LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
Operator : JU/CG
Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-041421

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	18	rVB	1230750	1494003	1.84%	0.815%
2	5.498	576	580	586	rVB	2624348	2480435	3.05%	1.353%
3	6.504	748	751	757	rBV2	3023596	2739670	3.37%	1.494%
4	6.869	810	813	817	rBV	2142082	1813472	2.23%	0.989%
5	7.428	901	908	911	rBV	1821170	1487510	1.83%	0.811%
6	8.157	1026	1032	1035	rBV	2874305	2364915	2.91%	1.290%
7	9.233	1211	1215	1218	rBV	3294609	2433462	2.99%	1.327%
8	9.916	1328	1331	1334	rVB	2421742	1907073	2.35%	1.040%
9	10.704	1460	1465	1469	rBV	1298276	1054004	1.30%	0.575%
10	11.410	1581	1585	1587	rBV	1692743	1674824	2.06%	0.913%
11	11.433	1587	1589	1592	rVB	1486631	1142900	1.41%	0.623%
12	11.816	1648	1654	1657	rBV	21694702	21711677	26.71%	11.840%
13	12.533	1766	1776	1777	rBV2	33070670	81285945	100.00%	44.329%
14	12.551	1777	1779	1783	rVV2	35066825	38545648	47.42%	21.021%
15	12.610	1786	1789	1791	rVV	11861584	9862754	12.13%	5.379%
16	12.627	1791	1792	1796	rVB	1554523	1241362	1.53%	0.677%
17	12.863	1826	1832	1841	rVB	1696347	2166924	2.67%	1.182%
18	13.004	1852	1856	1859	rBV	1947296	1599781	1.97%	0.872%
19	13.251	1893	1898	1903	rVB3	1055116	1464784	1.80%	0.799%
20	13.327	1908	1911	1914	rBV	1227419	1011725	1.24%	0.552%
21	13.998	2022	2025	2028	rBV	1091476	892296	1.10%	0.487%
22	14.057	2031	2035	2038	rBV2	1617790	2028335	2.50%	1.106%
23	15.551	2285	2289	2292	rBV2	797516	967013	1.19%	0.527%

