LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.457	569	573	577	rBV	1452758	1381954	2.84%	0.853%
2	6.469	741	745	752	rBV	1465044	1354369	2.79%	0.836%
3	6.851	807	810	817	rVB	1135112	898313	1.85%	0.555%
4	7.410	897	905	908	rBV	1087727	907751	1.87%	0.560%
5	8.134	1023	1028	1032	rBV	1240920	1058500	2.18%	0.654%
6	9.204	1207	1210	1214	rBV	1573436	1379306	2.84%	0.852%
7	9.886	1322	1326	1329	rBV	1263493	957392	1.97%	0.591%
8	10.669	1455	1459	1463	rBV	1004520	800900	1.65%	0.495%
9	11.369	1575	1578	1581	rBV	1147213	903844	1.86%	0.558%
10	11.780	1642	1648	1651	rBV	20140494	23024583	47.38%	14.216%
11	11.916	1666	1671	1677	rBV	954708	1026327	2.11%	0.634%
12	12.480	1759	1767	1769	rBV	23361298	48597197	100.00%	30.005%
13	12.510	1769	1772	1776	rVV2	33958141	45606569	93.85%	28.159%
14	12.575	1779	1783	1786	rVV	13016736	10691822	22.00%	6.601%
15	12.639	1786	1794	1802	rVV	3504859	5911248	12.16%	3.650%
16	12.963	1845	1849	1852	rBV	1724394	1424730	2.93%	0.880%
17	13.145	1874	1880	1885	rBV5	521421	1010697	2.08%	0.624%
18	13.210	1885	1891	1897	rVB	1176571	1285870	2.65%	0.794%
19	13.292	1901	1905	1906	rBV	1134651	1052468	2.17%	0.650%
20	13.310	1906	1908	1913	rVV2	1420475	1907791	3.93%	1.178%
21	13.357	1913	1916	1920	rVV	1290535	1853847	3.81%	1.145%
22	13.398	1920	1923	1928	rVV4	693254	1431045	2.94%	0.884%
23	13.451	1929	1932	1935	rVV	812641	995124	2.05%	0.614%
24	13.498	1938	1940	1945	rVB	987322	943063	1.94%	0.582%
25	13.721	1972	1978	1981	rVB2	2258905	2883844	5.93%	1.781%
26	13.957	2015	2018	2022	rVB	1181724	964066	1.98%	0.595%
27	14.010	2023	2027	2030	rBV	1095327	1094279	2.25%	0.676%
28	15.474	2272	2276	2279	rBV	563308	614159	1.26%	0.379%

Sum of corrected areas: 161961058

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Instrument :
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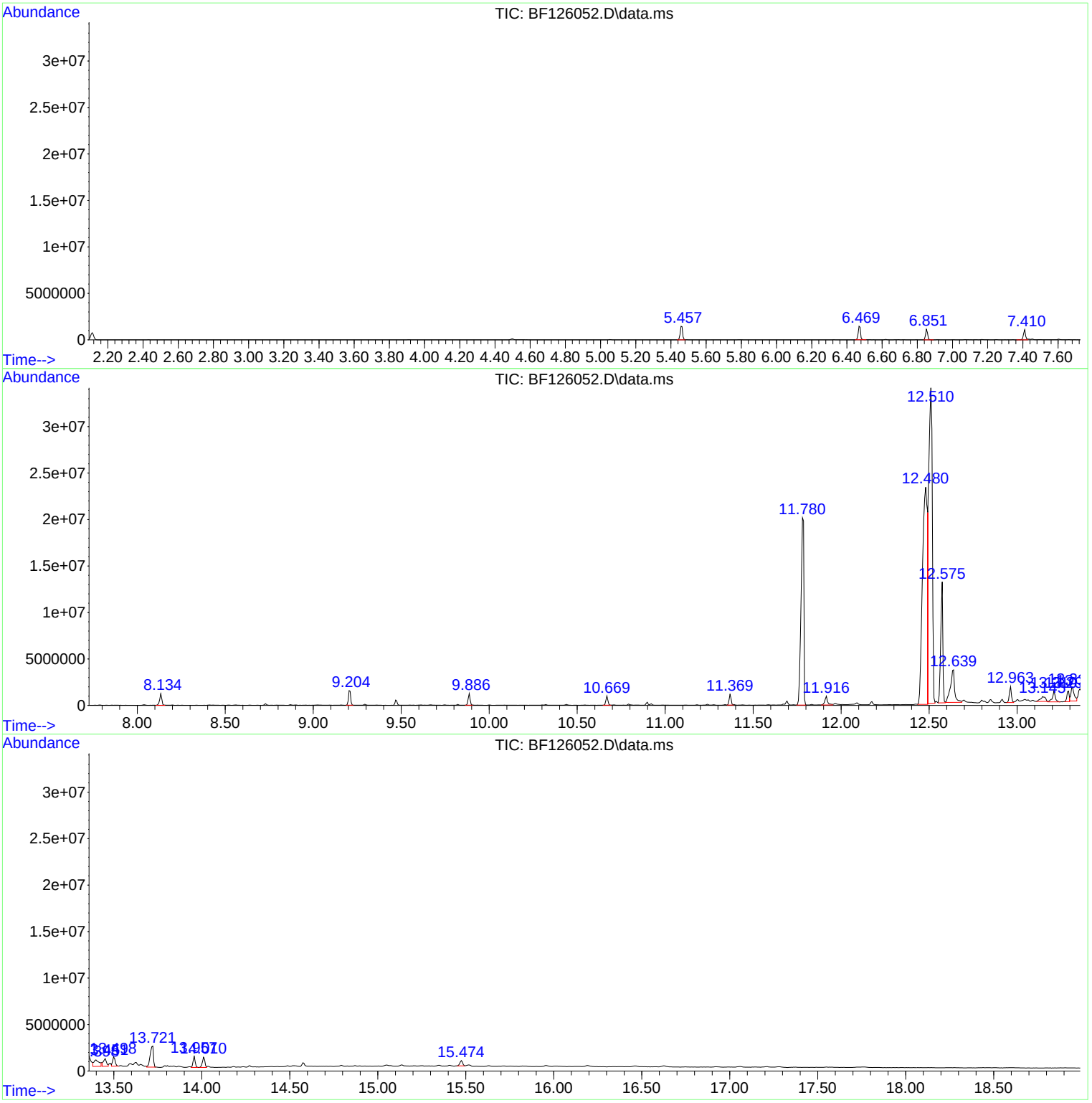
ClientSampleId :
TR-4-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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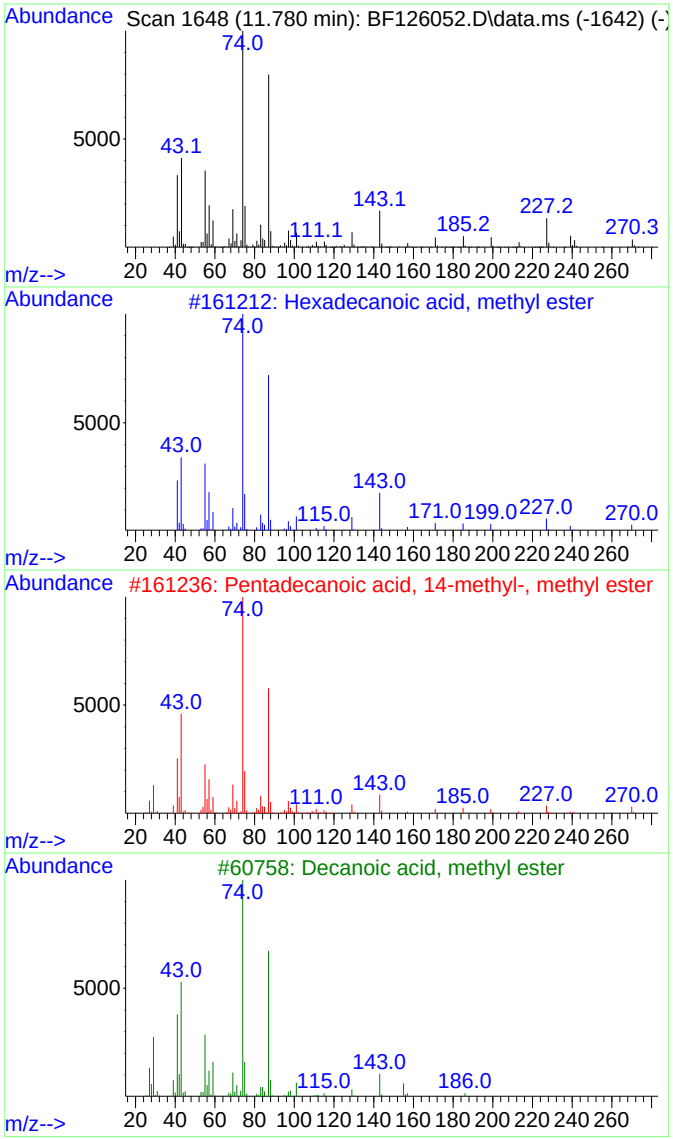
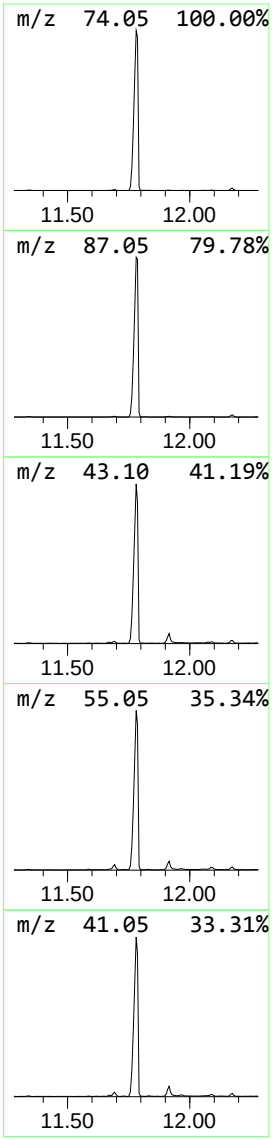
****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	509.48 ng	23024600	Phenanthrene-d10	11.369

