39137	2.45%	0.298%
23	18.671	2578	2584	2588	rBV4	42368	90246	5.65%	0.688%
24	18.959	2630	2633	2638	rBV2	16858	23588	1.48%	0.180%
25	19.012	2640	2642	2650	rVB6	27935	42735	2.68%	0.326%
26	19.364	2698	2702	2703	rBV3	45483	61865	3.88%	0.472%
27	19.523	2724	2729	2736	rBV	86367	155252	9.73%	1.184%
28	19.647	2745	2750	2755	rVB	228794	334251	20.94%	2.548%
29	20.005	2807	2811	2818	rVB	399208	581357	36.42%	4.433%
30	20.187	2837	2842	2847	rBV	1167278	1596154	100.00%	12.170%
31	20.792	2942	2945	2949	rVB2	49670	60775	3.81%	0.463%
32	21.903	3126	3134	3139	rBV2	372370	993507	62.24%	7.575%
33	21.956	3140	3143	3151	rVB	178560	275488	17.26%	2.100%
34	23.413	3387	3391	3398	rVB3	110115	201368	12.62%	1.535%
35	24.235	3524	3531	3550	rVB	265048	1177436	73.77%	8.977%
36	25.164	3683	3689	3699	rVB2	215050	623698	39.08%	4.755%

