

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
 Data File : BP009620.D
 Acq On : 30 Mar 2022 15:59
 Operator : CG/JU
 Sample : N2150-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 337

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_P\Methods\8270E-BP031722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.223	38	40	58	rVB	33657	112164	1.34%	0.124%
2	4.875	316	321	329	rVB	57625	95722	1.14%	0.106%
3	5.346	393	401	417	rBV	2544619	4314872	51.52%	4.758%
4	6.928	659	670	692	rBV	2485265	4585755	54.76%	5.056%
5	7.734	800	807	816	rBV	699038	1201472	14.35%	1.325%
6	8.893	990	1004	1022	rBV	1747428	3294333	39.34%	3.632%
7	10.528	1274	1282	1297	rBV	930266	1723110	20.58%	1.900%
8	13.004	1695	1703	1718	rBV	3780307	5893052	70.37%	6.498%
9	14.104	1884	1890	1899	rVB	120125	209351	2.50%	0.231%
10	14.387	1931	1938	1945	rBV	1273621	2020790	24.13%	2.228%
11	14.451	1945	1949	1958	rVB	53803	91316	1.09%	0.101%
12	15.440	2113	2117	2129	rVB	76412	137171	1.64%	0.151%
13	15.669	2149	2156	2163	rBV2	36969	116678	1.39%	0.129%
14	15.887	2183	2193	2202	rBV	3223610	4988411	59.57%	5.500%
15	16.557	2302	2307	2316	rBV5	93801	222240	2.65%	0.245%
16	16.704	2328	2332	2340	rVB4	36068	87738	1.05%	0.097%
17	17.151	2401	2408	2412	rBV	1596816	2440982	29.15%	2.692%
18	17.192	2412	2415	2423	rVV	859391	1208216	14.43%	1.332%
19	17.287	2423	2431	2436	rVB	225971	371718	4.44%	0.410%
20	17.563	2471	2478	2489	rBV2	97180	240612	2.87%	0.265%
21	18.028	2552	2557	2559	rBV	142841	203003	2.42%	0.224%
22	18.063	2559	2563	2571	rVB2	544897	918070	10.96%	1.012%
23	18.151	2575	2578	2582	rVB	85759	114792	1.37%	0.127%
