

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
 Data File : BG060731.D
 Acq On : 2 Apr 2024 1:43
 Operator : MA/JU
 Sample : P1879-13 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HS-01(0-6)

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.106	14	20	28	rBV2	27334	65110	3.64%	0.380%
2	3.182	28	33	42	rVB	78830	141004	7.89%	0.824%
3	3.693	115	120	130	rVB	18153	38031	2.13%	0.222%
4	5.544	427	435	445	rBV	455398	760872	42.58%	4.446%
5	7.119	694	703	712	rBV	548531	944819	52.87%	5.521%
6	7.959	838	846	854	rVB	327616	570139	31.90%	3.332%
7	9.110	1032	1042	1050	rBV	318988	550999	30.83%	3.220%
8	10.755	1315	1322	1329	rBV	473902	855637	47.88%	5.000%
9	10.802	1329	1330	1340	rVB	22232	33222	1.86%	0.194%
10	11.496	1443	1448	1455	rVB2	16665	31872	1.78%	0.186%
11	12.418	1598	1605	1611	rBV2	21119	40644	2.27%	0.238%
12	12.630	1637	1641	1646	rVB2	18353	27755	1.55%	0.162%
13	13.211	1733	1740	1748	rVB	849573	1309130	73.25%	7.650%
14	13.775	1827	1836	1841	rVB7	10296	24028	1.34%	0.140%
15	13.916	1853	1860	1865	rBV3	20541	40003	2.24%	0.234%
16	14.146	1894	1899	1903	rBV5	13818	20806	1.16%	0.122%
17	14.310	1921	1927	1933	rBV2	34189	64063	3.58%	0.374%
18	14.586	1964	1974	1981	rBV	690258	1101638	61.64%	6.438%
19	14.998	2039	2044	2050	rVV8	13747	25824	1.45%	0.151%
20	15.068	2051	2056	2061	rVB4	14123	21543	1.21%	0.126%
21	15.632	2148	2152	2159	rBV	32095	48506	2.71%	0.283%
22	16.073	2220	2227	2236	rBV	617856	935879	52.37%	5.469%
23	16.320	2264	2269	2280	rVB	13304	34246	1.92%	0.200%
24	16.637	2321	2323	2329	rVB6	16050	19962	1.12%	0.117%
25	16.983	2378	2382	2389	rVB2	22417	42547	2.38%	0.249%
26	17.154	2407	2411	2419	rVB	40651	72990	4.08%	0.427%
27	17.336	2436	2442	2446	rBV	825030	1276064	71.40%	7.457%
28	17.377	2446	2449	2455	rVB	482988	641859	35.92%	3.751%
29	17.465	2460	2464	2470	rVB	49320	74431	4.16%	0.435%
30	17.859	2529	2531	2535	rVB2	24507	25622	1.43%	0.150%
31	17.918	2537	2541	2545	rVB2	39773	60610	3.39%	0.354%
32	18.211	2586	2591	2594	rBV	149496	233389	13.06%	1.364%
33	18.264	2594	2600	2607	rVB2	190558	382165	21.38%	2.233%
34	18.405	2619	2624	2627	rBV2	151079	253431	14.18%	1.481%
35	18.441	2628	2630	2638	rVB	107312	149694	8.38%	0.875%
36	18.711	2673	2676	2680	rBV	67179	107397	6.01%	0.628%

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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	19.011	2724	2727	2730	rBV	60603	71891	4.02%	0.420%
38	19.134	2743	2748	2752	rBV	132346	210910	11.80%	1.232%
39	19.263	2767	2770	2778	rBV4	71318	134264	7.51%	0.785%
40	19.387	2787	2791	2797	rBV	507898	710841	39.78%	4.154%
41	19.751	2848	2853	2862	rVB	738596	1104142	61.78%	6.452%
42	19.956	2884	2888	2903	rVB	1301812	1787089	100.00%	10.443%
43	20.403	2961	2964	2969	rBV	153094	195148	10.92%	1.140%
44	20.538	2985	2987	2991	rBV	111462	132832	7.43%	0.776%
45	21.596	3161	3167	3172	rBV2	785189	1739393	97.33%	10.164%

