

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
 Data File : BM029628.D
 Acq On : 24 Apr 2021 00:22
 Operator : CG/JU
 Sample : M2117-01 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PL-01-042121

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-BM042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029628.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	393	399	410	rBV	218747	335258	14.62%	1.794%
2	6.816	662	668	683	rBV	196597	332665	14.51%	1.780%
3	7.634	800	807	817	rBV	356123	561614	24.50%	3.005%
4	8.793	997	1004	1012	rBV	112652	203941	8.90%	1.091%
5	10.416	1269	1280	1286	rBV	428765	733178	31.98%	3.923%
6	11.851	1517	1524	1529	rBV3	13842	26971	1.18%	0.144%
7	12.087	1555	1564	1570	rVB5	11794	26722	1.17%	0.143%
8	12.898	1694	1702	1709	rBV	370550	570257	24.87%	3.051%
9	13.110	1732	1738	1744	rBV2	22232	37200	1.62%	0.199%
10	13.739	1841	1845	1849	rBV2	20331	32023	1.40%	0.171%
11	13.998	1883	1889	1898	rBV	51819	96530	4.21%	0.516%
12	14.122	1905	1910	1917	rBV6	15439	36842	1.61%	0.197%
13	14.192	1917	1922	1927	rVV	33535	45433	1.98%	0.243%
14	14.281	1930	1937	1943	rVV	695286	1026013	44.75%	5.490%
15	14.345	1944	1948	1955	rVB	37041	59445	2.59%	0.318%
16	14.681	1995	2005	2013	rBV	26815	65323	2.85%	0.350%
17	14.810	2023	2027	2036	rBV8	13662	27663	1.21%	0.148%
18	15.145	2080	2084	2090	rVB2	41990	56430	2.46%	0.302%
19	15.328	2111	2115	2119	rBV	49820	71615	3.12%	0.383%
20	15.551	2148	2153	2161	rVB6	22825	39834	1.74%	0.213%
21	15.769	2185	2190	2199	rVB	299266	448674	19.57%	2.401%
22	16.010	2226	2231	2233	rBV	61376	87830	3.83%	0.470%
23	16.798	2362	2365	2369	rVV	48095	51725	2.26%	0.277%
24	16.845	2370	2373	2385	rVB3	50056	86313	3.76%	0.462%
25	17.028	2398	2404	2408	rBV	789971	1208307	52.70%	6.465%
26	17.069	2408	2411	2418	rVV	348805	485757	21.19%	2.599%
27	17.157	2422	2426	2432	rVB	163490	235669	10.28%	1.261%
28	17.433	2470	2473	2481	rVB	27699	47941	2.09%	0.257%
29	17.533	2487	2490	2495	rBV4	47298	63394	2.76%	0.339%
30	17.704	2515	2519	2525	rVB	179136	230764	10.07%	1.235%
31	17.898	2548	2552	2554	rBV	62990	82726	3.61%	0.443%
