

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
 Data File : BP019690.D
 Acq On : 13 Feb 2024 22:14
 Operator : MA/JU
 Sample : P1421-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 72-11977

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-BP013124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019690.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	400	407	425	rBV	961320	1454245	43.40%	4.473%
2	7.081	671	679	690	rBV	917463	1542113	46.03%	4.743%
3	7.905	812	819	828	rBV	297255	478145	14.27%	1.471%
4	9.075	1010	1018	1031	rBV	616038	1051166	31.37%	3.233%
5	10.704	1286	1295	1301	rBV	383041	665560	19.86%	2.047%
6	10.757	1301	1304	1311	rVB	46696	70228	2.10%	0.216%
7	12.363	1572	1577	1585	rVB	21747	36355	1.09%	0.112%
8	13.169	1706	1714	1726	rBV	1628232	2507560	74.84%	7.712%
9	14.263	1892	1900	1909	rBV	22850	39971	1.19%	0.123%
10	14.540	1939	1947	1953	rBV	611271	924093	27.58%	2.842%
11	14.604	1953	1958	1966	rVB	169734	264961	7.91%	0.815%
12	14.939	2009	2015	2024	rBV	53760	94602	2.82%	0.291%
13	15.545	2113	2118	2122	rBV	117049	169503	5.06%	0.521%
14	15.592	2122	2126	2136	rVB	125616	190624	5.69%	0.586%
15	15.751	2150	2153	2158	rVB4	25765	34648	1.03%	0.107%
16	16.034	2194	2201	2210	rBV	1464367	2196119	65.55%	6.754%
17	16.563	2286	2291	2295	rBV	42035	76716	2.29%	0.236%
18	16.963	2354	2359	2362	rBV2	37657	62235	1.86%	0.191%
19	17.116	2381	2385	2393	rVB	46243	70932	2.12%	0.218%
20	17.298	2410	2416	2419	rBV	740606	1076346	32.13%	3.310%
21	17.339	2419	2423	2429	rVB	954804	1348478	40.25%	4.147%
22	17.433	2434	2439	2444	rVV	295194	436991	13.04%	1.344%
