

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
 Data File : BM036111.D
 Acq On : 04 Aug 2022 22:49
 Operator : CG/JU
 Sample : N4032-01 10X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SU-03-080322

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.422	390	397	405	rBV	495604	745150	1.98%	0.639%
2	7.034	664	671	680	rVB	500224	787070	2.09%	0.675%
3	7.858	802	811	819	rBV	1712127	2675074	7.10%	2.294%
4	9.028	1004	1010	1018	rBV	306735	521109	1.38%	0.447%
5	10.663	1278	1288	1303	rBV	2395937	4093836	10.87%	3.511%
6	13.128	1700	1707	1716	rBV	846553	1232141	3.27%	1.057%
7	14.498	1934	1940	1947	rBV	3687601	5383164	14.30%	4.617%
8	15.986	2186	2193	2200	rBV	635193	928274	2.47%	0.796%
9	17.245	2400	2407	2411	rBV	4178010	5962711	15.84%	5.114%
10	17.916	2516	2521	2527	rBV	8149198	9920044	26.35%	8.508%
11	19.069	2710	2717	2719	rBV	24957650	37651846	100.00%	32.294%
12	19.098	2719	2722	2732	rVB2	19908765	27133337	72.06%	23.272%
13	19.222	2739	2743	2749	rVB	5118773	6133429	16.29%	5.261%
14	19.298	2753	2756	2761	rVB	387556	479315	1.27%	0.411%
