LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099306.D
Acq On : 10 Oct 2017 18:03
Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	507	510	525	rBV	330311	436025	2.25%	0.722%
2	5.487	574	578	587	rBV	2126726	2141180	11.04%	3.547%
3	6.140	685	689	693	rBV	1797169	1682139	8.68%	2.786%
4	6.498	745	750	753	rBV	1930727	2121048	10.94%	3.514%
5	6.563	757	761	765	rVB	1507943	1264269	6.52%	2.094%
6	6.639	769	774	777	rBV	2246366	2226485	11.48%	3.688%
7	6.863	809	812	816	rBV	695456	559821	2.89%	0.927%
8	7.022	835	839	842	rVV	2066611	1732504	8.94%	2.870%
9	7.428	904	908	911	rBV	1315031	1335202	6.89%	2.212%
10	8.145	1026	1030	1032	rBV	931249	741531	3.82%	1.228%
11	9.222	1208	1213	1216	rBV	2680014	2338749	12.06%	3.874%
12	9.610	1275	1279	1284	rBV	358524	282859	1.46%	0.469%
13	9.898	1325	1328	1332	rBV2	792494	713463	3.68%	1.182%
14	10.692	1459	1463	1466	rBV	1188733	1054928	5.44%	1.747%
15	10.898	1495	1498	1501	rBV	362684	256155	1.32%	0.424%
16	11.386	1577	1581	1584	rBV	694574	610411	3.15%	1.011%
17	11.692	1631	1633	1638	rVV	986687	798442	4.12%	1.323%
18	11.786	1641	1649	1652	rVB	5077933	6793439	35.04%	11.253%
19	11.927	1667	1673	1680	rBV	683841	844629	4.36%	1.399%
20	12.092	1698	1701	1706	rVB	289675	248685	1.28%	0.412%
21	12.174	1711	1715	1719	rVB	263900	245480	1.27%	0.407%
22	12.510	1758	1772	1776	rBV3	5354597	19386944	100.00%	32.114%
23	12.574	1779	1783	1786	rVV	4324499	4437495	22.89%	7.351%
24	12.633	1789	1793	1799	rVV	739442	1136330	5.86%	1.882%
25	12.704	1802	1805	1810	rVB2	214938	231683	1.20%	0.384%
26	12.980	1845	1852	1854	rBV	1819999	1875277	9.67%	3.106%
27	13.210	1886	1891	1897	rVB	773831	904115	4.66%	1.498%
28	13.286	1900	1904	1913	rBV	789722	868555	4.48%	1.439%
29	13.386	1918	1921	1922	rBV	297024	268677	1.39%	0.445%
30	13.727	1973	1979	1982	rBV2	674162	1007948	5.20%	1.670%
31	13.863	1999	2002	2004	rVB	312922	276381	1.43%	0.458%
32	13.957	2015	2018	2022	rBV	439050	382954	1.98%	0.634%
33	14.033	2028	2031	2040	rVB	544086	701840	3.62%	1.163%
34	15.515	2278	2283	2288	rVB	340275	462642	2.39%	0.766%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 60368285

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
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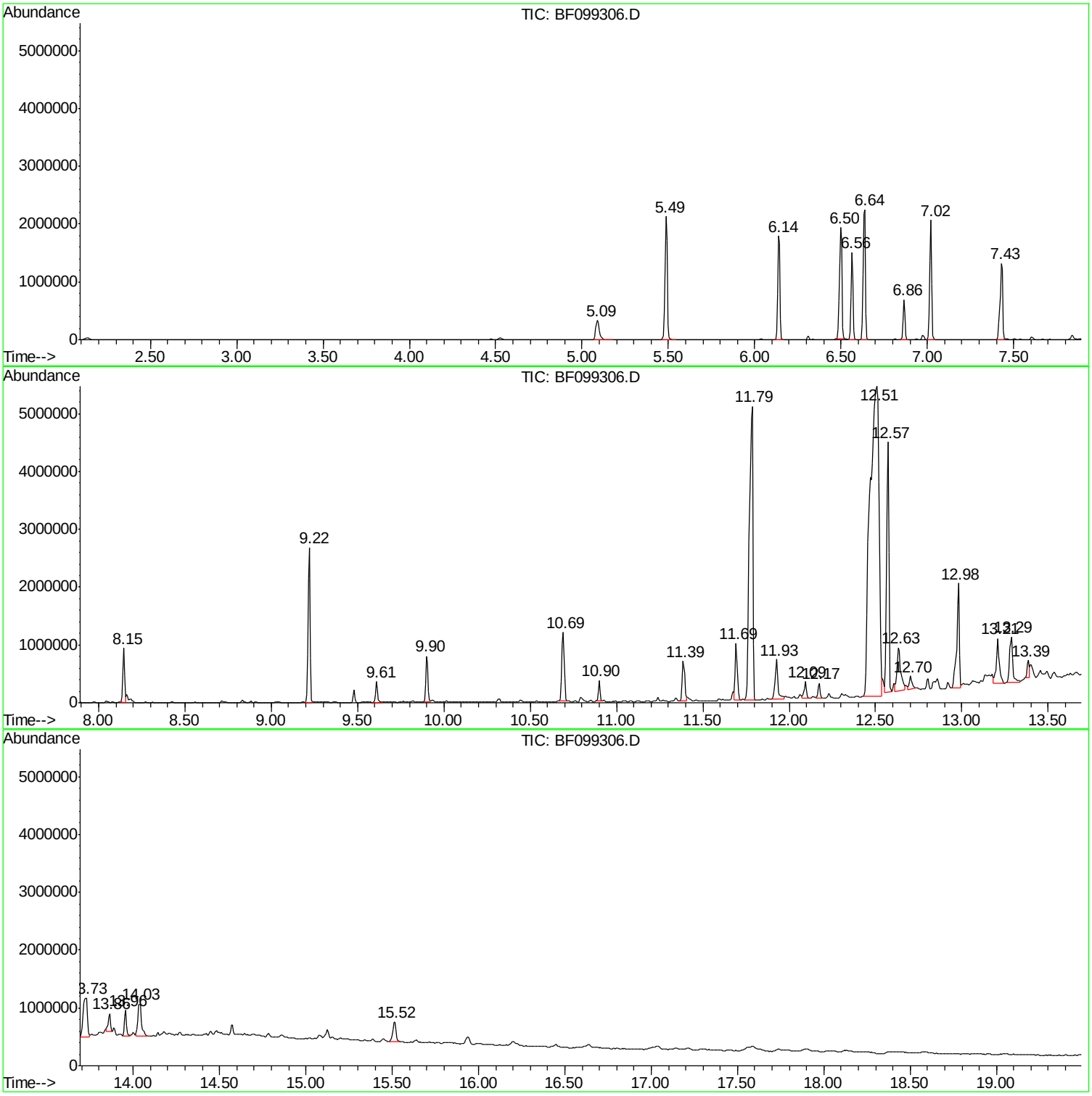
Instrument :
BNA_F
ClientSampleId :
TR-05-100517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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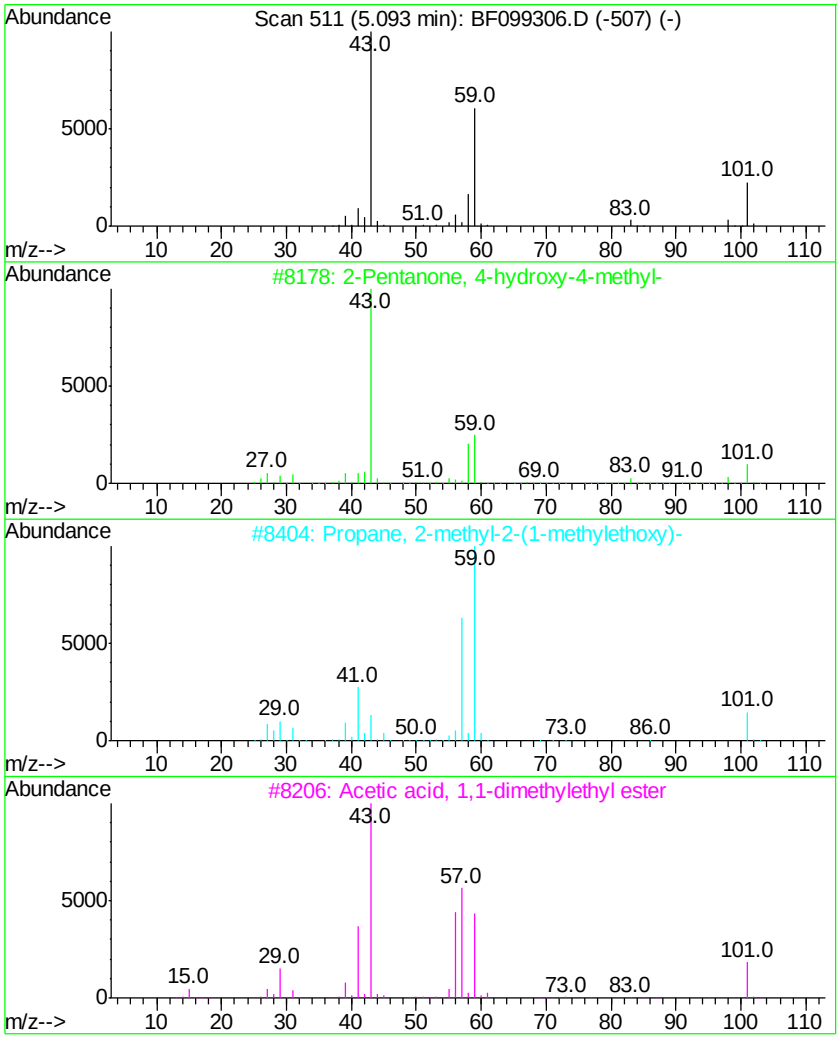
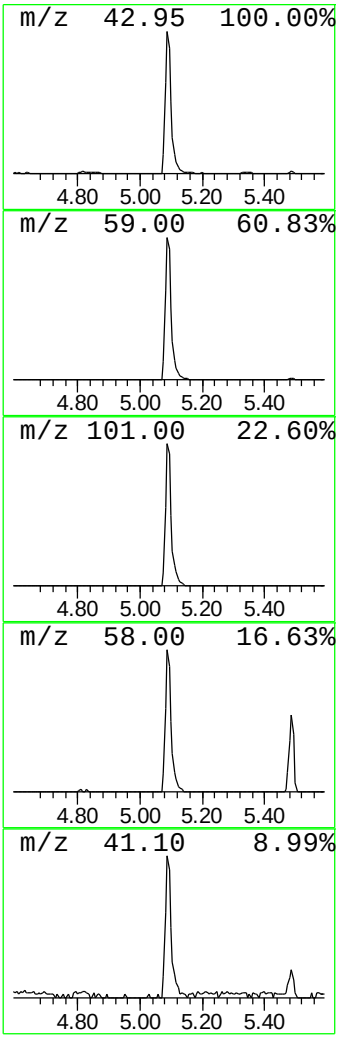
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	15.58 ng	436025	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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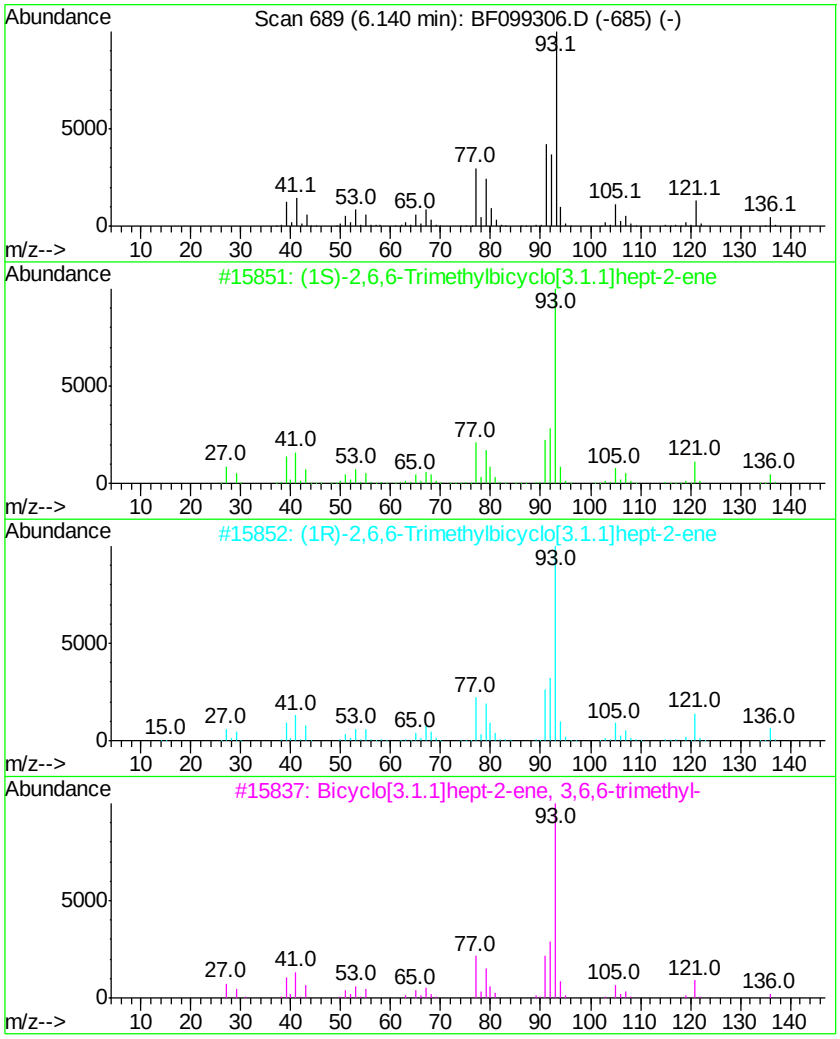
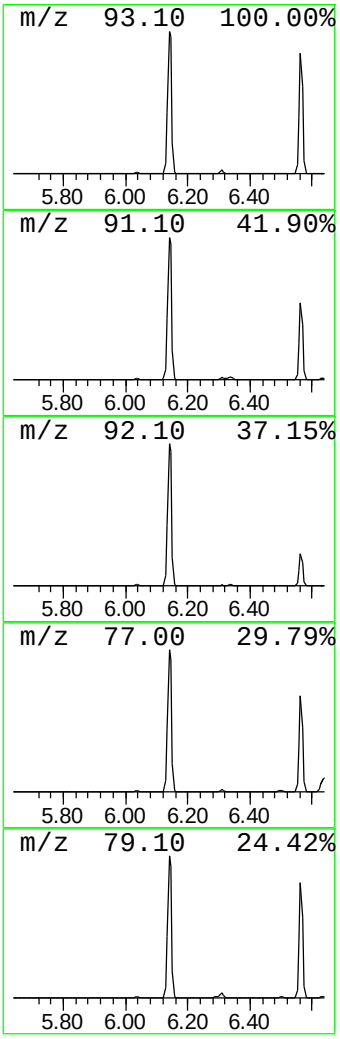
****

