

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
 Data File : BM029715.D
 Acq On : 29 Apr 2021 18:46
 Operator : CG/JU
 Sample : M2190-01 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 NB-08-042721

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-BM043021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	386	392	403	rBV	346599	510871	6.96%	1.679%
2	6.775	655	661	677	rBV	299320	514180	7.00%	1.690%
3	7.593	792	800	809	rBV	235776	379990	5.17%	1.249%
4	8.751	990	997	1013	rBV	182150	332022	4.52%	1.091%
5	10.375	1266	1273	1290	rVB	282778	484076	6.59%	1.591%
6	12.857	1689	1695	1707	rBV	644835	936463	12.75%	3.078%
7	14.245	1923	1931	1939	rBV	466998	699090	9.52%	2.298%
8	15.733	2178	2184	2196	rBV	478753	705498	9.61%	2.319%
9	16.986	2392	2397	2402	rBV	560511	815601	11.11%	2.681%
10	17.033	2402	2405	2411	rVB	59574	82520	1.12%	0.271%
11	17.674	2508	2514	2525	rBV	2092368	2442835	33.26%	8.029%
12	17.904	2548	2553	2563	rBV2	243706	368790	5.02%	1.212%
13	18.827	2704	2710	2712	rBV	6009366	7343879	100.00%	24.137%
14	18.857	2712	2715	2725	rVB2	5733973	7140584	97.23%	23.469%
15	18.986	2733	2737	2742	rBV	1016912	1191875	16.23%	3.917%