15	19.663	2812	2818	2827	rVB2	349544	725024	1.93%	0.622%
16	19.863	2848	2852	2857	rBV	1120743	1325407	3.52%	1.137%
17	20.210	2908	2911	2918	rVB3	435423	668118	1.77%	0.573%
18	20.321	2926	2930	2933	rBV	456232	525725	1.40%	0.451%
19	20.486	2954	2958	2963	rBV	623327	754331	2.00%	0.647%
20	21.268	3088	3091	3094	rBV	449429	485615	1.29%	0.417%
21	21.421	3112	3117	3121	rBV	3529959	4438274	11.79%	3.807%
22	23.780	3513	3518	3528	rVB2	2092223	4022598	10.68%	3.450%

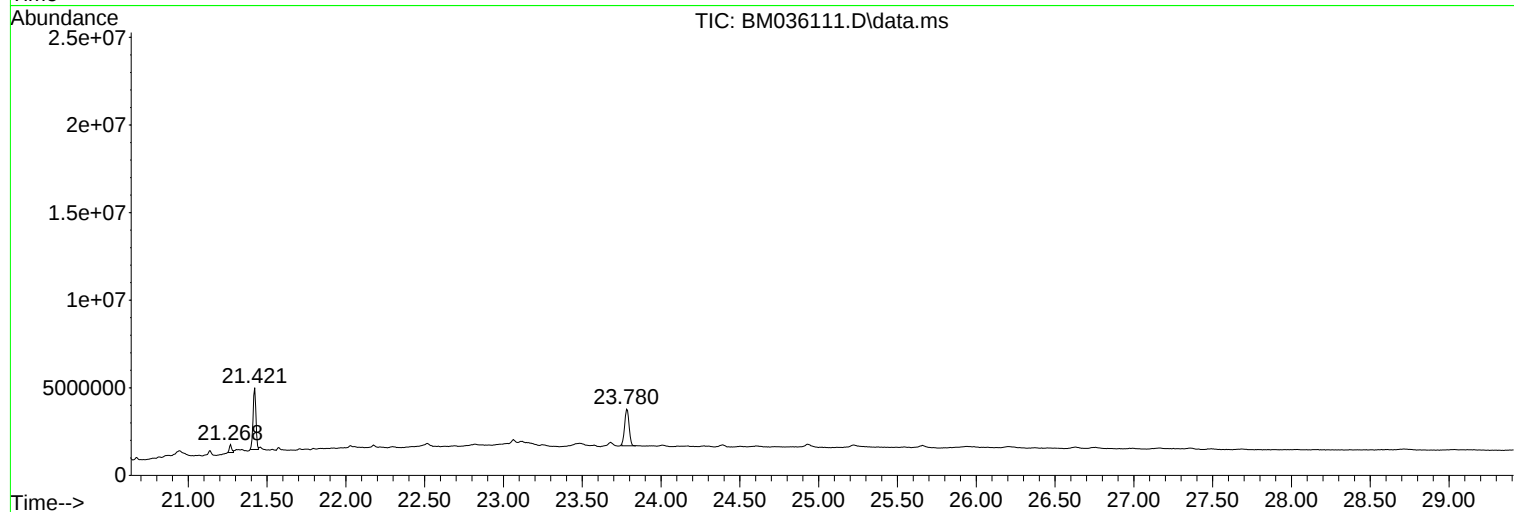
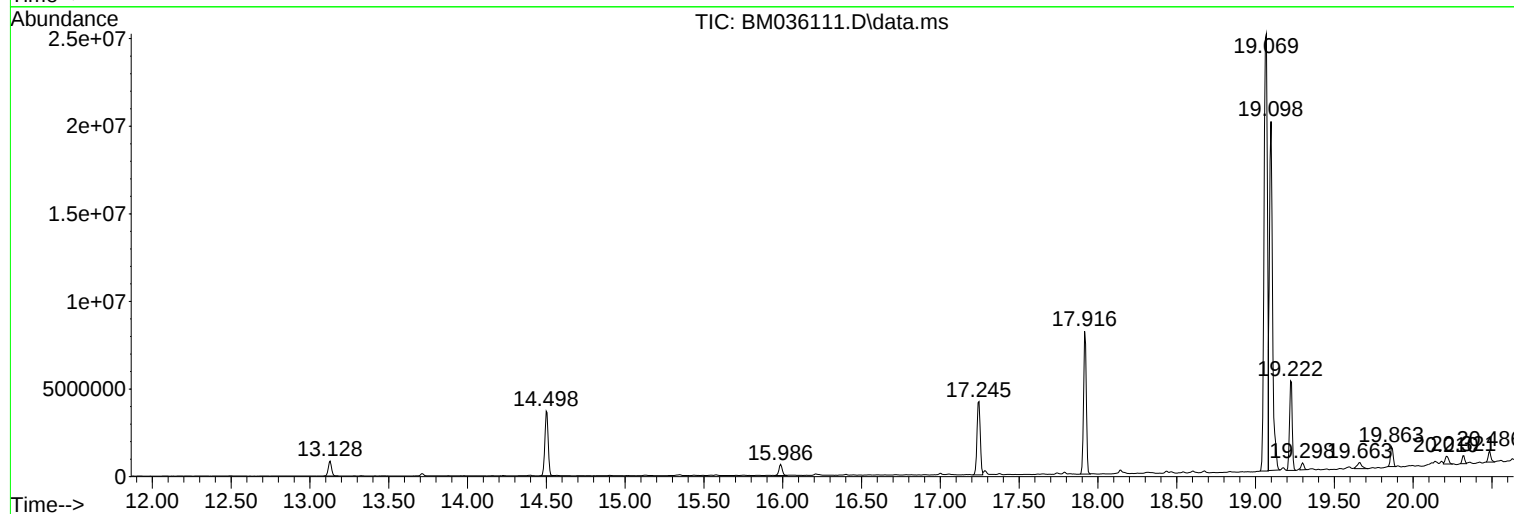
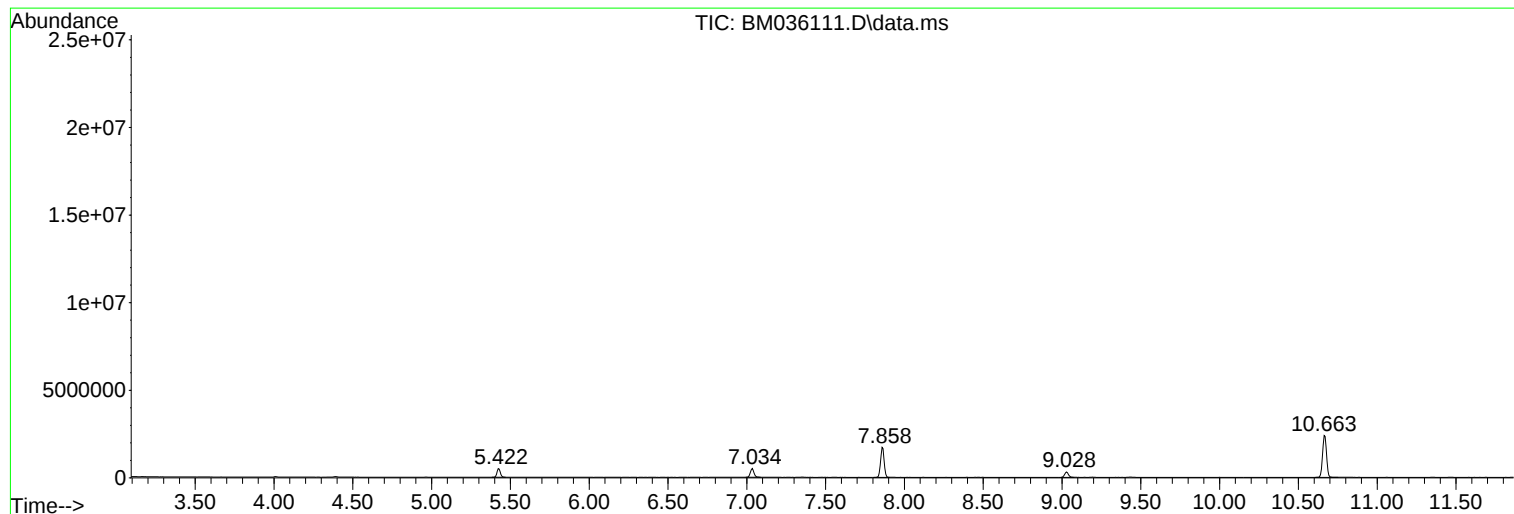
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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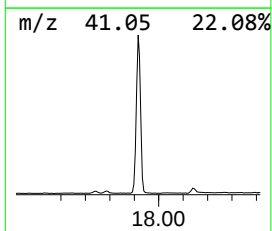
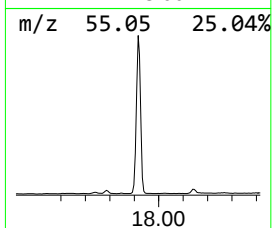
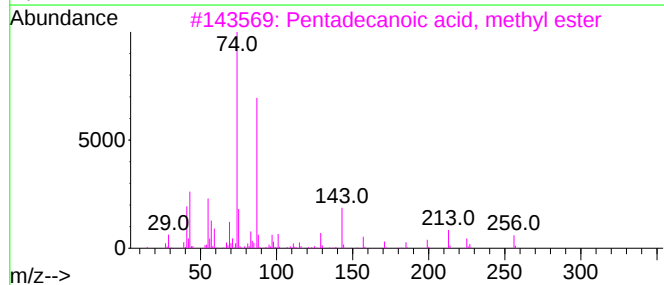
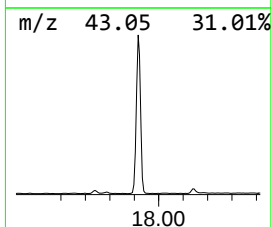
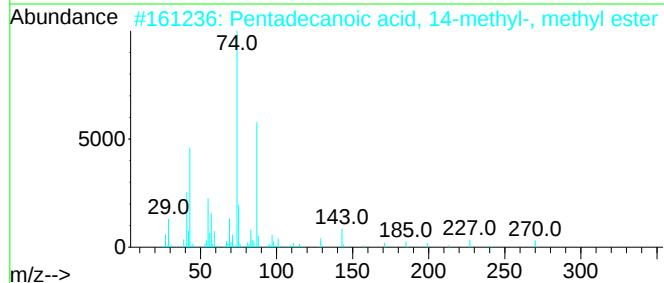
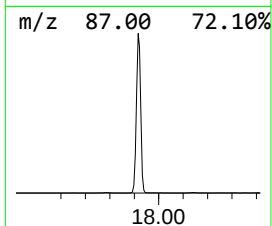
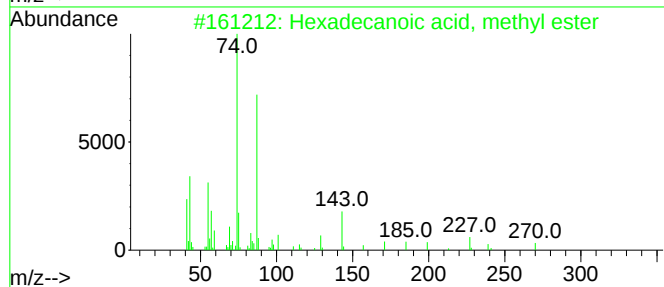
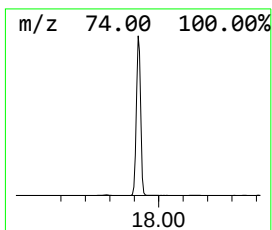
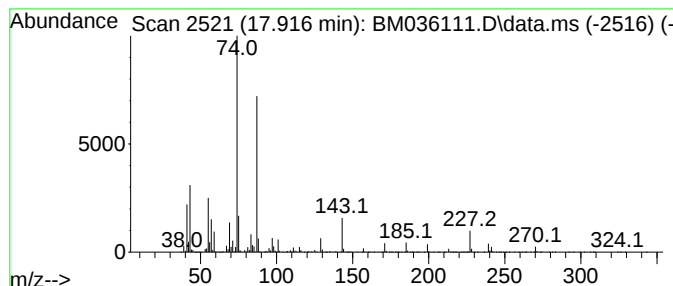