Sum of corrected areas: 183370512

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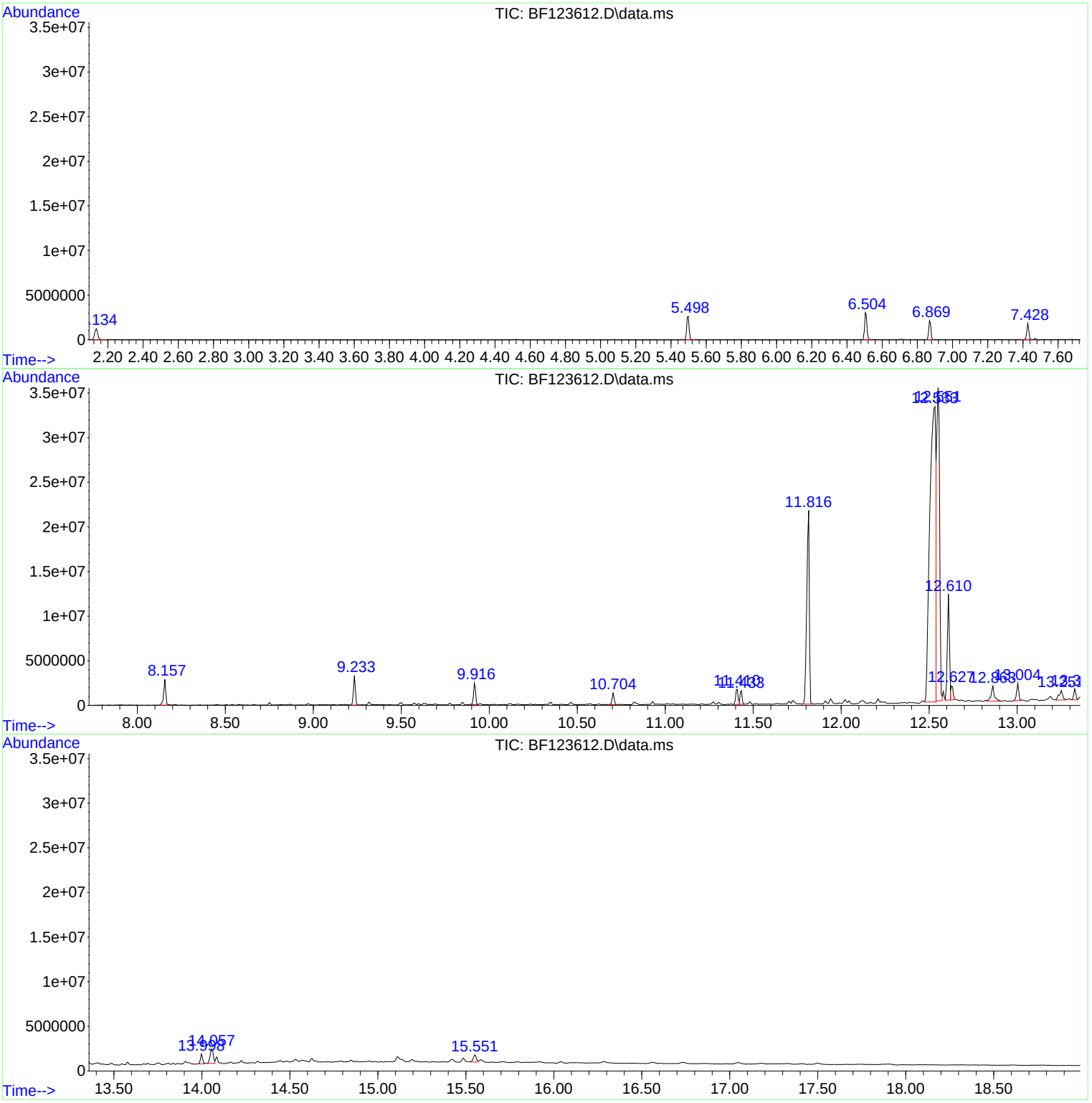
Instrument :
BNA_F
ClientSampleId :
TR-05-041421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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Data File : BF123612.D
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Instrument :
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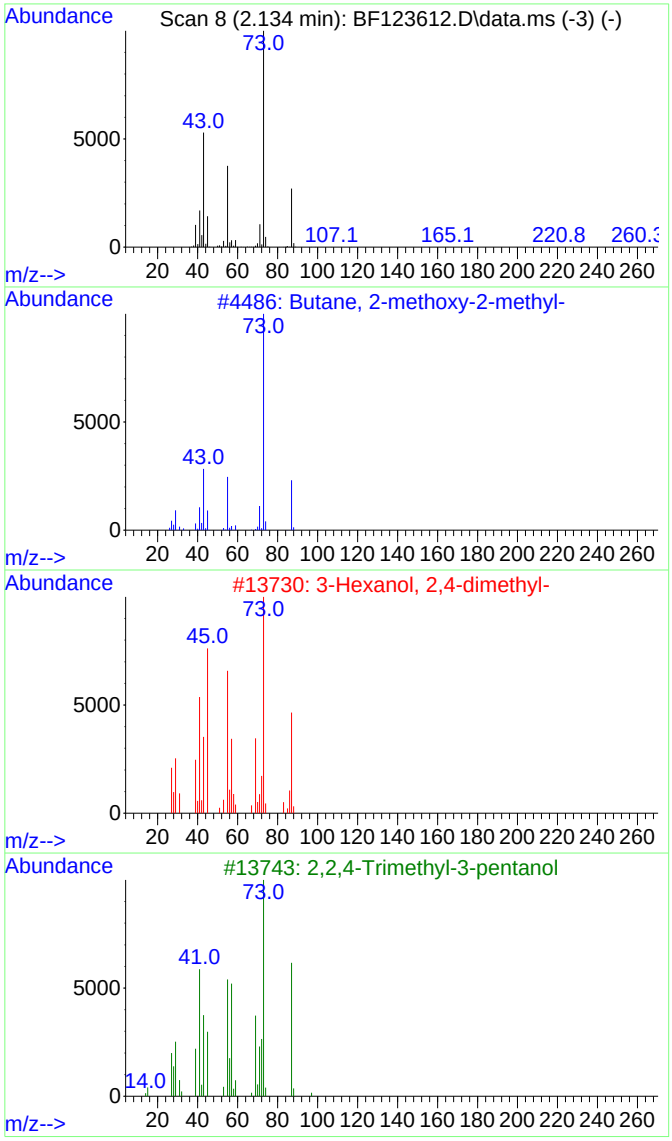
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