16	19.057	2742	2749	2759	rBV2	213655	596808	8.13%	1.962%
17	19.186	2767	2771	2786	rVB2	150550	247286	3.37%	0.813%
18	19.410	2805	2809	2820	rVB	163308	273787	3.73%	0.900%
19	19.621	2840	2845	2851	rBV	1277622	1601578	21.81%	5.264%
20	19.980	2902	2906	2909	rBV2	71018	92421	1.26%	0.304%
21	20.086	2918	2924	2927	rBV2	85403	124478	1.69%	0.409%
22	20.127	2927	2931	2937	rVV3	133027	250618	3.41%	0.824%
23	20.186	2937	2941	2949	rVV3	138409	242115	3.30%	0.796%
24	20.251	2949	2952	2957	rVV3	55693	76973	1.05%	0.253%
25	20.392	2973	2976	2982	rVB3	83565	113831	1.55%	0.374%
26	20.704	3025	3029	3034	rVB5	43296	73832	1.01%	0.243%
27	20.904	3059	3063	3068	rBV4	150191	223316	3.04%	0.734%
28	21.033	3082	3085	3088	rBV2	76255	84174	1.15%	0.277%
29	21.174	3103	3109	3113	rBV	894360	1251439	17.04%	4.113%
30	21.209	3113	3115	3123	rVB	108835	136850	1.86%	0.450%
31	23.350	3473	3479	3486	rBV2	620566	1087931	14.81%	3.576%

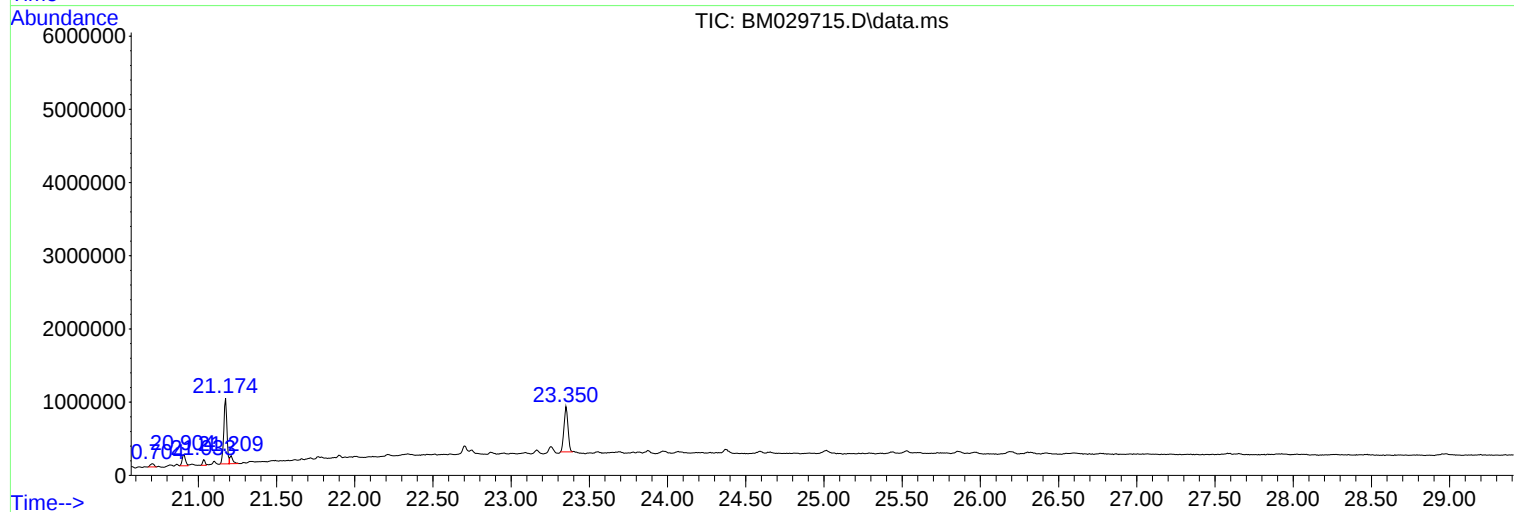
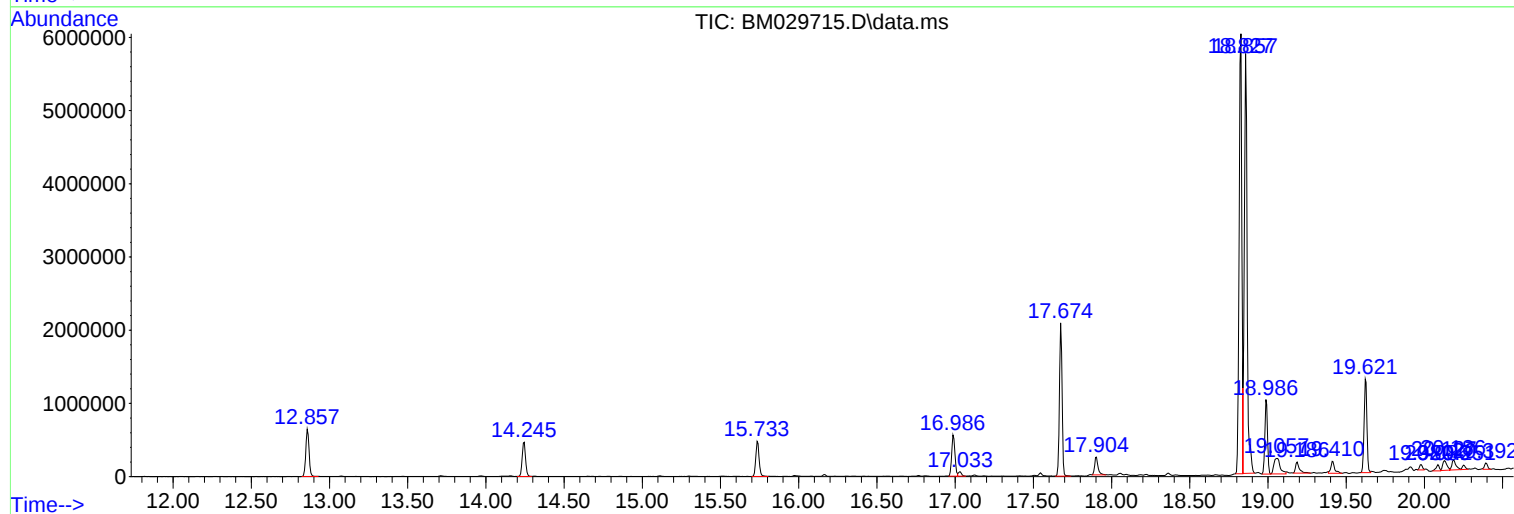
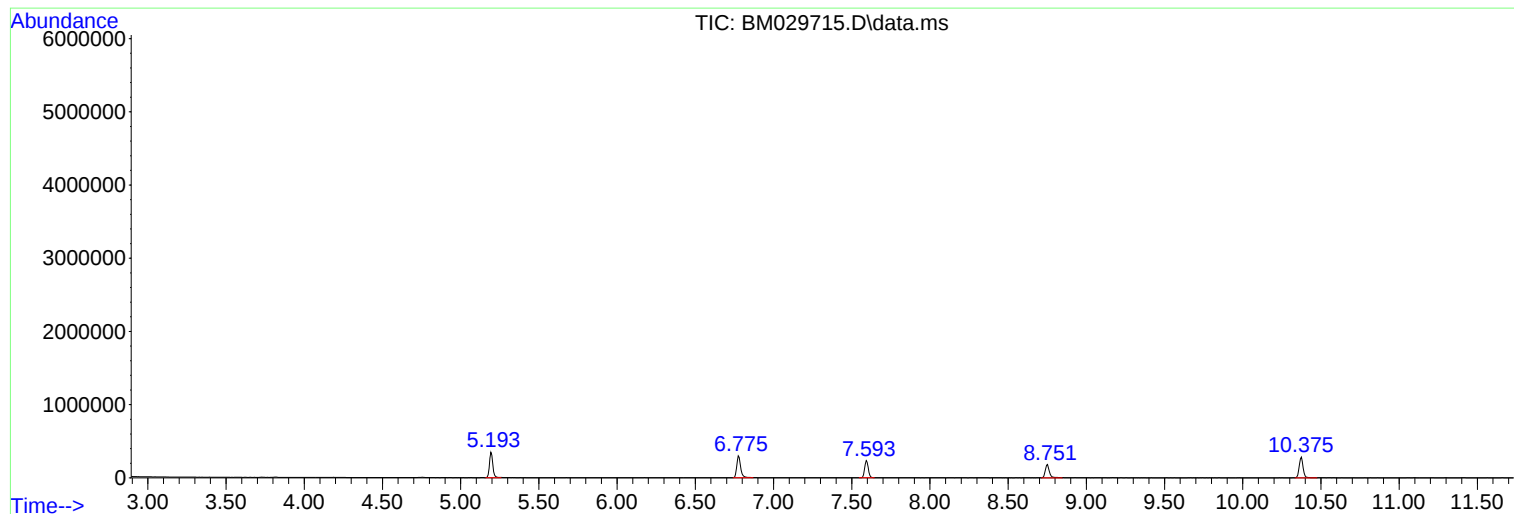
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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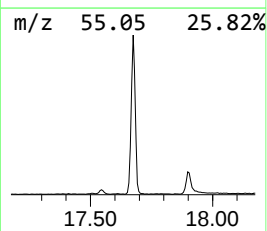
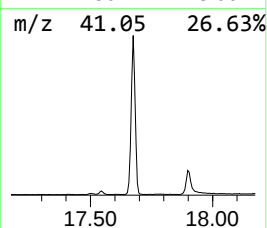
