

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
 Data File : BG054193.D
 Acq On : 1 Jul 2022 16:16
 Operator : CG/JU
 Sample : N3558-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 72-11998

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-BG061322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.633	375	382	393	rVB	177845	299640	23.40%	3.689%
2	7.225	645	653	667	rBV	190721	345013	26.94%	4.247%
3	8.065	789	796	803	rBV	56778	98347	7.68%	1.211%
4	9.223	986	993	1003	rBV	122953	231419	18.07%	2.849%
5	10.874	1266	1274	1279	rBV	82651	148765	11.62%	1.831%
6	10.927	1279	1283	1292	rVB	13361	22859	1.78%	0.281%
7	12.525	1548	1555	1561	rBB	11698	19506	1.52%	0.240%
8	13.312	1682	1689	1698	rBB	419656	679590	53.07%	8.366%
9	14.693	1914	1924	1930	rBV	154779	251659	19.65%	3.098%
10	14.752	1930	1934	1941	rVB	30188	50707	3.96%	0.624%
11	15.087	1984	1991	2000	rBV	43119	65445	5.11%	0.806%
12	15.739	2094	2102	2110	rBV	57375	92683	7.24%	1.141%
13	16.179	2170	2177	2189	rBV2	388926	632233	49.37%	7.783%
14	16.409	2208	2216	2221	rBV5	11108	24232	1.89%	0.298%
15	17.090	2326	2332	2340	rVB2	36001	55751	4.35%	0.686%
16	17.184	2340	2348	2352	rBV6	7353	13211	1.03%	0.163%
17	17.249	2352	2359	2365	rVB2	11013	22667	1.77%	0.279%
18	17.437	2384	2391	2394	rBV	214344	330870	25.84%	4.073%
19	17.478	2394	2398	2408	rVB	171383	272076	21.25%	3.349%
20	17.566	2408	2413	2418	rBV	13463	19565	1.53%	0.241%
21	18.095	2499	2503	2508	rBV2	16435	21768	1.70%	0.268%
22	18.201	2518	2521	2530	rBV7	13374	31601	2.47%	0.389%
23	18.318	2536	2541	2545	rBV2	81884	124728	9.74%	1.536%
