

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
 Data File : BG056412.D
 Acq On : 24 Jan 2023 21:13
 Operator : CG/JU
 Sample : 01266-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-219

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.330	341	347	356	rBB	116966	180347	7.01%	0.910%
2	5.818	421	430	440	rBV	487299	786838	30.60%	3.971%
3	7.263	671	676	684	rBB2	21872	32762	1.27%	0.165%
4	7.439	697	706	720	rBV	494767	864270	33.62%	4.362%
5	8.291	844	851	858	rBV	117698	201664	7.84%	1.018%
6	9.466	1043	1051	1061	rVB	291625	523978	20.38%	2.645%
7	11.123	1325	1333	1339	rBV	168561	298708	11.62%	1.508%
8	11.170	1339	1341	1348	rVB2	18517	29025	1.13%	0.146%
9	13.532	1736	1743	1752	rBV	1205384	1768328	68.78%	8.925%
10	14.907	1969	1977	1983	rVV	299866	483873	18.82%	2.442%
11	14.972	1983	1988	1993	rVB	20152	28664	1.11%	0.145%
12	15.301	2037	2044	2050	rVB	14843	26434	1.03%	0.133%
13	15.947	2148	2154	2163	rVB	34853	53219	2.07%	0.269%
14	16.241	2199	2204	2210	rVB2	41263	63908	2.49%	0.323%
15	16.388	2222	2229	2236	rBV	870904	1283382	49.92%	6.478%
16	16.946	2312	2324	2329	rBV5	13695	33424	1.30%	0.169%
17	17.357	2390	2394	2399	rBV5	14833	25811	1.00%	0.130%
18	17.645	2436	2443	2446	rBV	405332	625527	24.33%	3.157%
19	17.686	2446	2450	2456	rVB	301264	446783	17.38%	2.255%
20	17.774	2456	2465	2472	rBV	96003	164160	6.39%	0.829%
21	18.039	2505	2510	2517	rBV3	16134	39460	1.53%	0.199%
22	18.368	2561	2566	2575	rBV3	13901	33927	1.32%	0.171%
23	18.491	2582	2587	2594	rBV2	92881	209723	8.16%	1.059%
24	18.556	2594	2598	2603	rVB2	57639	88913	3.46%	0.449%
25	18.638	2608	2612	2616	rVB	32839	43087	1.68%	0.217%
26	18.708	2618	2624	2628	rBV2	85550	167428	6.51%	0.845%
27	18.996	2669	2673	2678	rBV2	41409	78942	3.07%	0.398%
28	19.225	2709	2712	2717	rBV6	25724	44659	1.74%	0.225%
29	19.419	2738	2745	2749	rBV6	55870	152767	5.94%	0.771%
30	19.560	2765	2769	2774	rBV2	28049	50546	1.97%	0.255%
31	19.613	2775	2778	2782	rVV3	36494	58204	2.26%	0.294%
32	19.678	2783	2789	2794	rVB	860844	1191666	46.35%	6.015%
33	20.001	2840	2844	2846	rBV2	129865	199850	7.77%	1.009%
34	20.036	2846	2850	2857	rVB	703511	1000343	38.91%	5.049%
35	20.218	2876	2881	2886	rVB	2059612	2571025	100.00%	12.977%
36	20.271	2887	2890	2895	rBV4	36235	64532	2.51%	0.326%

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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	20.524	2930	2933	2940	rVB2	155421	220119	8.56%	1.111%
38	20.618	2945	2949	2953	rBV	120852	169977	6.61%	0.858%
39	21.928	3164	3172	3177	rBV3	481514	1394639	54.24%	7.039%
40	21.981	3177	3181	3190	rVB	325991	610342	23.74%	3.081%
41	23.127	3370	3376	3388	rVB	476745	890014	34.62%	4.492%
42	24.272	3562	3571	3579	rBV	257148	957408	37.24%	4.832%
43	25.042	3695	3702	3716	rVB2	157762	474092	18.44%	2.393%
44	25.201	3720	3729	3742	rVB	217955	639368	24.87%	3.227%
45	25.365	3749	3757	3765	rVB2	191929	540667	21.03%	2.729%