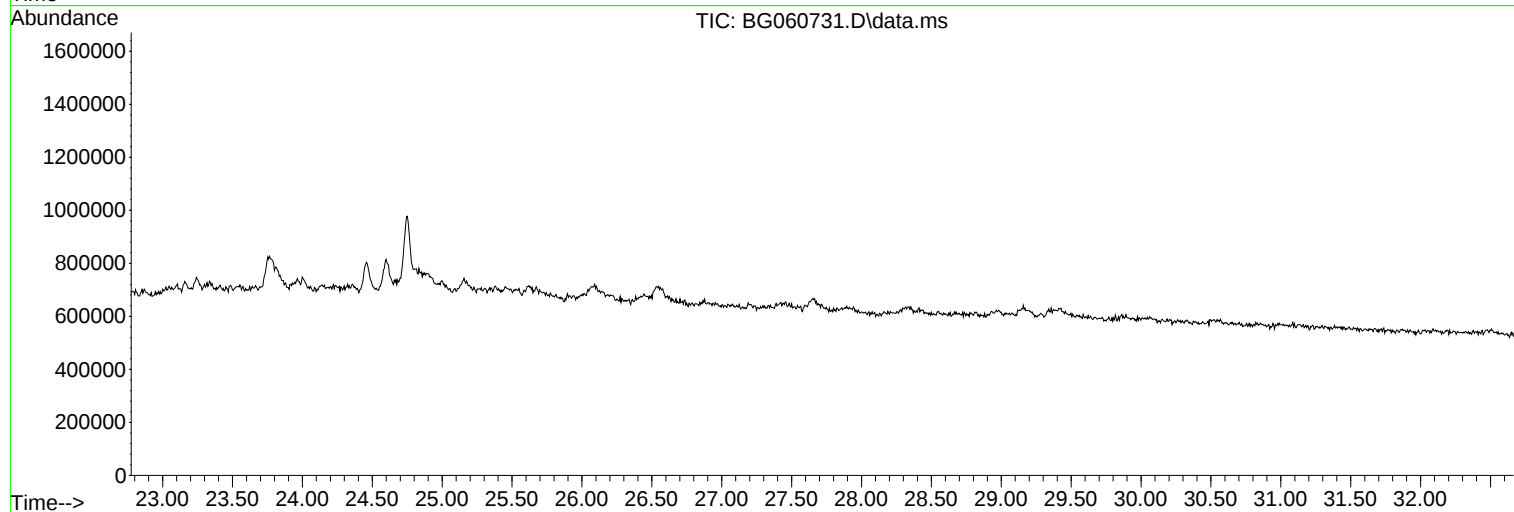
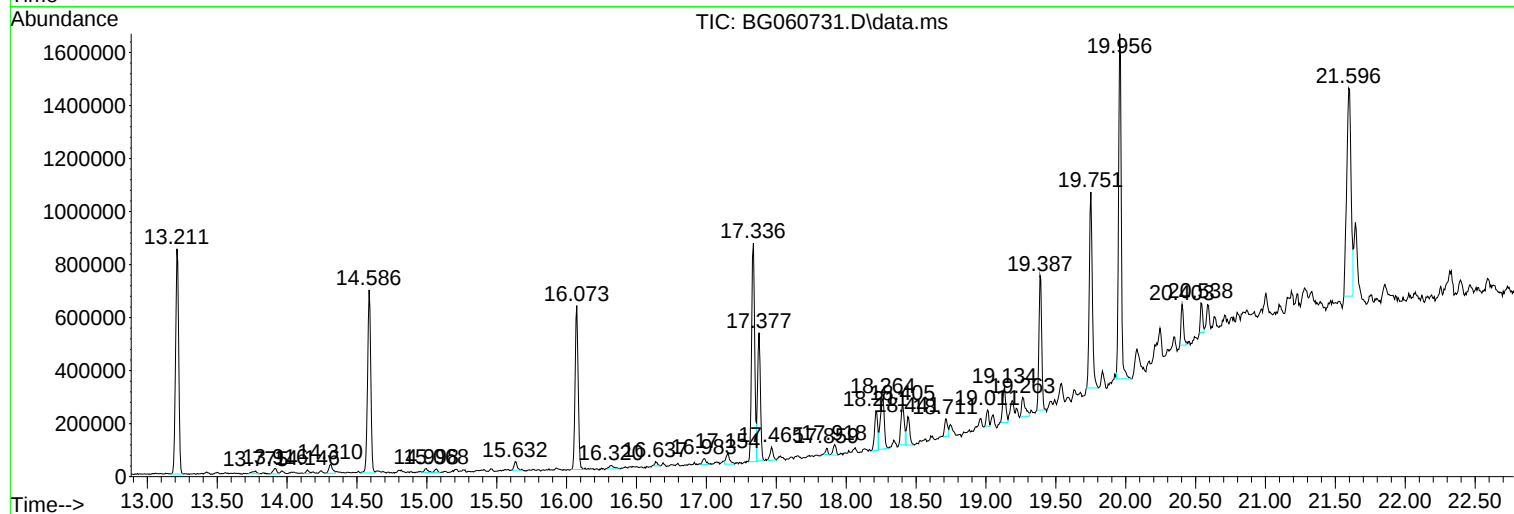
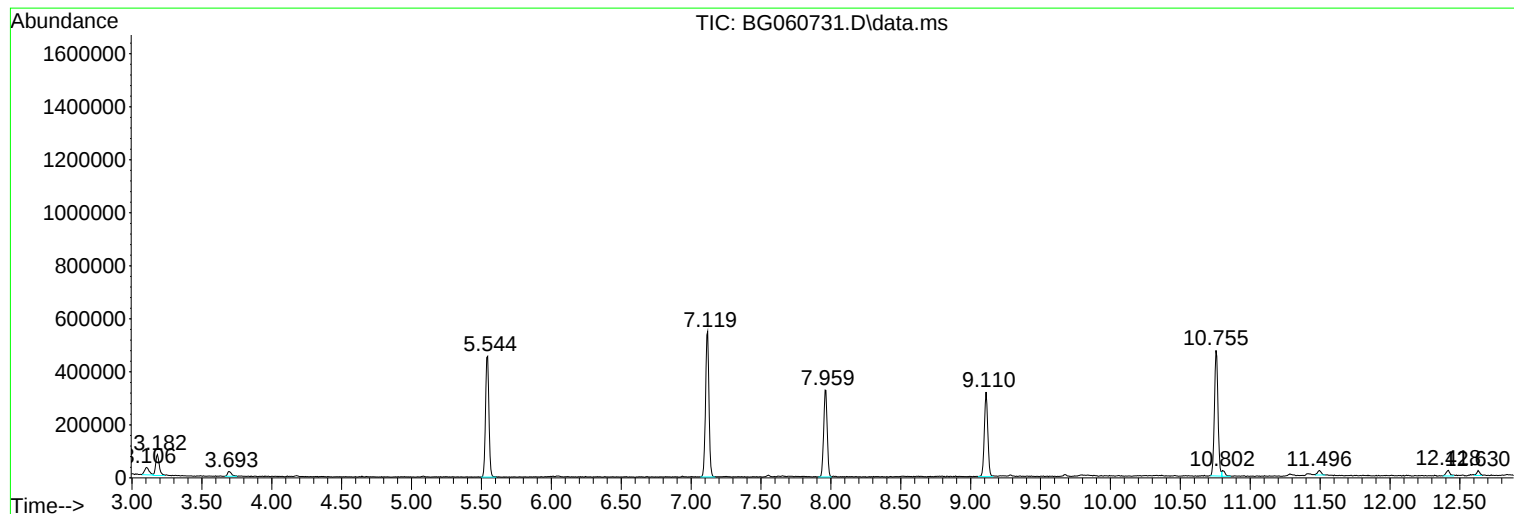
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HS-01(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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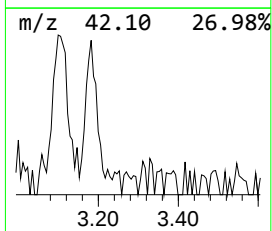
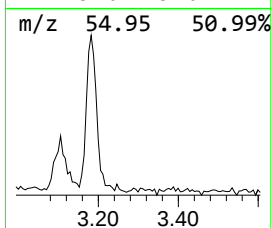
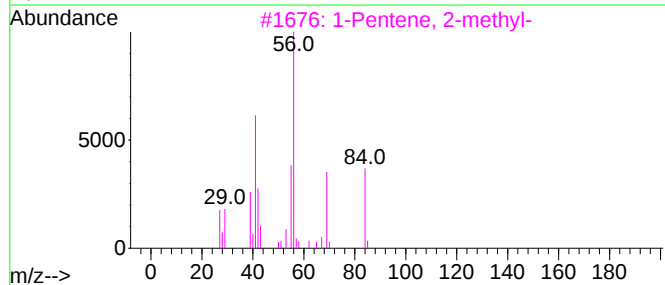
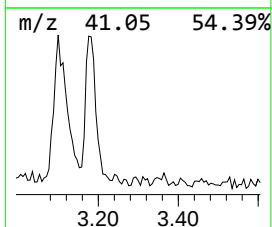
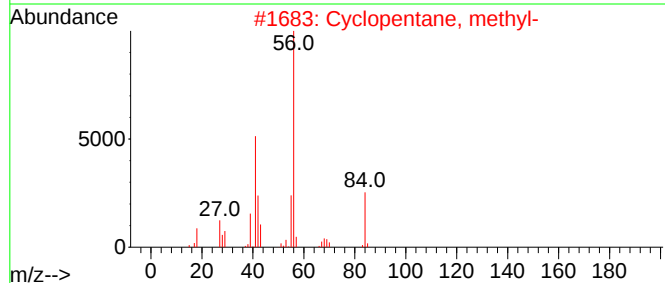
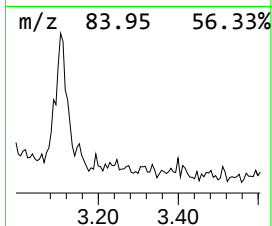
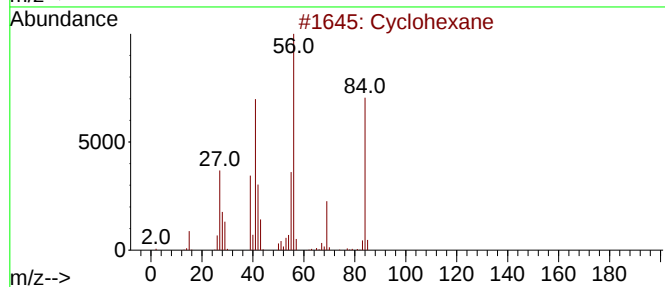
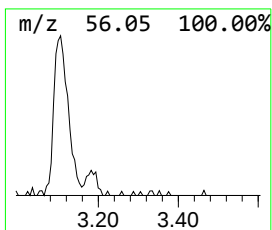
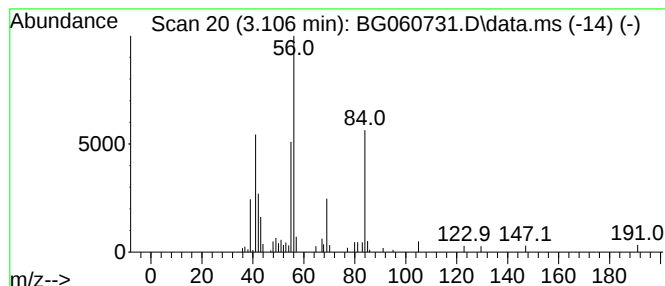
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.106	2.28 ng	65110	1,4-Dichlorobenzene-d4	7.959