32	17.933	2554	2558	2569	rVB2	151285	329288	14.36%	1.762%
33	18.092	2580	2585	2589	rBV4	112673	198786	8.67%	1.064%
34	18.227	2605	2608	2611	rBV	39570	46750	2.04%	0.250%
35	18.404	2635	2638	2641	rVB	39941	47181	2.06%	0.252%
36	18.851	2706	2714	2717	rBV2	808150	1084549	47.30%	5.803%

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Instrument :
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ClientSampleId :
PL-01-042121

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	18.886	2717	2720	2724	rVB	700226	806128	35.16%	4.313%
38	19.021	2739	2743	2747	rBV	139711	173696	7.58%	0.929%
39	19.086	2749	2754	2762	rVV	850707	1265524	55.20%	6.771%
40	19.445	2812	2815	2825	rVB	726054	1070352	46.68%	5.727%
41	19.657	2847	2851	2855	rVB	716270	840713	36.67%	4.498%
42	20.045	2914	2917	2921	rBV	118471	153240	6.68%	0.820%
43	21.204	3109	3114	3118	rBV2	1347455	2292734	100.00%	12.267%
44	21.245	3118	3121	3128	rVB	499633	681624	29.73%	3.647%
45	22.745	3372	3376	3381	rBV	513477	1002396	43.72%	5.363%
46	23.404	3484	3488	3494	rVB	794478	1282926	55.96%	6.864%

