

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
 Data File : BG048409.D
 Acq On : 17 Mar 2021 22:30
 Operator : CG/JU
 Sample : M1691-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FK-GF-02-068-A

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-BG031621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.195	311	316	323	rBV	39399	65802	2.07%	0.277%
2	5.665	389	396	405	rBV	962445	1546127	48.57%	6.513%
3	7.263	660	668	678	rBV	1006423	1765818	55.47%	7.438%
4	8.115	806	813	820	rBV	262000	448134	14.08%	1.888%
5	9.278	1003	1011	1020	rBV	641639	1163725	36.56%	4.902%
6	10.935	1285	1293	1300	rBV	338649	611724	19.22%	2.577%
7	13.379	1701	1709	1717	rBV	1591837	2461757	77.33%	10.370%
8	14.196	1841	1848	1852	rBV2	22772	43530	1.37%	0.183%
9	14.754	1936	1943	1949	rVV	544787	830795	26.10%	3.500%
10	14.819	1949	1954	1962	rVB2	41215	70232	2.21%	0.296%
11	15.148	2006	2010	2016	rVB3	25927	43025	1.35%	0.181%
12	15.794	2116	2120	2128	rBV4	38504	63972	2.01%	0.269%
13	16.241	2189	2196	2203	rBV	1346361	1998683	62.78%	8.419%
14	16.476	2230	2236	2239	rBV8	16724	36247	1.14%	0.153%
15	17.151	2348	2351	2358	rVB5	23579	42092	1.32%	0.177%
16	17.245	2361	2367	2373	rVV10	21187	50511	1.59%	0.213%
17	17.328	2377	2381	2384	rVB2	21313	32717	1.03%	0.138%
18	17.504	2405	2411	2415	rBV	622793	949740	29.83%	4.001%
19	17.545	2415	2418	2425	rVV	451049	664019	20.86%	2.797%
20	17.639	2427	2434	2438	rVB	69363	118873	3.73%	0.501%
21	17.903	2476	2479	2484	rVB	28058	40088	1.26%	0.169%
22	18.385	2556	2561	2565	rBV3	316464	437357	13.74%	1.842%
23	18.432	2565	2569	2574	rVB2	101920	162237	5.10%	0.683%
24	18.509	2579	2582	2588	rVB4	27012	47290	1.49%	0.199%
25	18.573	2588	2593	2597	rBV4	110562	226765	7.12%	0.955%
26	18.873	2640	2644	2647	rBV	64426	95471	3.00%	0.402%
27	18.914	2647	2651	2658	rVB2	95279	154373	4.85%	0.650%
28	19.167	2691	2694	2698	rVB3	22922	37228	1.17%	0.157%
29	19.290	2711	2715	2719	rBV2	54972	98423	3.09%	0.415%
30	19.431	2736	2739	2747	rVB4	33928	46223	1.45%	0.195%
31	19.554	2754	2760	2766	rBV	752518	1048020	32.92%	4.415%
32	19.648	2773	2776	2781	rBV7	75806	108173	3.40%	0.456%
33	19.883	2812	2816	2818	rBV2	115251	167911	5.27%	0.707%
34	19.919	2818	2822	2830	rVB	651402	934964	29.37%	3.938%
35	20.113	2849	2855	2860	rBV	2506015	3183421	100.00%	13.410%
36	20.506	2920	2922	2927	rVB	57459	60792	1.91%	0.256%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.423	3074	3078	3089	rVB7	237880	454697	14.28%	1.915%
38	21.511	3090	3093	3099	rVB4	104918	154820	4.86%	0.652%
39	21.799	3134	3142	3147	rBV2	666369	1564802	49.15%	6.591%
40	21.846	3147	3150	3160	rVB	277584	447213	14.05%	1.884%
41	24.078	3526	3530	3538	rBV2	95505	223784	7.03%	0.943%
42	24.983	3679	3684	3695	rVB2	140657	374014	11.75%	1.575%
43	25.148	3705	3712	3720	rVB	267241	664290	20.87%	2.798%

