LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129932.D
Acq On : 20 Aug 2022 03:26
Operator : CG\JU
Sample : N4240-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

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_F\Methods\8270-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129932.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	460	463	484	rVB	281414	385832	1.69%	0.539%
2	5.422	530	533	554	rBV	3354155	3574781	15.63%	4.991%
3	6.445	702	707	721	rBV	3663093	3548648	15.52%	4.954%
4	6.787	761	765	771	rBV	1111163	950822	4.16%	1.327%
5	7.357	857	862	865	rBV	2584887	2287228	10.00%	3.193%
6	8.069	979	983	986	rBV	1518159	1252126	5.48%	1.748%
7	9.139	1161	1165	1168	rBV	4500338	4088809	17.88%	5.708%
8	9.822	1277	1281	1284	rBV	1611626	1256953	5.50%	1.755%
9	10.616	1412	1416	1427	rBV	2384084	2027163	8.86%	2.830%
10	11.310	1530	1534	1537	rBV	1200762	1020655	4.46%	1.425%
11	11.698	1595	1600	1603	rBV	7520068	6359470	27.81%	8.878%
12	11.839	1621	1624	1630	rBV3	246539	237480	1.04%	0.332%
13	12.398	1710	1719	1721	rBV	12579525	22869296	100.00%	31.928%
14	12.422	1721	1723	1727	rVV2	12556666	11917502	52.11%	16.638%
15	12.457	1727	1729	1731	rVV	289657	232889	1.02%	0.325%
16	12.486	1731	1734	1738	rVB	3900016	3257090	14.24%	4.547%
17	12.533	1738	1742	1752	rBV2	746542	1282801	5.61%	1.791%
18	12.763	1777	1781	1788	rVB	262607	334325	1.46%	0.467%
19	12.898	1798	1804	1807	rBV	3129224	2752964	12.04%	3.843%
20	13.210	1853	1857	1860	rBV	288949	267770	1.17%	0.374%
21	13.874	1967	1970	1975	rBV	327062	276583	1.21%	0.386%
22	13.957	1980	1984	1987	rBV2	859310	889343	3.89%	1.242%
23	15.415	2229	2232	2237	rVB	493750	557896	2.44%	0.779%