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	87
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	50
5			Cyclopentanone	84	C5H8O	000120-92-3	47



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BNA_G
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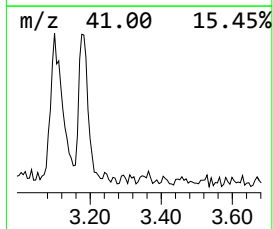
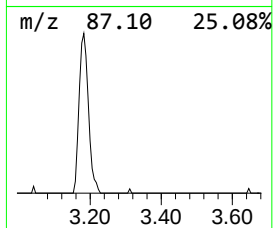
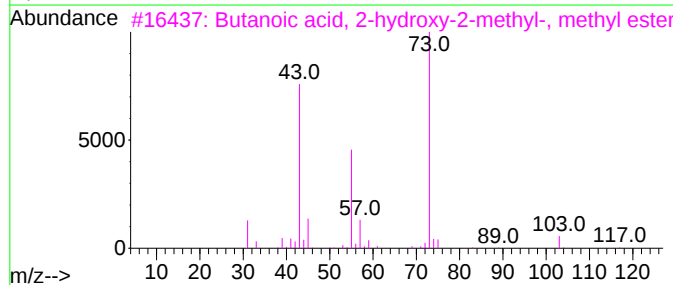
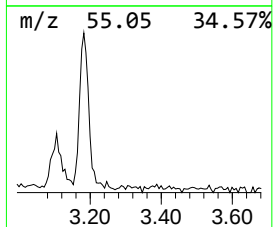
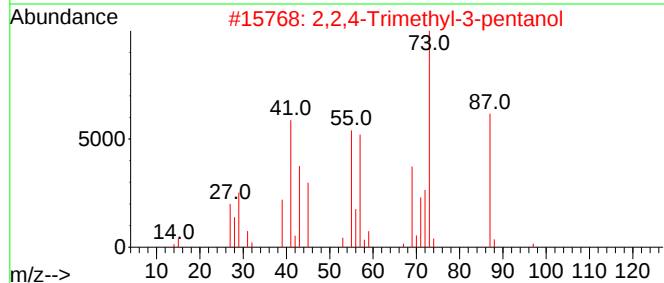
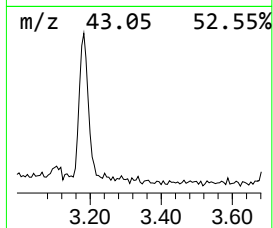
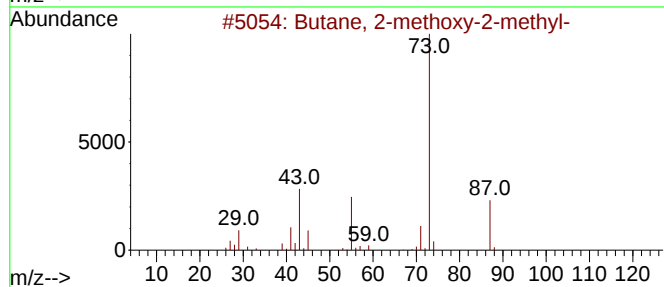
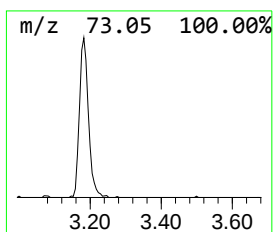
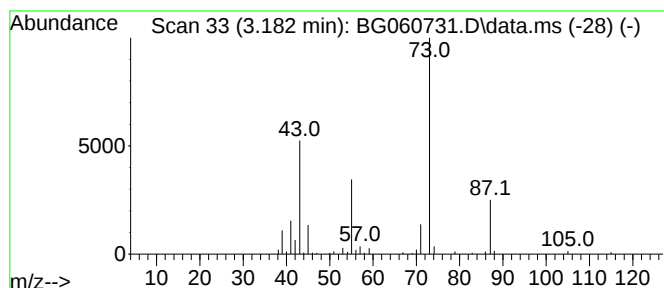
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.182	4.95 ng	141004	1,4-Dichlorobenzene-d4	7.959