24	18.216	2583	2589	2593	rBV2	342397	571032	6.82%	0.630%
25	18.328	2603	2608	2612	rBV2	191605	327152	3.91%	0.361%
26	18.375	2612	2616	2629	rVB4	274957	577088	6.89%	0.636%
27	18.516	2636	2640	2643	rBV	158209	190588	2.28%	0.210%
28	18.557	2643	2647	2652	rVB	152576	210704	2.52%	0.232%
29	18.804	2685	2689	2692	rBV2	71846	96147	1.15%	0.106%
30	18.898	2700	2705	2714	rBV2	351173	859428	10.26%	0.948%
31	19.057	2728	2732	2739	rBV	252308	424176	5.07%	0.468%
32	19.175	2747	2752	2759	rVB	3406793	4766471	56.92%	5.256%
33	19.275	2766	2769	2771	rBV	71986	89663	1.07%	0.099%
34	19.304	2771	2774	2781	rVB2	127767	251973	3.01%	0.278%
35	19.416	2790	2793	2796	rBV	93806	104623	1.25%	0.115%
36	19.534	2803	2813	2821	rVB	2912707	5279979	63.05%	5.822%

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Peak Location: TOP

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37	19.604	2821	2825	2831	rVB2	154766	265639	3.17%	0.293%
38	19.733	2839	2847	2852	rBV	6455496	8374629	100.00%	9.234%
39	19.857	2862	2868	2874	rBV3	217160	540592	6.46%	0.596%
40	20.022	2885	2896	2902	rBV	613844	1349738	16.12%	1.488%
41	20.116	2908	2912	2916	rBV	607239	845161	10.09%	0.932%
42	20.175	2917	2922	2925	rVV2	341252	556444	6.64%	0.614%
43	20.310	2942	2945	2949	rBV	291017	426143	5.09%	0.470%
44	20.357	2950	2953	2957	rVB2	212054	290934	3.47%	0.321%
45	20.757	3018	3021	3028	rVB	302610	443739	5.30%	0.489%
46	20.916	3045	3048	3052	rBV2	338722	421501	5.03%	0.465%
47	20.957	3052	3055	3057	rVV	239691	274362	3.28%	0.303%
48	20.992	3057	3061	3067	rVB2	934883	1428901	17.06%	1.576%
49	21.263	3101	3107	3111	rBV2	3158961	6561285	78.35%	7.235%
50	21.304	3111	3114	3123	rVB	2639692	3339348	39.87%	3.682%