23	17.492	2444	2449	2454	rVB	35809	65151	1.94%	0.200%
24	17.692	2477	2483	2496	rBV3	403729	689496	20.58%	2.121%
25	18.169	2559	2564	2565	rBV	89310	119621	3.57%	0.368%
26	18.198	2565	2569	2578	rVB2	443954	743303	22.19%	2.286%
27	18.292	2581	2585	2589	rVB	54901	78449	2.34%	0.241%
28	18.351	2590	2595	2599	rBV2	189724	314327	9.38%	0.967%
29	18.610	2635	2639	2643	rBV	330834	397316	11.86%	1.222%
30	18.651	2643	2646	2650	rVV	89445	104931	3.13%	0.323%
31	18.692	2650	2653	2657	rVB2	38973	51967	1.55%	0.160%
32	18.928	2689	2693	2699	rBV	156128	230418	6.88%	0.709%
33	19.139	2726	2729	2734	rVB	96799	113194	3.38%	0.348%
34	19.310	2752	2758	2763	rBV	1429955	1915689	57.18%	5.892%
35	19.363	2765	2767	2772	rVV2	60579	79896	2.38%	0.246%
36	19.433	2775	2779	2786	rVB3	194441	298832	8.92%	0.919%

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Sampling : 1

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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	19.633	2808	2813	2814	rBV	303493	404067	12.06%	1.243%
38	19.663	2814	2818	2826	rVB	1119903	1703217	50.84%	5.238%
39	19.863	2847	2852	2857	rBV	2817421	3350425	100.00%	10.304%
40	20.145	2896	2900	2904	rVB2	213510	277621	8.29%	0.854%
41	20.210	2908	2911	2914	rVV	203320	256697	7.66%	0.789%
42	20.245	2914	2917	2921	rVB	221000	266557	7.96%	0.820%
43	20.622	2978	2981	2984	rBV	101621	106000	3.16%	0.326%
44	21.080	3056	3059	3062	rBV	113037	137560	4.11%	0.423%
45	21.116	3062	3065	3070	rVB2	255734	348435	10.40%	1.072%
46	21.386	3105	3111	3115	rBV3	1073549	2135230	63.73%	6.567%
47	21.427	3115	3118	3129	rVB	591473	884203	26.39%	2.719%
48	23.080	3394	3399	3403	rBV	347965	782710	23.36%	2.407%