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	32
4			4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	25
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25



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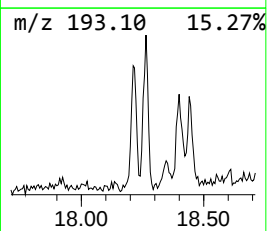
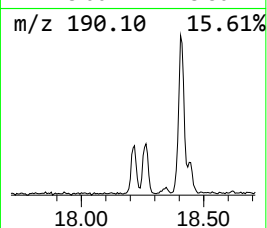
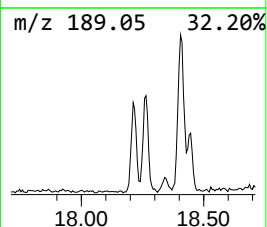
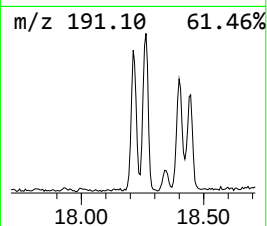
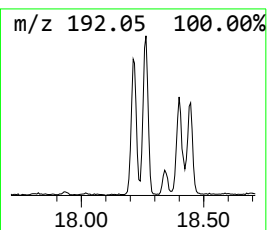
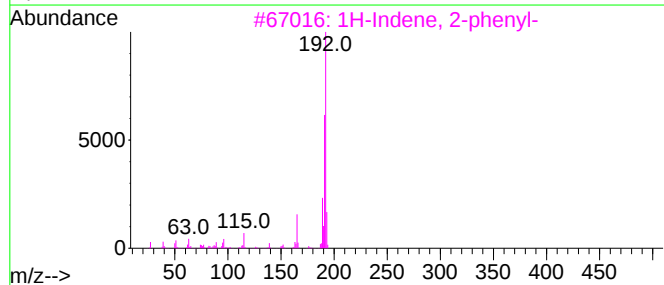
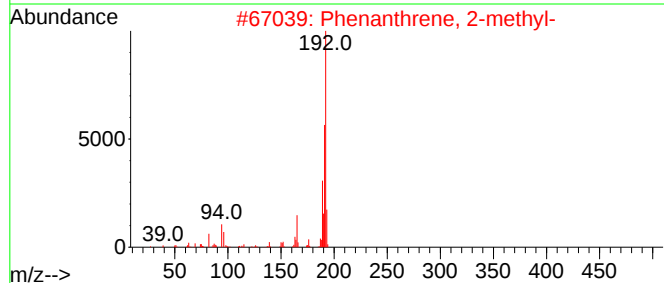
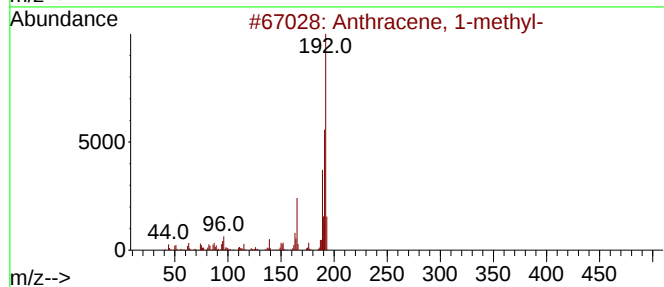
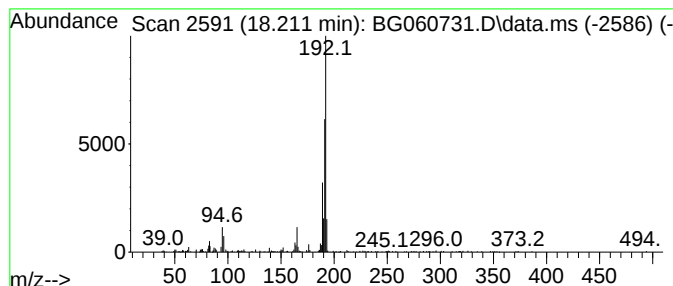
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	3.66 ng	233389	Phenanthrene-d10	17.336