51	21.386	3123	3128	3133	rBV	5133425	7343241	87.68%	8.097%
52	22.927	3384	3390	3394	rBV	1528052	3265724	39.00%	3.601%
53	23.439	3472	3477	3485	rVB	742502	1530760	18.28%	1.688%
54	23.539	3489	3494	3501	rBV	856985	1704796	20.36%	1.880%
55	23.645	3506	3512	3519	rBV2	1624780	3387775	40.45%	3.736%

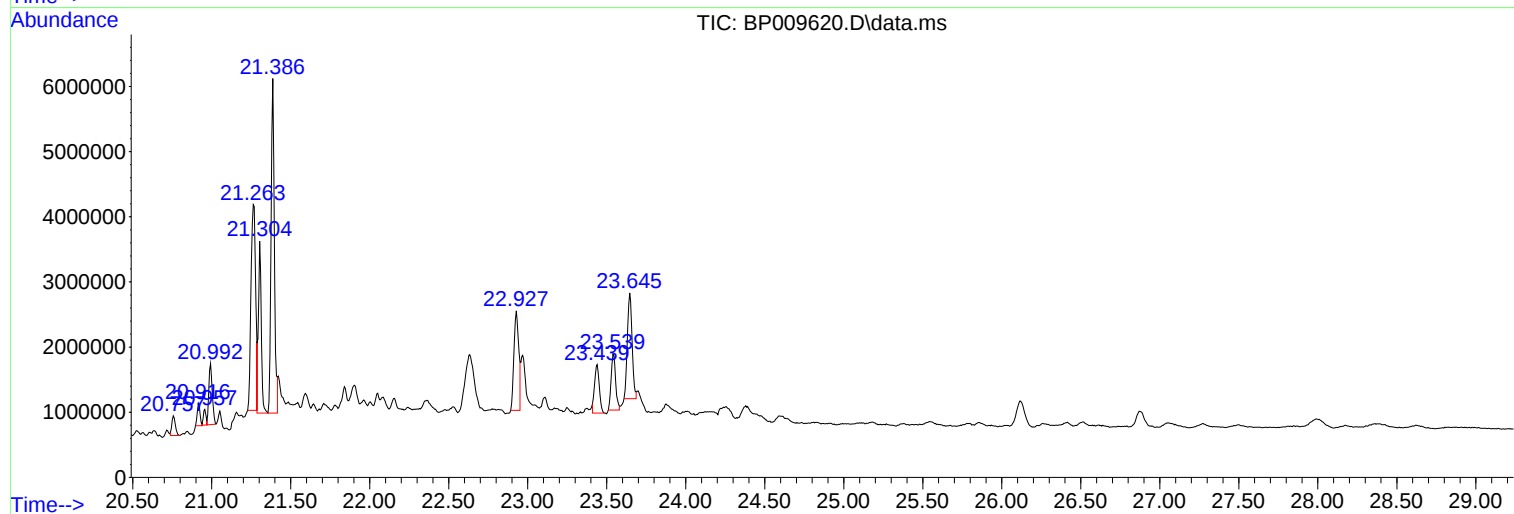
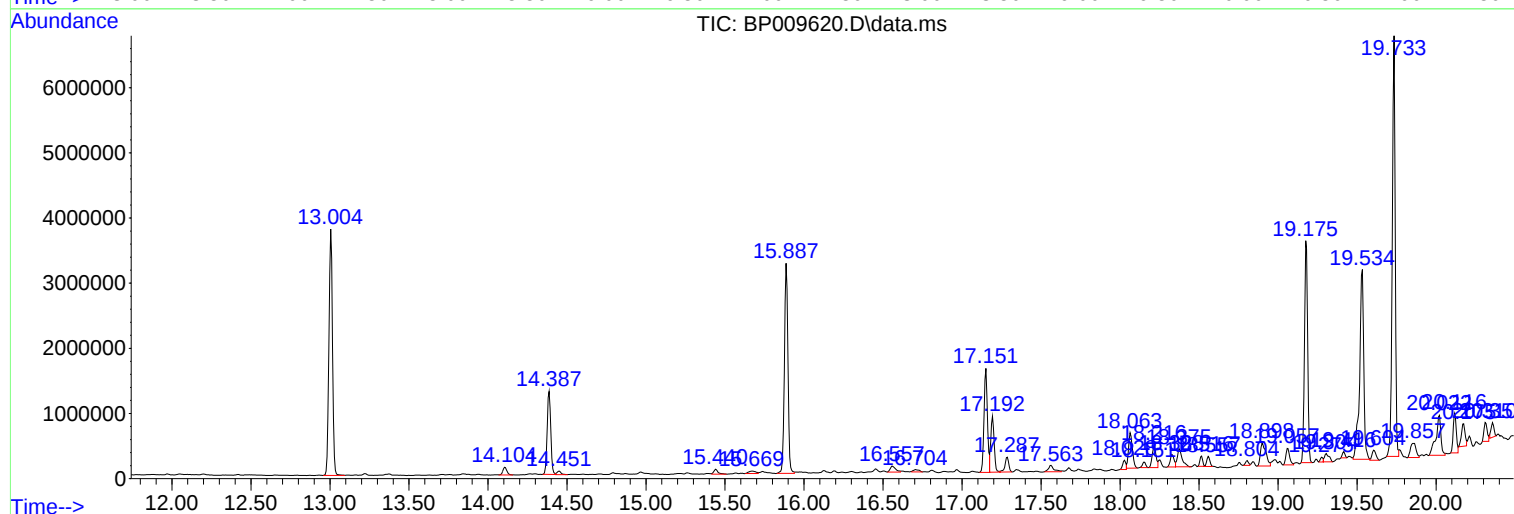
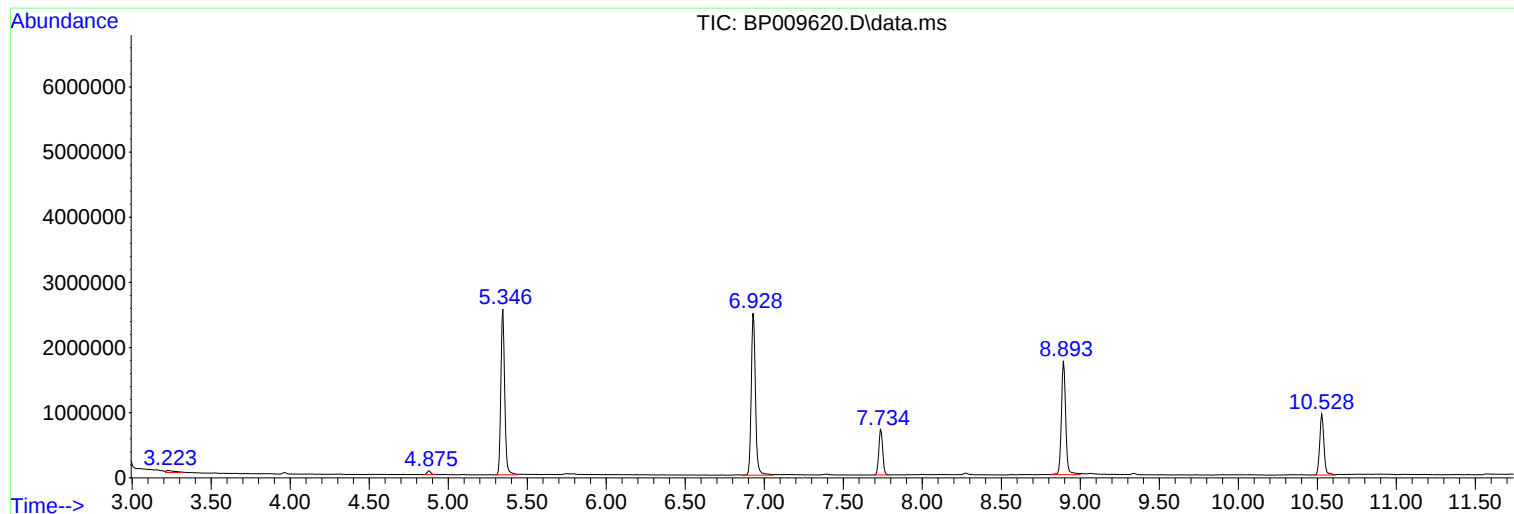
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 5 Sample Multiplier: 1

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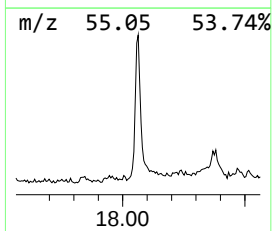
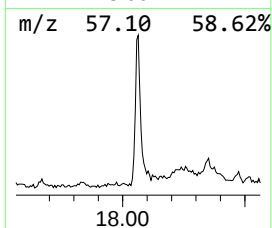
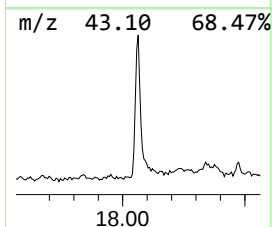
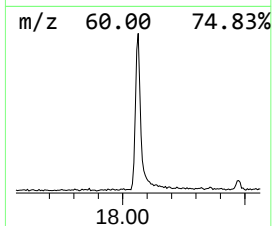
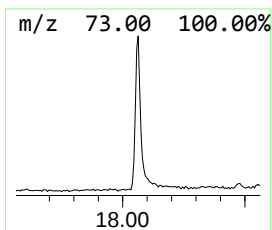
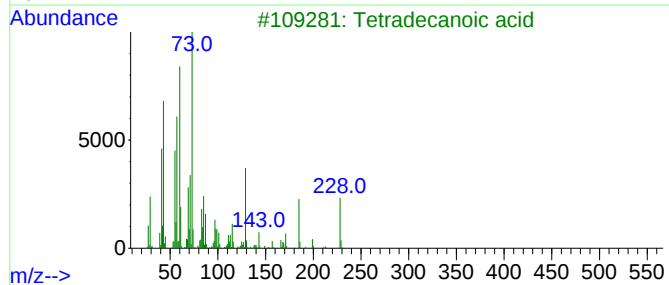
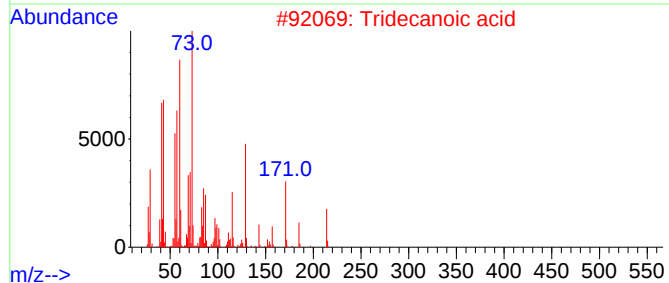
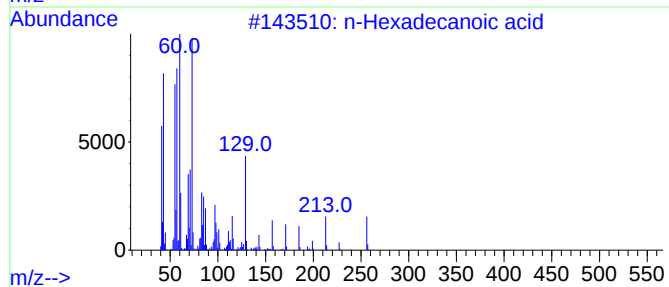
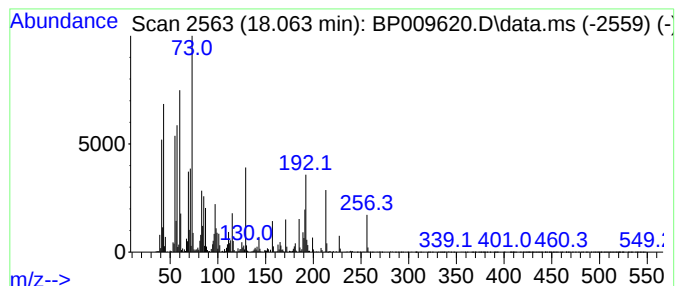
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	7.52 ng	918070	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



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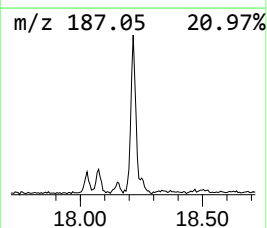
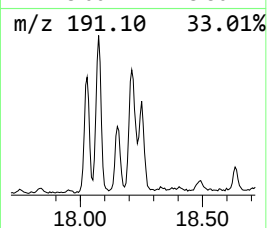
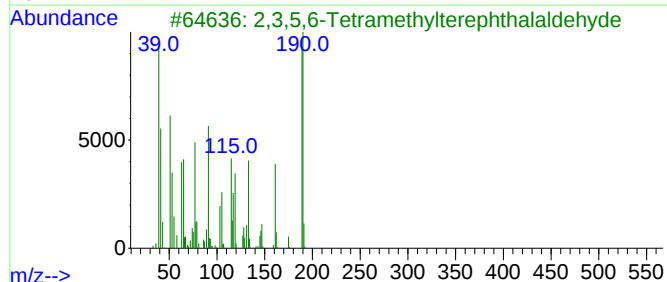
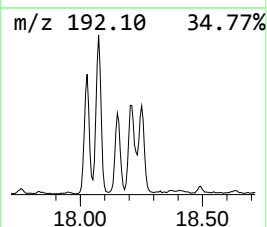
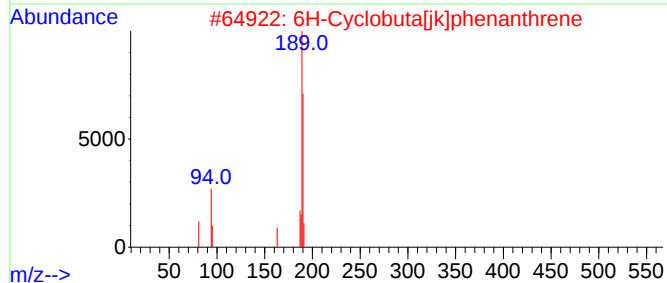
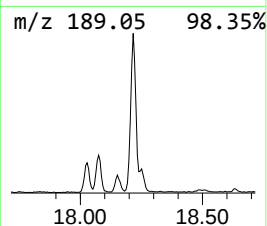
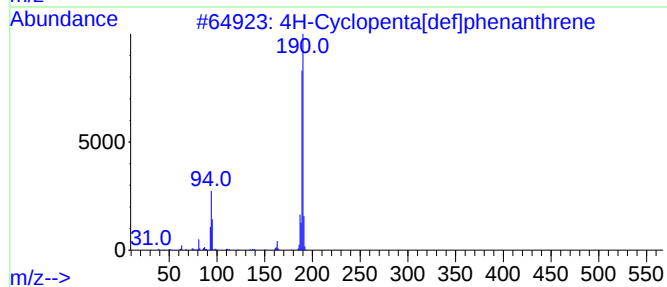
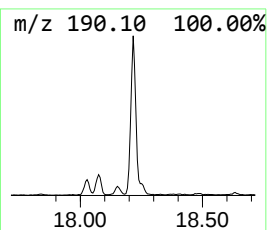
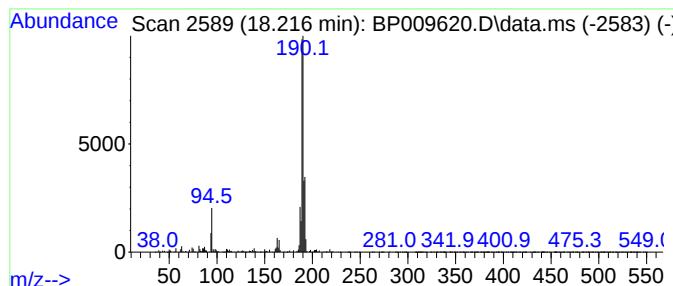
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	4.68 ng	571032	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
5			Methyl diselenide	190	C2H6Se2	007101-31-7	46



