

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
 Data File : BG050496.D
 Acq On : 7 Oct 2021 23:55
 Operator : CG/JU
 Sample : M4134-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-01

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050496.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.797	385	393	402	rBV	823506	1386838	53.39%	7.248%
2	7.395	656	665	675	rBV	860437	1528136	58.83%	7.986%
3	8.259	805	812	818	rBV	228352	389490	14.99%	2.035%
4	9.428	1002	1011	1019	rBV	530119	960733	36.98%	5.021%
5	10.826	1242	1249	1263	rBV	241689	402181	15.48%	2.102%
6	11.085	1284	1293	1300	rBV	295997	555371	21.38%	2.902%
7	13.500	1697	1704	1711	rBV	1245048	1982393	76.31%	10.360%
8	14.875	1929	1938	1944	rBV	478383	750985	28.91%	3.925%
9	16.355	2183	2190	2200	rVB	927541	1408223	54.21%	7.359%
10	17.618	2398	2405	2409	rBV	553755	877808	33.79%	4.587%
11	17.660	2409	2412	2418	rVB	148914	214343	8.25%	1.120%
12	17.748	2421	2427	2433	rVV	36916	55555	2.14%	0.290%
13	18.259	2509	2514	2518	rBV2	25827	34010	1.31%	0.178%
14	18.347	2524	2529	2536	rBV5	11824	27002	1.04%	0.141%
15	18.476	2543	2551	2557	rBV3	129760	252800	9.73%	1.321%
16	18.535	2557	2561	2568	rVV	77187	124189	4.78%	0.649%
17	18.617	2570	2575	2579	rVV3	27575	44875	1.73%	0.235%
18	18.676	2580	2585	2590	rVV4	68161	152653	5.88%	0.798%
