LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080222\
Data File : BF129522.D
Acq On : 02 Aug 2022 23:14
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.510	544	548	558	rBV	3200328	2952929	3.18%	1.584%
2	6.522	716	720	723	rBV	3380800	2870007	3.09%	1.539%
3	7.440	872	876	879	rBV	2275368	1833449	1.98%	0.983%
4	8.157	995	998	1001	rBV	1414571	1088030	1.17%	0.584%
5	9.234	1177	1181	1184	rVB	3475086	2980680	3.21%	1.599%
6	9.916	1293	1297	1300	rVB	1174036	964580	1.04%	0.517%
7	10.704	1428	1431	1435	rBV	1647185	1466982	1.58%	0.787%
8	11.427	1552	1554	1560	rVB	1189788	959594	1.03%	0.515%
9	11.810	1611	1619	1622	rBV	16319478	26288518	28.34%	14.100%
10	11.969	1638	1646	1652	rVV2	2811220	4895179	5.28%	2.626%
11	12.022	1652	1655	1662	rVV3	562572	1007326	1.09%	0.540%
12	12.551	1724	1745	1746	rBV3	21881104	92746381	100.00%	49.745%
13	12.610	1750	1755	1757	rVV	14142098	16566860	17.86%	8.886%
14	12.657	1757	1763	1773	rVV3	5696684	14661164	15.81%	7.864%
15	12.869	1795	1799	1807	rVB2	1206792	2410566	2.60%	1.293%
16	13.004	1816	1822	1825	rBV	2608583	2857675	3.08%	1.533%
17	13.180	1847	1852	1855	rBV5	663146	1192461	1.29%	0.640%
18	13.227	1858	1860	1867	rVB2	1518071	1922584	2.07%	1.031%
19	13.304	1869	1873	1876	rBV2	2243245	2234807	2.41%	1.199%
20	13.469	1896	1901	1905	rVV2	795620	966812	1.04%	0.519%
21	13.974	1983	1987	1990	rBV	2187325	1958185	2.11%	1.050%
22	14.051	1996	2000	2003	rBV2	1073321	1619382	1.75%	0.869%