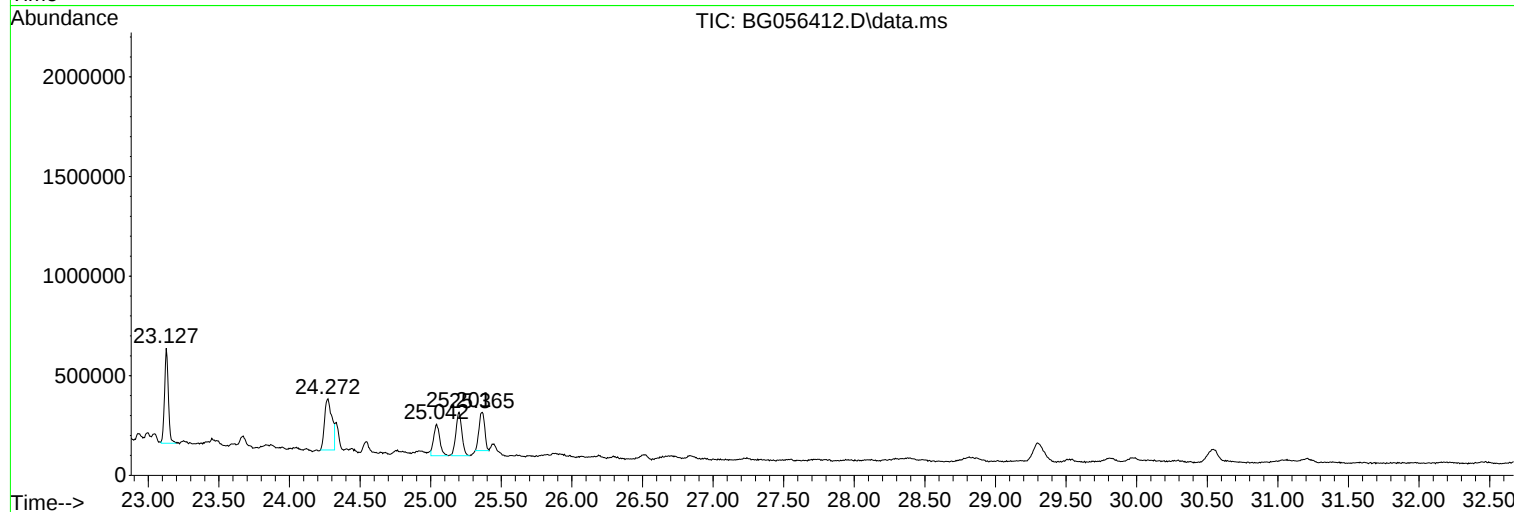
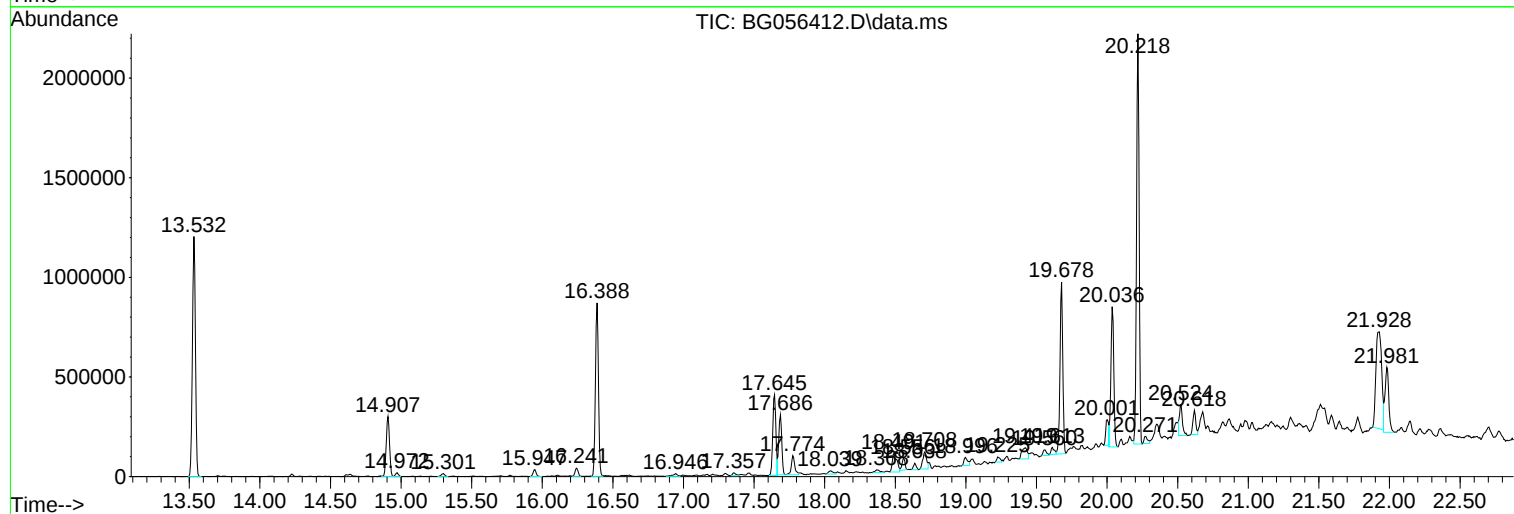
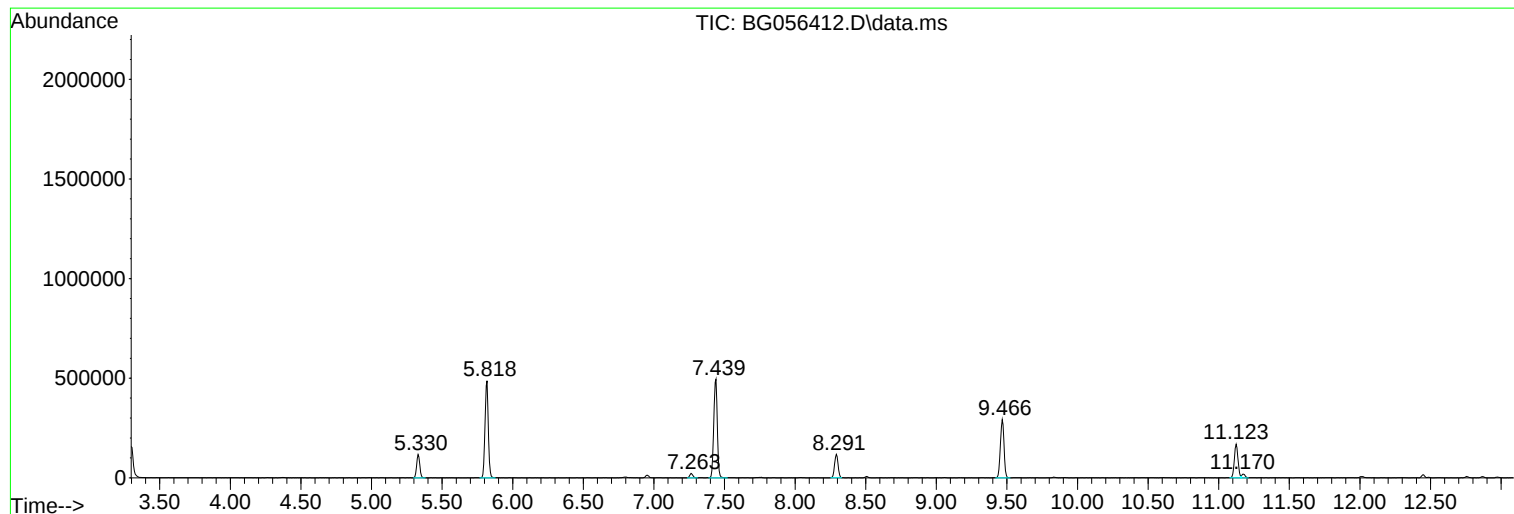
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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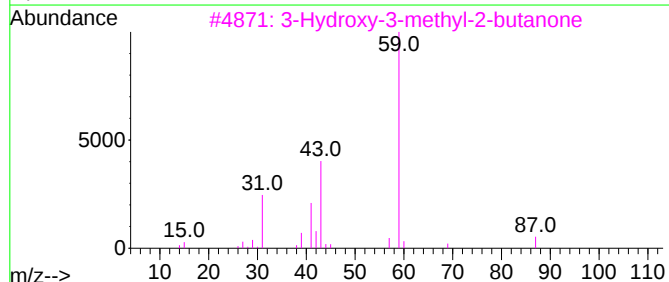
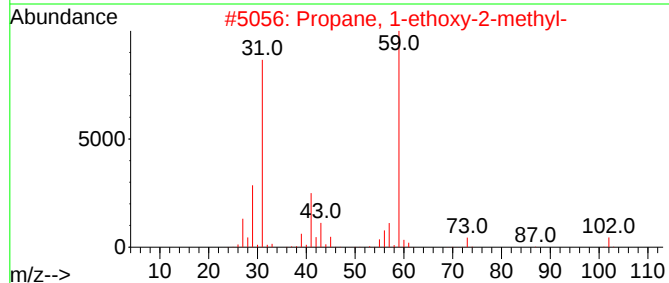
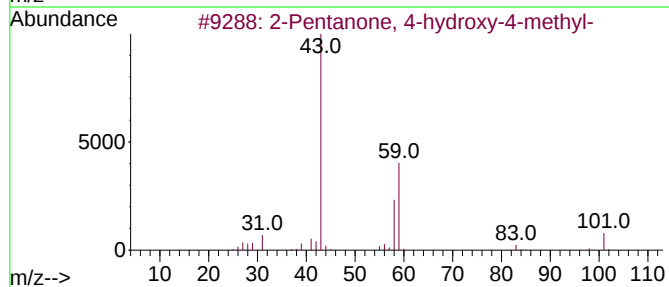
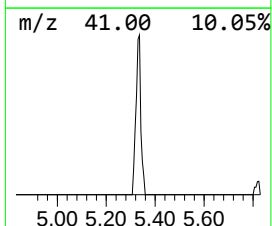
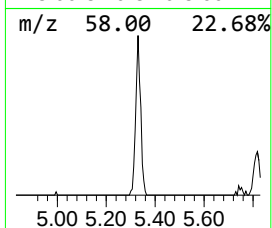
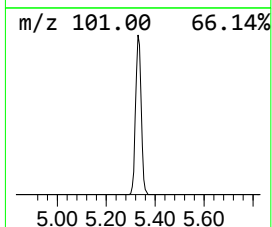
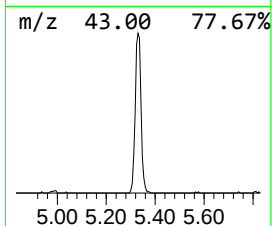
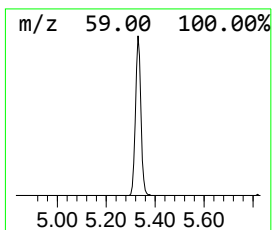
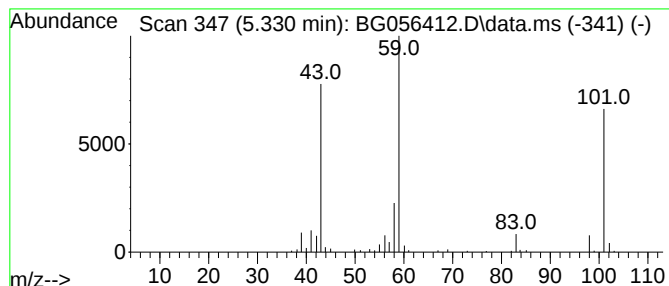
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.330 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.330	17.89 ng	180347	1,4-Dichlorobenzene-d4	8.291