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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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

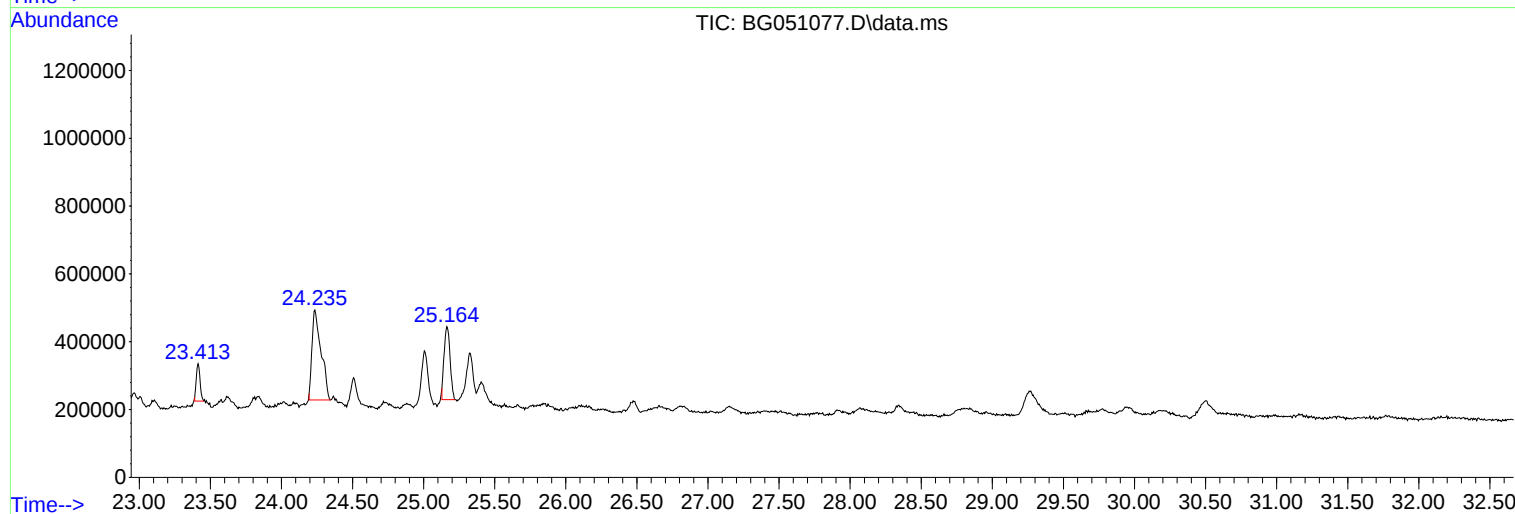
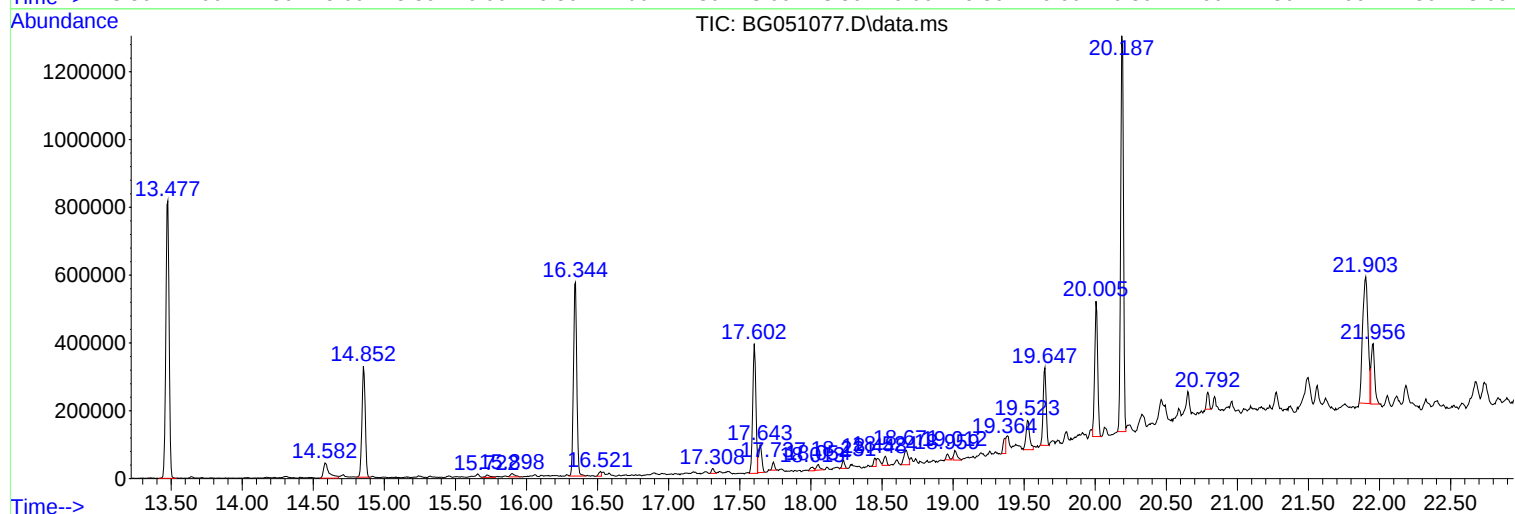
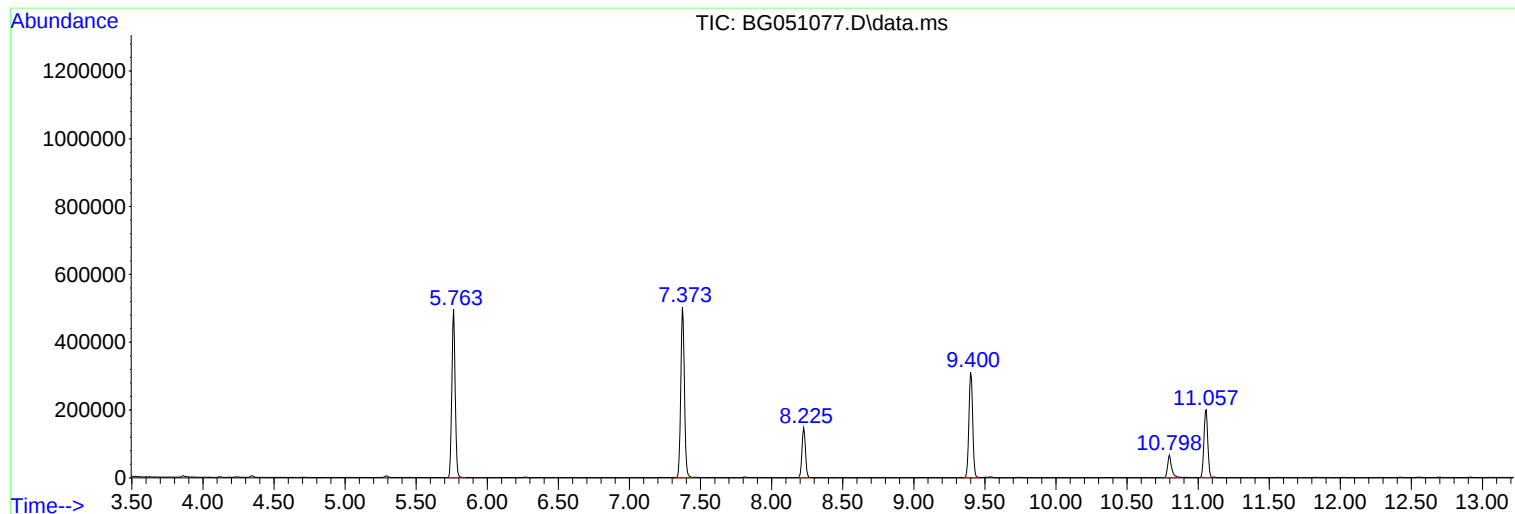
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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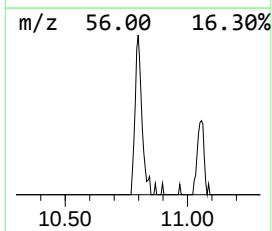
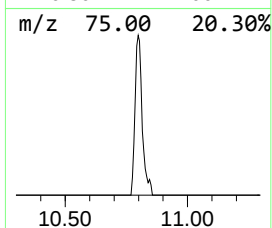
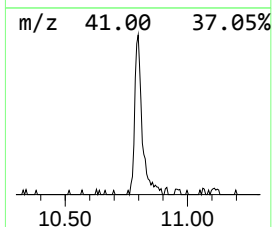
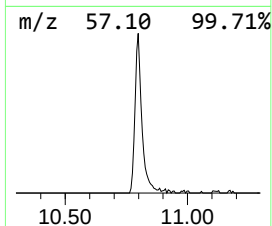
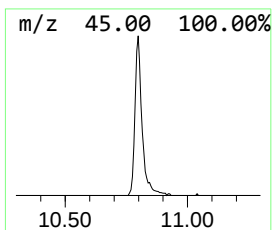
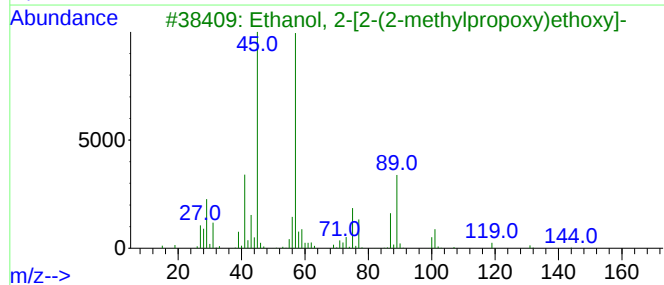
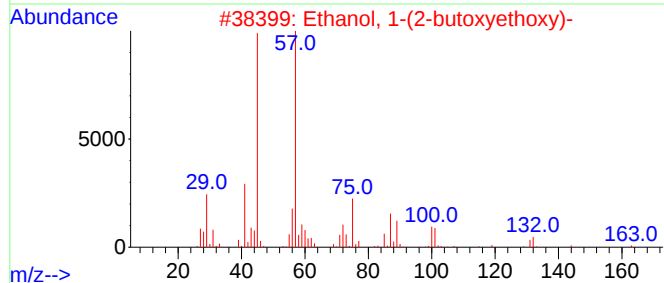
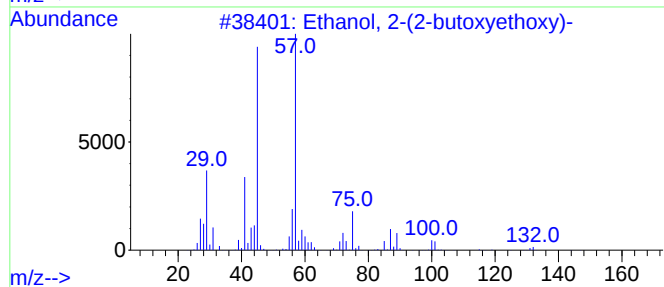
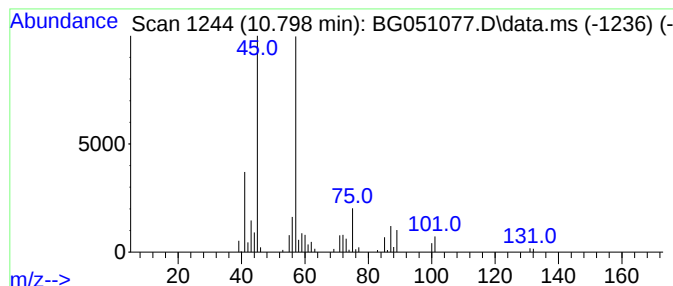