24	18.359	2545	2548	2556	rVB3	24669	41765	3.26%	0.514%
25	18.430	2556	2560	2565	rBV7	10294	22079	1.72%	0.272%
26	18.506	2569	2573	2577	rBV2	22062	39652	3.10%	0.488%
27	18.624	2588	2593	2596	rBV3	22769	40920	3.20%	0.504%
28	18.806	2621	2624	2627	rBV	14381	17585	1.37%	0.216%
29	18.853	2627	2632	2638	rBV3	51591	117041	9.14%	1.441%
30	19.246	2695	2699	2704	rBV4	34759	70037	5.47%	0.862%
31	19.487	2732	2740	2745	rBV	303754	542044	42.33%	6.673%
32	19.587	2753	2757	2760	rBV5	45701	73605	5.75%	0.906%
33	19.816	2792	2796	2798	rBV2	82614	117811	9.20%	1.450%
34	19.852	2798	2802	2810	rVB	215127	359097	28.04%	4.421%
35	20.045	2827	2835	2840	rVB	865639	1280618	100.00%	15.765%
36	20.339	2883	2885	2890	rVB3	77248	102851	8.03%	1.266%

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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-BG061322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.798	2960	2963	2966	rBV	80939	93777	7.32%	1.154%
38	21.714	3112	3119	3124	rBV2	243761	570213	44.53%	7.020%
39	22.895	3315	3320	3333	rVB2	190565	381960	29.83%	4.702%
40	24.975	3666	3674	3685	rVB2	133683	397527	31.04%	4.894%

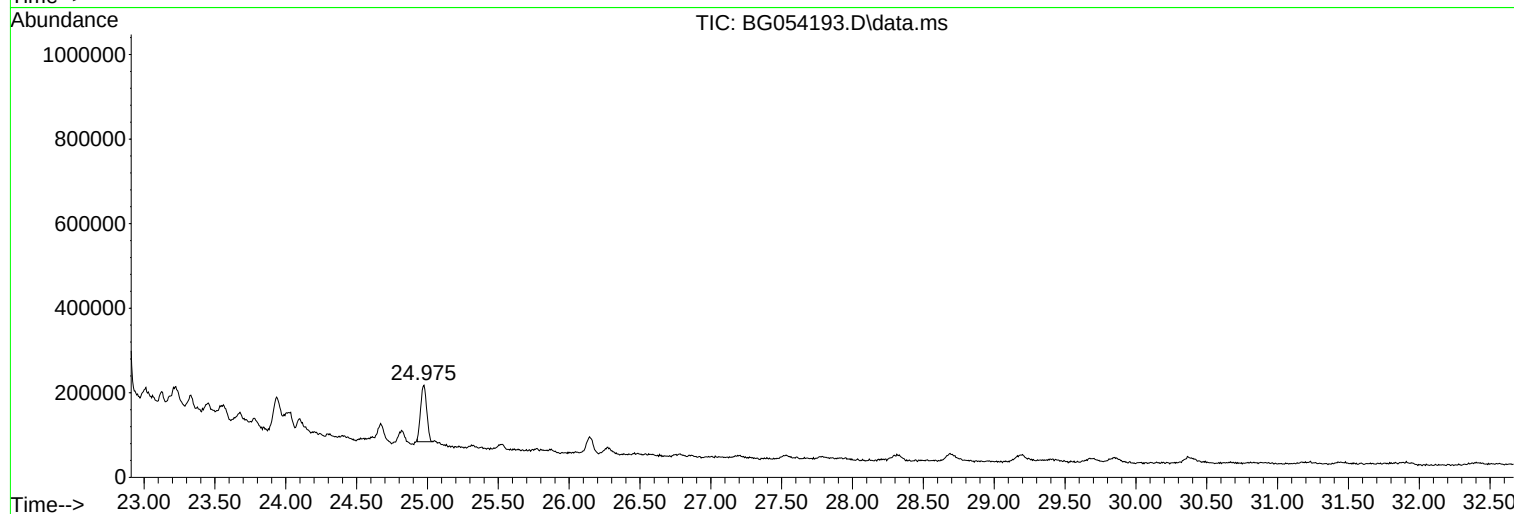
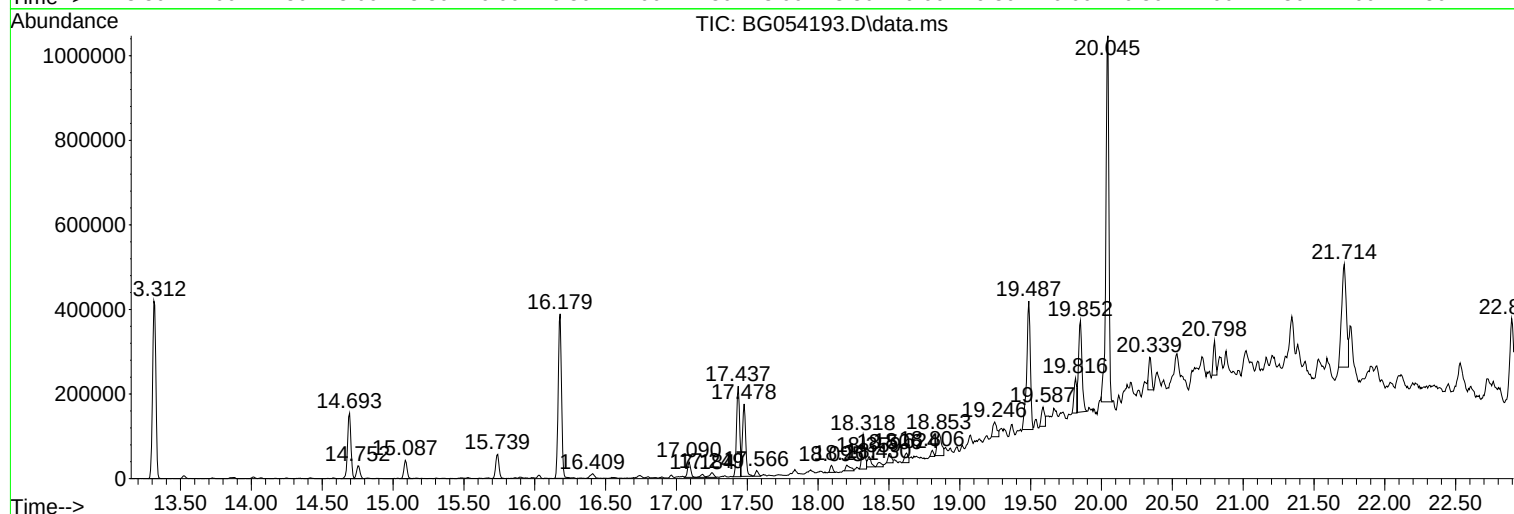
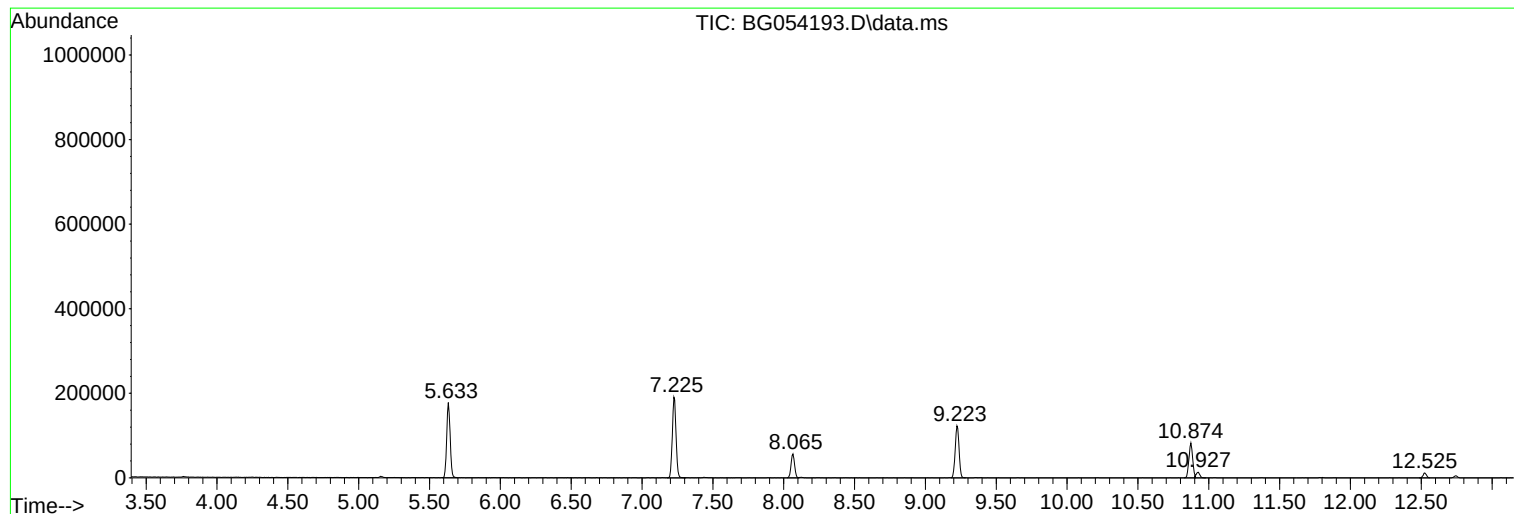
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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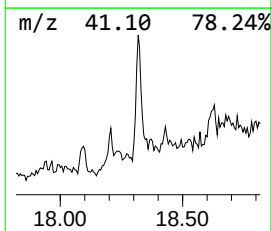
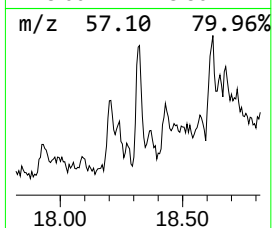
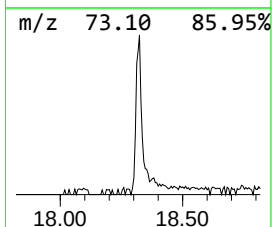
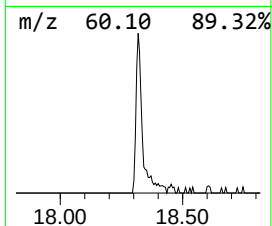
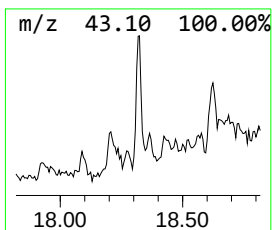