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39	
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32	
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32	
4	Guanidine	59	CH5N3	000113-00-8	25	
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23	



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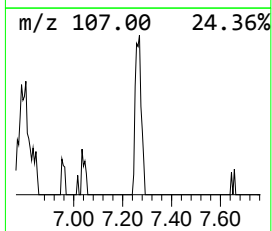
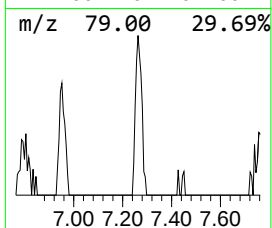
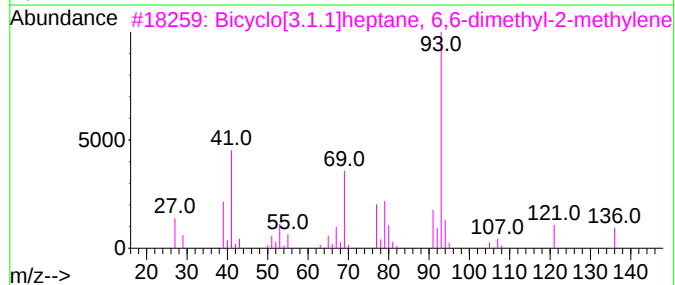
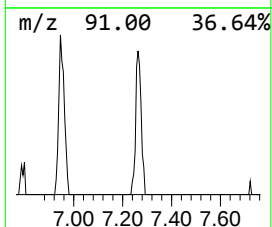
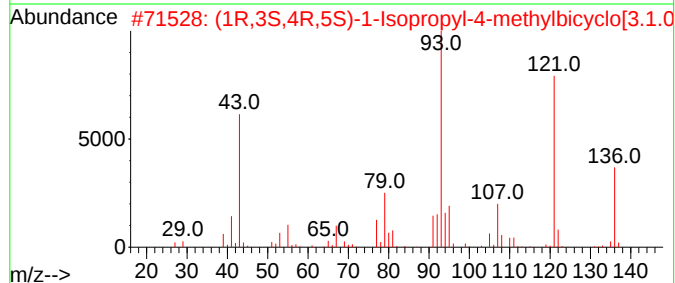
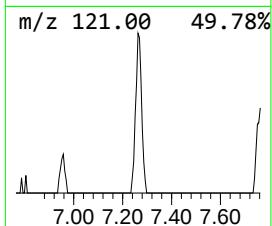
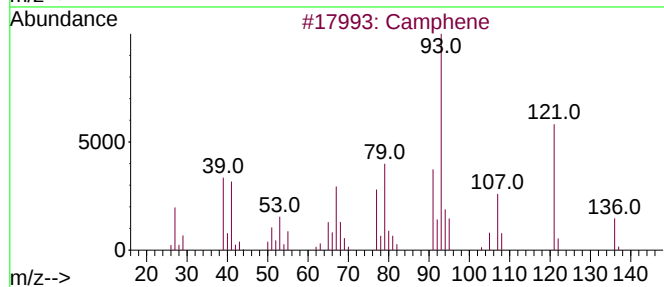
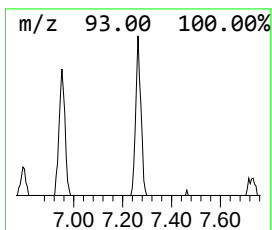
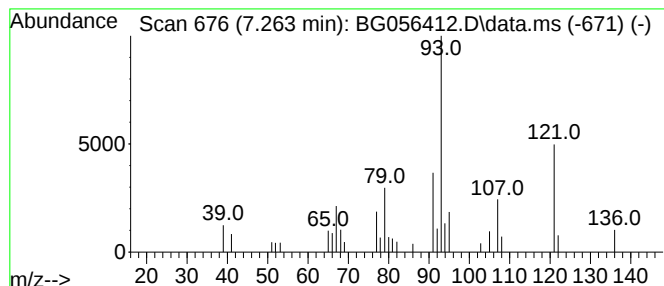
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Camphene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.263	3.25 ng	32762	1,4-Dichlorobenzene-d4	8.291

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	94
2			(1R,3S,4R,5S)-1-Isopropyl-4-meth...	196	C12H20O2	062181-91-3	72
3			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	64
4			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	62
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	58



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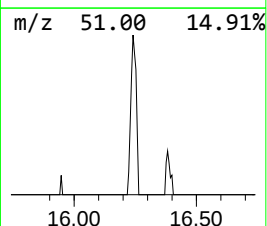
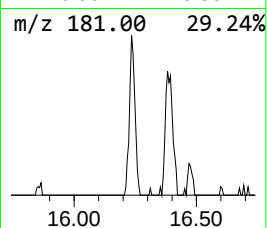
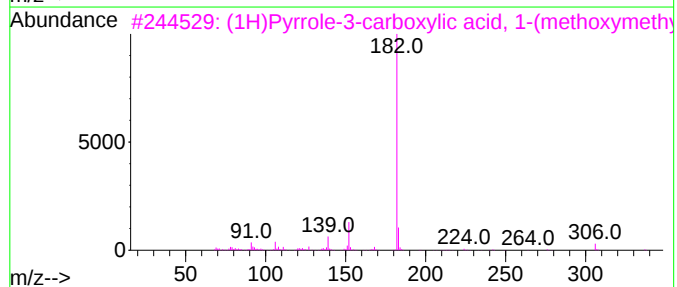
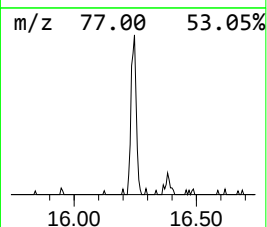
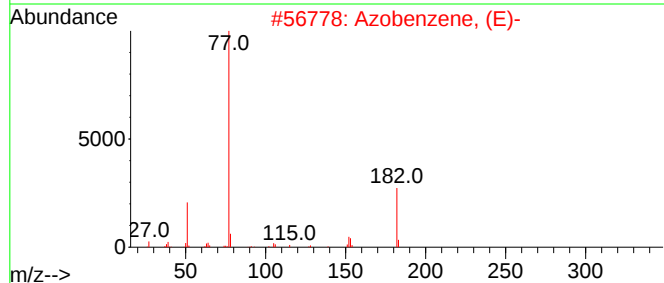
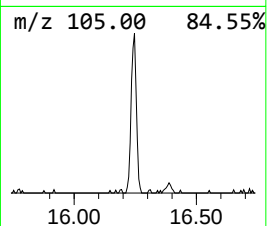
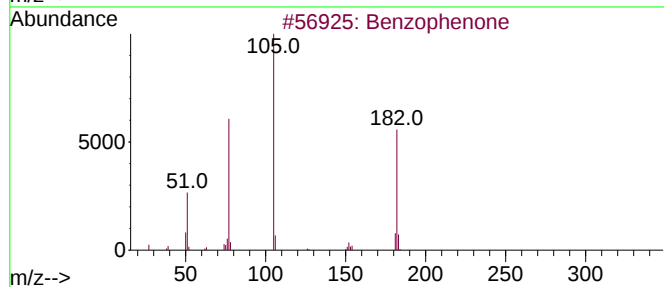
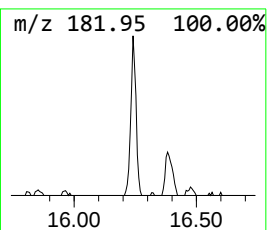
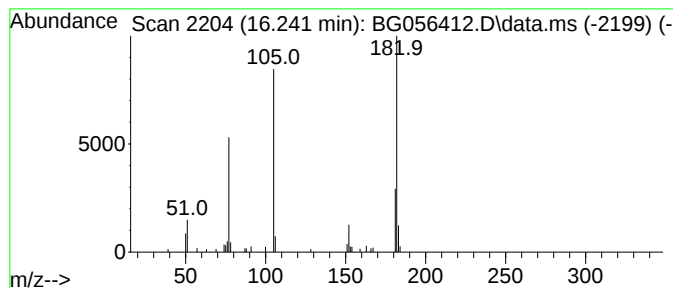
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.241	2.64 ng	63908	Acenaphthene-d10	14.907