Peak Number 2 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	60.10 ng	1682140	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	96
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
4	.alpha.-Pinene	136	C10H16	000080-56-8	94
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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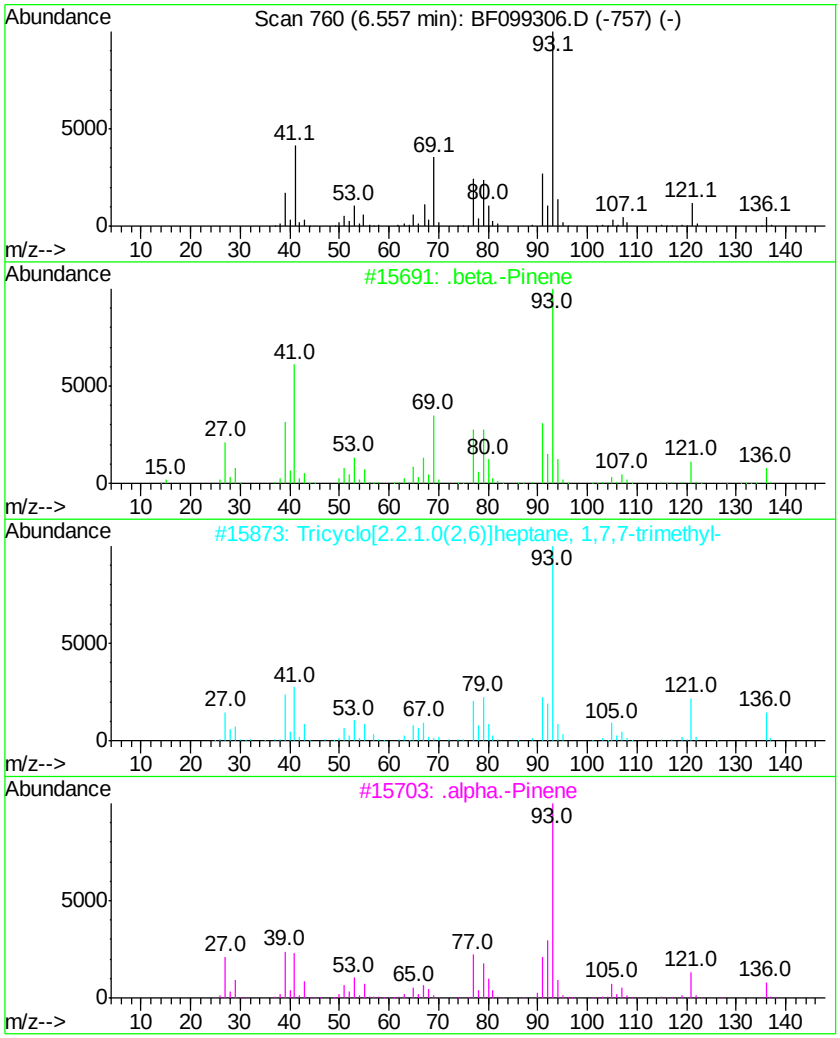
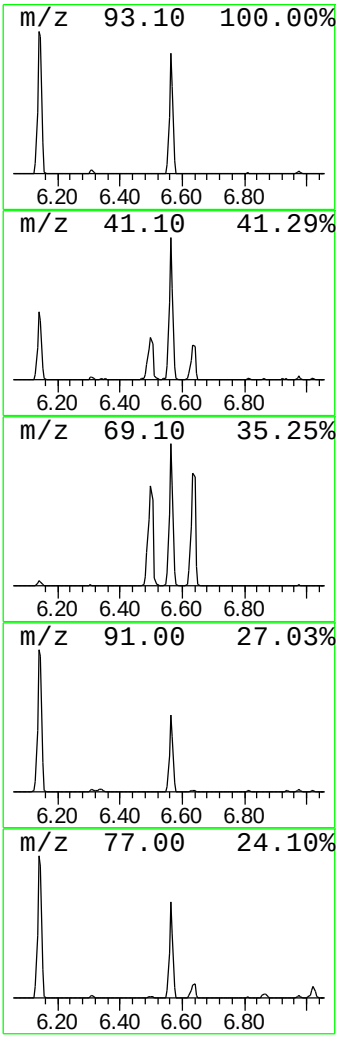
****

Peak Number 3 .beta.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	45.17 ng	1264270	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	93
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
3	.alpha.-Pinene	136	C10H16	000080-56-8	87
4	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	87
5	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	87