Sum of corrected areas: 186444151

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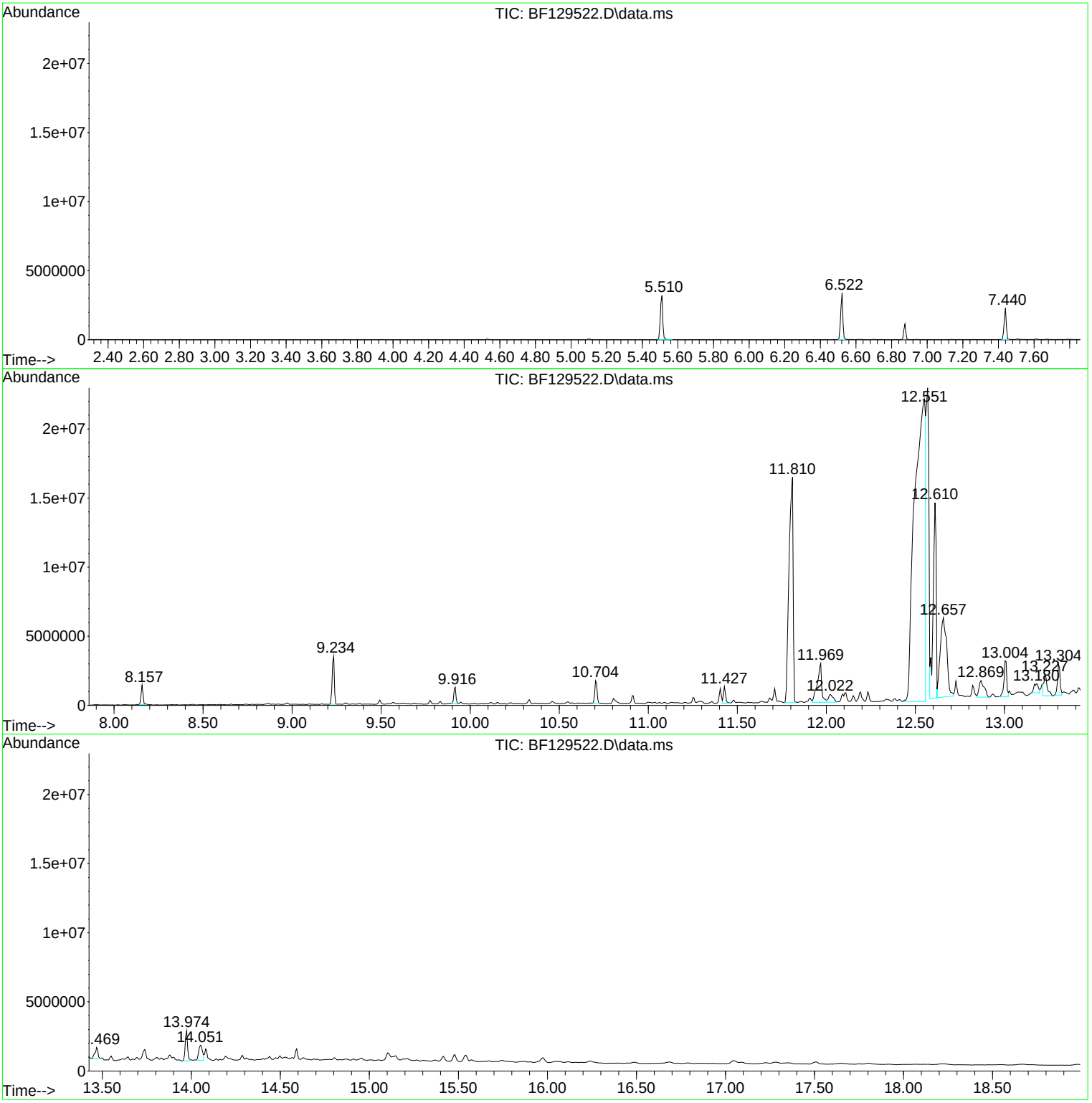
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF080222\
Data File : BF129522.D
Acq On : 02 Aug 2022 23:14
Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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BNA_F
ClientSampleId :
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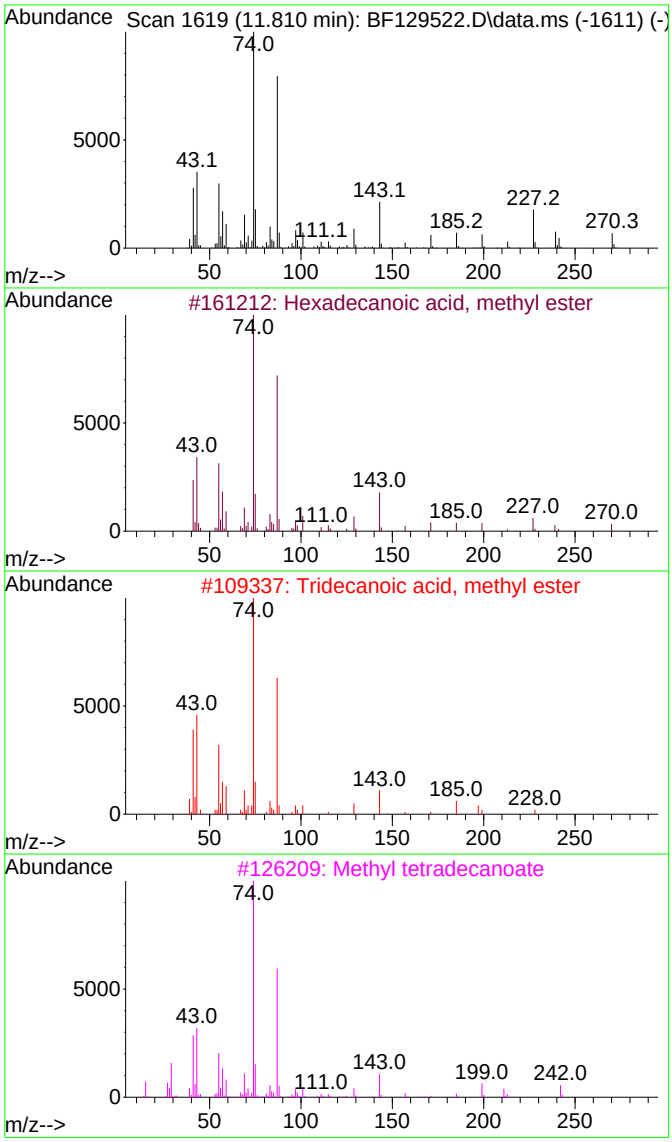
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

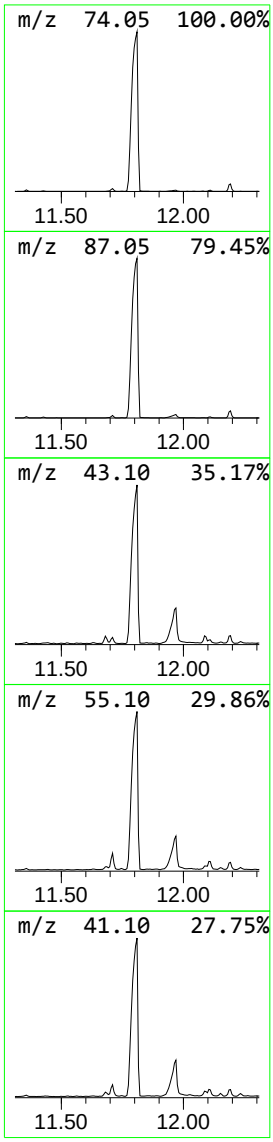
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	547.91 ng	26288500	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	83
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80





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Data File : BF129522.D
Acq On : 02 Aug 2022 23:14
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Sample : N3979-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