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	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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ClientSampleId :
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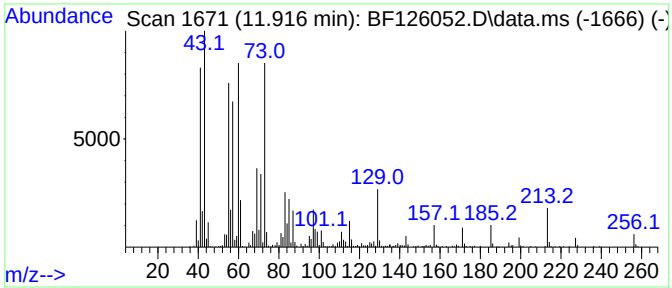
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

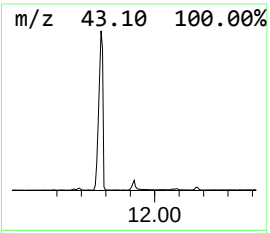
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

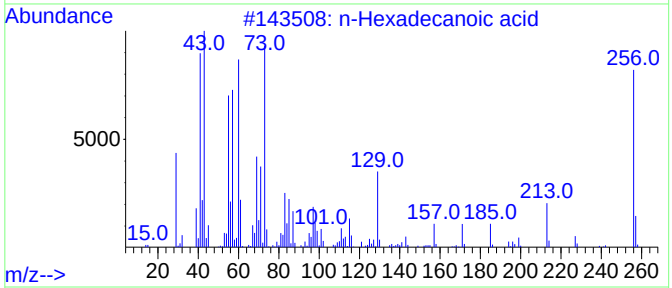
****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 10

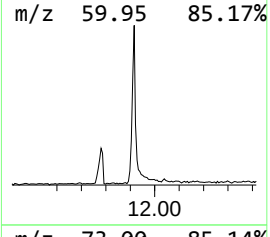
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	22.71 ng	1026330	Phenanthrene-d10	11.369

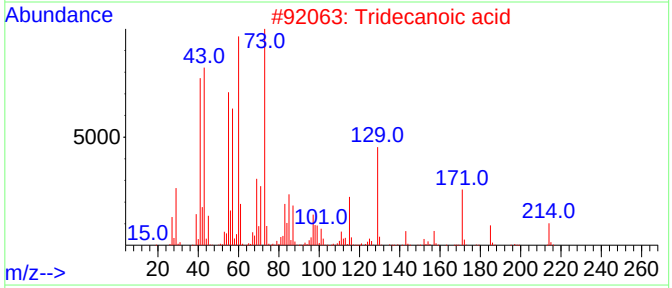
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	76

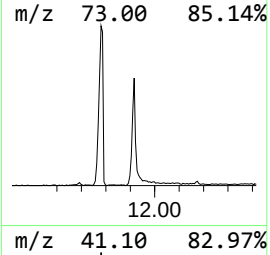


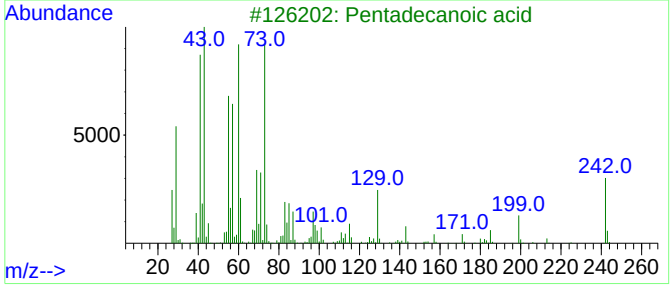


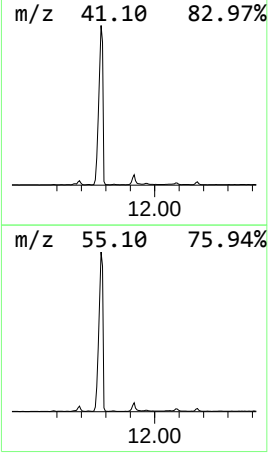












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Acq On : 4 Nov 2021 18:35
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Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

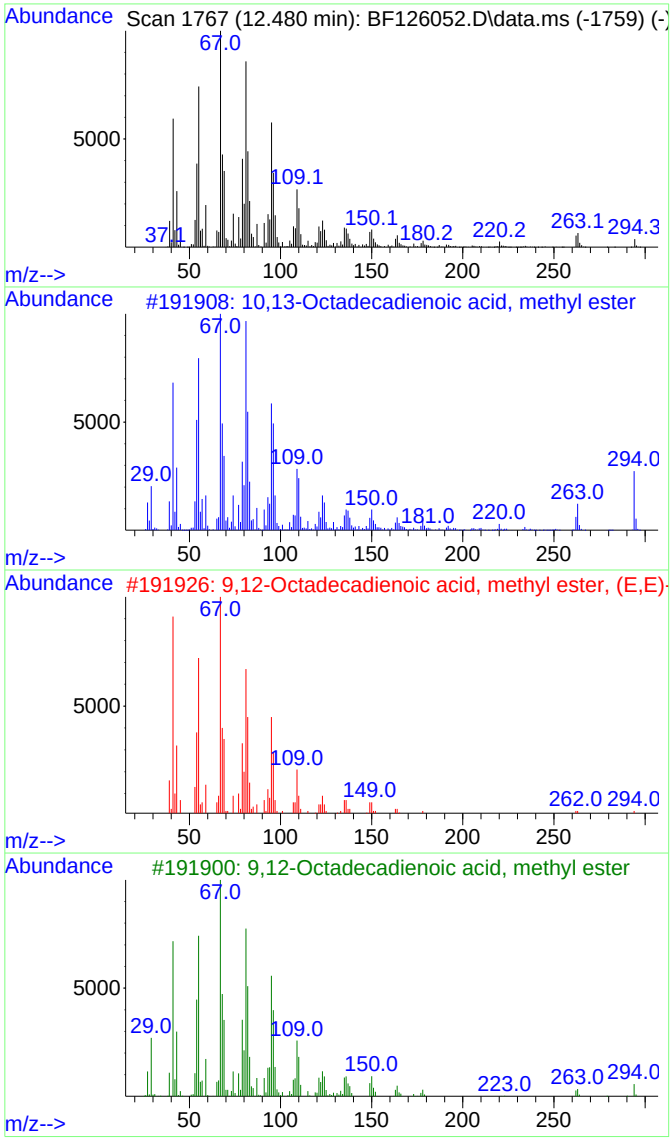
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