Library Search Compound Report

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Instrument :
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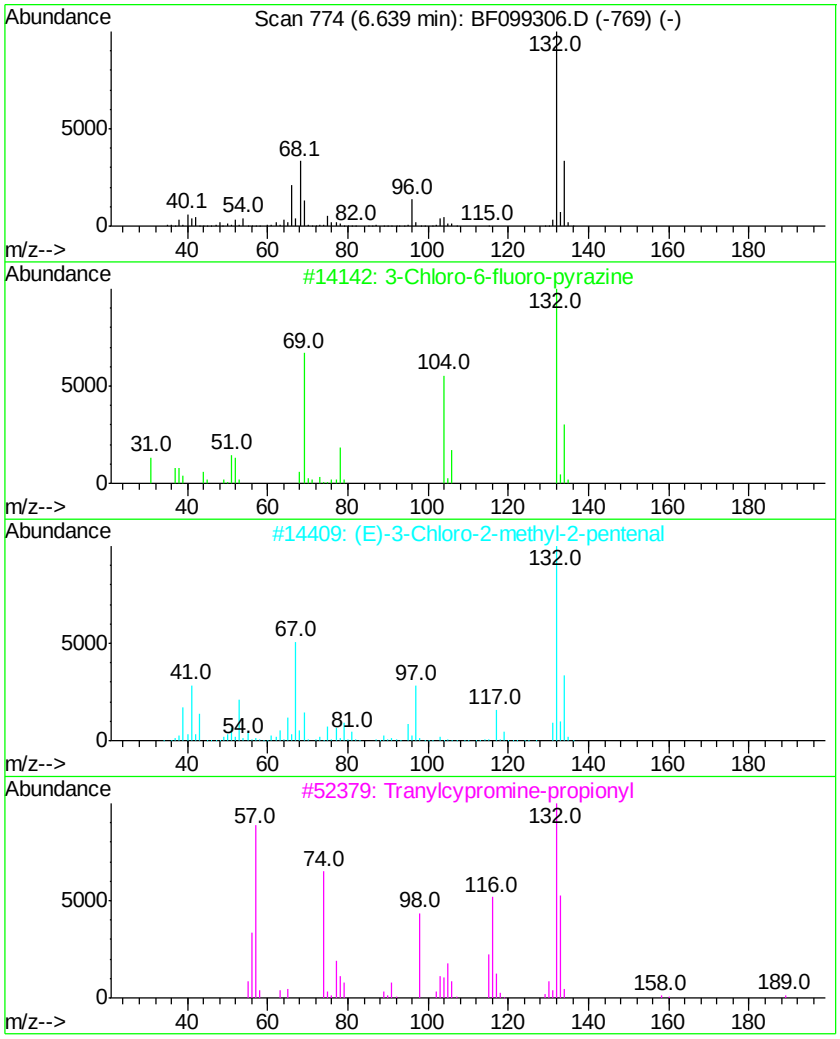
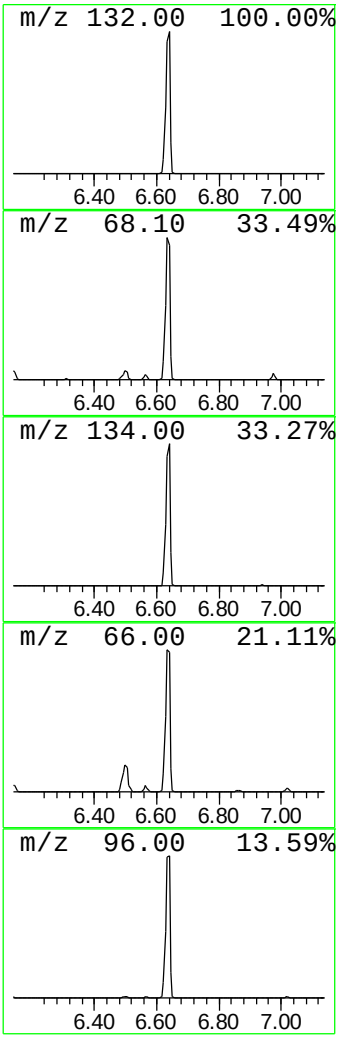
****

Peak Number 4 unknown6.64 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	79.54 ng	2226490	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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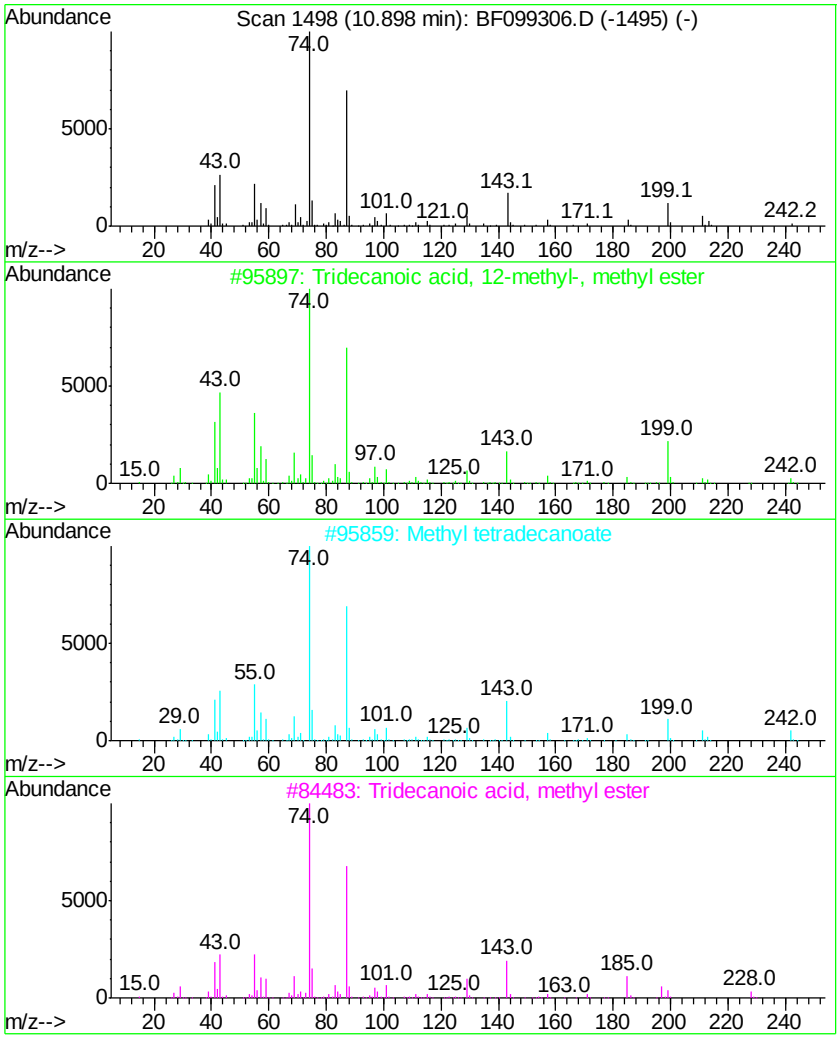
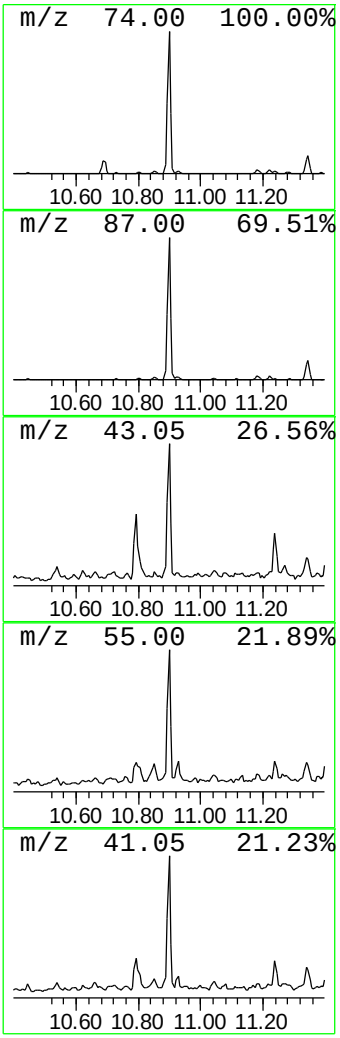
****

Peak Number 6 Tridecanoic acid, 12-methyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	8.39 ng	256155	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	92
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	80





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

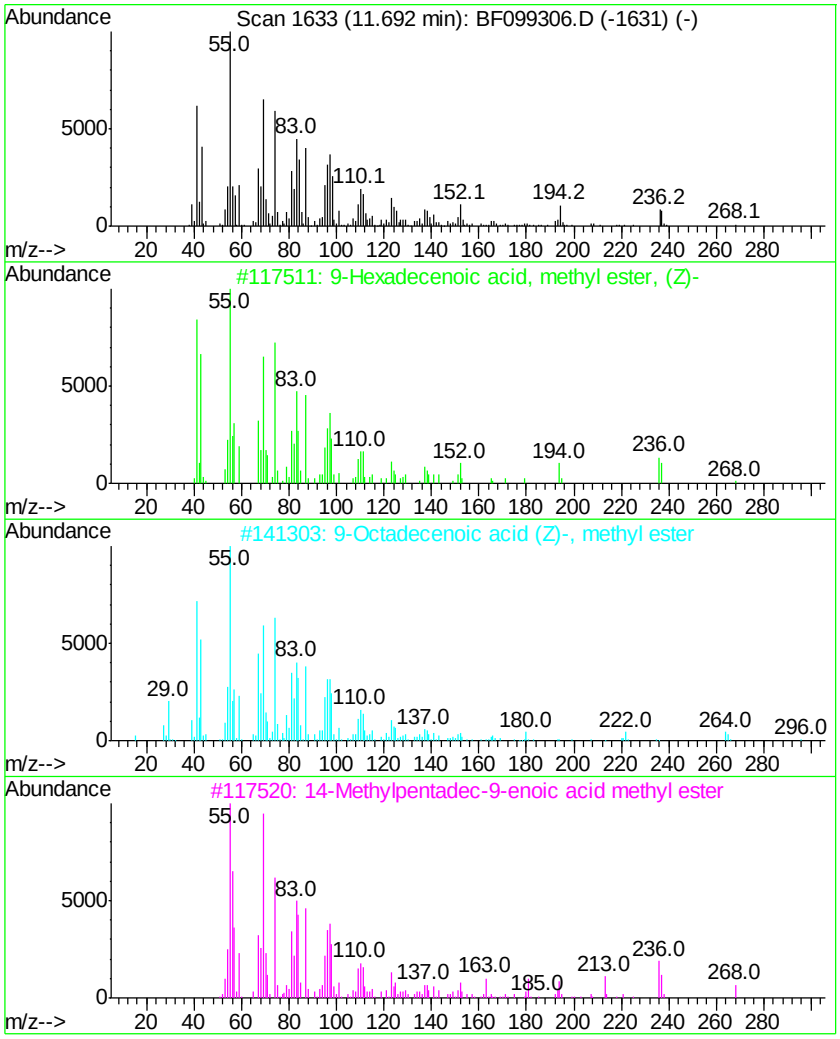
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

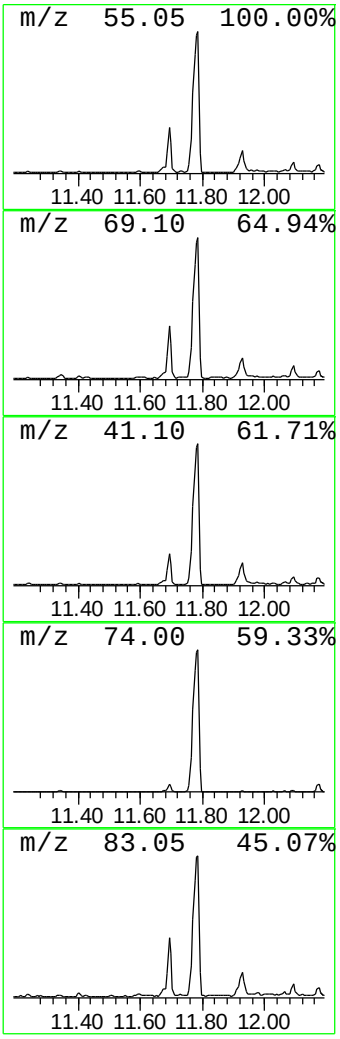
****

Peak Number 7 9-Hexadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	26.16 ng	798442	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
3	14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	93
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	91
5	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	91