49	23.704	3500	3505	3512	rBV	398703	792959	23.67%	2.439%
50	23.815	3518	3524	3530	rBV	520706	1074795	32.08%	3.306%

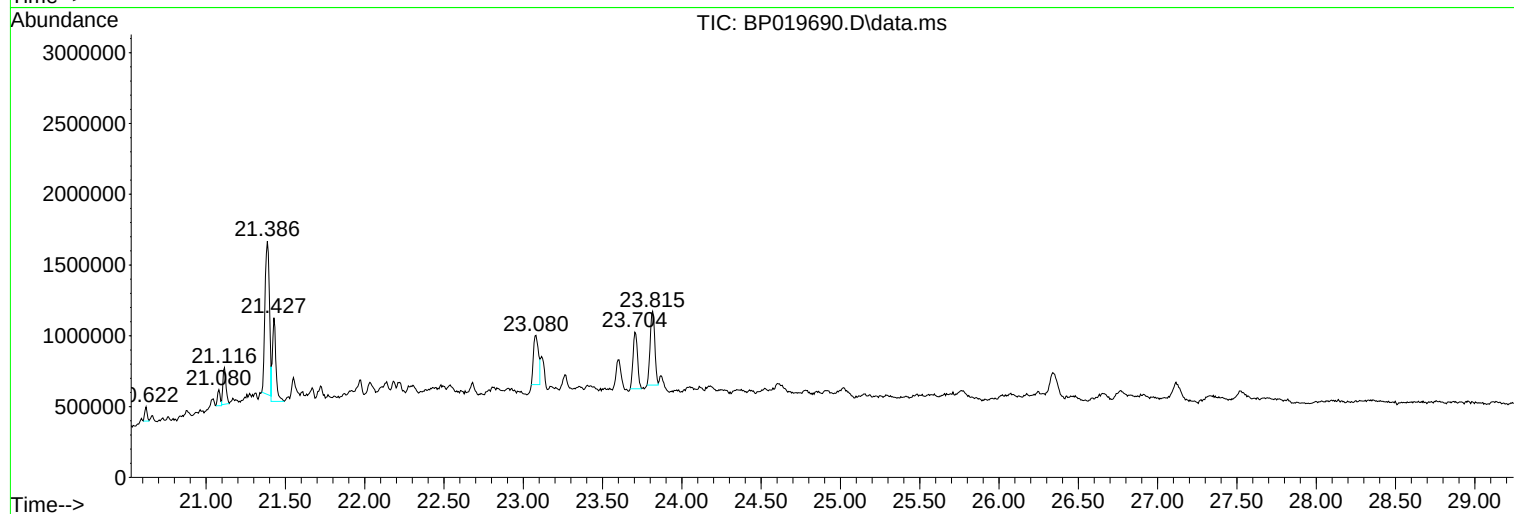
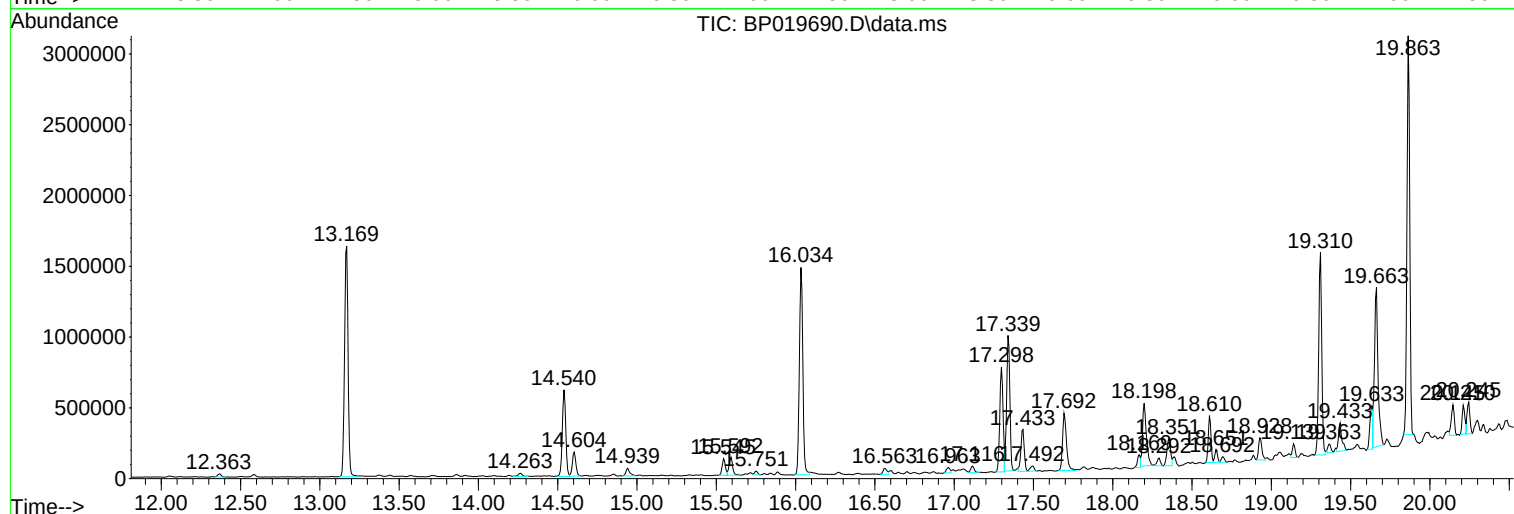
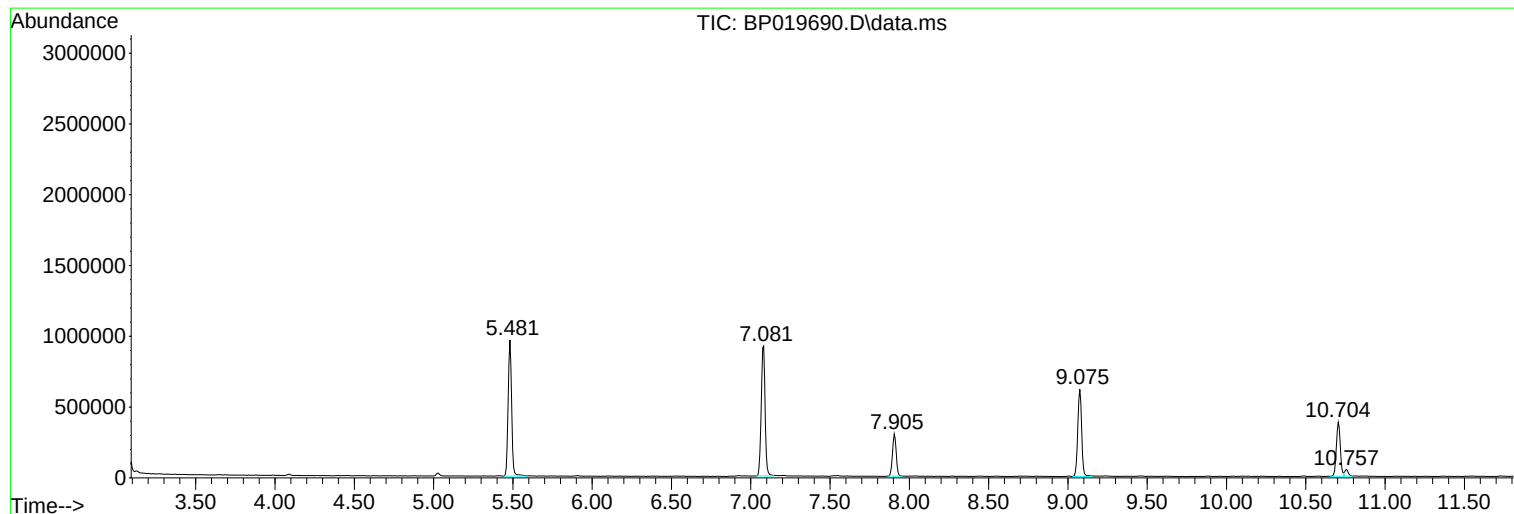
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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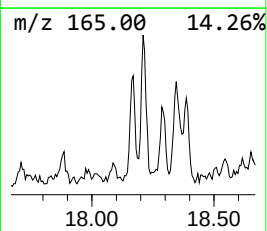
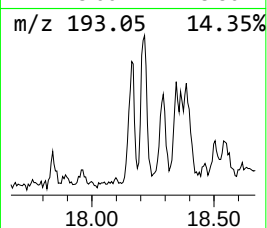
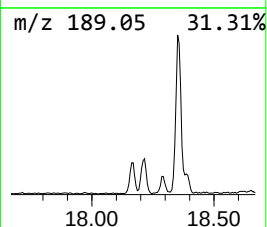
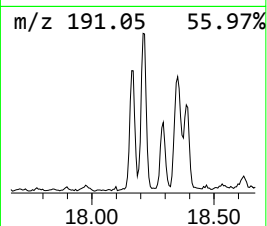
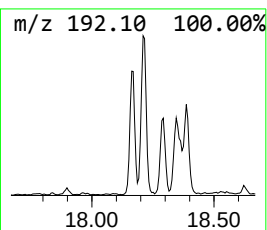
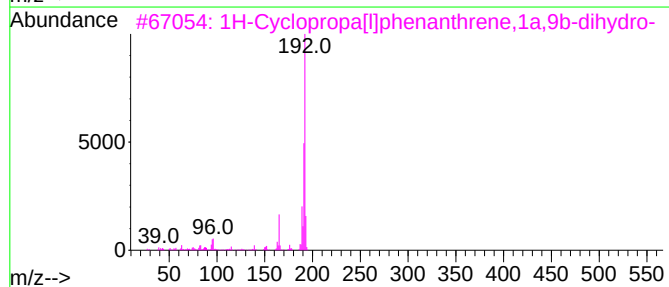
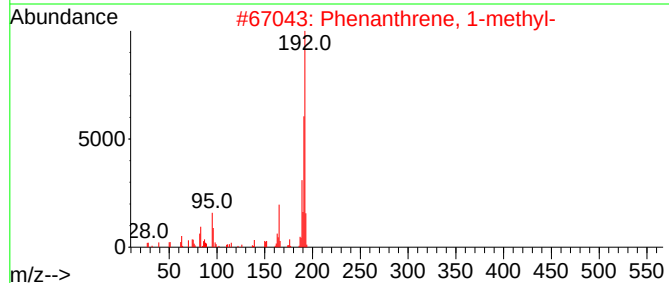
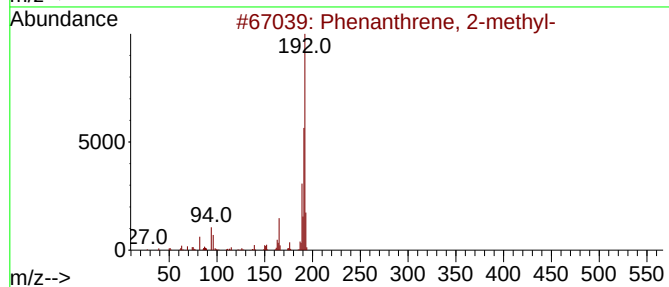
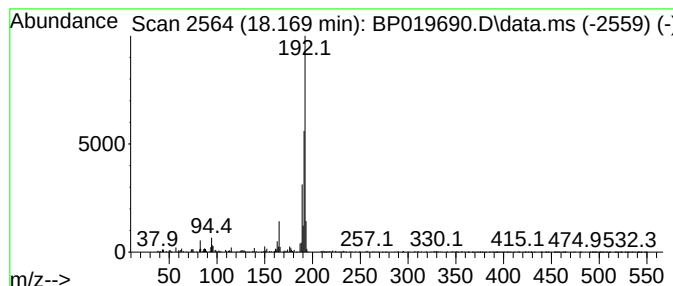
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	2.22 ng	119621	Phenanthrene-d10	17.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3		1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
5		Anthracene, 2-methyl-	192	C15H12	000613-12-7	91



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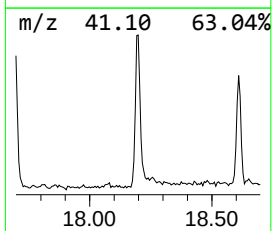
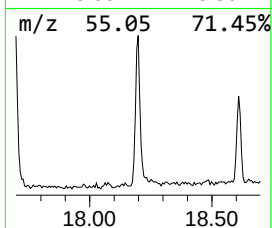
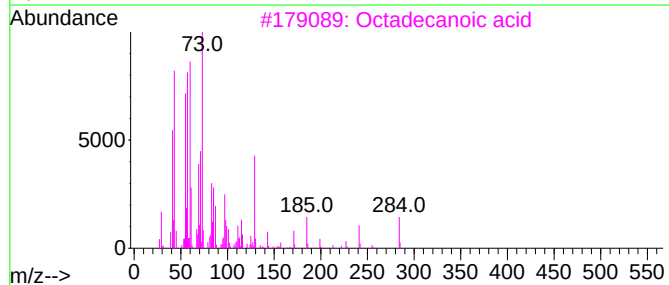
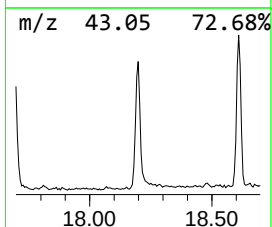
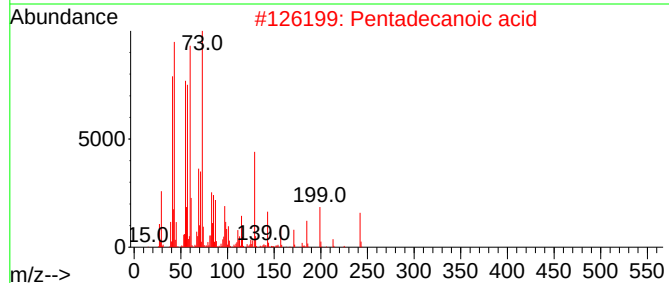
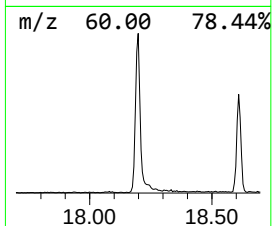
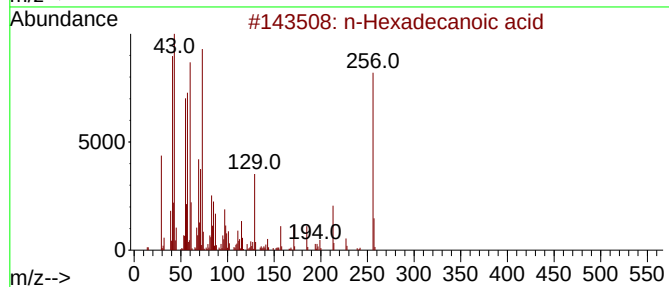
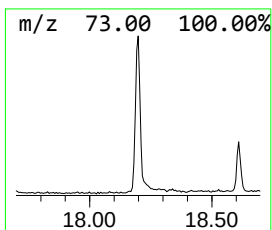
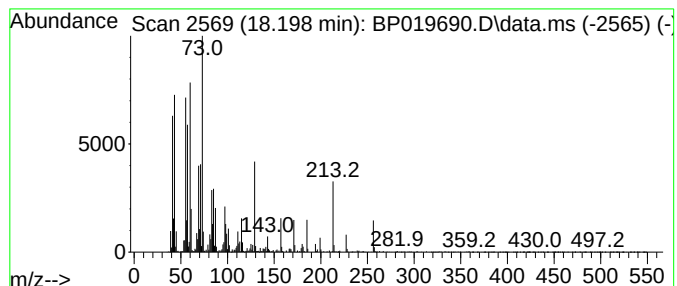
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	13.81 ng	743303	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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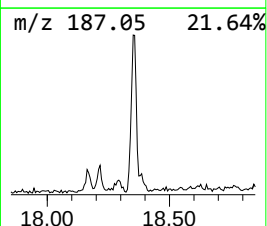