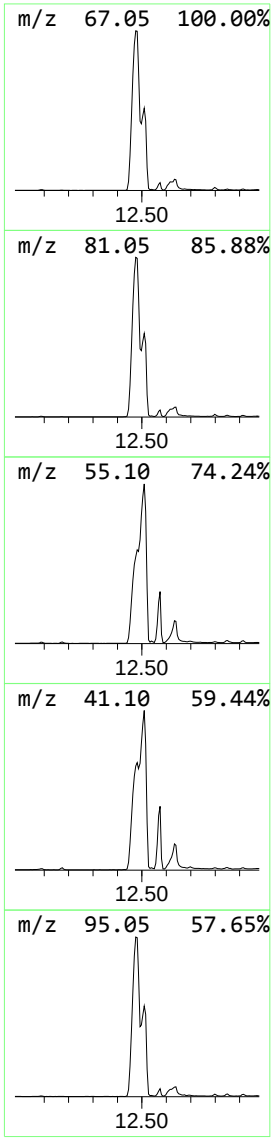
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	1075.34 ng	48597200	Phenanthrene-d10	11.369

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	002566-97-4	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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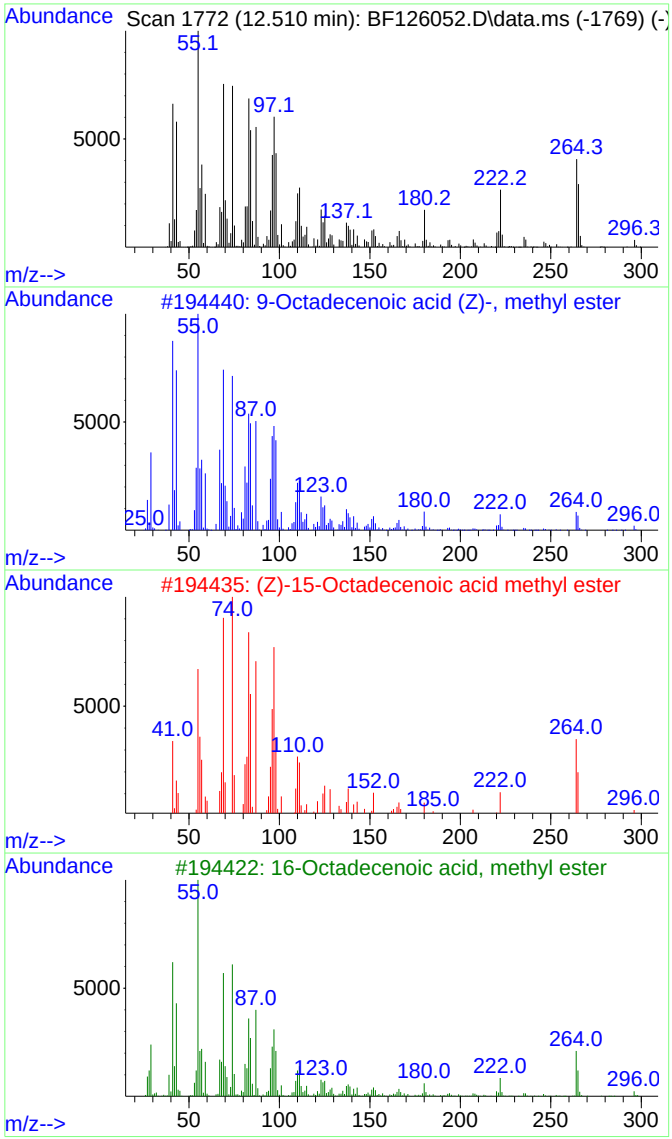
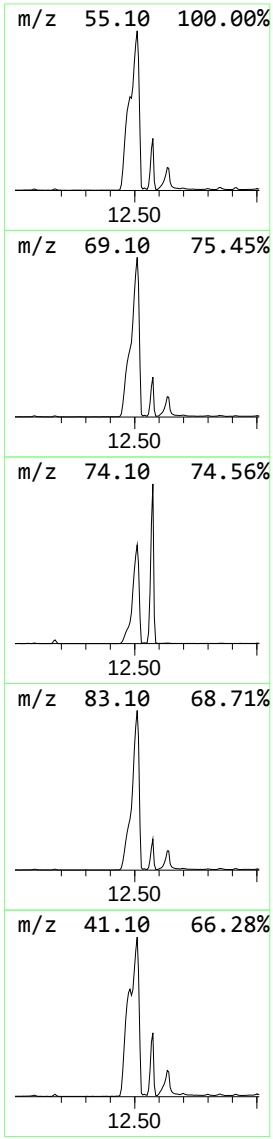
****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	1009.17 ng	45606600	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	95
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
5	3-Octadecenoic acid, methyl ester	296	C19H36O2	056599-33-8	91