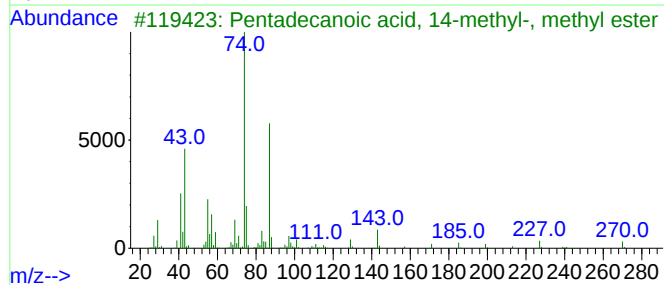
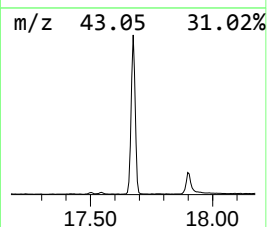
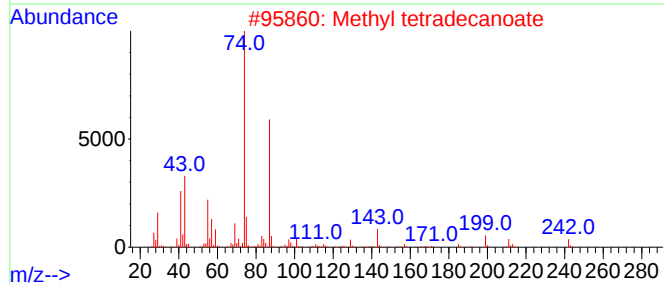
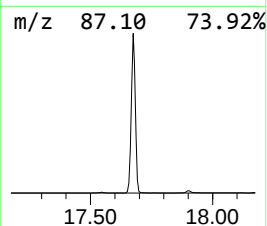
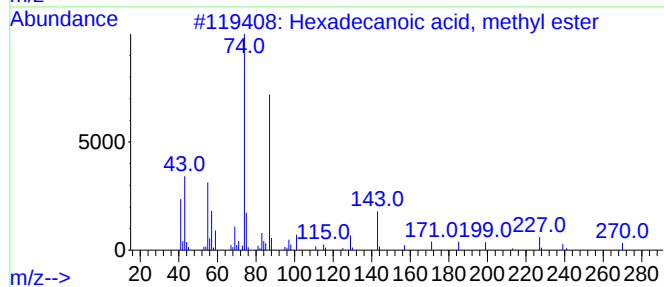
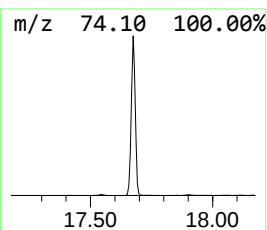
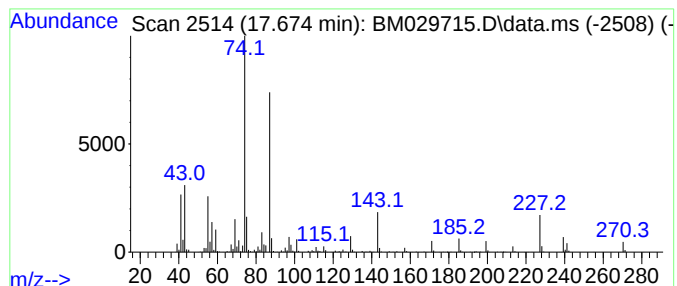
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.674	59.90 ng	2442840	Phenanthrene-d10	16.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87



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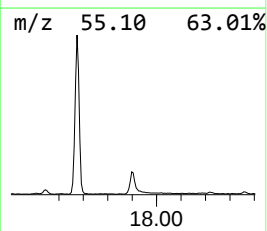
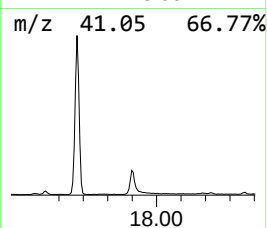
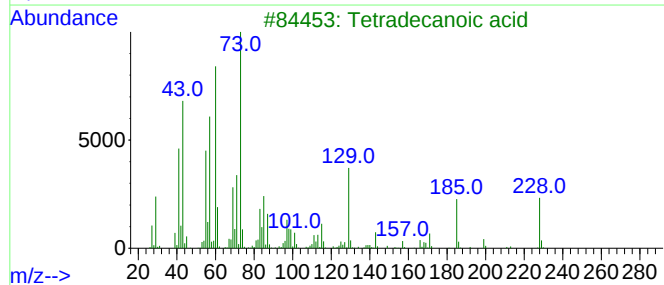
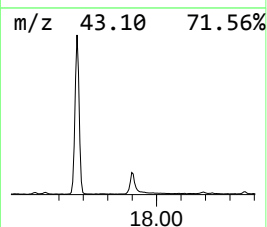
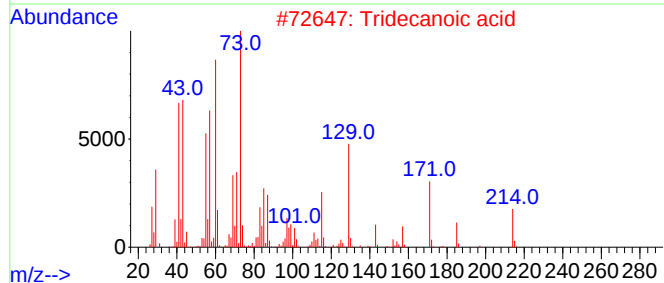
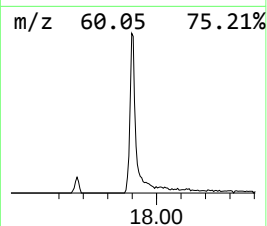
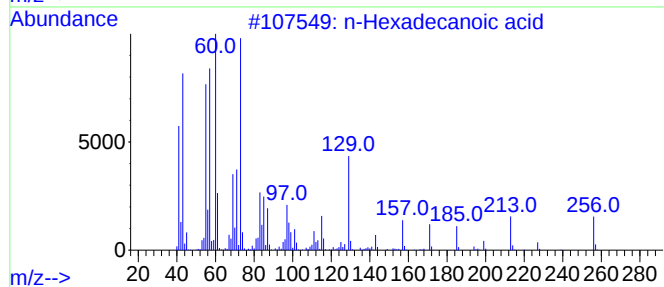
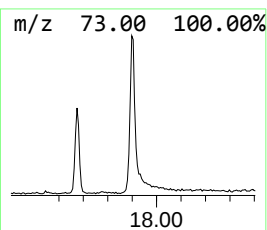
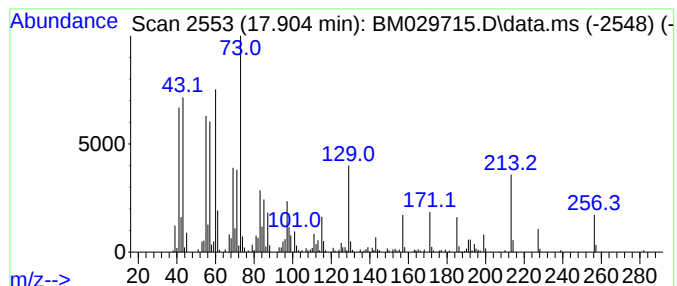
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.904	9.04 ng	368790	Phenanthrene-d10	16.986

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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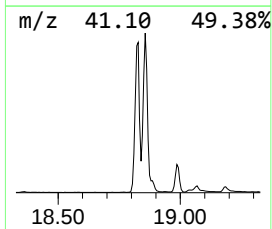
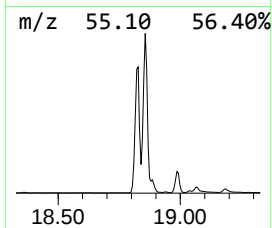
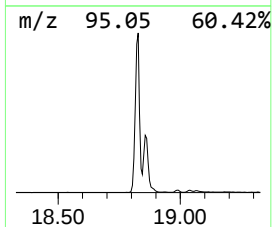