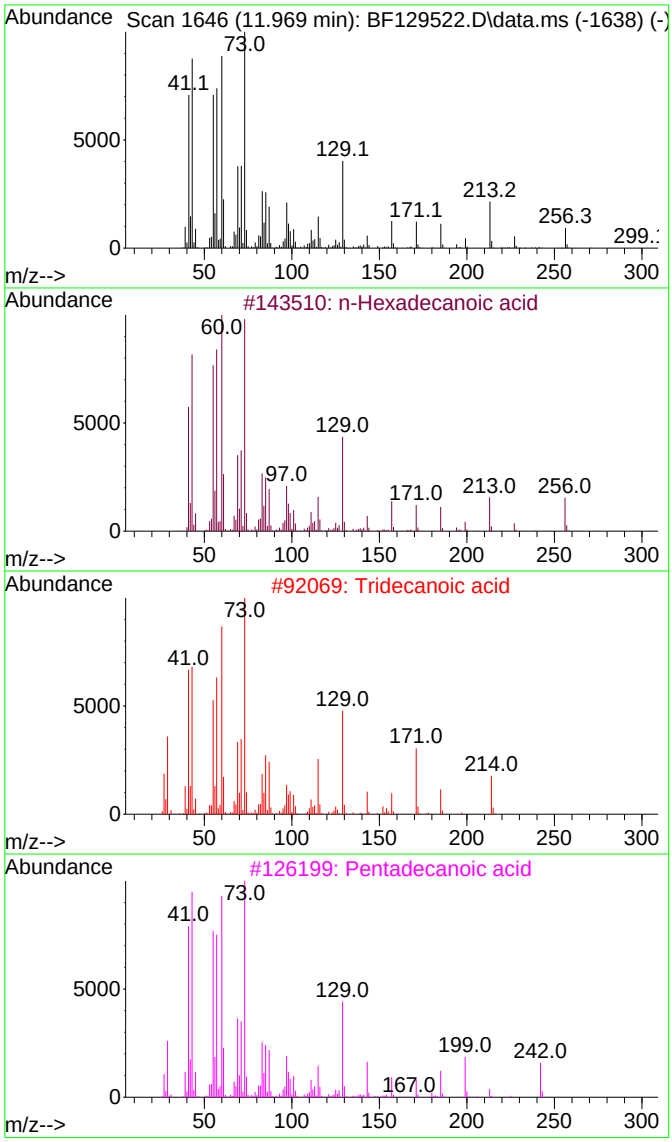
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

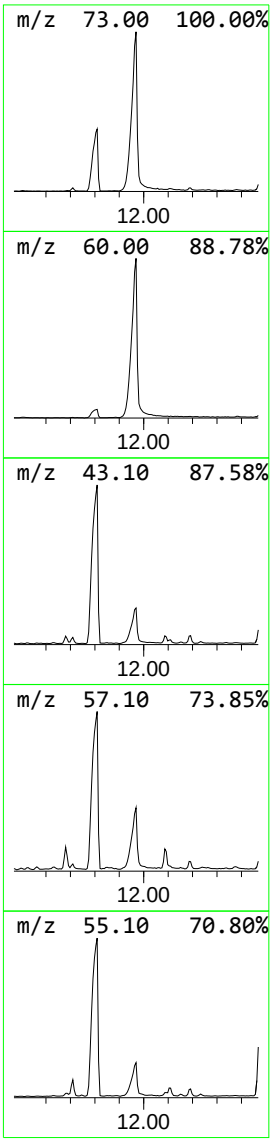
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	102.03 ng	4895180	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BF129522.D
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Operator : CG\JU
Sample : N3979-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-06-072922

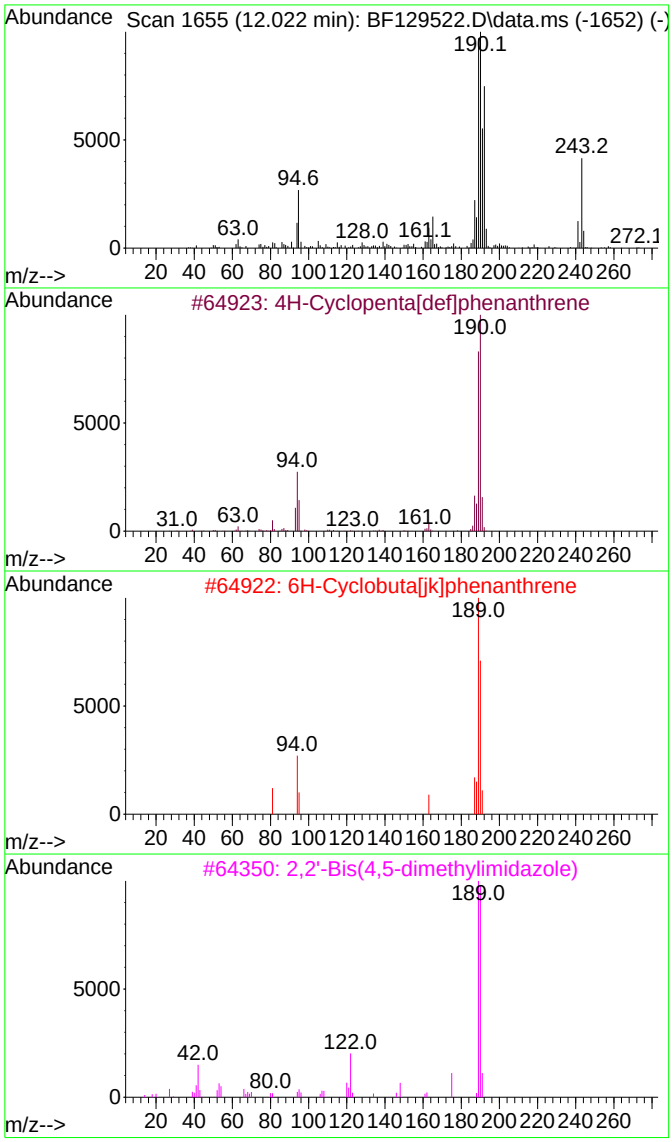
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