19	18.717	2590	2592	2597	rVB	45394	56549	2.18%	0.296%
20	18.976	2631	2636	2640	rBV2	35937	52787	2.03%	0.276%
21	19.017	2640	2643	2650	rVB5	19989	34681	1.34%	0.181%
22	19.217	2674	2677	2682	rVB4	23664	31270	1.20%	0.163%
23	19.269	2682	2686	2690	rBV	26880	34317	1.32%	0.179%
24	19.311	2690	2693	2700	rVB	20119	27662	1.06%	0.145%
25	19.393	2701	2707	2713	rBV	72422	148178	5.70%	0.774%
26	19.446	2713	2716	2720	rVV5	14930	25997	1.00%	0.136%
27	19.528	2726	2730	2738	rBV7	31073	79857	3.07%	0.417%
28	19.657	2746	2752	2757	rBV	337052	489569	18.85%	2.558%
29	19.734	2758	2765	2774	rVB3	71469	128310	4.94%	0.671%
30	19.980	2801	2807	2809	rBV2	59078	97855	3.77%	0.511%
31	20.016	2809	2813	2820	rVV	353494	552069	21.25%	2.885%
32	20.080	2820	2824	2829	rVB	33825	53364	2.05%	0.279%
33	20.204	2839	2845	2851	rBV	1863992	2597685	100.00%	13.575%
34	20.345	2862	2869	2874	rBV3	39441	97359	3.75%	0.509%
35	20.497	2887	2895	2901	rVB2	70769	164087	6.32%	0.858%
36	20.603	2909	2913	2916	rBV2	35723	52183	2.01%	0.273%

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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

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37	20.662	2919	2923	2927	rVB	60436	87379	3.36%	0.457%
38	20.803	2943	2947	2951	rBV	55785	86032	3.31%	0.450%
39	20.850	2951	2955	2964	rVB5	57297	109574	4.22%	0.573%