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	7.01 ng	130076	Naphthalene-d8	11.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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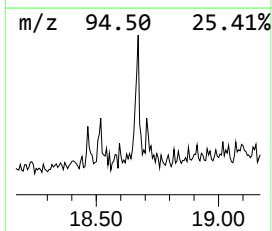
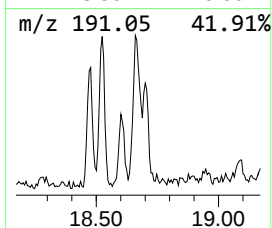
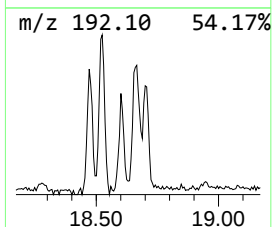
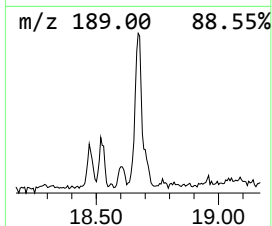
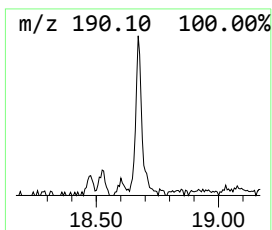
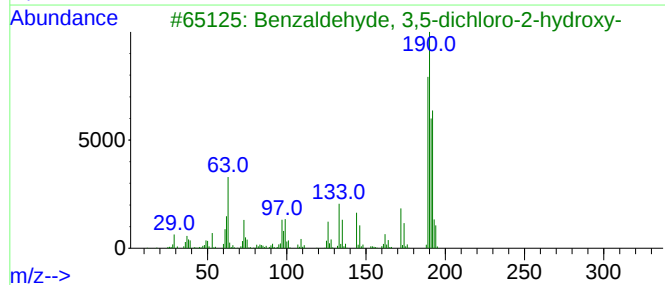
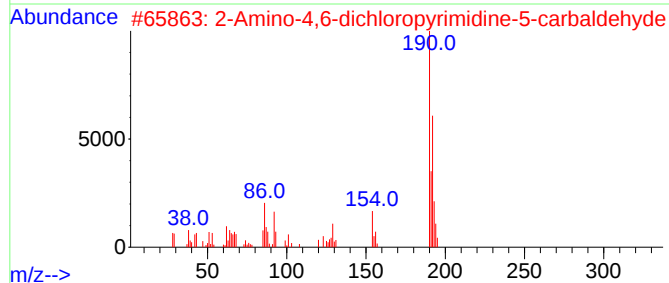
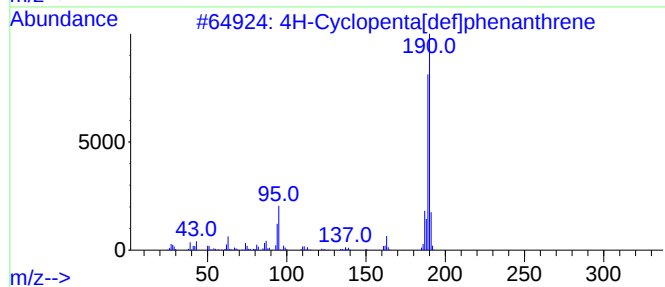
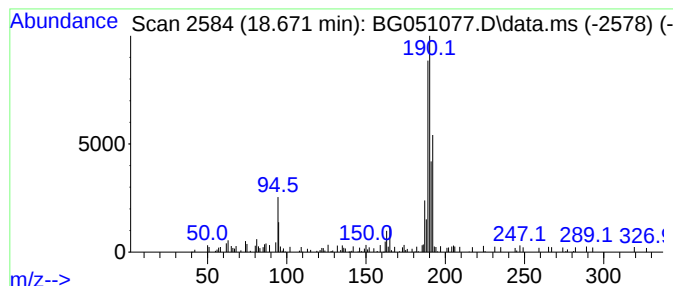
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.671	3.02 ng	90246	Phenanthrene-d10		17.602	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	58
2	2-Amino-4,6-dichloropyrimidine-5...		191	C5H3Cl2N3O	005604-46-6	38
3	Benzaldehyde, 3,5-dichloro-2-hyd...		190	C7H4Cl2O2	000090-60-8	38