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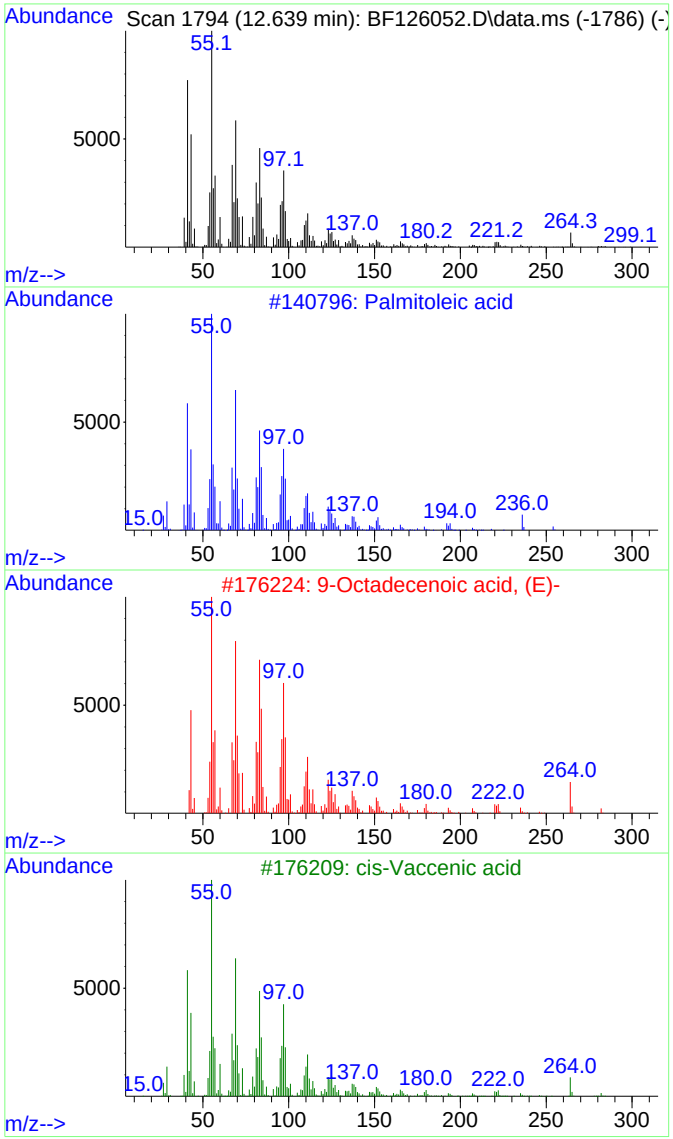
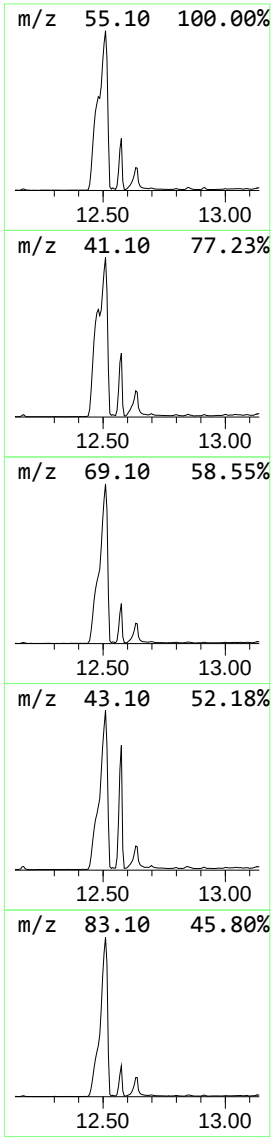
****

Peak Number 5 Palmitoleic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	130.80 ng	5911250	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	90
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
4	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	87
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87





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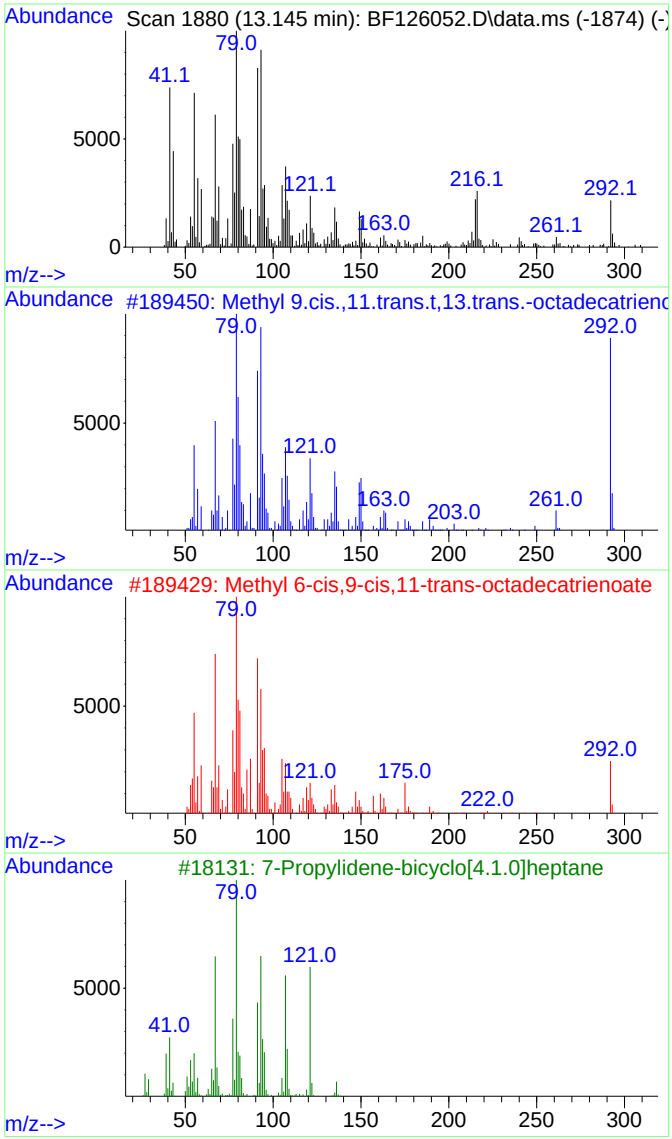
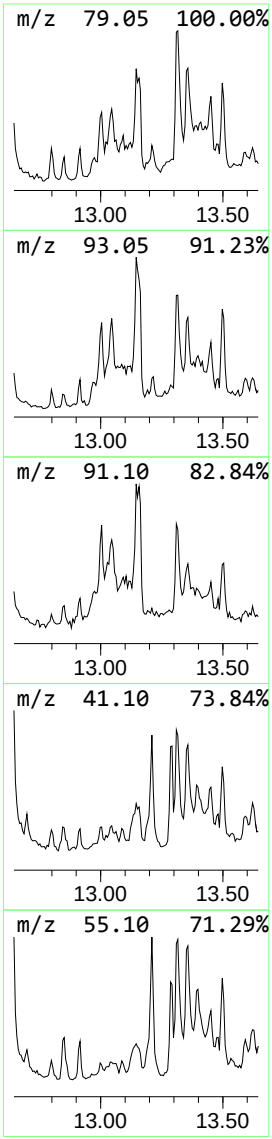
****
Peak Number 6 Methyl 9.cis.,11.trans.t,13... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	18.47 ng	1010700	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	95
2	Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	83
3	7-Propylidene-bicyclo[4.1.0]heptane	136	C10H16	082253-09-6	70
4	9,12,15-Octadecatrienoic acid, e...	306	C20H34O2	001191-41-9	70
5	6,9,12-Octadecatrienoic acid, me...	292	C19H32O2	002676-41-7	62





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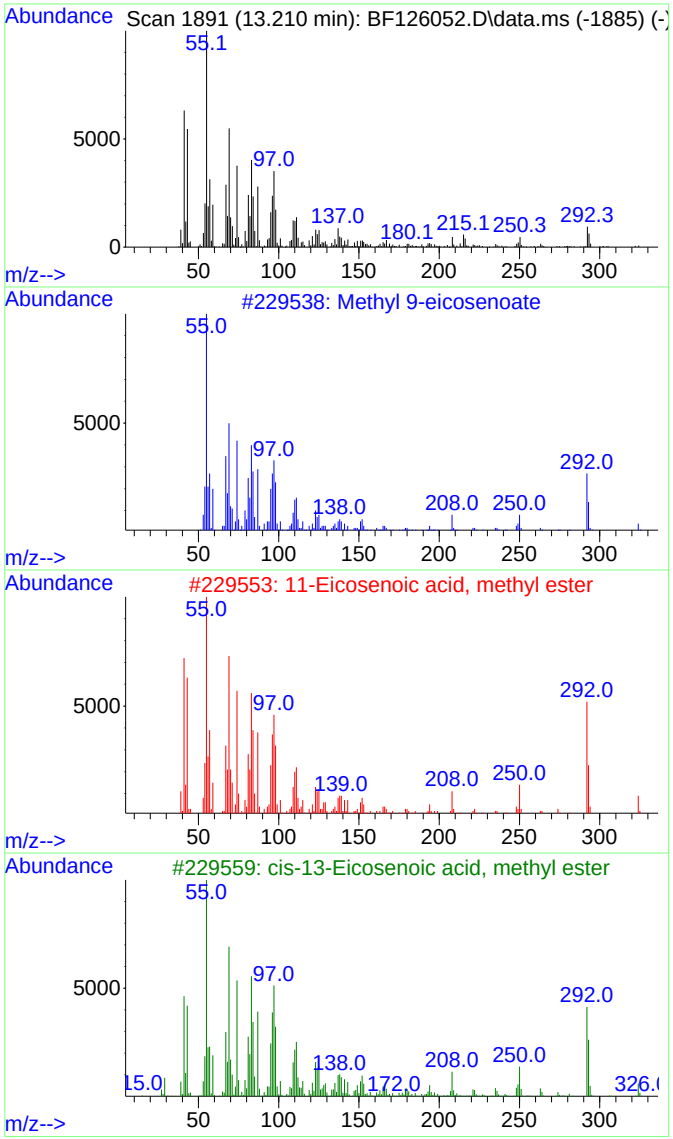
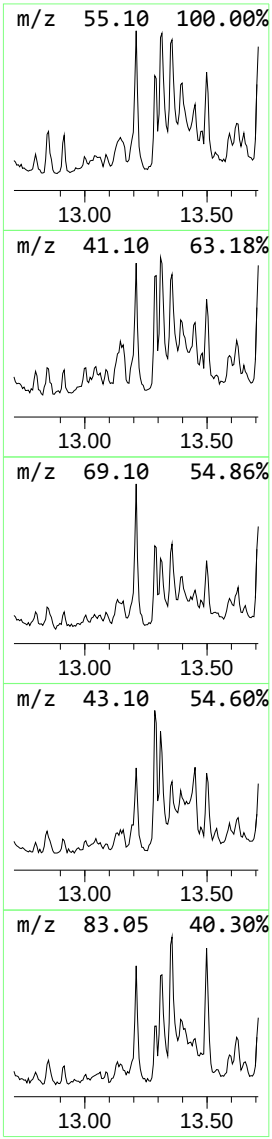
****