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.916	33.27 ng	9920040	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	80



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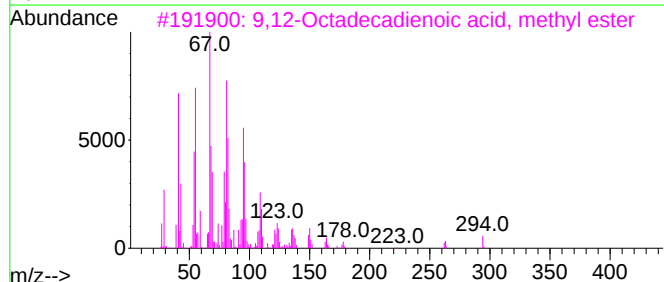
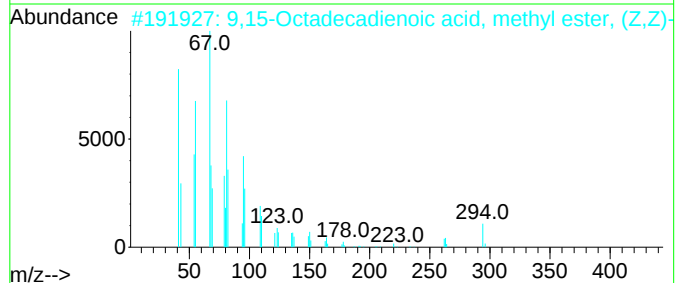
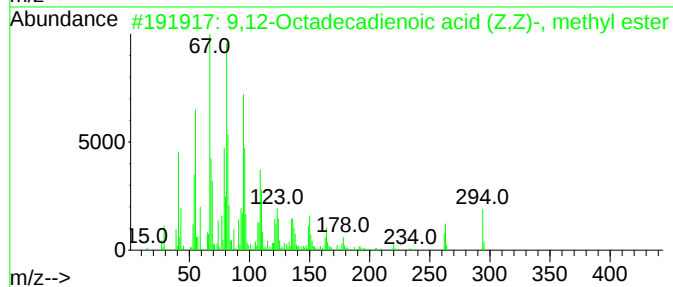
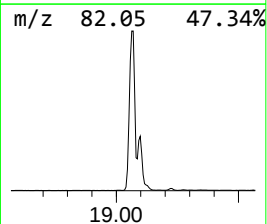
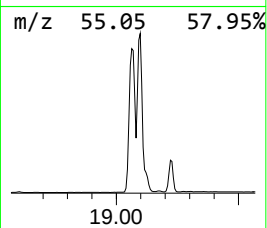
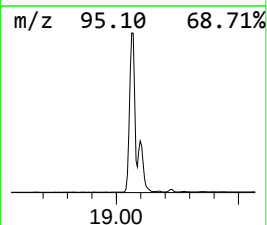
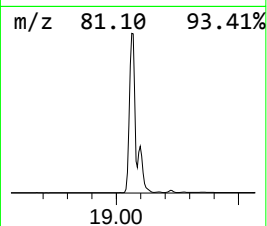
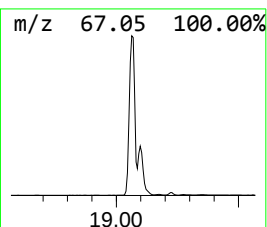
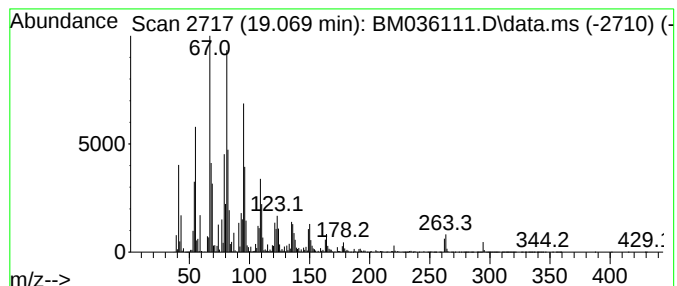
Instrument :
BNA_M
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.069	126.29 ng	37651800	Phenanthrene-d10	17.245
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		9,12-Octadecadienoic acid (Z,Z)-...	294 C19H34O2	000112-63-0 99
2		9,15-Octadecadienoic acid, methy...	294 C19H34O2	017309-05-6 99
3		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002462-85-3 99
4		10,13-Octadecadienoic acid, meth...	294 C19H34O2	056554-62-2 99
5		8,11-Octadecadienoic acid, methy...	294 C19H34O2	056599-58-7 99



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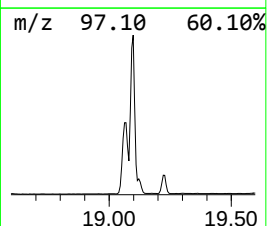