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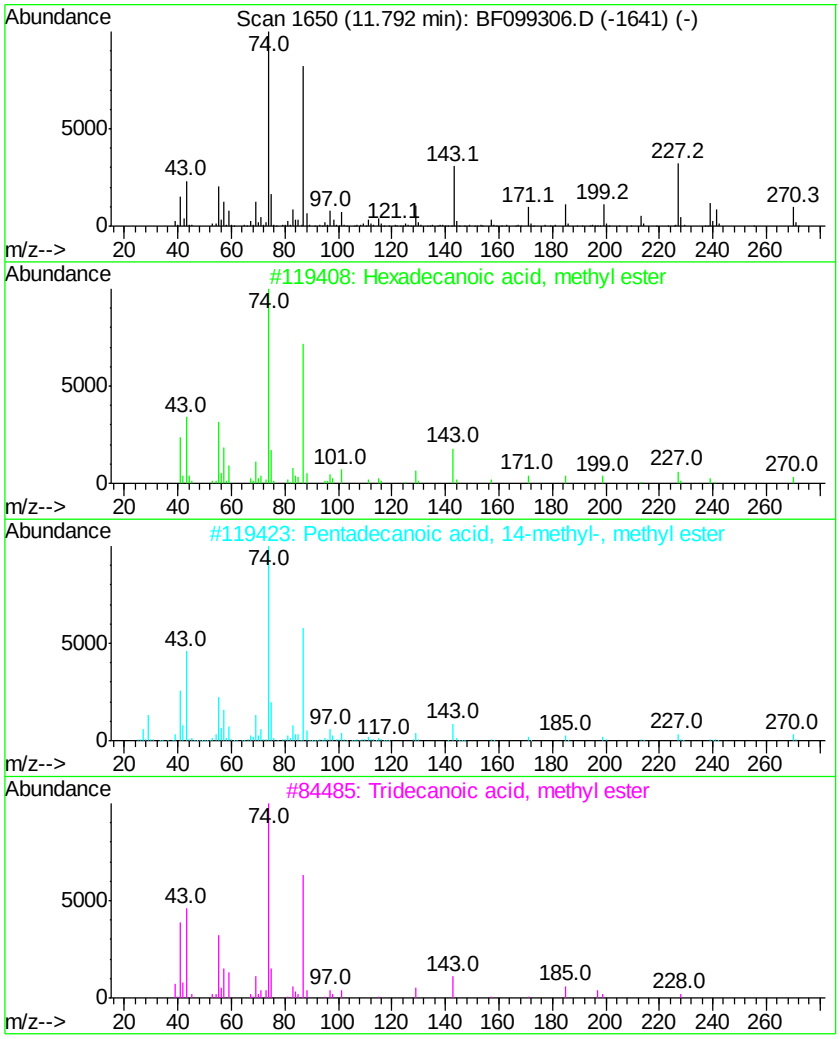
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

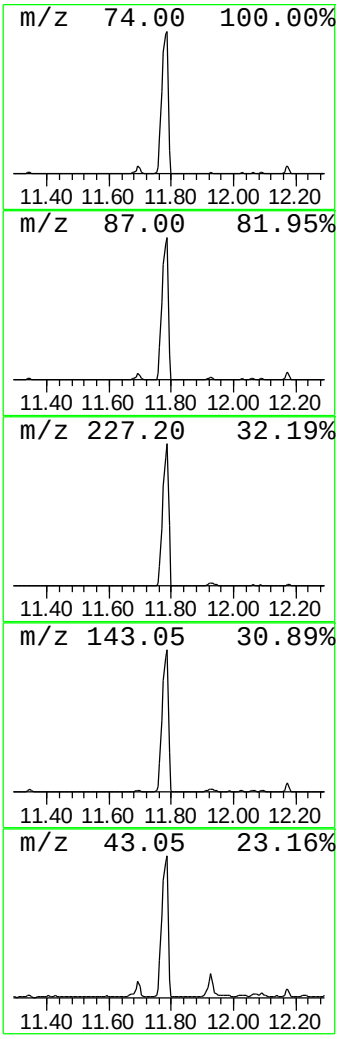
****

Peak Number 8 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	222.59 ng	6793440	Phenanthrene-d10	11.39

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	92
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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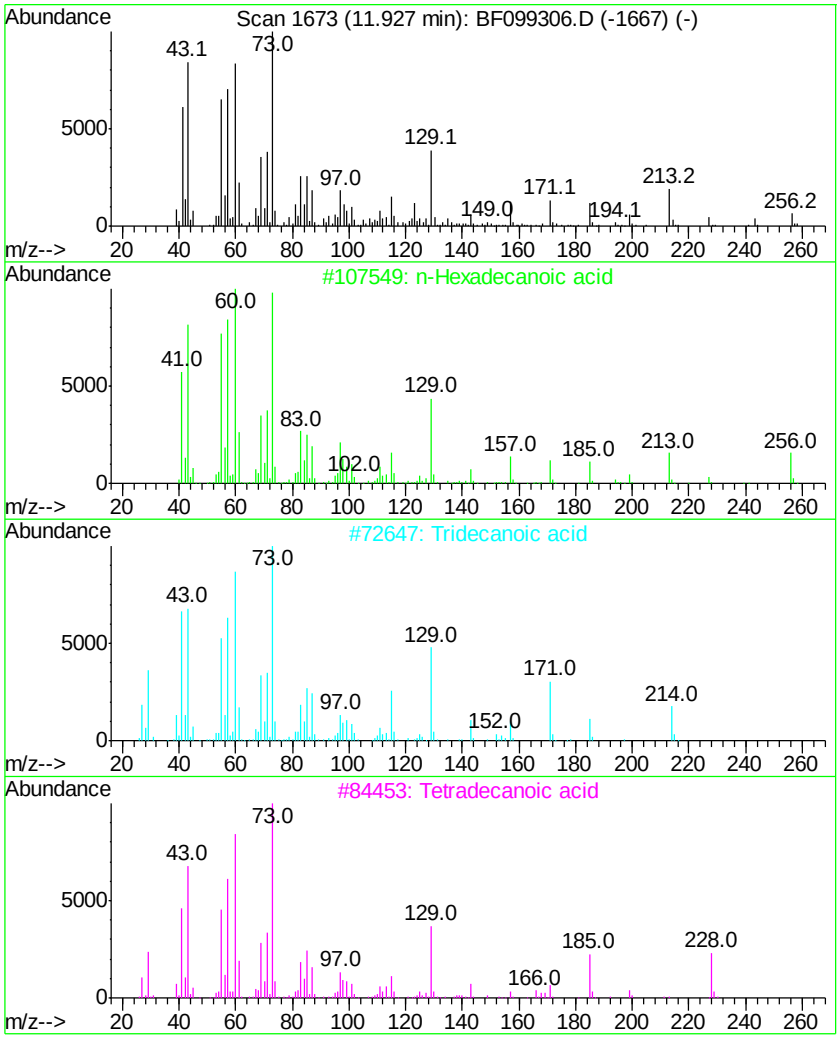
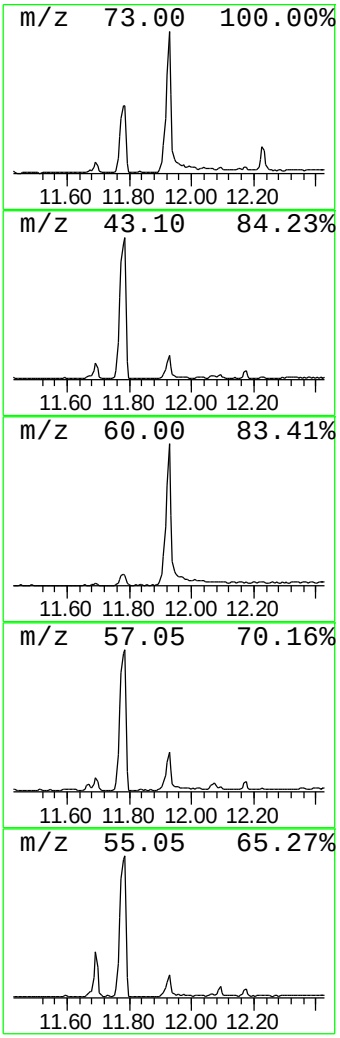
Peak Number 9 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	27.67 ng	844629	Phenanthrene-d10	11.39

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

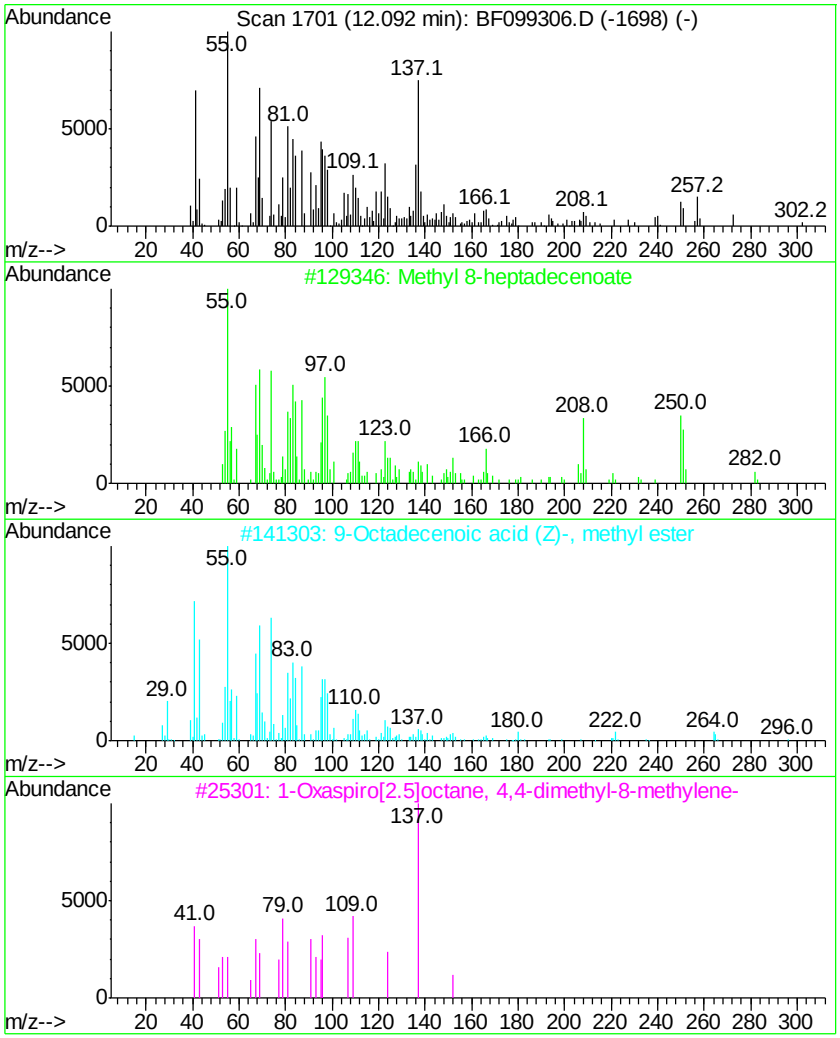
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