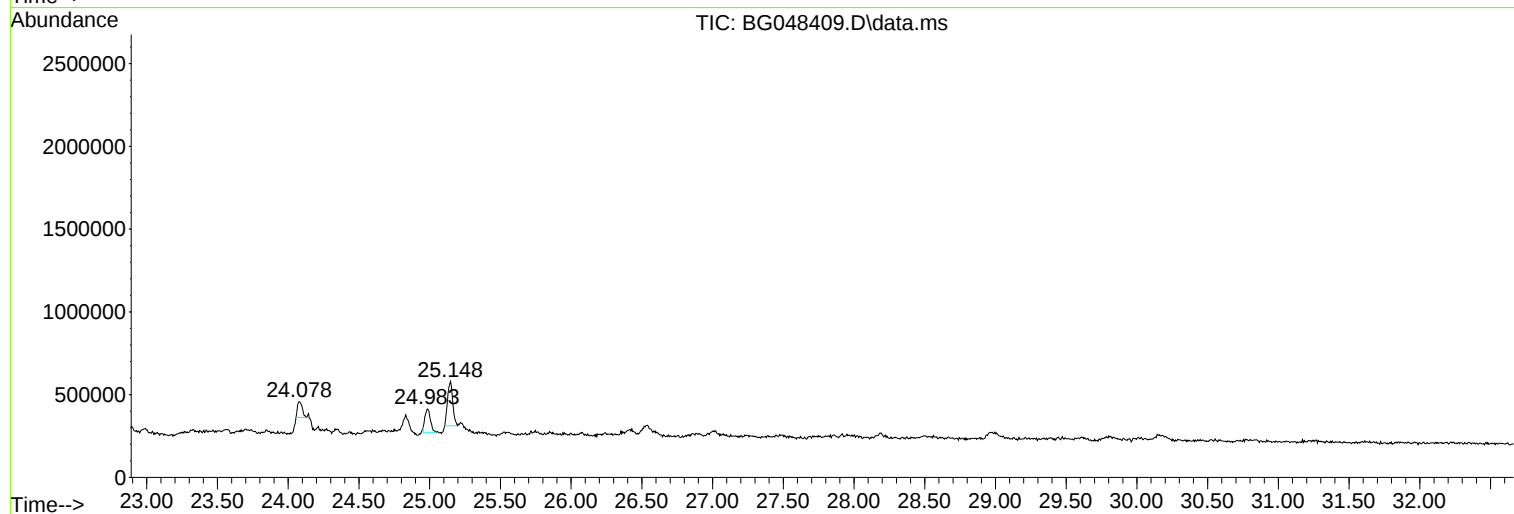
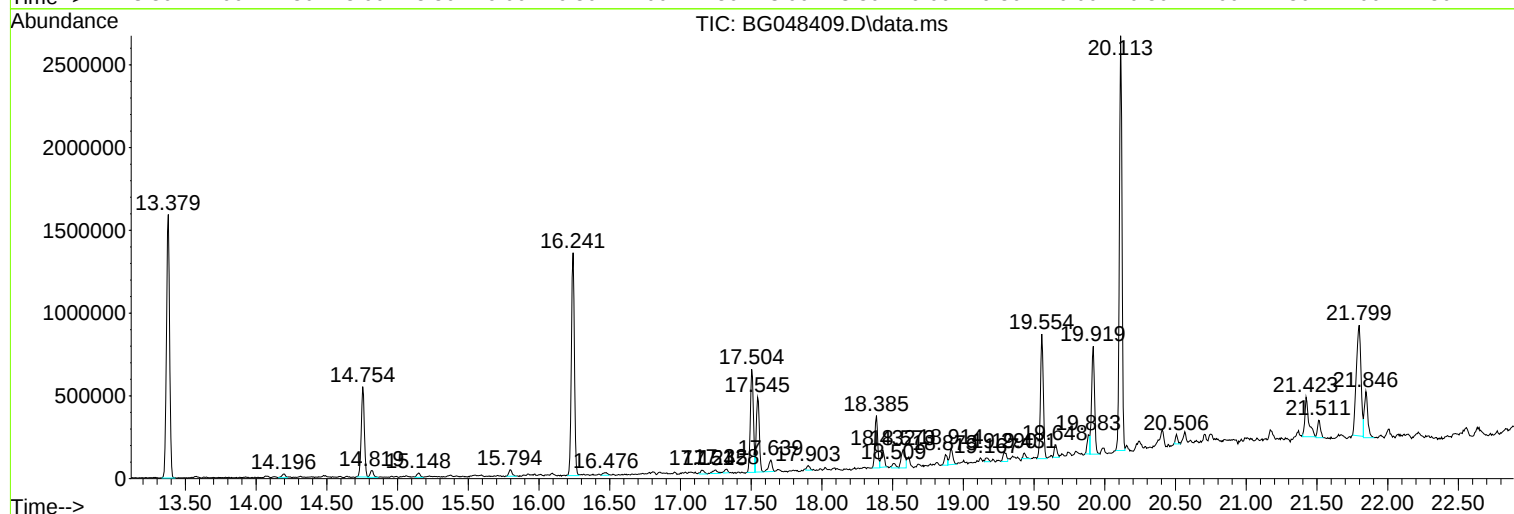
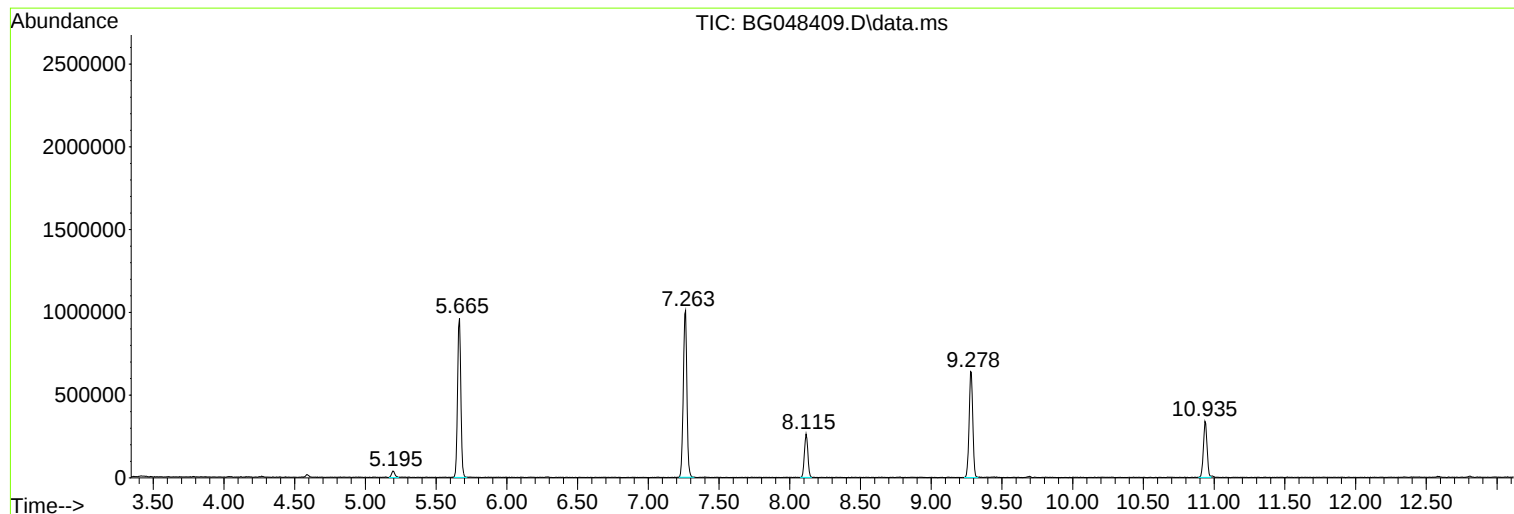
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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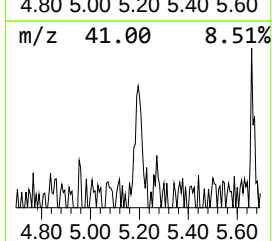
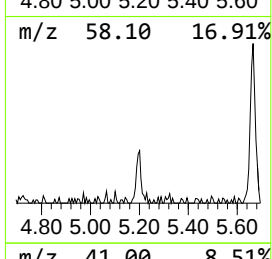
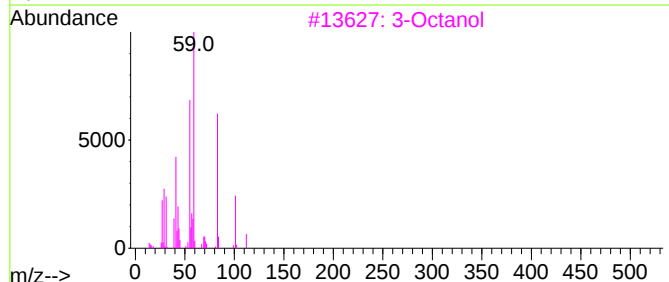
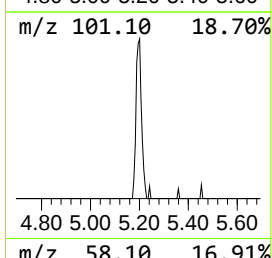
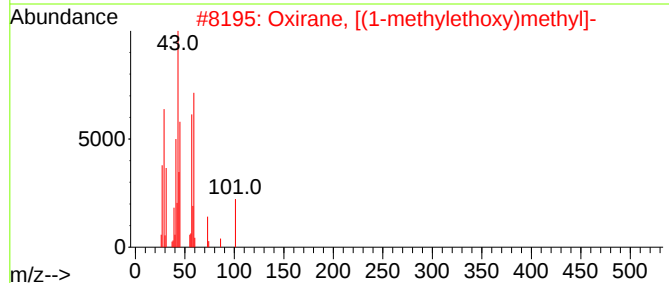
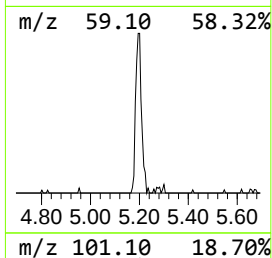
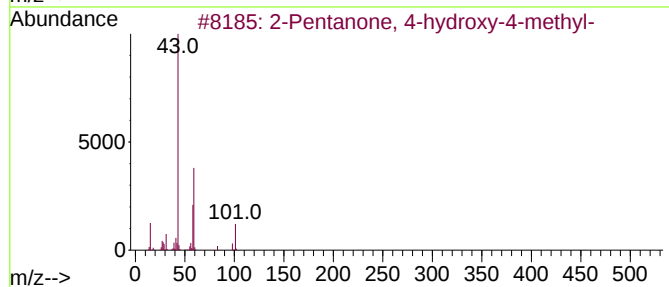
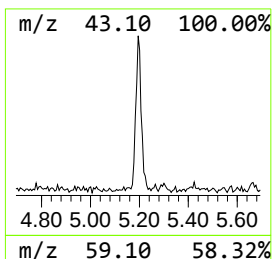
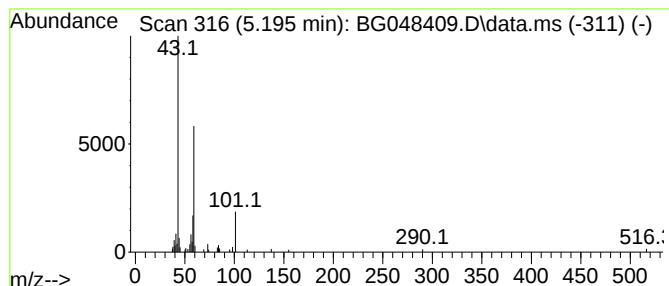
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	2.94 ng	65802	1,4-Dichlorobenzene-d4	8.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	39		
3	3-Octanol	130	C8H18O	000589-98-0	38		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
5	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	28		