40	21.279	3025	3028	3034	rVB	41551	69440	2.67%	0.363%
41	21.520	3065	3069	3074	rVB	90067	134170	5.16%	0.701%
42	21.913	3128	3136	3142	rBV2	501893	1146798	44.15%	5.993%
43	21.966	3142	3145	3152	rVB	143116	221268	8.52%	1.156%
44	24.240	3525	3532	3539	rBV2	74118	247723	9.54%	1.295%
45	25.010	3658	3663	3672	rVB3	51685	139240	5.36%	0.728%
46	25.163	3683	3689	3699	rVB2	73067	201444	7.75%	1.053%
47	25.327	3708	3717	3728	rBV3	267106	820763	31.60%	4.289%

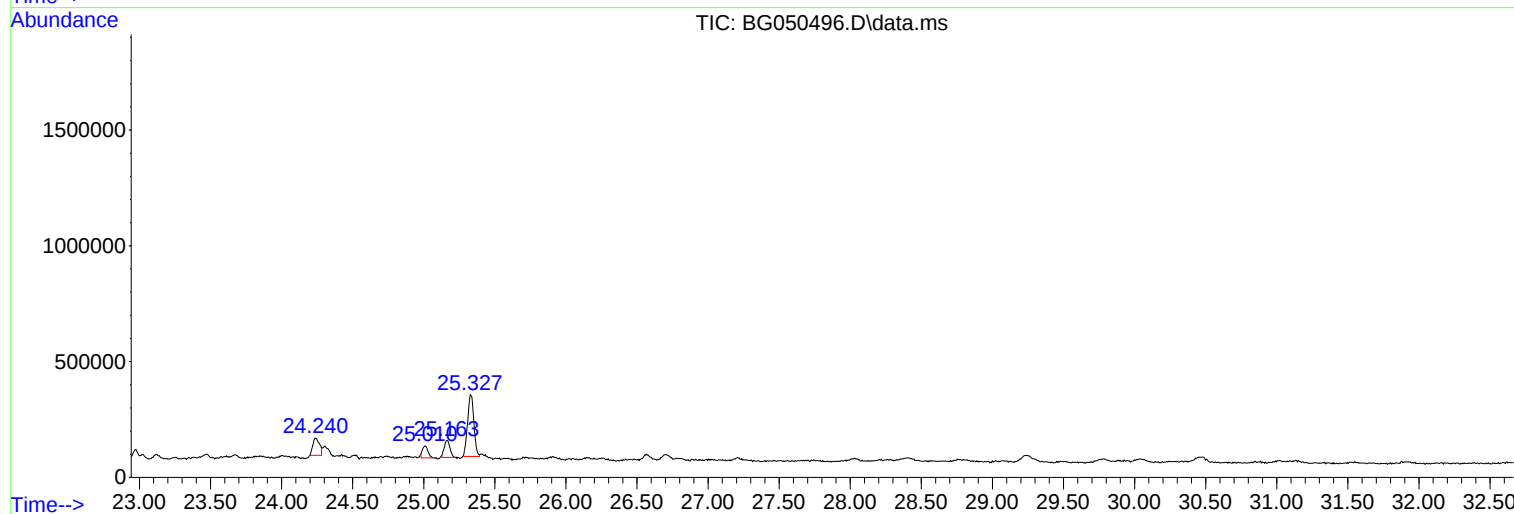
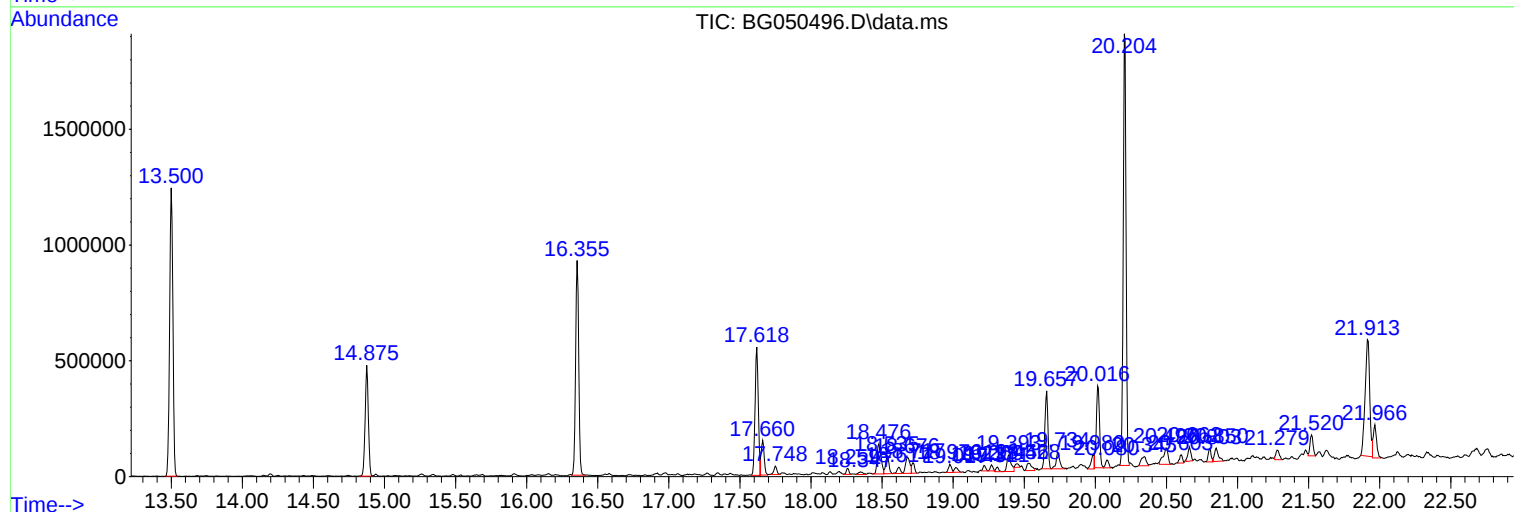
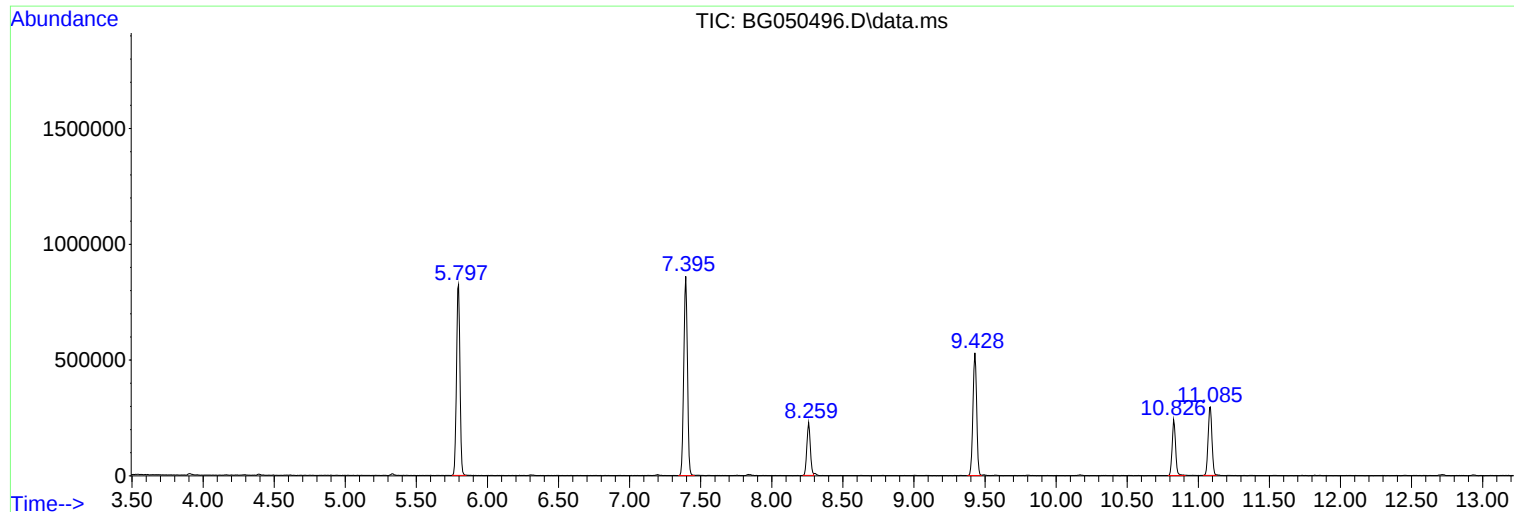
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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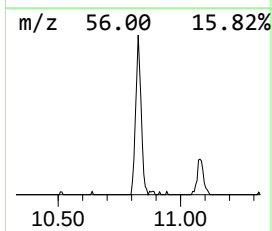
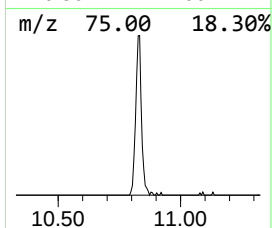
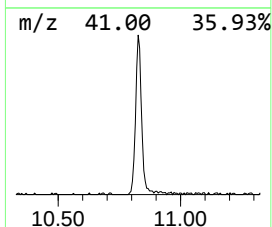
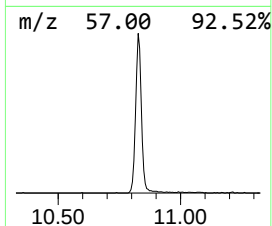
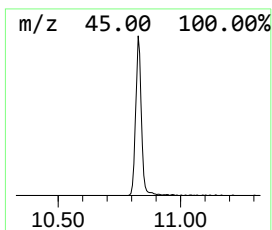
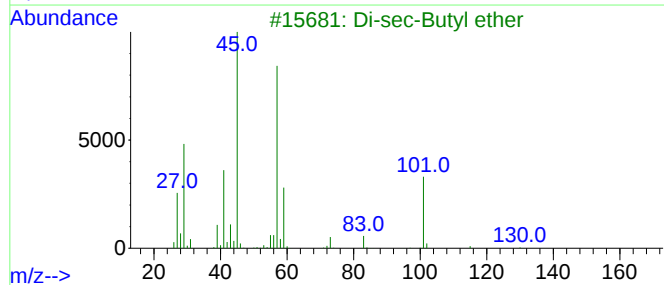
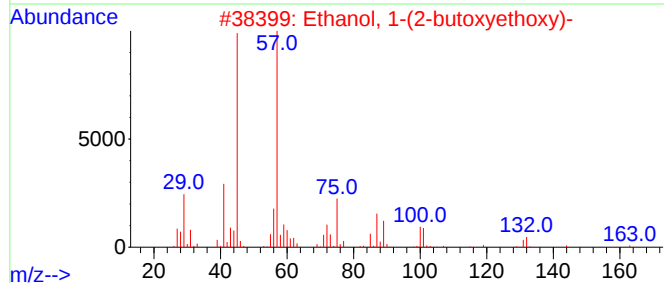
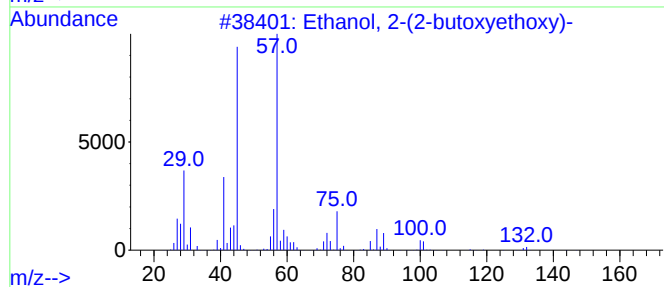
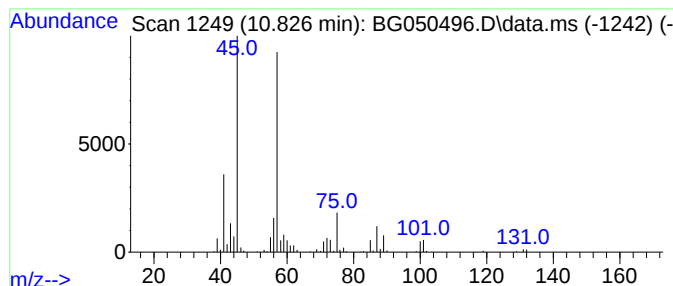
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
10.826	14.48 ng	402181	Naphthalene-d8	11.085

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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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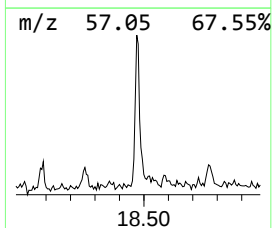