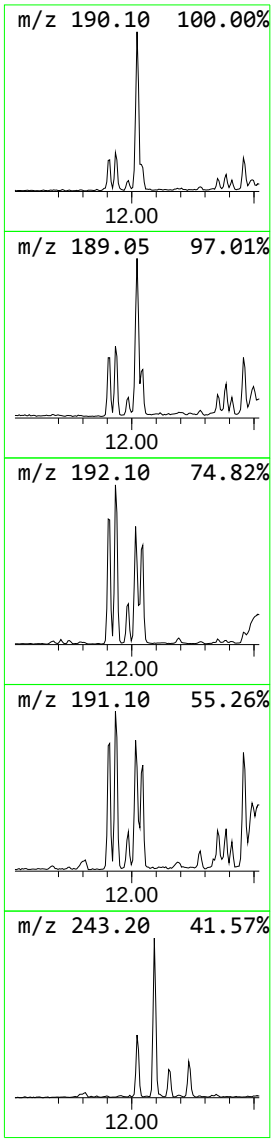
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	20.99 ng	1007330	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	27
4	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	25
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	20





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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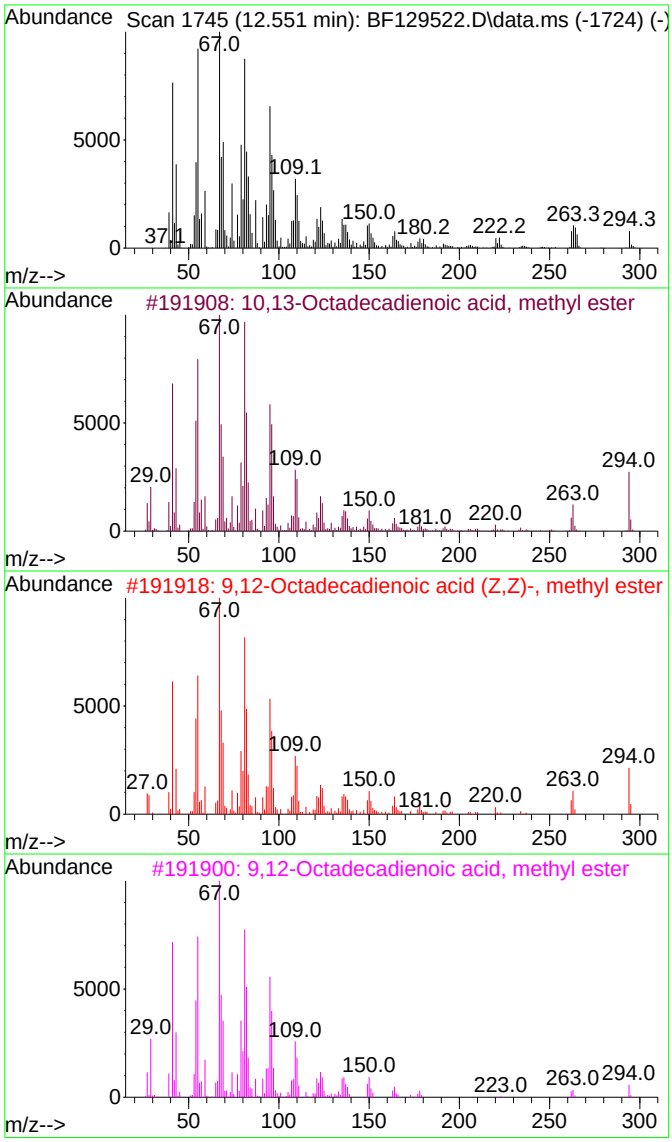
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

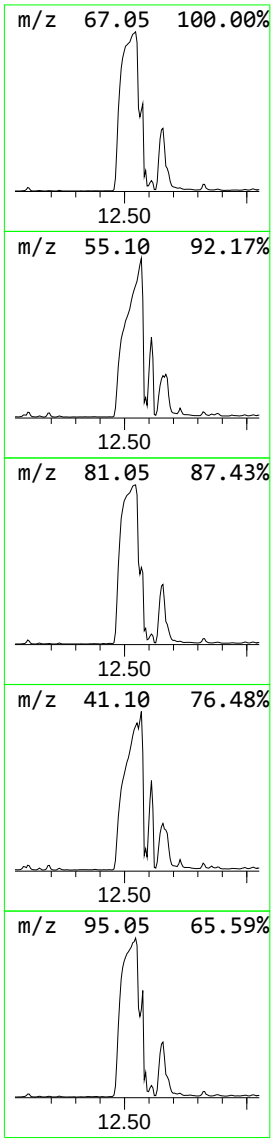
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	1933.03 ng	92746400	Phenanthrene-d10	11.404