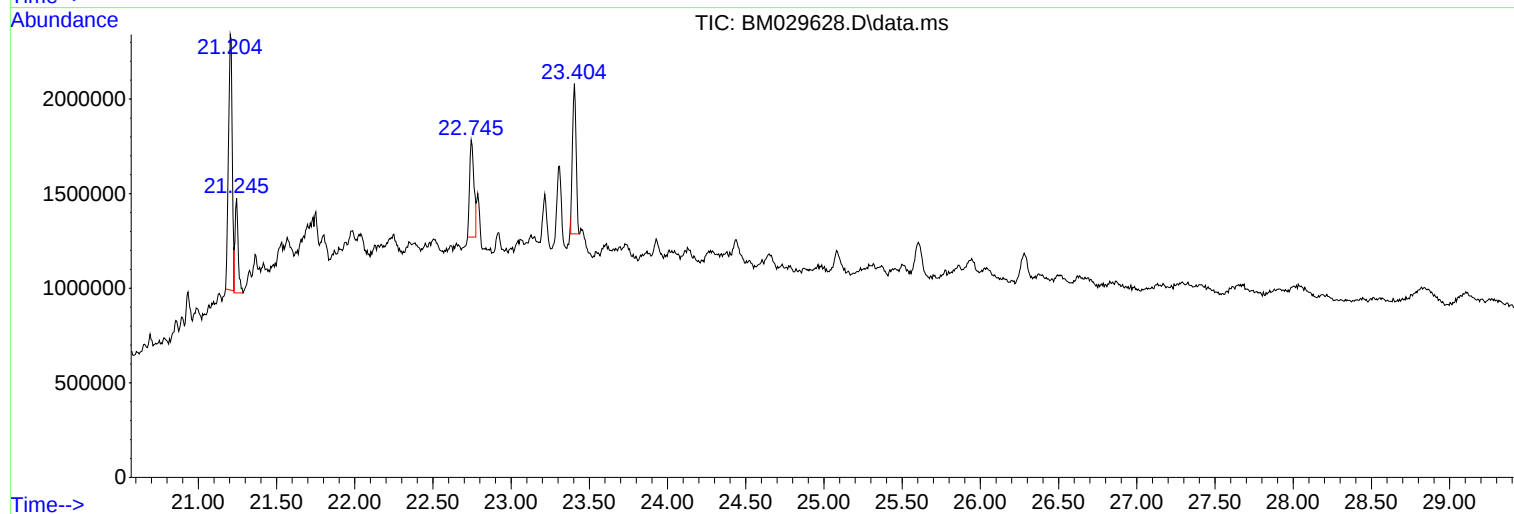
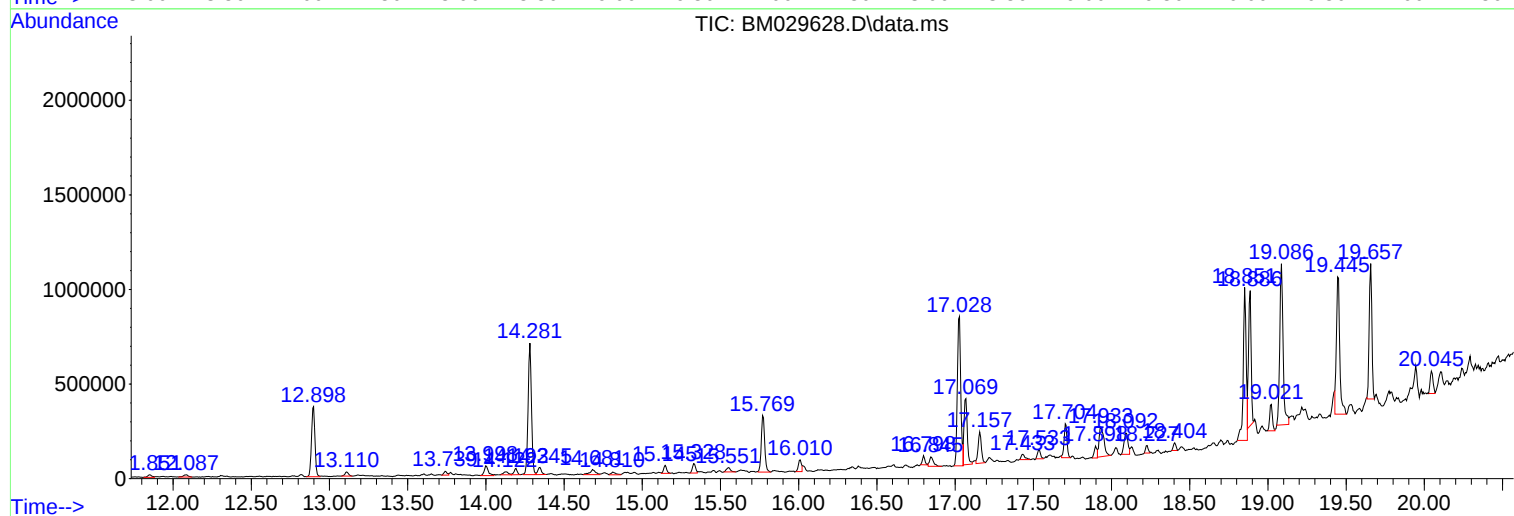
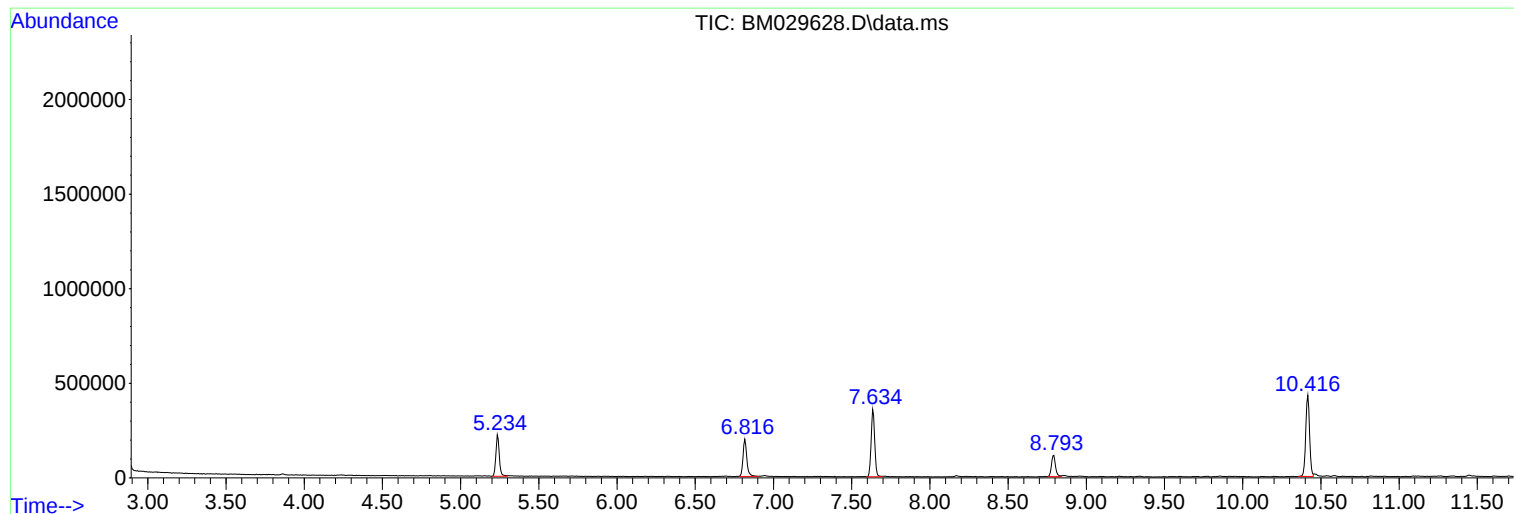
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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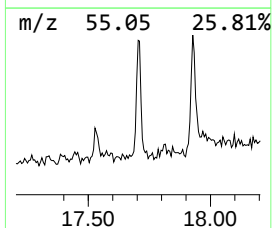
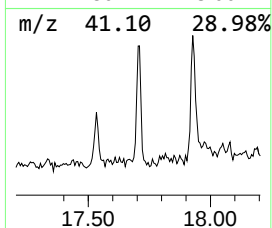
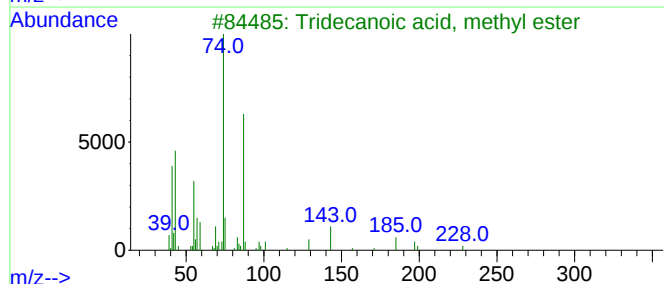
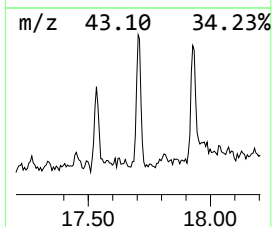
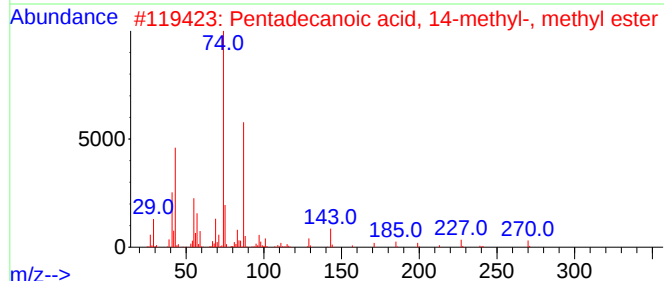
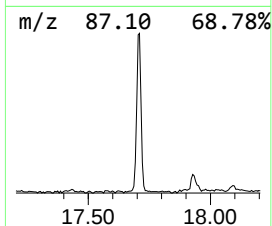
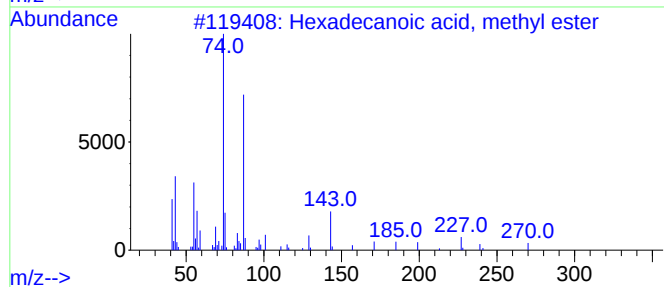
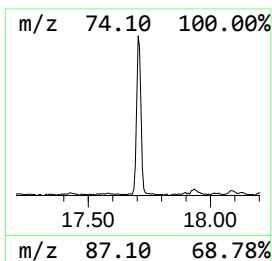
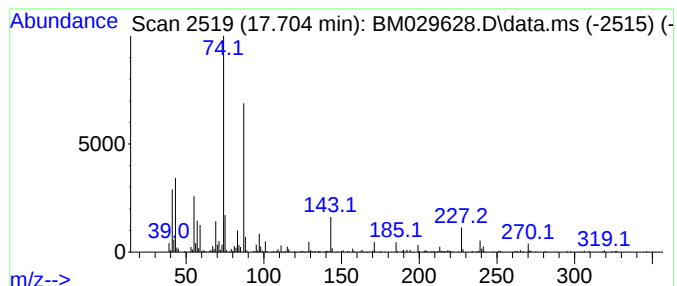
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.704	3.82 ng	230764	Phenanthrene-d10	17.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81



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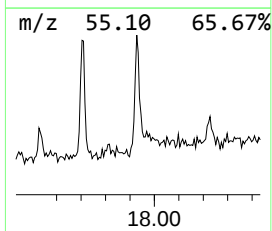
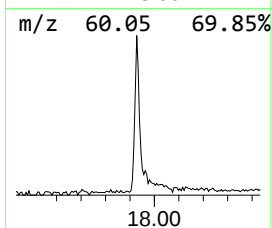
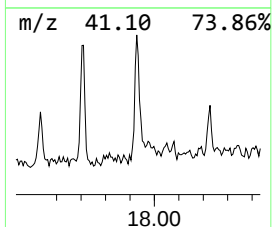
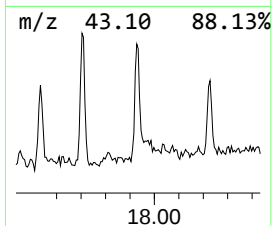
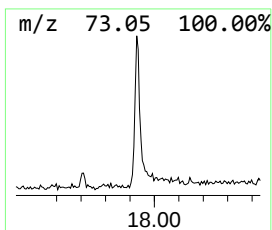