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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-068-A

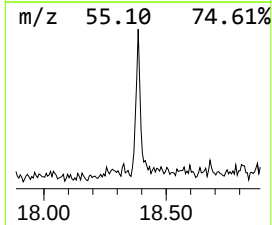
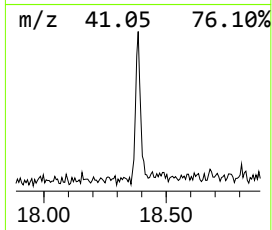
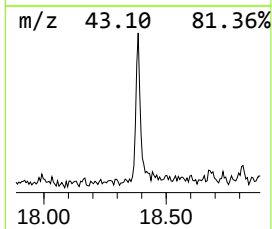
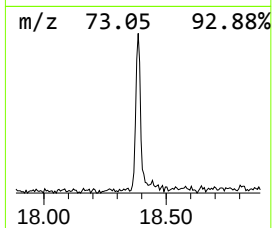
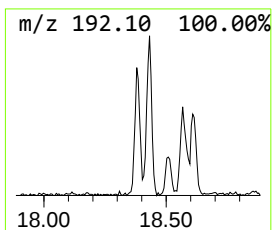
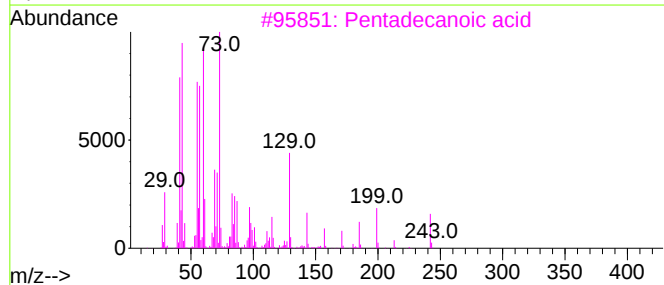
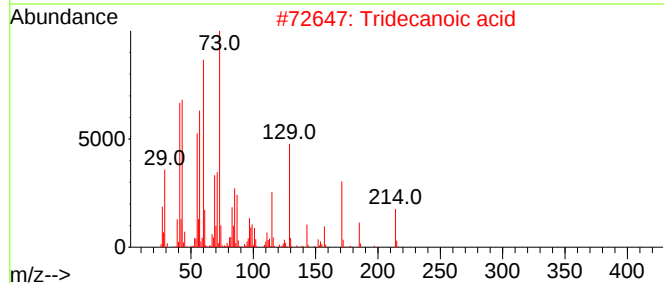
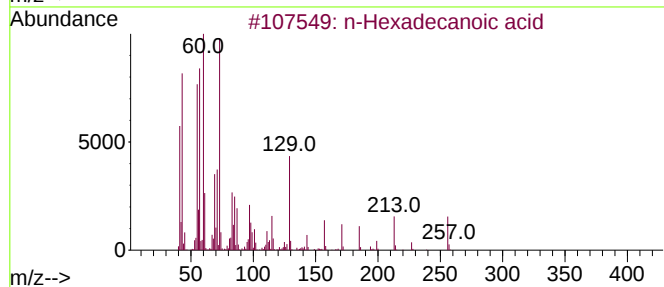
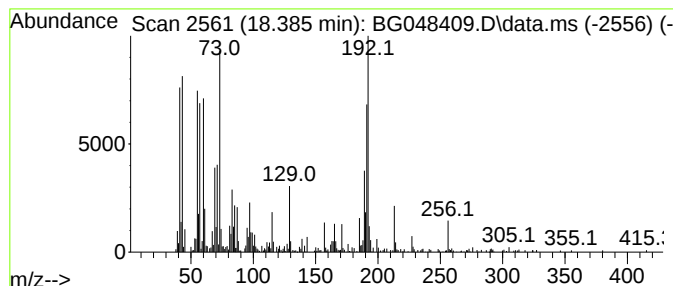
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	9.21 ng	437357	Phenanthrene-d10	17.504