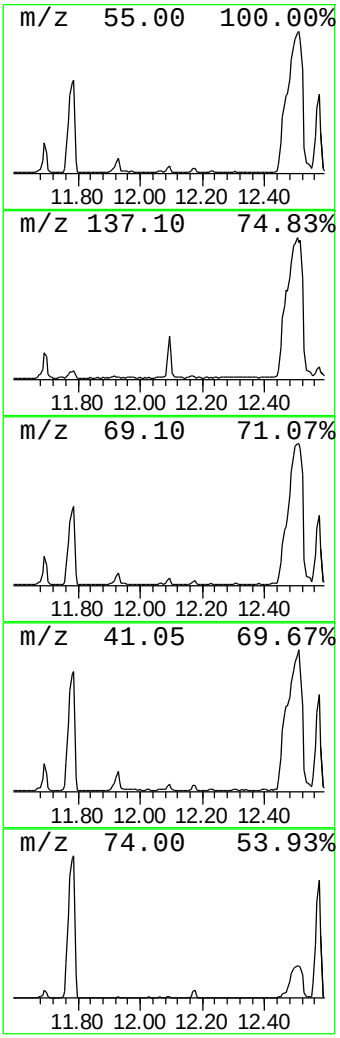
****

Peak Number 10 unknown12.09 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	8.15 ng	248685	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 8-heptadecenoate	282	C18H34O2	1000336-36-4	46
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	46
3	1-Oxaspiro[2.5]octane, 4,4-dimet...	152	C10H16O	054345-56-1	42
4	Methyl myristoleate	240	C15H28O2	056219-06-8	42
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	41





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099306.D
Acq On : 10 Oct 2017 18:03
Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

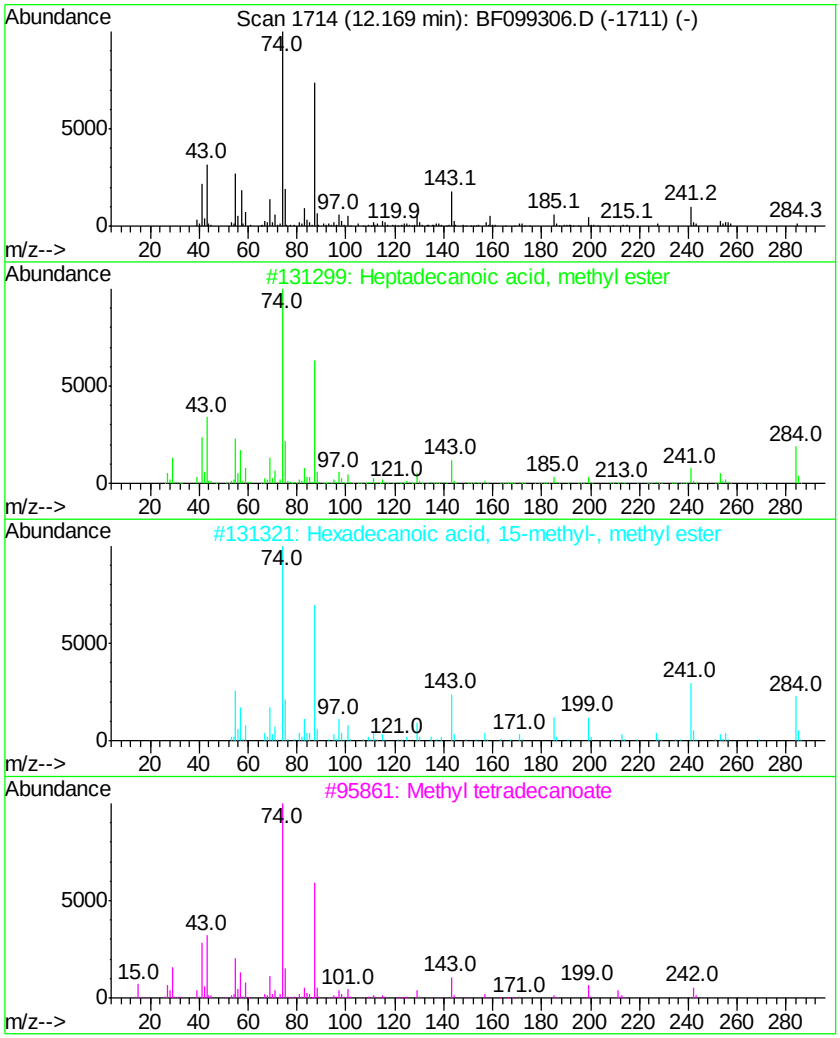
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

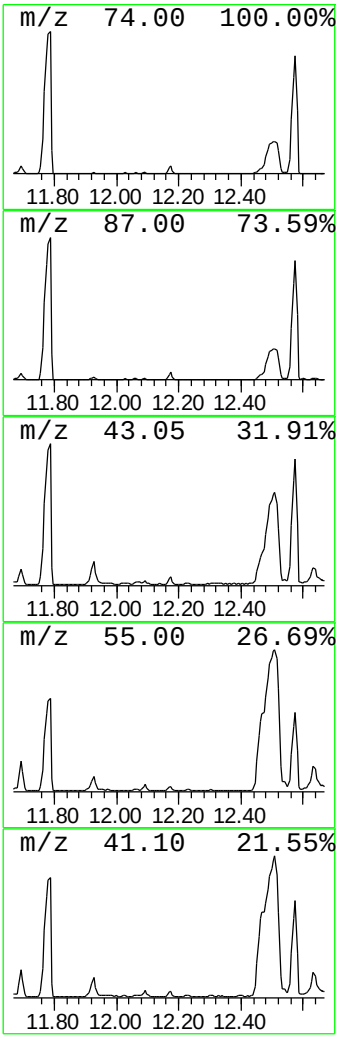
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptadecanoic acid, methyl ... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	8.04 ng	245480	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	97
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	97
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	74





Library Search Compound Report

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Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

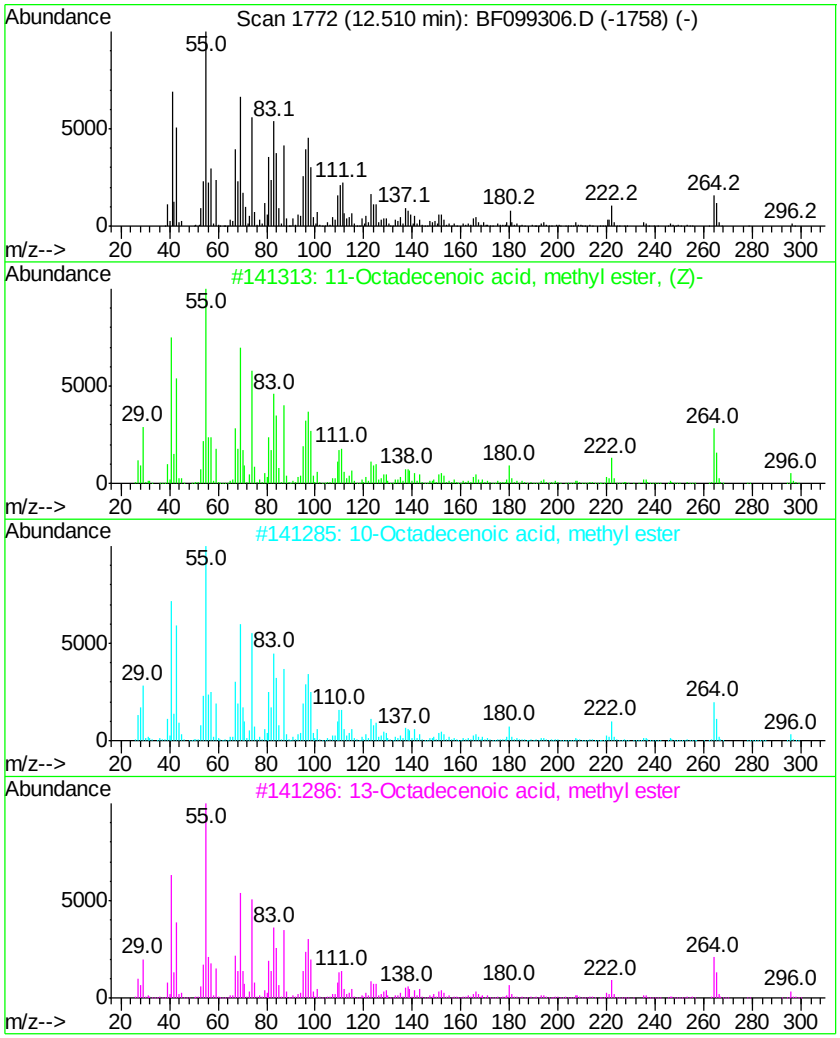
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

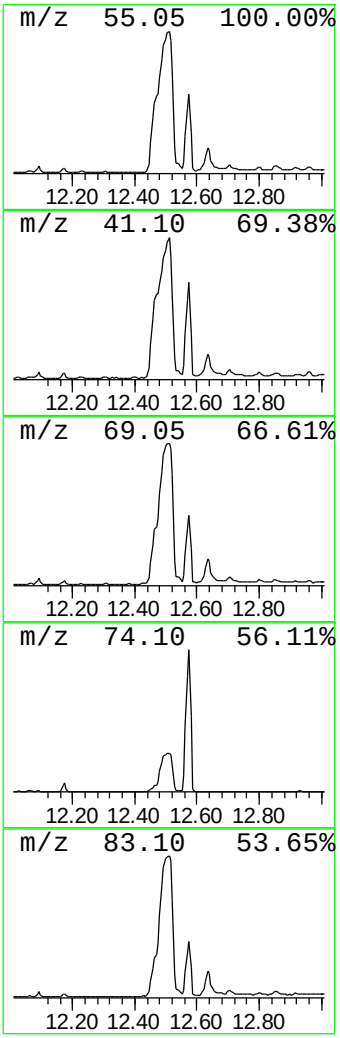
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 11-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	635.21 ng	19386900	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99