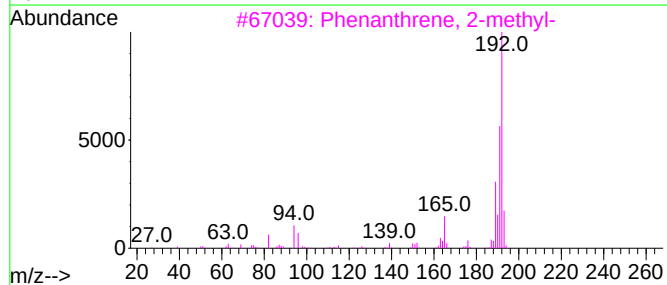
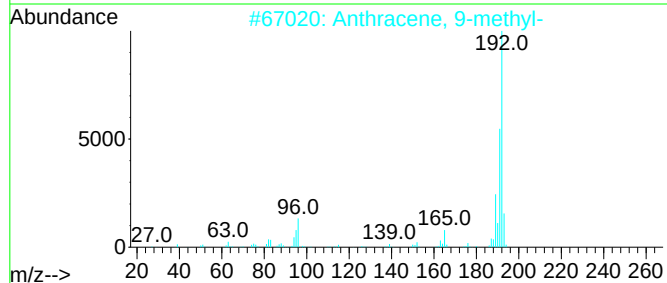
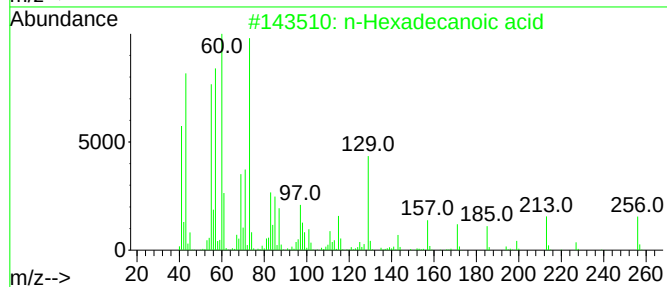
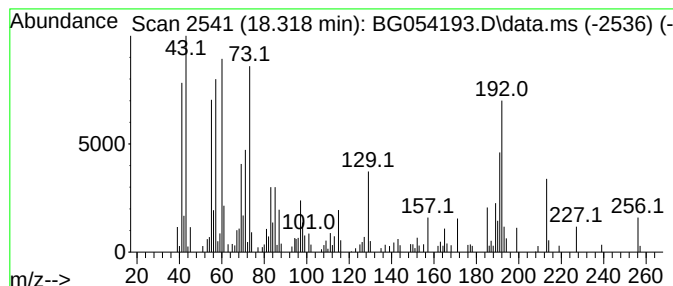
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.318	7.54 ng	124728	Phenanthrene-d10	17.437

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Anthracene, 9-methyl-	192	C15H12	000779-02-2	55
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53
4		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	53
5		Tridecanoic acid	214	C13H26O2	000638-53-9	46



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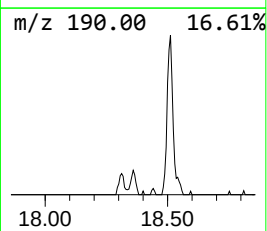
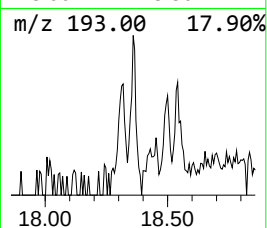
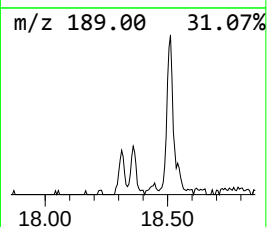
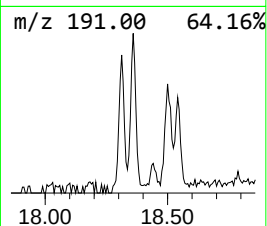
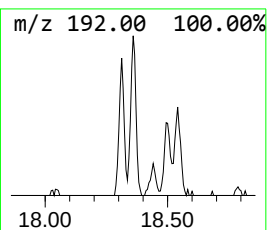
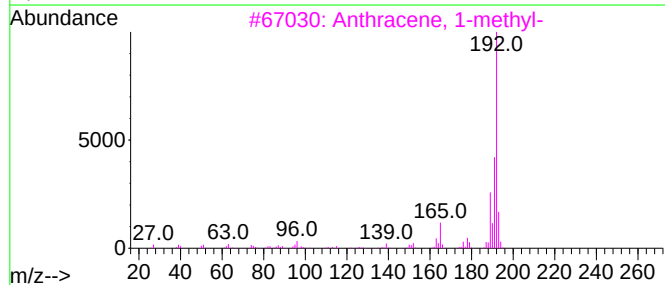
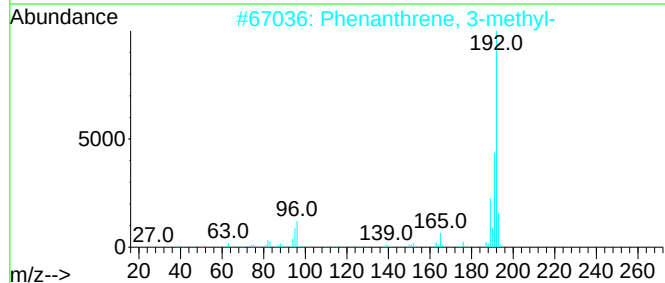
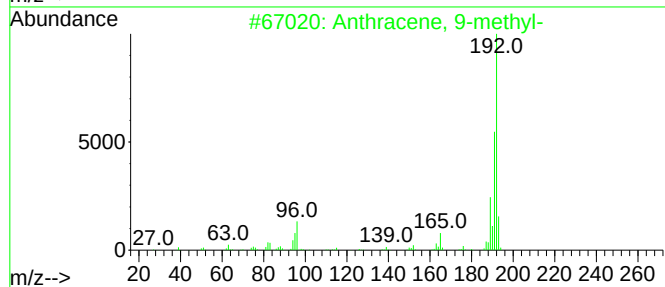
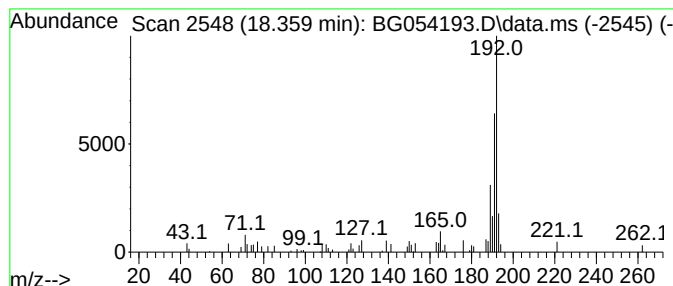
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Anthracene, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.359	2.52 ng	41765	Phenanthrene-d10	17.437

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 9-methyl-	192	C15H12	000779-02-2	76
2		Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	76
3		Anthracene, 1-methyl-	192	C15H12	000610-48-0	74
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	68
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	68



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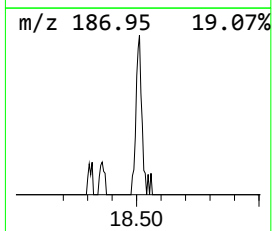