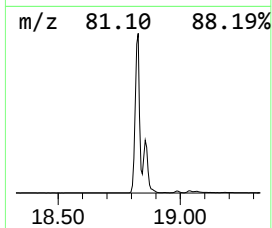
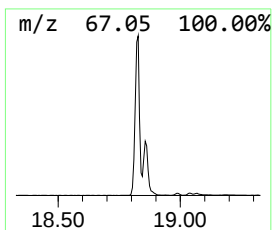
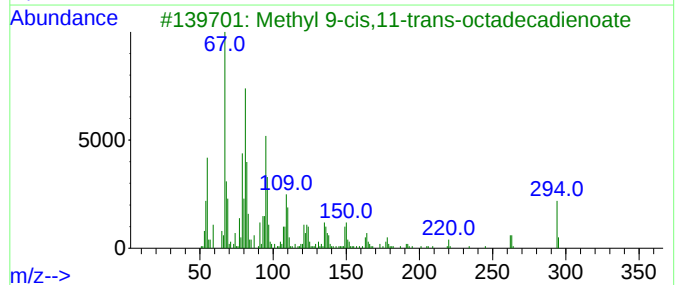
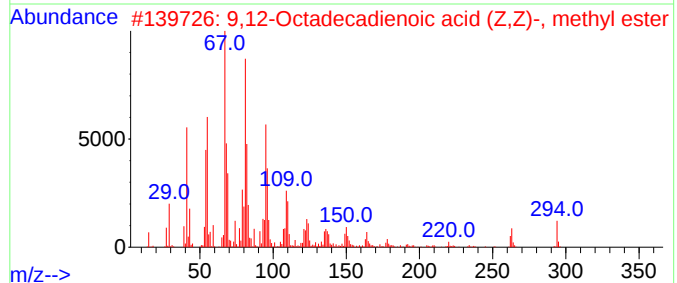
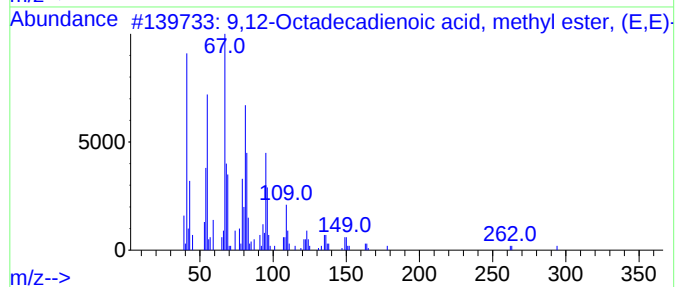
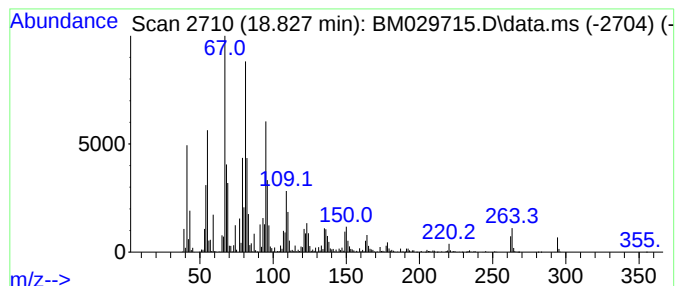
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.827	180.09 ng	7343880	Phenanthrene-d10	16.986	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98



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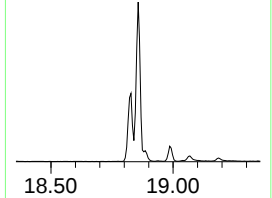
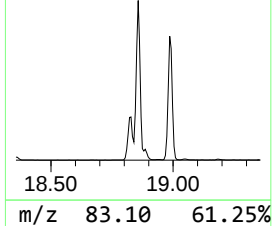
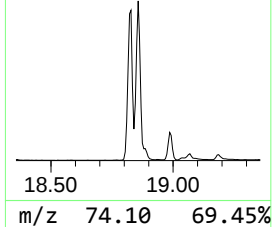
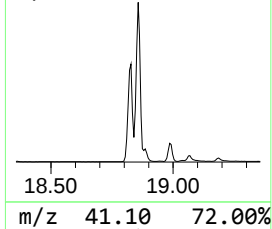
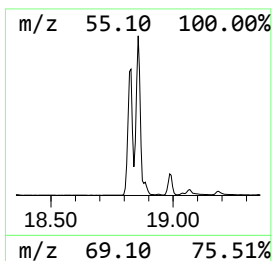
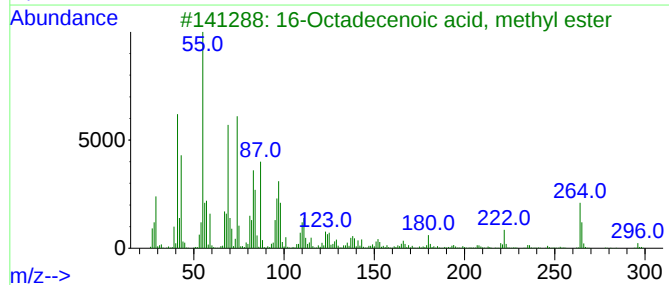
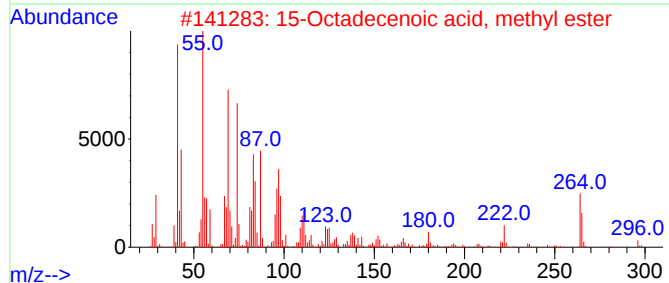
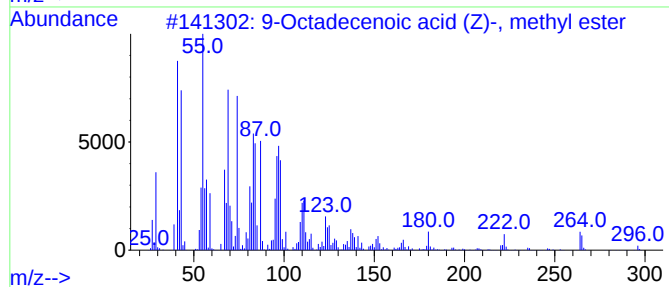
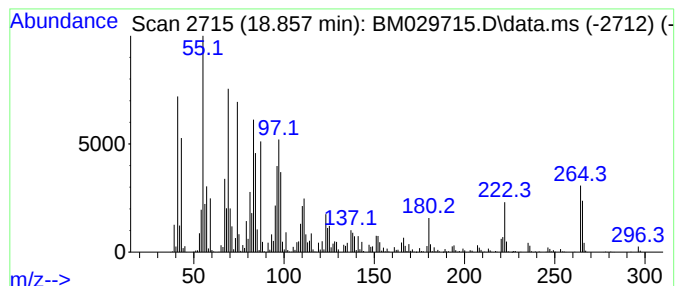
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Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.857	175.10 ng	7140580	Phenanthrene-d10	16.986	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99



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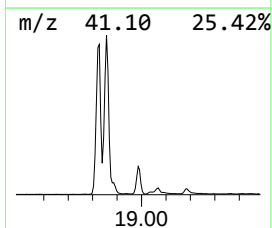
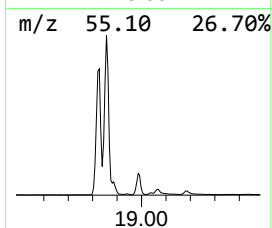