Sum of corrected areas: 71628426

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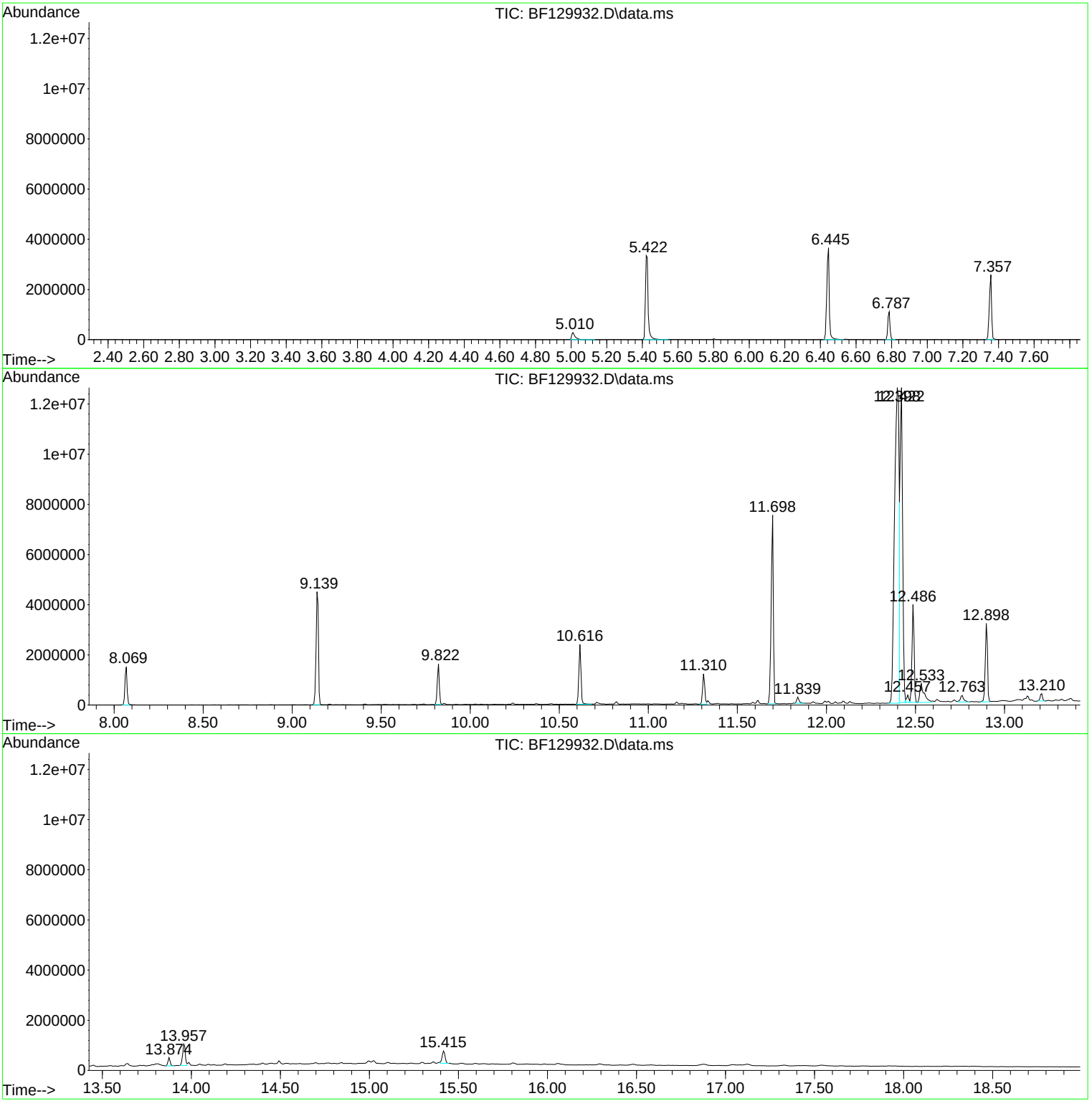
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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_F\Data\BF081922\
Data File : BF129932.D
Acq On : 20 Aug 2022 03:26
Operator : CG\JU
Sample : N4240-01
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ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
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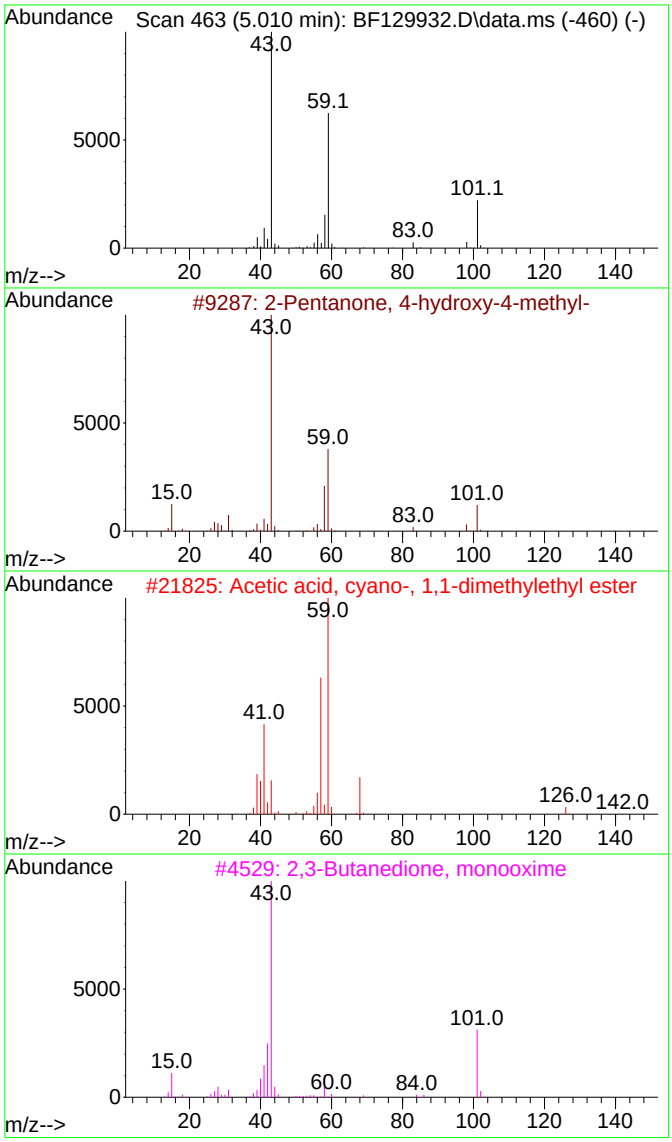
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

