

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
 Data File : BG056688.D
 Acq On : 21 Feb 2023 17:32
 Operator : CG/JU
 Sample : 01552-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-06-0-2.0

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-BG021523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056688.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.470	322	329	337	rBV	158222	260650	21.48%	2.942%
2	5.946	403	410	419	rBV	403975	661894	54.53%	7.471%
3	7.562	676	685	692	rBV	421421	736909	60.72%	8.318%
4	8.432	826	833	840	rBV	83721	144852	11.93%	1.635%
5	9.607	1025	1033	1046	rVB	241950	449165	37.01%	5.070%
6	11.275	1310	1317	1322	rBV	109283	197684	16.29%	2.231%
7	11.322	1322	1325	1331	rVB	9260	14675	1.21%	0.166%
8	13.667	1717	1724	1730	rBV	683003	1022864	84.28%	11.546%
9	15.036	1952	1957	1963	rVB2	167751	263302	21.69%	2.972%
10	15.100	1963	1968	1974	rBV	25523	38646	3.18%	0.436%
11	15.424	2018	2023	2028	rVB4	15979	25607	2.11%	0.289%
12	16.076	2127	2134	2139	rBV2	19364	33652	2.77%	0.380%
13	16.264	2157	2166	2172	rVB	34725	62671	5.16%	0.707%
14	16.369	2179	2184	2190	rVB2	22468	37441	3.08%	0.423%
15	16.510	2202	2208	2216	rBV	465463	723527	59.61%	8.167%
16	16.722	2241	2244	2250	rVB6	11638	18981	1.56%	0.214%
17	17.298	2335	2342	2344	rBV8	6241	12651	1.04%	0.143%
18	17.339	2345	2349	2357	rVV8	7296	18166	1.50%	0.205%
19	17.421	2358	2363	2369	rVV4	7847	13829	1.14%	0.156%