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 (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	99





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TIC Library : C:\Database\NIST20.L
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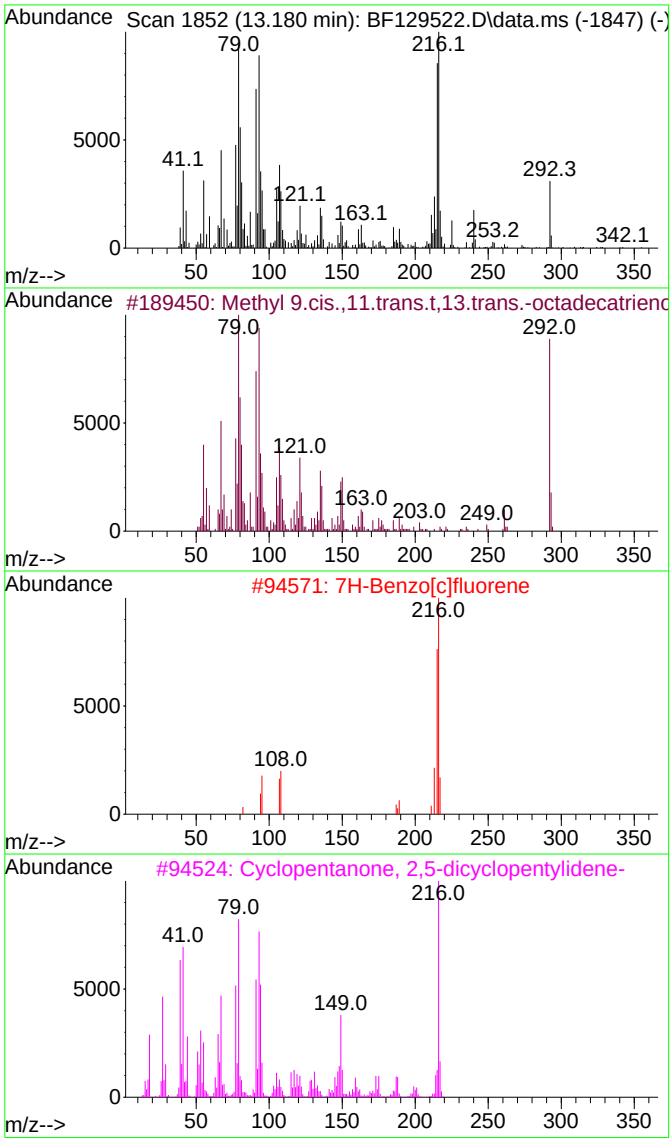
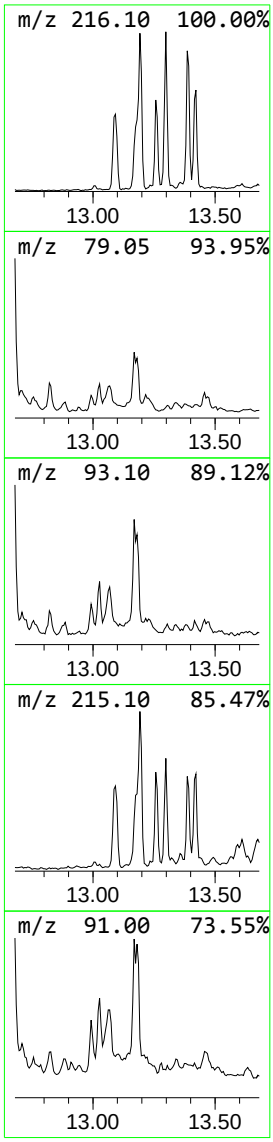
****

Peak Number 5 Methyl 9.cis.,11.trans.t,13... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	14.73 ng	1192460	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	78
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	49
3	Cyclopentanone, 2,5-dicyclopenty...	216	C15H20O	005682-82-6	45
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	42
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	38





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Instrument :
BNA_F
ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