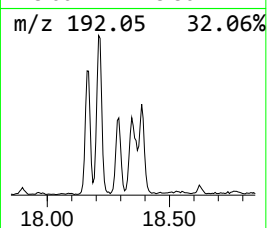
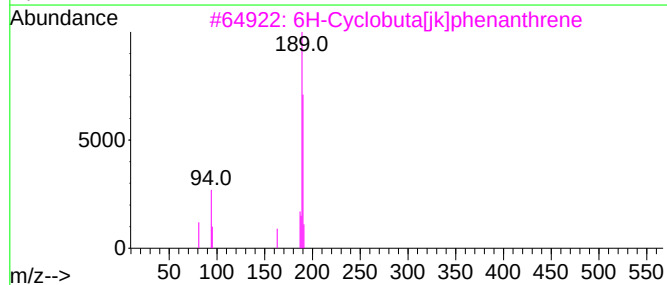
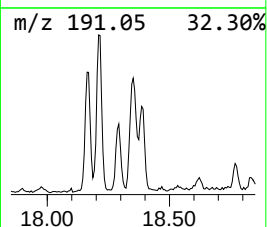
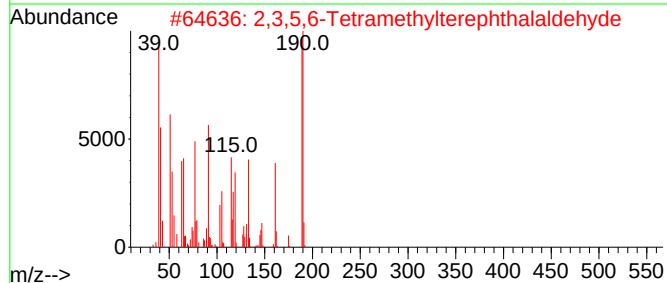
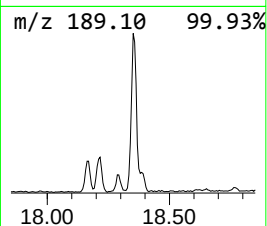
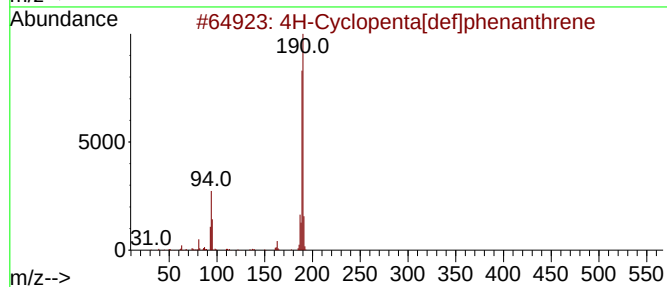
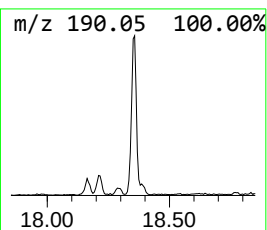
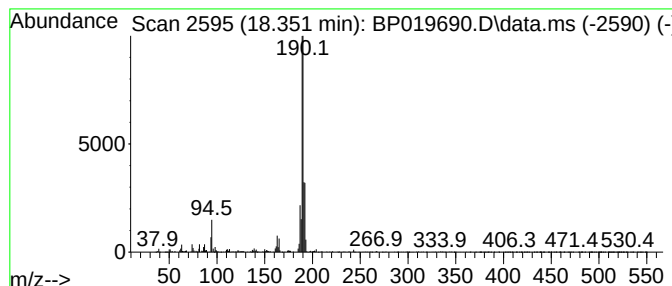
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	5.84 ng	314327	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



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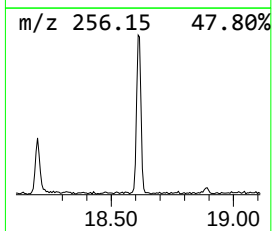
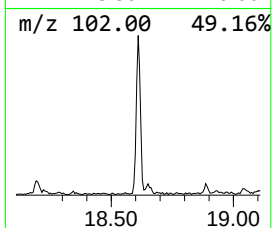
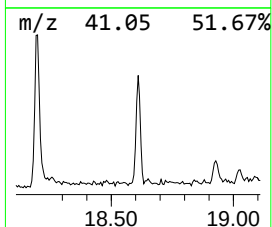
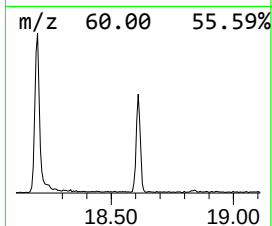
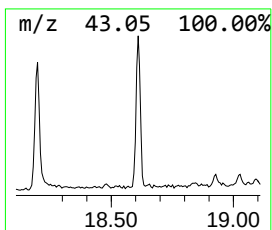
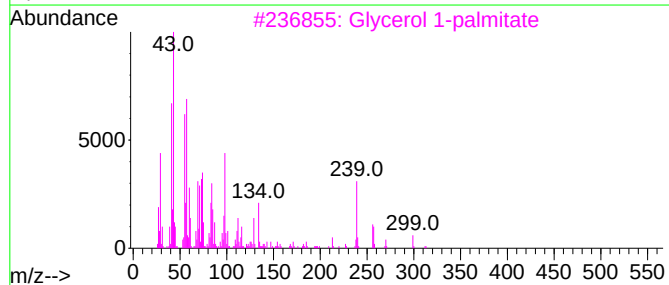
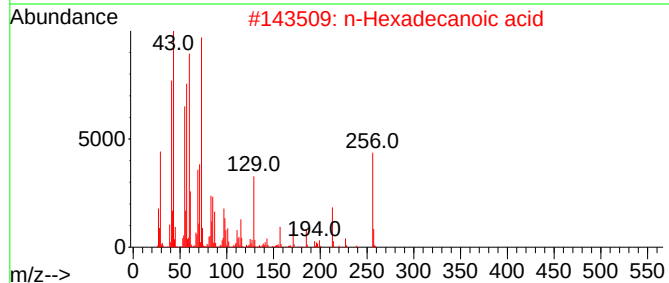
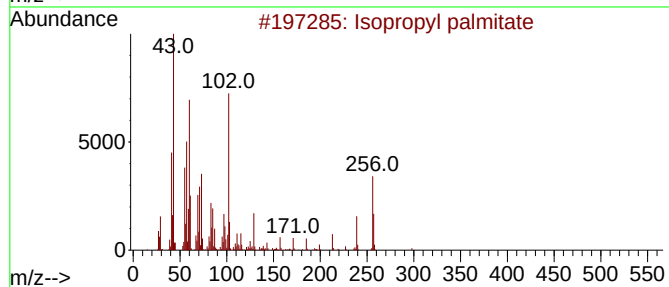
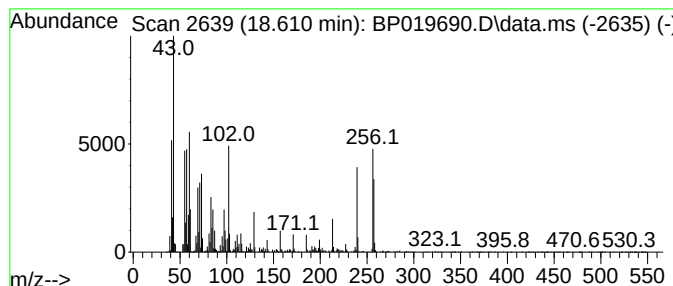
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl palmitate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.610	7.38 ng	397316	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	72
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
3			Glycerol 1-palmitate	330	C19H38O4	000542-44-9	38
4			Methyl isopropylidene-.beta.-d-a...	204	C9H16O5	1000129-88-1	16
5			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	16



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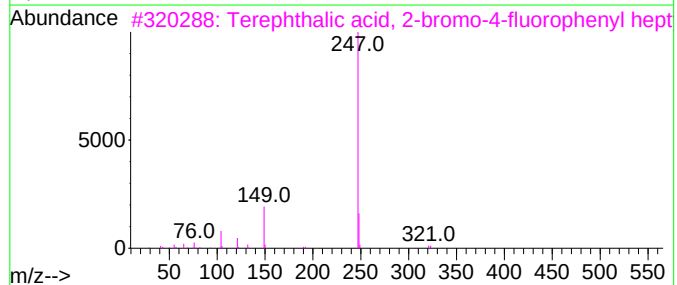
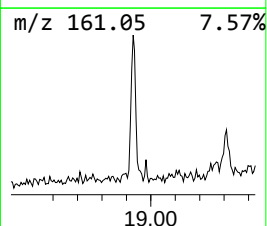
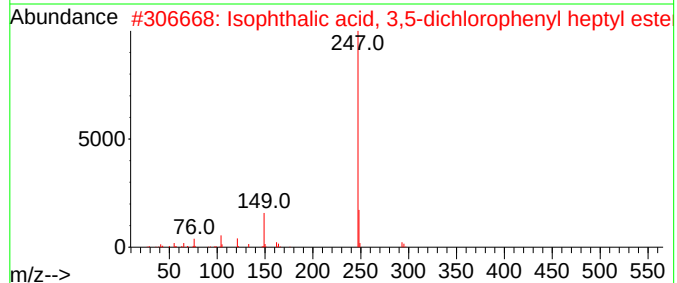
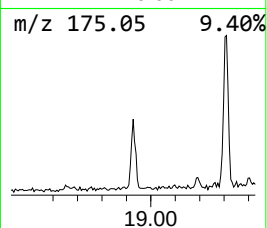
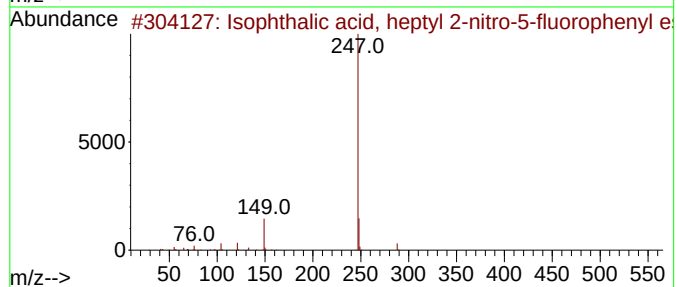
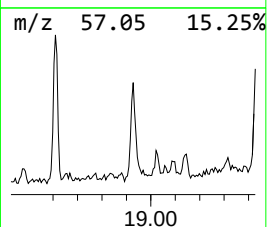