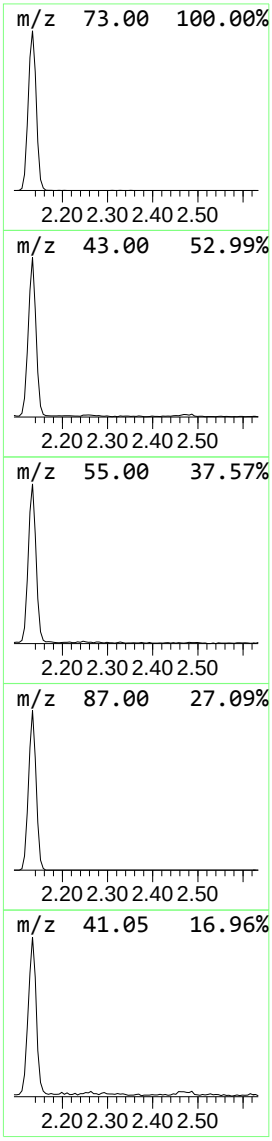
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	16.48 ng	1494000	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	45
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





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Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
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Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-041421

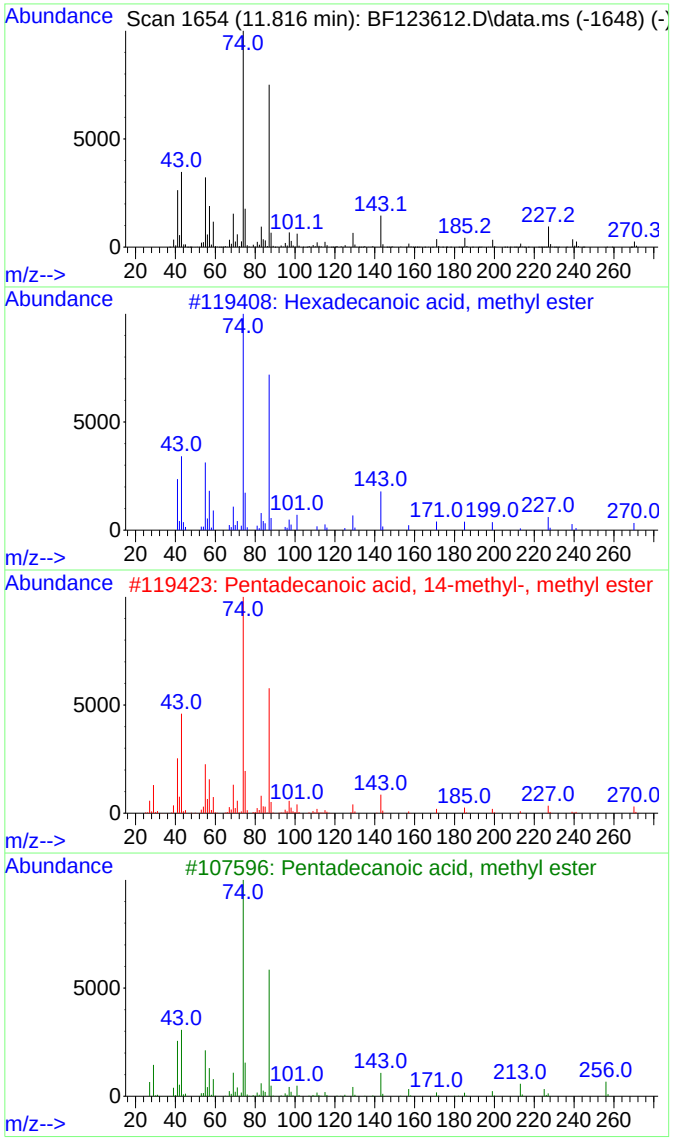
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