20	17.486	2370	2374	2378	rVV6	13130	20732	1.71%	0.234%
21	17.539	2380	2383	2387	rVV5	12258	17056	1.41%	0.193%
22	17.592	2387	2392	2398	rVV	15062	24498	2.02%	0.277%
23	17.774	2416	2423	2426	rBV	200367	299206	24.65%	3.377%
24	17.815	2426	2430	2436	rVB	185925	280880	23.14%	3.171%
25	17.903	2437	2445	2450	rBV	60765	102613	8.45%	1.158%
26	17.962	2450	2455	2458	rVB4	11219	17507	1.44%	0.198%
27	18.161	2483	2489	2496	rBV2	19849	43151	3.56%	0.487%
28	18.226	2498	2500	2507	rVB6	11967	19448	1.60%	0.220%
29	18.614	2561	2566	2569	rBV	67413	99979	8.24%	1.129%
30	18.684	2574	2578	2583	rVB2	42820	69488	5.73%	0.784%
31	18.767	2588	2592	2594	rBV	20106	24457	2.02%	0.276%
32	18.837	2598	2604	2607	rBV2	55186	96541	7.95%	1.090%
33	19.119	2649	2652	2656	rBV	23965	30254	2.49%	0.342%
34	19.530	2718	2722	2727	rBV3	26137	47729	3.93%	0.539%
35	19.801	2763	2768	2773	rBV	400965	556513	45.85%	6.282%
36	20.124	2819	2823	2825	rBV2	64595	99468	8.20%	1.123%

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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-BG021523.M
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37	20.159	2825	2829	2837	rVB	344974	519848	42.83%	5.868%
38	20.341	2854	2860	2865	rBV	900740	1213716	100.00%	13.700%
39	22.086	3150	3157	3163	rBV3	194591	538687	44.38%	6.081%

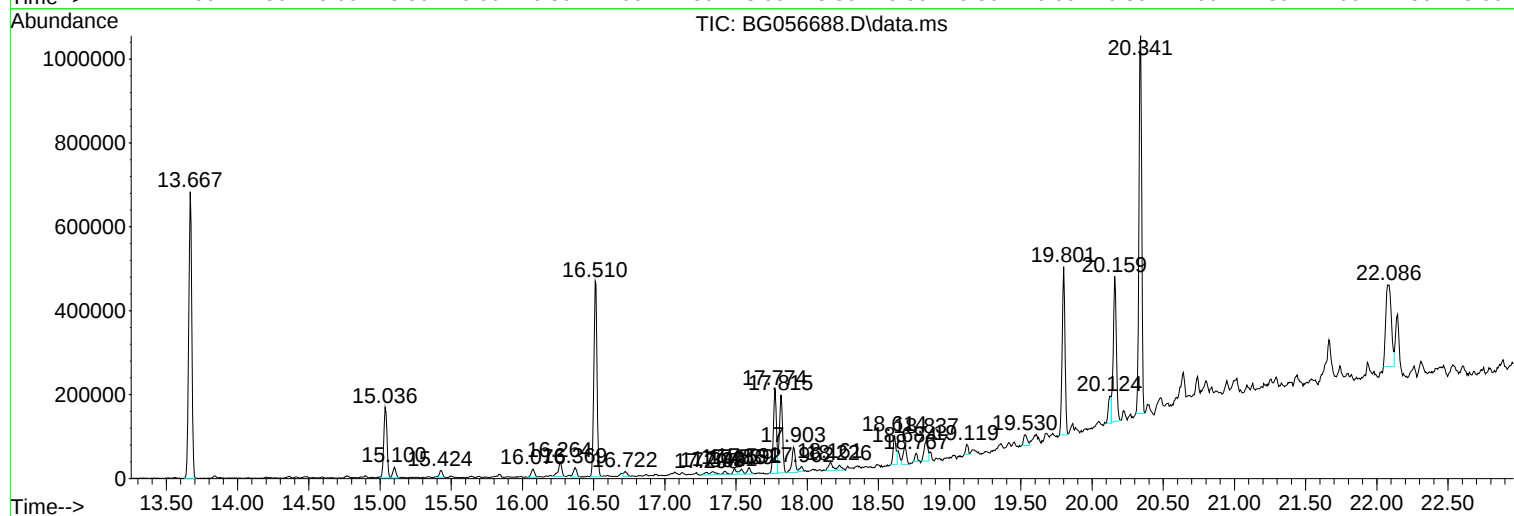
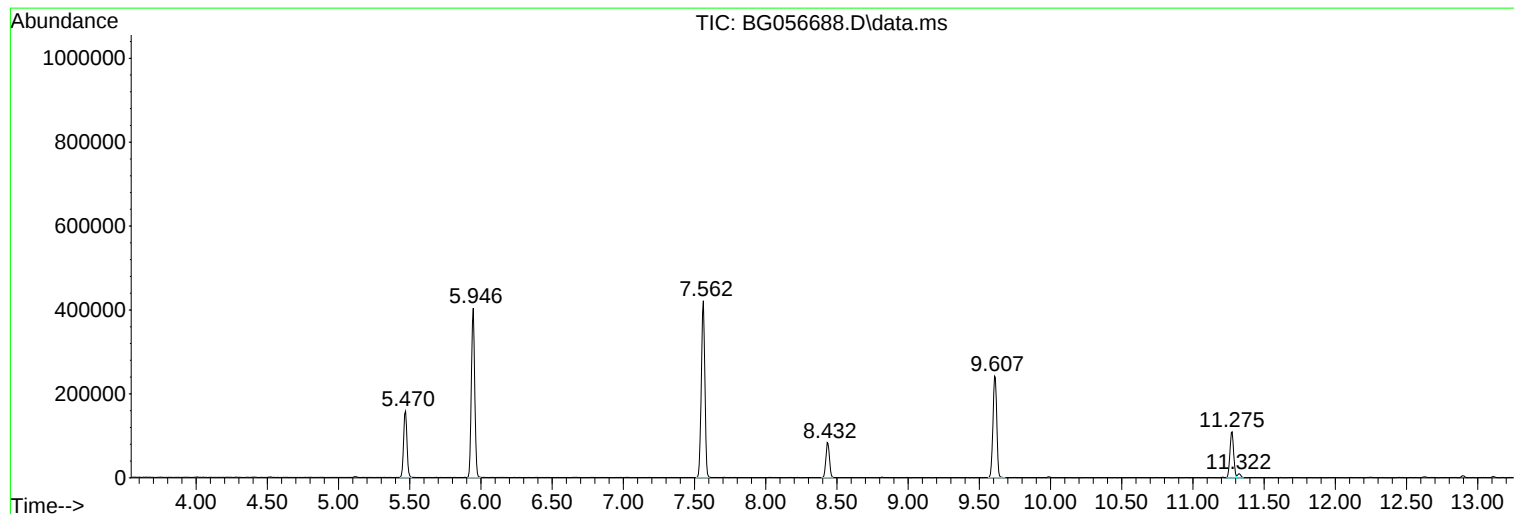
