

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
 Data File : BM042588.D
 Acq On : 04 Nov 2023 13:06
 Operator : MA/JU
 Sample : 05237-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 11TH-ST-1

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_M\Methods\8270-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.546	226	231	234	rBV2	16113	21822	1.07%	0.115%
2	4.999	304	308	313	rVB	14947	21220	1.04%	0.112%
3	5.446	378	384	396	rBV	747568	1083771	52.97%	5.729%
4	7.081	655	662	678	rBV	677847	1094419	53.50%	5.786%
5	7.910	797	803	812	rBV	197928	310712	15.19%	1.643%
6	9.110	998	1007	1019	rBV	429516	715214	34.96%	3.781%
7	10.734	1276	1283	1288	rBV	221435	371156	18.14%	1.962%
8	10.781	1288	1291	1300	rVB	26809	44111	2.16%	0.233%
9	12.392	1559	1565	1572	rBV	14545	24865	1.22%	0.131%
10	13.186	1694	1700	1710	rVB	821987	1196288	58.47%	6.324%
11	13.404	1733	1737	1743	rVB3	16386	25156	1.23%	0.133%
12	14.563	1929	1934	1940	rVV	317447	456650	22.32%	2.414%
13	14.628	1940	1945	1952	rVB2	53503	78085	3.82%	0.413%
14	14.963	1991	2002	2008	rBV2	36977	93479	4.57%	0.494%