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	90
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	43
3			(1H)Pyrrole-3-carboxylic acid, 1...	337	C16H19NO5S	155345-18-9	43
4			4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	43
5			Benzoic acid, 3,4-dimethoxy-	182	C9H10O4	000093-07-2	38



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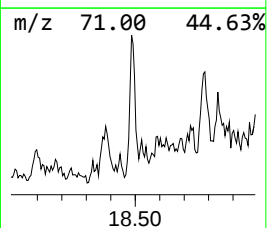
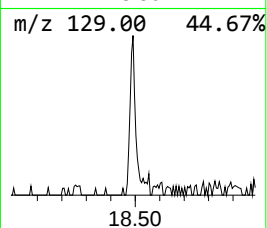
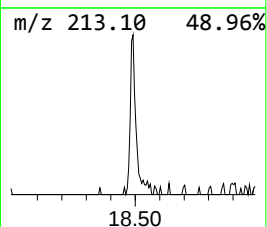
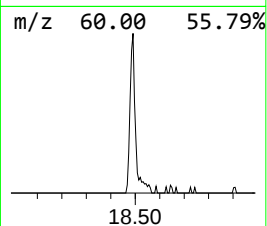
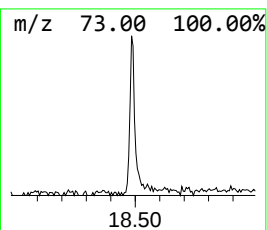
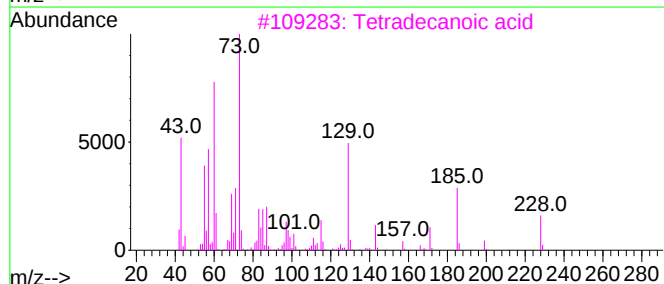
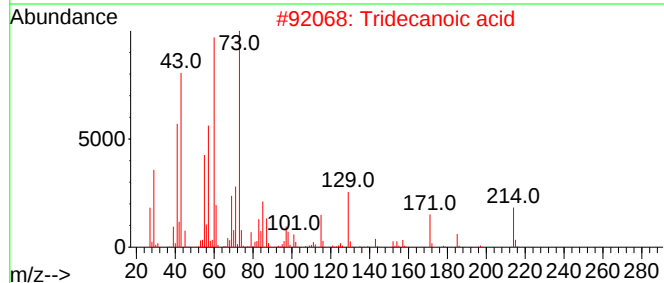
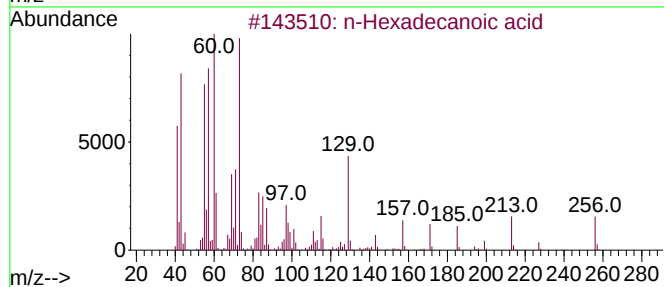
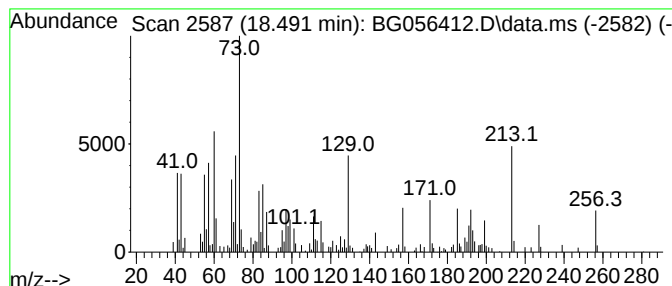
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.491	6.71 ng	209723	Phenanthrene-d10	17.645

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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	46
5			Undecanoic acid	186	C11H22O2	000112-37-8	35



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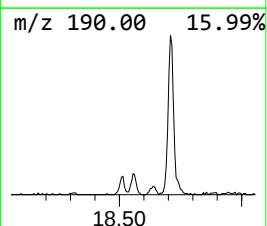
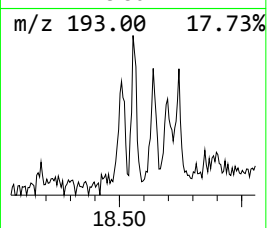
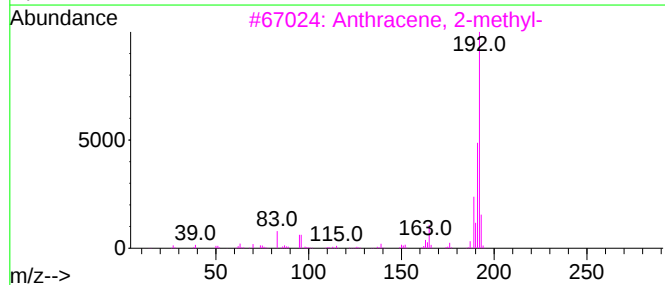
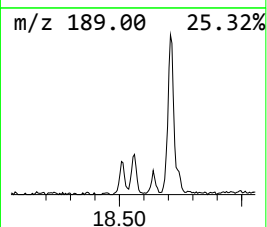
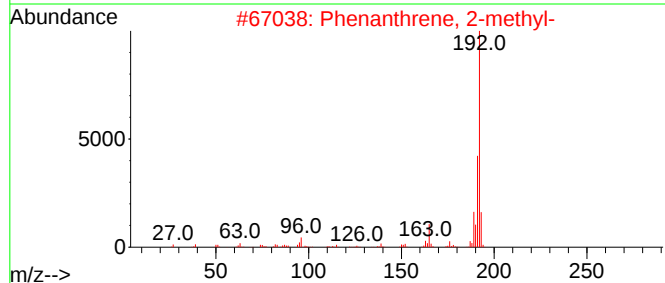
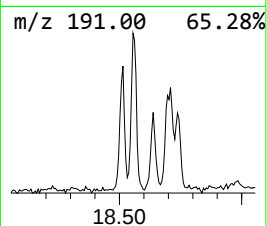
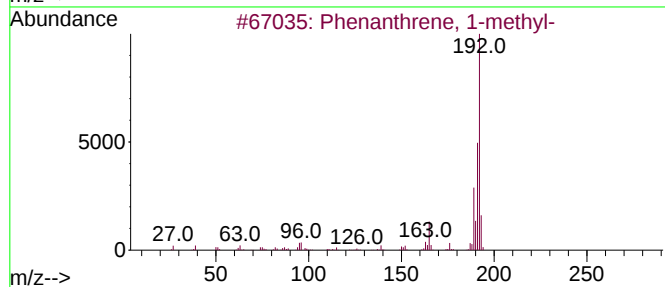
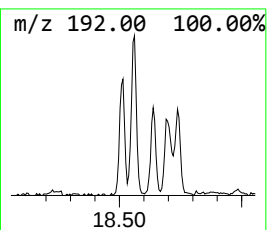
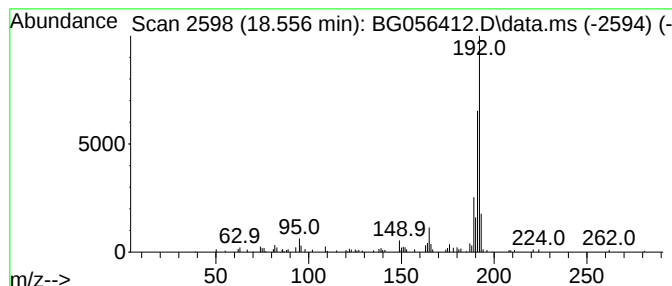
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.556	2.84 ng	88913	Phenanthrene-d10	17.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
Operator : CG/JU
Sample : 01266-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