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	90



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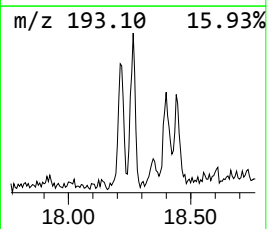
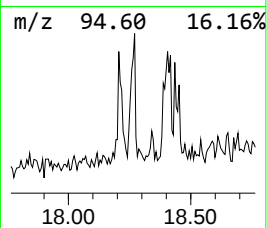
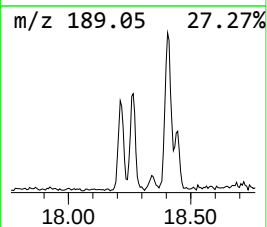
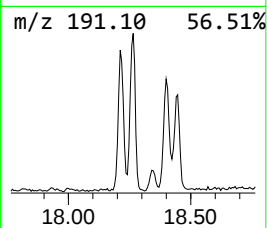
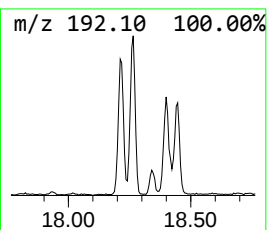
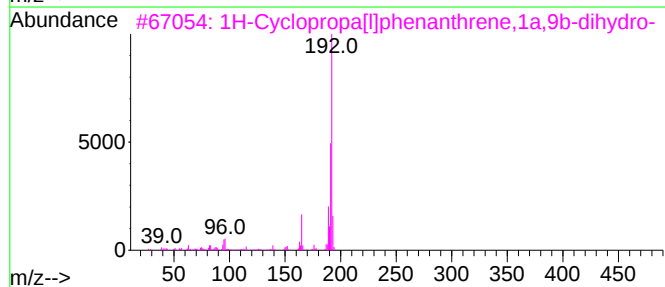
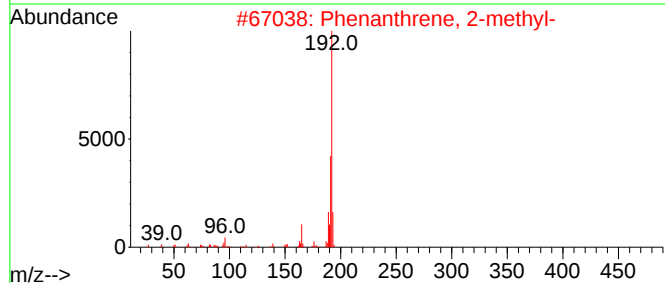
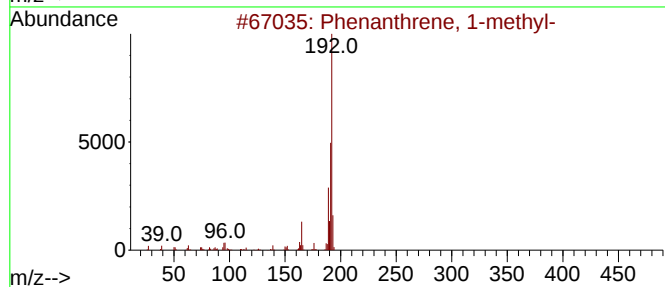
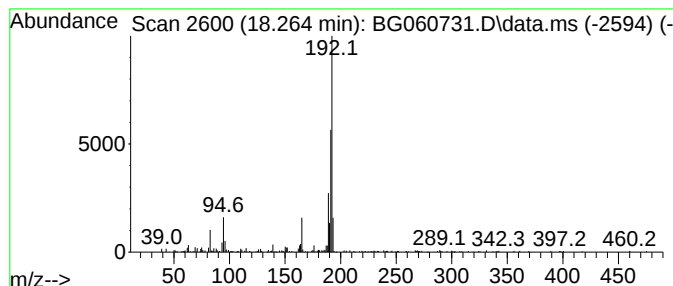
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.264	5.99 ng	382165	Phenanthrene-d10	17.336

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			1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	90



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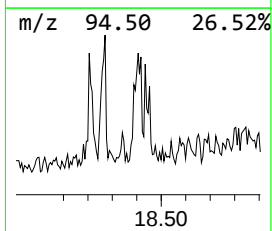
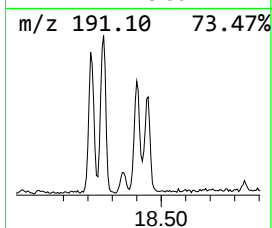
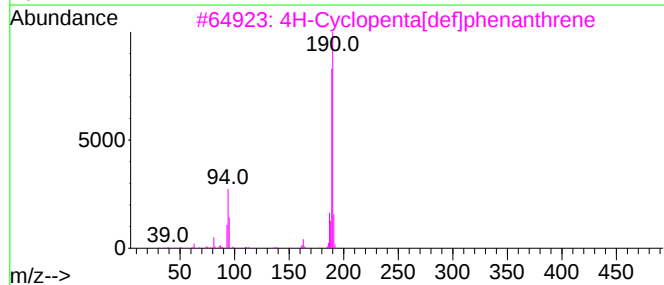
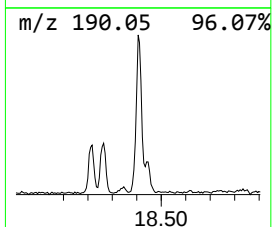
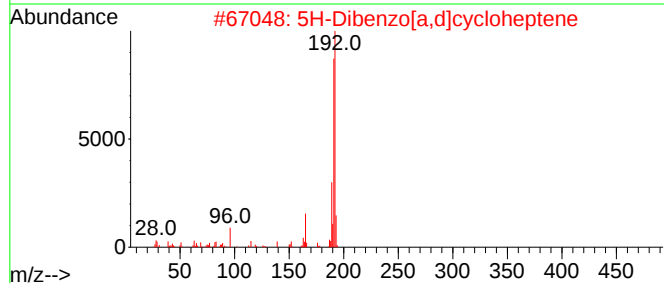
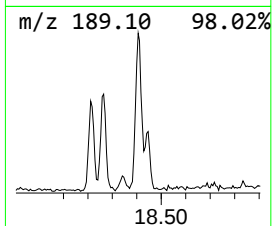
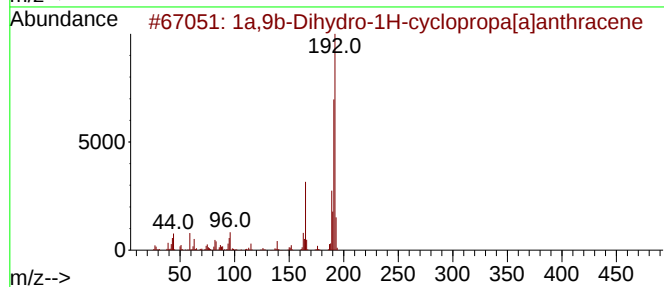
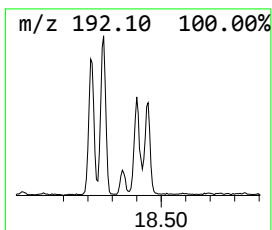
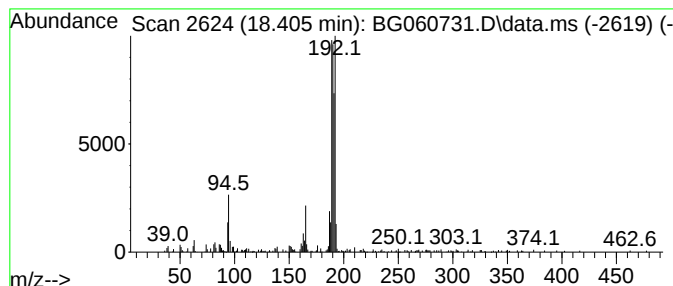
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown18.405 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.405	3.97 ng	253431	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	46		
2	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	46		
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	43		
4	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	43		
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	41		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060731.D
Acq On : 2 Apr 2024 1:43
Operator : MA/JU
Sample : P1879-13 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HS-01(0-6)