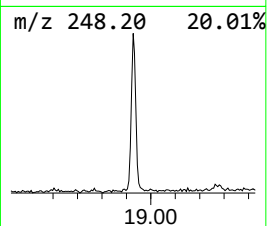
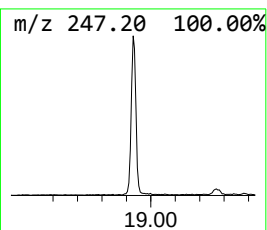
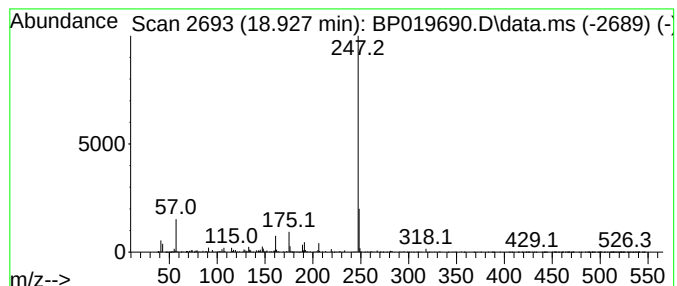
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Isophthalic acid, heptyl 2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.927	4.28 ng	230418	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isophthalic acid, heptyl 2-nitro...	403	C21H22FN06	1010344-42-2	53
2			Isophthalic acid, 3,5-dichloroph...	408	C21H22Cl2O4	1000356-58-6	53
3			Terephthalic acid, 2-bromo-4-flu...	436	C21H22BrF04	1000323-71-1	53
4			2-(Salicylideneamino)naphthalene	247	C17H13NO	001689-72-1	53
5			9H-Imidazo[1,2-a]benzimidazole, ...	247	C16H13N3	021431-82-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
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Acq On : 13 Feb 2024 22:14
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Sample : P1421-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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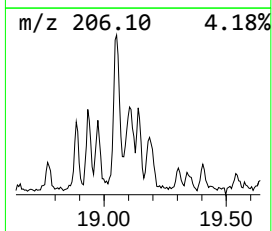
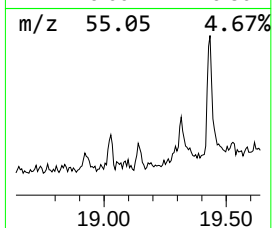
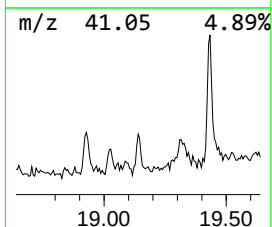
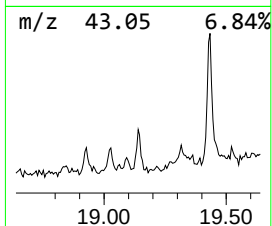
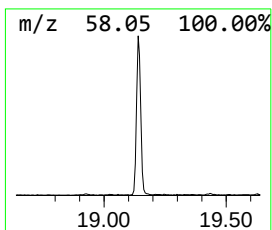
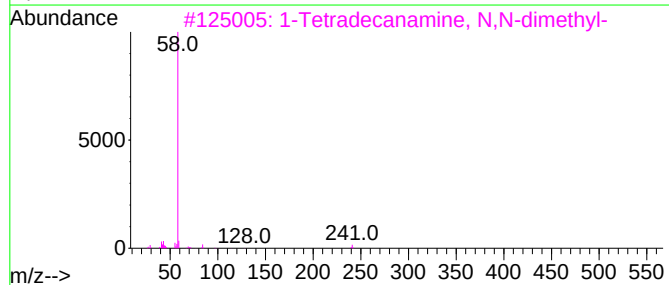
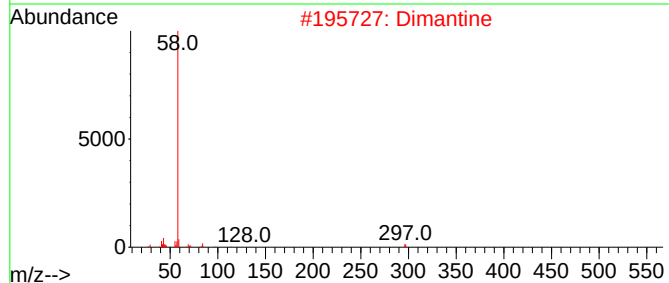
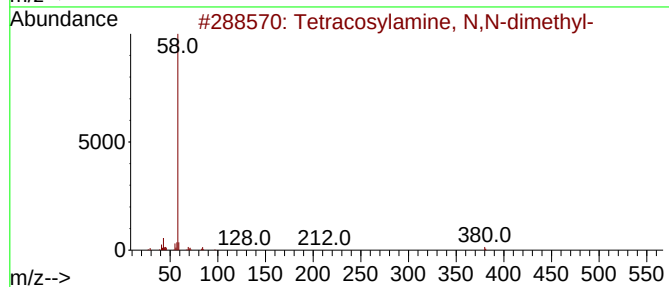
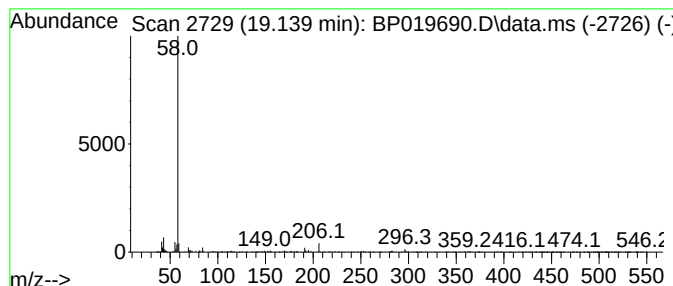
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetracosylamine, N,N-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.139	2.10 ng	113194	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosylamine, N,N-dimethyl-	381	C26H55N	1000406-30-7	64
2			Dimantine	297	C20H43N	000124-28-7	64