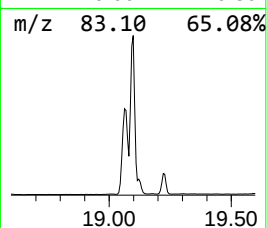
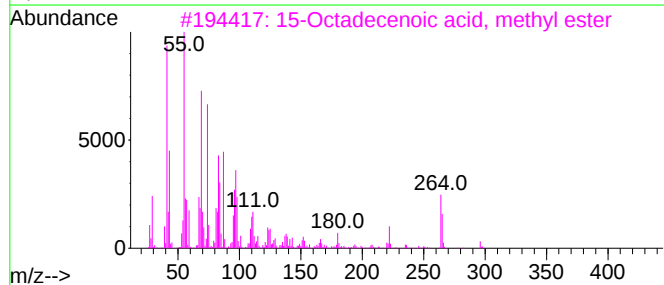
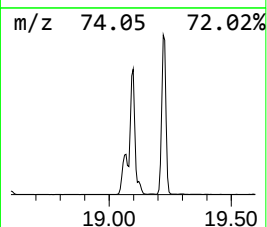
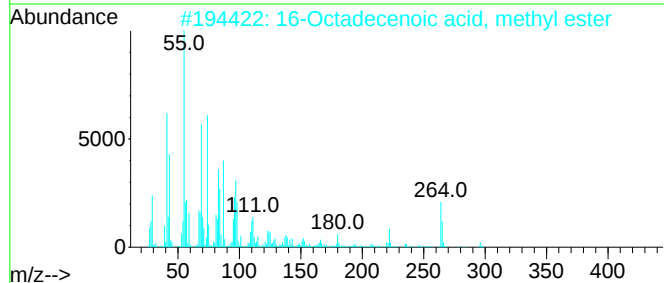
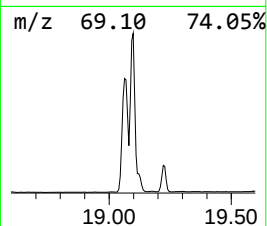
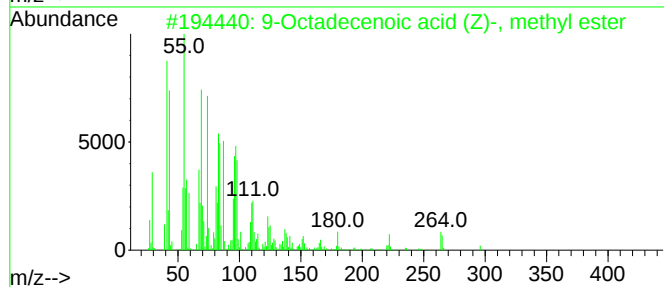
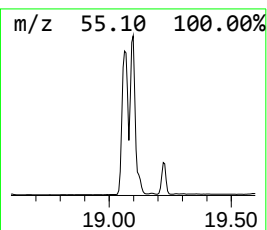
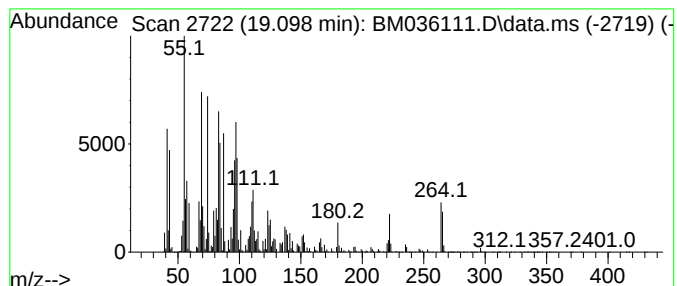
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BNA_M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.098	91.01 ng	27133300	Phenanthrene-d10	17.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	95



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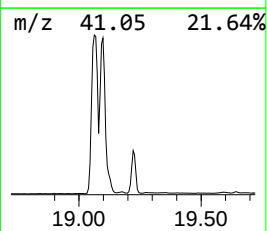
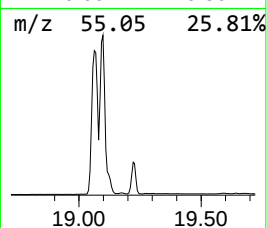
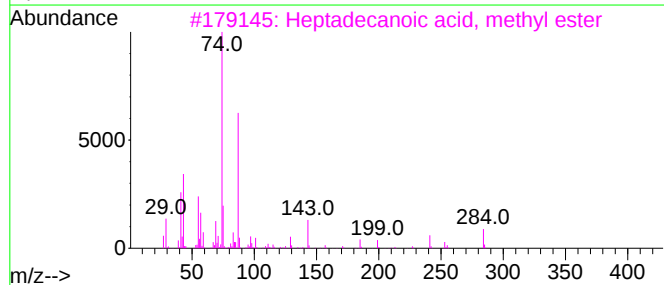
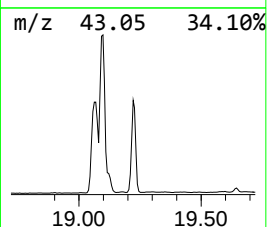
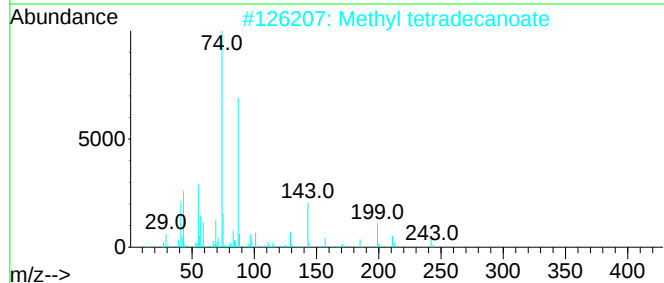
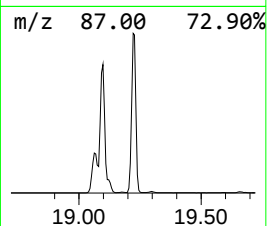
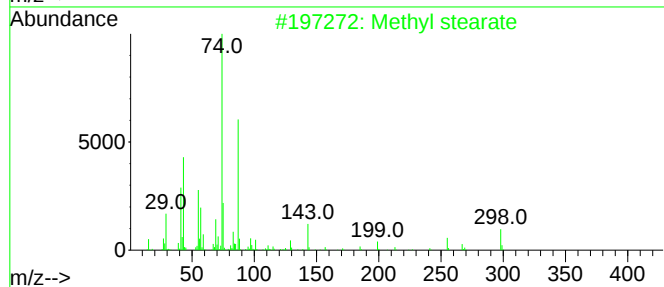
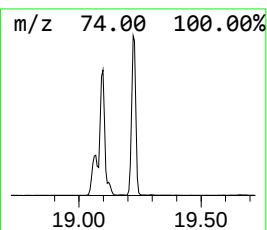
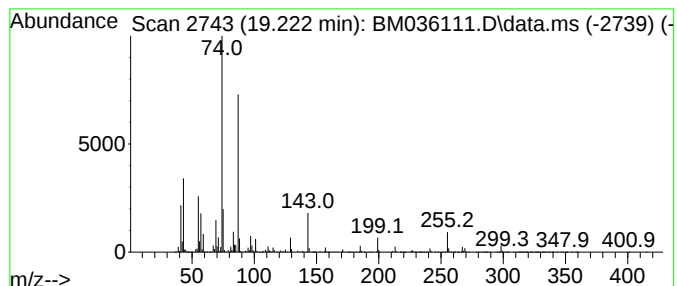
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	20.57 ng	6133430	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90