15	15.616	2107	2113	2121	rVB	53793	84296	4.12%	0.446%
16	15.898	2157	2161	2168	rVB3	17740	27237	1.33%	0.144%
17	16.057	2182	2188	2198	rBV	865189	1201103	58.71%	6.350%
18	16.604	2275	2281	2286	rVB5	13096	26669	1.30%	0.141%
19	16.669	2286	2292	2297	rBV6	15129	27709	1.35%	0.146%
20	16.980	2338	2345	2350	rBV	19077	35305	1.73%	0.187%
21	17.139	2367	2372	2378	rBV	24821	39708	1.94%	0.210%
22	17.316	2397	2402	2406	rBV	390620	558953	27.32%	2.955%
23	17.363	2406	2410	2417	rVB	499243	689376	33.70%	3.644%
24	17.451	2417	2425	2431	rBV	118071	179490	8.77%	0.949%
25	17.739	2470	2474	2482	rVB	56666	88110	4.31%	0.466%
26	18.168	2541	2547	2555	rBV2	883962	1286403	62.88%	6.801%
27	18.239	2555	2559	2569	rVV	96161	199663	9.76%	1.056%
28	18.316	2569	2572	2578	rVV	36326	60030	2.93%	0.317%
29	18.386	2578	2584	2588	rVV3	80437	153289	7.49%	0.810%
30	18.421	2588	2590	2599	rVB	36046	44772	2.19%	0.237%
31	18.692	2631	2636	2640	rVB	38517	53428	2.61%	0.282%
32	18.751	2642	2646	2651	rVB4	20969	31488	1.54%	0.166%
33	19.015	2688	2691	2698	rBV5	18057	30263	1.48%	0.160%