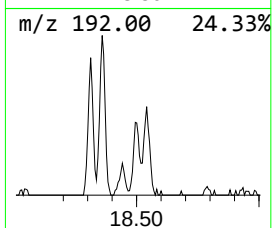
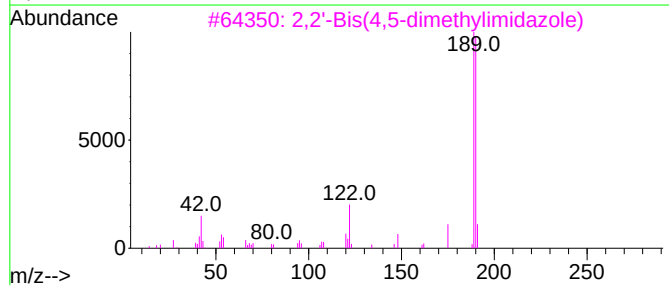
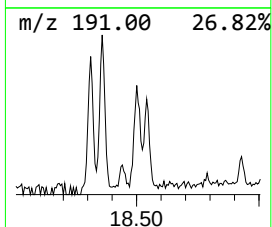
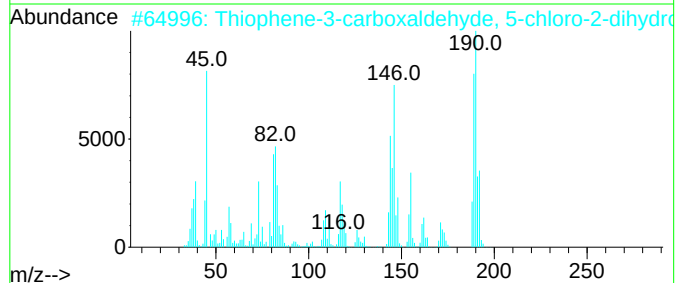
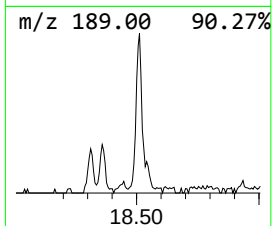
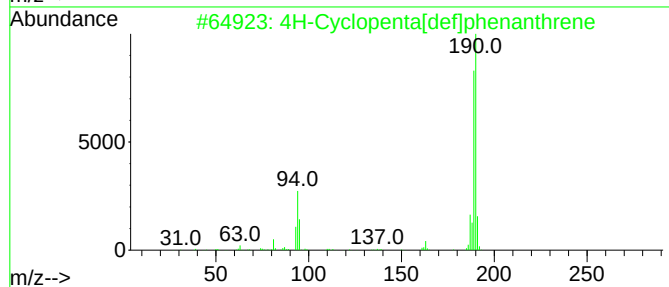
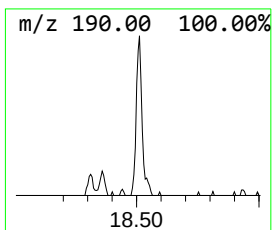
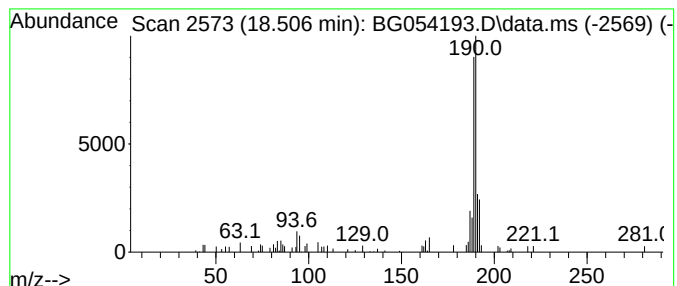
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	2.40 ng	39652	Phenanthrene-d10	17.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
4			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
5			Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25



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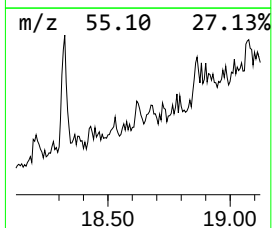
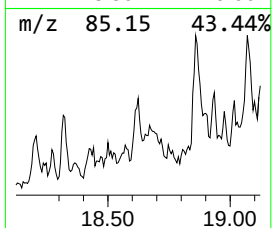
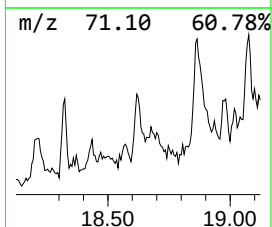
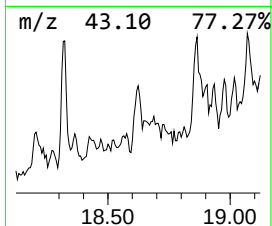
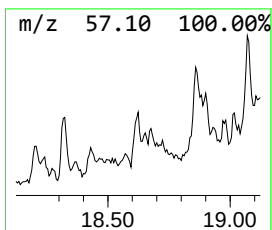
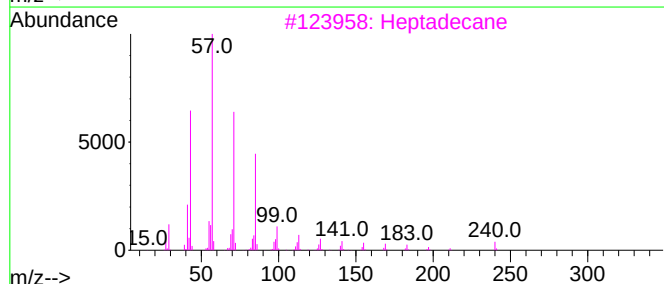
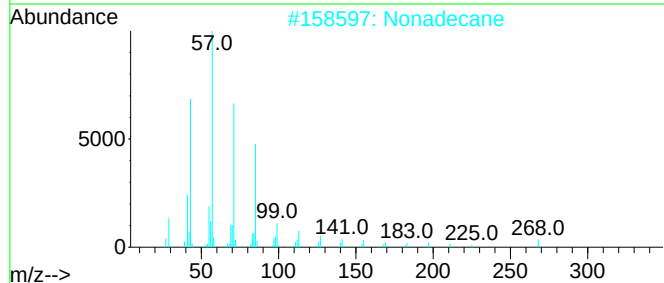
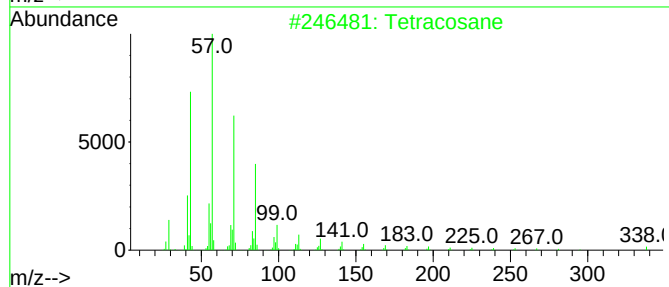
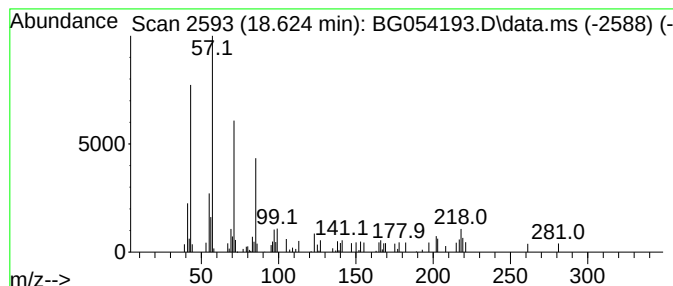
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.624	2.47 ng	40920	Phenanthrene-d10	17.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	72
2			Nonadecane	268	C19H40	000629-92-5	64
3			Heptadecane	240	C17H36	000629-78-7	64
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64



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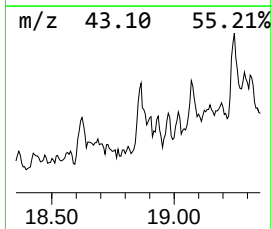
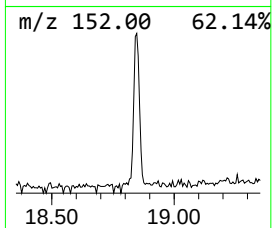
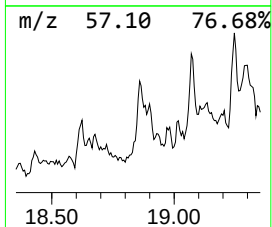
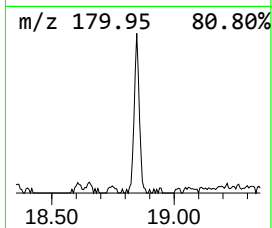
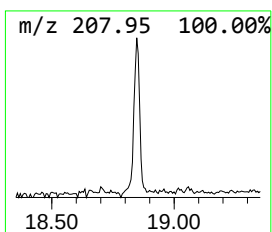