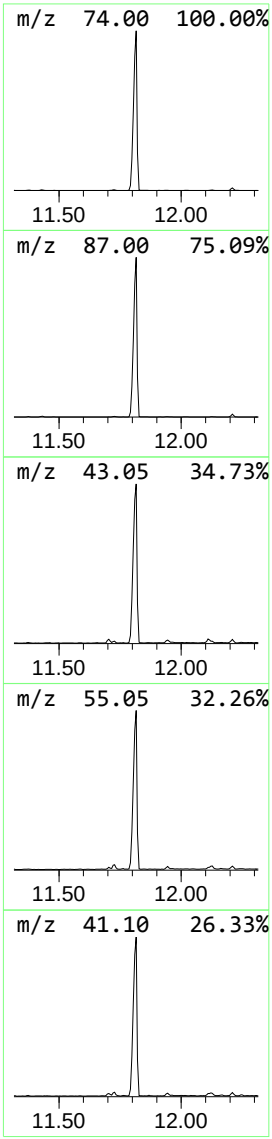
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	259.27 ng	21711700	Phenanthrene-d10	11.410

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	96
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
Operator : JU/CG
Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-041421

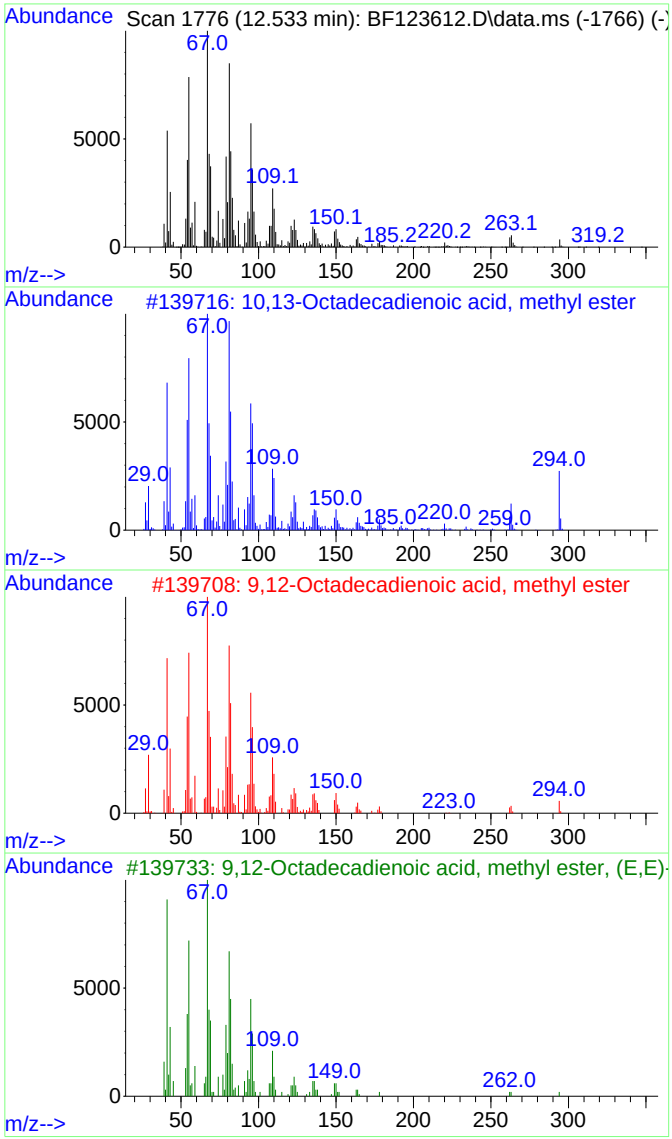
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

