

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
 Data File : BM028615.D
 Acq On : 29 Jan 2021 20:41
 Operator : CG/JU
 Sample : M1271-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RO-332

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-BM012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.540	57	60	72	rBV	9653	14746	1.80%	0.198%
2	5.475	383	389	398	rBV	317443	452562	55.32%	6.082%
3	7.110	660	667	676	rBV	308015	481885	58.91%	6.476%
4	7.534	735	739	745	rBV	5563	8759	1.07%	0.118%
5	7.928	800	806	813	rVB	100380	154991	18.95%	2.083%
6	9.104	999	1006	1014	rBV	191776	303865	37.14%	4.083%
7	10.739	1278	1284	1291	rVB	127566	210858	25.78%	2.834%
8	13.204	1696	1703	1710	rBV	451684	640823	78.33%	8.612%
9	14.033	1839	1844	1851	rVB	34593	45221	5.53%	0.608%
10	14.304	1883	1890	1895	rBV	16282	24299	2.97%	0.327%
11	14.580	1931	1937	1944	rVB	188059	265719	32.48%	3.571%
12	16.068	2184	2190	2196	rVB	355726	477253	58.34%	6.414%
13	16.298	2221	2229	2234	rBV2	5632	11717	1.43%	0.157%
14	17.315	2396	2402	2407	rBV	218727	295545	36.13%	3.972%
15	18.198	2545	2552	2567	rBV	98011	144768	17.70%	1.945%
16	19.239	2723	2729	2737	rBV	15901	24913	3.05%	0.335%
17	19.356	2744	2749	2756	rVB	63608	84294	10.30%	1.133%
18	19.462	2762	2767	2772	rBV2	55758	76334	9.33%	1.026%
19	19.509	2772	2775	2780	rVB2	9209	13142	1.61%	0.177%
20	19.621	2789	2794	2801	rVB4	5635	12382	1.51%	0.166%
21	19.686	2801	2805	2807	rBV2	17200	24487	2.99%	0.329%
22	19.721	2807	2811	2816	rVB	99625	131149	16.03%	1.762%
23	19.915	2839	2844	2849	rBV	668465	818062	100.00%	10.994%
24	19.962	2849	2852	2858	rVB	18862	23910	2.92%	0.321%
25	20.050	2860	2867	2872	rBV3	14112	31077	3.80%	0.418%
26	20.209	2882	2894	2899	rBV3	25500	82686	10.11%	1.111%
27	20.303	2907	2910	2914	rBV	14780	20401	2.49%	0.274%
28	20.362	2914	2920	2924	rVV3	17503	35812	4.38%	0.481%