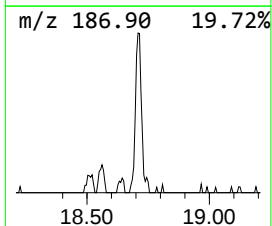
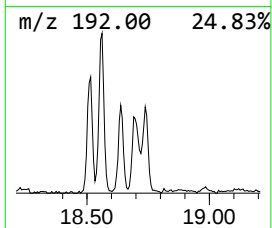
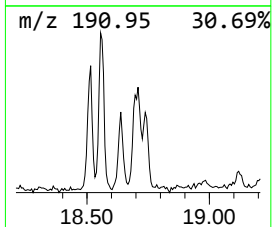
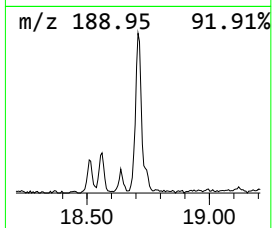
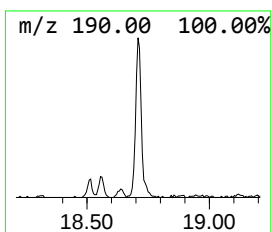
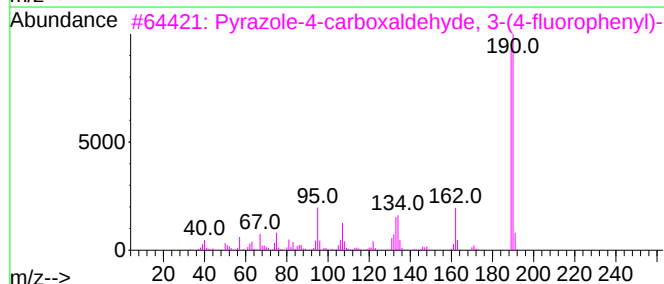
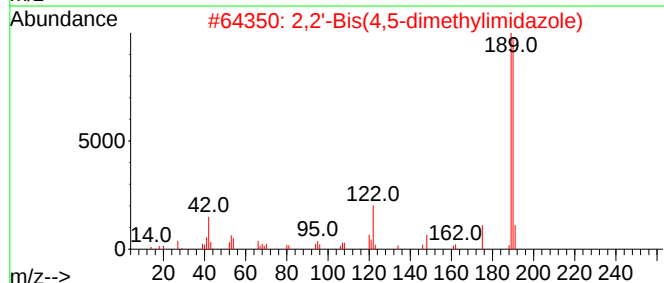
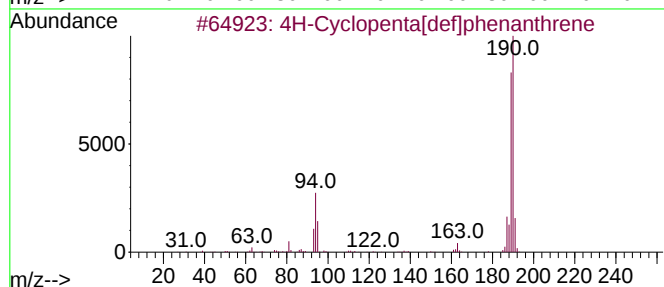
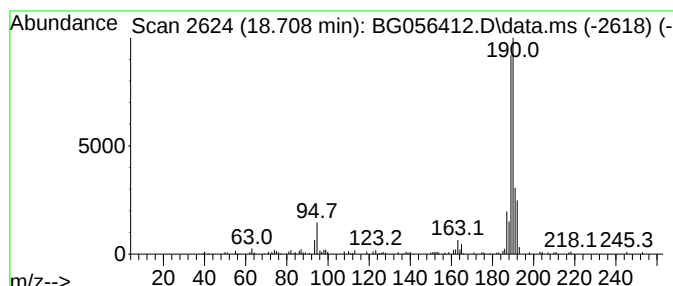
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.708	5.35 ng	167428	Phenanthrene-d10		17.645	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	91
2	2,2'-Bis(4,5-dimethylimidazole)		190	C10H14N4	069286-06-2	53
3	Pyrazole-4-carboxaldehyde, 3-(4-...		190	C10H7FN2O	306936-57-2	42
4	Thiophene-3-carboxaldehyde, 5-ch...		190	C5H4BClO3S	036155-87-0	40
5	Pyrimidine, 2-chloro-5-phenyl-		190	C10H7ClN2	022536-62-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
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Sample : 01266-01
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Instrument :
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ClientSampleId :
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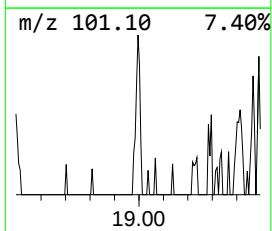
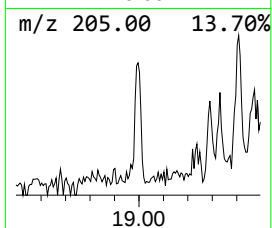
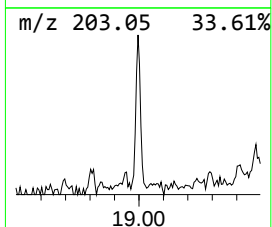
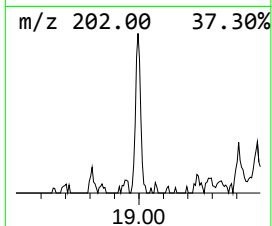
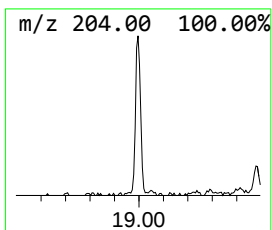
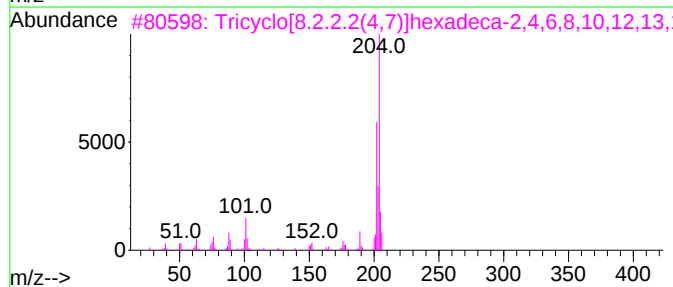
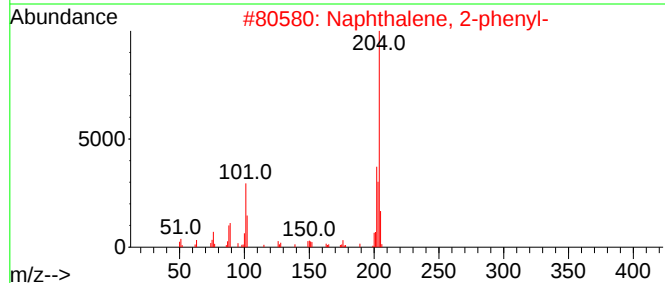
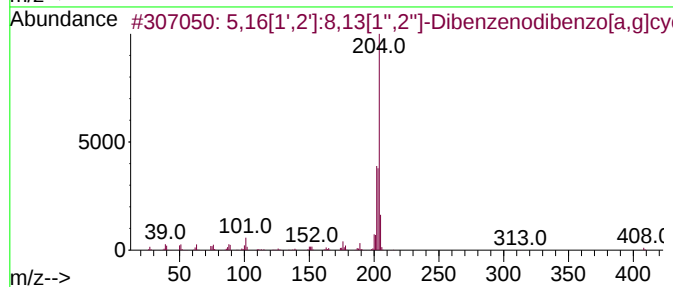
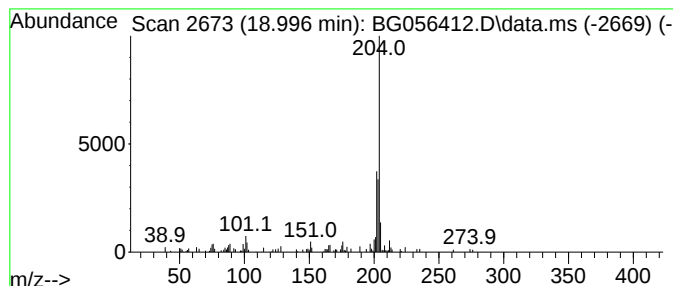
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5,16[1',2']:8,13[1'',2'']-D... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.996	2.52 ng	78942	Phenanthrene-d10	17.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	83		
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	64		
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	59		
4	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	58		
5	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	58		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
Operator : CG/JU
Sample : 01266-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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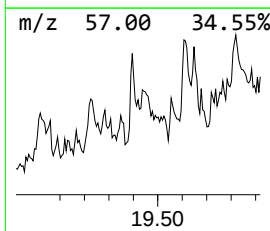
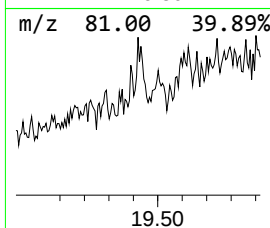
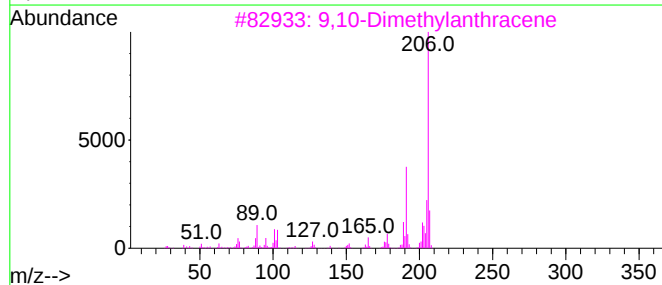
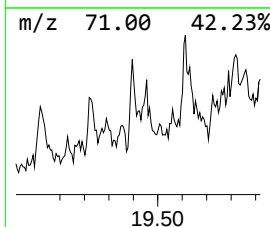
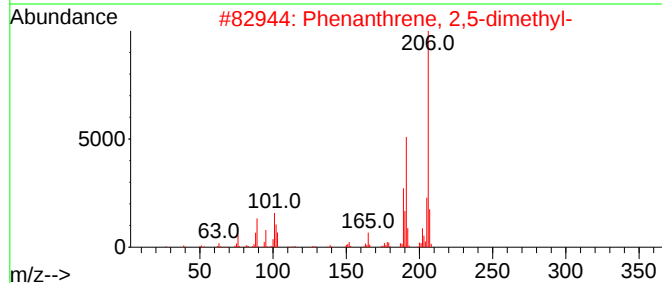
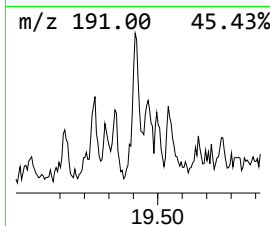
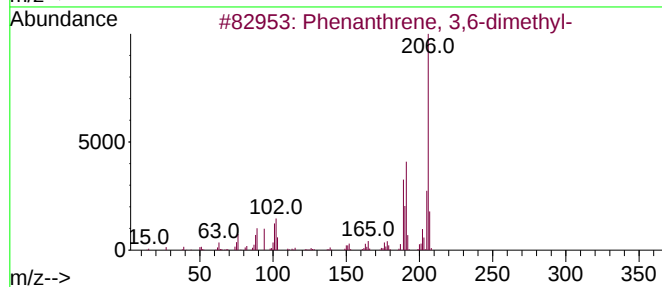
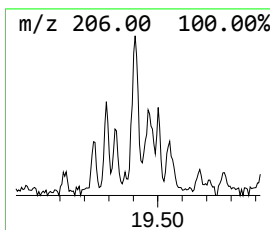
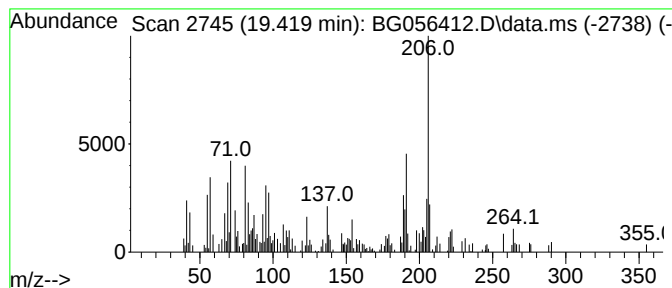
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.419	4.88 ng	152767	Phenanthrene-d10	17.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
3			9,10-Dimethylantracene	206	C16H14	000781-43-1	70
4			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	64
5			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
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Misc :
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Instrument :
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ClientSampleId :
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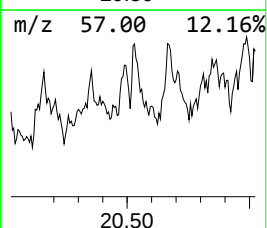
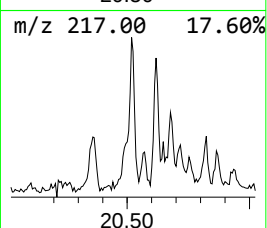
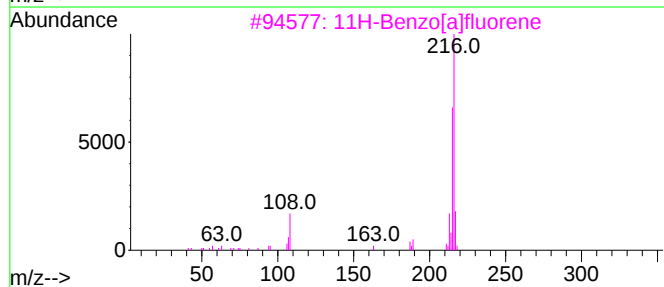
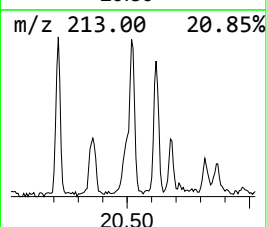
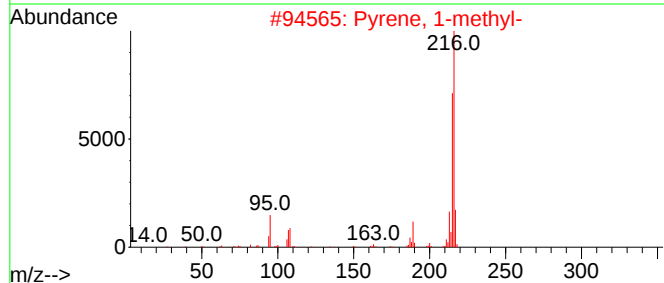
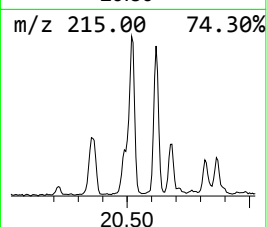
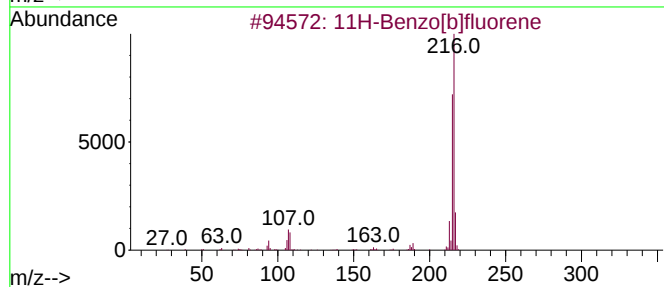
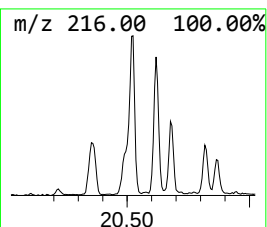
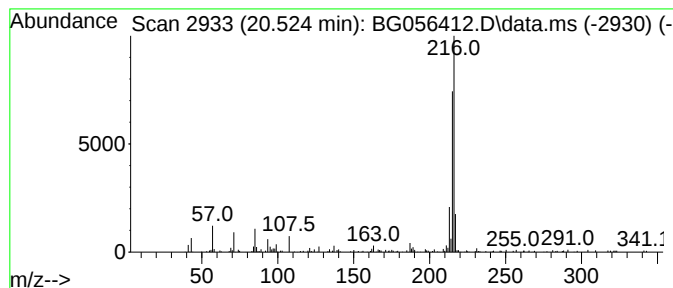
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.524	3.16 ng	220119	Chrysene-d12	21.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4		Pyrene, 2-methyl-	216	C17H12	003442-78-2	72
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
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Sample : 01266-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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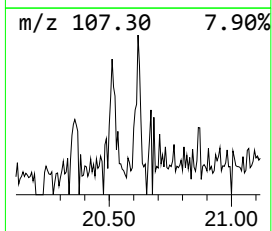
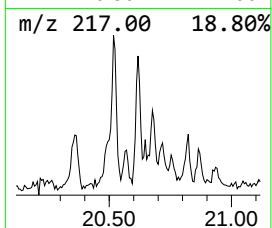
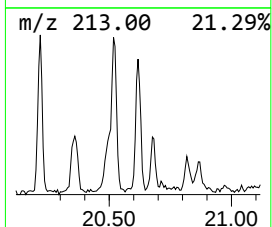
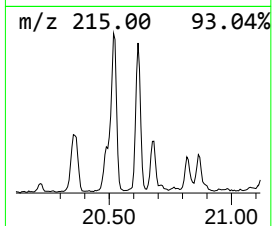
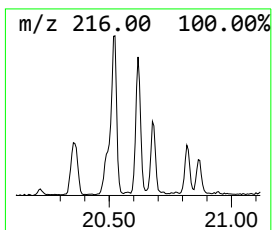
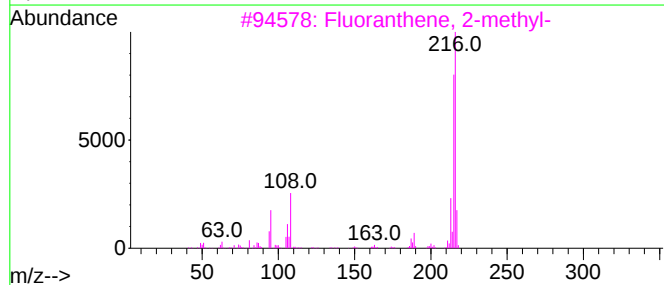
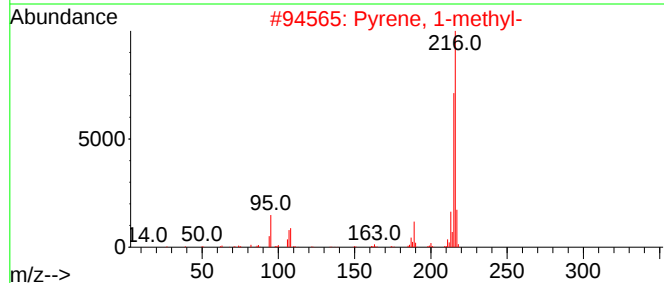
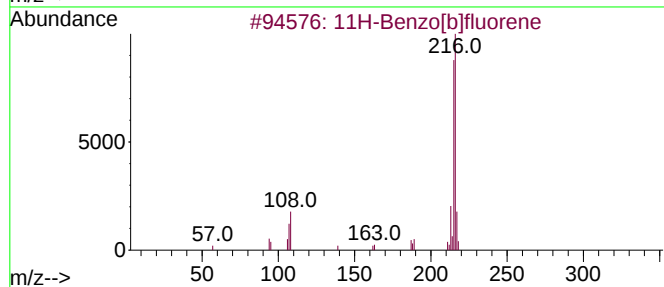
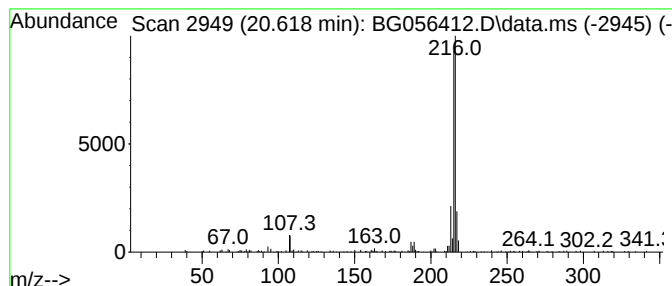
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.618	2.44 ng	169977	Chrysene-d12	21.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene		216	C17H12	000243-17-4	93
2	Pyrene, 1-methyl-		216	C17H12	002381-21-7	91
3	Fluoranthene, 2-methyl-		216	C17H12	033543-31-6	87
4	11H-Benzo[a]fluorene		216	C17H12	000238-84-6	86
5	1,3,5-Triazine-2,4,6-triamine, N...		216	C10H12N6	046731-79-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
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Sample : 01266-01
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ALS Vial : 11 Sample Multiplier: 1