3			1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	64
4			1-Heptadecanamine, N,N-dimethyl-	283	C19H41N	003002-57-1	64
5			Cetrimonium Bromide	363	C19H42BrN	000057-09-0	64



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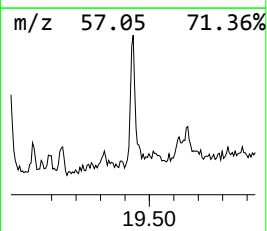
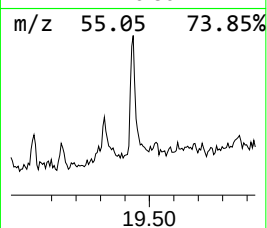
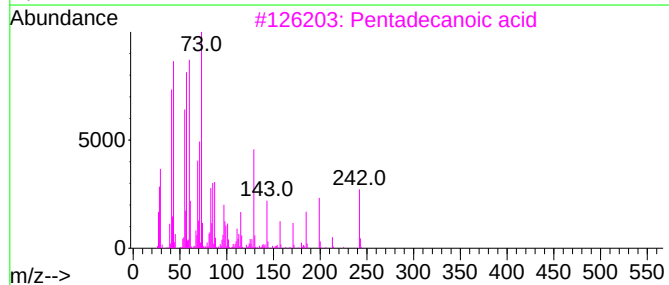
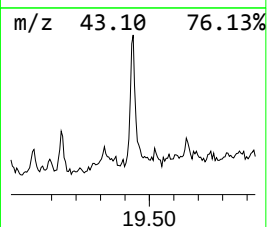
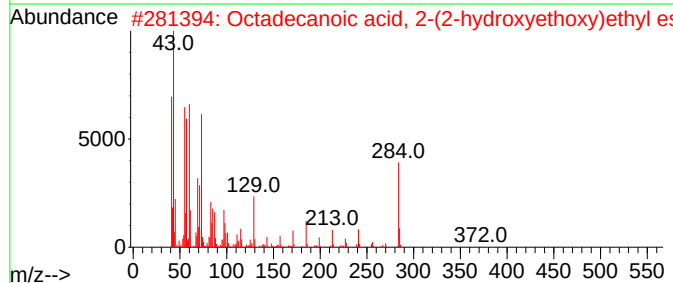
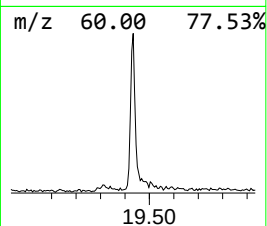
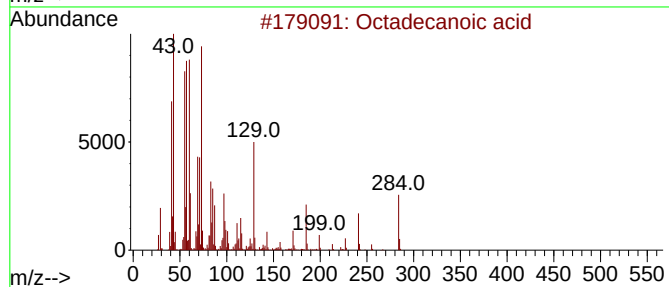
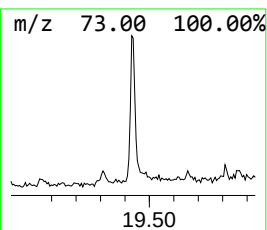
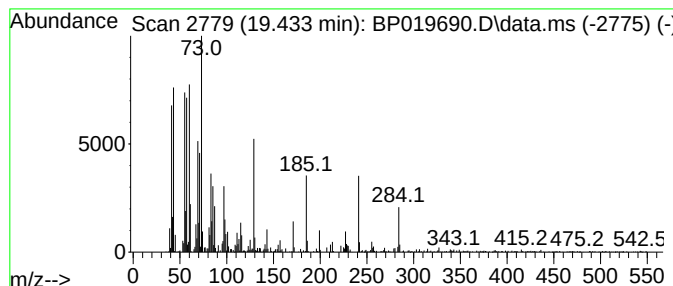
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	2.80 ng	298832	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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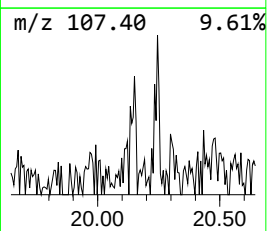
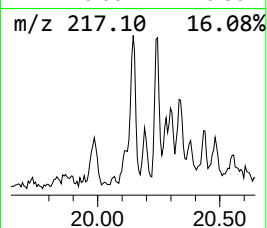
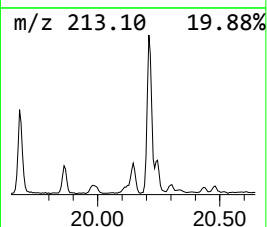
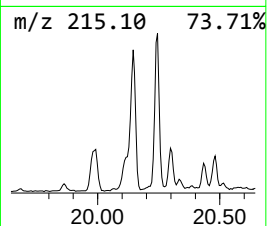
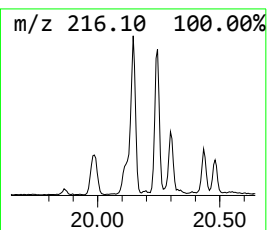
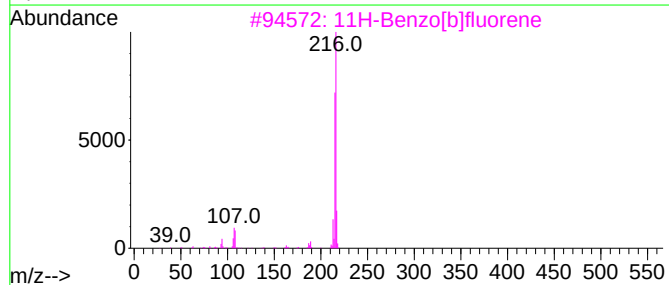
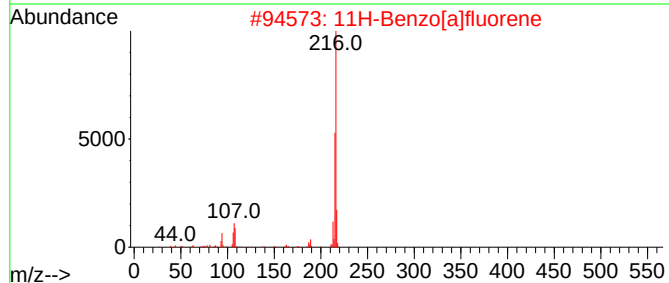
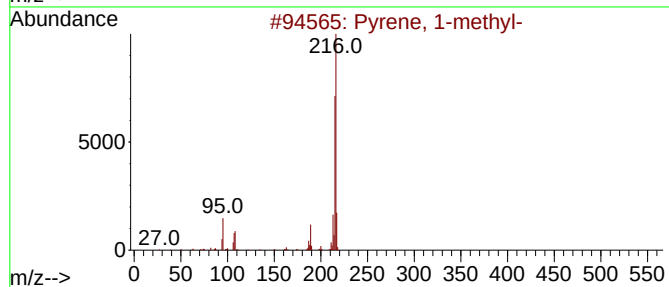
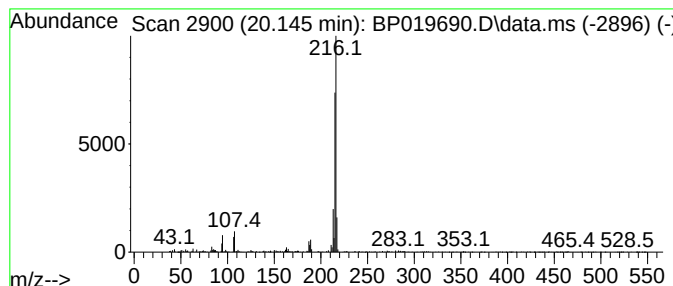
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.145	2.60 ng	277621	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019690.D
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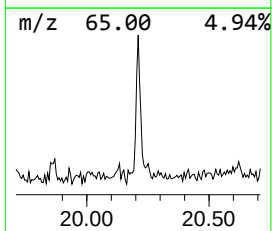
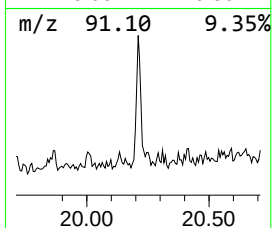
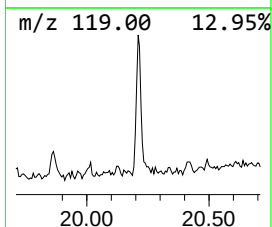
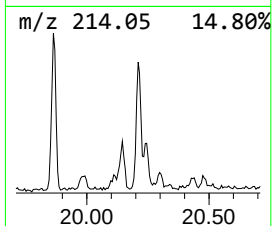
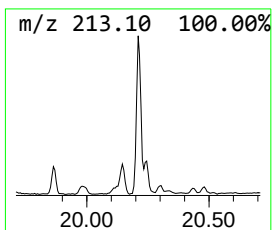
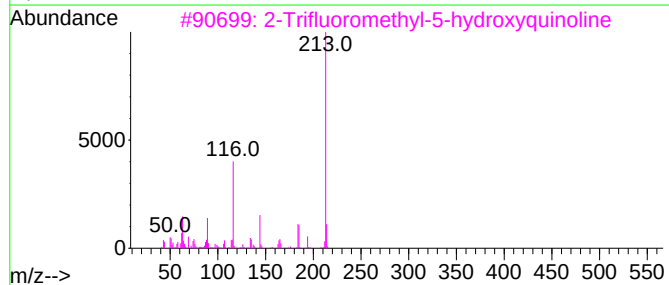
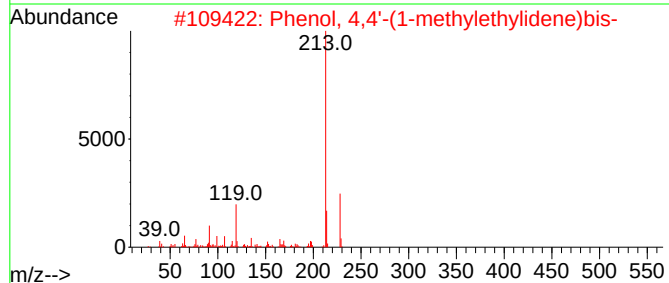