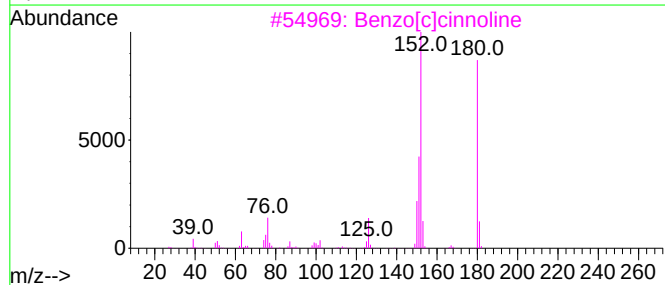
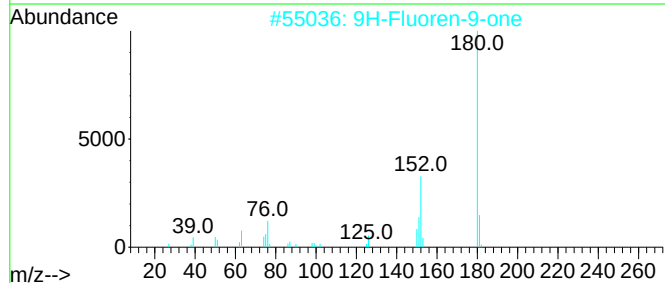
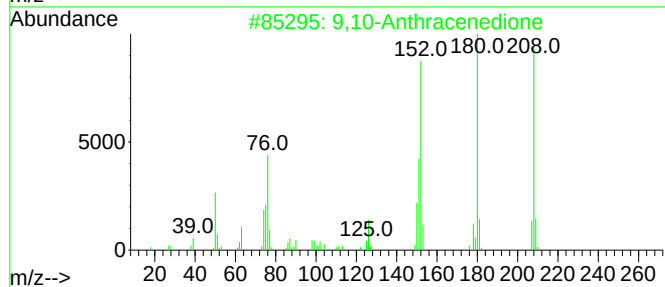
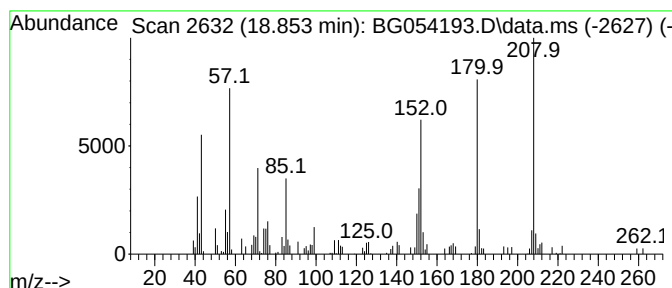
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,10-Anthracenedione Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.853	7.07 ng	117041	Phenanthrene-d10	17.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione			208	C14H8O2	000084-65-1	64
2	9H-Fluoren-9-one			180	C13H8O	000486-25-9	46
3	Benzo[c]cinnoline			180	C12H8N2	000230-17-1	41
4	Benzo[h]cinnoline			180	C12H8N2	000230-31-9	41
5	1H-Phenalen-1-one			180	C13H8O	000548-39-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
Data File : BG054193.D
Acq On : 1 Jul 2022 16:16
Operator : CG/JU
Sample : N3558-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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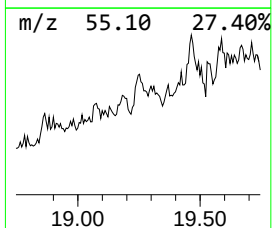
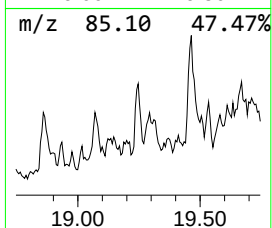
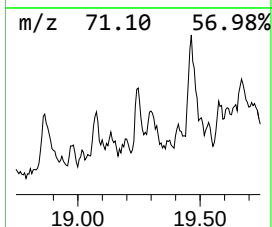
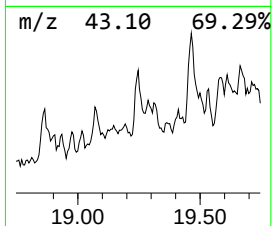
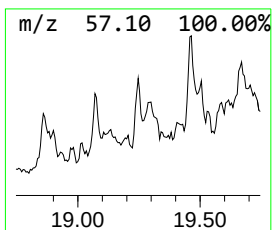
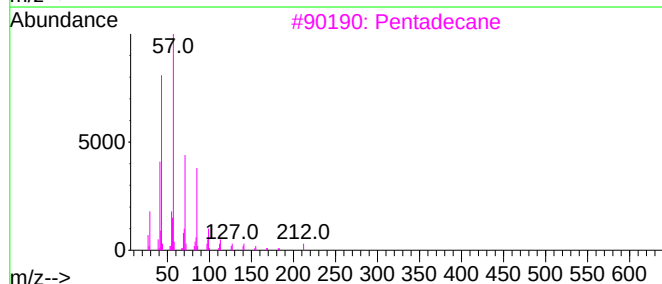
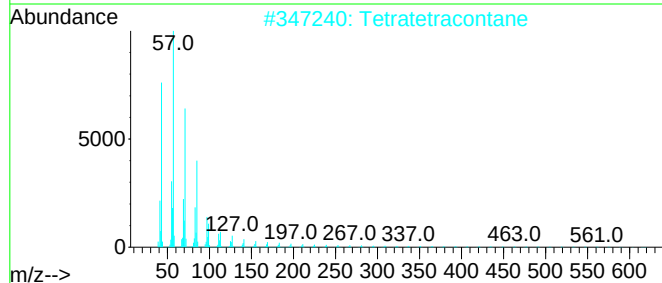
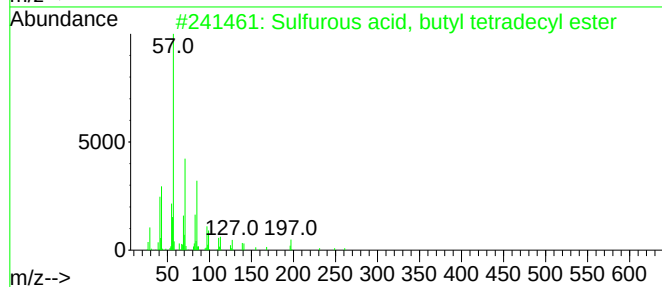
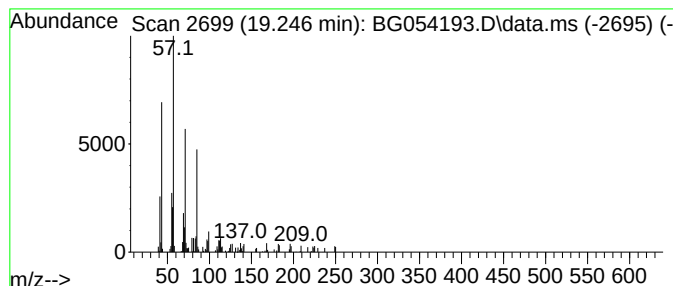
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Sulfurous acid, butyl tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.246	4.23 ng	70037	Phenanthrene-d10	17.437

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	86
2			Tetratetracontane	619	C44H90	007098-22-8	86
3			Pentadecane	212	C15H32	000629-62-9	86
4			Hexadecane	226	C16H34	000544-76-3	78