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	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	42
5			Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	42



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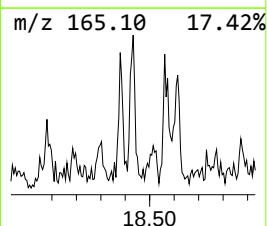
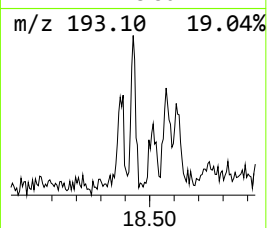
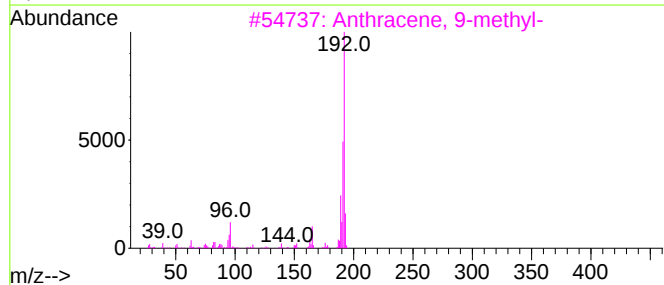
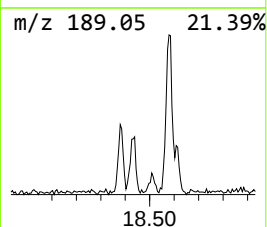
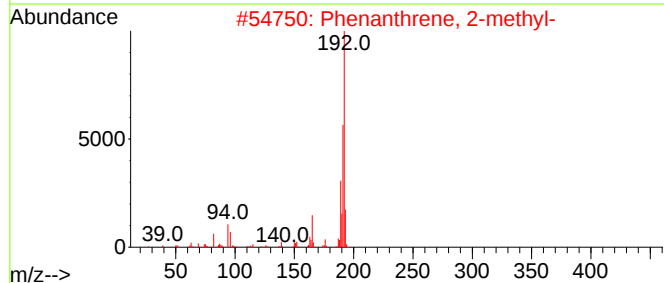
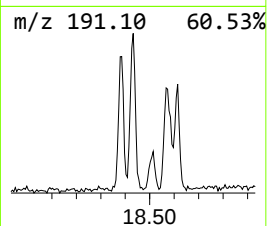
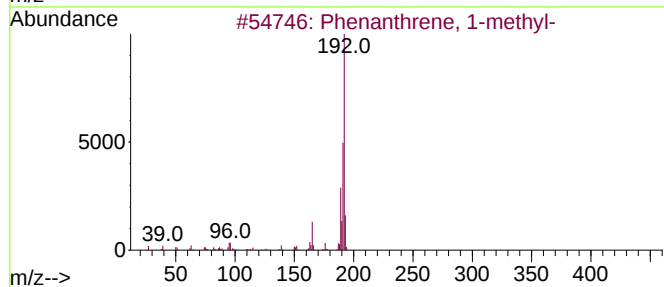
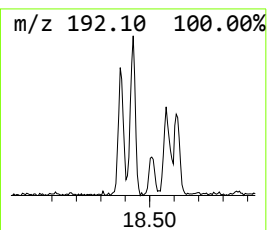
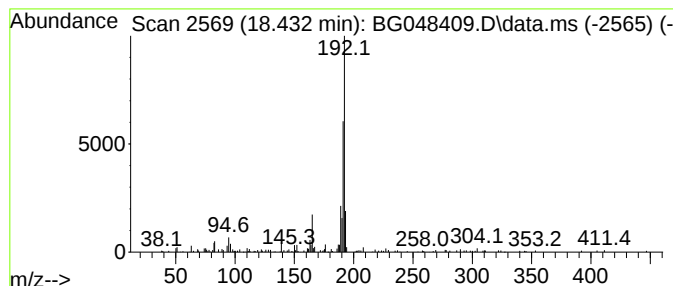
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.432	3.42 ng	162237	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
4			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	91
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91