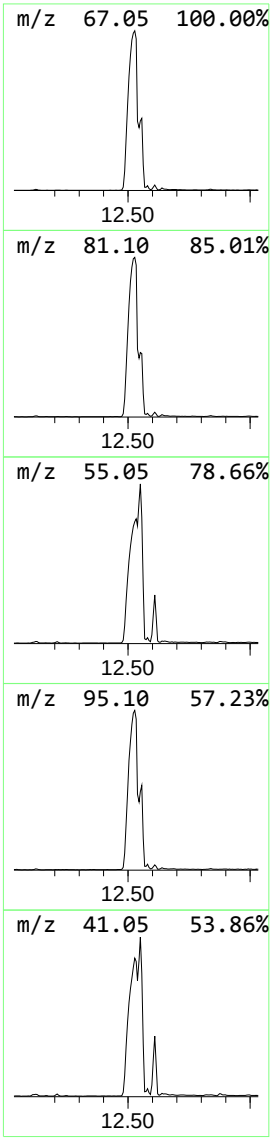
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	970.68 ng	81285900	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	97





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Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
Operator : JU/CG
Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-041421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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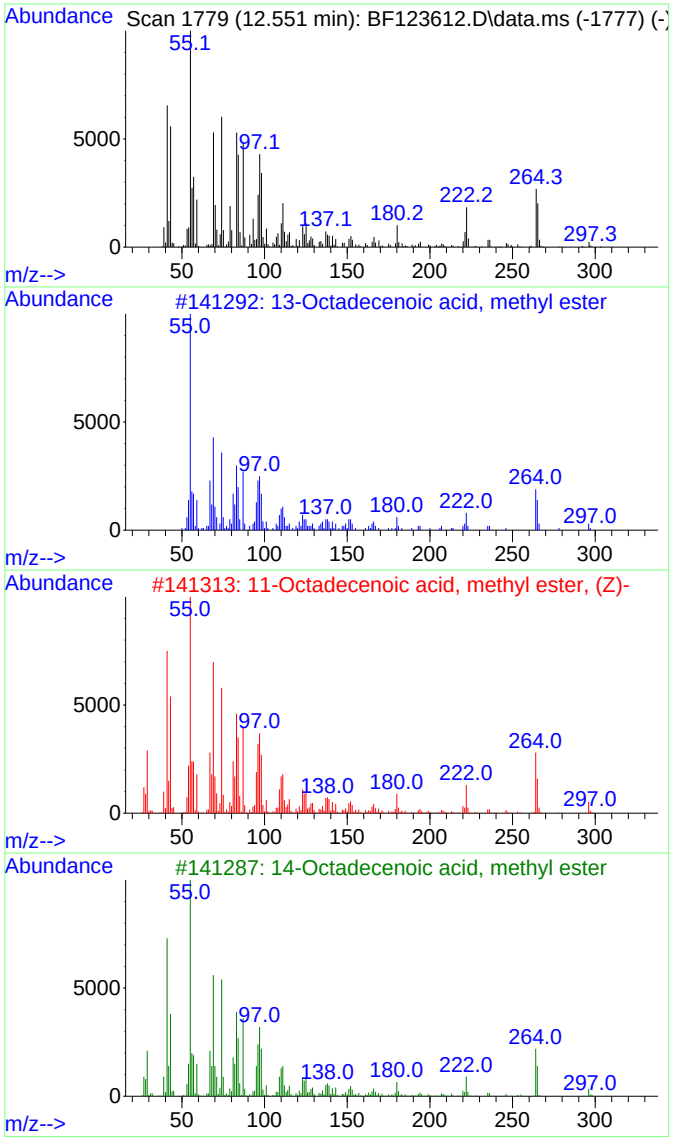
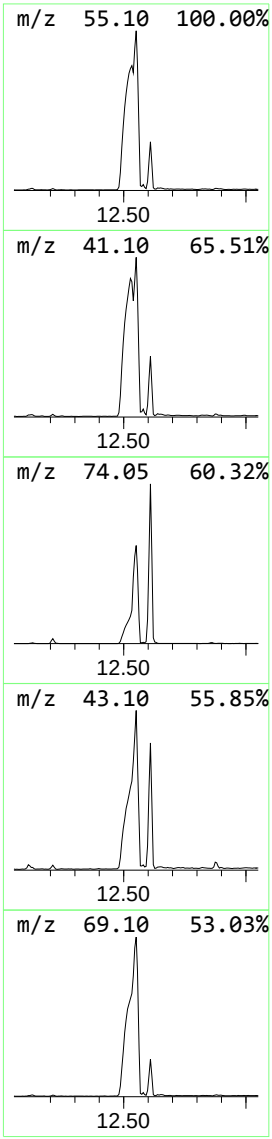
****
Peak Number 4 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	460.30 ng	38545600	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	87
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	87
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	86
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	83