Peak Number 7 Methyl 9-eicosenoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	23.50 ng	1285870	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	99
2	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
3	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	87
4	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	87
5	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	86





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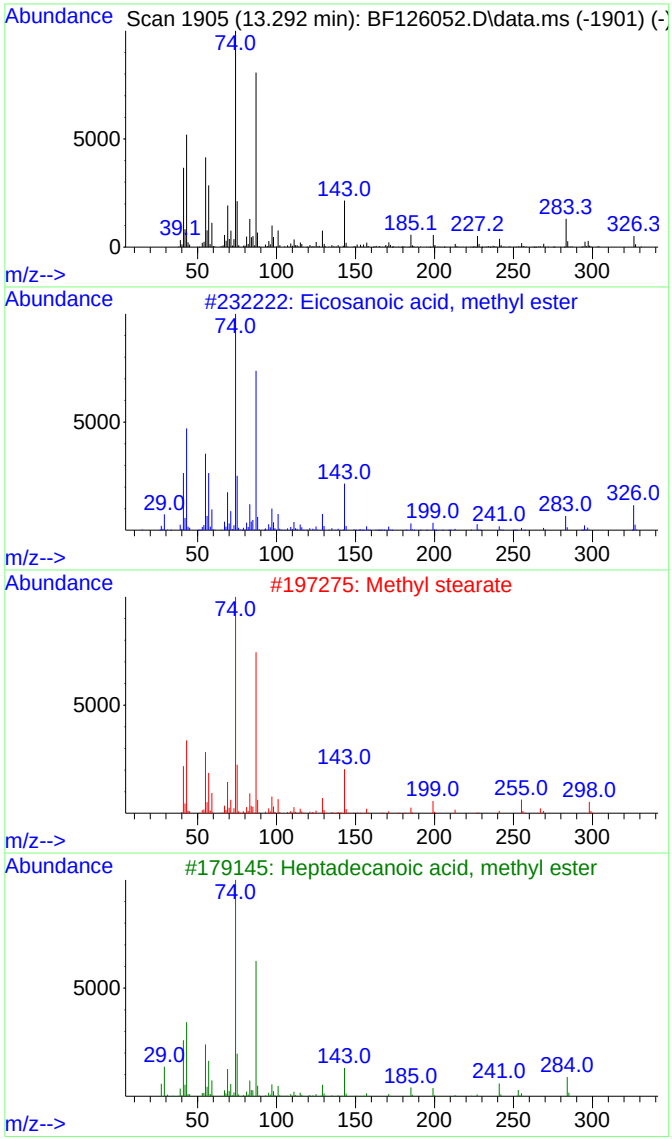
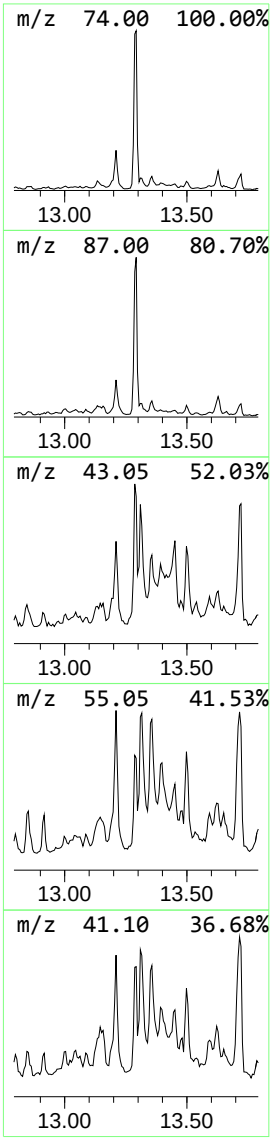
****
Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	19.24 ng	1052470	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Methyl stearate	298	C19H38O2	000112-61-8	94
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91





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Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

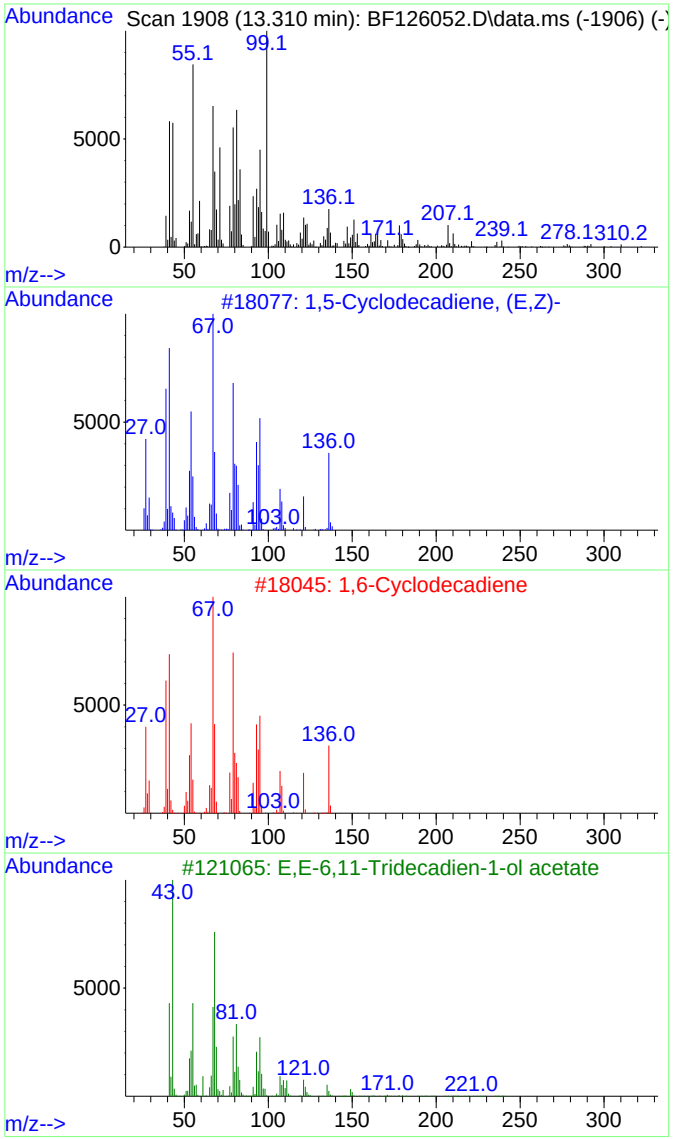
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