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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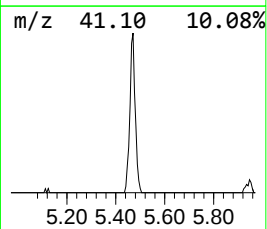
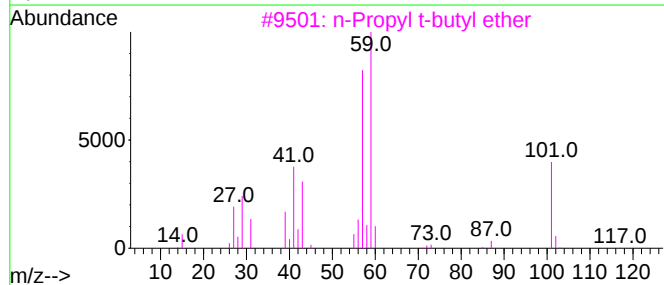
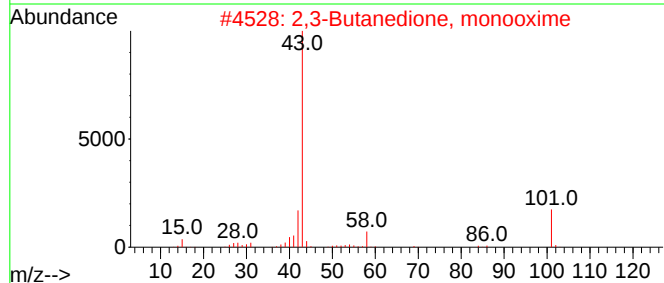
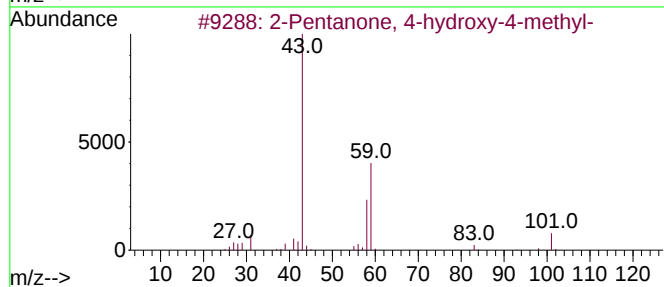
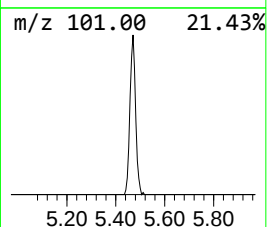
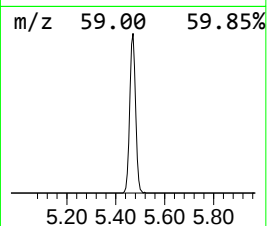
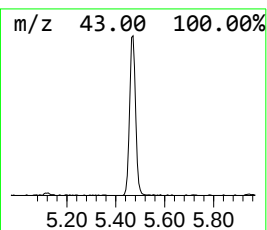
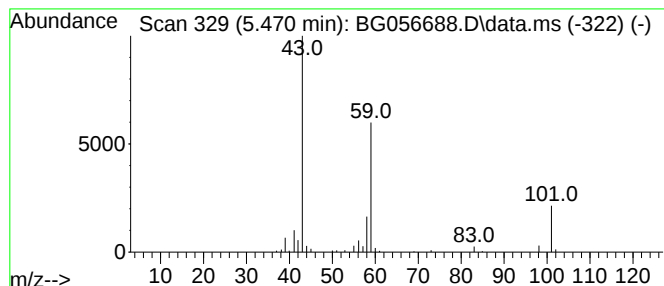
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.470	35.99 ng	260650	1,4-Dichlorobenzene-d4	8.438

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4			Acetone	58	C3H6O	000067-64-1	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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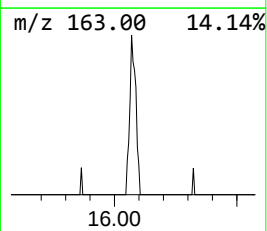
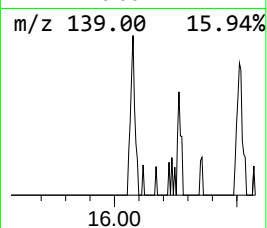
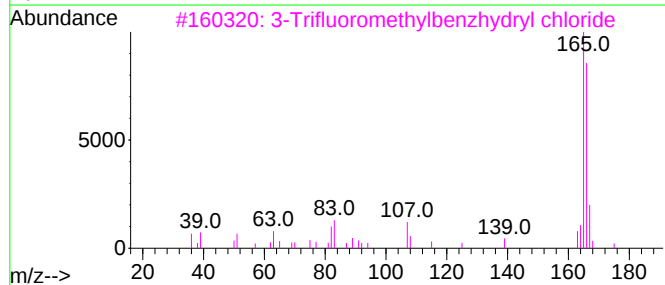
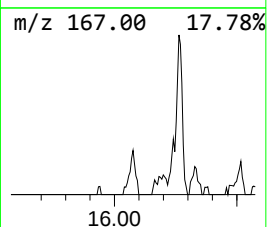
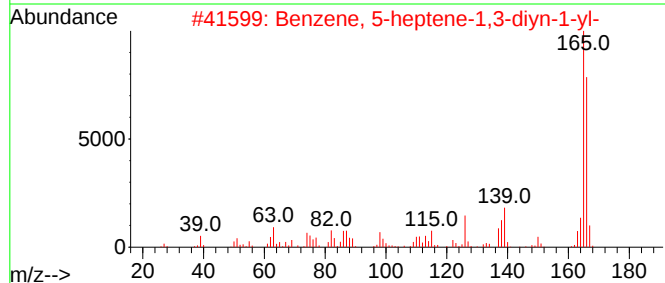
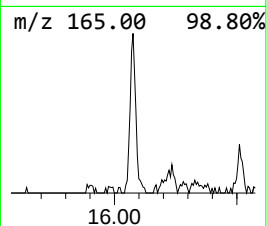
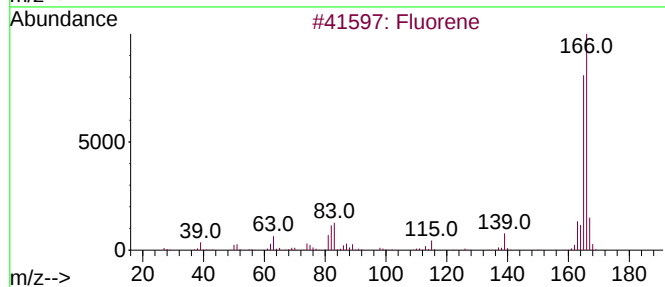
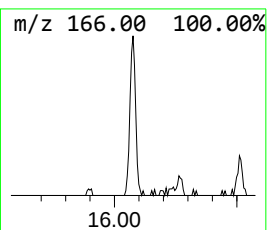
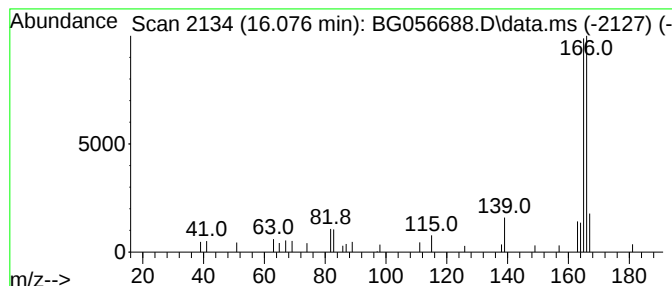
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Peak Number 2 Benzene, 5-heptene-1,3-diyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.076	2.56 ng	33652	Acenaphthene-d10	15.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluorene	166	C13H10	000086-73-7	91
2			Benzene, 5-heptene-1,3-diyn-1-yl-	166	C13H10	013678-98-3	86
3			3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	50