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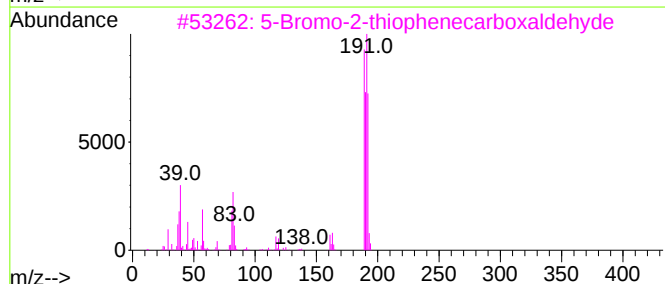
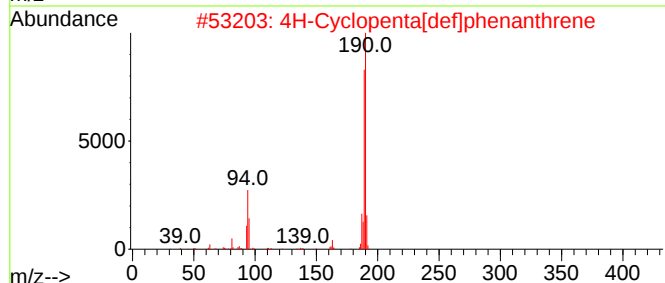
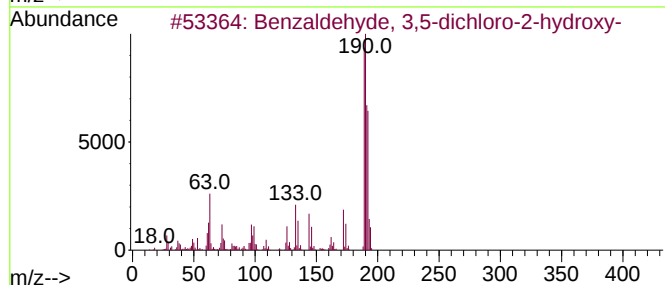
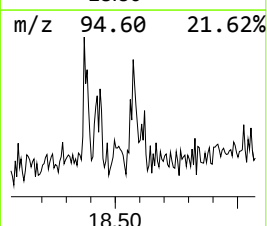
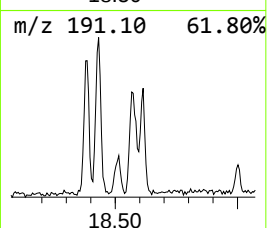
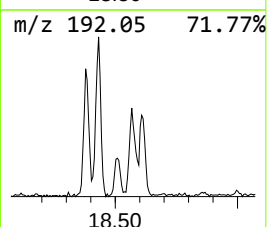
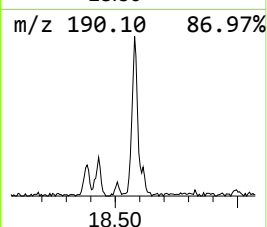
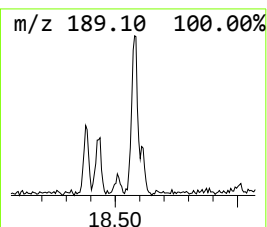
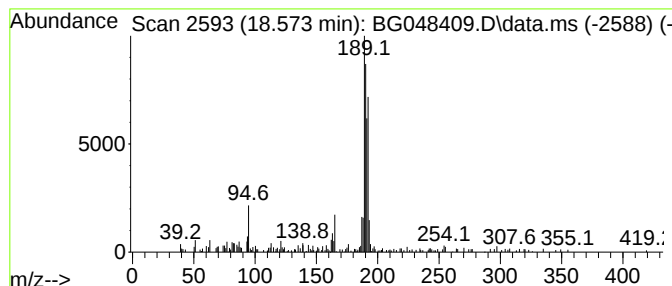
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Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.573	4.78 ng	226765	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	80
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3			5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
5			Methyl diselenide	190	C2H6Se2	007101-31-7	38



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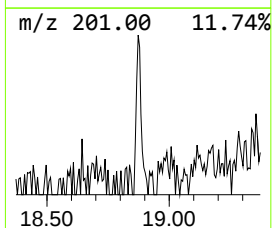
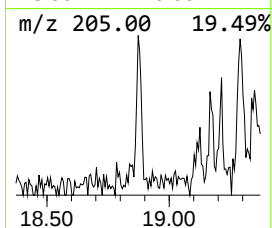
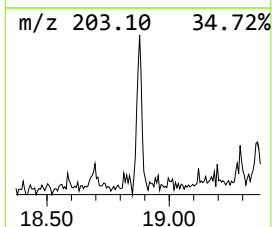
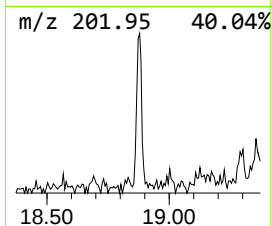
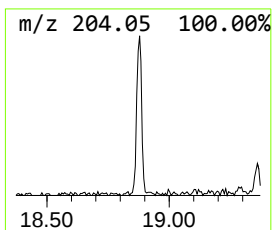
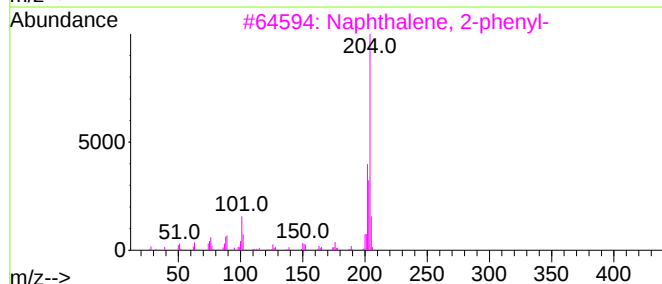
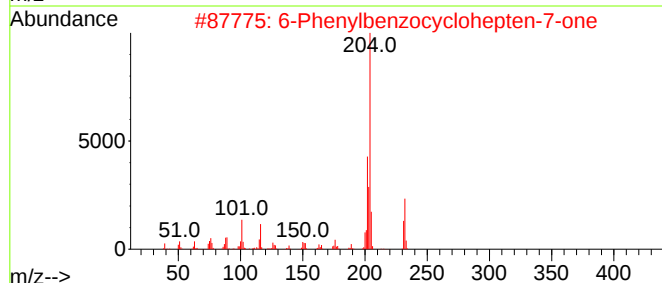
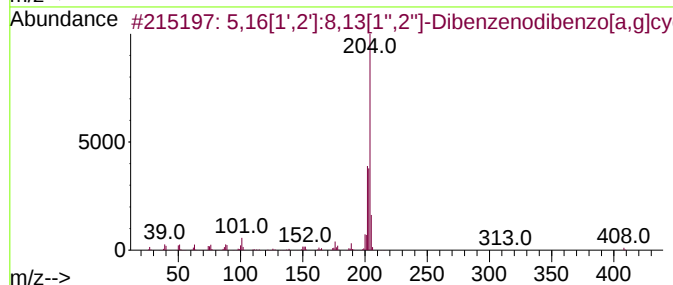
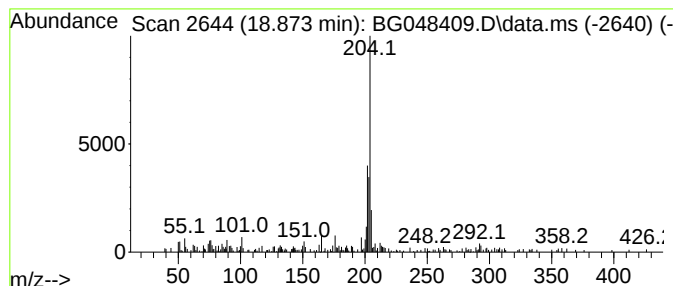
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.873	2.01 ng	95471	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	74		
2	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	64		
3	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	64		
4	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	58		
5	Benzene, 1,1'-(1-buten-3-yne-1,4...	204	C16H12	013141-45-2	55		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048409.D
Acq On : 17 Mar 2021 22:30
Operator : CG/JU
Sample : M1691-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-068-A