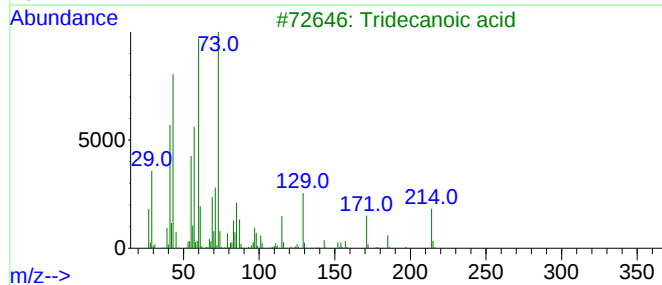
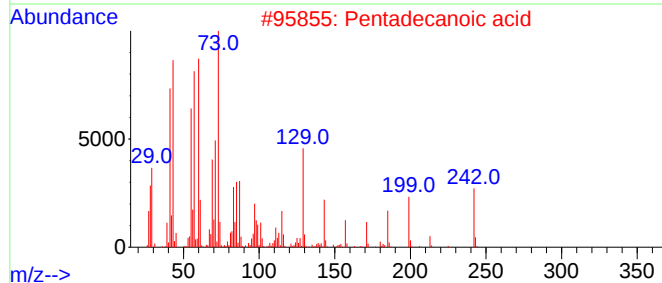
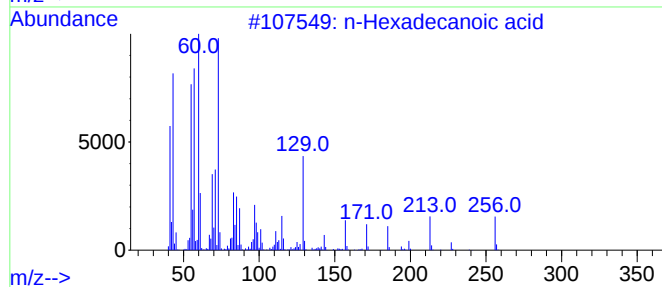
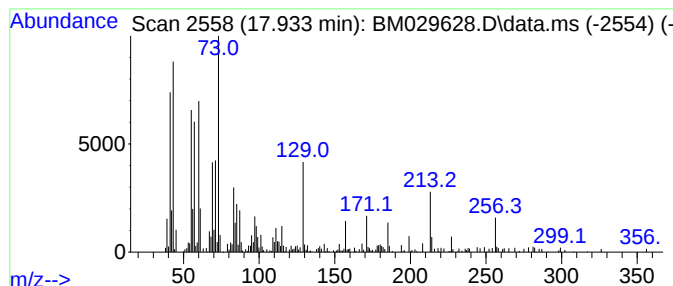
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	5.45 ng	329288	Phenanthrene-d10	17.028

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	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Octadecanoic acid	284	C18H36O2	000057-11-4	70



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ALS Vial : 16 Sample Multiplier: 1

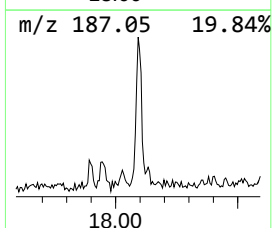
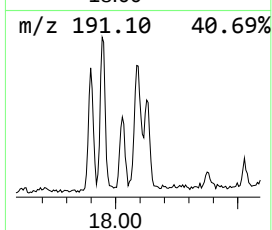
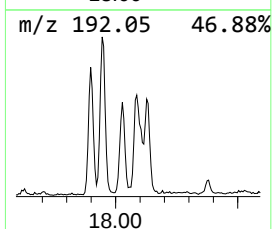
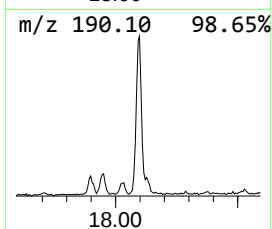
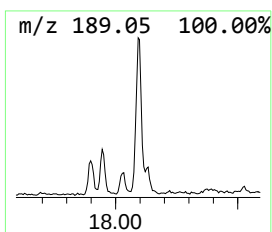
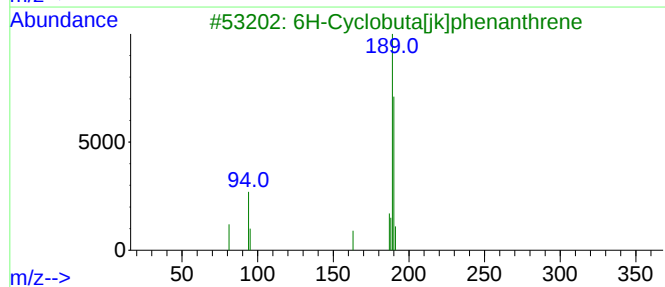
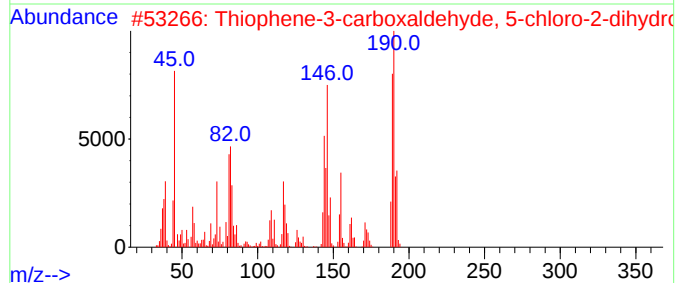
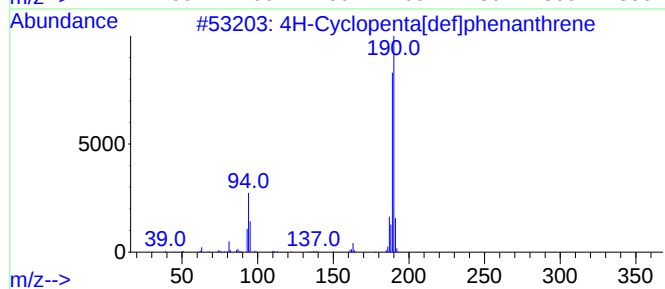
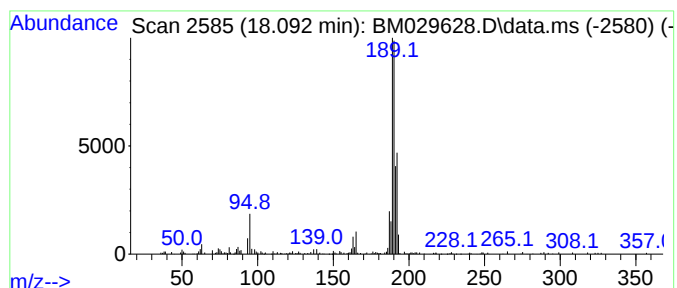
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.092	3.29 ng	198786	Phenanthrene-d10		17.028	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene		190	C15H10	000203-64-5	70