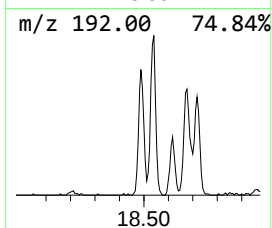
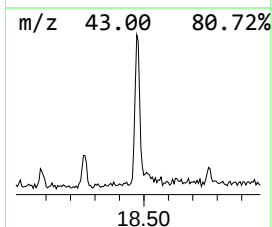
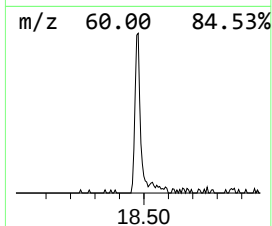
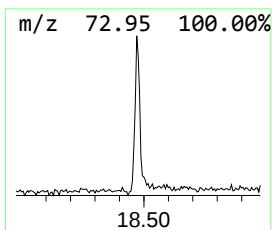
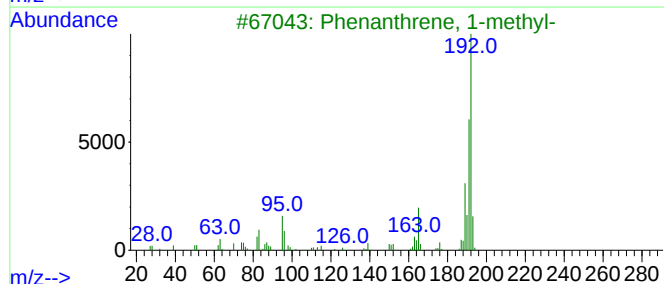
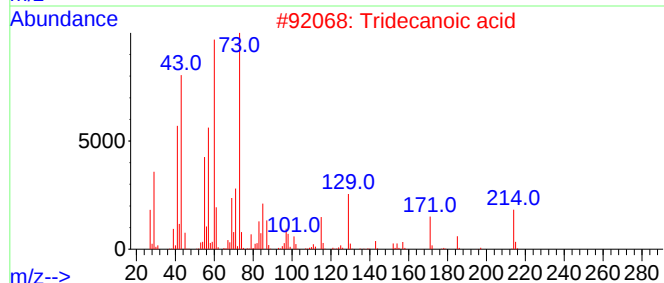
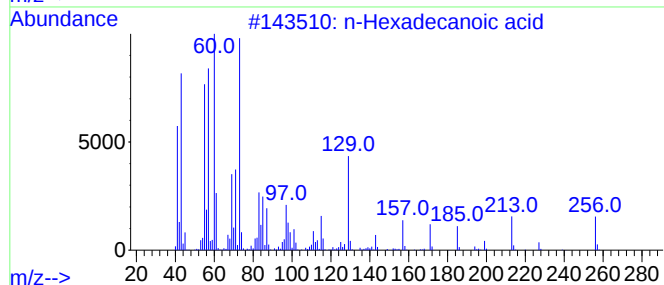
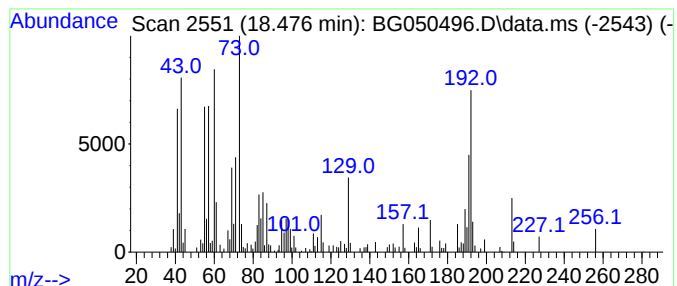
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.476	5.76 ng	252800	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	84
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	64



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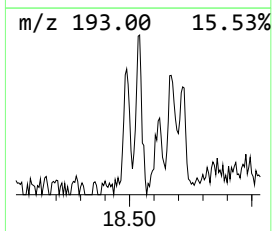
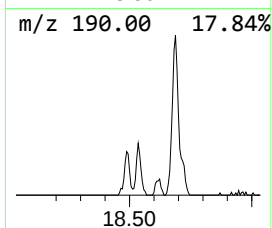
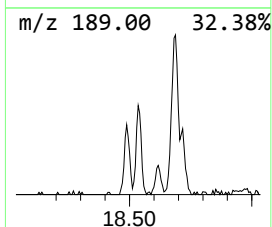
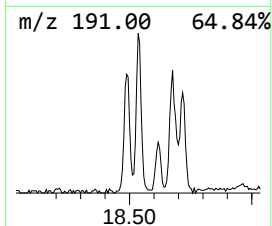
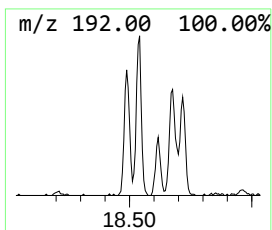
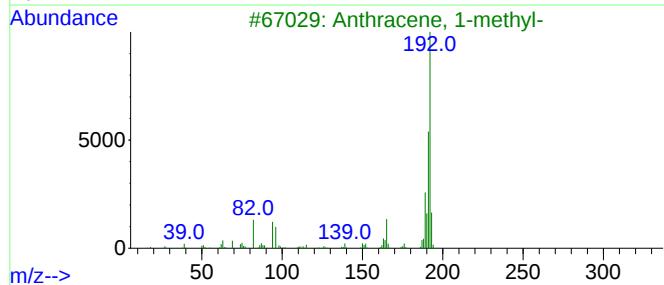
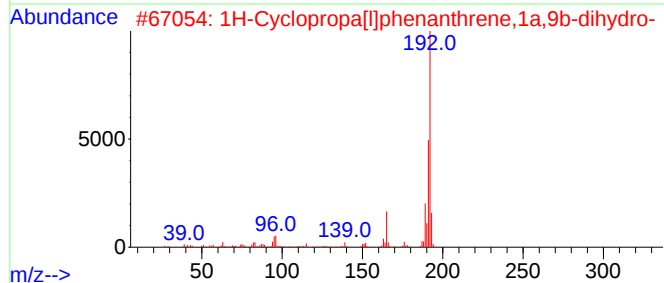
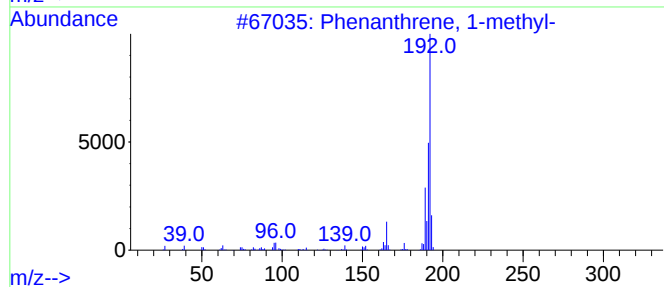
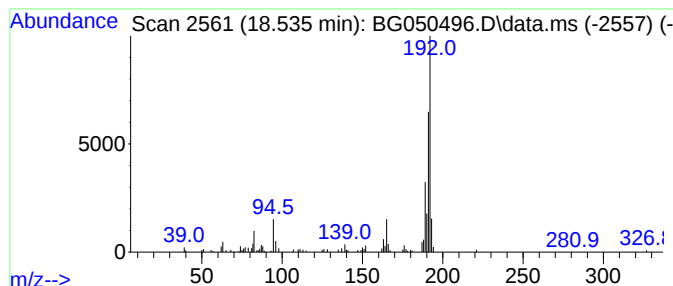
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.535	2.83 ng	124189	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	95
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93



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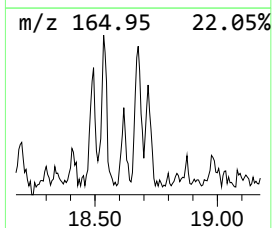
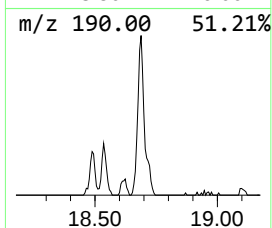
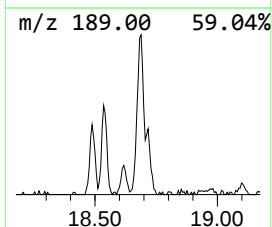