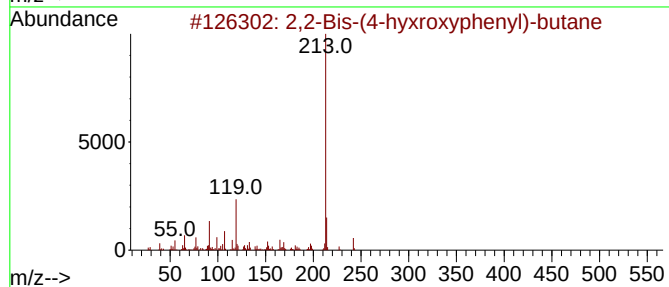
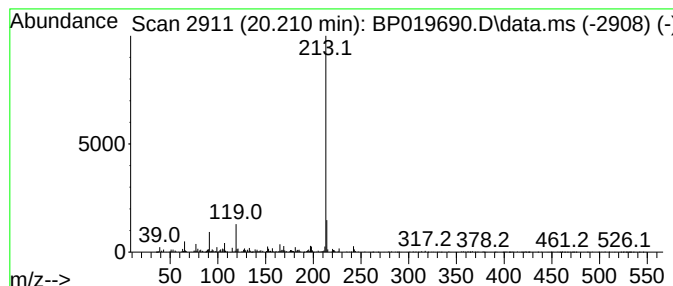
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,2-Bis-(4-hydroxyphenyl)-b... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.210	2.40 ng	256697	Chrysene-d12	21.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	90
2		Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	72
3		2-Trifluoromethyl-5-hydroxyquinoline	213	C10H6F3NO	041958-06-9	59
4		Indole, 6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	58
5		5-Methyl-4-(trifluoromethyl)pyrrole	213	C9H6F3N3	1192656-81-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019690.D
Acq On : 13 Feb 2024 22:14
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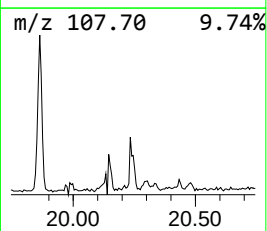
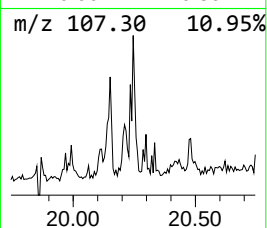
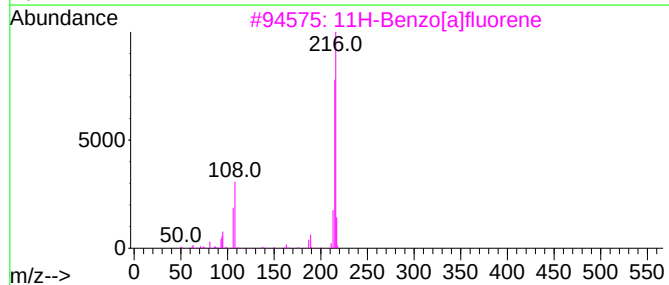
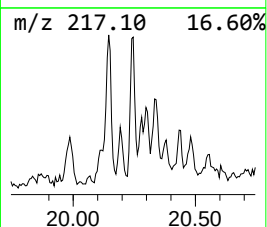
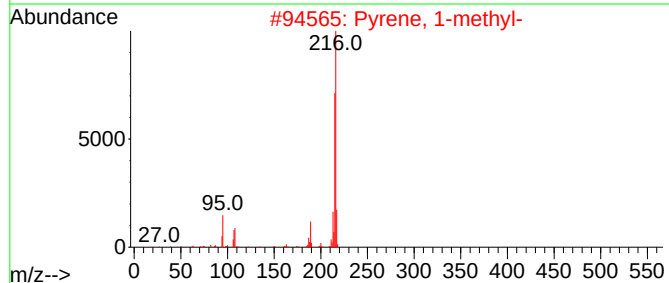
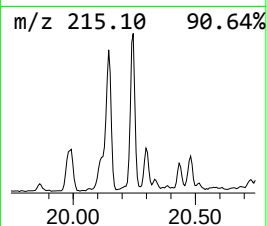
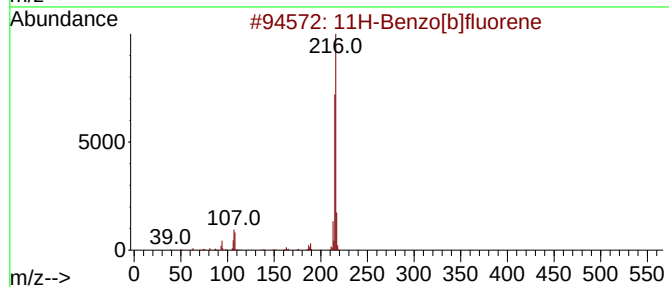
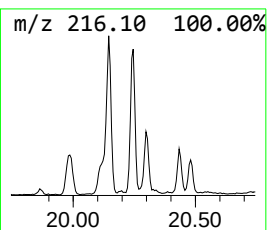
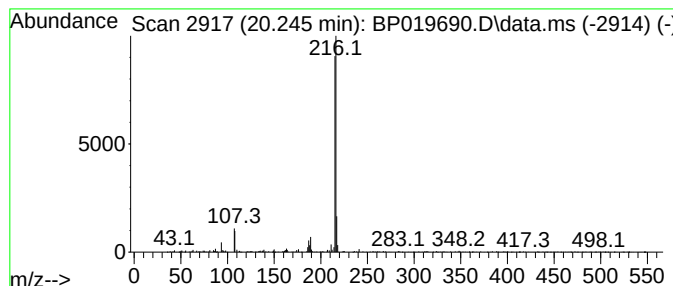
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.245	2.50 ng	266557	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
4			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	80
5			Pyridin-3-ol, 2-(4-nitrophenyl)-	216	C11H8N2O3	030820-89-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
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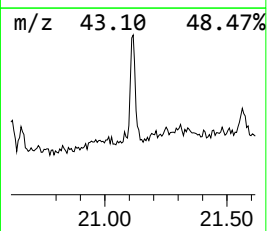
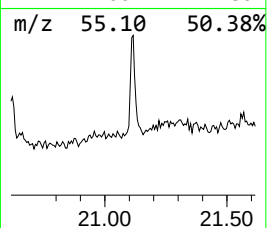
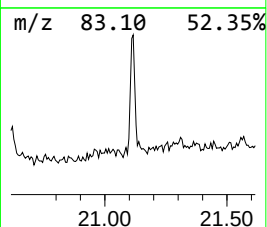
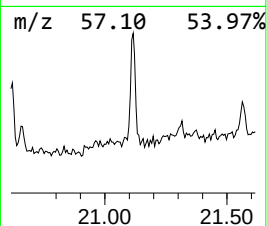