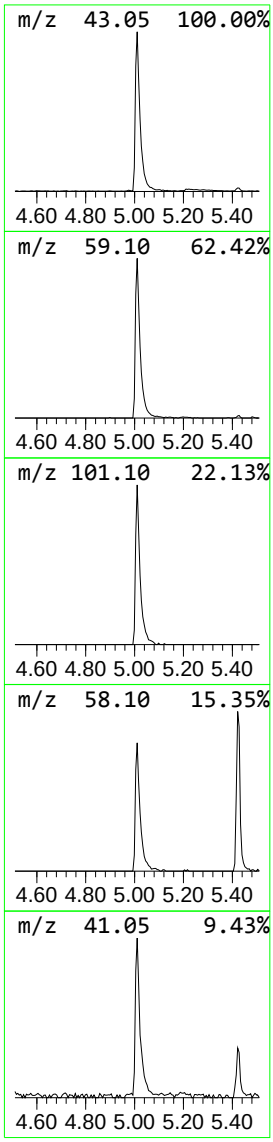
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	8.12 ng	385832	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF129932.D
Acq On : 20 Aug 2022 03:26
Operator : CG\JU
Sample : N4240-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

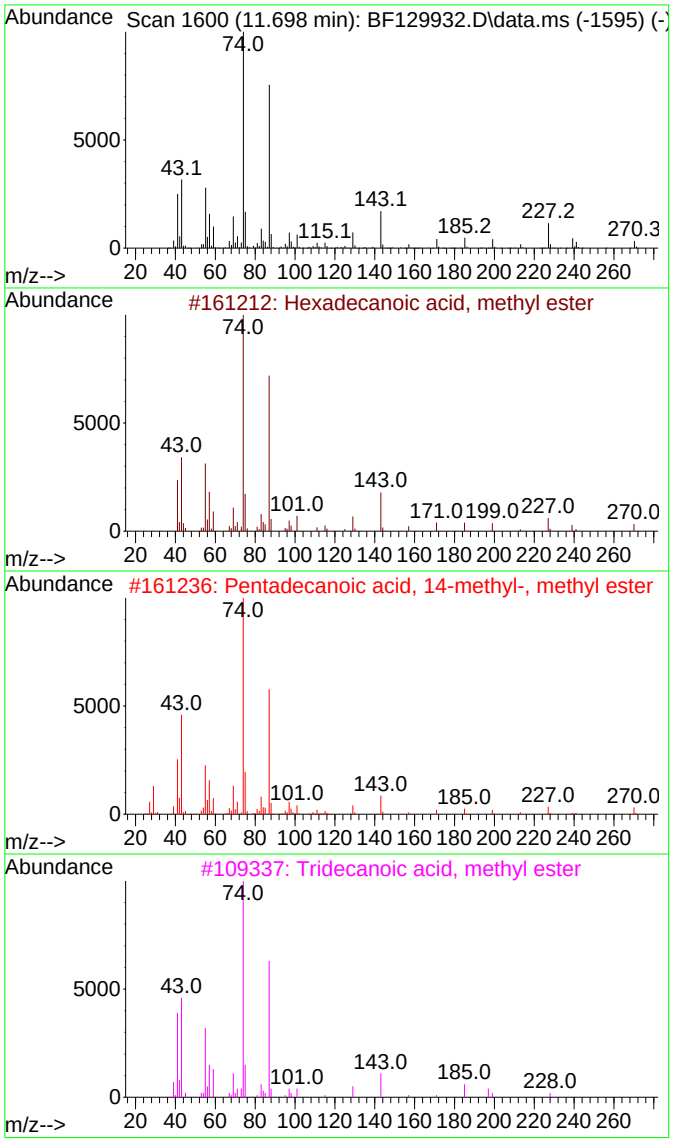
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

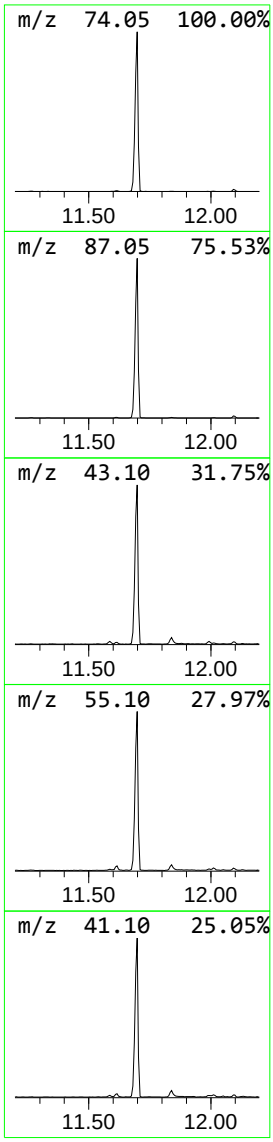
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	124.61 ng	6359470	Phenanthrene-d10	11.310

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	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Data File : BF129932.D
Acq On : 20 Aug 2022 03:26
Operator : CG\JU
Sample : N4240-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