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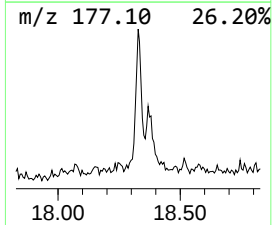
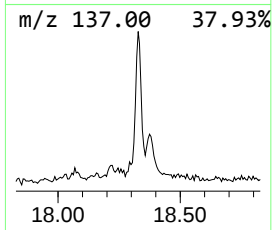
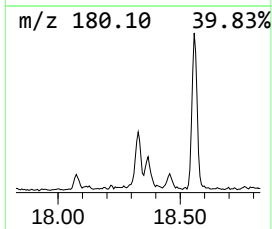
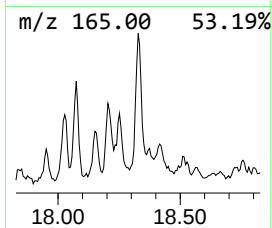
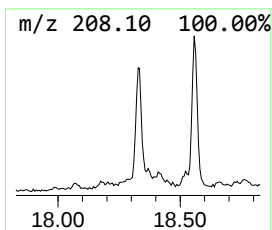
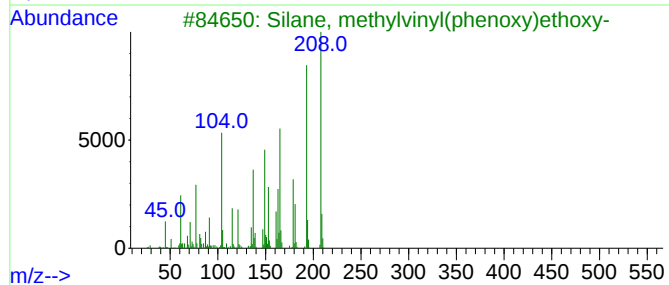
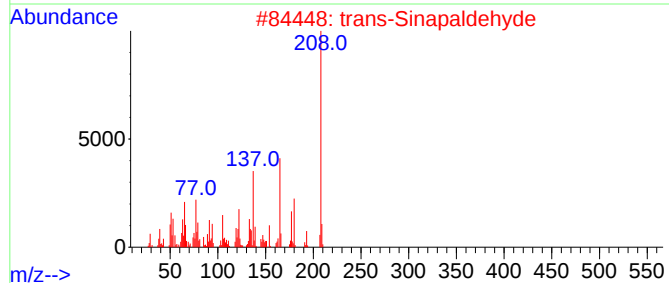
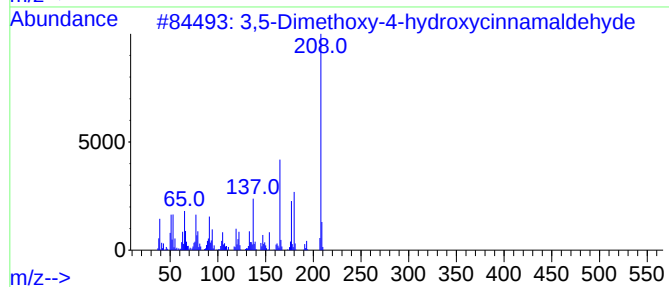
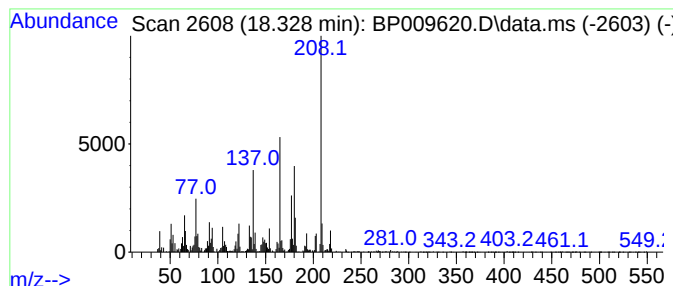
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.328	2.68 ng	327152	Phenanthrene-d10	17.151

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,5-Dimethoxy-4-hydroxycinnamal... 208	C11H12O4		087345-53-7	93
2		trans-Sinapaldehyde 208	C11H12O4		004206-58-0	83
3		Silane, methylvinyl(phenoxy)ethoxy- 208	C11H16O2Si		1000416-92-4	58
4		1,3,5-Trimethoxy-2-propenylbenzene 208	C12H16O3		005273-94-9	45
5		.beta.-Asarone 208	C12H16O3		005273-86-9	43



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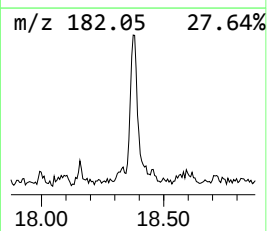
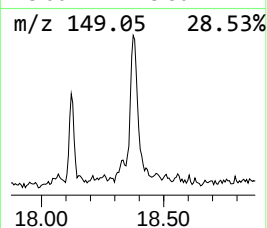
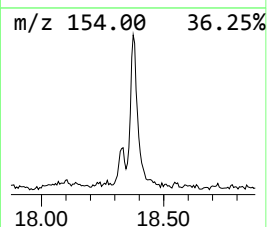
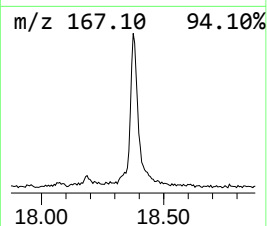
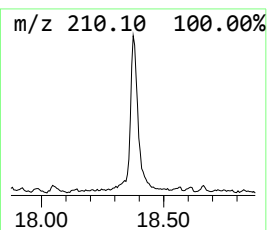
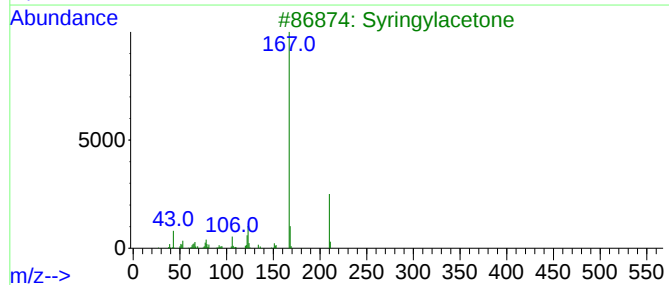
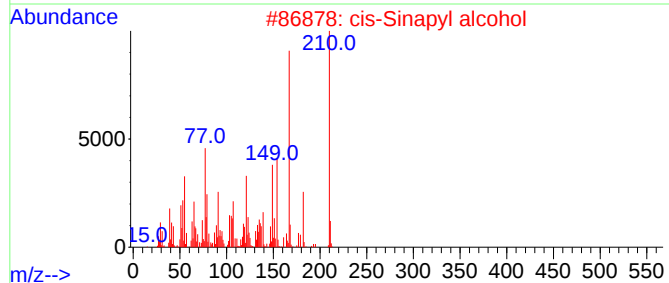
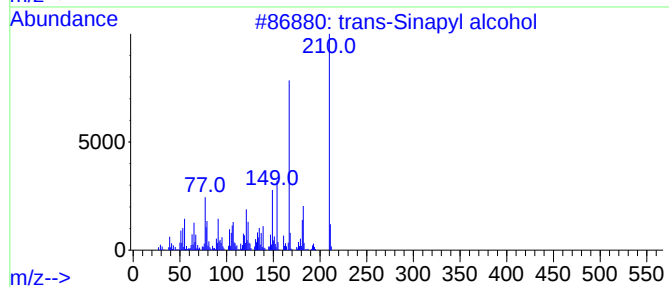
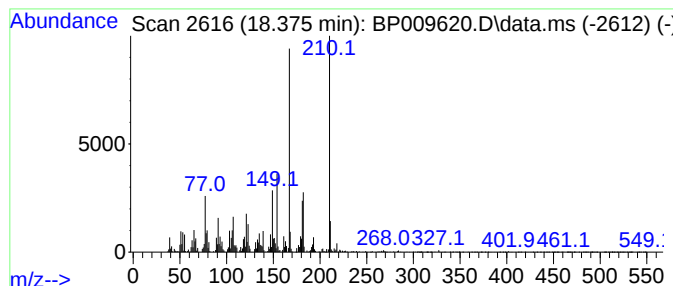
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 trans-Sinapyl alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.375	4.73 ng	577088	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	94
2			cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	87
3			Syringylacetone	210	C11H14O4	019037-58-2	58