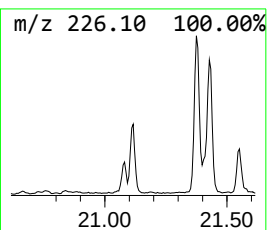
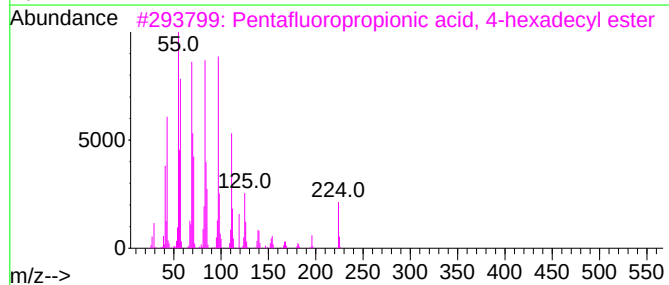
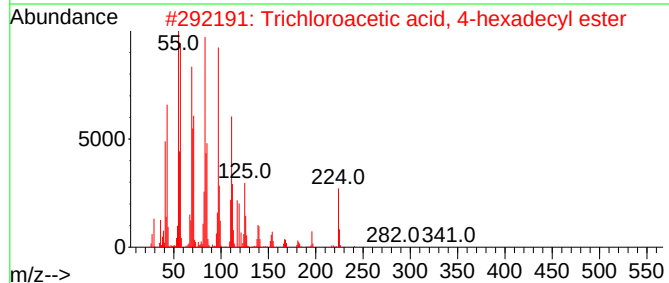
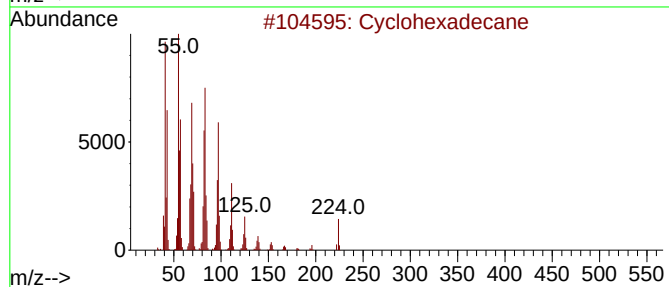
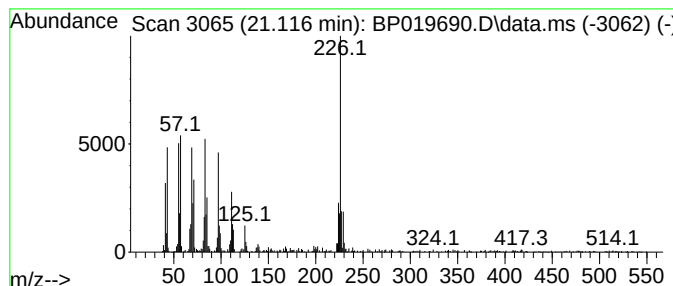
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown21.116 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	3.26 ng	348435	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	45
2			Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	43
3			Pentafluoropropionic acid, 4-hex...	388	C19H33F5O2	1000283-04-1	38
4			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	35
5			Chloroacetic acid, 4-hexadecyl e...	318	C18H35ClO2	1000282-93-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019690.D
Acq On : 13 Feb 2024 22:14
Operator : MA/JU
Sample : P1421-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
72-11977

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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
Phenanthrene, 2...	18.169	2.2	ng	119621	4	17.298	1076350	20.0
n-Hexadecanoic ...	18.198	13.8	ng	743303	4	17.298	1076350	20.0
4H-Cyclopenta[d...	18.351	5.8	ng	314327	4	17.298	1076350	20.0
Isopropyl palmi...	18.610	7.4	ng	397316	4	17.298	1076350	20.0
Isophthalic aci...	18.927	4.3	ng	230418	4	17.298	1076350	20.0
Tetracosylamine...	19.139	2.1	ng	113194	4	17.298	1076350	20.0
Octadecanoic acid	19.433	2.8	ng	298832	5	21.392	2135230	20.0
Pyrene, 1-methyl-	20.145	2.6	ng	277621	5	21.392	2135230	20.0
2,2-Bis-(4-hyxr...	20.210	2.4	ng	256697	5	21.392	2135230	20.0
11H-Benzo[b]flu...	20.245	2.5	ng	266557	5	21.392	2135230	20.0
unknown21.116	21.116	3.3	ng	348435	5	21.392	2135230	20.0