4			6H-Purine-6-thione, 1,9-dihydro-...	166	C6H6N4S	001006-20-8	37
5			5-Amino-2-Mercaptobenzimidazole	165	C7H7N3S	002818-66-8	32



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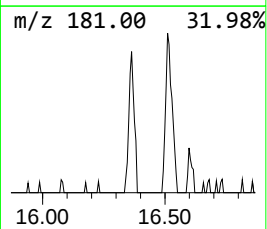
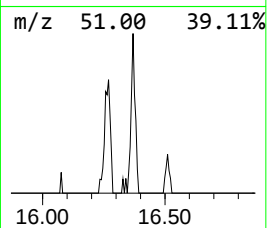
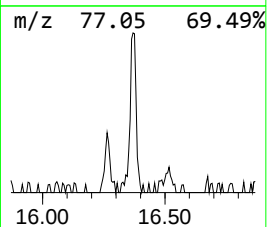
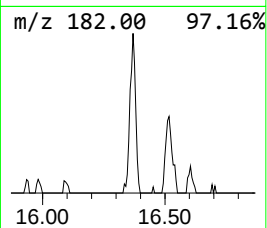
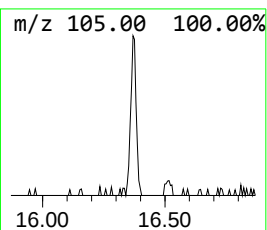
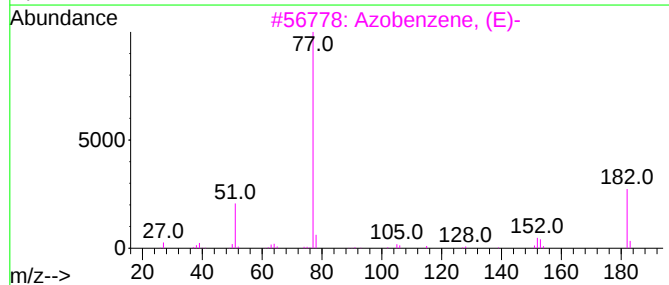
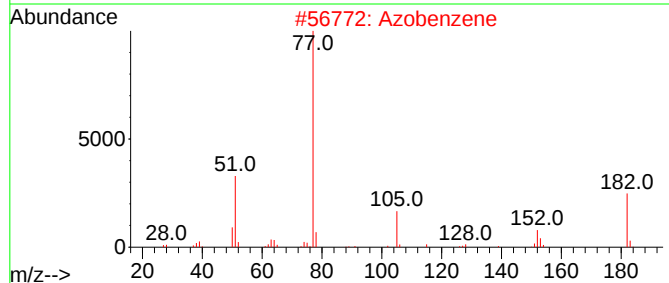
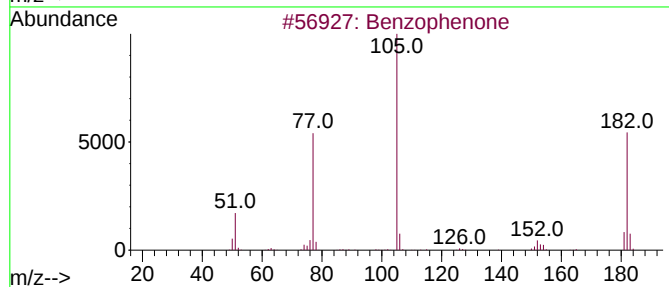
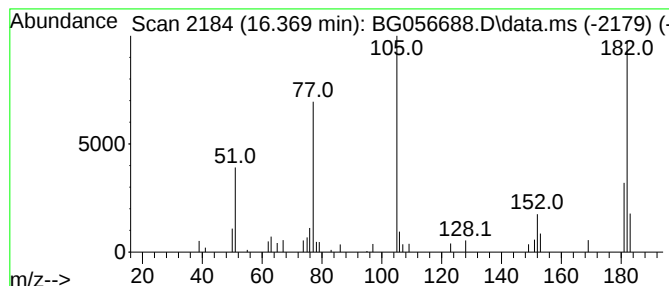
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.369	2.84 ng	37441	Acenaphthene-d10	15.036

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	87
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
4			4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	45
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	43



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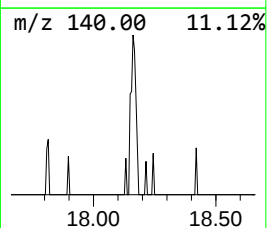
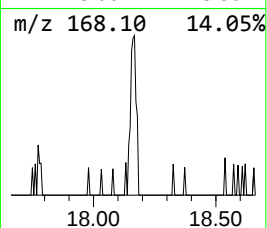
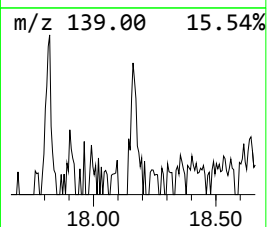
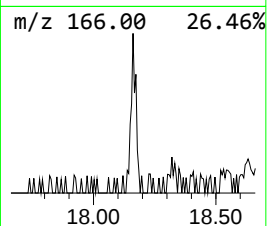
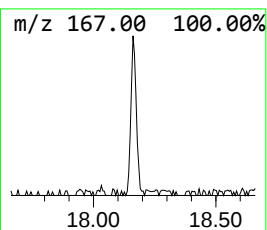
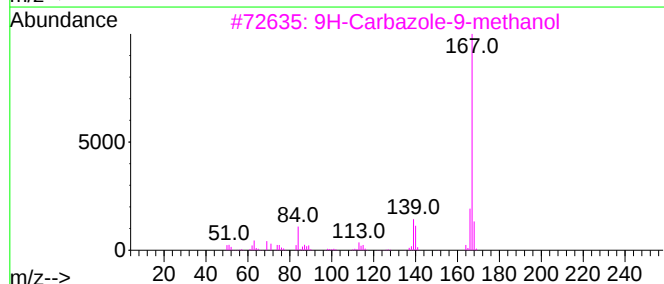
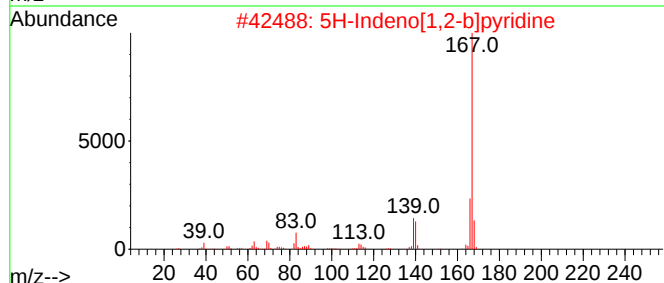
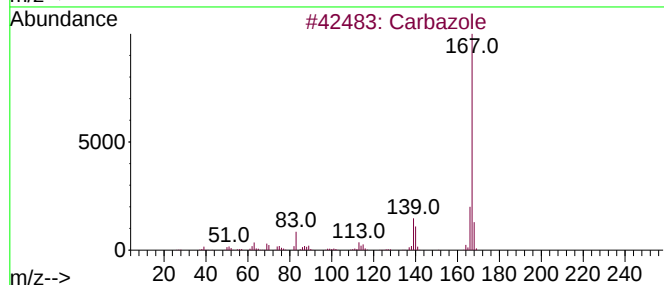
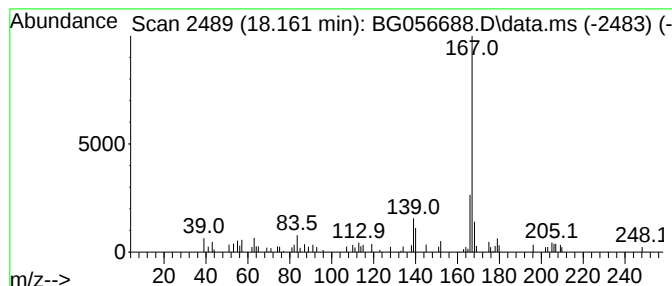