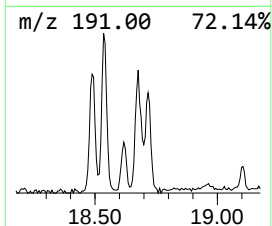
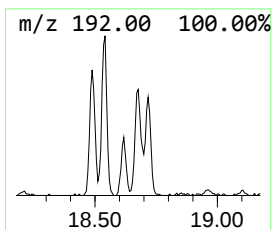
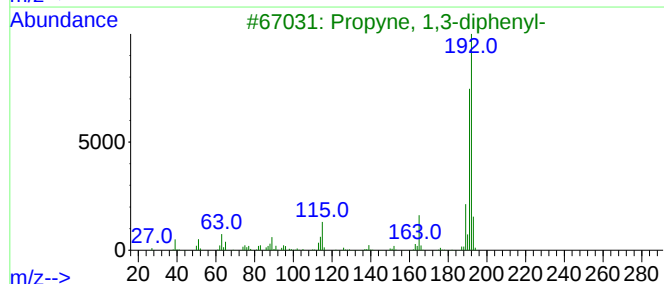
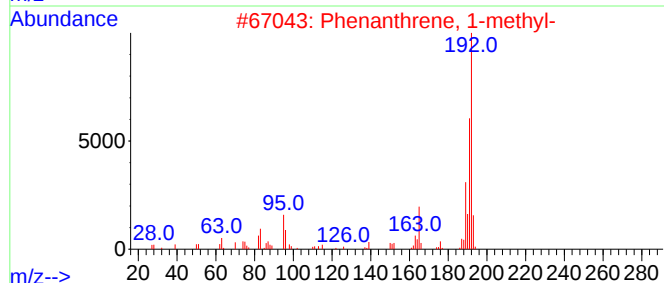
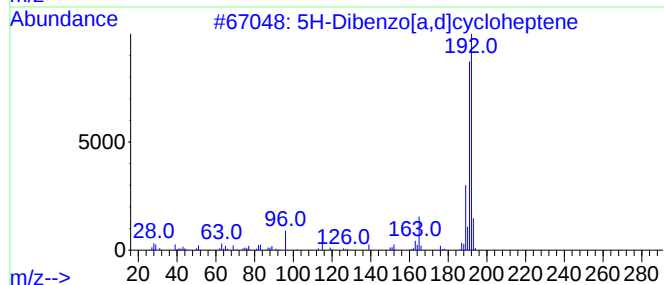
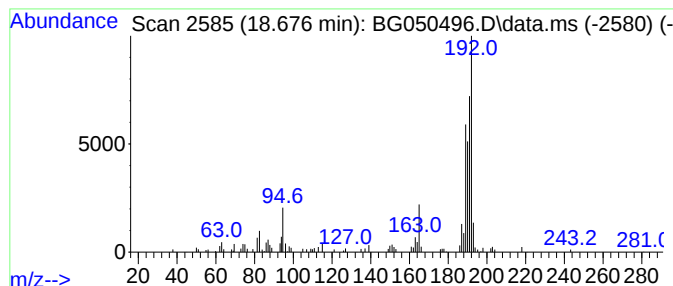
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5H-Dibenzo[a,d]cycloheptene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.676	3.48 ng	152653	Phenanthrene-d10	17.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	60
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
3		Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	60
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	58
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	53



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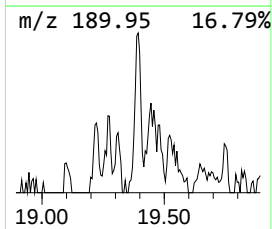
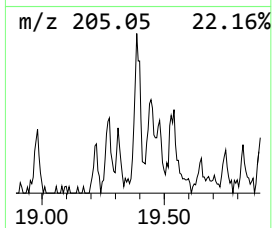
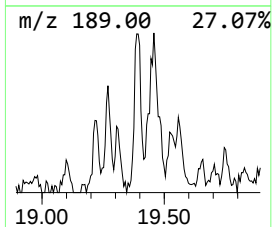
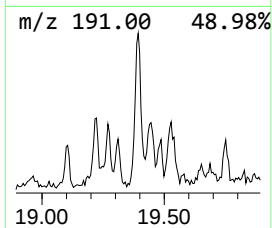
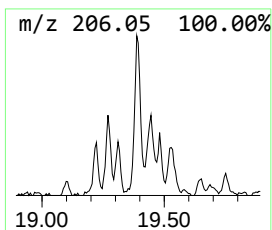
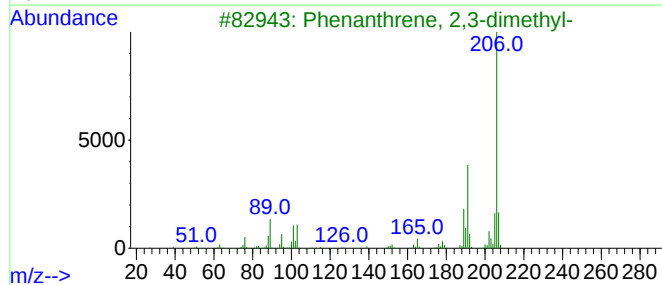
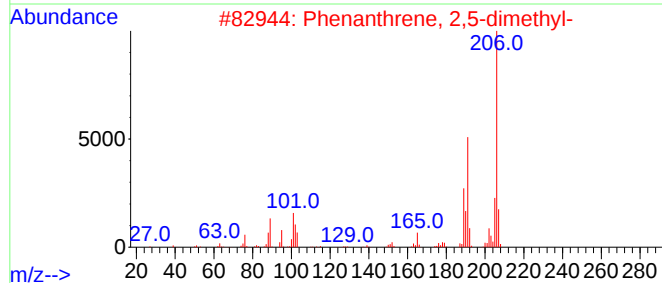
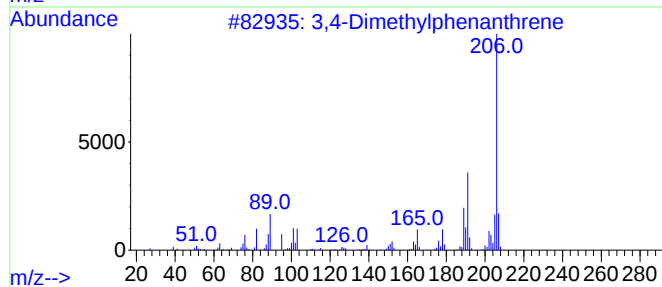
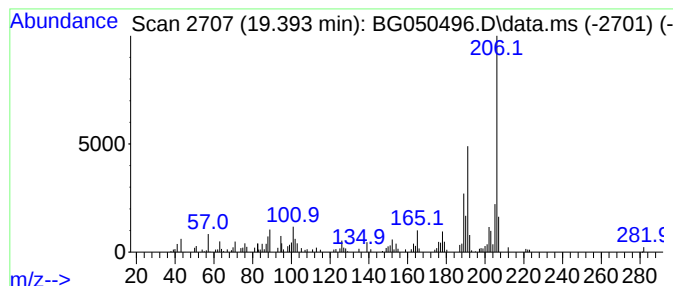
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3,4-Dimethylphenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.393	3.38 ng	148178	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