34	19.092	2700	2704	2709	rBV2	31163	50250	2.46%	0.266%
35	19.262	2730	2733	2737	rVB2	16600	21991	1.07%	0.116%
36	19.304	2737	2740	2741	rBV2	25240	26537	1.30%	0.140%

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Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	19.374	2747	2752	2757	rVB	696605	887103	43.36%	4.690%
38	19.445	2759	2764	2776	rBV	383447	580492	28.37%	3.069%
39	19.704	2802	2808	2810	rBV3	111348	180003	8.80%	0.952%
40	19.739	2810	2814	2821	rVV	556041	731722	35.77%	3.868%
41	19.804	2821	2825	2830	rVB2	29972	46152	2.26%	0.244%
42	19.933	2840	2847	2854	rBV	1637293	2045831	100.00%	10.815%
43	20.045	2863	2866	2868	rBV2	32606	43470	2.12%	0.230%
44	20.227	2894	2897	2902	rVB	87944	118293	5.78%	0.625%
45	20.327	2911	2914	2917	rBV2	58401	64809	3.17%	0.343%
46	20.527	2945	2948	2951	rBV	34248	40896	2.00%	0.216%
47	20.980	3022	3025	3029	rBV	42057	57150	2.79%	0.302%
48	21.157	3049	3055	3063	rBV4	197820	447929	21.89%	2.368%
49	21.362	3087	3090	3092	rBV	49867	57775	2.82%	0.305%
50	21.498	3106	3113	3117	rBV2	690628	1283352	62.73%	6.784%