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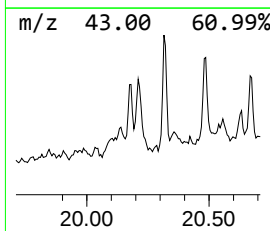
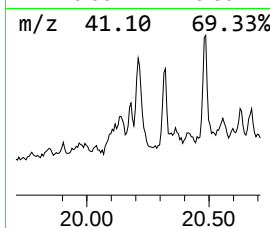
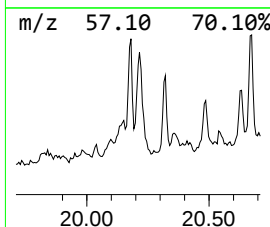
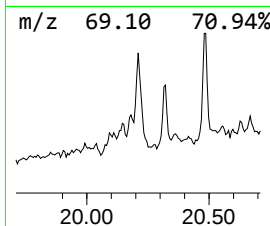
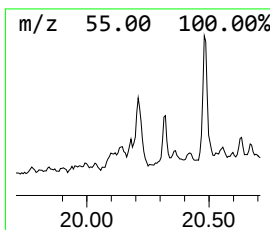
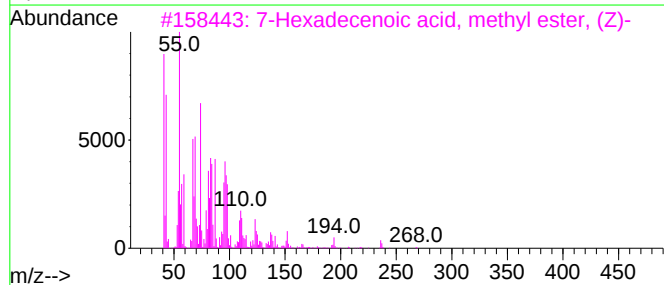
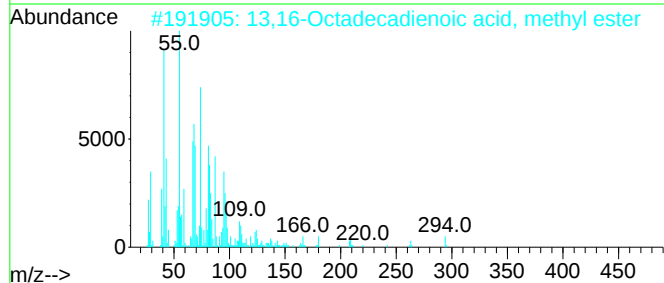
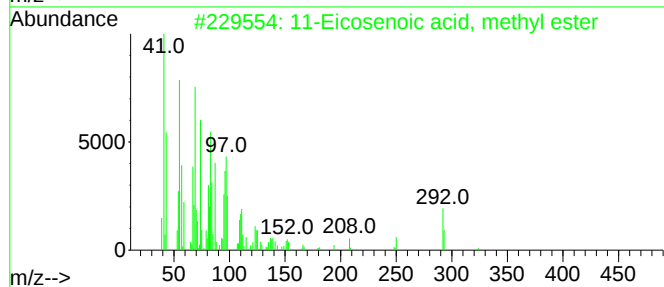
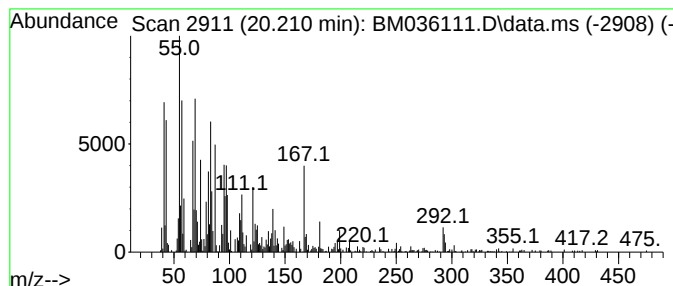
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Peak Number 6 11-Eicosenoic acid, methyl ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.210	3.01 ng	668118	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	95
2			13,16-Octadecadienoic acid, meth...	294	C19H34O2	056846-99-2	60
3			7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	55
4			13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	52
5			Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	50



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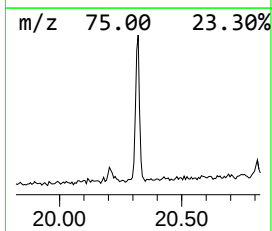
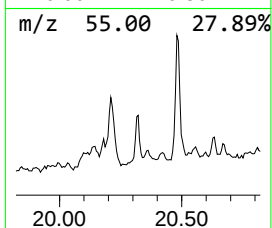