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Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
Operator : JU/CG
Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-041421

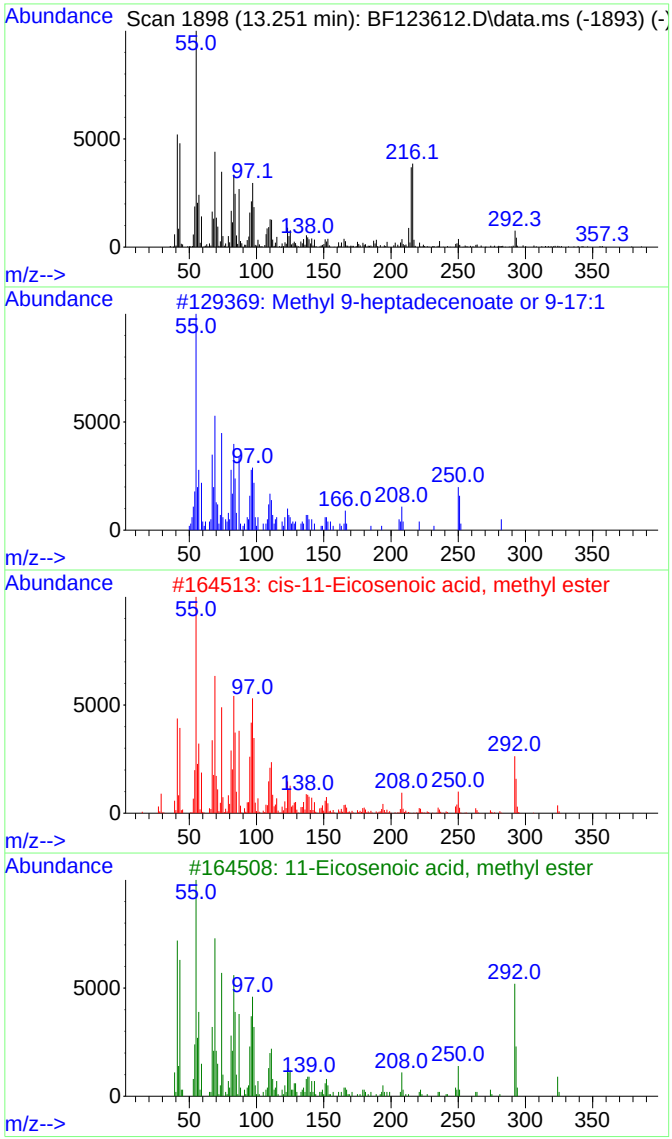
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

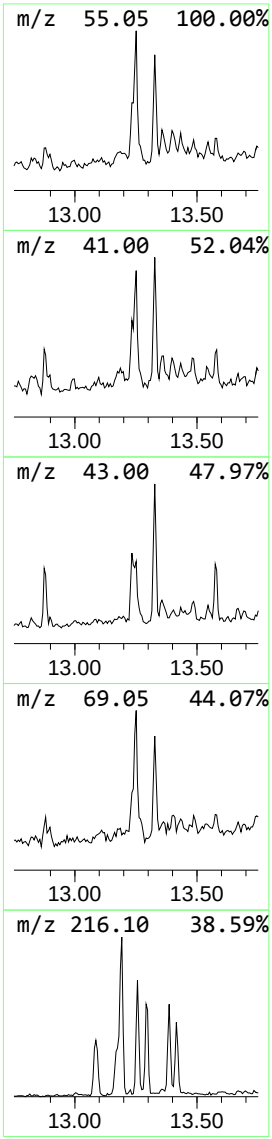
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methyl 9-heptadecenoate or ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	14.44 ng	1464780	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	87
2	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	60
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	53
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	50
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	50