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Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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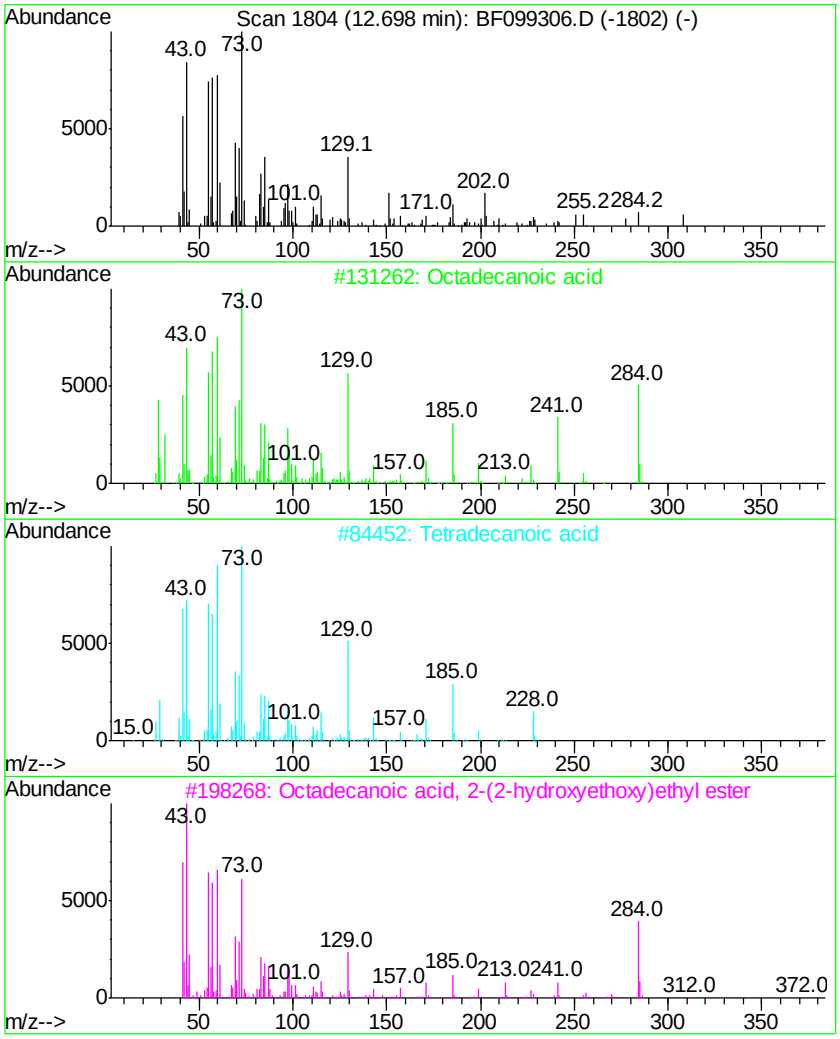
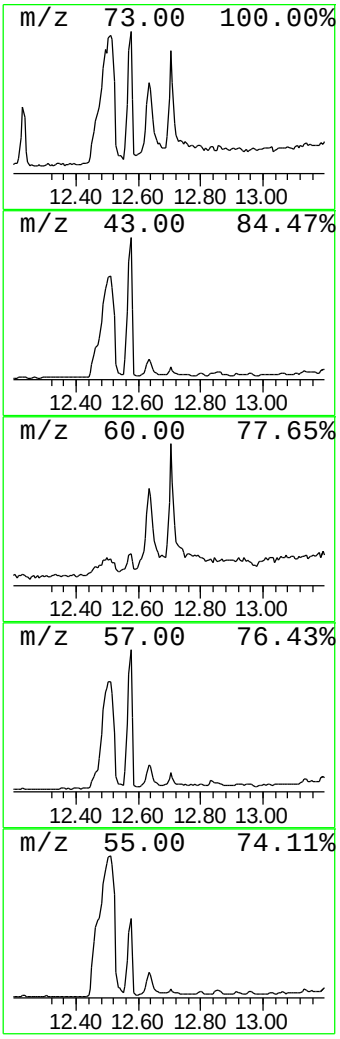
****

Peak Number 13 Octadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	7.59 ng	231683	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

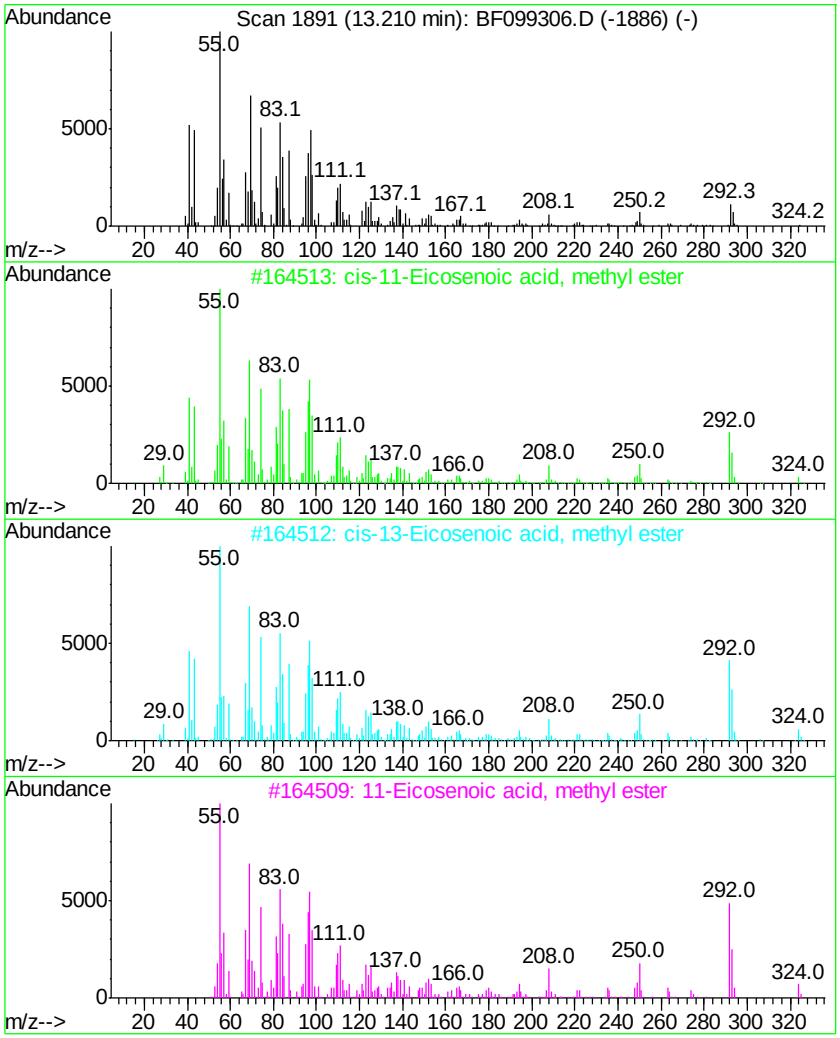
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

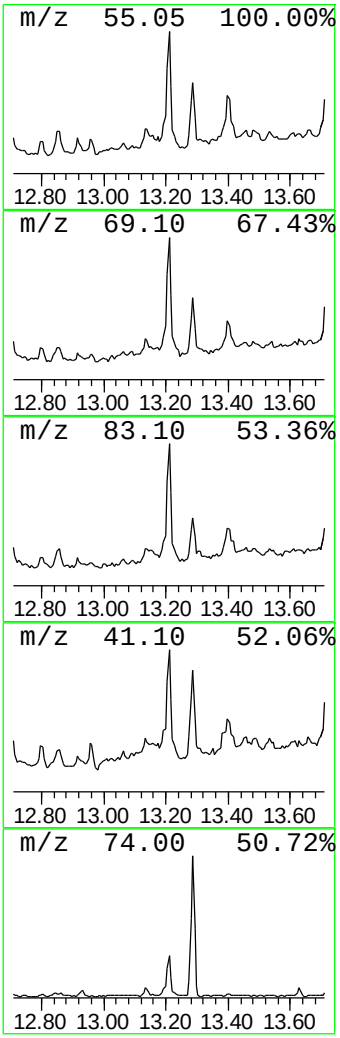
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 cis-11-Eicosenoic acid, met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	25.76 ng	904115	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	99
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	99
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	91
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91





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Data File : BF099306.D
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Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-100517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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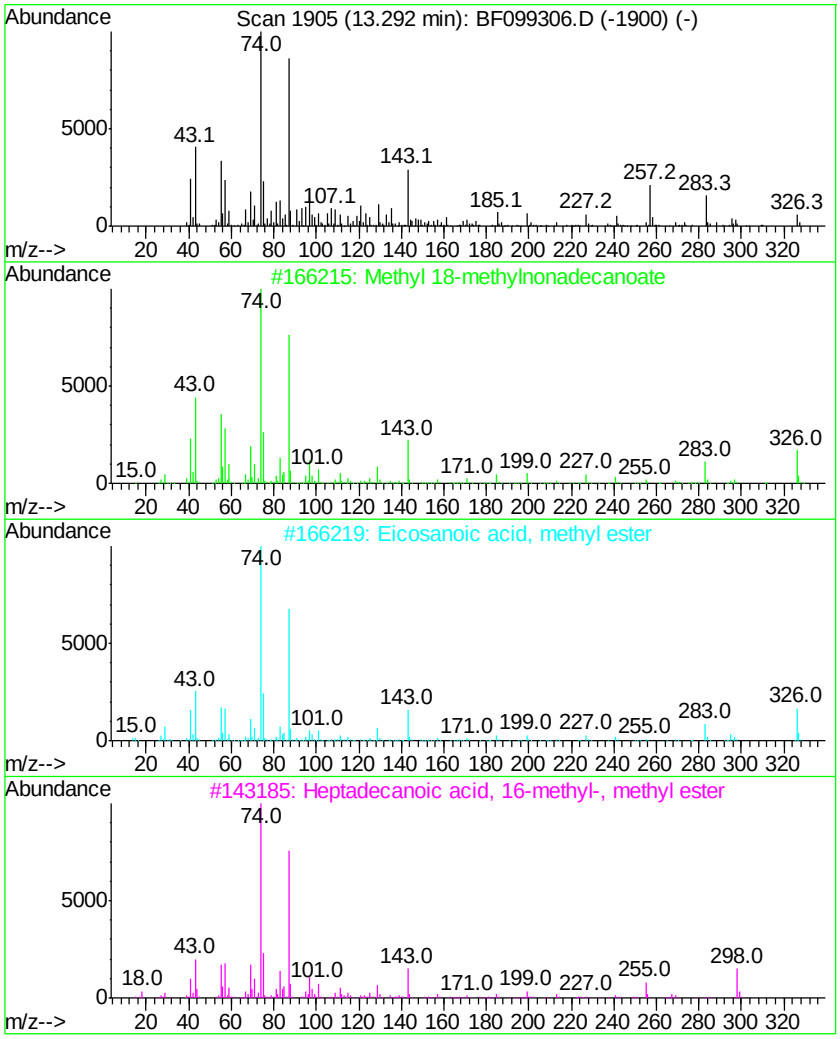
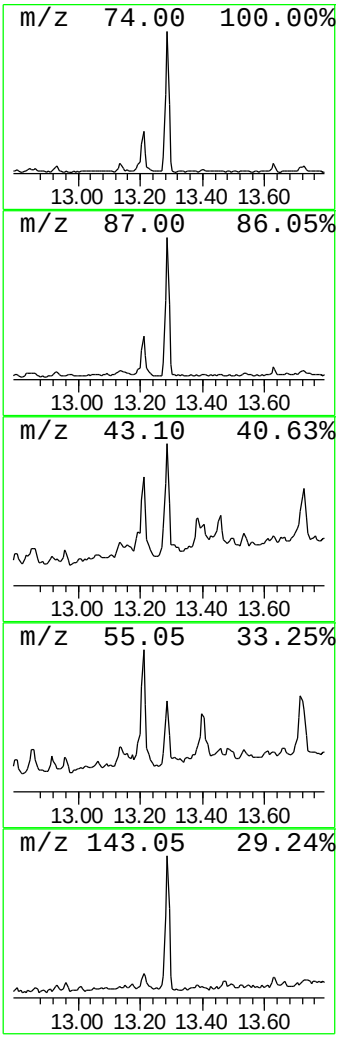
****