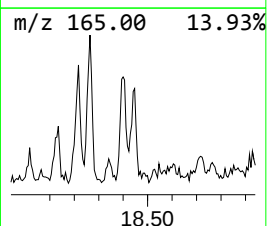
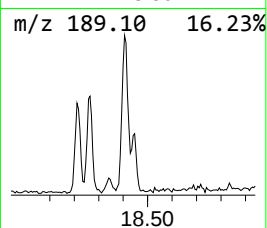
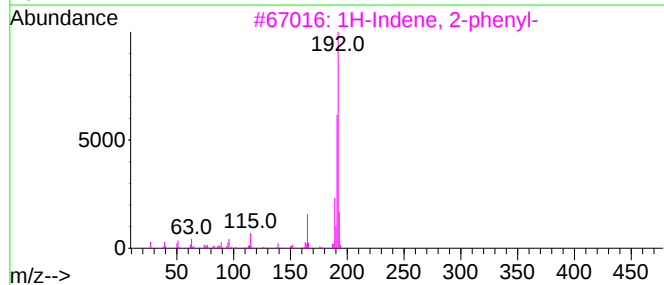
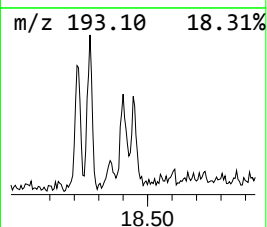
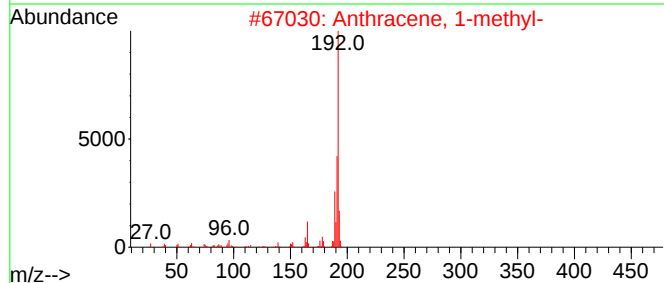
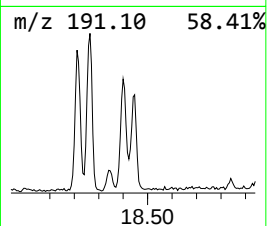
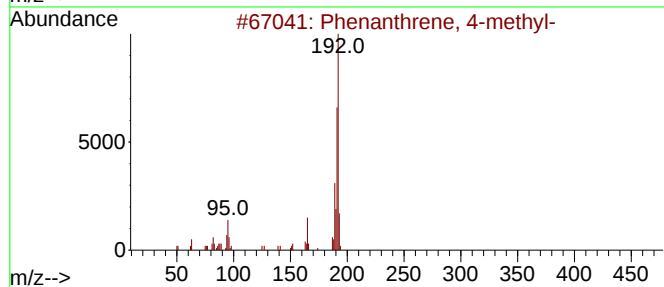
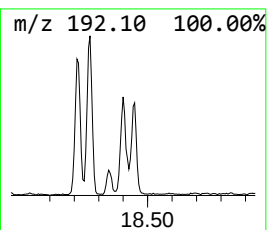
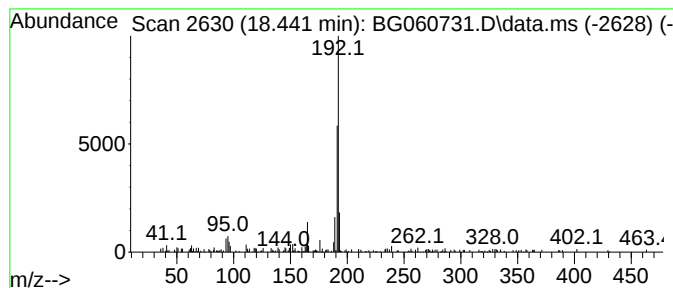
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.441	2.35 ng	149694	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
3			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	87
4			1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	87
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060731.D
Acq On : 2 Apr 2024 1:43
Operator : MA/JU
Sample : P1879-13 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HS-01(0-6)