4			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	52
5			Imidazo[4,5-e][1,4]diazepin-8(1H...	210	C8H10N4O5	1000142-41-3	43



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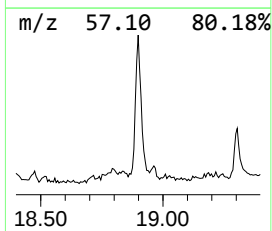
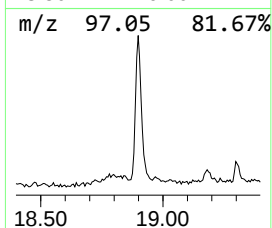
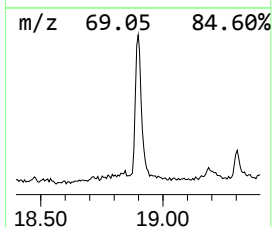
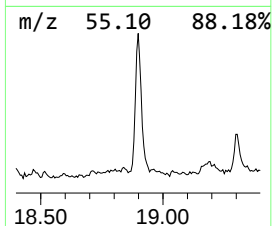
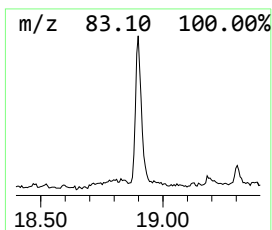
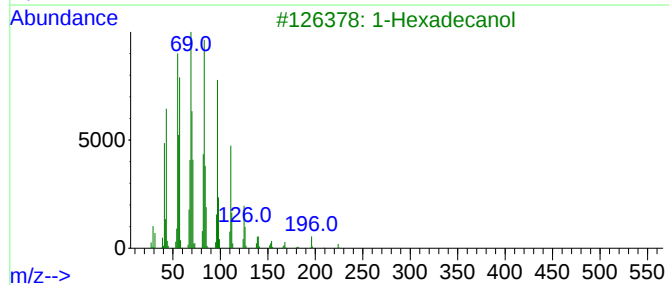
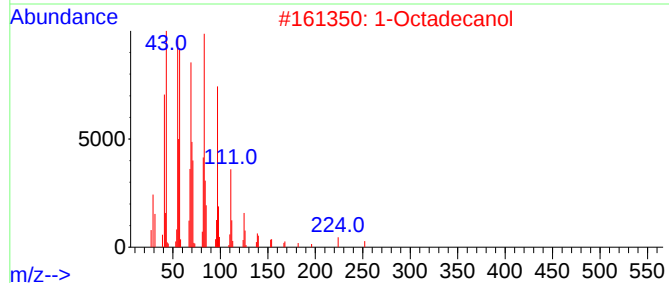
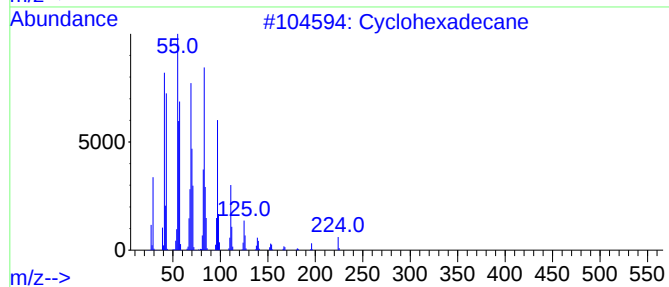
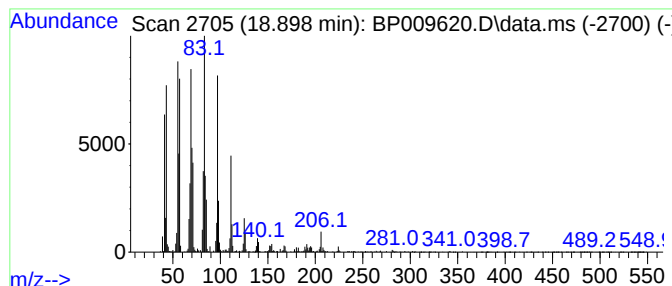
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.898	7.04 ng	859428	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			1-Octadecanol	270	C18H38O	000112-92-5	94
3			1-Hexadecanol	242	C16H34O	036653-82-4	94
4			Cetene	224	C16H32	000629-73-2	93
5			1-Heptadecene	238	C17H34	006765-39-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
337

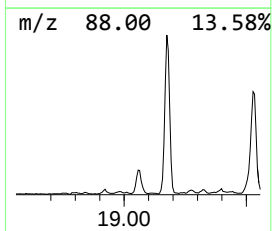
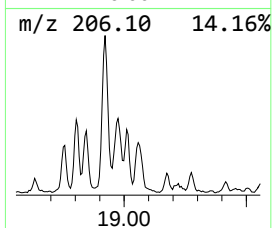
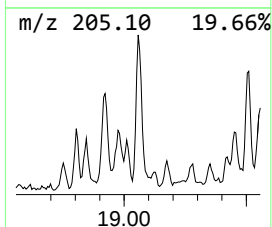
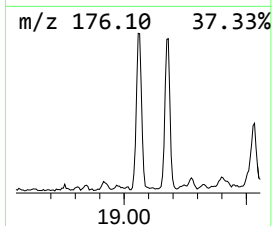
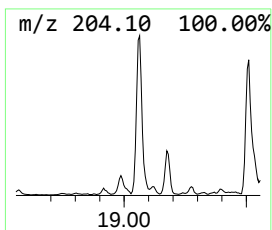
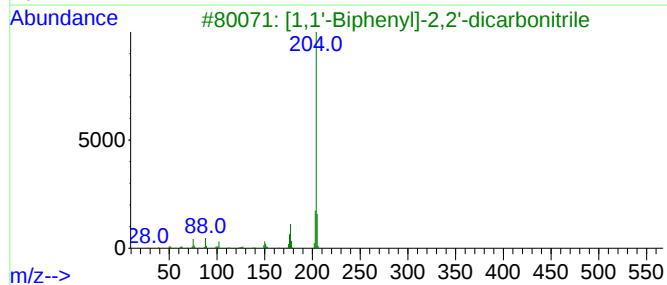
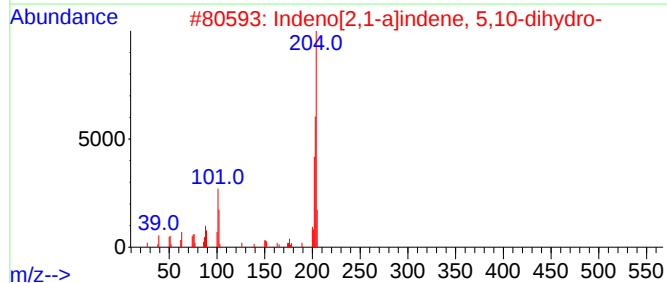
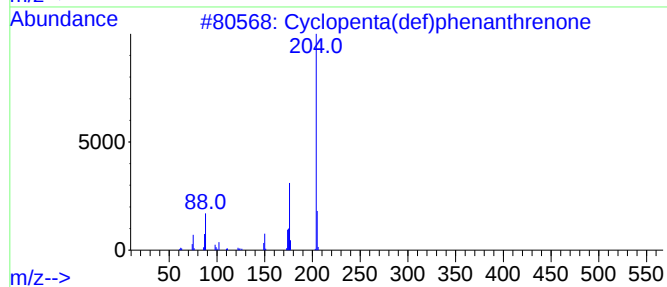
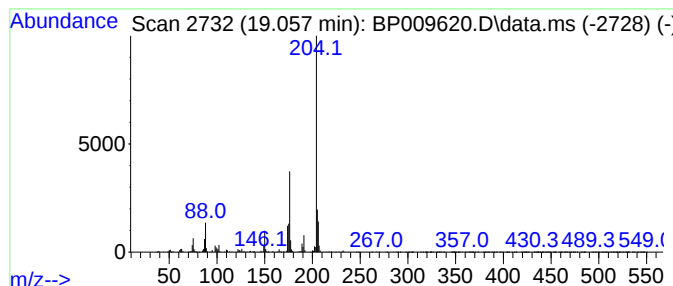
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.057	3.48 ng	424176	Phenanthrene-d10	17.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	96
2			Indeno[2,1-a]indene, 5,10-dihydro-	204	C16H12	006543-29-9	53
3			[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	52
4			Multifidin, 4TMS derivative	547	C23H49NO6Si4	1000480-87-0	50