3			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	94
4			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
Data File : BG050496.D
Acq On : 7 Oct 2021 23:55
Operator : CG/JU
Sample : M4134-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-01

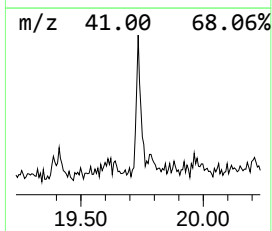
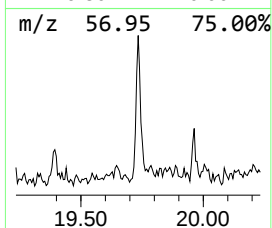
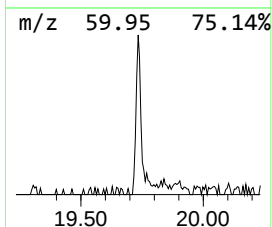
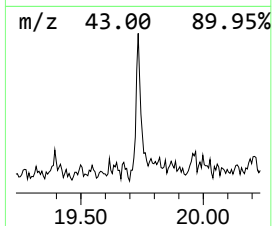
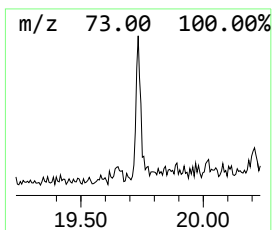
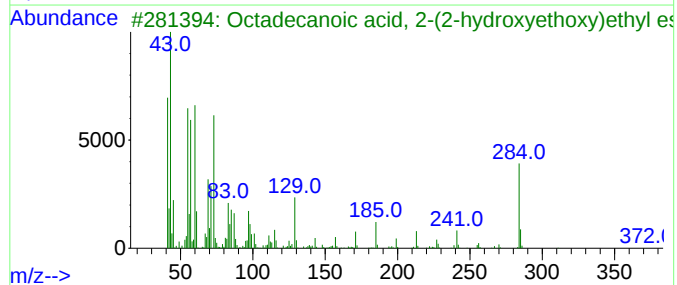
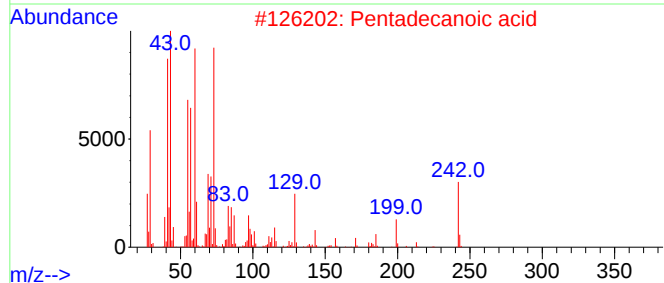
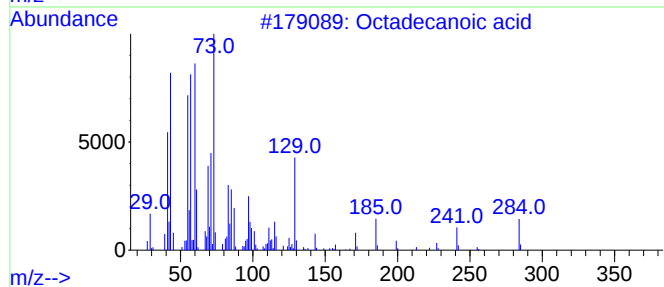
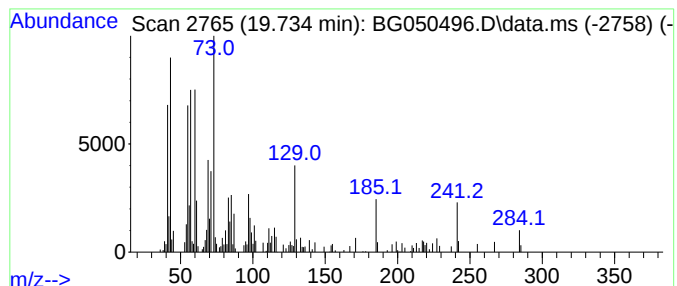
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.734	2.92 ng	128310	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
Data File : BG050496.D
Acq On : 7 Oct 2021 23:55
Operator : CG/JU
Sample : M4134-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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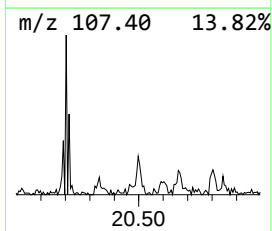
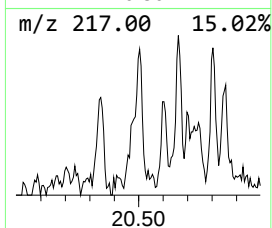
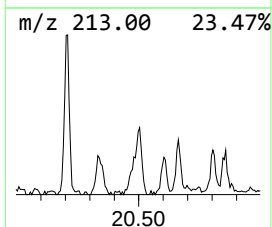
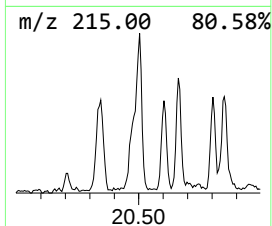
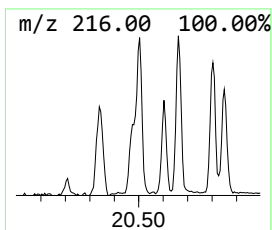
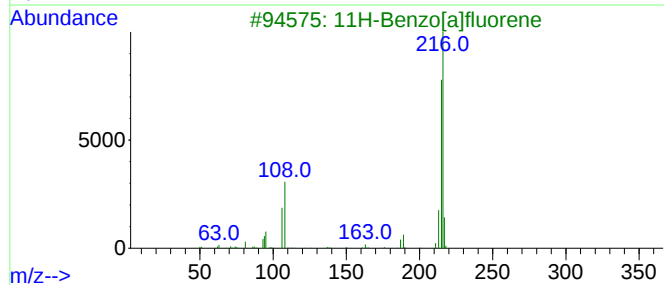
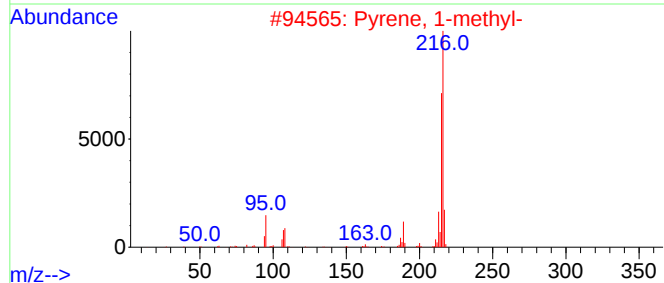
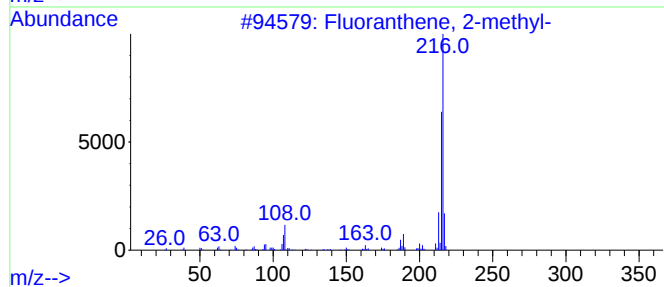
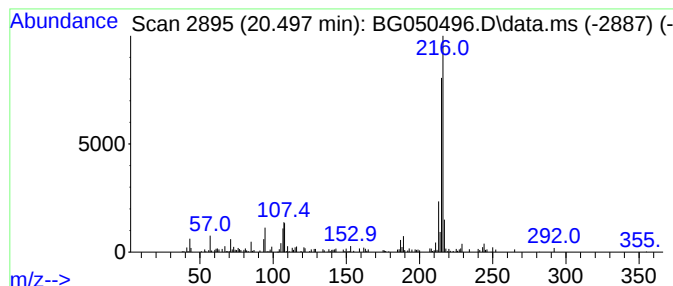