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5H-Indeno[1,2-b]pyridine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	2.88 ng	43151	Phenanthrene-d10	17.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbazole	167	C12H9N	000086-74-8	93
2			5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	87
3			9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	80
4			9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	72
5			2-Azafluorene	167	C12H9N	000244-40-6	64



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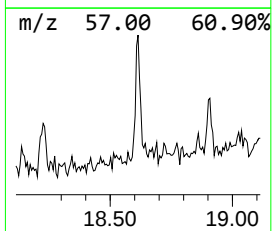
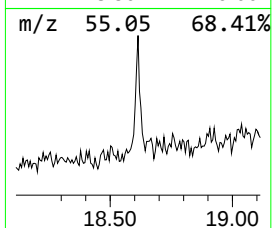
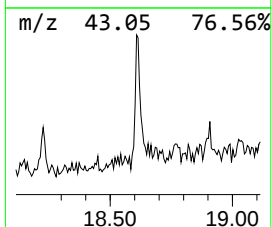
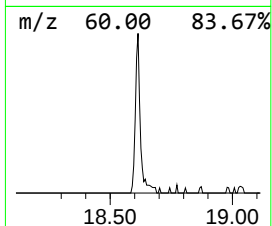
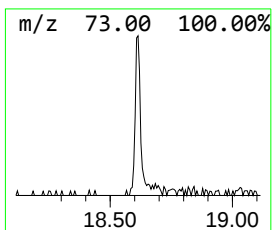
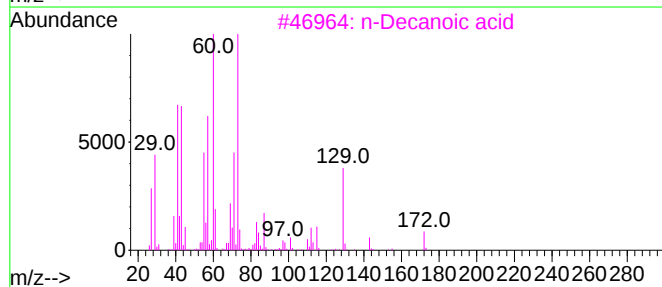
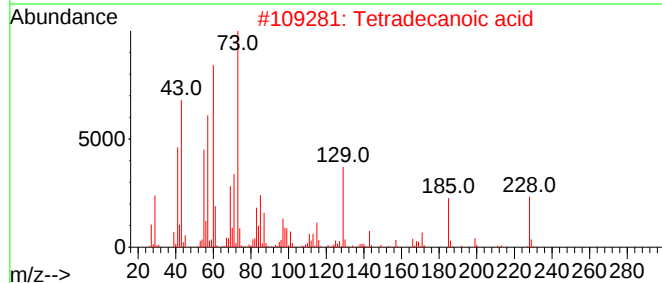
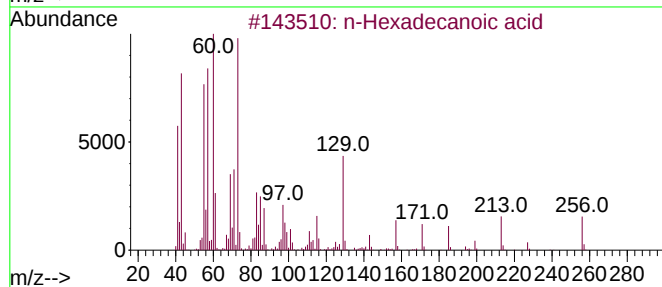
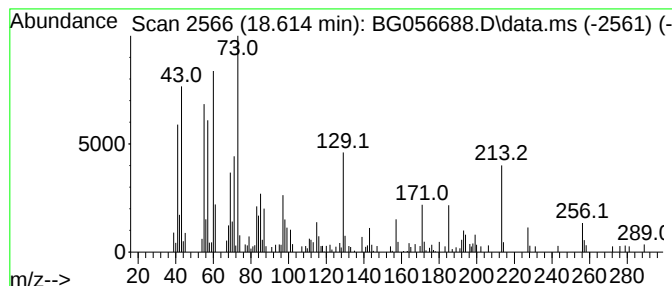
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.614	6.68 ng	99979	Phenanthrene-d10	17.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3			n-Decanoic acid	172	C10H20O2	000334-48-5	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
Data File : BG056688.D
Acq On : 21 Feb 2023 17:32
Operator : CG/JU
Sample : 01552-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

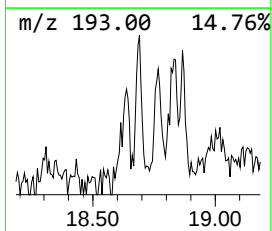
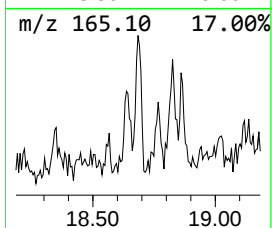
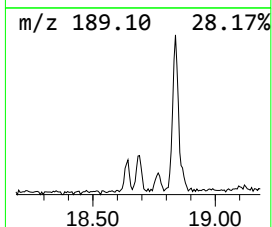
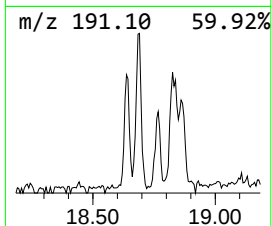
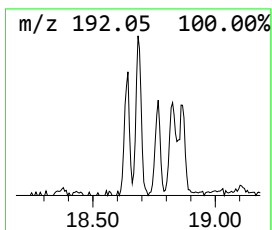
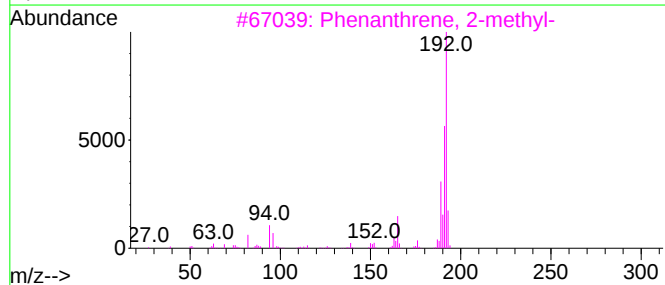