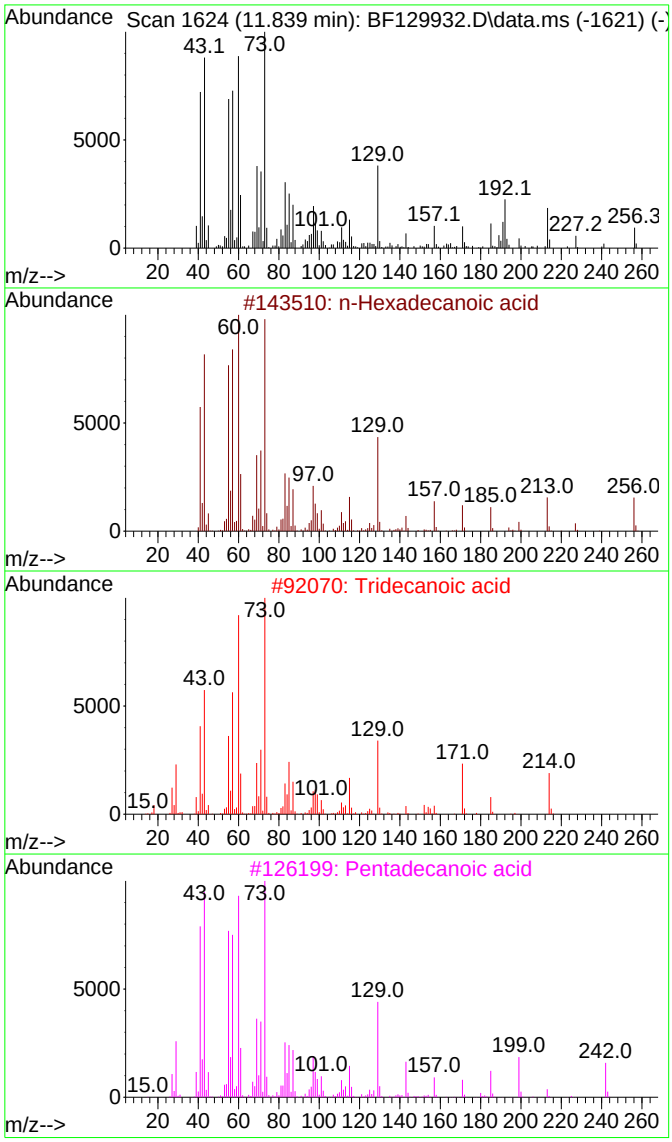
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

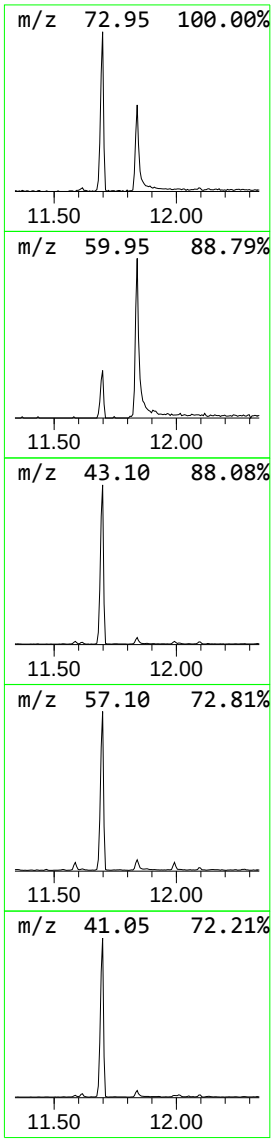
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.65 ng	237480	Phenanthrene-d10	11.310

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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Acq On : 20 Aug 2022 03:26
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Sample : N4240-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