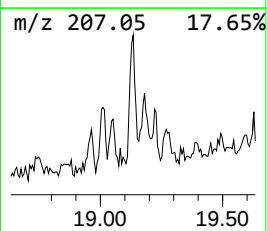
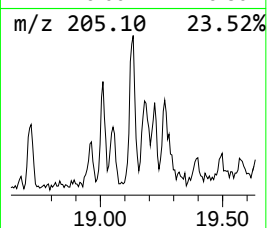
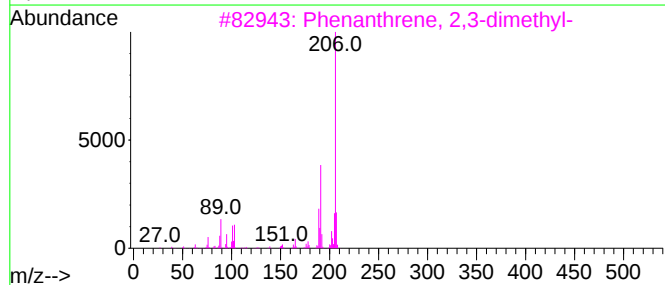
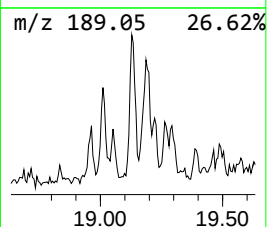
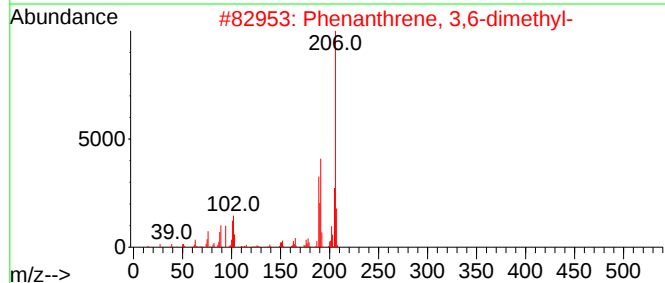
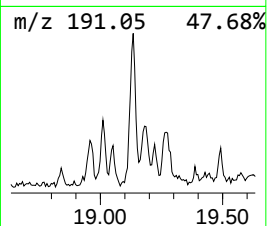
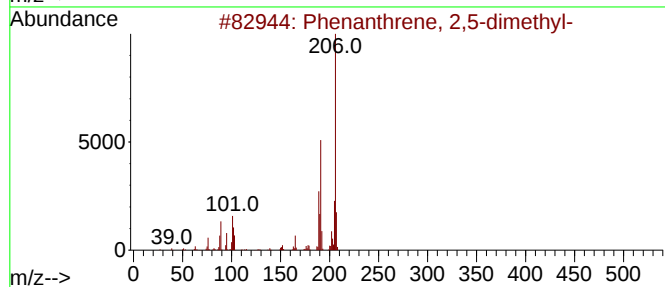
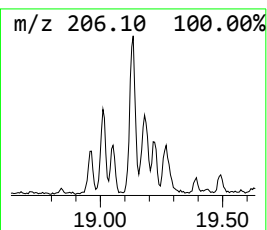
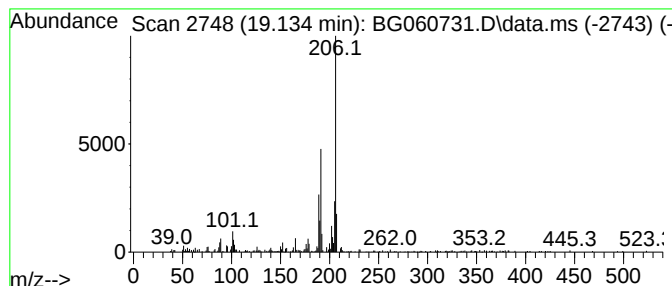
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.134	3.31 ng	210910	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
2			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
3			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
4			9,10-Dimethylantracene	206	C16H14	000781-43-1	93
5			di-p-Tolylacetylene	206	C16H14	002789-88-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060731.D
Acq On : 2 Apr 2024 1:43
Operator : MA/JU
Sample : P1879-13 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HS-01(0-6)

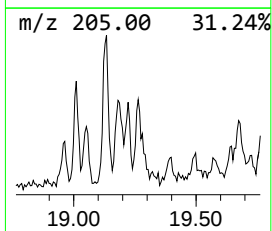
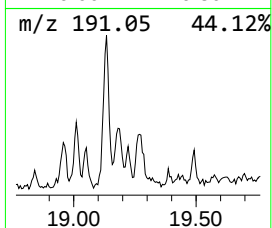
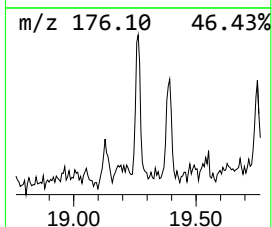
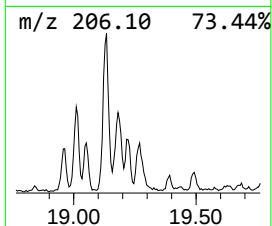
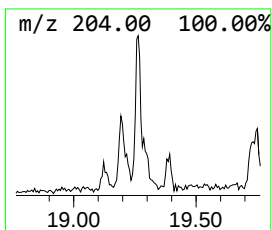
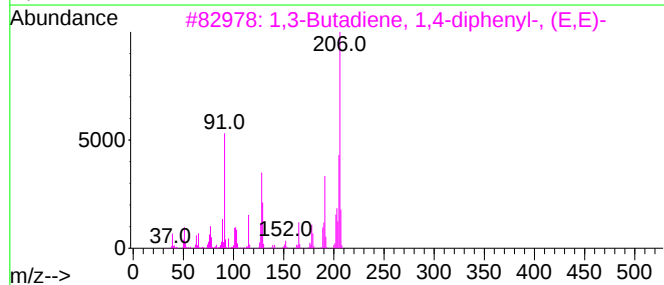
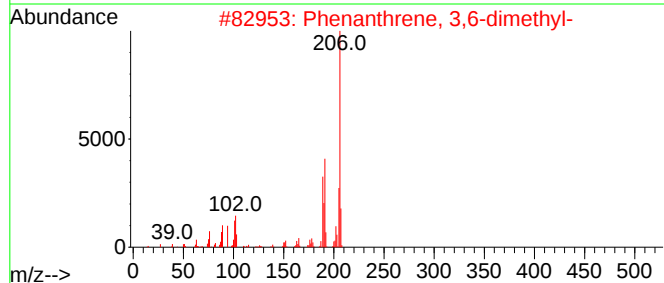
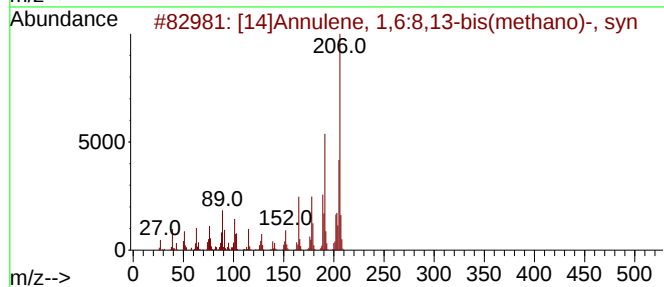
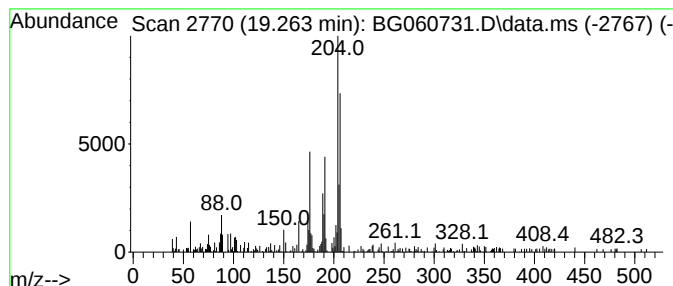
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 [14]Annulene, 1,6:8,13-bis(...) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.263	2.10 ng	134264	Phenanthrene-d10	17.336