2	Thiophene-3-carboxaldehyde, 5-ch...		190	C5H4BClO3S	036155-87-0	53
3	6H-Cyclobuta[jk]phenanthrene		190	C15H10	083469-43-6	52
4	Benzaldehyde, 3,5-dichloro-2-hyd...		190	C7H4Cl2O2	000090-60-8	43
5	Pyrazole-4-carboxaldehyde, 3-(4-...		190	C10H7FN2O	306936-57-2	43



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ClientSampleId :
PL-01-042121

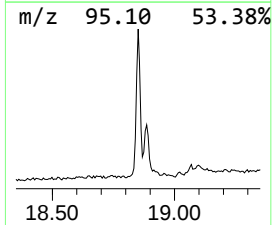
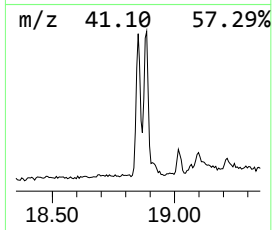
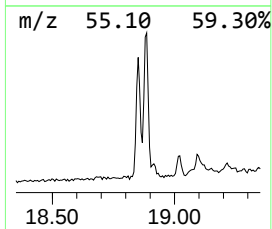
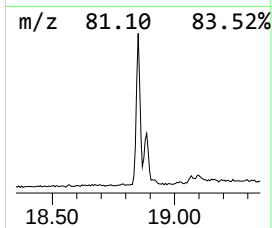
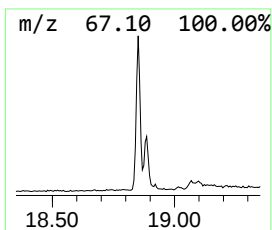
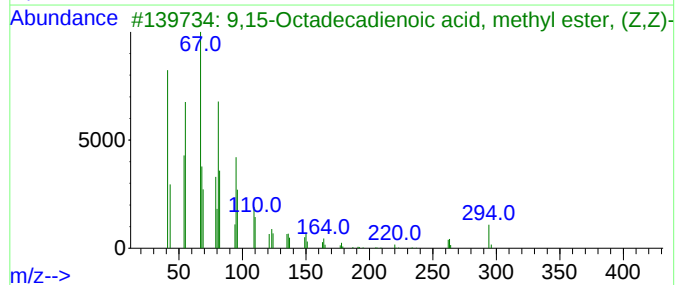
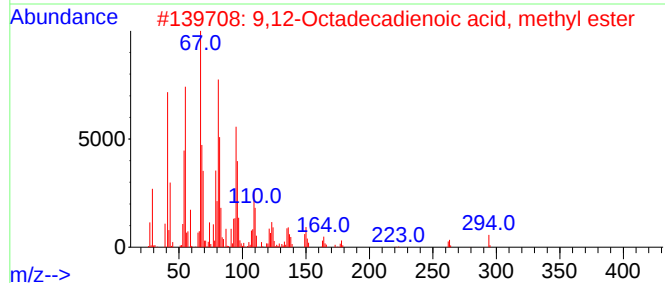
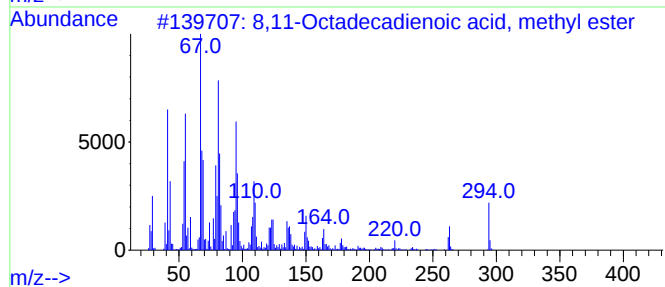
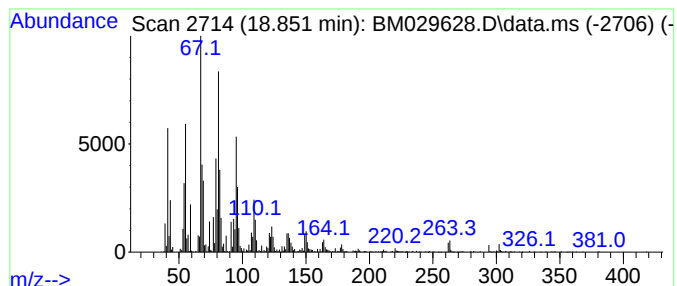
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 8,11-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	17.95 ng	1084550	Phenanthrene-d10	17.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
2			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99



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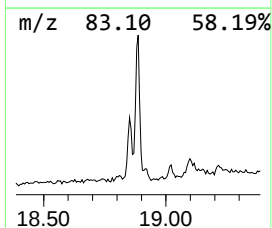