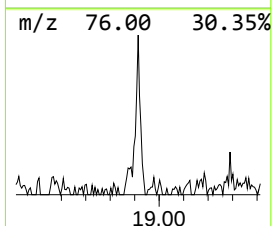
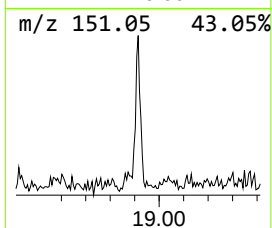
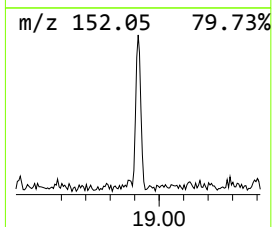
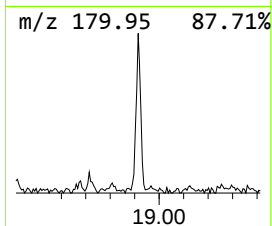
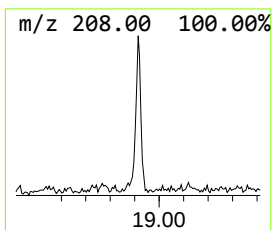
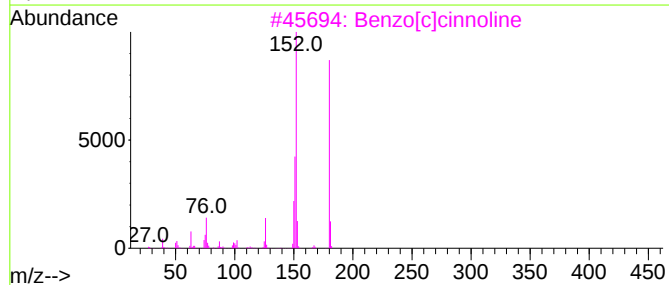
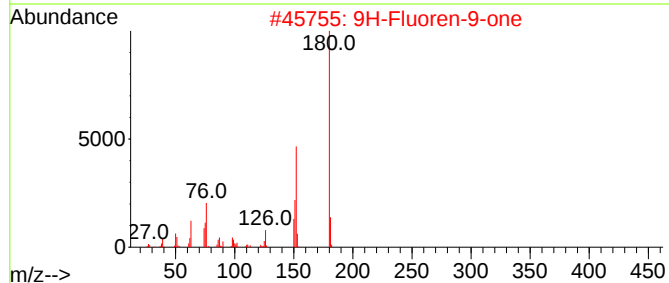
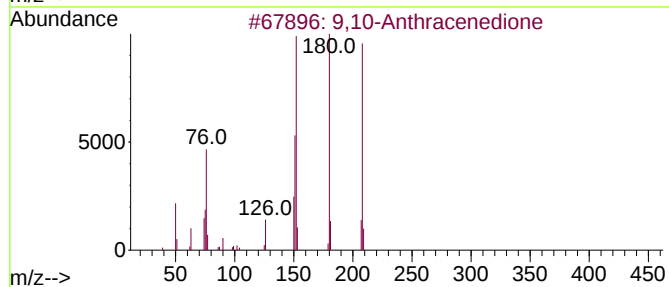
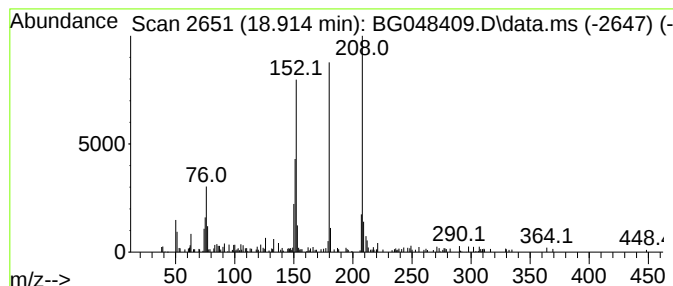
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9,10-Anthracenedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.914	3.25 ng	154373	Phenanthrene-d10	17.504

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,10-Anthracenedione	208	C14H8O2	000084-65-1	90
2		9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
3		Benzo[c]cinnoline	180	C12H8N2	000230-17-1	62
4		1,3-Benzenedicarboxaldehyde, 2,4...	180	C9H8O4	010209-57-1	53
5		1,4-Anthracenedione	208	C14H8O2	000635-12-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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Operator : CG/JU
Sample : M1691-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-GF-02-068-A