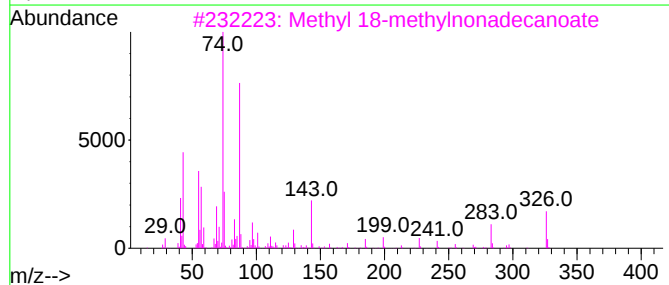
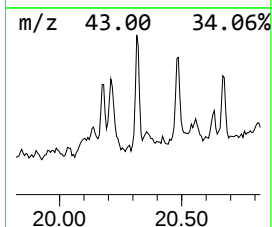
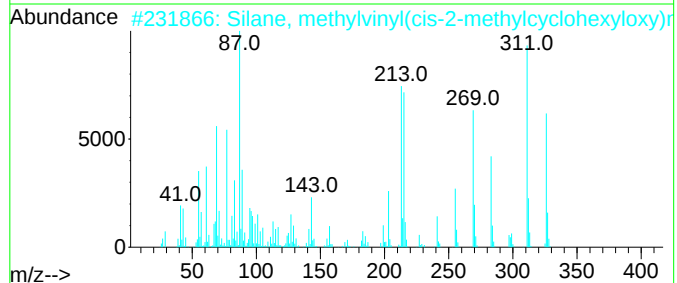
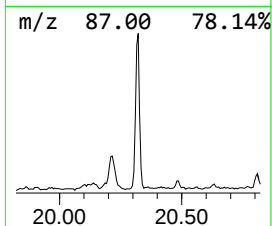
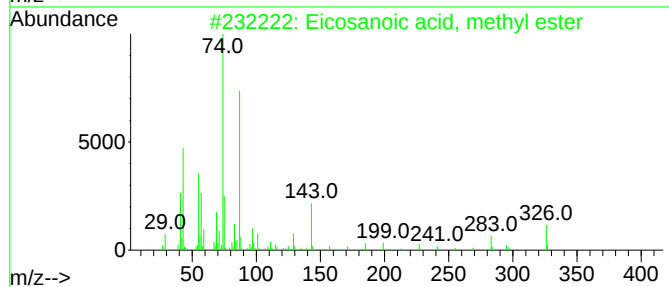
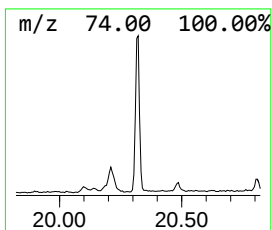
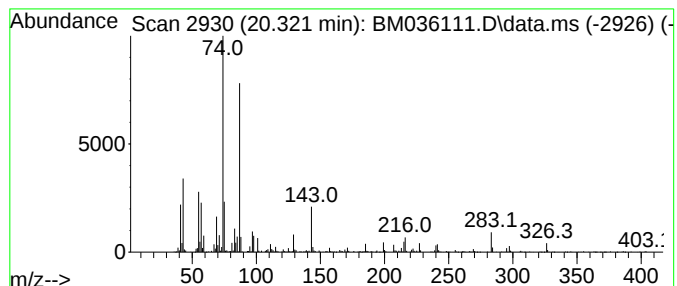
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BNA_M
ClientSampleId :
SU-03-080322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.322	2.37 ng	525725	Chrysene-d12	21.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Silane, methylvinyl(cis-2-methyl...	326	C19H38O2Si	1000421-05-3	95
3	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	95
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036111.D
Acq On : 04 Aug 2022 22:49
Operator : CG/JU
Sample : N4032-01 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-03-080322

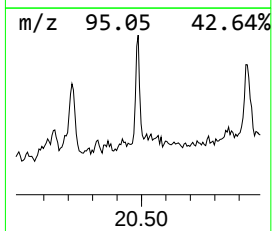
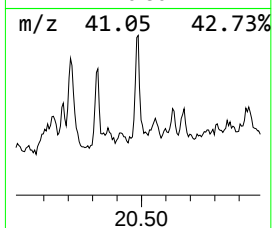
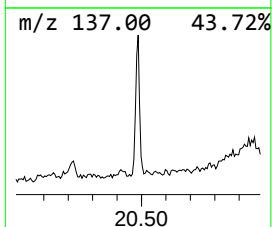
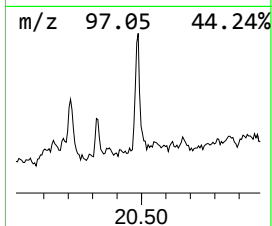
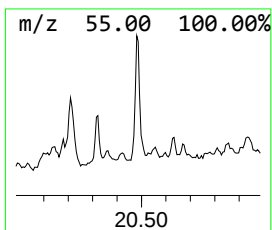
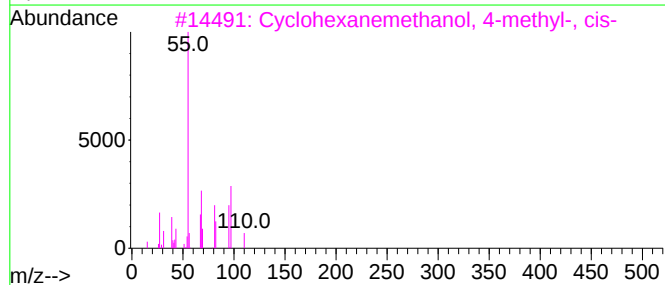