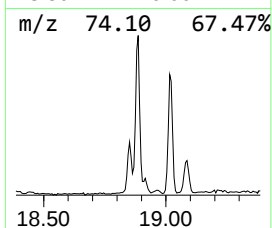
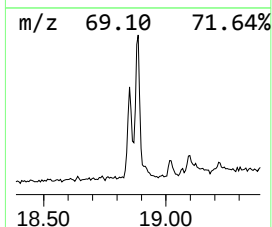
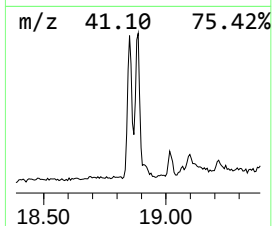
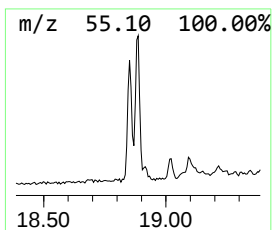
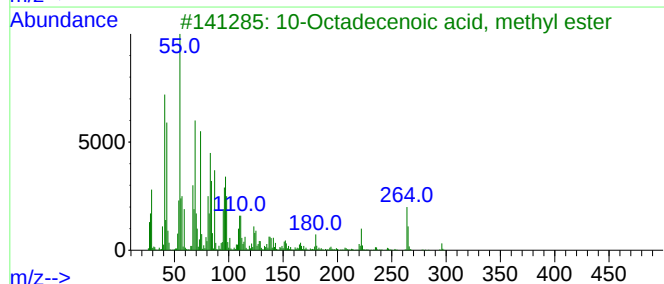
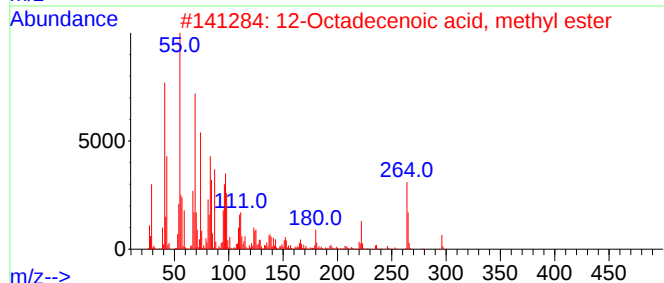
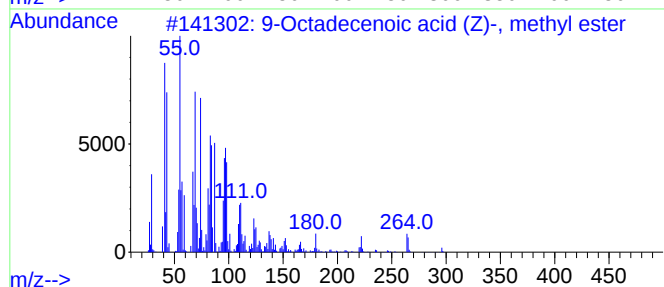
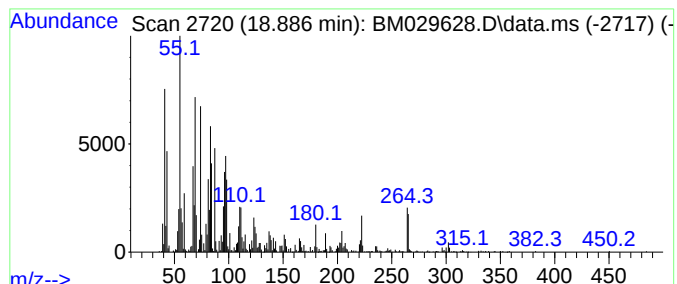
Instrument :
BNA_M
ClientSampleId :
PL-01-042121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.886	13.34 ng	806128	Phenanthrene-d10	17.028	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029628.D
Acq On : 24 Apr 2021 00:22
Operator : CG/JU
Sample : M2117-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-01-042121

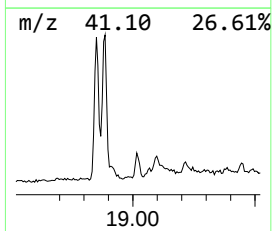
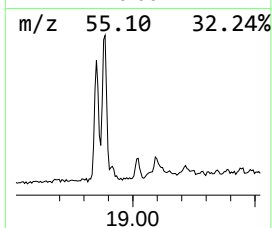
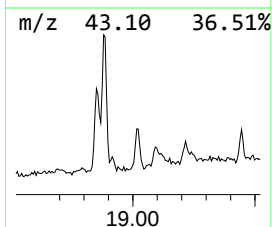
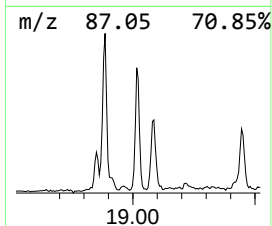
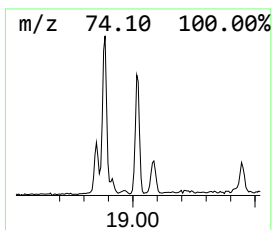
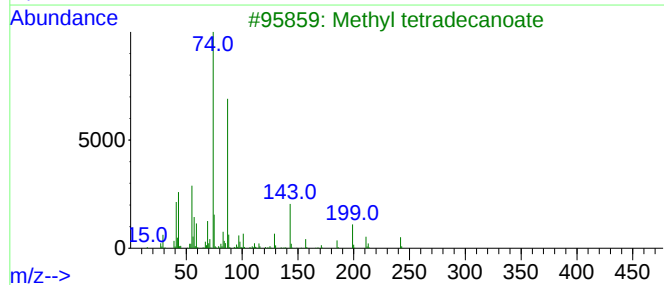
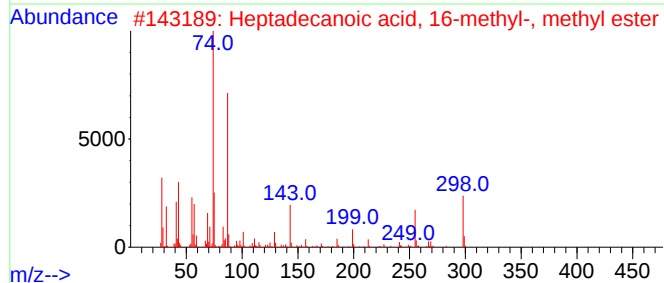
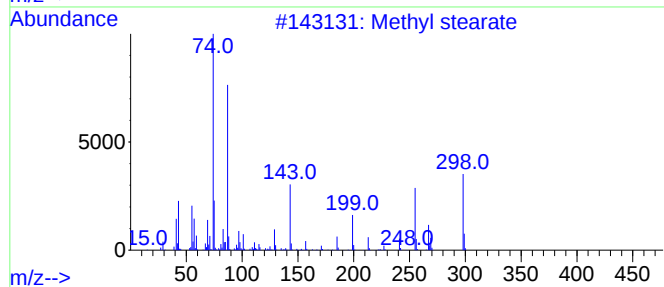