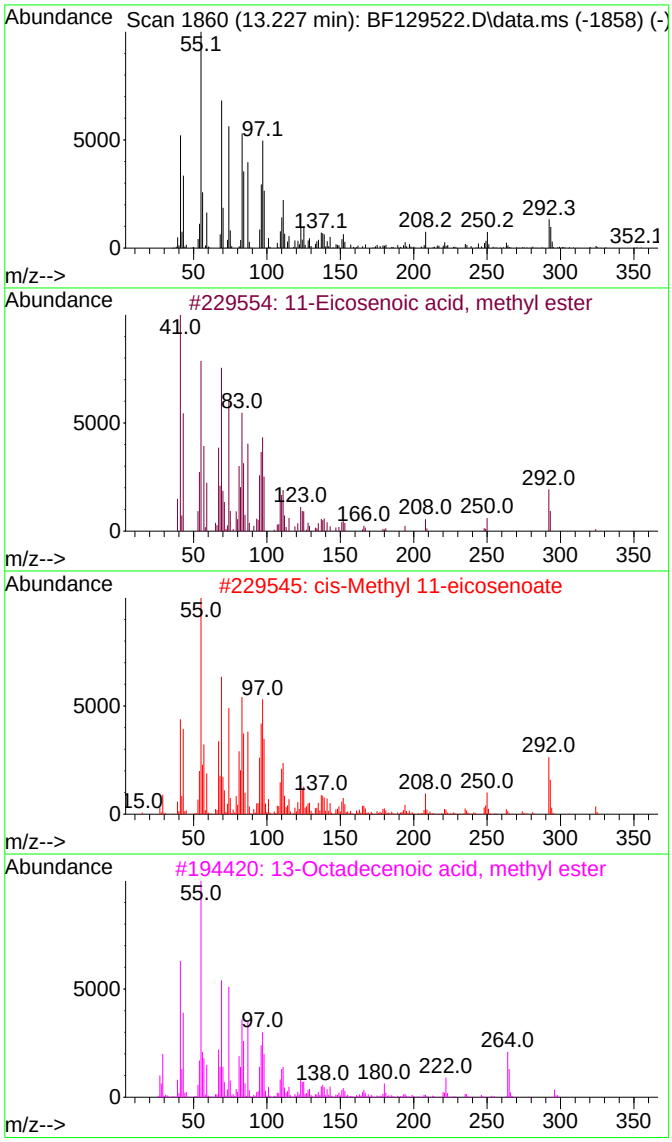
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

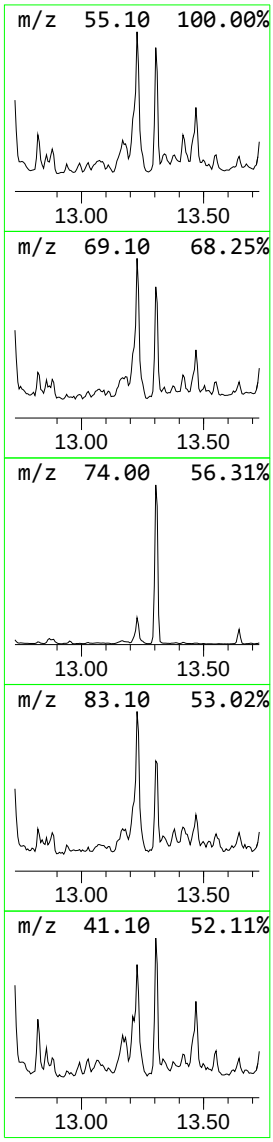
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	23.74 ng	1922580	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	94
2	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	74
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	72
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	72





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Instrument :
BNA_F
ClientSampleId :
TR-06-072922

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

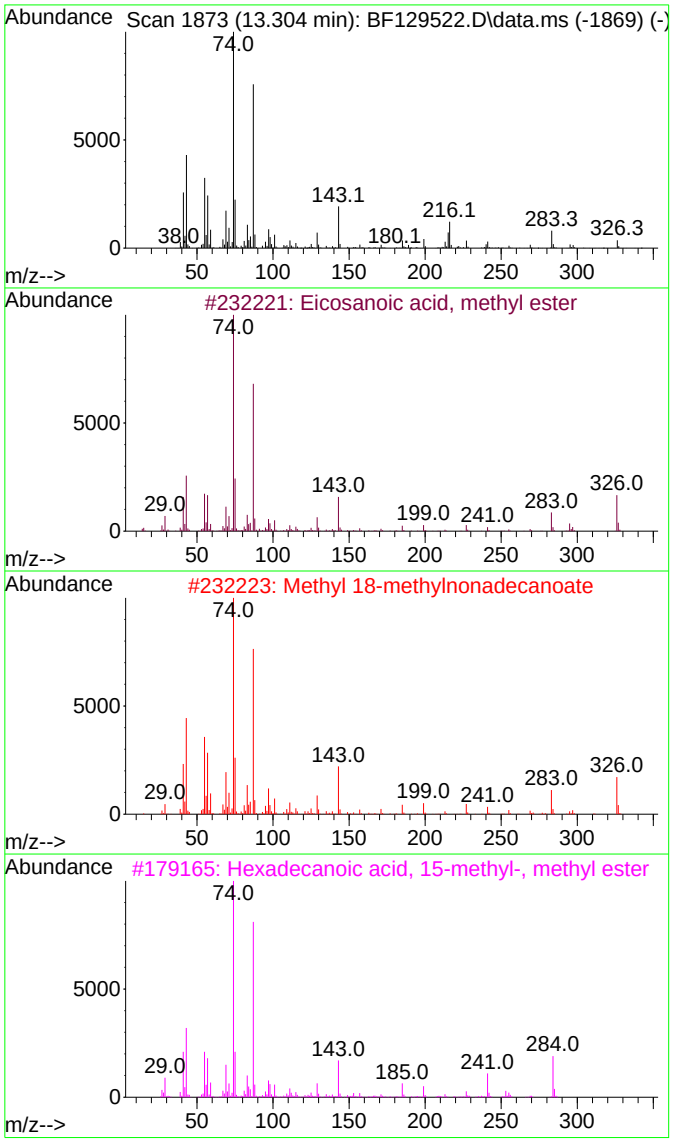
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