51	21.533	3117	3119	3125	rVB	305049	354486	17.33%	1.874%
52	23.168	3393	3397	3403	rBV	190544	422555	20.65%	2.234%
53	23.803	3501	3505	3513	rVB	182143	341259	16.68%	1.804%
54	23.915	3518	3524	3530	rBV	381706	759940	37.15%	4.017%

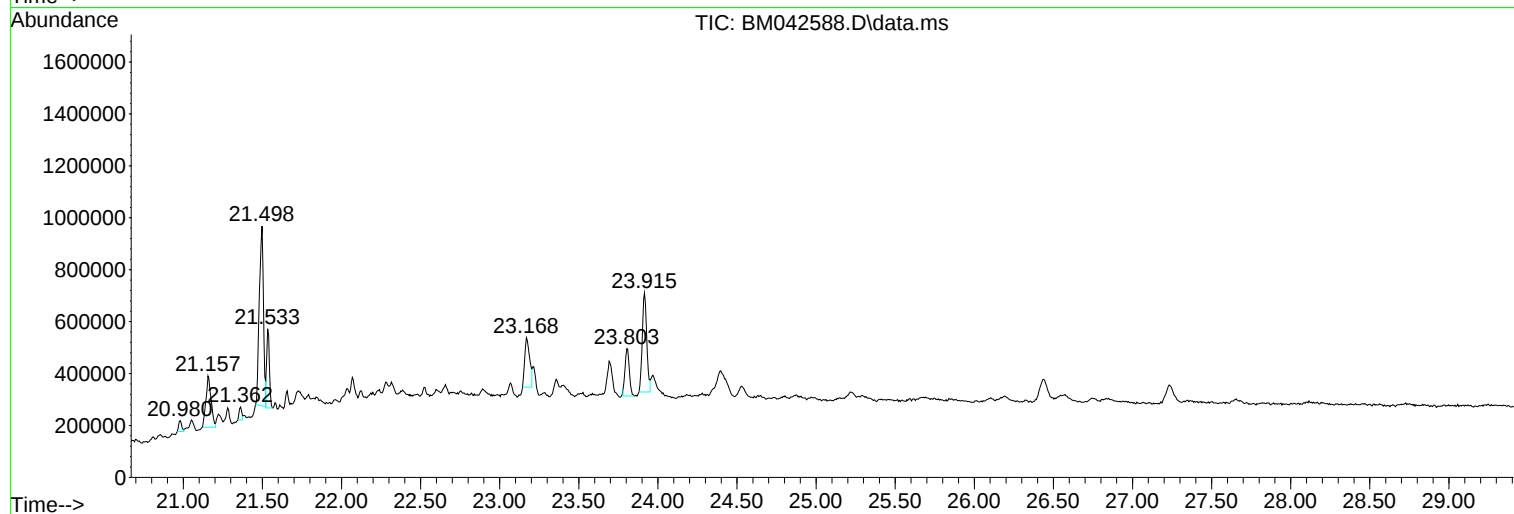
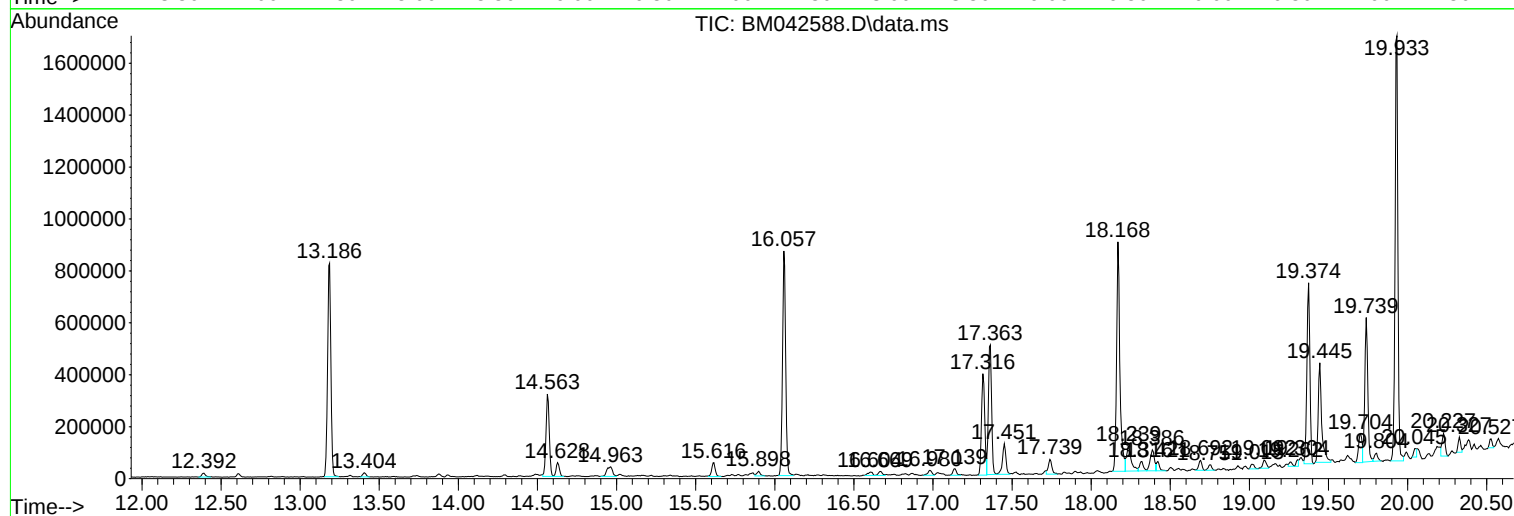
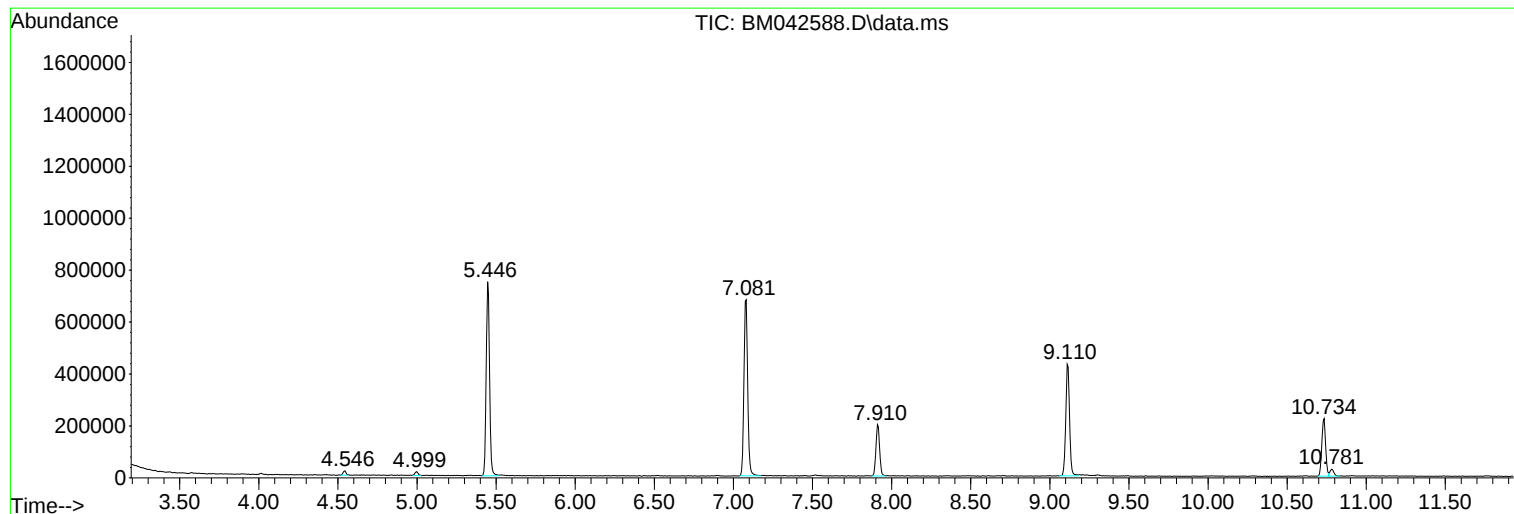
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042588.D
Acq On : 04 Nov 2023 13:06
Operator : MA/JU
Sample : 05237-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

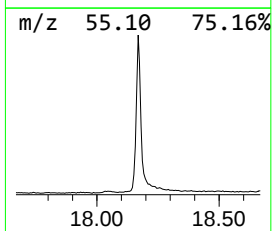
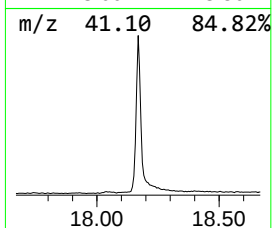
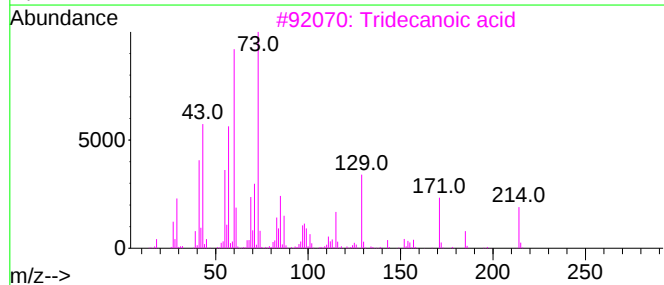
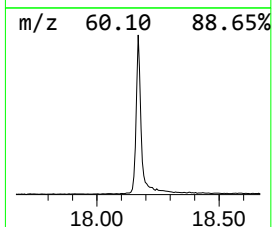
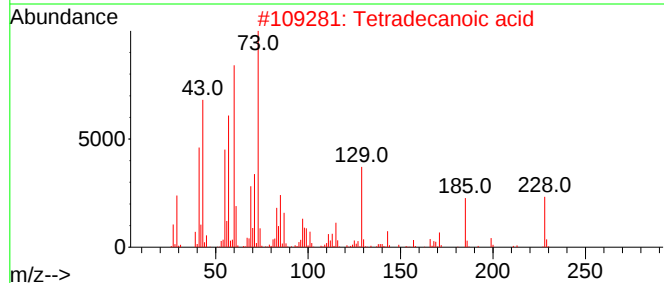
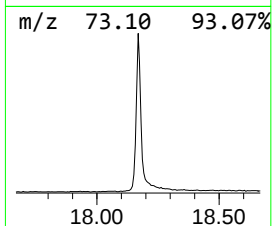
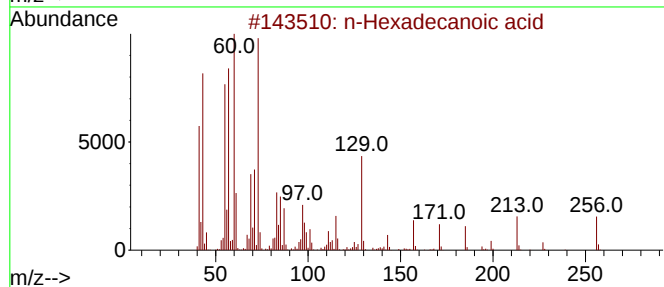
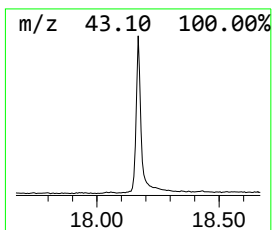
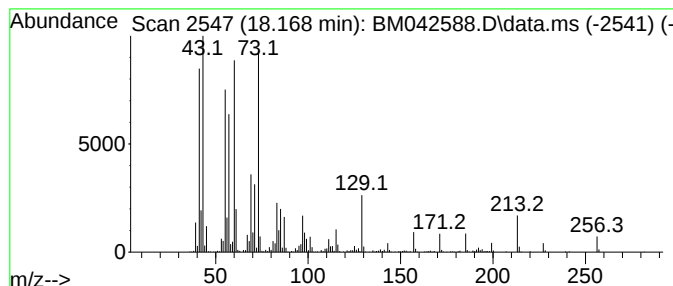
Instrument :
BNA_M
ClientSampleId :
11TH-ST-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.169	46.03 ng	1286400	Phenanthrene-d10		17.316	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	95