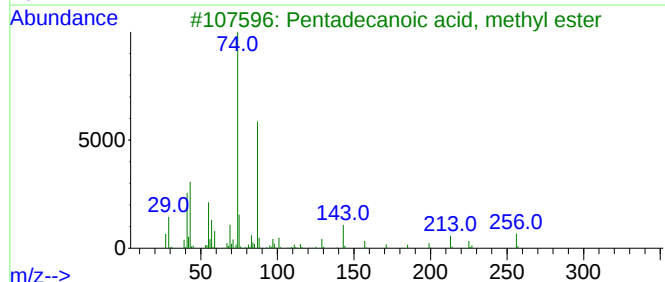
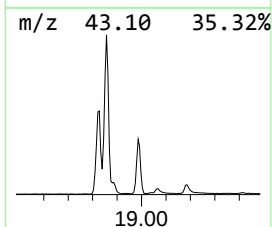
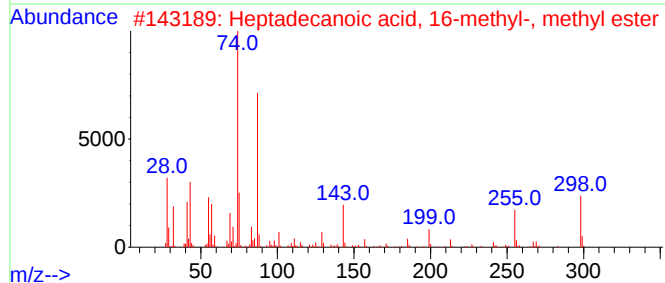
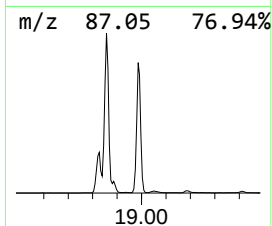
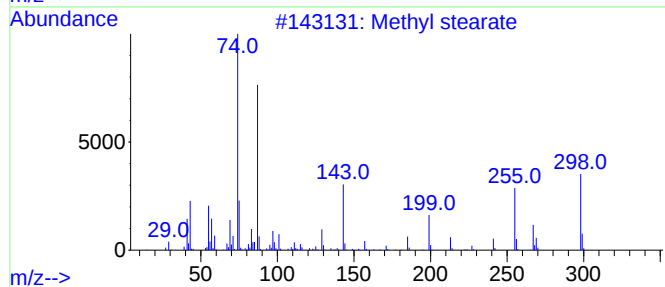
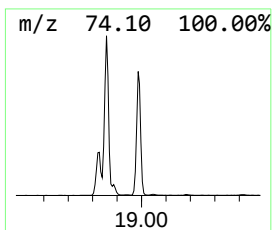
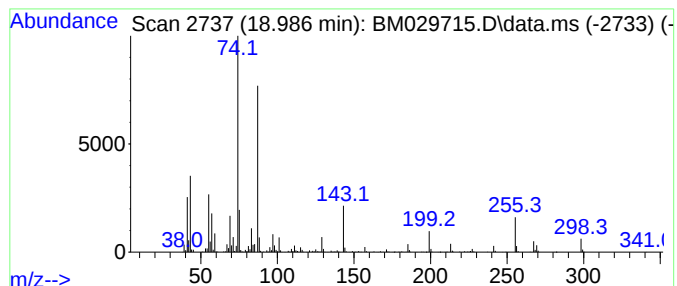
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Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	29.23 ng	1191880	Phenanthrene-d10	16.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	83



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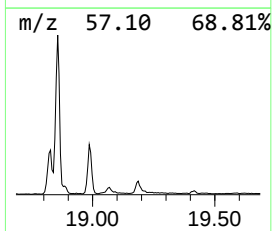
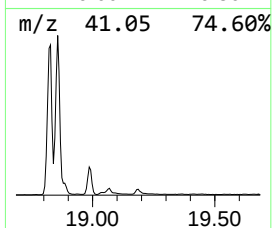
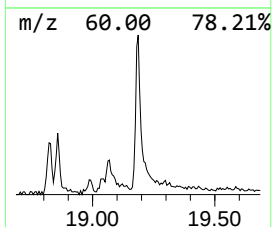
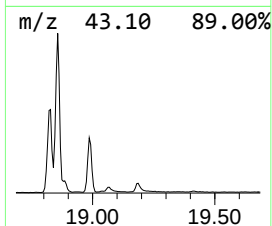
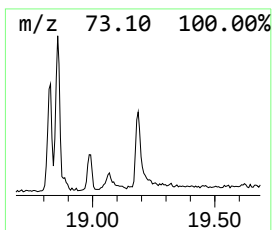
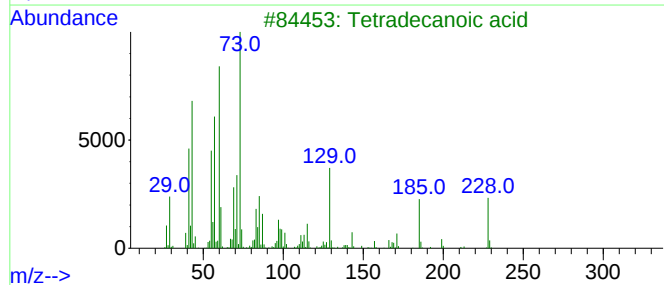
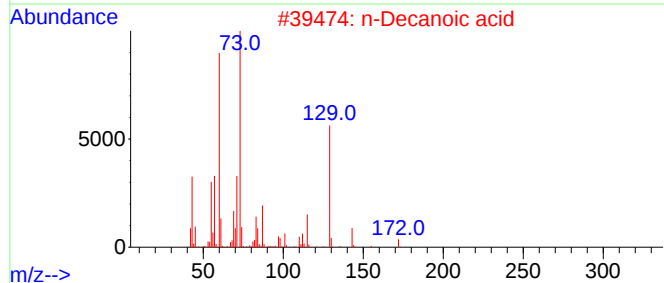
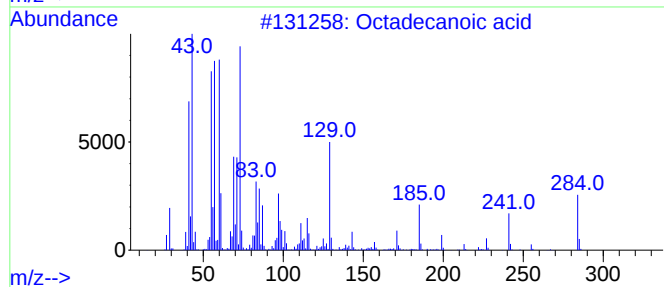
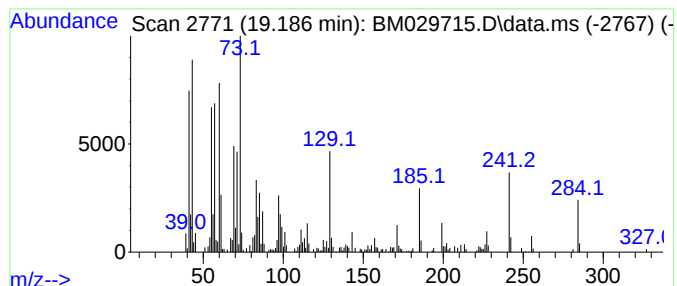
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	3.95 ng	247286	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029715.D
Acq On : 29 Apr 2021 18:46
Operator : CG/JU
Sample : M2190-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-08-042721