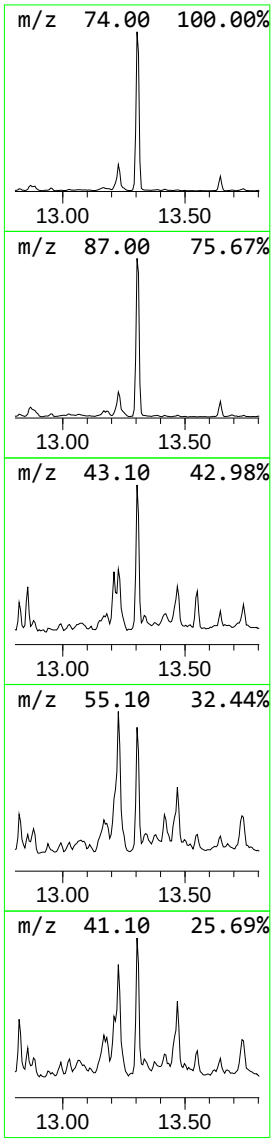
****

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.304	27.60 ng	2234810	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	98
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90





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Instrument :
BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

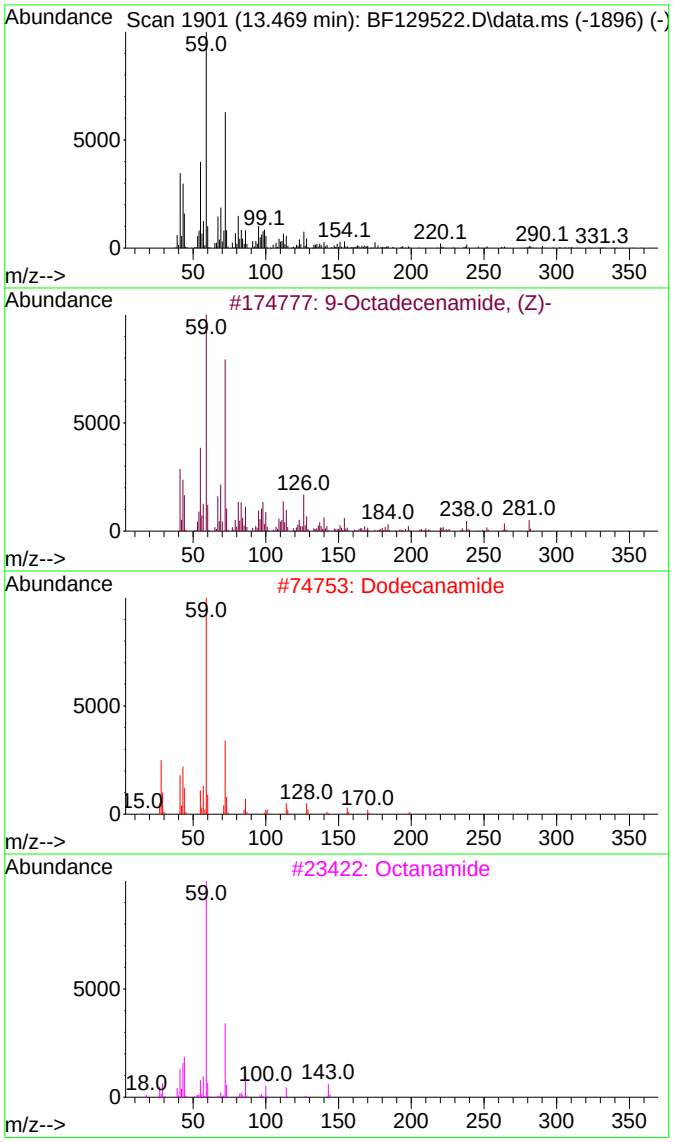
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

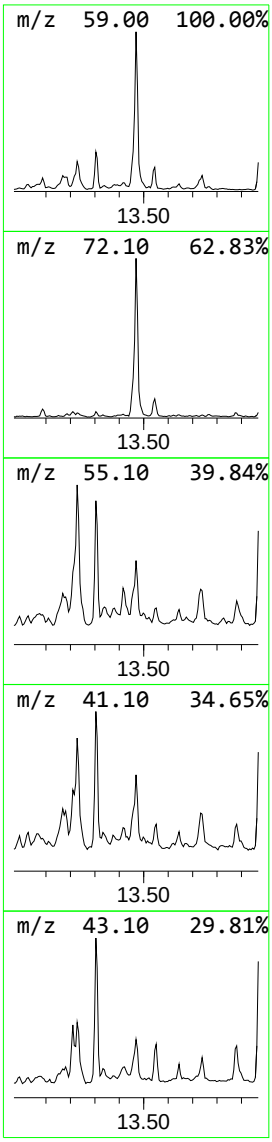
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	11.94 ng	966812	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Dodecanamide	199	C12H25NO	001120-16-7	53
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Hexadecanamide	255	C16H33NO	000629-54-9	53
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53