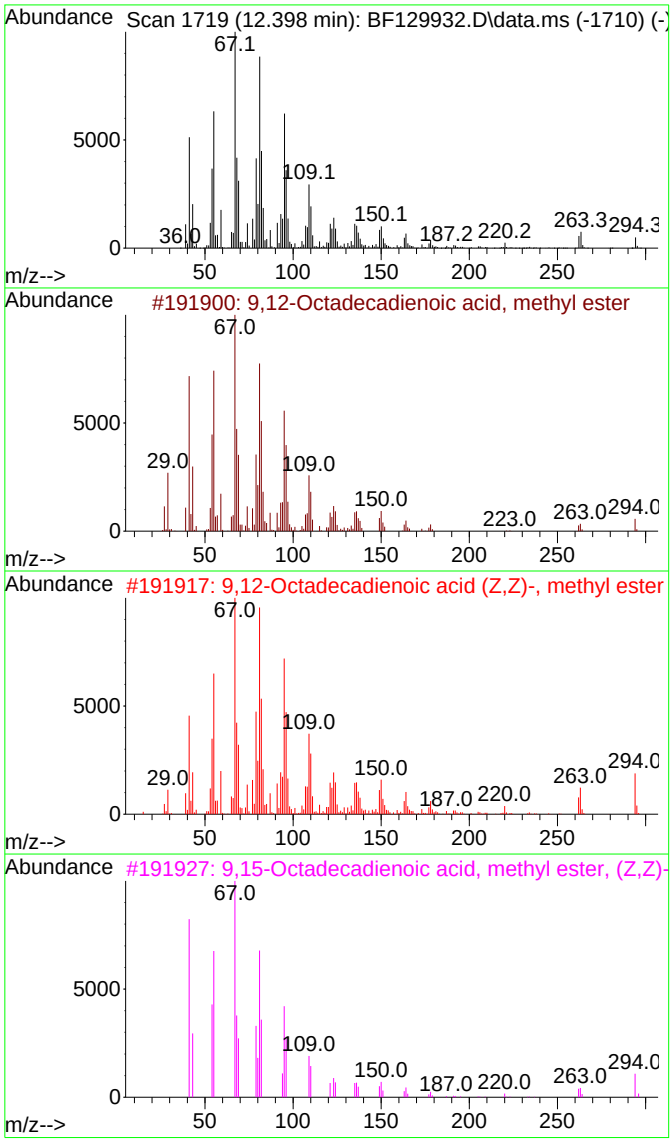
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

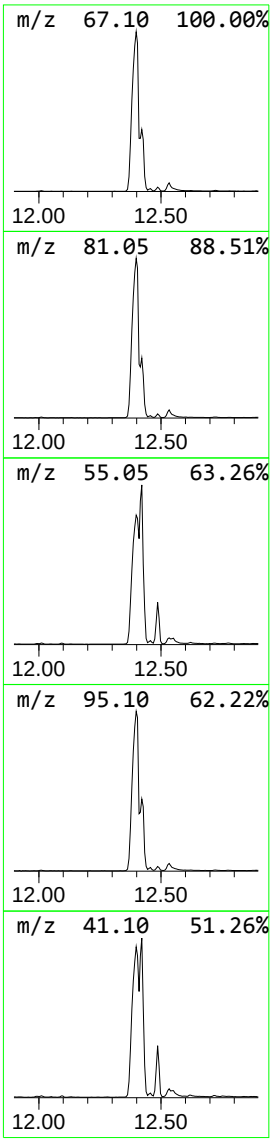
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	448.13 ng	22869300	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99





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Data File : BF129932.D
Acq On : 20 Aug 2022 03:26
Operator : CG\JU
Sample : N4240-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-081722

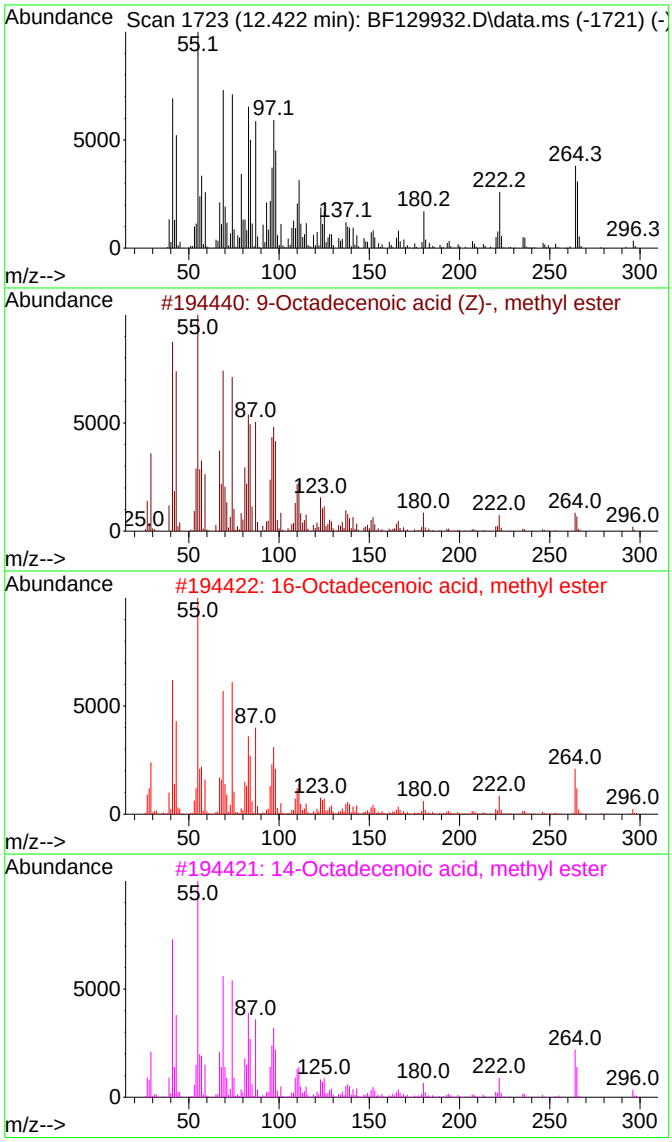
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