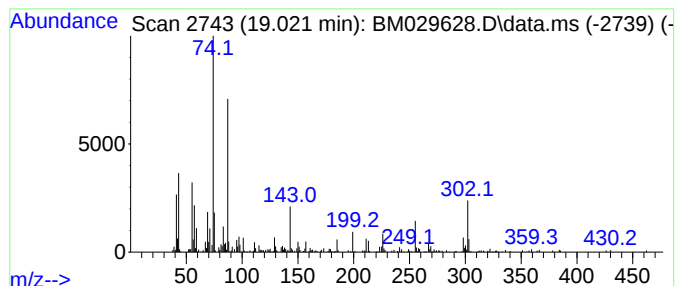
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.022	2.88 ng	173696	Phenanthrene-d10	17.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	99
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	97
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	72
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	70
5			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042321\
Data File : BM029628.D
Acq On : 24 Apr 2021 00:22
Operator : CG/JU
Sample : M2117-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PL-01-042121

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.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
Hexadecanoic ac...	17.704	3.8	ng	230764	4	17.028	1208310	20.0
n-Hexadecanoic ...	17.933	5.5	ng	329288	4	17.028	1208310	20.0
4H-Cyclopenta[d...]	18.092	3.3	ng	198786	4	17.028	1208310	20.0
8,11-Octadecadi...	18.851	17.9	ng	1084550	4	17.028	1208310	20.0
9-Octadecenoic ...	18.886	13.3	ng	806128	4	17.028	1208310	20.0
Methyl stearate	19.022	2.9	ng	173696	4	17.028	1208310	20.0