5			3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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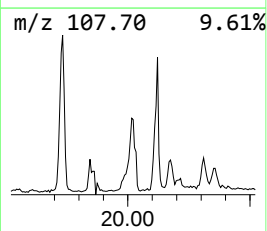
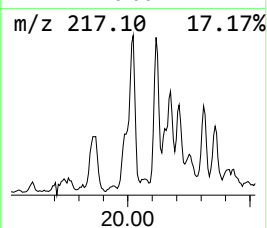
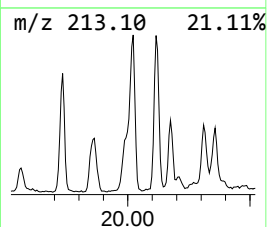
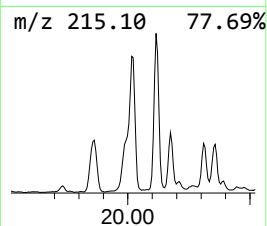
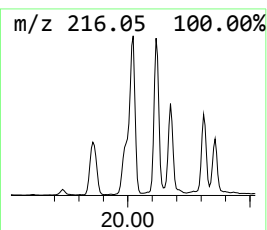
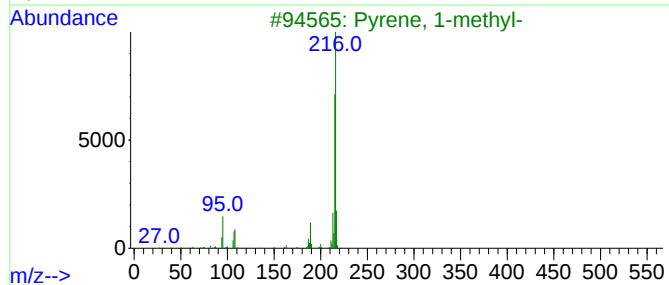
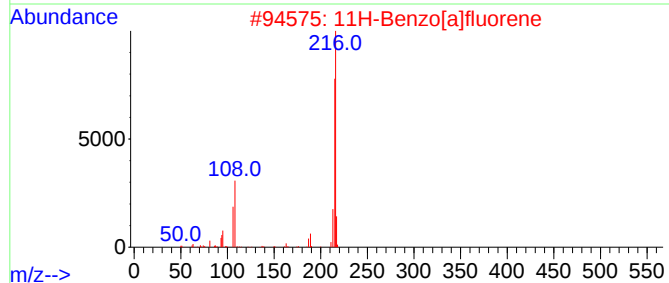
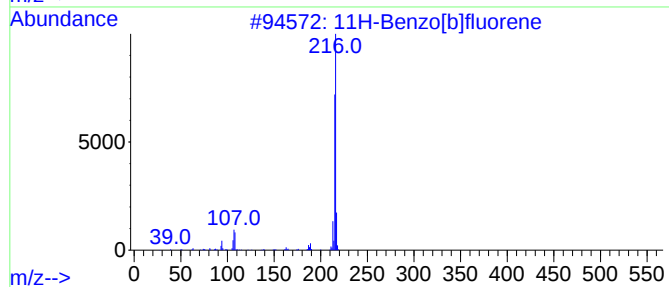
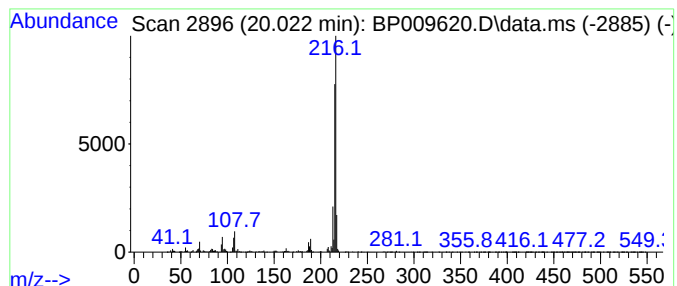
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.022	4.11 ng	1349740	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
5			Pyrene, 2-methyl-	216	C17H12	003442-78-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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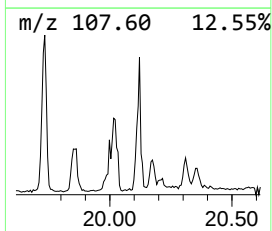
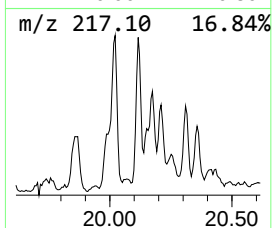
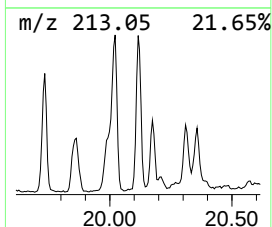
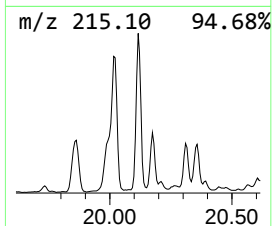
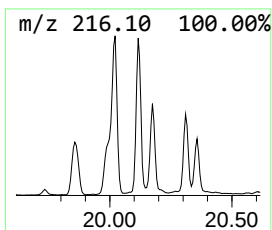
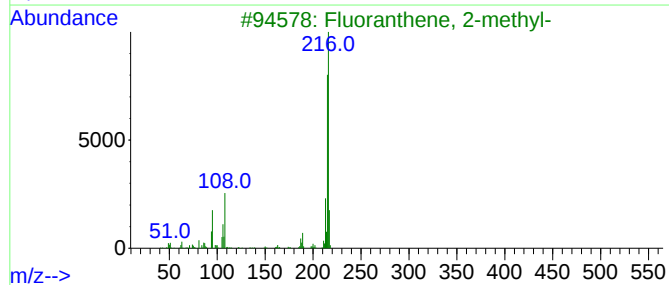
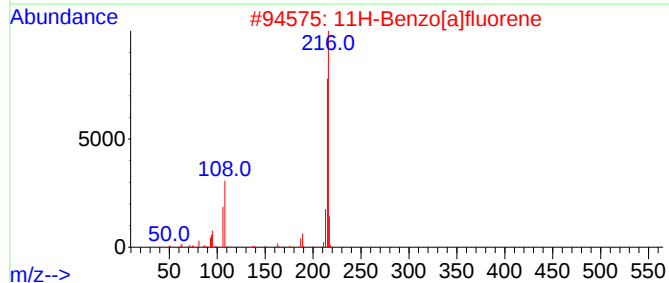
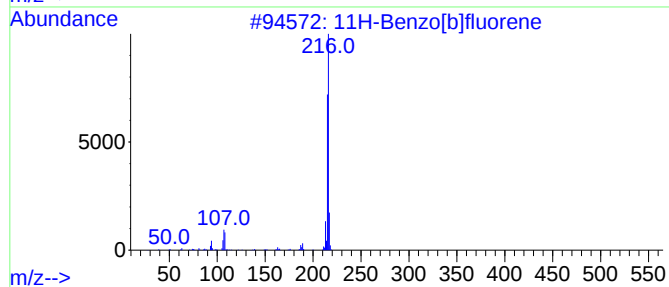
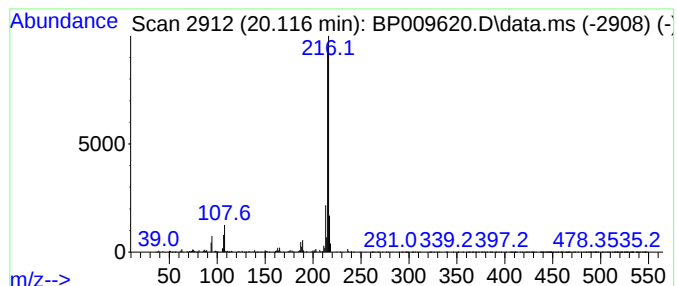
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.116	2.58 ng	845161	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	62
5			Pyrene, 1-methyl-	216	C17H12	002381-21-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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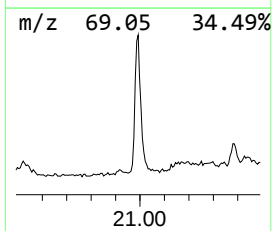
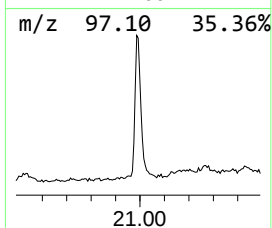
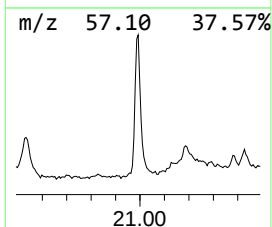
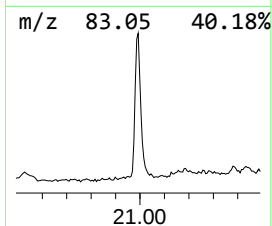
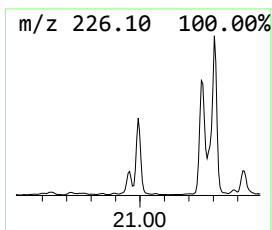
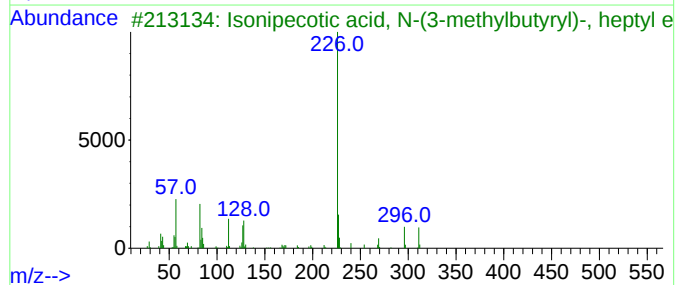