5			Heptadecane	240	C17H36	000629-78-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
Data File : BG054193.D
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Sample : N3558-01
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Instrument :
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ClientSampleId :
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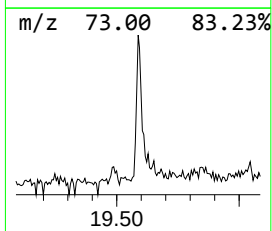
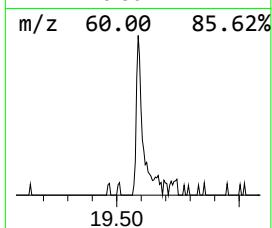
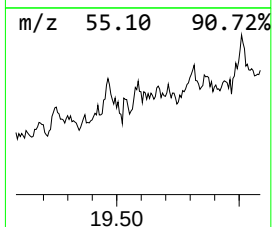
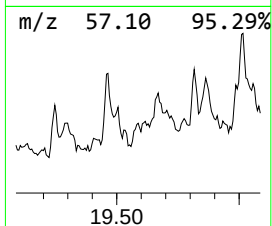
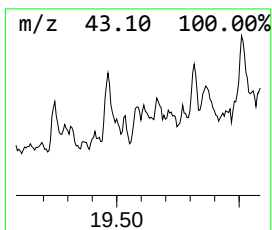
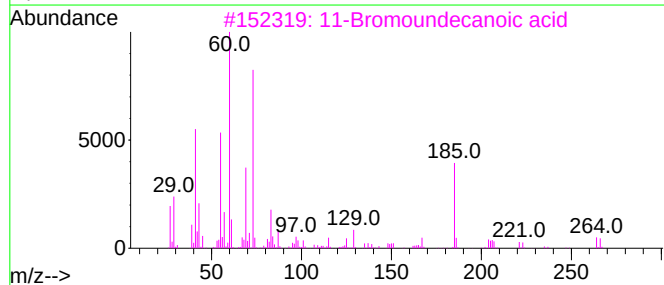
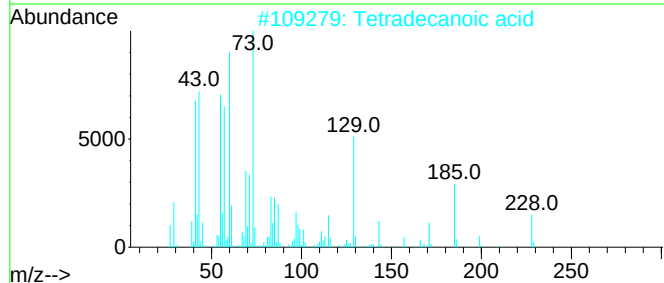
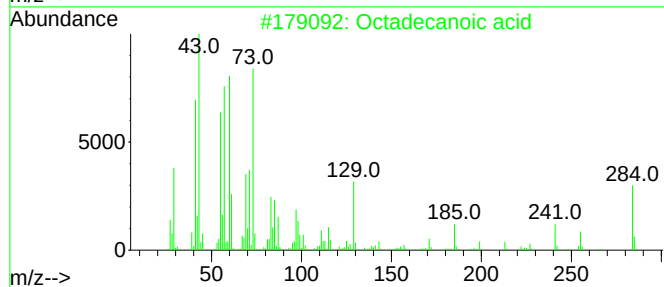
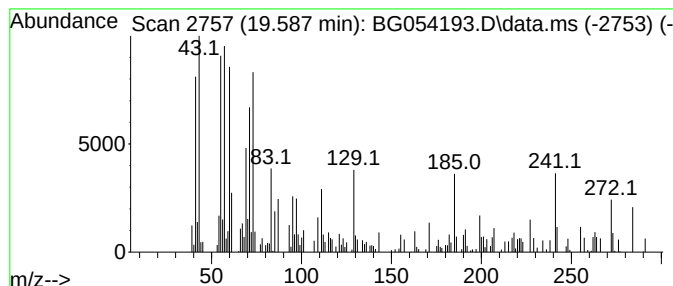
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.587	2.58 ng	73605	Chrysene-d12	21.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	62
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
3			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
4			Dodecanoic acid	200	C12H24O2	000143-07-7	35
5			n-Decanoic acid	172	C10H20O2	000334-48-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
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Operator : CG/JU
Sample : N3558-01
Misc :
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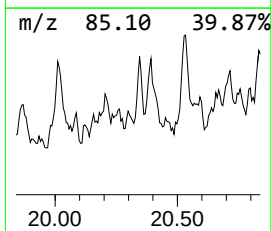
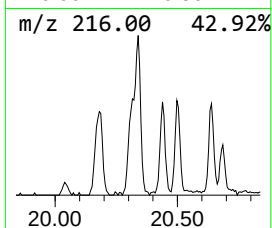
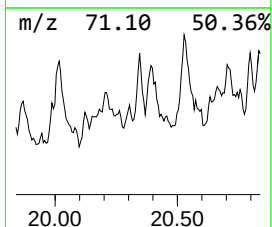
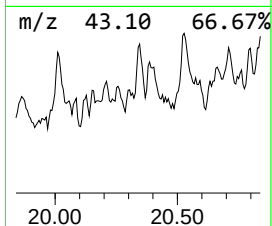
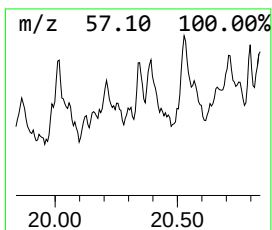
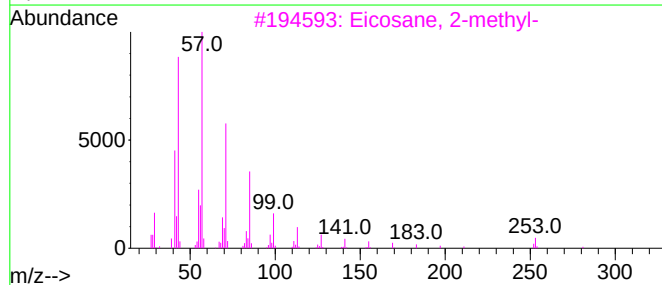