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	64
2		Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	50
3		1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	46
4		Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	46
5		1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060731.D
Acq On : 2 Apr 2024 1:43
Operator : MA/JU
Sample : P1879-13 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HS-01(0-6)

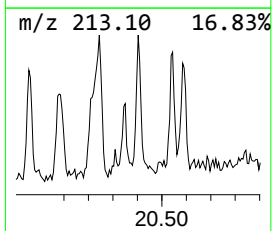
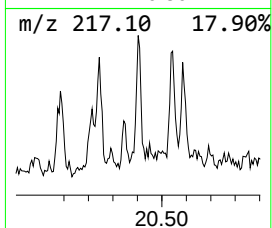
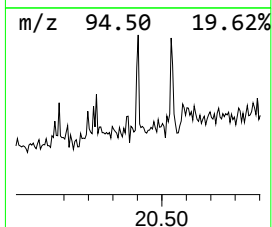
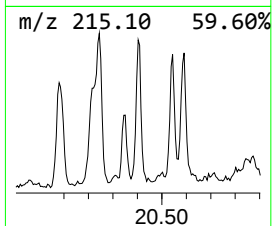
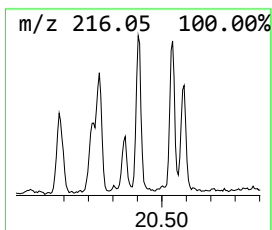
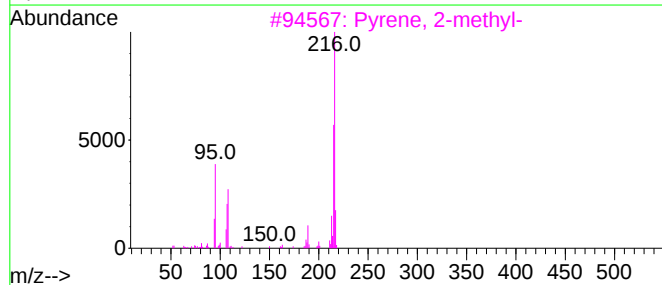
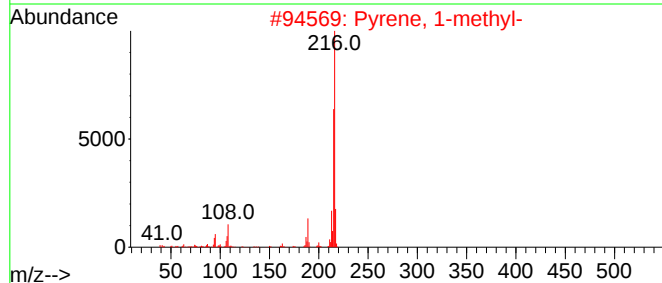
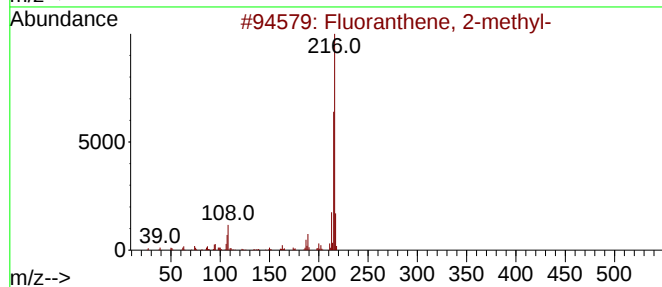
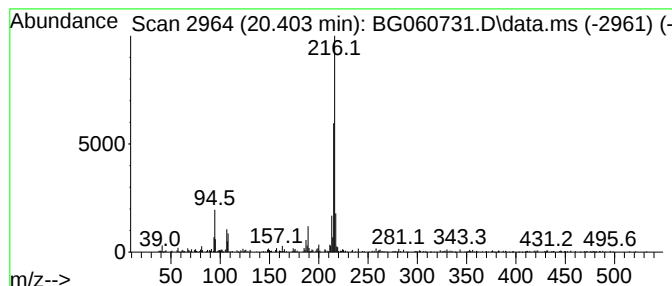
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Fluoranthene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.403	2.24 ng	195148	Chrysene-d12	21.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	96
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	96
4			Pyrene, 4-methyl-	216	C17H12	003353-12-6	93
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
Data File : BG060731.D
Acq On : 2 Apr 2024 1:43
Operator : MA/JU
Sample : P1879-13 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HS-01(0-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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
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Butane, 2-metho...	3.182	5.0	ng	141004	1	7.959	570139	20.0
Anthracene, 1-m...	18.211	3.7	ng	233389	4	17.336	1276060	20.0
Phenanthrene, 1...	18.264	6.0	ng	382165	4	17.336	1276060	20.0
unknown18.405	18.405	4.0	ng	253431	4	17.336	1276060	20.0
Phenanthrene, 4...	18.441	2.4	ng	149694	4	17.336	1276060	20.0
Phenanthrene, 2...	19.134	3.3	ng	210910	4	17.336	1276060	20.0
[14]Annulene, 1...	19.263	2.1	ng	134264	4	17.336	1276060	20.0
Fluoranthene, 2...	20.403	2.2	ng	195148	5	21.602	1739390	20.0