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Fluoranthene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.497	2.86 ng	164087	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	89
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
Data File : BG050496.D
Acq On : 7 Oct 2021 23:55
Operator : CG/JU
Sample : M4134-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-01

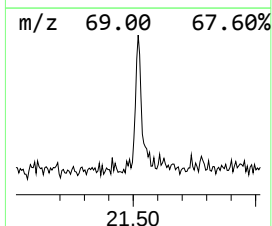
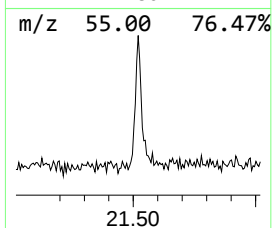
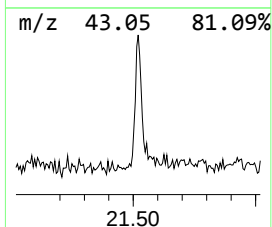
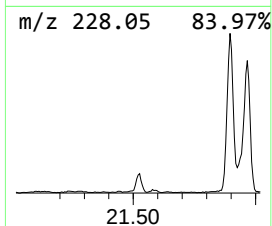
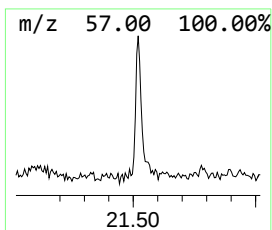
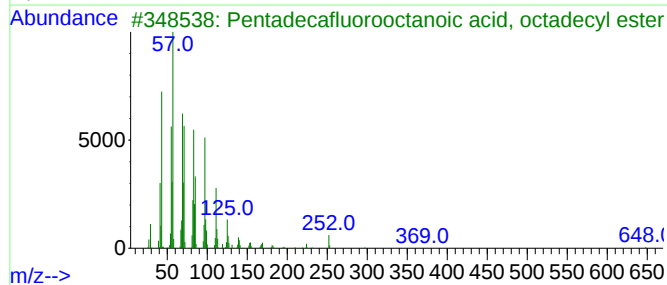
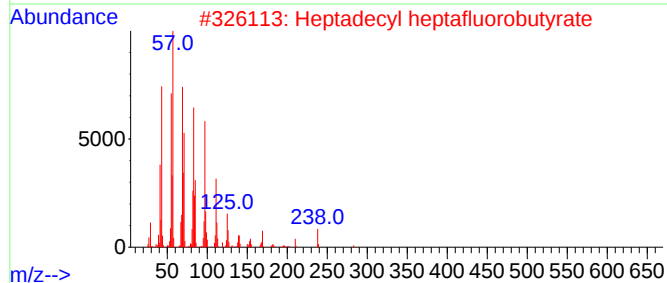
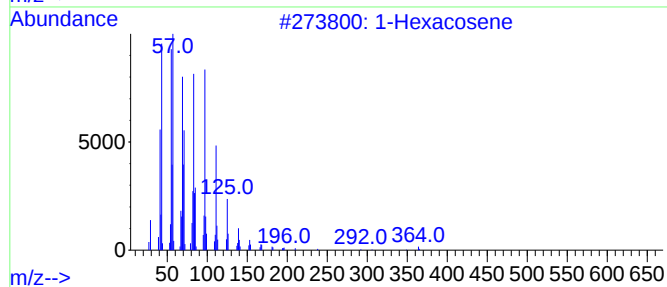
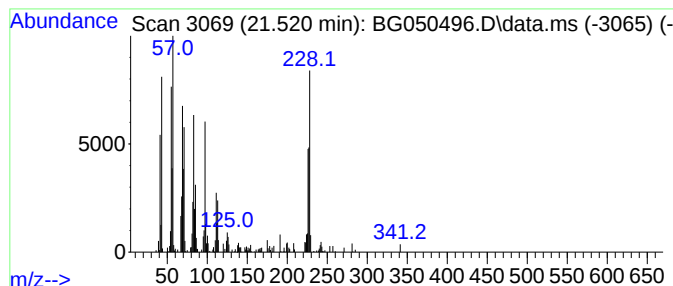
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexacosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.520	2.34 ng	134170	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	50
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	50
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	45
4	Oxirane, [(dodecyloxy)methyl]-			242	C15H30O2	002461-18-9	45
5	1-Octadecanol			270	C18H38O	000112-92-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
Data File : BG050496.D
Acq On : 7 Oct 2021 23:55
Operator : CG/JU
Sample : M4134-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP-01