Peak Number 15 Methyl 18-methylnonadecanoate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	24.75 ng	868555	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	98
2	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87





Library Search Compound Report

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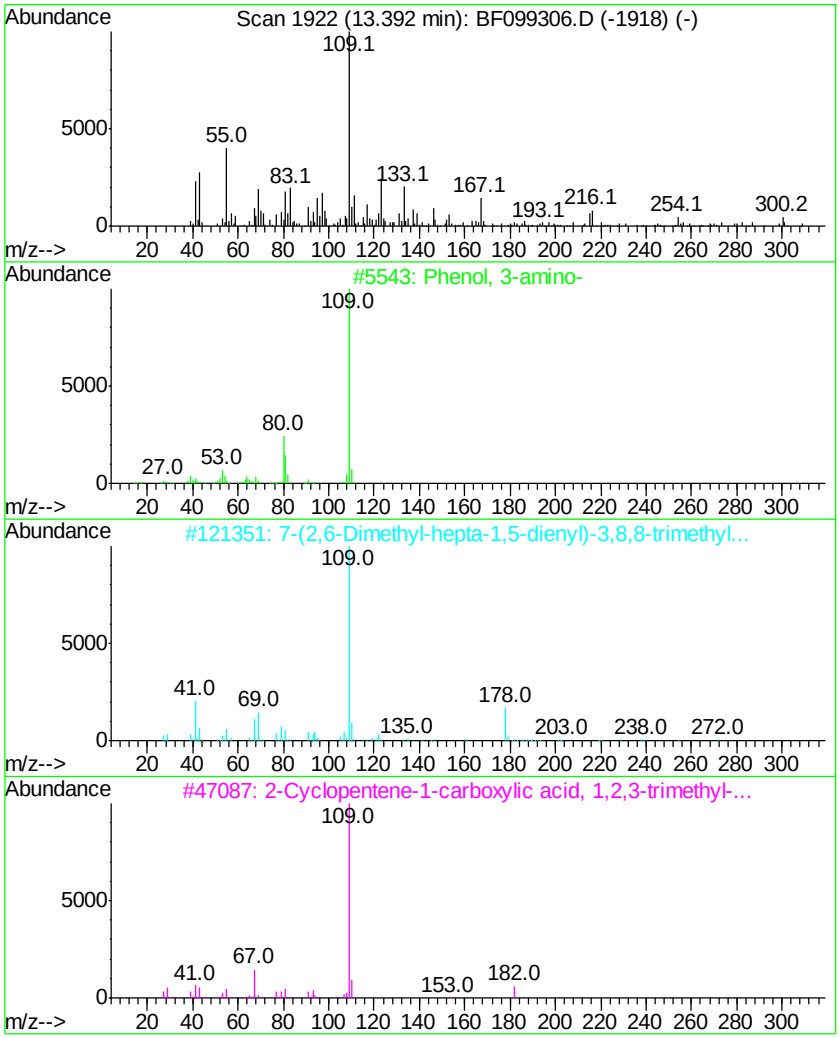
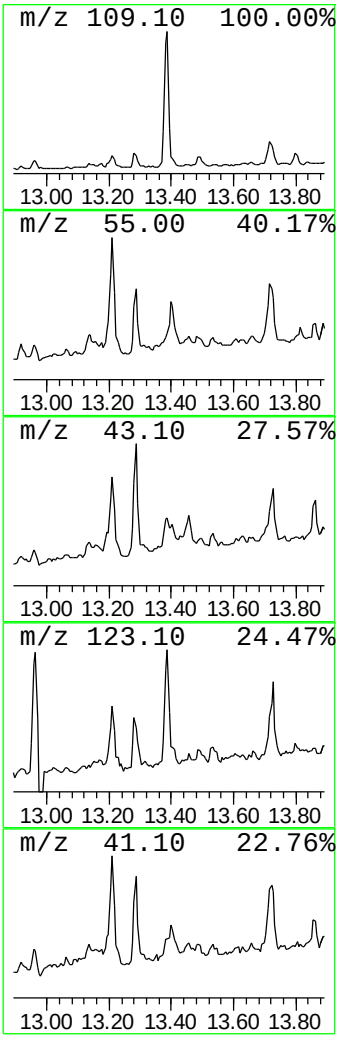
****

Peak Number 16 Phenol, 3-amino- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	7.66 ng	268677	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-amino-	109	C6H7NO	000591-27-5	52
2	7-(2,6-Dimethyl-hepta-1,5-dienyl...	272	C20H32	1000190-62-8	50
3	2-Cyclopentene-1-carboxylic acid...	182	C11H18O2	029915-95-5	50
4	Ketone, isopropylidenecyclopropy...	124	C8H12O	029765-67-1	42
5	Ethanone, 1-(1,3-dimethyl-3-cycl...	152	C10H16O	051733-68-7	42





Library Search Compound Report

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Operator : SJ/JU
Sample : I5714-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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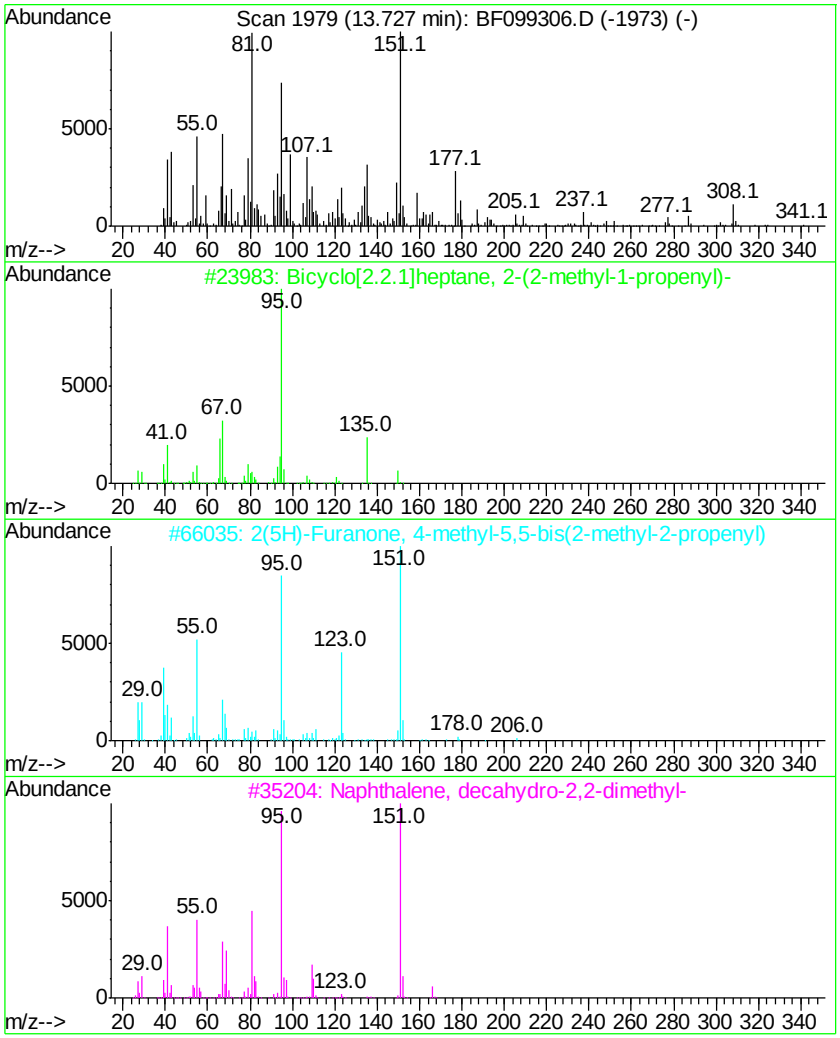
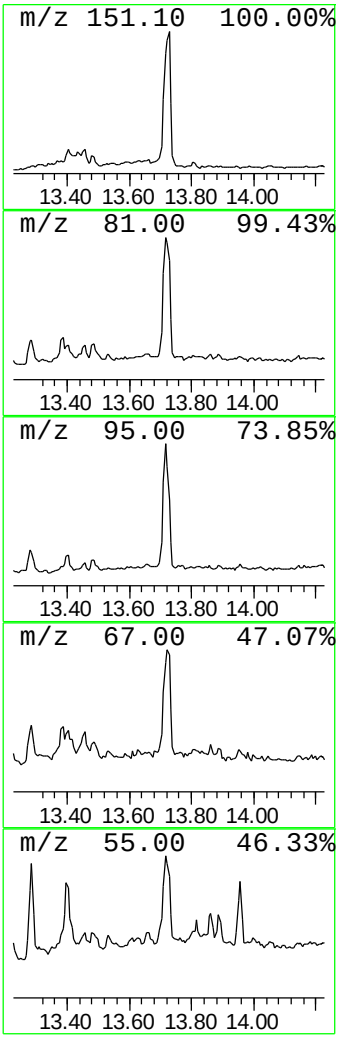
****

Peak Number 17 unknown13.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	28.72 ng	1007950	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2-(2-meth...	150	C11H18	061142-27-6	27
2	2(5H)-Furanone, 4-methyl-5,5-bis...	206	C13H18O2	099202-98-9	25
3	Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	25
4	Butyric acid, 4-(3-oxo-3H-benzo[...	237	C11H11NO3S	1000315-94-4	11
5	2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	11