29	20.403	2924	2927	2931	rVB2	8550	11380	1.39%	0.153%
30	20.503	2940	2944	2947	rBV	20524	25299	3.09%	0.340%
31	20.550	2948	2952	2956	rVV3	11156	16403	2.01%	0.220%
32	20.950	3017	3020	3025	rVB2	13300	16946	2.07%	0.228%
33	21.109	3044	3047	3051	rBV	15657	21509	2.63%	0.289%
34	21.162	3051	3056	3059	rBV2	109658	150513	18.40%	2.023%
35	21.362	3086	3090	3094	rVB	62796	68849	8.42%	0.925%
36	21.456	3100	3106	3111	rBV2	331830	577401	70.58%	7.759%

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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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37	21.497	3111	3113	3122	rVB2	84893	101613	12.42%	1.366%
38	21.609	3129	3132	3138	rBV	27564	41568	5.08%	0.559%
39	21.774	3156	3160	3164	rBV2	20456	32822	4.01%	0.441%
40	23.039	3369	3375	3380	rBV	171554	390449	47.73%	5.247%
41	23.209	3401	3404	3409	rVB	40521	60131	7.35%	0.808%
42	23.521	3452	3457	3463	rVB	107844	189430	23.16%	2.546%
43	23.615	3468	3473	3480	rVB	144548	255140	31.19%	3.429%
44	23.715	3484	3490	3495	rBV2	184146	339393	41.49%	4.561%
45	26.003	3873	3879	3891	rVB	80209	230816	28.21%	3.102%

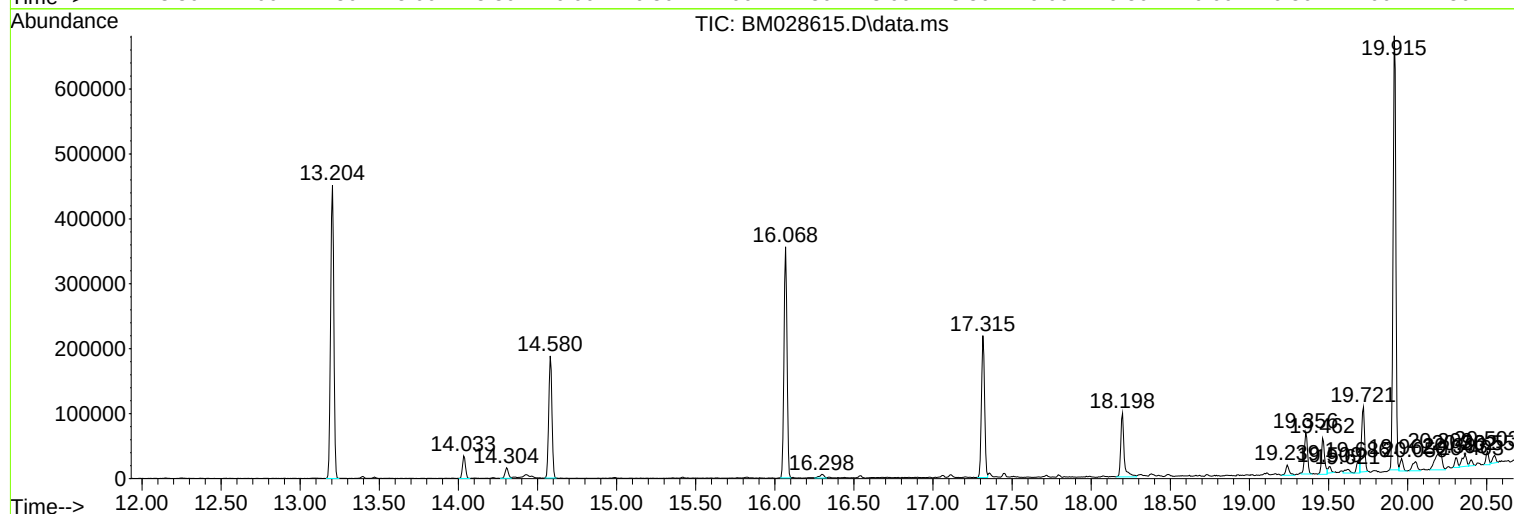
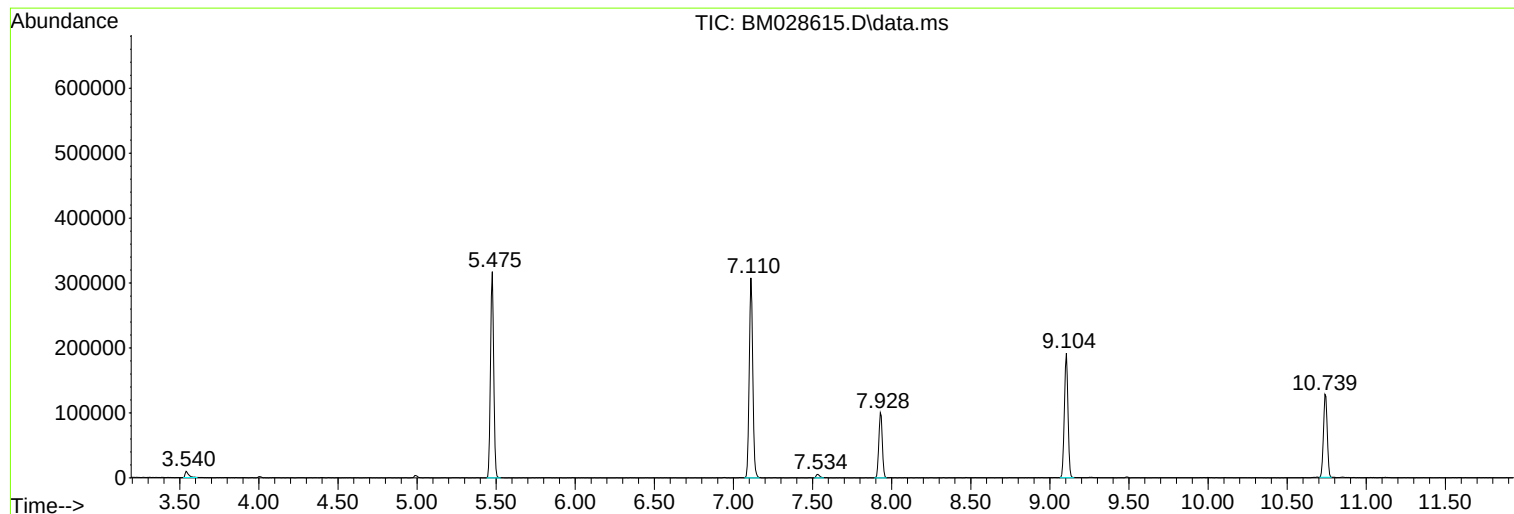
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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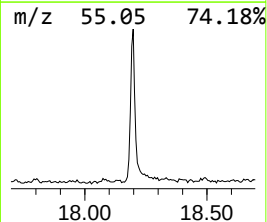
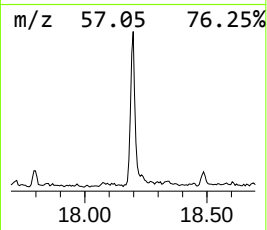
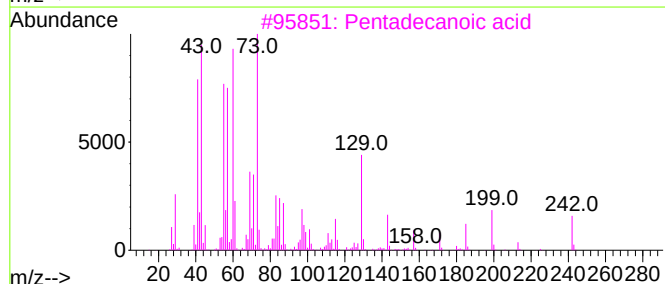
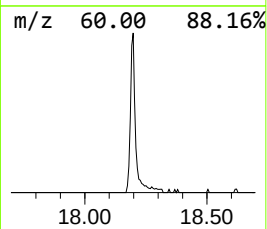
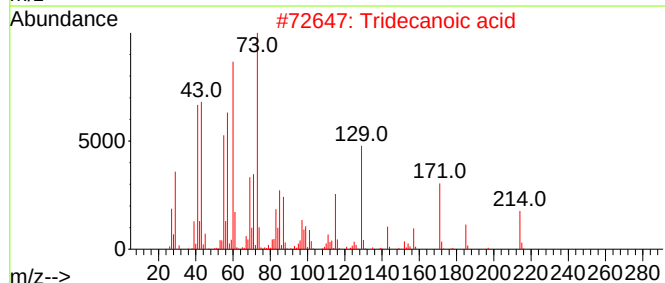
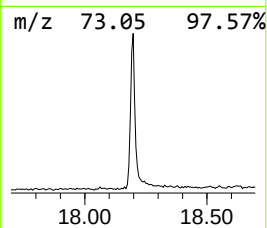
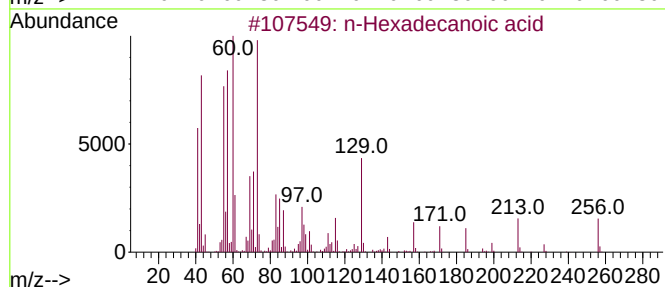
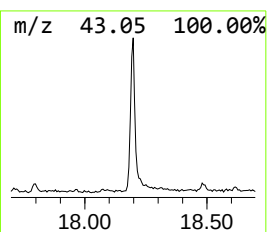
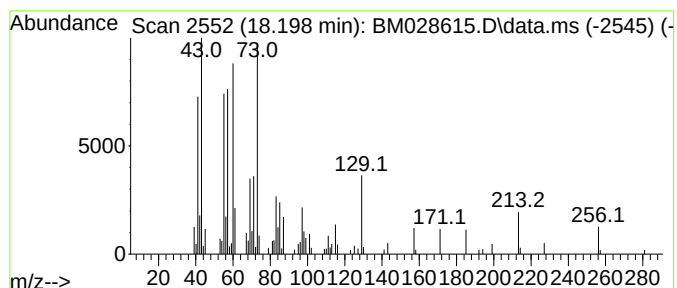
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	9.80 ng	144768	Phenanthrene-d10	17.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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Misc :
ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
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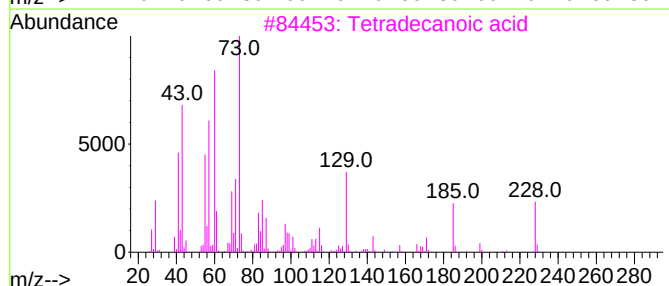
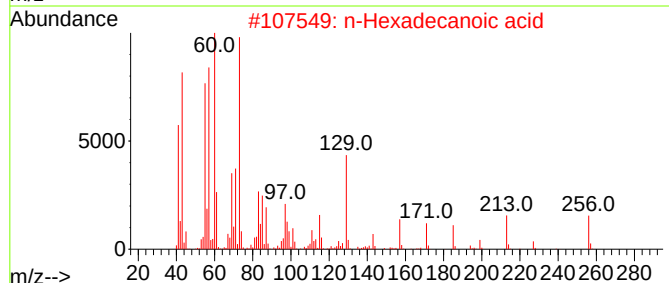
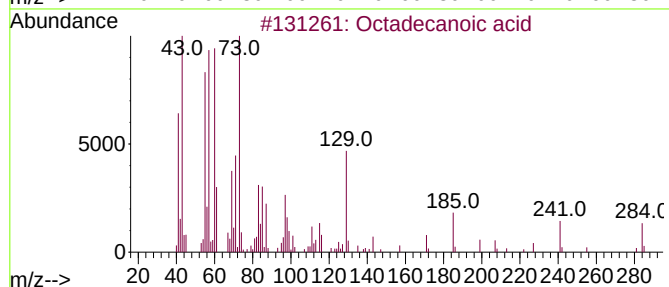
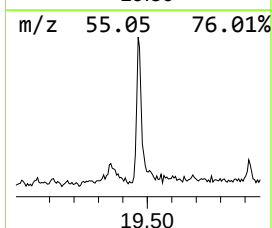
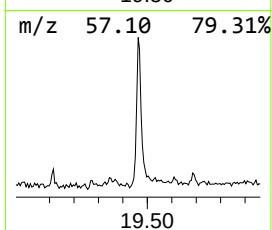
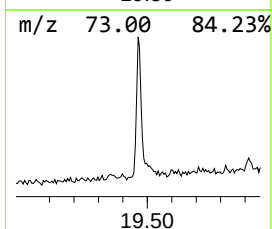
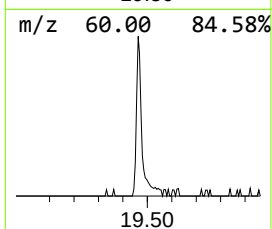
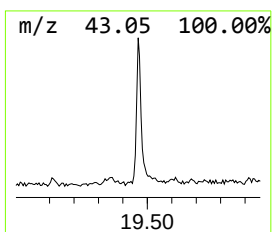
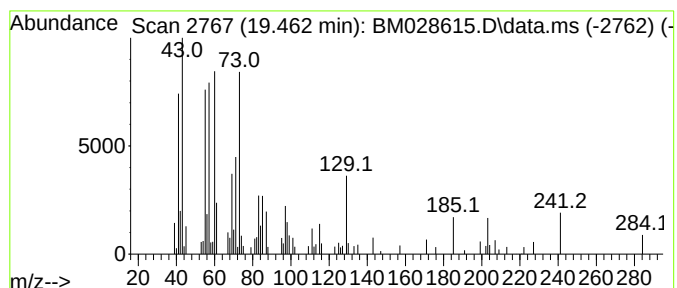
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	2.64 ng	76334	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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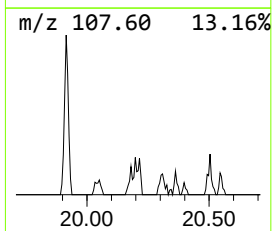
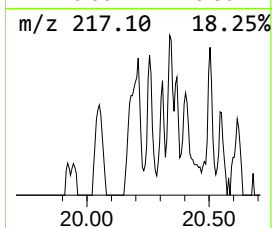
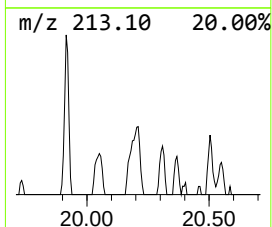
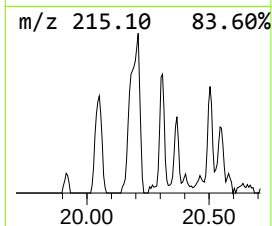
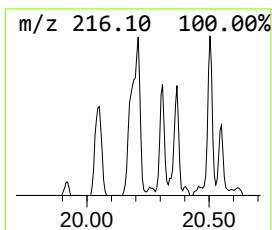
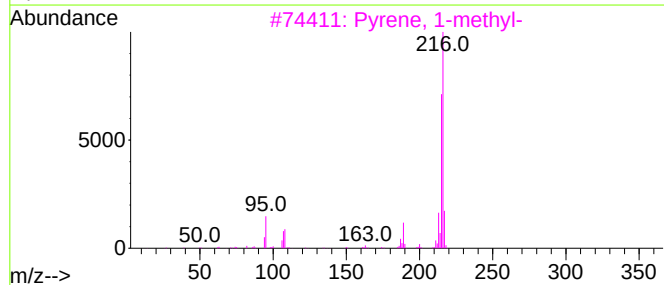
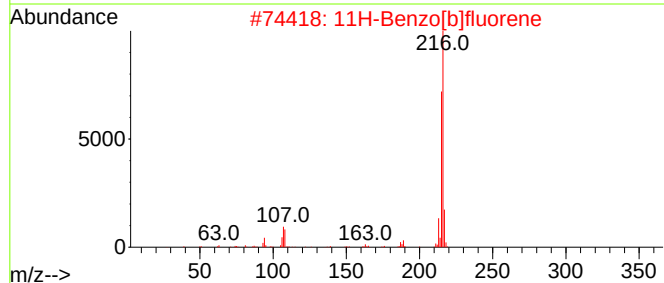