3	Tridecanoic acid		214	C13H26O2	000638-53-9	94
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	Undecanoic acid		186	C11H22O2	000112-37-8	78



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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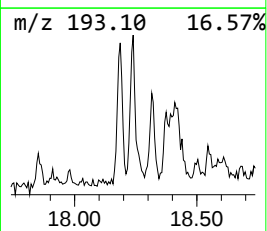
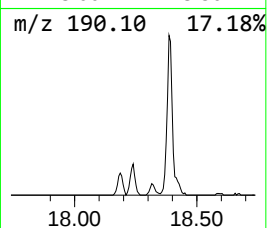
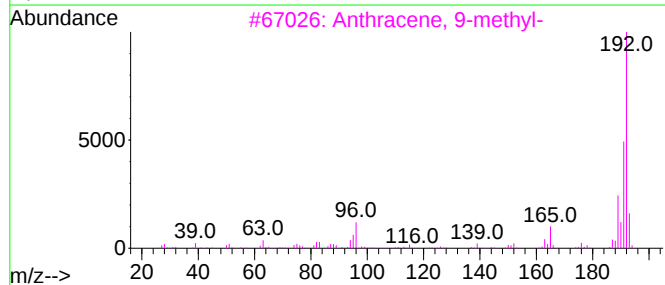
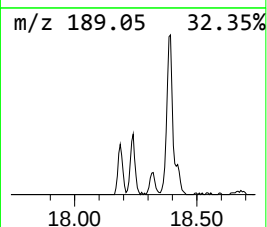
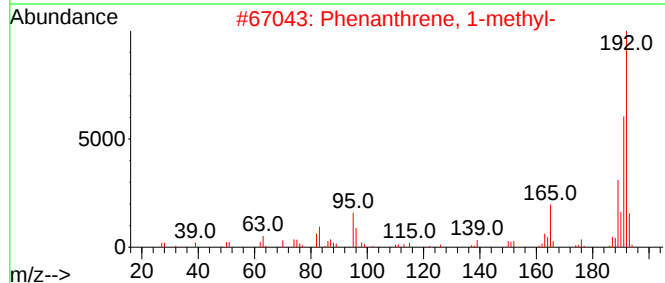
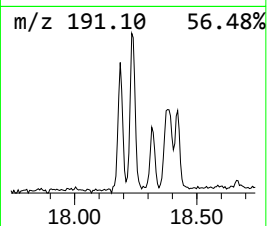
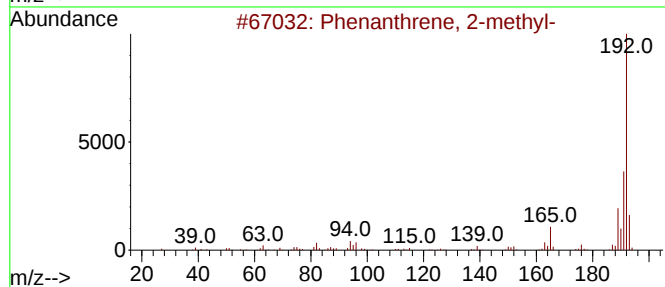
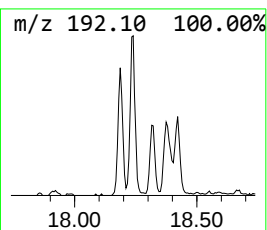
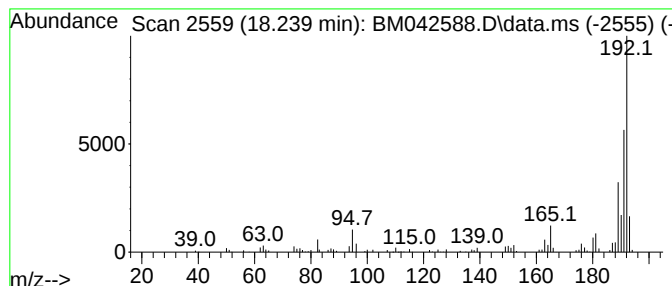
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	7.14 ng	199663	Phenanthrene-d10	17.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3			Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91



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Misc :
ALS Vial : 5 Sample Multiplier: 1

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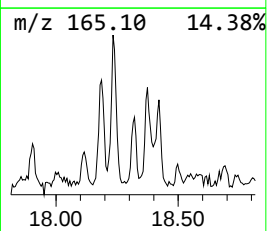
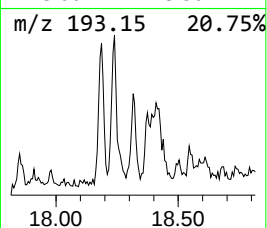