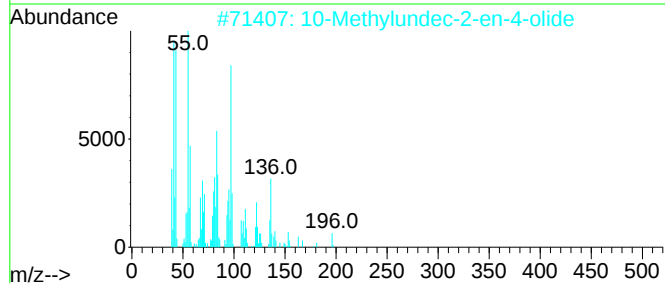
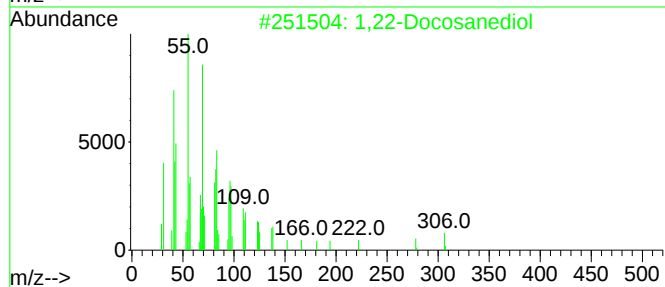
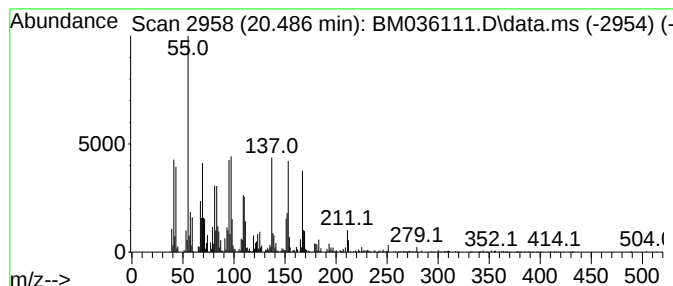
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.486 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.486	3.40 ng	754331	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,22-Docosanediol			342	C22H46O2	022513-81-1	25
2	10-Methylundec-2-en-4-olide			196	C12H20O2	1000370-40-9	15
3	Cyclohexanemethanol, 4-methyl-, ...			128	C8H16O	003937-48-2	12
4	6-Nitroundec-5-ene			199	C11H21NO2	1000192-40-3	12
5	2-(4-Nitrobutyryl)cyclooctanone			241	C12H19NO4	079630-93-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036111.D
Acq On : 04 Aug 2022 22:49
Operator : CG/JU
Sample : N4032-01 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-03-080322

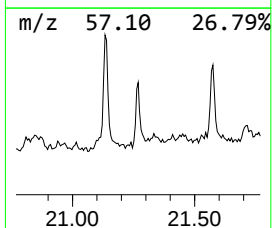
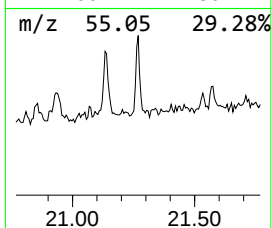
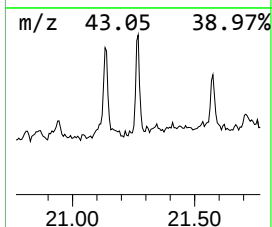
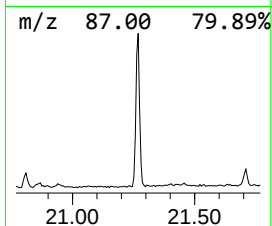
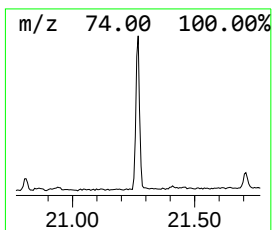
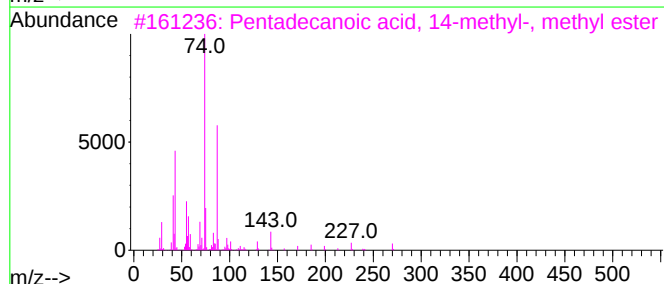
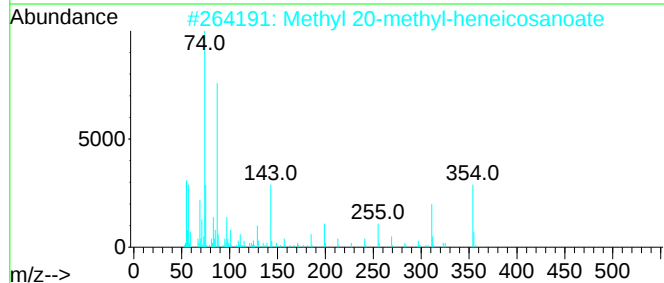