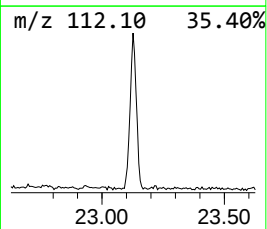
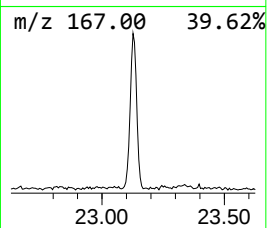
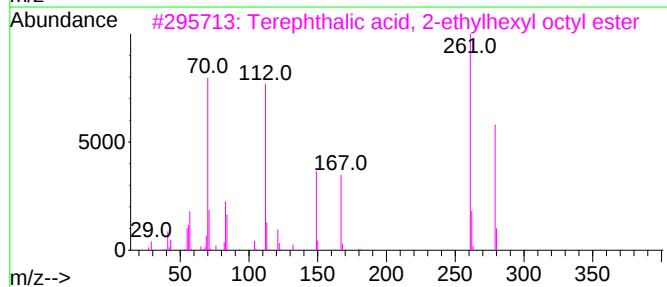
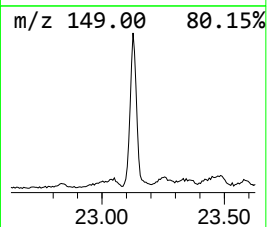
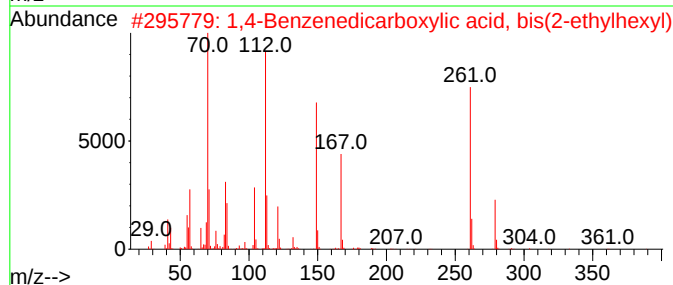
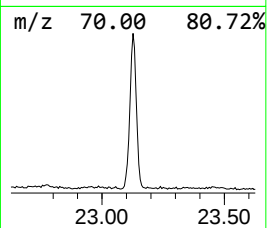
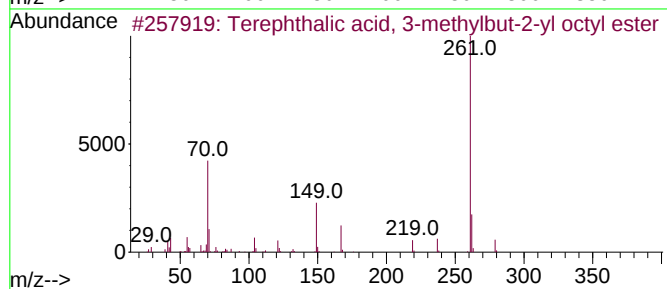
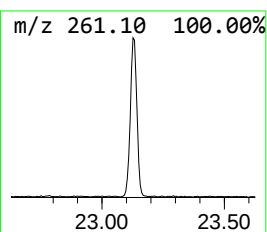
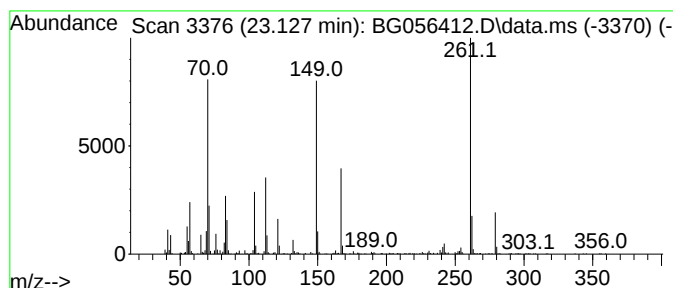
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Terephthalic acid, 3-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.127	12.76 ng	890014	Chrysene-d12	21.934	
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, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	52
4	Terephthalic acid, octyl 2,3,4-t...	408	C22H23F3O4	1010415-80-4	46
5	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
Operator : CG/JU
Sample : 01266-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-219