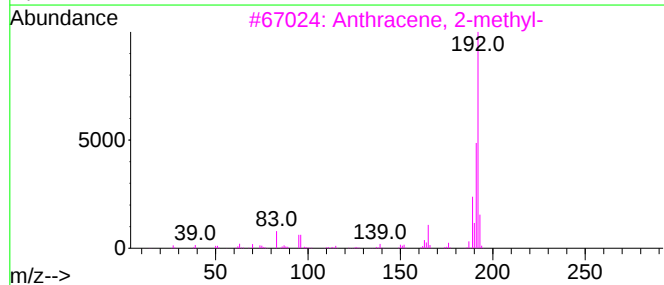
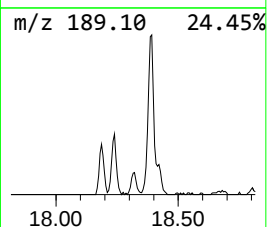
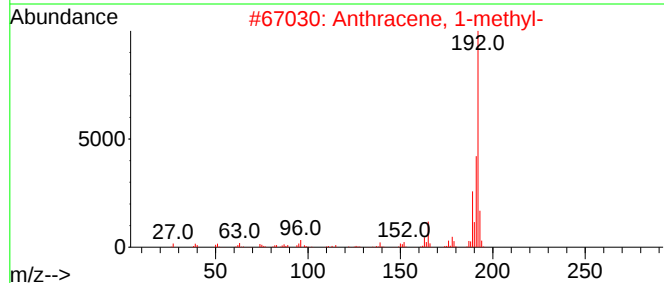
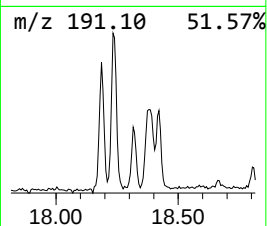
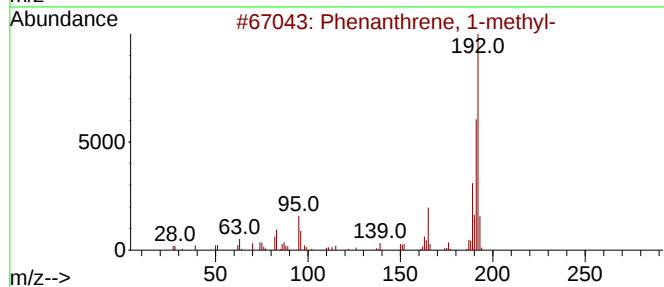
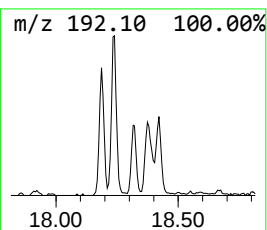
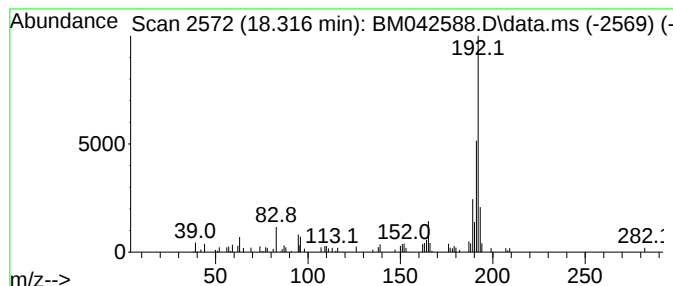
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.316	2.15 ng	60030	Phenanthrene-d10	17.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



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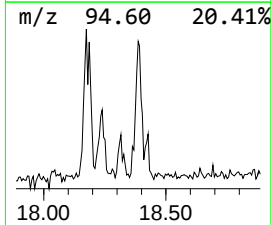
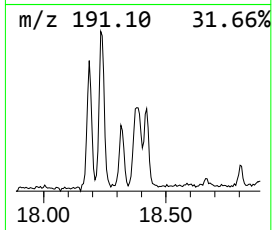
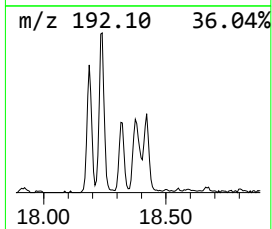
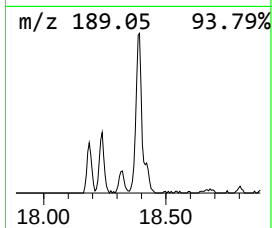
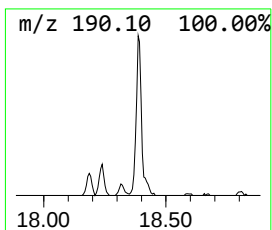
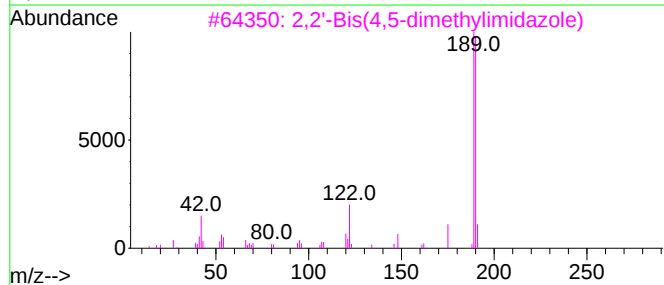
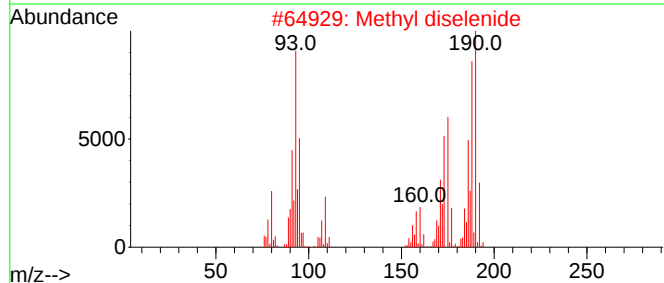
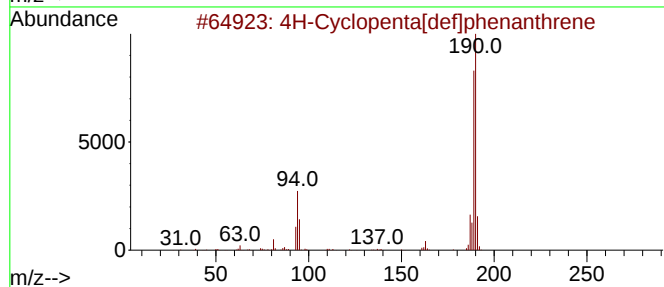
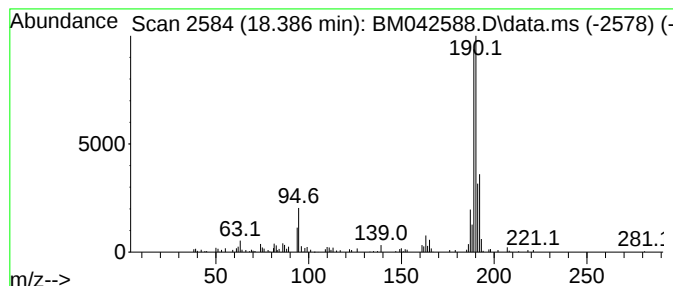
Instrument :
BNA_M
ClientSampleId :
11TH-ST-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.386	5.48 ng	153289	Phenanthrene-d10	17.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Methyl diselenide	190	C2H6Se2	007101-31-7	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	33