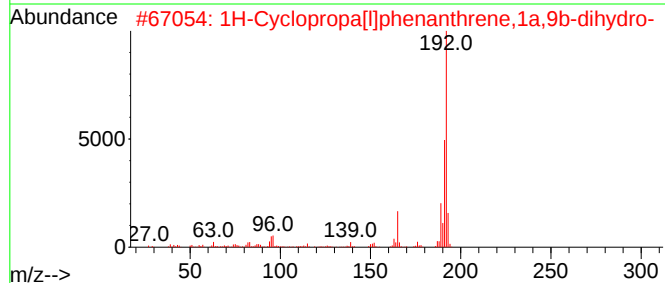
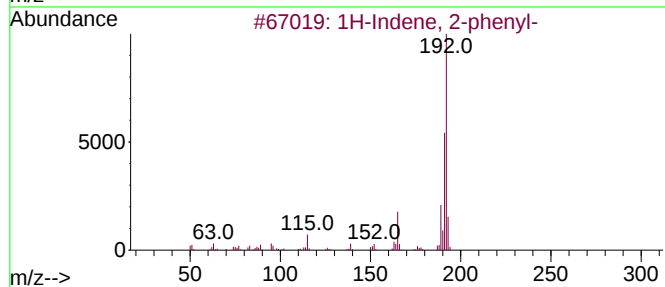
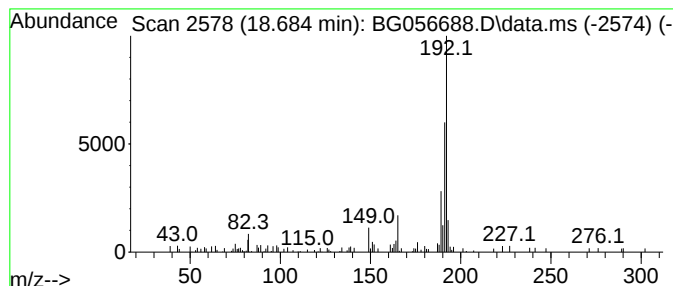
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1H-Indene, 2-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.684	4.64 ng	69488	Phenanthrene-d10	17.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
2		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	90
3		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
Data File : BG056688.D
Acq On : 21 Feb 2023 17:32
Operator : CG/JU
Sample : 01552-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

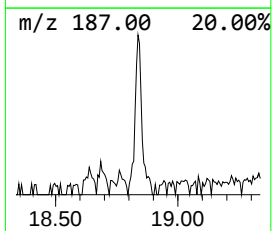
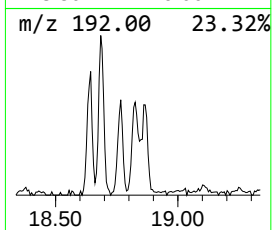
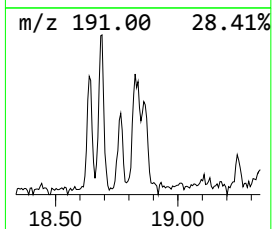
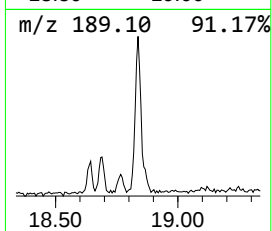
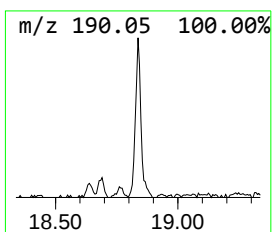
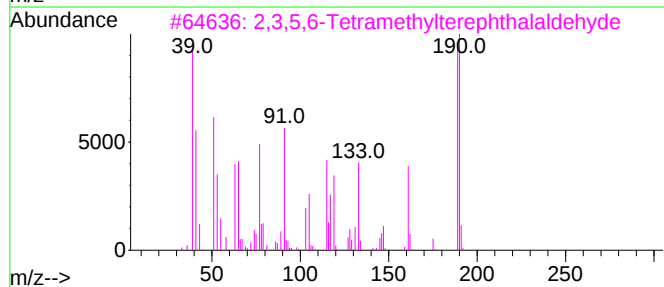
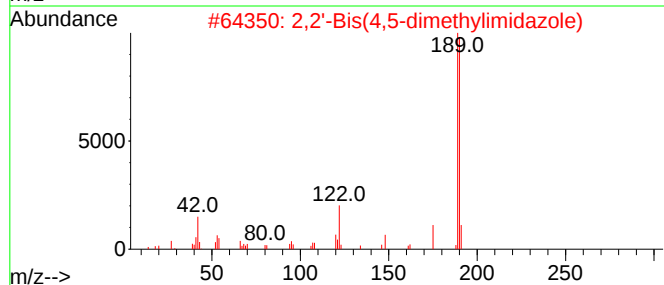
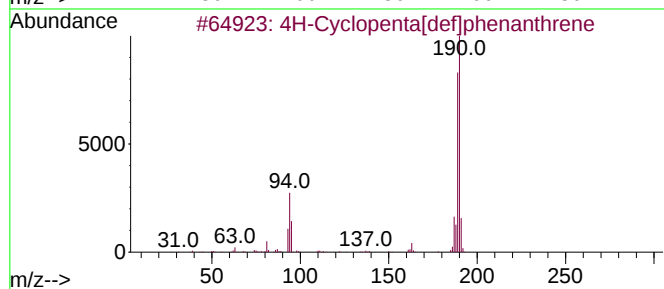
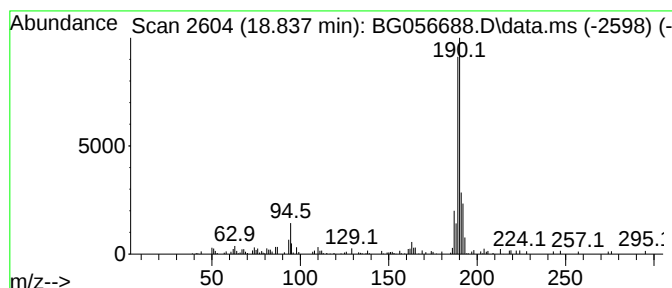
Instrument :
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ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
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 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.837	6.45 ng	96541	Phenanthrene-d10	17.774	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	53
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	Phenol, 4-(2-thienylmethyl)-	190	C11H10O5	091680-55-6	36