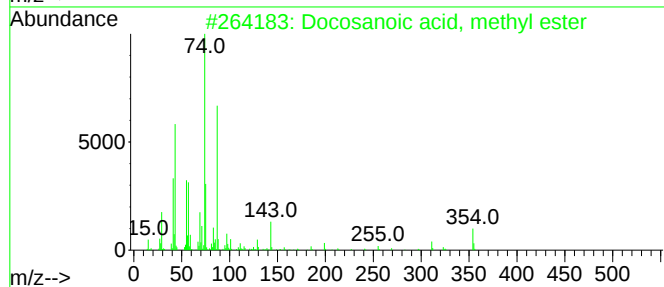
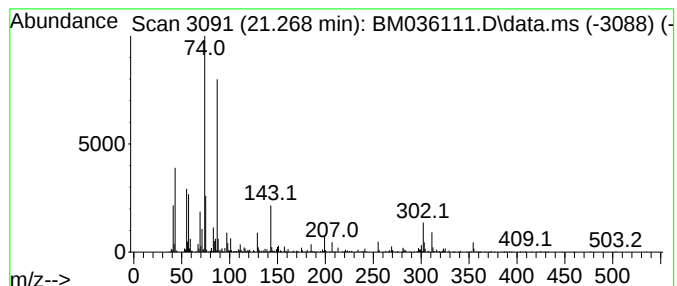
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.269	2.19 ng	485615	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	97
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4			Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	87
5			Methyl stearate	298	C19H38O2	000112-61-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036111.D
Acq On : 04 Aug 2022 22:49
Operator : CG/JU
Sample : N4032-01 10X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SU-03-080322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	17.916	33.3	ng	9920040	4	17.245	5962710	20.0
9,12-Octadecadi...	19.069	126.3	ng	37651800	4	17.245	5962710	20.0
9-Octadecenoic ...	19.098	91.0	ng	27133300	4	17.245	5962710	20.0
Methyl stearate	19.221	20.6	ng	6133430	4	17.245	5962710	20.0
11-Eicosenoic a...	20.210	3.0	ng	668118	5	21.421	4438270	20.0
Eicosanoic acid...	20.322	2.4	ng	525725	5	21.421	4438270	20.0
unknown20.486	20.486	3.4	ng	754331	5	21.421	4438270	20.0
Docosanoic acid...	21.269	2.2	ng	485615	5	21.421	4438270	20.0