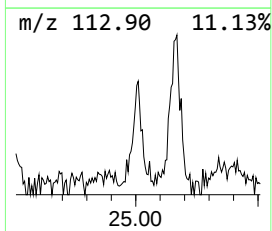
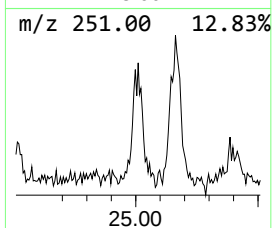
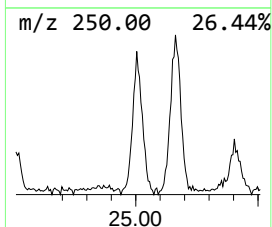
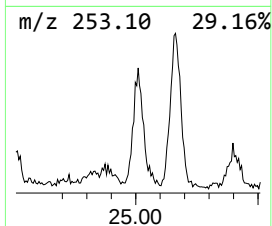
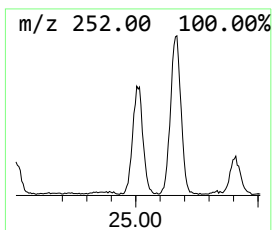
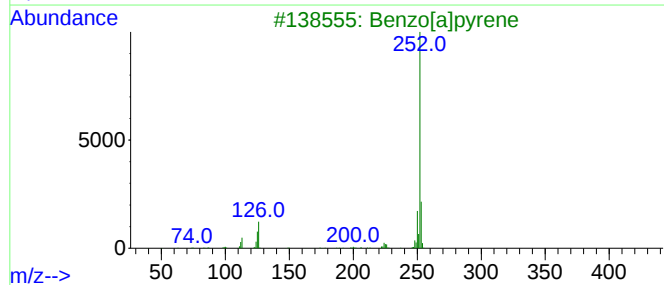
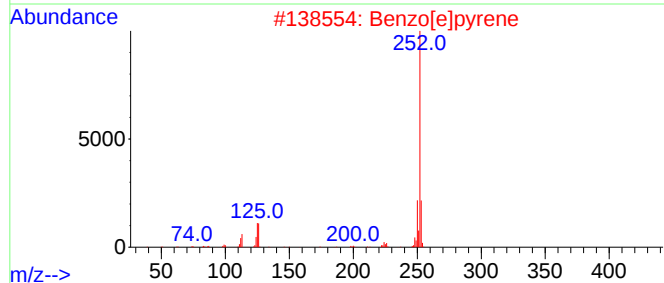
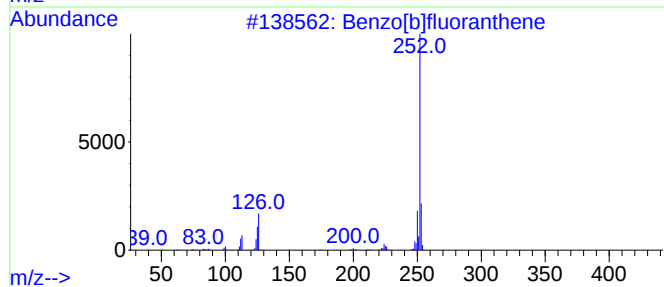
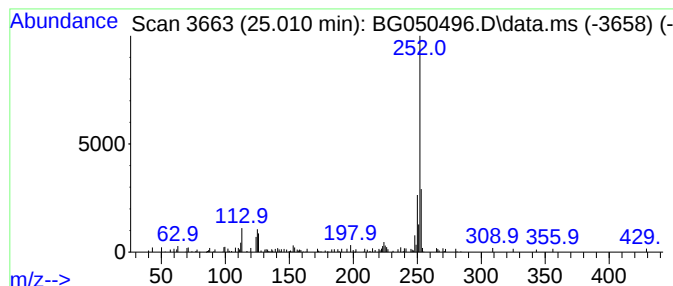
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.010	3.39 ng	139240	Perylene-d12	25.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	81
4			Perylene	252	C20H12	000198-55-0	74
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100721\
Data File : BG050496.D
Acq On : 7 Oct 2021 23:55
Operator : CG/JU
Sample : M4134-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
Ethanol, 2-(2-b...	10.826	14.5	ng	402181	2	11.085	555371	20.0
n-Hexadecanoic ...	18.476	5.8	ng	252800	4	17.619	877808	20.0
Phenanthrene, 1...	18.535	2.8	ng	124189	4	17.619	877808	20.0
5H-Dibenzo[a,d]...	18.676	3.5	ng	152653	4	17.619	877808	20.0
3,4-Dimethylphe...	19.393	3.4	ng	148178	4	17.619	877808	20.0
Octadecanoic acid	19.734	2.9	ng	128310	4	17.619	877808	20.0
Fluoranthene, 2...	20.497	2.9	ng	164087	5	21.919	1146800	20.0
1-Hexacosene	21.520	2.3	ng	134170	5	21.919	1146800	20.0
Benzo[e]pyrene	25.010	3.4	ng	139240	6	25.327	820763	20.0