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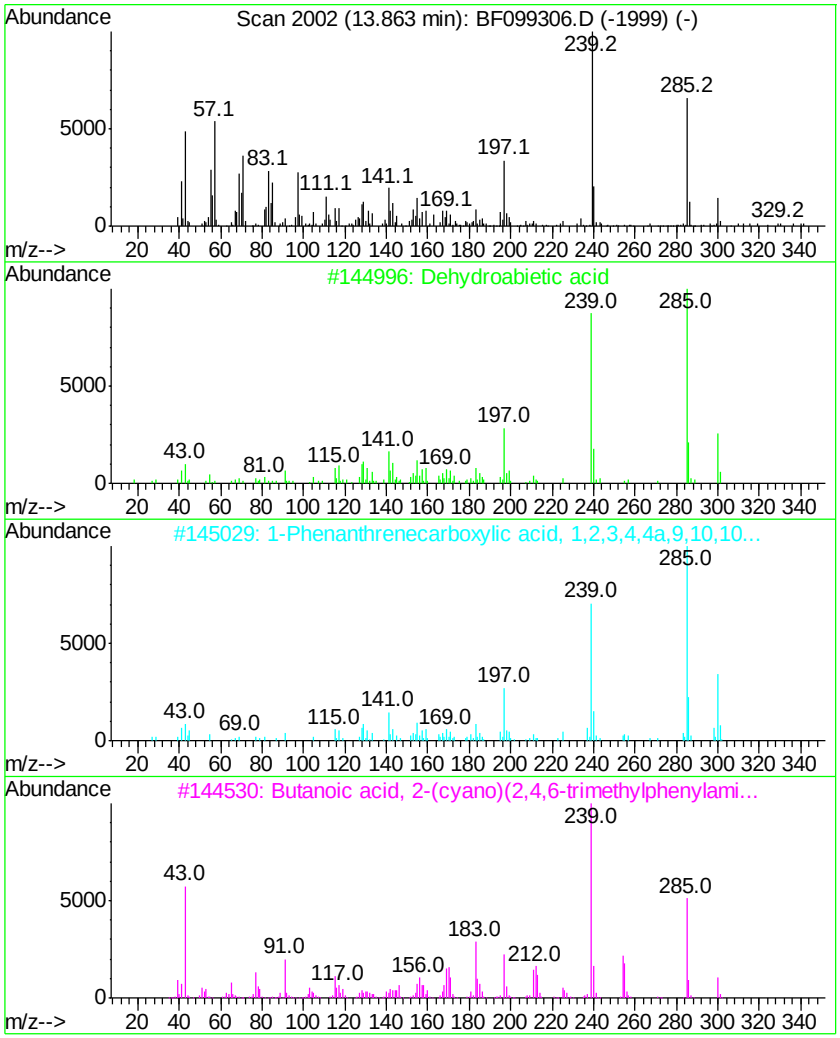
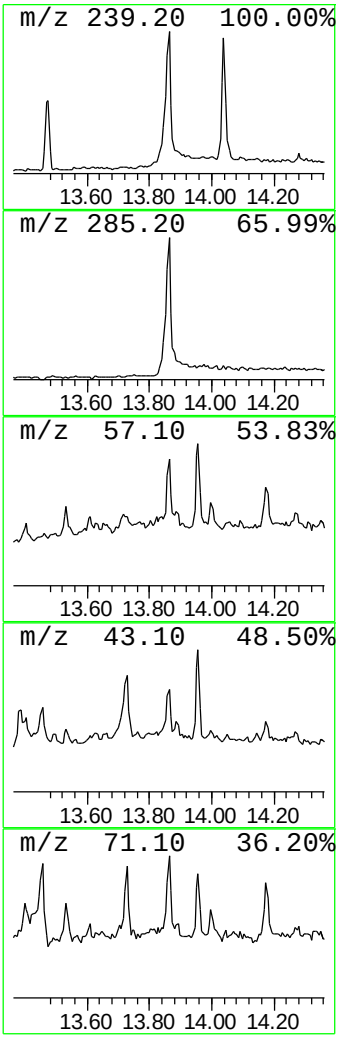
****

Peak Number 18 Dehydroabietic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.88 ng	276381	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydroabietic acid	300	C20H28O2	001740-19-8	90
2	1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	89
3	Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	62
4	trans-1,2-Bis(methyldichlorosily...	252	C4H8Cl4Si2	065899-10-7	60
5	Dibenzo[b,f]oxepin-3-amine, 6-me...	239	C15H13NO2	1000338-08-4	38





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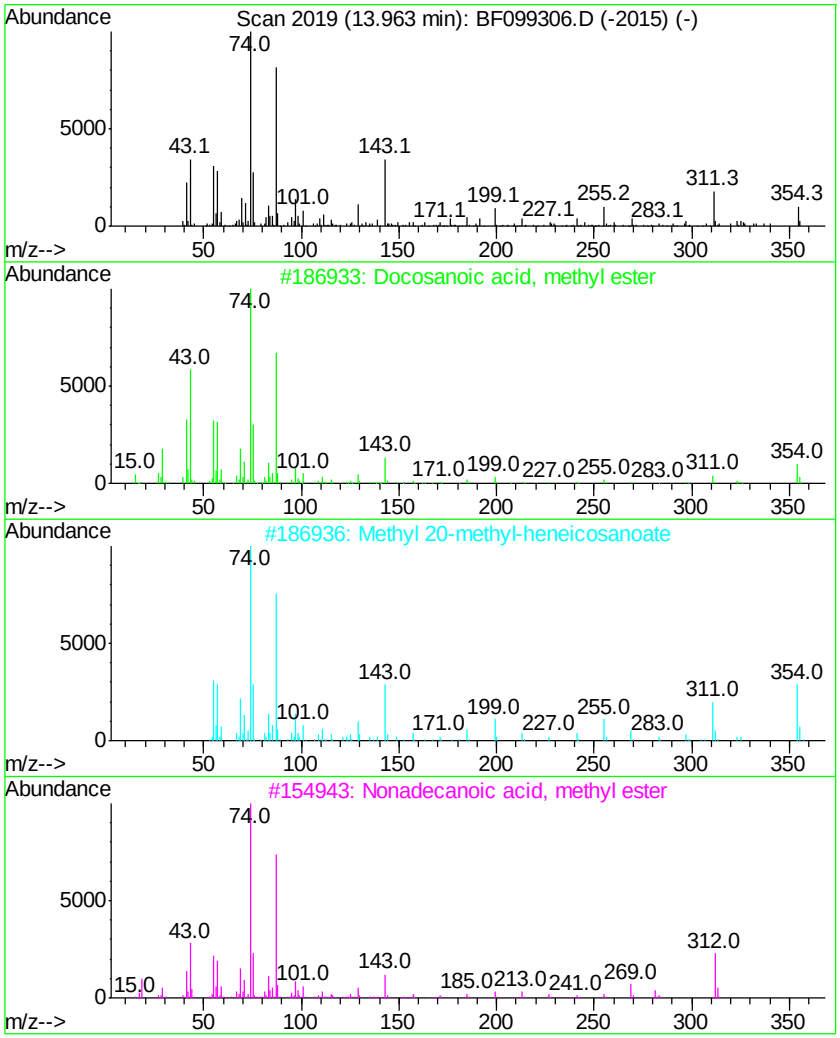
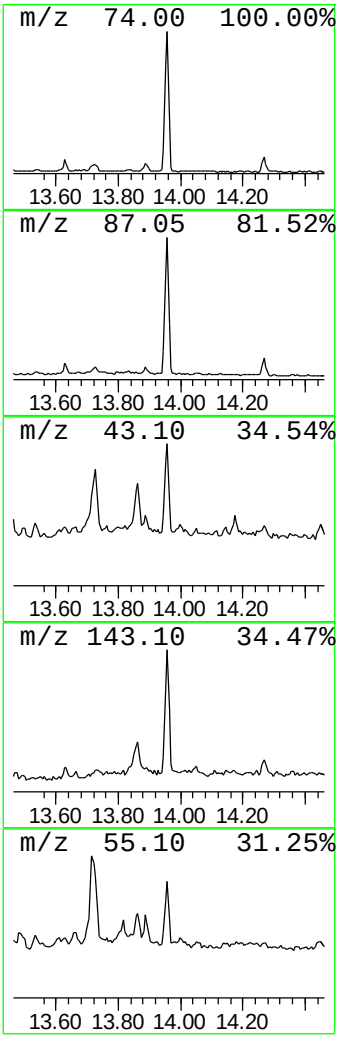
****
Peak Number 19 Docosanoic acid, methyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	10.91 ng	382954	Chrysene-d12	14.04

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	95
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	95
4	Methyl stearate	298	C19H38O2	000112-61-8	83
5	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	83





Tentatively Identified Compound (LSC) summary

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Data File : BF099306.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	15.6	ng	436025	1	6.86	559821	20.0
(1S)-2,6,6-Trimet...	6.14	60.1	ng	1682140	1	6.86	559821	20.0
.beta.-Pinene	6.56	45.2	ng	1264270	1	6.86	559821	20.0
unknown6.64	6.64	79.5	ng	2226490	1	6.86	559821	20.0
Tridecanoic acid,...	10.90	8.4	ng	256155	4	11.39	610411	20.0
9-Hexadecenoic ac...	11.69	26.2	ng	798442	4	11.39	610411	20.0
Hexadecanoic acid...	11.79	222.6	ng	6793440	4	11.39	610411	20.0
n-Hexadecanoic acid	11.93	27.7	ng	844629	4	11.39	610411	20.0
unknown12.09	12.09	8.2	ng	248685	4	11.39	610411	20.0
Heptadecanoic aci...	12.17	8.0	ng	245480	4	11.39	610411	20.0
11-Octadecenoic a...	12.51	635.2	ng	19386900	4	11.39	610411	20.0
Octadecanoic acid	12.70	7.6	ng	231683	4	11.39	610411	20.0
cis-11-Eicosenoic...	13.21	25.8	ng	904115	5	14.04	701840	20.0
Methyl 18-methyln...	13.29	24.8	ng	868555	5	14.04	701840	20.0
Phenol, 3-amino-	13.39	7.7	ng	268677	5	14.04	701840	20.0
unknown13.73	13.73	28.7	ng	1007950	5	14.04	701840	20.0
Dehydroabietic acid	13.86	7.9	ng	276381	5	14.04	701840	20.0
Docosanoic acid, ...	13.96	10.9	ng	382954	5	14.04	701840	20.0