4	9H-1,2,5-Thiadiazolo[3,4-g]-1,5-...		232	C10H8N4OS	1000277-07-6	27
5	Carbonic acid, butyl 2-formyl-4,...		290	C12H12Cl2O4	1000331-42-2	25



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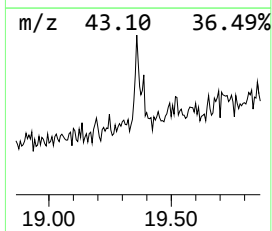
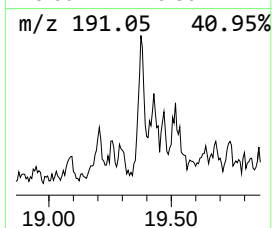
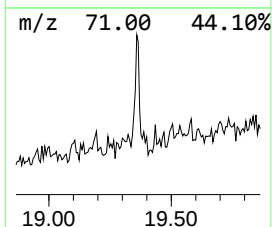
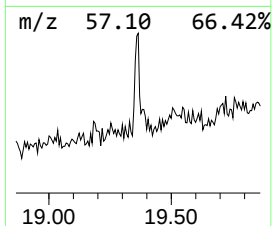
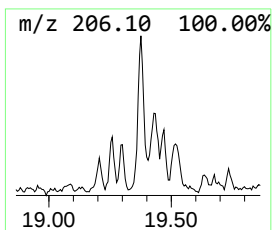
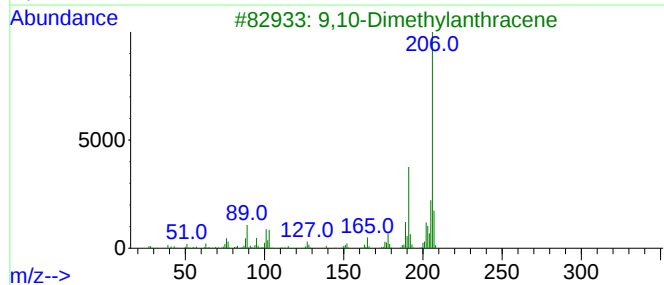
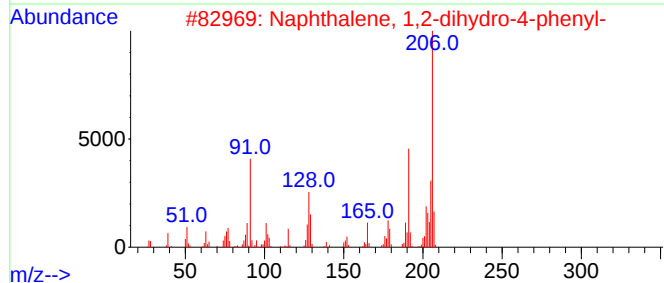
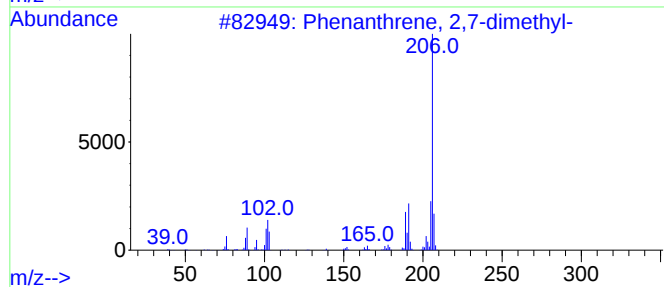
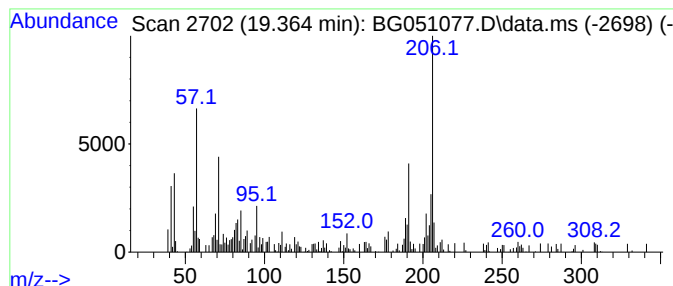
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 2,7-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.365	2.07 ng	61865	Phenanthrene-d10	17.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	60