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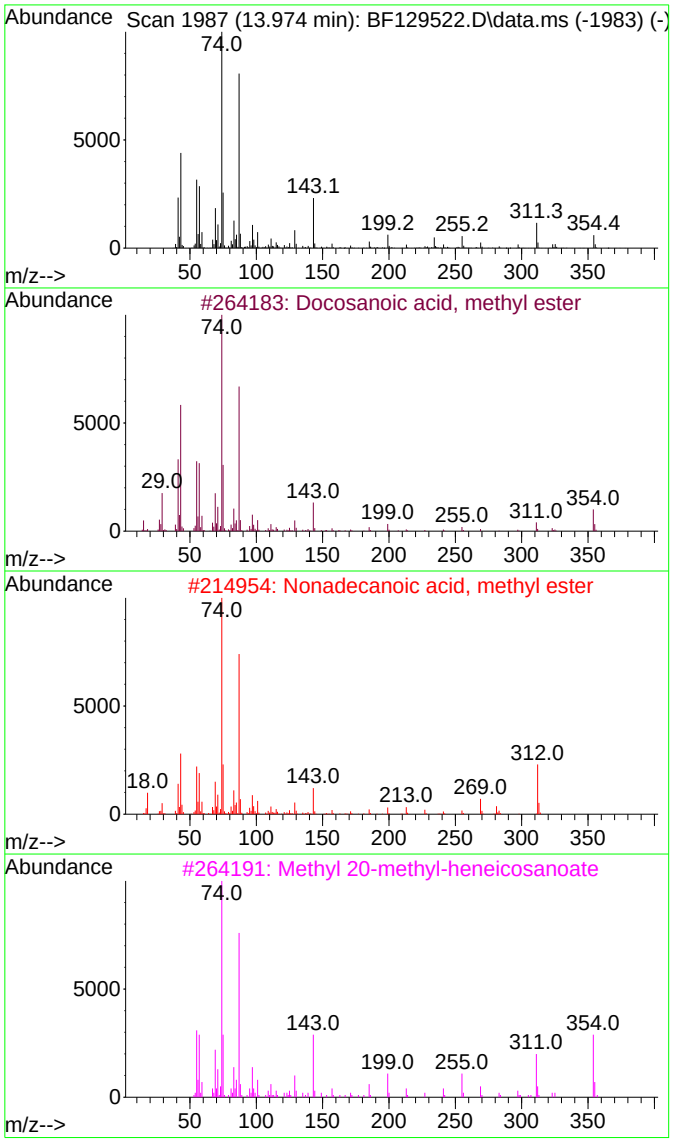
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

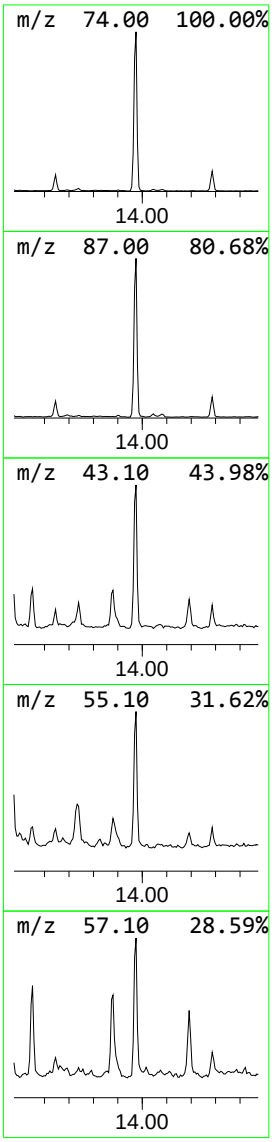
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	24.18 ng	1958190	Chrysene-d12	14.057

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	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90
4	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
5	Octadecanoic acid, 17-methyl-, m...	312	C20H40O2	055124-97-5	87





Tentatively Identified Compound (LSC) summary

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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
Hexadecanoic ac...	11.810	547.9	ng	26288500	4	11.404	959594	20.0
n-Hexadecanoic ...	11.969	102.0	ng	4895180	4	11.404	959594	20.0
4H-Cyclopenta[d...	12.022	21.0	ng	1007330	4	11.404	959594	20.0
10,13-Octadecad...	12.551	1933.0	ng	92746400	4	11.404	959594	20.0
Methyl 9.cis.,1...	13.180	14.7	ng	1192460	5	14.057	1619380	20.0
11-Eicosenoic a...	13.227	23.7	ng	1922580	5	14.057	1619380	20.0
Eicosanoic acid...	13.304	27.6	ng	2234810	5	14.057	1619380	20.0
9-Octadecenamid...	13.469	11.9	ng	966812	5	14.057	1619380	20.0
Docosanoic acid...	13.974	24.2	ng	1958190	5	14.057	1619380	20.0