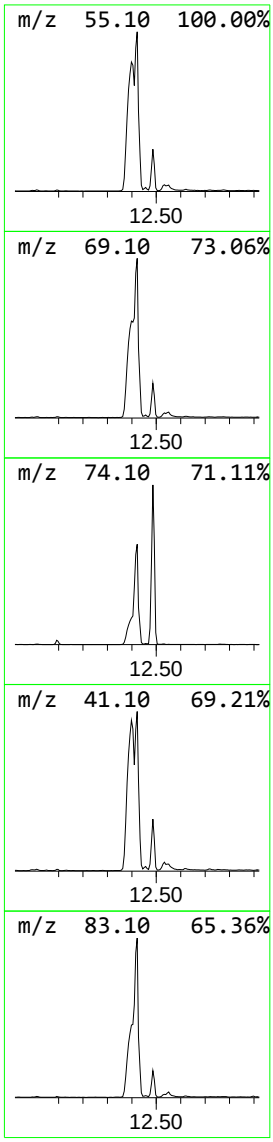
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	233.53 ng	11917500	Phenanthrene-d10	11.310

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	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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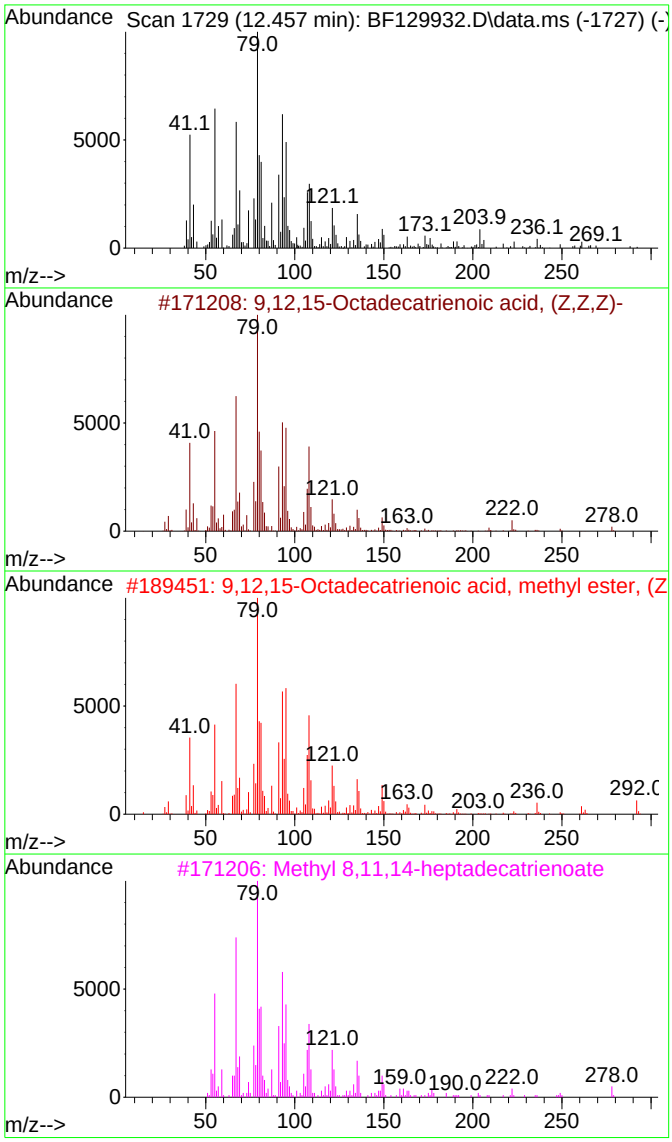
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