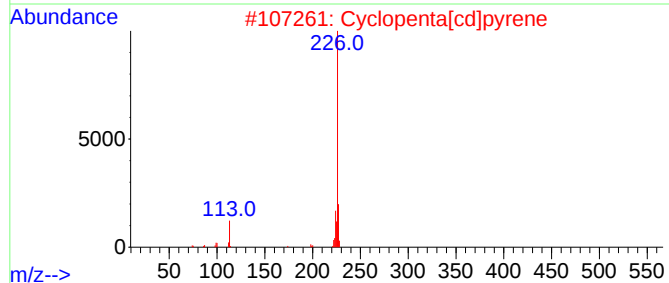
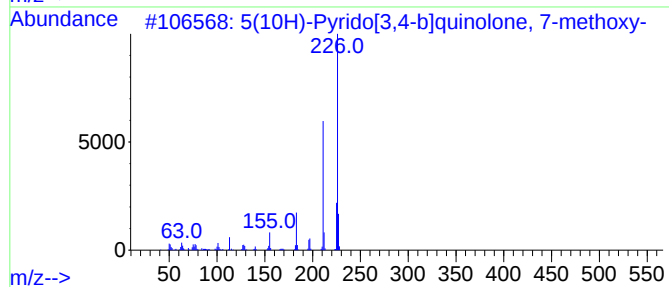
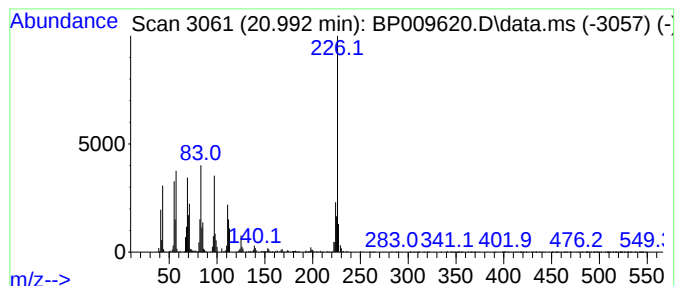
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown20.992 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.992	4.36 ng	1428900	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5(10H)-Pyrido[3,4-b]quinolone, 7...	226	C13H10N2O2	1000256-99-5	35		
2	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	27		
3	Isonipecotic acid, N-(3-methylbu...	311	C18H33NO3	1000360-99-1	25		
4	4-Amino-5-(4-chlorophenyl)-4H-1,...	226	C8H7ClN4S	1010476-96-9	25		
5	benzenamine, 4-(2-benzothiazolyl)-	226	C13H10N2S	1000400-93-4	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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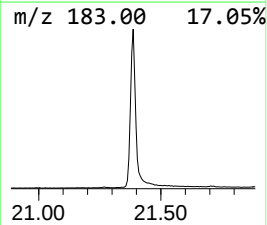
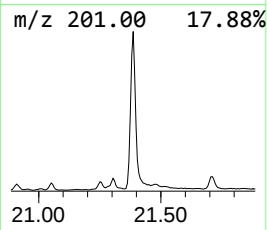
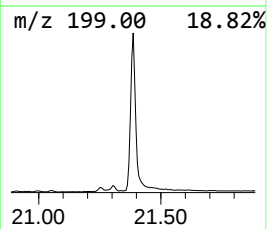
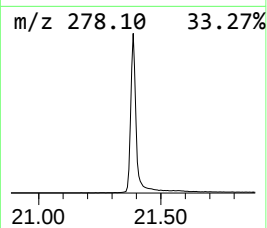
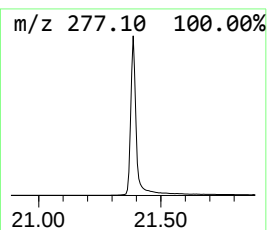
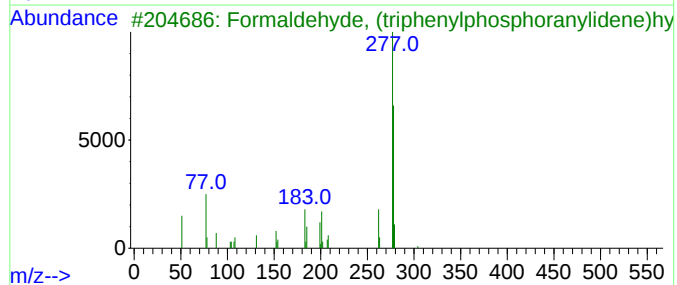
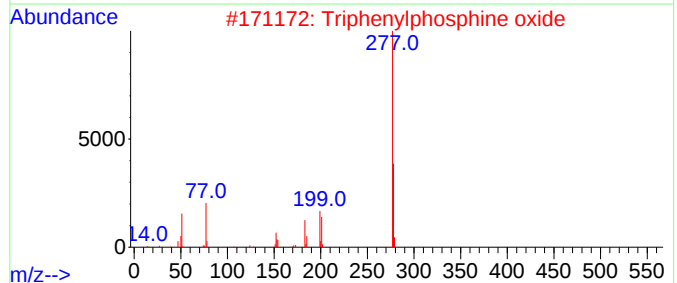
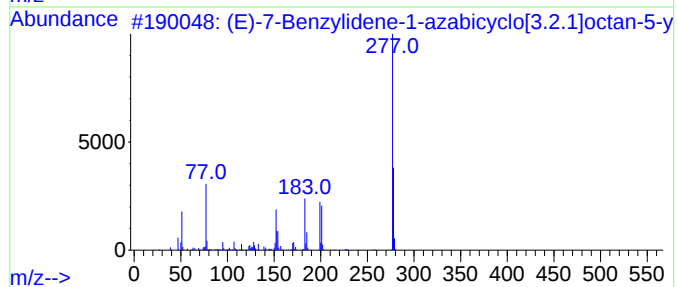
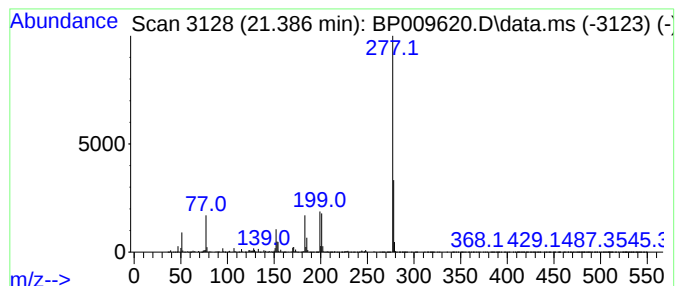
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 (E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.386	22.38 ng	7343240	Chrysene-d12	21.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3.2.1]octan-5-yl	293	C15H19NO3S	1000483-83-4	91		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	86		
3	Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	47		
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	42		
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