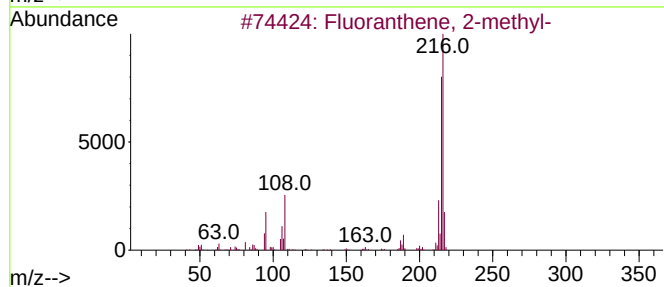
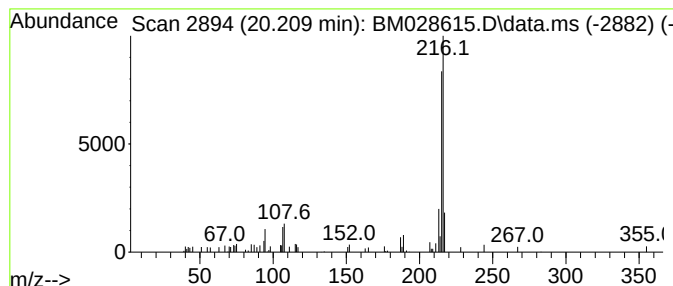
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Fluoranthene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.209	2.86 ng	82686	Chrysene-d12	21.456

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3		Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	86



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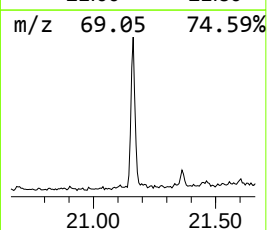
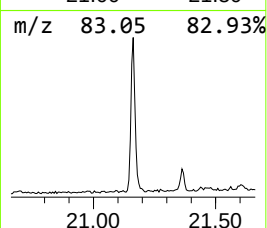
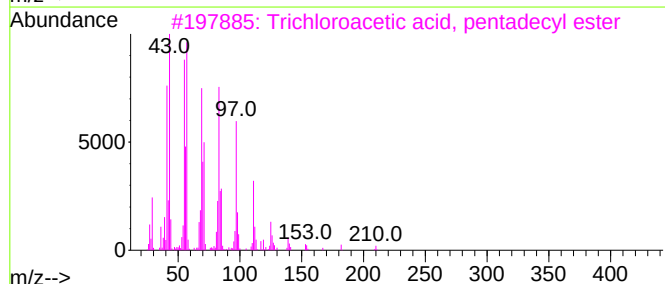
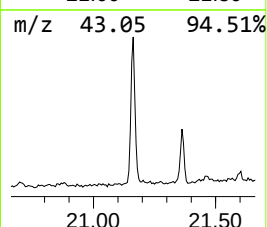
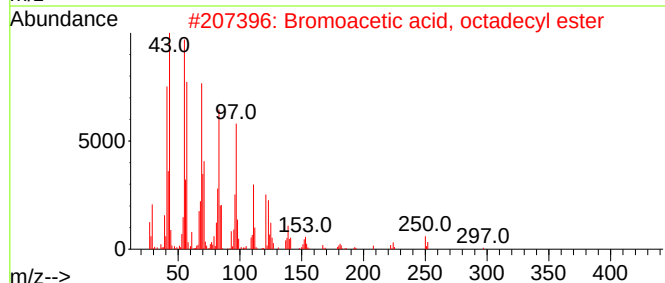
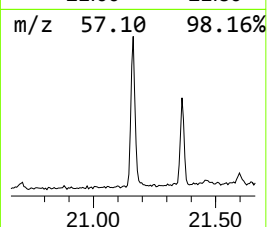
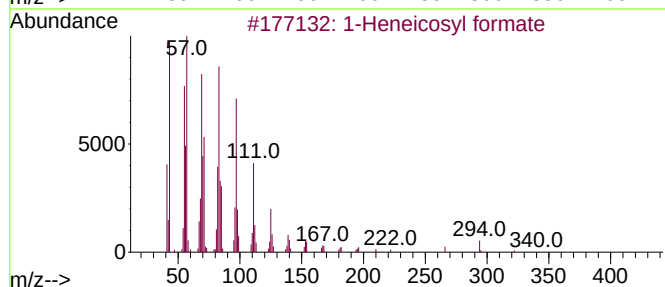
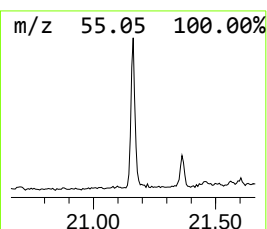
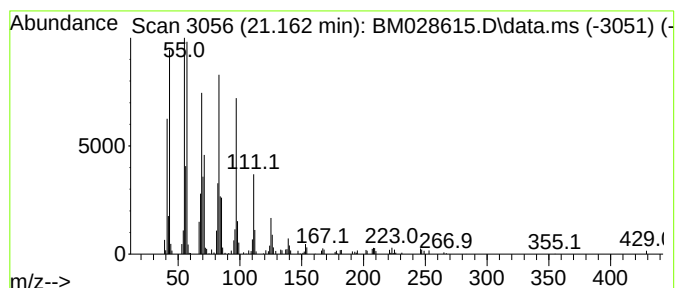
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	5.21 ng	150513	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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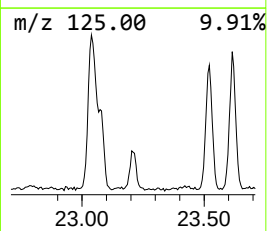