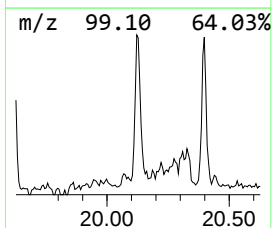
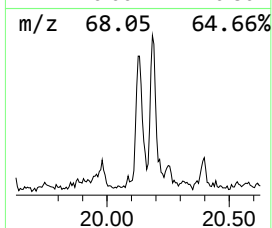
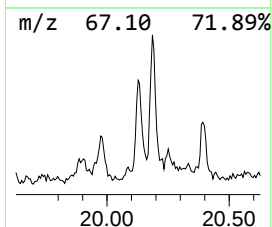
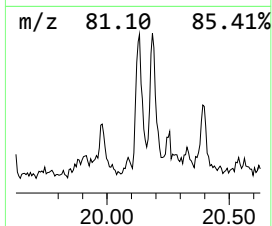
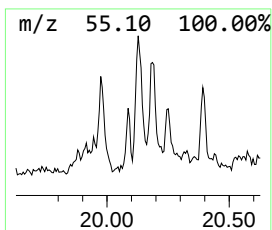
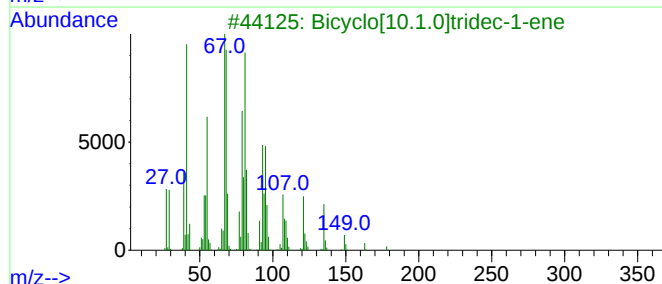
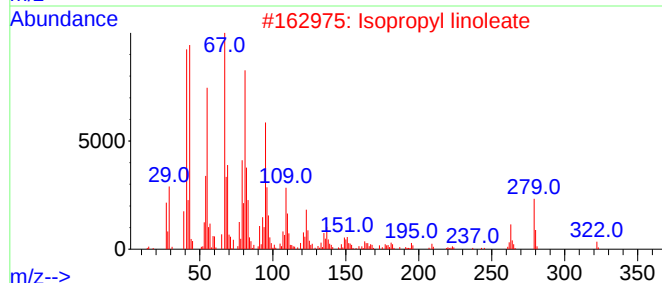
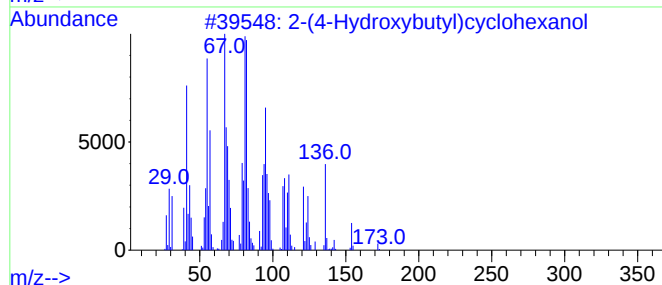
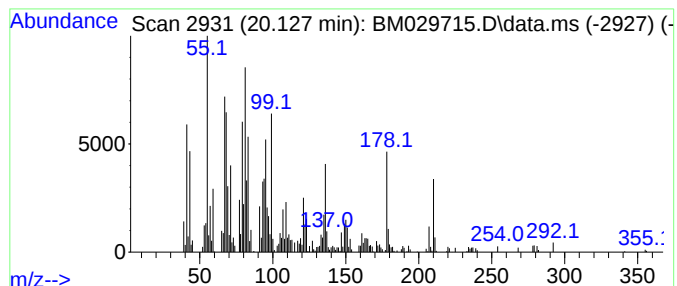
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-(4-Hydroxybutyl)cyclohexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.127	4.01 ng	250618	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Hydroxybutyl)cyclohexanol	172	C10H20O2	1000185-44-6	70		
2	Isopropyl linoleate	322	C21H38O2	022882-95-7	38		
3	Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	38		
4	1,2-Dioctylcyclopropene	264	C19H36	001089-40-3	38		
5	But-2-ynoic acid, 1,7,7-trimethy...	220	C14H20O2	091404-80-7	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029715.D
Acq On : 29 Apr 2021 18:46
Operator : CG/JU
Sample : M2190-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-08-042721

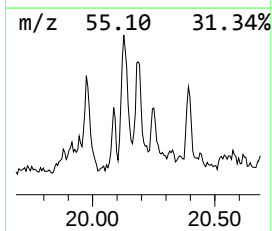
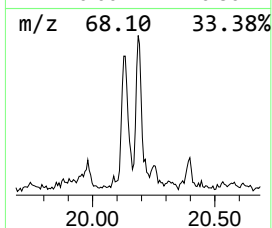
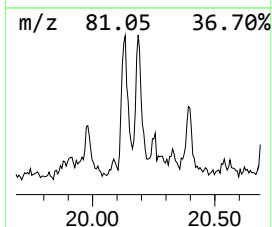