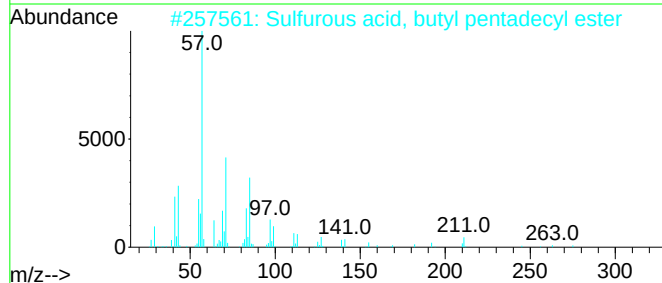
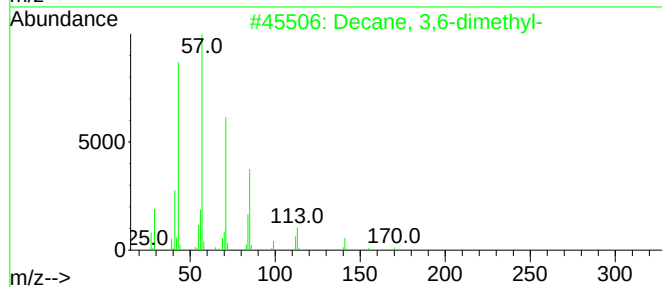
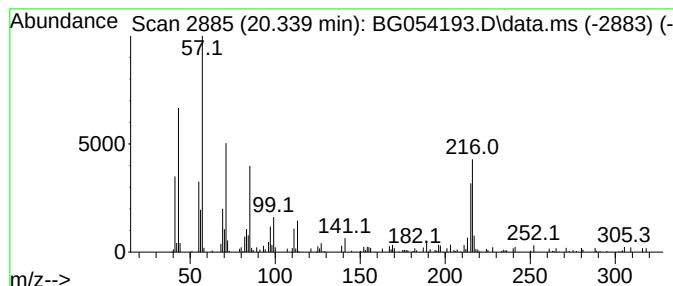
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Decane, 3,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.339	3.61 ng	102851	Chrysene-d12	21.714	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	60
2	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	58
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	52
4	Heptacosane	380	C27H56	000593-49-7	52
5	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
Data File : BG054193.D
Acq On : 1 Jul 2022 16:16
Operator : CG/JU
Sample : N3558-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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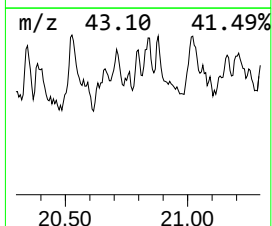
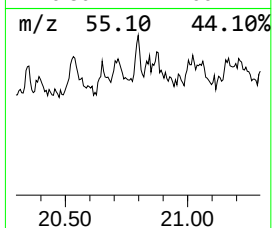
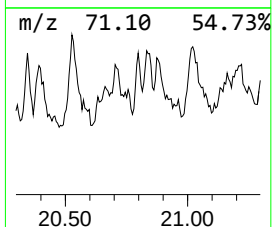
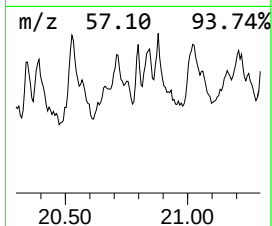
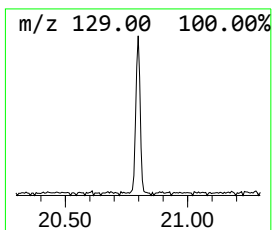
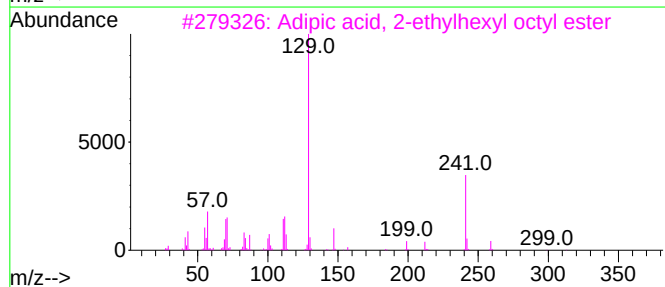
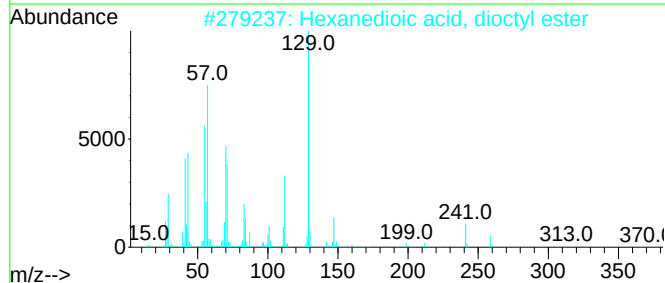
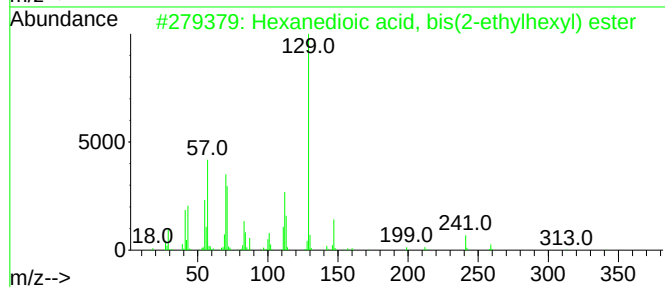
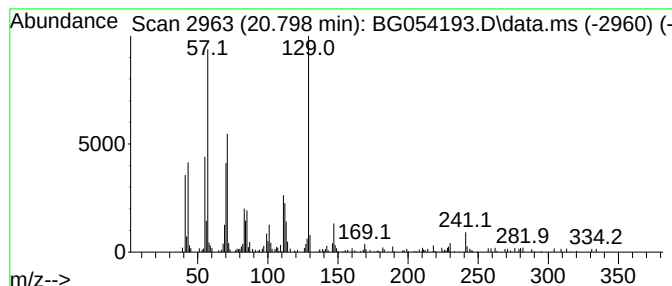
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.797	3.29 ng	93777	Chrysene-d12	21.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	68
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	68
3			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	59
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	43
5			Adipic acid, 2-methylpent-3-yl o...	342	C20H38O4	1000353-56-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