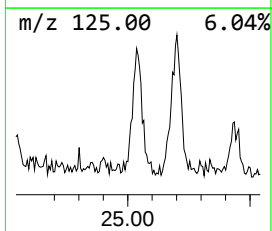
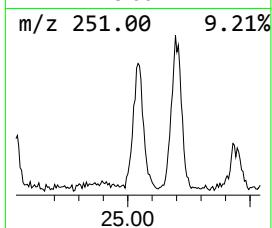
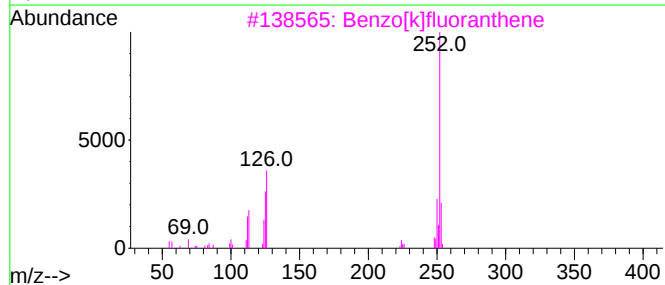
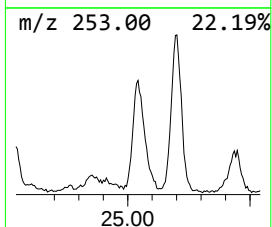
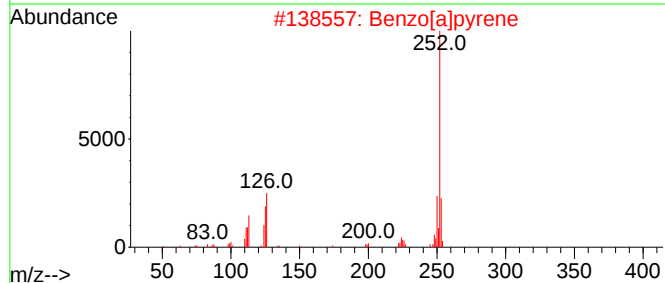
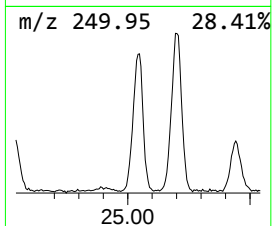
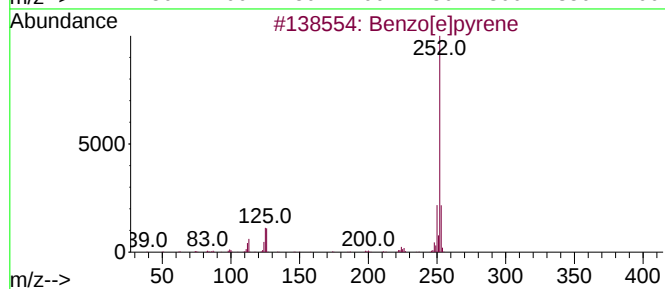
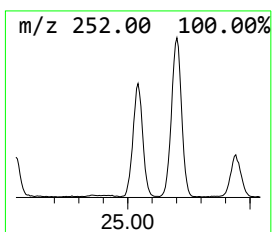
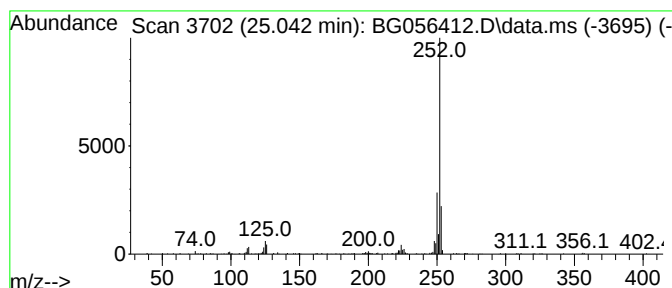
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.042	17.54 ng	474092	Perylene-d12	25.365