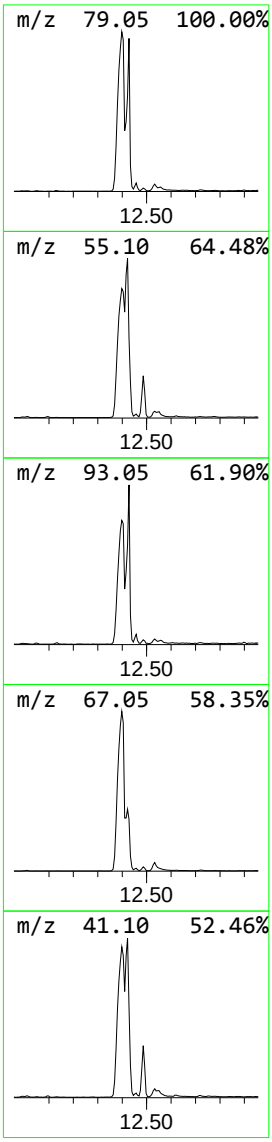
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12,15-Octadecatrienoic ac... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	4.56 ng	232889	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	90
2	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	90
3	Methyl 8,11,14-heptadecatrienoate	278	C18H30O2	1000336-35-1	90
4	1,8,11,14-Heptadecatetraene, (Z,...	232	C17H28	010482-53-8	86
5	9,12,15-Octadecatrien-1-ol, (Z,Z...	264	C18H32O	000506-44-5	83





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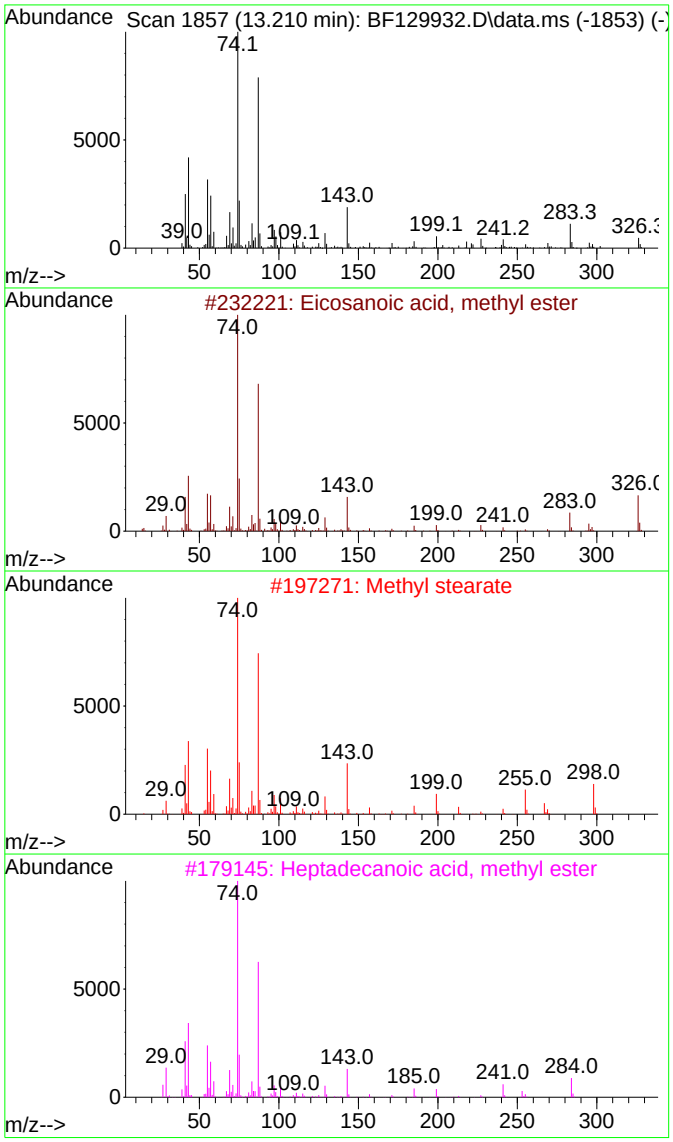
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

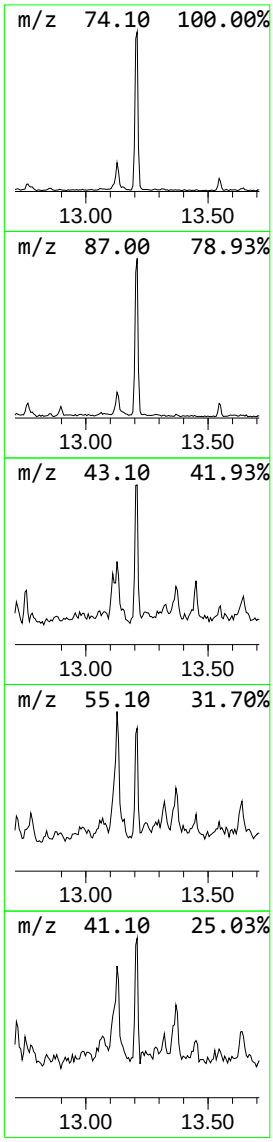
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	6.02 ng	267770	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Methyl stearate	298	C19H38O2	000112-61-8	93
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	83
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83