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Acq On : 1 Jul 2022 16:16
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Sample : N3558-01
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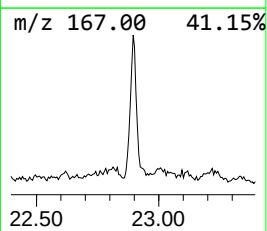
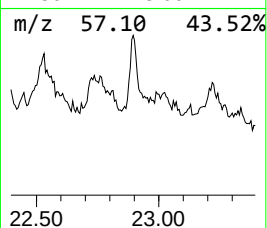
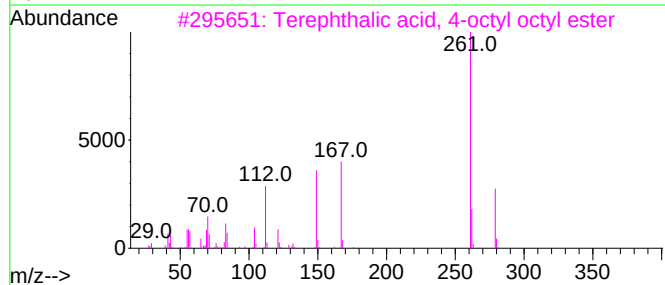
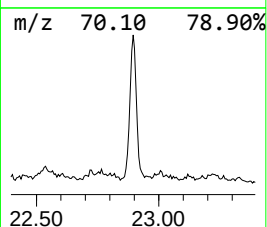
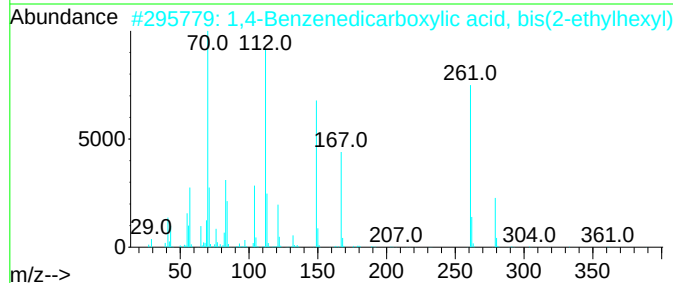
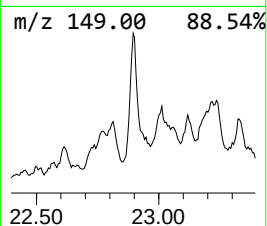
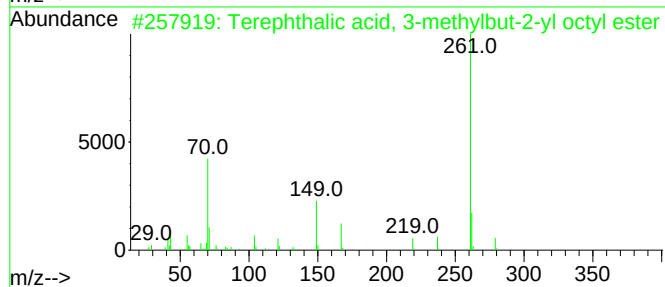
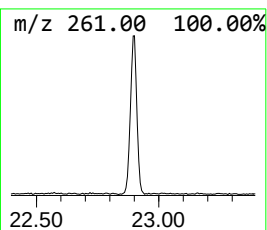
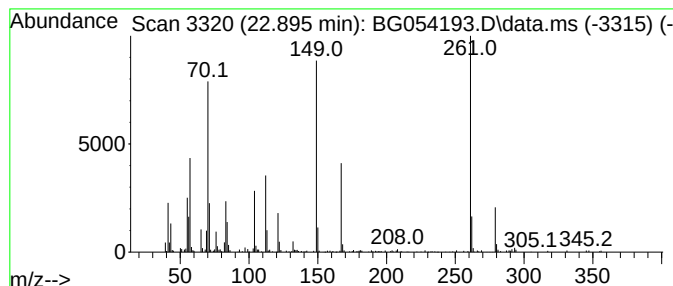
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Terephthalic acid, 3-methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.895	13.40 ng	381960	Chrysene-d12	21.714

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	43
4			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	38
5			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070122\
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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Anthracene, 9-m...	18.359	2.5	ng	41765	4	17.437	330870	20.0
4H-Cyclopenta[d...	18.506	2.4	ng	39652	4	17.437	330870	20.0
Tetracosane	18.624	2.5	ng	40920	4	17.437	330870	20.0
9,10-Anthracene...	18.853	7.1	ng	117041	4	17.437	330870	20.0
Sulfurous acid,...	19.246	4.2	ng	70037	4	17.437	330870	20.0
Octadecanoic acid	19.587	2.6	ng	73605	5	21.714	570213	20.0
Decane, 3,6-dim...	20.339	3.6	ng	102851	5	21.714	570213	20.0
Hexanedioic aci...	20.797	3.3	ng	93777	5	21.714	570213	20.0
Terephthalic ac...	22.895	13.4	ng	381960	5	21.714	570213	20.0