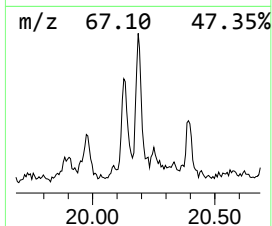
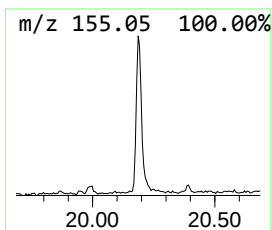
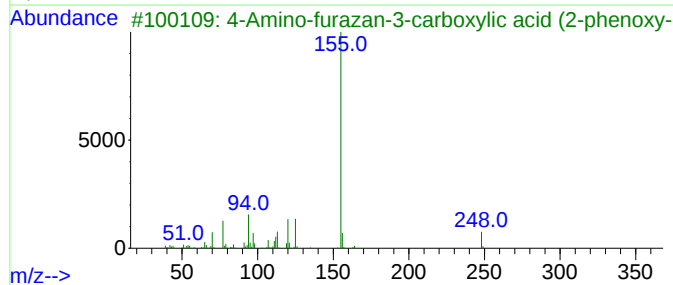
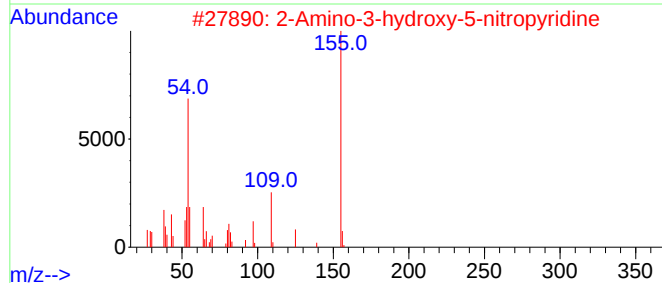
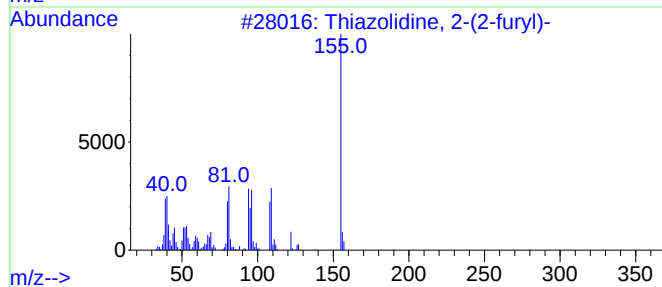
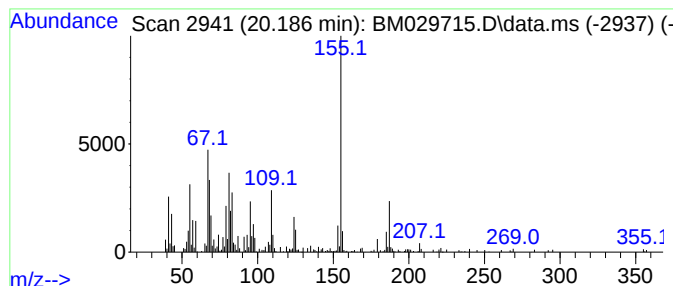
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.186 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.186	3.87 ng	242115	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiazolidine, 2-(2-furyl)-	155	C7H9NOS	051859-60-0	43
2			2-Amino-3-hydroxy-5-nitropyridine	155	C5H5N3O3	1000289-29-0	38
3			4-Amino-furazan-3-carboxylic aci...	248	C11H12N4O3	1000275-80-2	35
4			1,2-Cyclohexanedicarboxylic acid...	434	C20H25Cl3O4	1000339-81-1	35
5			Fumaric acid, isobutyl 2-methyla...	226	C12H18O4	1000330-54-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029715.D
Acq On : 29 Apr 2021 18:46
Operator : CG/JU
Sample : M2190-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-08-042721

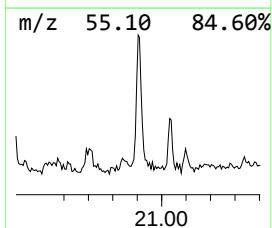
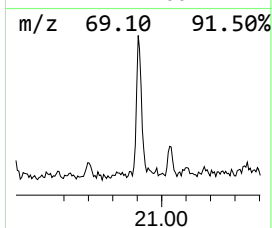
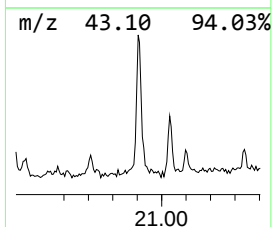
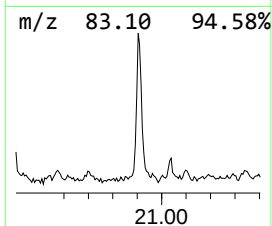
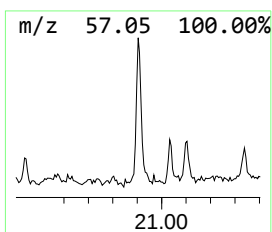
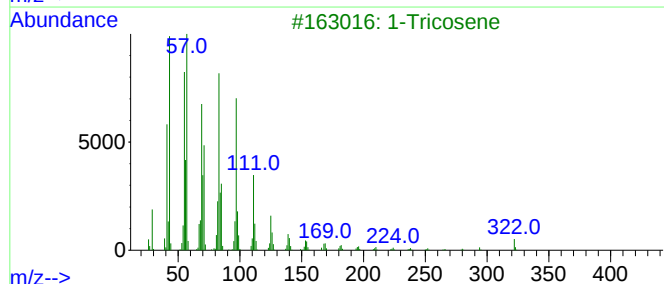