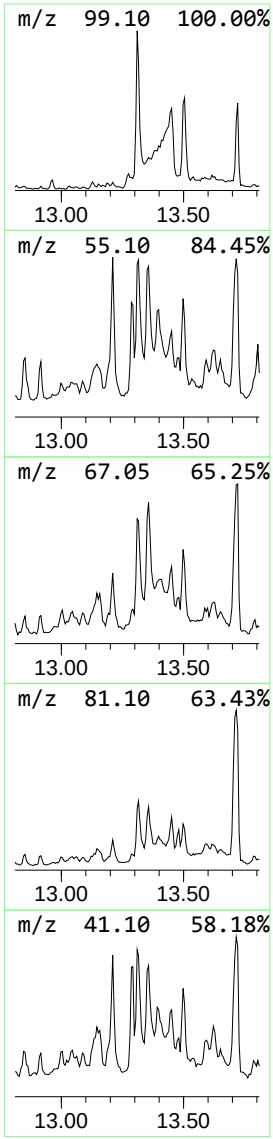
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,5-Cyclodecadiene, (E,Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.310	34.87 ng	1907790	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Cyclodecadiene, (E,Z)-	136	C10H16	001124-78-3	60
2	1,6-Cyclodecadiene	136	C10H16	007049-13-0	59
3	E,E-6,11-Tridecadien-1-ol acetate	238	C15H26O2	1000130-97-2	46
4	2H-Benzocyclohepten-2-one, 1,4a,...	178	C12H18O	017429-26-4	43
5	(Z,Z,Z)-6,12,15-Octadecatrienoic...	292	C19H32O2	1010427-70-2	38





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Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

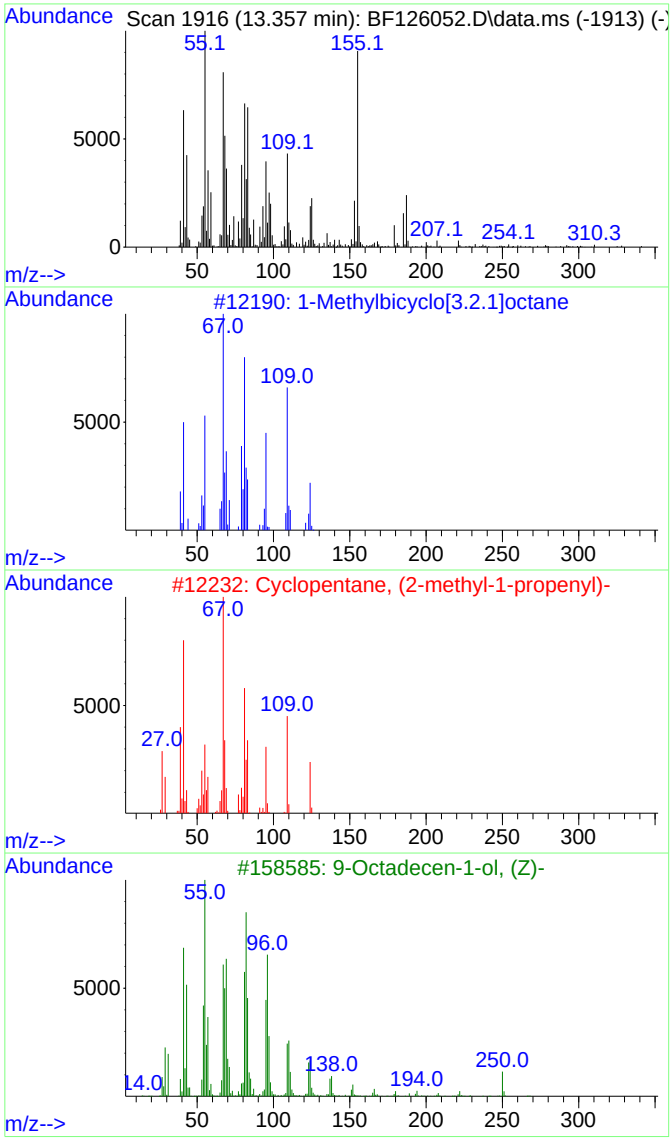
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

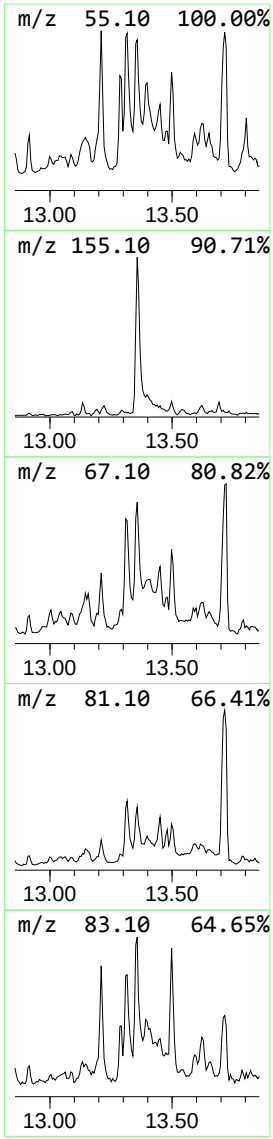
****

Peak Number 10 unknown13.357 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	33.88 ng	1853850	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylbicyclo[3.2.1]octane	124	C9H16	119972-41-7	41
2	Cyclopentane, (2-methyl-1-propen...	124	C9H16	053366-57-7	41
3	9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	38
4	cis-Dihydrocarvone	152	C10H16O	003792-53-8	38
5	[3-(Aminomethyl)-5-methylcyclohe...	157	C9H19NO	498531-57-0	35





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Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

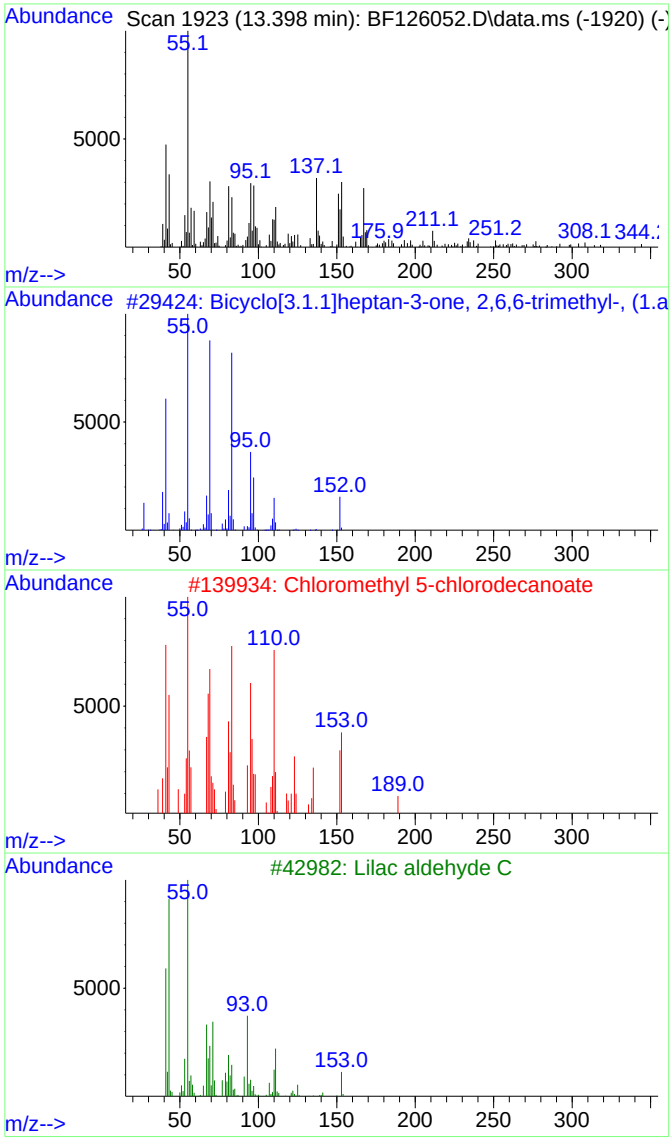
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