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	91
2			Benzo[a]pyrene	252	C20H12	000050-32-8	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012423\
Data File : BG056412.D
Acq On : 24 Jan 2023 21:13
Operator : CG/JU
Sample : 01266-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-219

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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
unknown5.330	5.330	17.9	ng	180347	1	8.291	201664	20.0
Camphene	7.263	3.3	ng	32762	1	8.291	201664	20.0
Benzophenone	16.241	2.6	ng	63908	3	14.907	483873	20.0
n-Hexadecanoic ...	18.491	6.7	ng	209723	4	17.645	625527	20.0
Phenanthrene, 1...	18.556	2.8	ng	88913	4	17.645	625527	20.0
4H-Cyclopenta[d...	18.708	5.3	ng	167428	4	17.645	625527	20.0
5,16[1',2']:8,1...	18.996	2.5	ng	78942	4	17.645	625527	20.0
Phenanthrene, 3...	19.419	4.9	ng	152767	4	17.645	625527	20.0
11H-Benzo[b]flu...	20.524	3.2	ng	220119	5	21.934	1394640	20.0
Pyrene, 1-methyl-	20.618	2.4	ng	169977	5	21.934	1394640	20.0
Terephthalic ac...	23.127	12.8	ng	890014	5	21.934	1394640	20.0
Benzo[e]pyrene	25.042	17.5	ng	474092	6	25.365	540667	20.0