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-041421

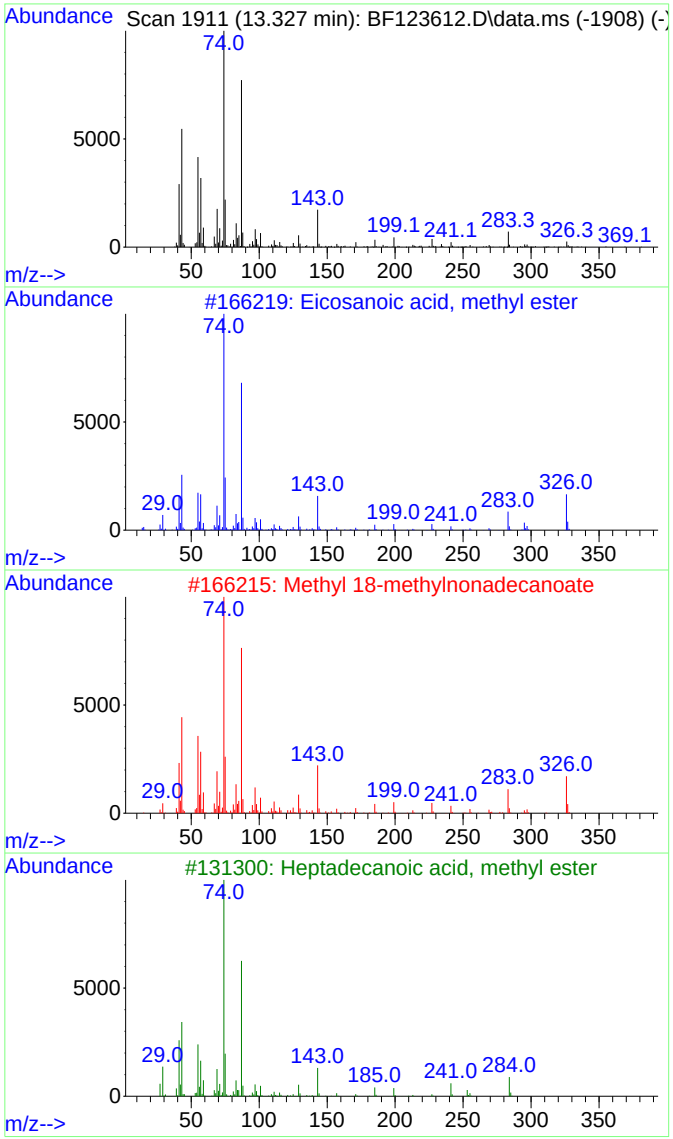
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

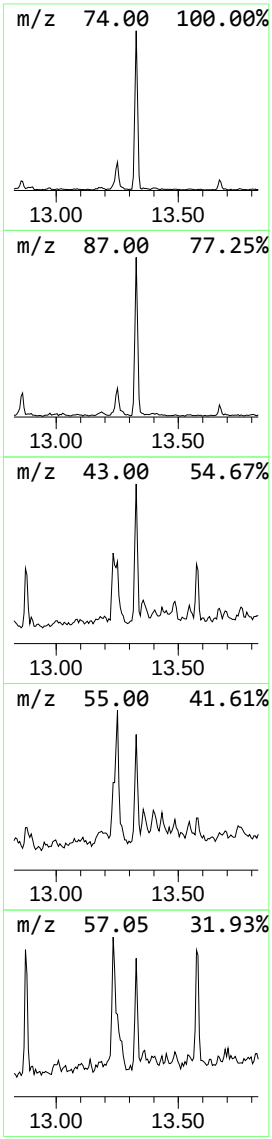
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	9.98 ng	1011730	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	96
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	95
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
5	Methyl stearate	298	C19H38O2	000112-61-8	87





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Data File : BF123612.D
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Sample : M2044-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-041421