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Acq On : 30 Mar 2022 15:59
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Sample : N2150-05
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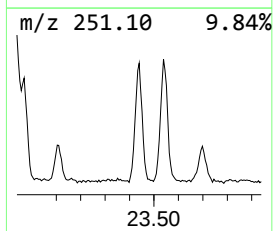
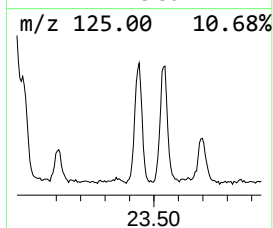
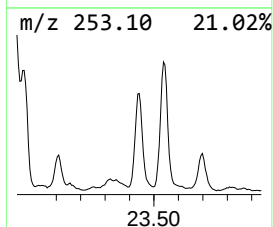
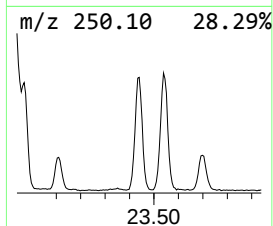
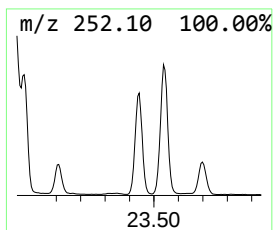
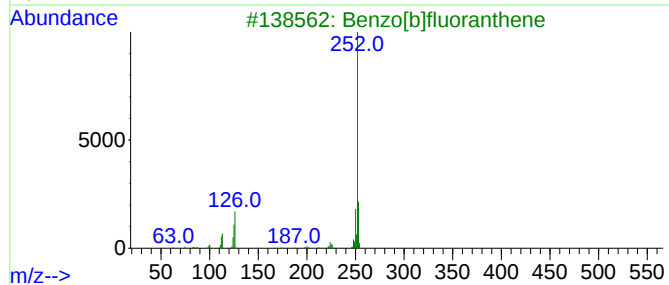
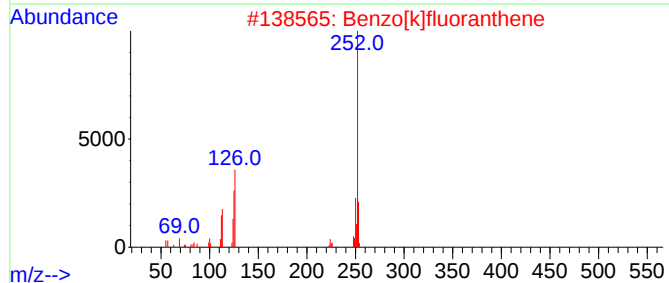
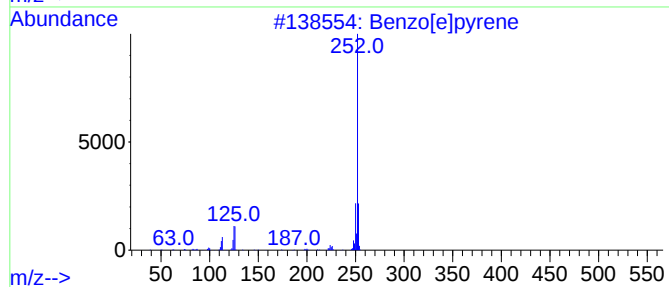
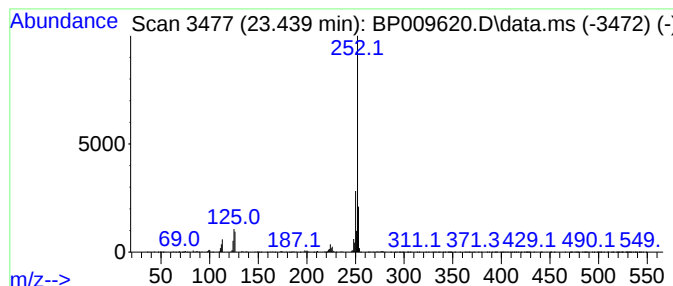
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.439	9.04 ng	1530760	Perylene-d12	23.645	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033022\
Data File : BP009620.D
Acq On : 30 Mar 2022 15:59
Operator : CG/JU
Sample : N2150-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
337

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.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
n-Hexadecanoic ...	18.063	7.5	ng	918070	4	17.151	2440980	20.0
4H-Cyclopenta[d]...	18.216	4.7	ng	571032	4	17.151	2440980	20.0
3,5-Dimethoxy-4...	18.328	2.7	ng	327152	4	17.151	2440980	20.0
trans-Sinapyl a...	18.375	4.7	ng	577088	4	17.151	2440980	20.0
Cyclohexadecane	18.898	7.0	ng	859428	4	17.151	2440980	20.0
Cyclopenta(def)...	19.057	3.5	ng	424176	4	17.151	2440980	20.0
11H-Benzo[b]flu...	20.022	4.1	ng	1349740	5	21.269	6561290	20.0
11H-Benzo[a]flu...	20.116	2.6	ng	845161	5	21.269	6561290	20.0
unknown20.992	20.992	4.4	ng	1428900	5	21.269	6561290	20.0
(E)-7-Benzylide...	21.386	22.4	ng	7343240	5	21.269	6561290	20.0
Benzo[e]pyrene	23.439	9.0	ng	1530760	6	23.645	3387780	20.0