5	1-Aminocyclopentanecarboxylic ac...	297	C11H17Cl2NO4	1000329-17-6	27



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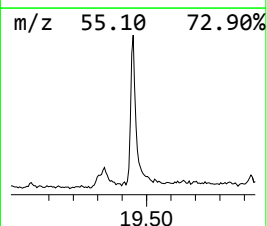
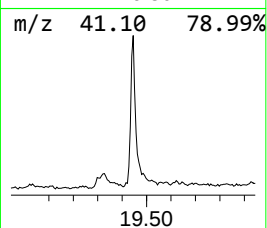
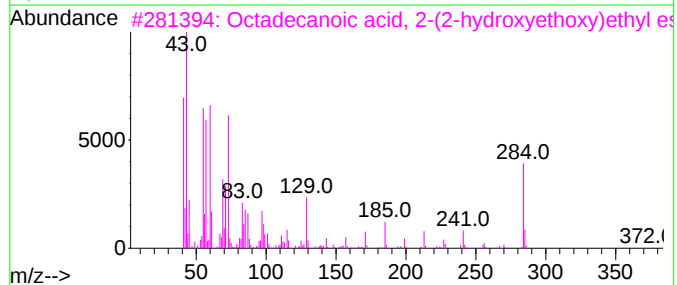
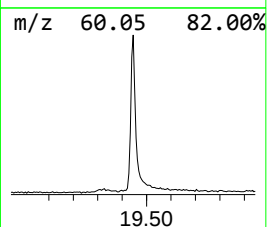
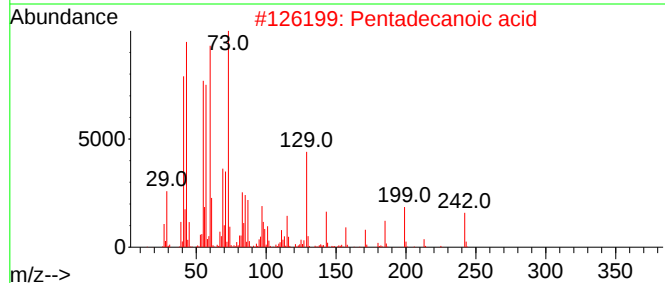
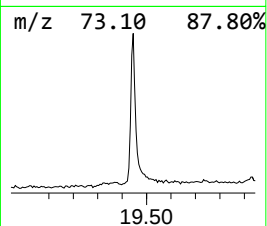
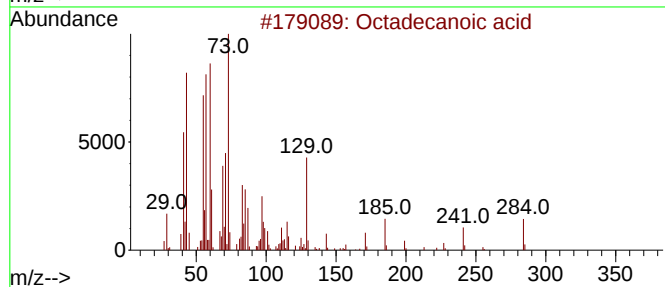
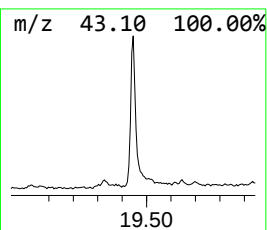
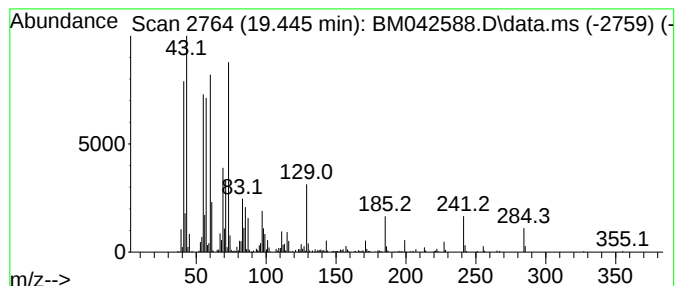
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	9.05 ng	580492	Chrysene-d12	21.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042588.D
Acq On : 04 Nov 2023 13:06
Operator : MA/JU
Sample : 05237-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
11TH-ST-1

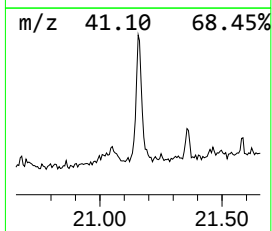
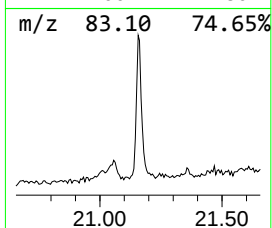
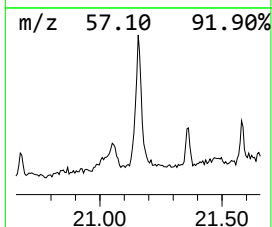
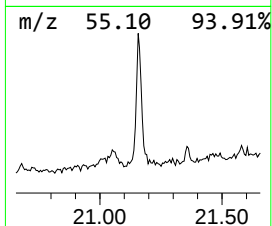
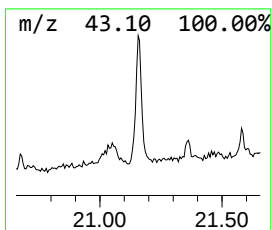
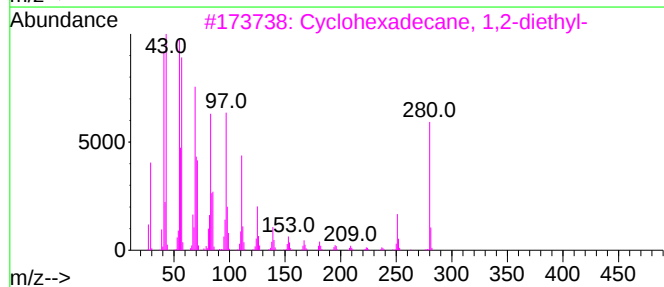