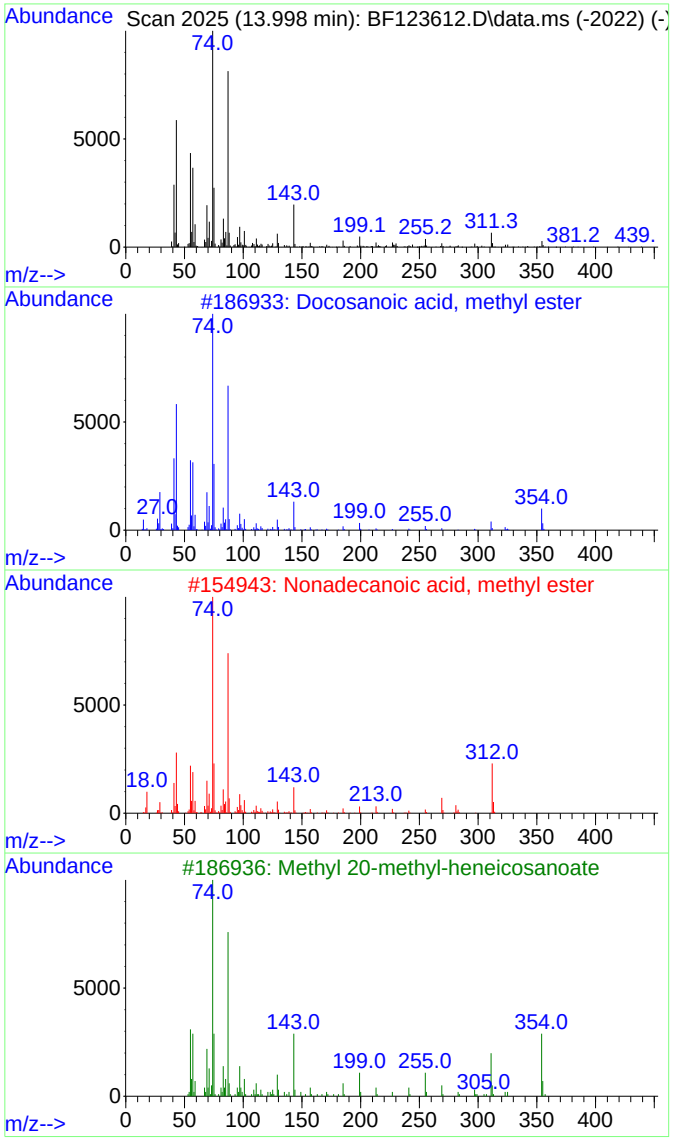
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

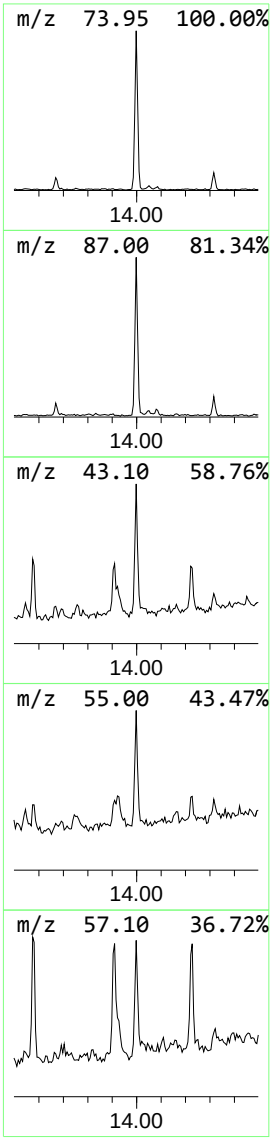
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Docosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	8.80 ng	892296	Chrysene-d12	14.063

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	91
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
4	Methyl stearate	298	C19H38O2	000112-61-8	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90





Tentatively Identified Compound (LSC) summary

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Data File : BF123612.D
Acq On : 17 Apr 2021 2:08
Operator : JU/CG
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Misc :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.134	16.5	ng	1494000	1	6.869	1813470	20.0
Hexadecanoic ac...	11.816	259.3	ng	21711700	4	11.410	1674820	20.0
10,13-Octadecad...	12.533	970.7	ng	81285900	4	11.410	1674820	20.0
13-Octadecenoic...	12.551	460.3	ng	38545600	4	11.410	1674820	20.0
Methyl 9-heptad...	13.251	14.4	ng	1464780	5	14.063	2028340	20.0
Eicosanoic acid...	13.327	10.0	ng	1011730	5	14.063	2028340	20.0
Docosanoic acid...	13.998	8.8	ng	892296	5	14.063	2028340	20.0