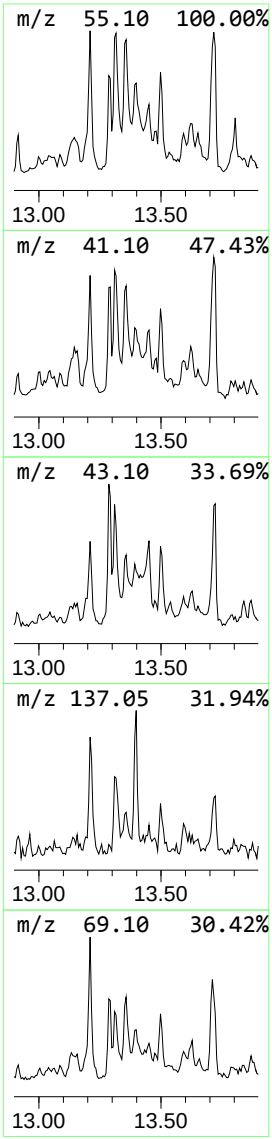
****

Peak Number 11 unknown13.398 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	26.16 ng	1431050	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
2	Chloromethyl 5-chlorodecanoate	254	C11H20Cl2O2	080418-82-2	22
3	Lilac aldehyde C	168	C10H16O2	053447-48-6	14
4	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	14
5	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

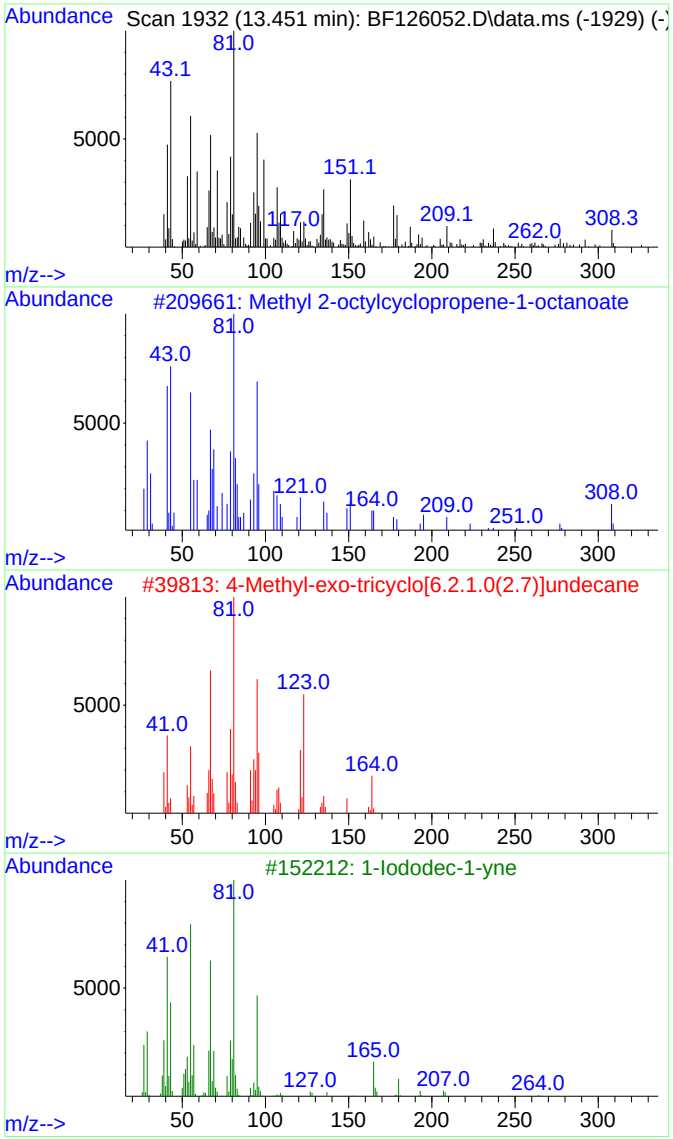
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

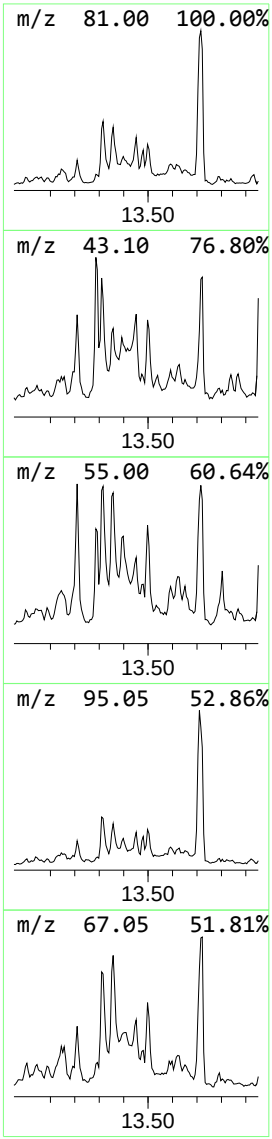
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Methyl 2-octylcyclopropene-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	18.19 ng	995124	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	64
2	4-Methyl-exo-tricyclo[6.2.1.0(2....	164	C12H20	1000215-29-8	38
3	1-Iododec-1-yne	264	C10H17I	067826-81-7	27
4	2-Octynoic acid, methyl ester	154	C9H14O2	000111-12-6	27
5	1,3,7-Octatriene, 2,7-dimethyl-	136	C10H16	036638-38-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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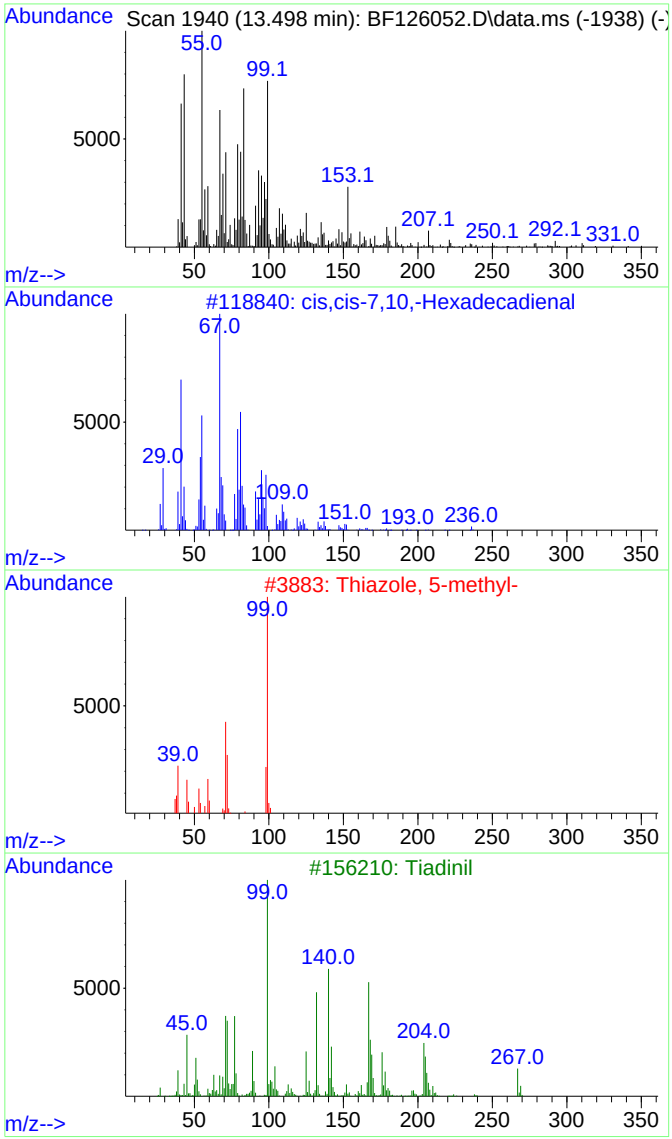
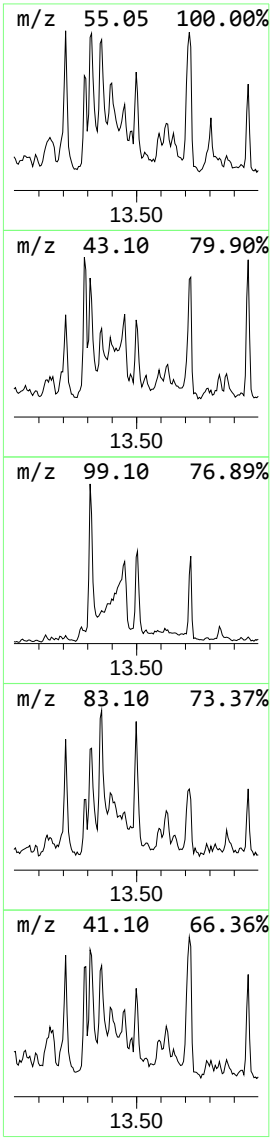
Peak Number 13 unknown13.498 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	17.24 ng	943063	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,cis-7,10,-Hexadecadienal	236	C16H28O	056829-23-3	44
2	Thiazole, 5-methyl-	99	C4H5NS	003581-89-3	30
3	Tiadinil	267	C11H10ClN3OS	223580-51-6	25
4	6-Iodohexanal	226	C6H11IO	1000411-49-9	22
5	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