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
Data File : BG056688.D
Acq On : 21 Feb 2023 17:32
Operator : CG/JU
Sample : 01552-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

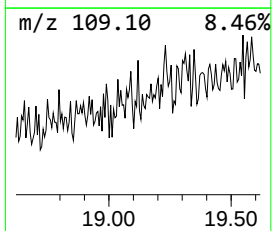
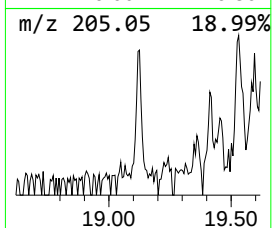
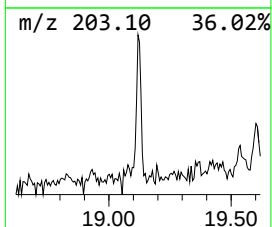
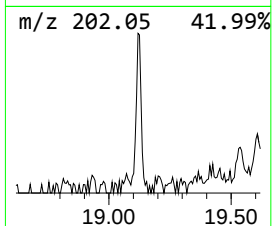
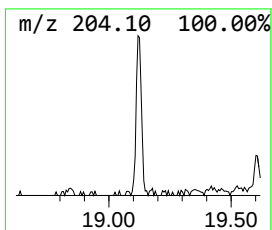
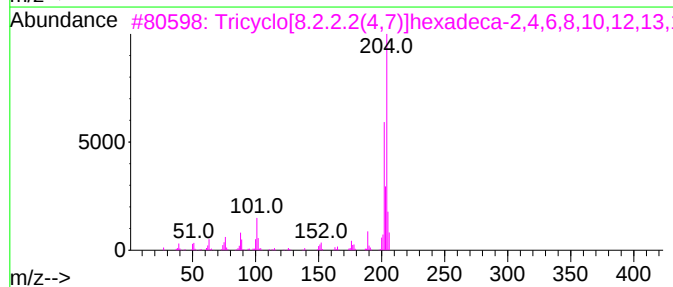
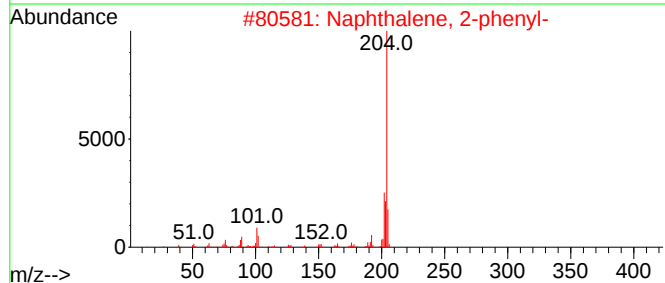
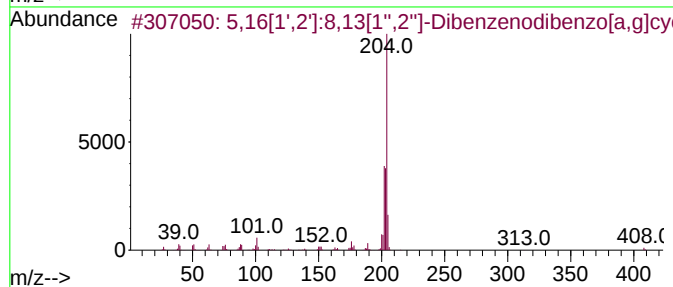
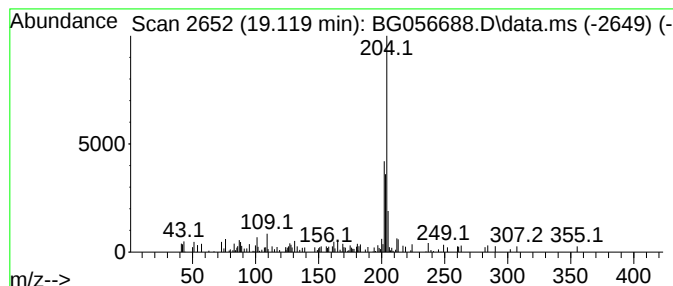
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ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
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 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.119	2.02 ng	30254	Phenanthrene-d10	17.774	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	80
2	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	60
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	53
4	[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	47
5	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
Data File : BG056688.D
Acq On : 21 Feb 2023 17:32
Operator : CG/JU
Sample : 01552-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

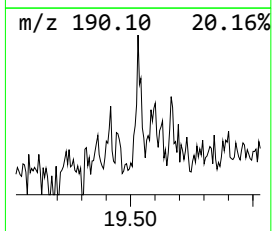
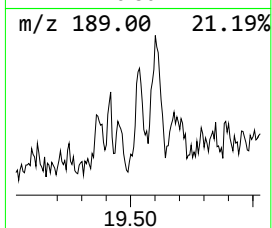
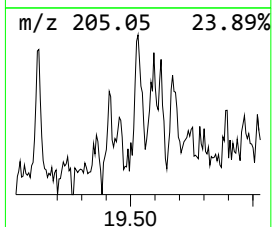
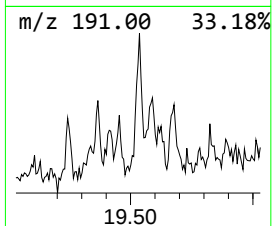
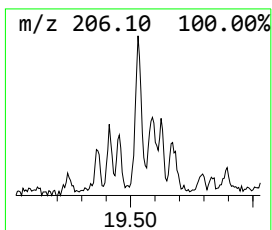