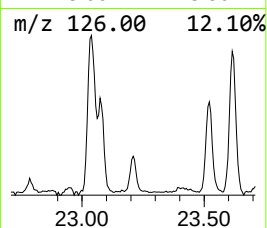
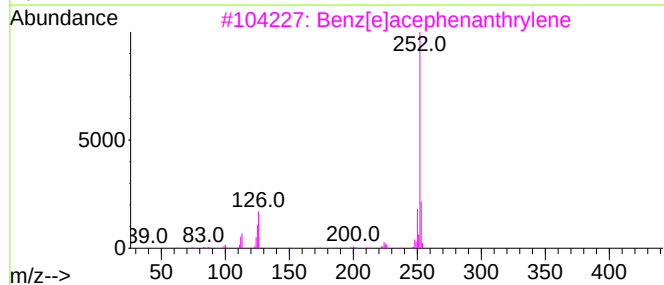
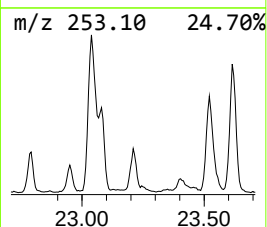
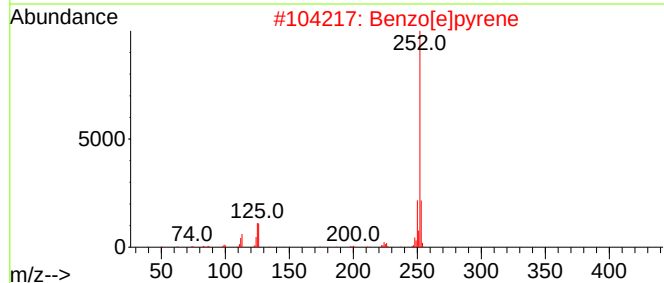
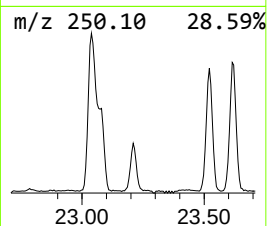
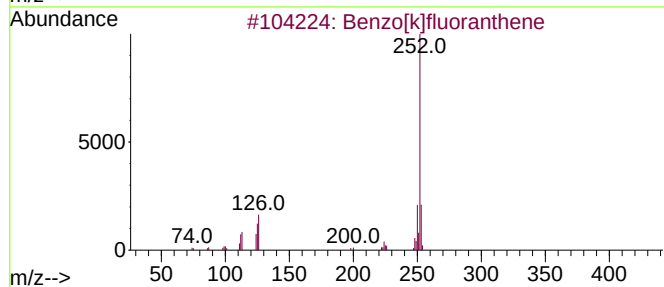
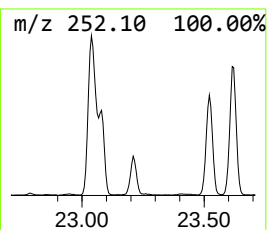
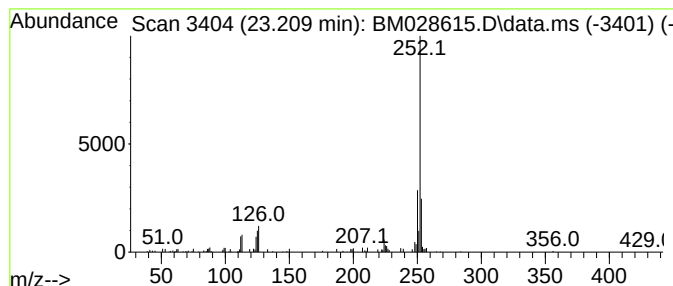
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.209	3.54 ng	60131	Perylene-d12	23.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028615.D
Acq On : 29 Jan 2021 20:41
Operator : CG/JU
Sample : M1271-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-332

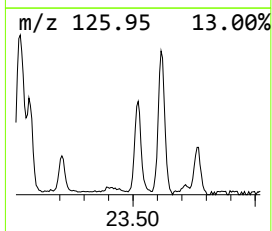
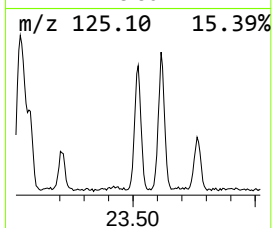
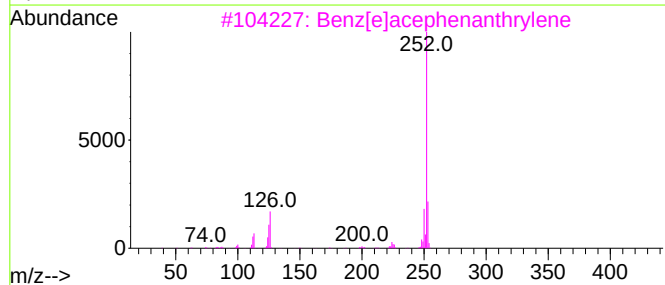
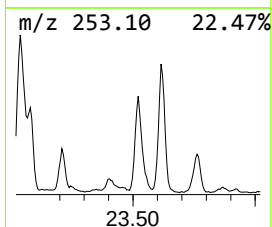
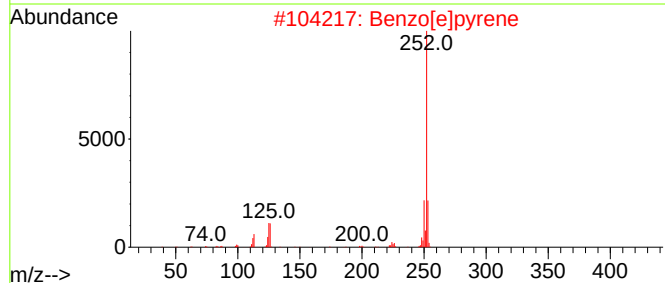
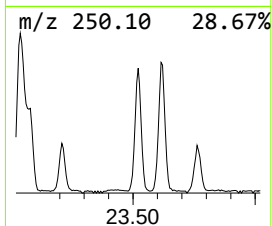
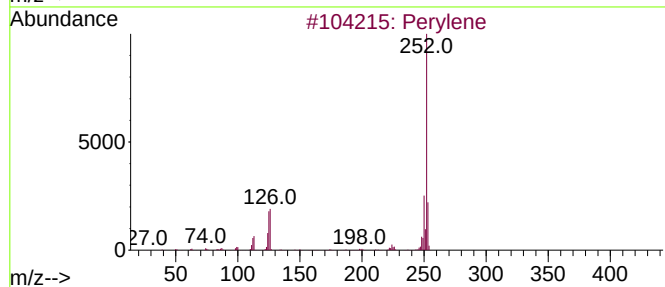