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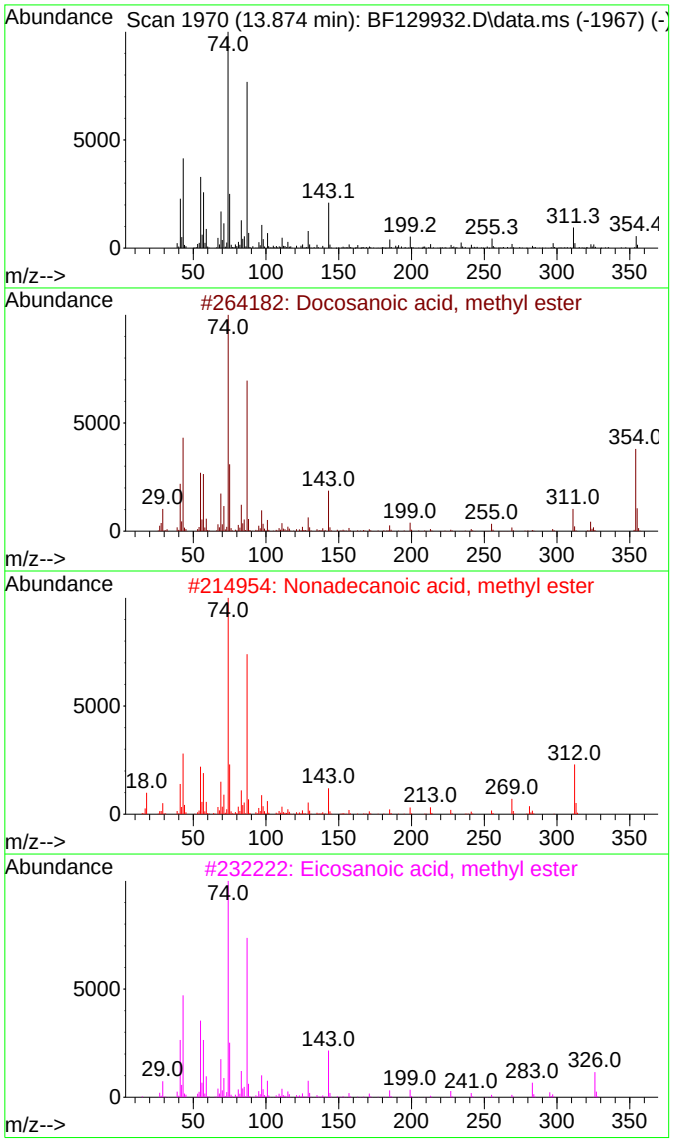
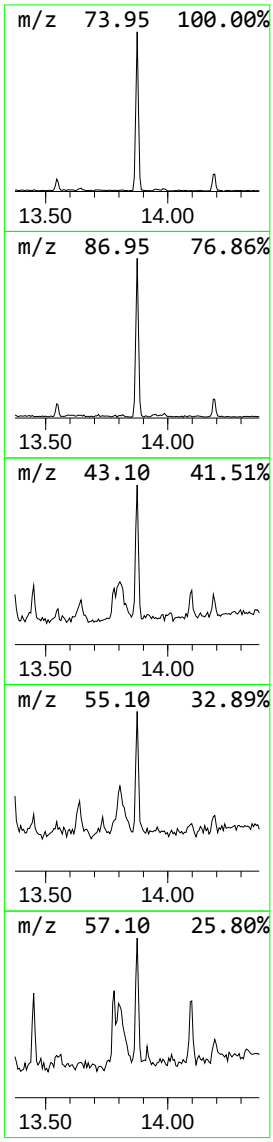
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.22 ng	276583	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	95
3	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90
5	Methyl stearate	298	C19H38O2	000112-61-8	87





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.010	8.1	ng	385832	1	6.787	950822	20.0
Hexadecanoic ac...	11.698	124.6	ng	6359470	4	11.310	1020660	20.0
n-Hexadecanoic ...	11.839	4.7	ng	237480	4	11.310	1020660	20.0
9,12-Octadecadi...	12.398	448.1	ng	22869300	4	11.310	1020660	20.0
9-Octadecenoic ...	12.422	233.5	ng	11917500	4	11.310	1020660	20.0
9,12,15-Octadec...	12.457	4.6	ng	232889	4	11.310	1020660	20.0
Eicosanoic acid...	13.210	6.0	ng	267770	5	13.957	889343	20.0
Docosanoic acid...	13.874	6.2	ng	276583	5	13.957	889343	20.0