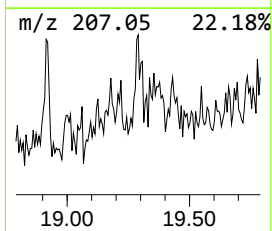
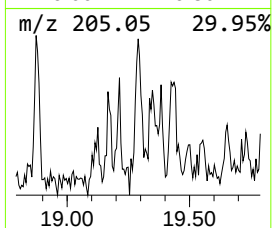
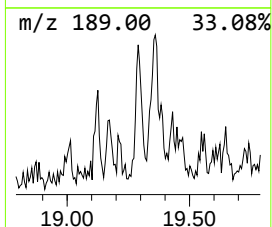
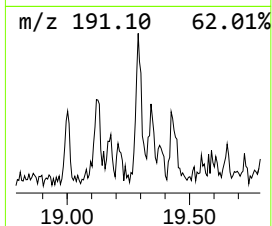
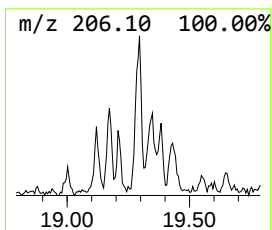
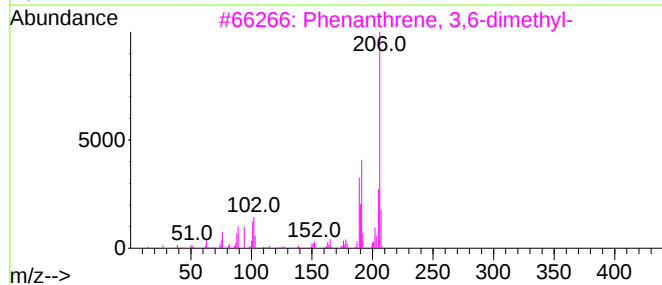
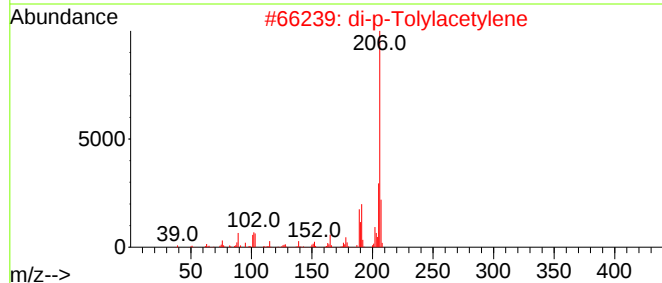
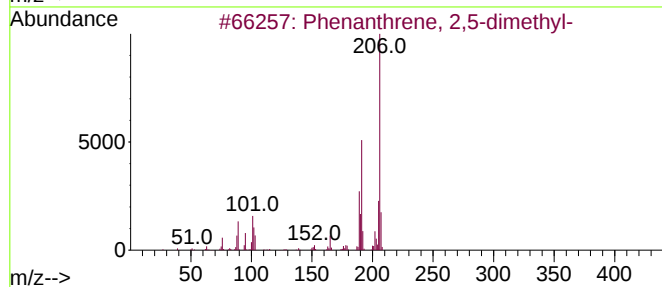
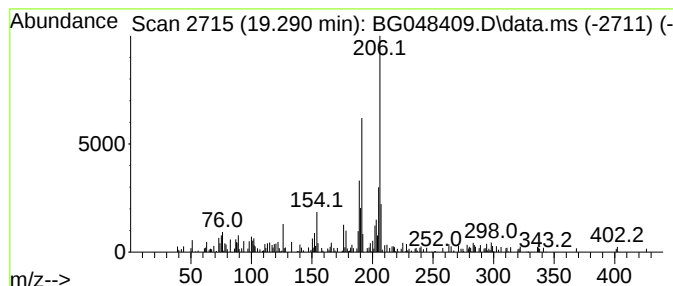
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.290	2.07 ng	98423	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	89
3			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	87
4			9,10-Dimethylanthracene	206	C16H14	000781-43-1	76
5			Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048409.D
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Operator : CG/JU
Sample : M1691-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-GF-02-068-A

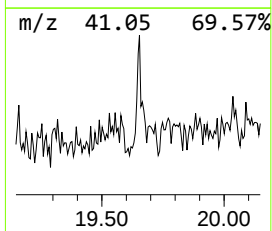
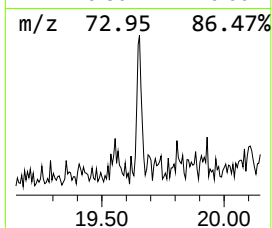
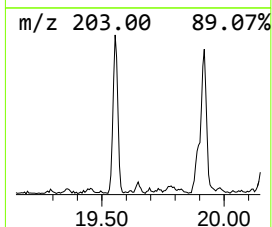
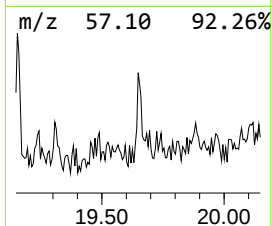
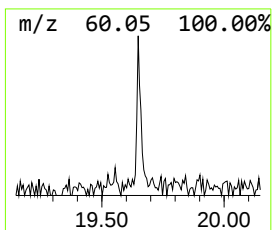
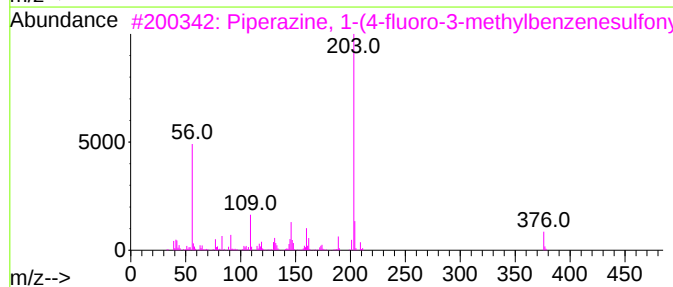
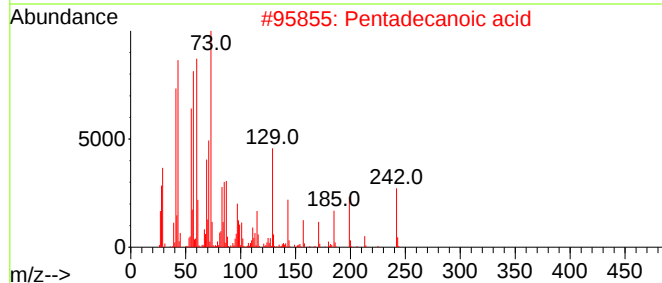
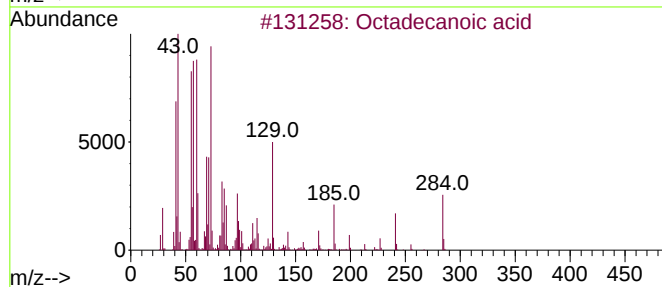
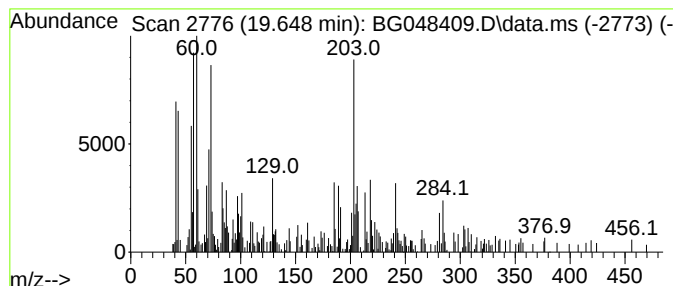
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown19.648 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.648	2.28 ng	108173	Phenanthrene-d10	17.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	42
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	30
3			Piperazine, 1-(4-fluoro-3-methyl...	376	C20H25FN2O2S	1000304-50-7	30
4			Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	30
5			9,11-Dimethyltetracyclo[7.3.1.0(...	218	C16H26	053263-99-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048409.D
Acq On : 17 Mar 2021 22:30
Operator : CG/JU
Sample : M1691-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-GF-02-068-A