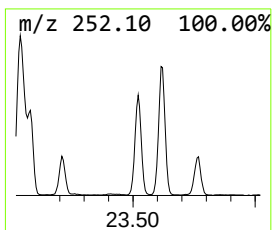
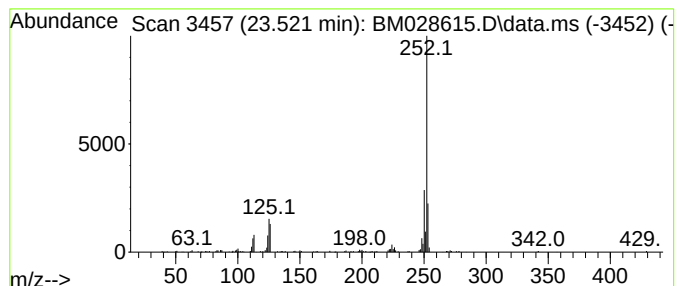
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.521	11.16 ng	189430	Perylene-d12	23.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	99
2			Benzo[e]pyrene	252	C20H12	000192-97-2	99
3			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	98
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012921\
Data File : BM028615.D
Acq On : 29 Jan 2021 20:41
Operator : CG/JU
Sample : M1271-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-332

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.198	9.8	ng	144768	4	17.315	295545	20.0
Octadecanoic acid	19.462	2.6	ng	76334	5	21.456	577401	20.0
Fluoranthene, 2...	20.209	2.9	ng	82686	5	21.456	577401	20.0
1-Heneicosyl fo...	21.162	5.2	ng	150513	5	21.456	577401	20.0
Benzo[e]pyrene	23.209	3.5	ng	60131	6	23.715	339393	20.0
Perylene	23.521	11.2	ng	189430	6	23.715	339393	20.0