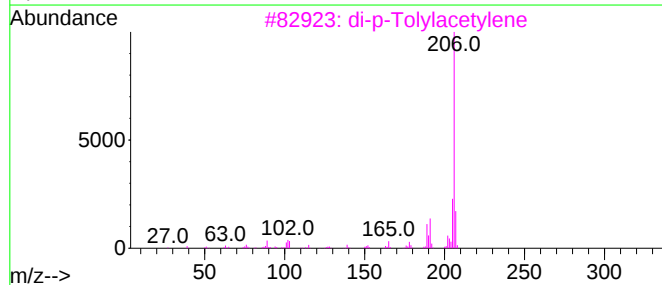
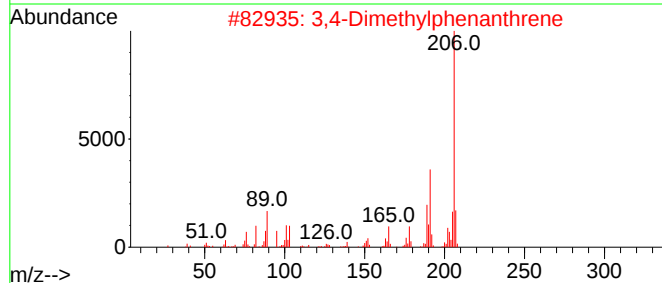
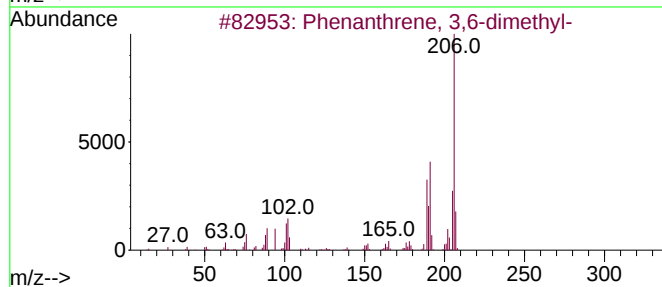
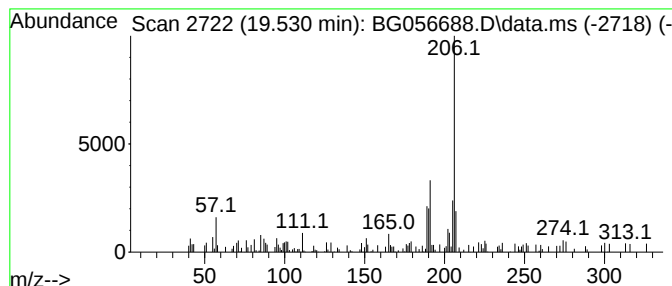
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phenanthrene, 3,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.531	3.19 ng	47729	Phenanthrene-d10		17.774	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-		206	C16H14	001576-67-6	83
2	3,4-Dimethylphenanthrene		206	C16H14	1000452-24-5	81
3	di-p-Tolylacetylene		206	C16H14	002789-88-0	74
4	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	72
5	9,10-Dimethylanthracene		206	C16H14	000781-43-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022123\
Data File : BG056688.D
Acq On : 21 Feb 2023 17:32
Operator : CG/JU
Sample : 01552-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG021523.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
2-Pentanone, 4-...	5.470	36.0	ng	260650	1	8.438	144852	20.0
Benzene, 5-hept...	16.076	2.6	ng	33652	3	15.036	263302	20.0
Benzophenone	16.369	2.8	ng	37441	3	15.036	263302	20.0
5H-Indeno[1,2-b...	18.162	2.9	ng	43151	4	17.774	299206	20.0
n-Hexadecanoic ...	18.614	6.7	ng	99979	4	17.774	299206	20.0
1H-Indene, 2-ph...	18.684	4.6	ng	69488	4	17.774	299206	20.0
4H-Cyclopenta[d...	18.837	6.5	ng	96541	4	17.774	299206	20.0
5,16[1',2']:8,1...	19.119	2.0	ng	30254	4	17.774	299206	20.0
Phenanthrene, 3...	19.531	3.2	ng	47729	4	17.774	299206	20.0