2			Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	55
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	55
4			1,4-Diphenyl-1,3-butadiene	206	C16H14	000886-65-7	50
5			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	46



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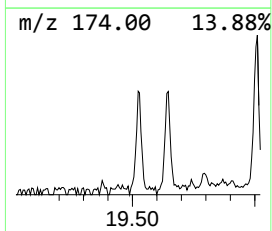
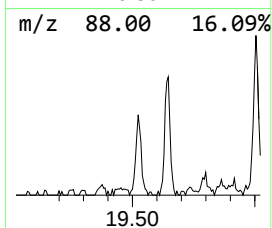
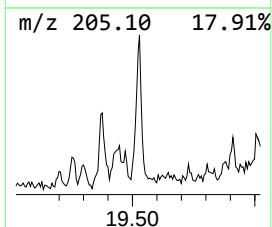
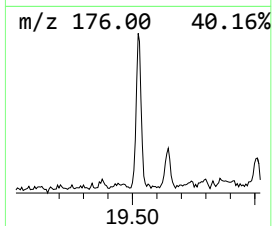
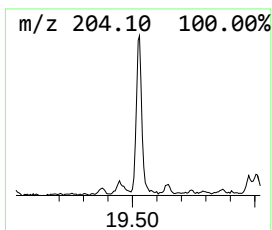
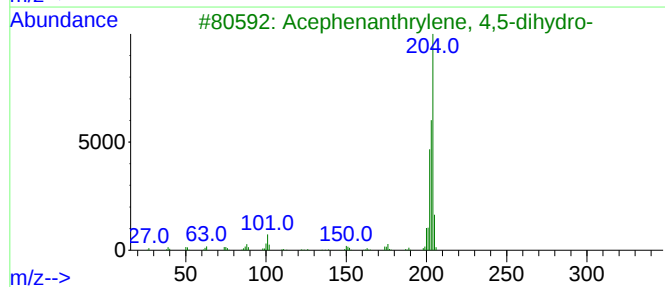
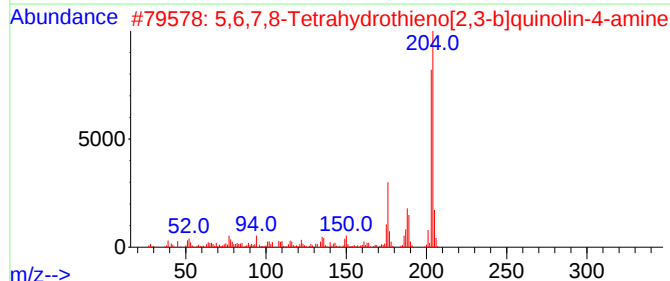
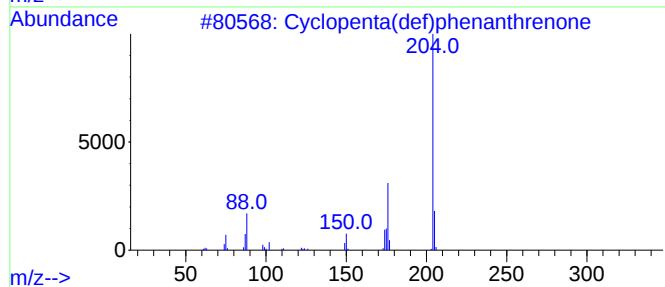
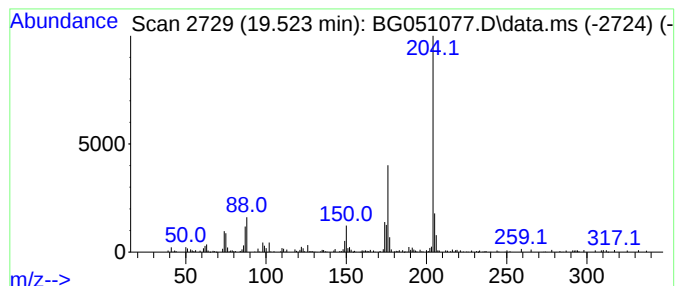
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopenta(def)phenanthrenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.523	5.20 ng	155252	Phenanthrene-d10		17.602	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone		204	C15H8O	005737-13-3	96