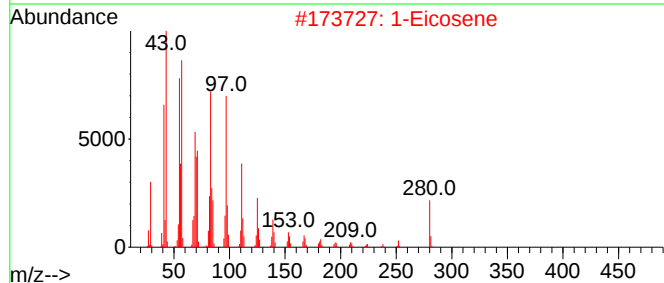
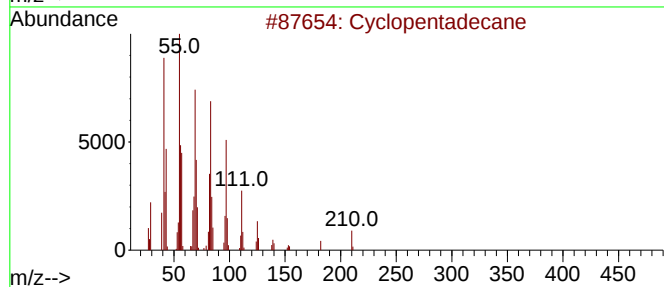
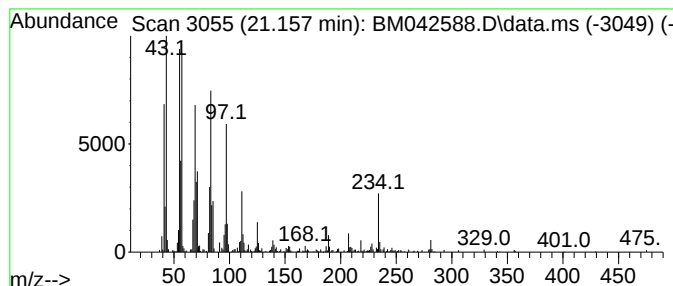
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.157	6.98 ng	447929	Chrysene-d12	21.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			1-Eicosene	280	C20H40	003452-07-1	94
3			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	93
5			E-14-Hexadecenal	238	C16H30O	330207-53-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042588.D
Acq On : 04 Nov 2023 13:06
Operator : MA/JU
Sample : 05237-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
11TH-ST-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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 ...	18.169	46.0	ng	1286400	4	17.316	558953	20.0
Phenanthrene, 2...	18.239	7.1	ng	199663	4	17.316	558953	20.0
Phenanthrene, 1...	18.316	2.1	ng	60030	4	17.316	558953	20.0
4H-Cyclopenta[d...	18.386	5.5	ng	153289	4	17.316	558953	20.0
Octadecanoic acid	19.445	9.1	ng	580492	5	21.498	1283350	20.0
Cyclopentadecane	21.157	7.0	ng	447929	5	21.498	1283350	20.0