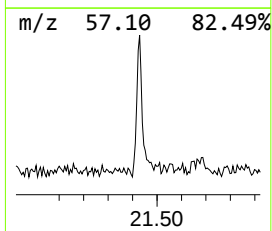
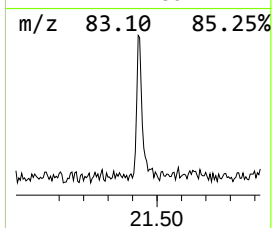
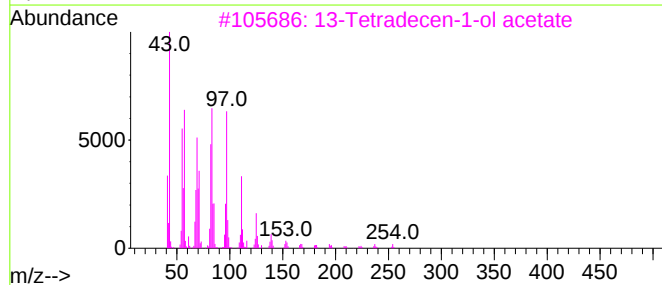
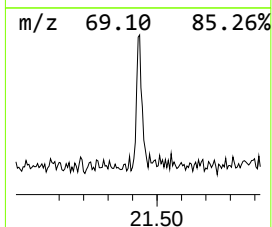
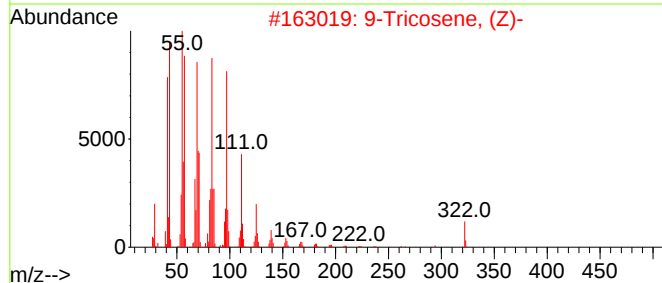
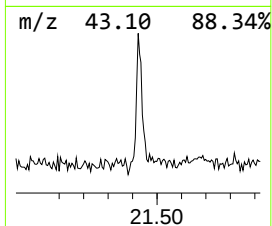
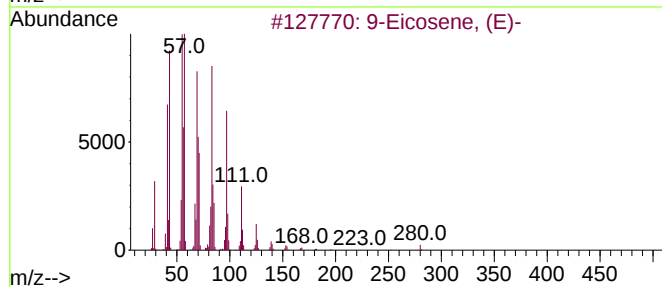
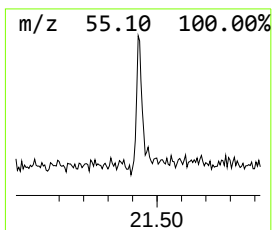
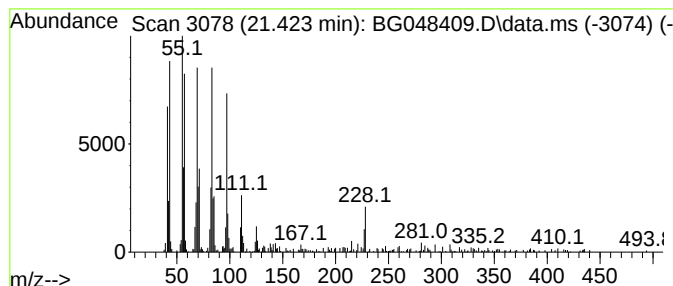
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 9-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.423	5.81 ng	454697	Chrysene-d12	21.799

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-		280	C20H40	074685-29-3	93
2	9-Tricosene, (Z)-		322	C23H46	027519-02-4	91
3	13-Tetradecen-1-ol acetate		254	C16H30O2	056221-91-1	86
4	Cyclotetracosane		336	C24H48	000297-03-0	76
5	n-Nonadecanol-1		284	C19H40O	001454-84-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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Acq On : 17 Mar 2021 22:30
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Sample : M1691-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-GF-02-068-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.195	2.9	ng	65802	1	8.115	448134	20.0
n-Hexadecanoic ...	18.385	9.2	ng	437357	4	17.504	949740	20.0
Phenanthrene, 1...	18.432	3.4	ng	162237	4	17.504	949740	20.0
Benzaldehyde, 3...	18.573	4.8	ng	226765	4	17.504	949740	20.0
5,16[1',2']:8,1...	18.873	2.0	ng	95471	4	17.504	949740	20.0
9,10-Anthracene...	18.914	3.3	ng	154373	4	17.504	949740	20.0
Phenanthrene, 2...	19.290	2.1	ng	98423	4	17.504	949740	20.0
unknown19.648	19.648	2.3	ng	108173	4	17.504	949740	20.0
9-Eicosene, (E)-	21.423	5.8	ng	454697	5	21.799	1564800	20.0