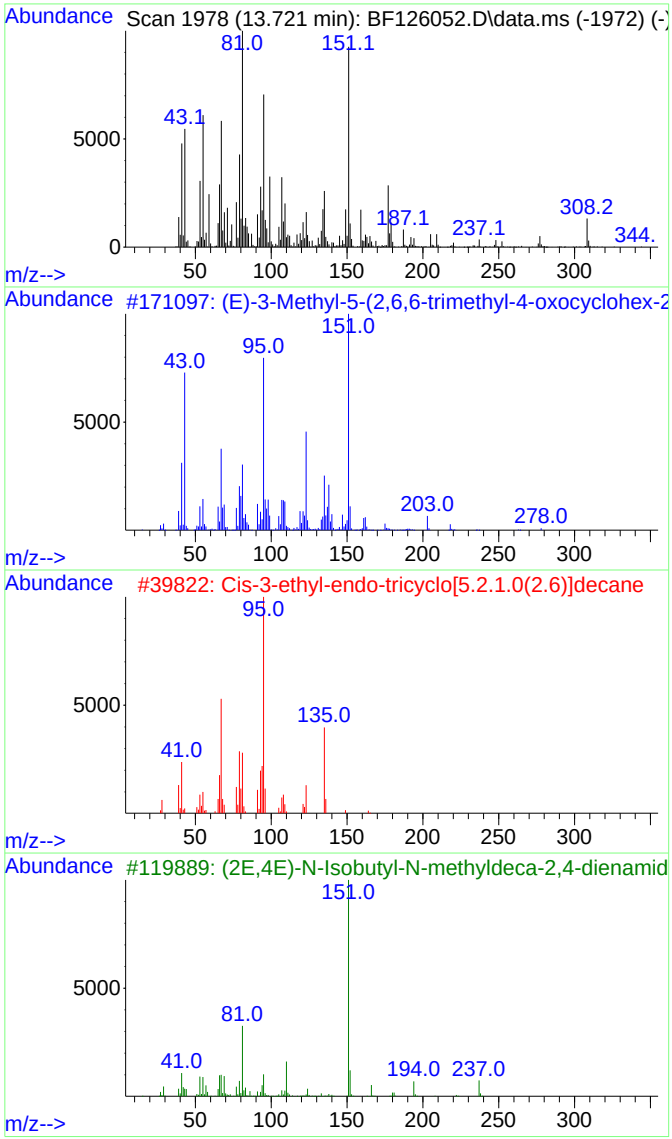
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

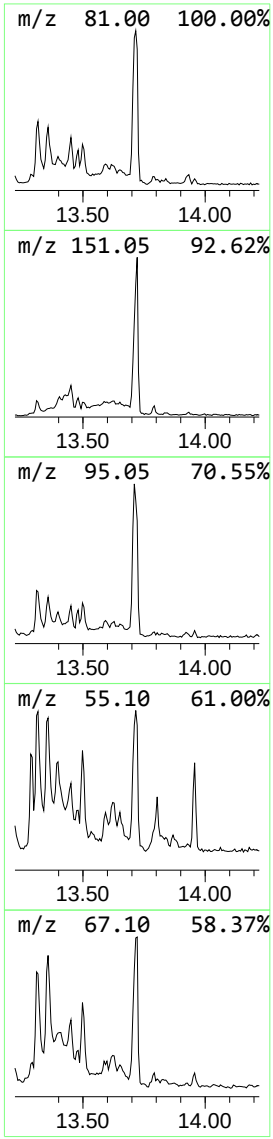
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 (E)-3-Methyl-5-(2,6,6-trime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.722	52.71 ng	2883840	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Methyl-5-(2,6,6-trimethyl-...	278	C17H26O3	1000495-80-8	55
2	Cis-3-ethyl-endo-tricyclo[5.2.1....	164	C12H20	1010215-29-1	38
3	(2E,4E)-N-Isobutyl-N-methyldeca-...	237	C15H27NO	1472057-16-1	30
4	4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	30
5	2,6-Diamino-8-azapurine	151	C4H5N7	018620-97-8	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110421\
Data File : BF126052.D
Acq On : 4 Nov 2021 18:35
Operator : JU/CG
Sample : M4500-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-110321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Hexadecanoic ac...	11.780	509.5	ng	23024600	4	11.369	903844	20.0
n-Hexadecanoic ...	11.916	22.7	ng	1026330	4	11.369	903844	20.0
10,13-Octadecad...	12.480	1075.3	ng	48597200	4	11.369	903844	20.0
9-Octadecenoic ...	12.510	1009.2	ng	45606600	4	11.369	903844	20.0
Palmitoleic acid	12.639	130.8	ng	5911250	4	11.369	903844	20.0
Methyl 9.cis.,1...	13.145	18.5	ng	1010700	5	14.010	1094280	20.0
Methyl 9-eicose...	13.210	23.5	ng	1285870	5	14.010	1094280	20.0
Eicosanoic acid...	13.292	19.2	ng	1052470	5	14.010	1094280	20.0
1,5-Cyclodecadi...	13.310	34.9	ng	1907790	5	14.010	1094280	20.0
unknown13.357	13.357	33.9	ng	1853850	5	14.010	1094280	20.0
unknown13.398	13.398	26.2	ng	1431050	5	14.010	1094280	20.0
Methyl 2-octylc...	13.451	18.2	ng	995124	5	14.010	1094280	20.0
unknown13.498	13.498	17.2	ng	943063	5	14.010	1094280	20.0
(E)-3-Methyl-5-...	13.722	52.7	ng	2883840	5	14.010	1094280	20.0