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...		204	C11H12N2S	122914-50-5	64
3	Acephenanthrylene, 4,5-dihydro-		204	C16H12	006232-48-0	43
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile		204	C14H8N2	001591-30-6	43
5	Tetracyano-p-quinodimethane		204	C12H4N4	001518-16-7	43



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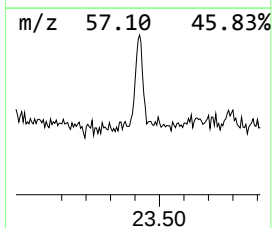
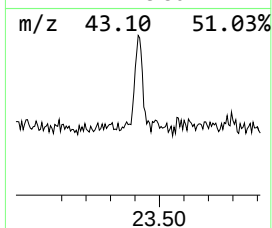
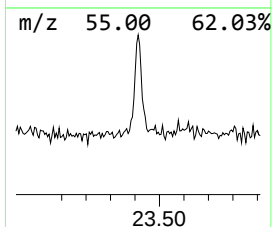
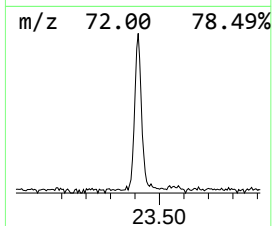
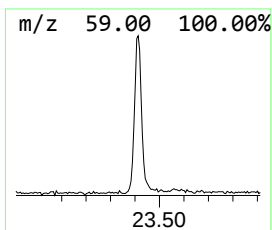
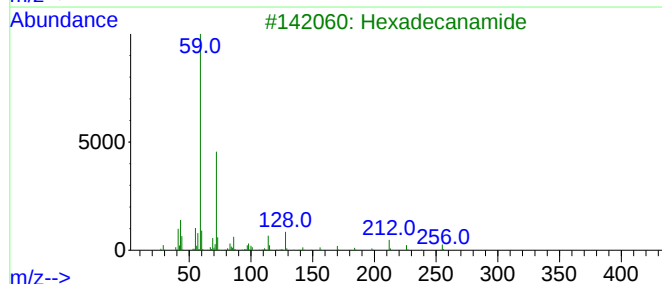
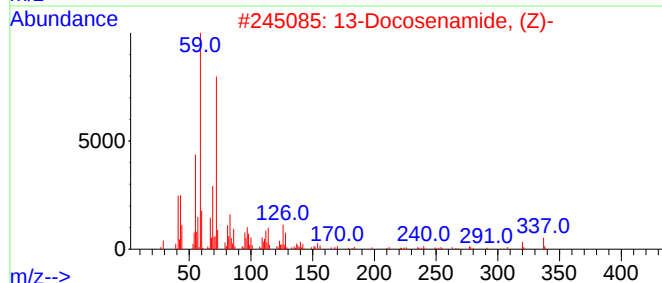
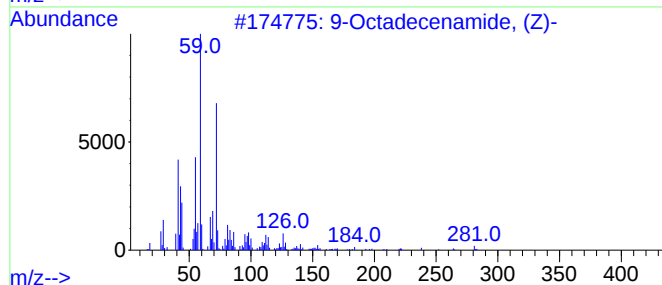
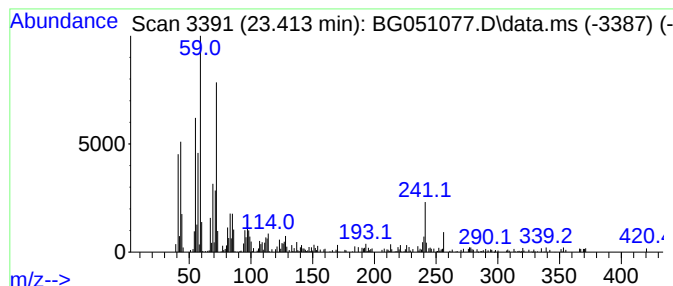
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.413	4.05 ng	201368	Chrysene-d12	21.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
3			Hexadecanamide	255	C16H33NO	000629-54-9	43
4			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	43
5			7-Nonenamide	155	C9H17NO	090949-53-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051077.D
Acq On : 16 Nov 2021 21:59
Operator : CG/JU
Sample : M4625-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-03-111021

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.798	7.0	ng	130076	2	11.057	371152	20.0
4H-Cyclopenta[d...	18.671	3.0	ng	90246	4	17.602	596757	20.0
Phenanthrene, 2...	19.365	2.1	ng	61865	4	17.602	596757	20.0
Cyclopenta(def)...	19.523	5.2	ng	155252	4	17.602	596757	20.0
9-Octadecenamid...	23.413	4.0	ng	201368	5	21.903	993507	20.0