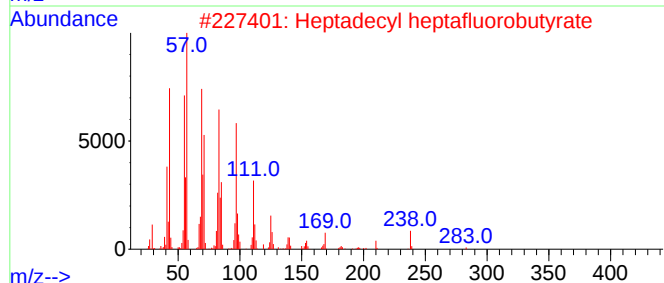
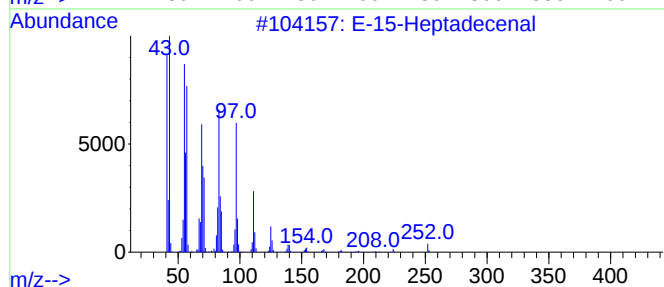
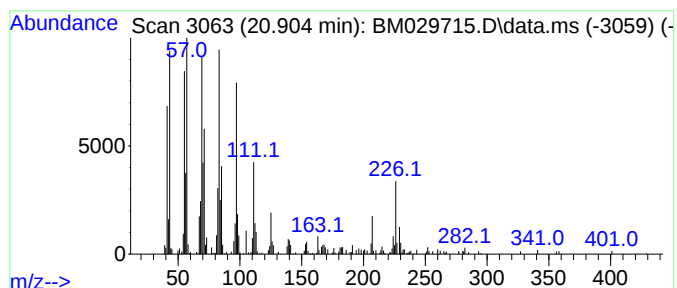
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-15-Heptadecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	3.57 ng	223316	Chrysene-d12	21.174

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Tricosene	322	C23H46	018835-32-0	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029715.D
Acq On : 29 Apr 2021 18:46
Operator : CG/JU
Sample : M2190-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-08-042721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.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...	17.674	59.9	ng	2442840	4	16.986	815601	20.0
n-Hexadecanoic ...	17.904	9.0	ng	368790	4	16.986	815601	20.0
9,12-Octadecadi...	18.827	180.1	ng	7343880	4	16.986	815601	20.0
9-Octadecenoic ...	18.857	175.1	ng	7140580	4	16.986	815601	20.0
Methyl stearate	18.986	29.2	ng	1191880	4	16.986	815601	20.0
Octadecanoic acid	19.186	4.0	ng	247286	5	21.174	1251440	20.0
2-(4-Hydroxybut...	20.127	4.0	ng	250618	5	21.174	1251440	20.0
unknown20.186	20.186	3.9	ng	242115	5	21.174	1251440	20.0
E-15-Heptadecenal	20.904	3.6	ng	223316	5	21.174	1251440	20.0