LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106354.D
Acq On : 12 Jun 2018 19:36
Operator : JU/SJ
Sample : J3415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37COMP

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-BF061118.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	5.207	484	488	494	rVB	210972	236623	2.99%	0.532%
2	5.595	550	554	557	rBV	2754498	2520545	31.89%	5.664%
3	6.595	719	724	727	rBV	2540588	2453397	31.04%	5.513%
4	6.742	745	749	752	rBV	2852635	2457934	31.10%	5.523%
5	6.972	785	788	792	rVB	1075874	867034	10.97%	1.948%
6	7.131	811	815	818	rBV	2331755	1965819	24.87%	4.418%
7	7.531	879	883	886	rBV	1683151	1513061	19.14%	3.400%
8	8.254	1002	1006	1009	rBV	1229265	966370	12.23%	2.172%
9	9.331	1185	1189	1192	rVB	2619255	2216222	28.04%	4.980%
10	9.719	1251	1255	1258	rBV	408648	298926	3.78%	0.672%
11	10.013	1301	1305	1309	rBV2	1097181	911561	11.53%	2.048%
12	10.801	1435	1439	1443	rBV	1738561	1409445	17.83%	3.167%
13	10.901	1453	1456	1462	rBV	76089	79567	1.01%	0.179%
14	11.507	1555	1559	1562	rBV	1048509	976826	12.36%	2.195%
15	11.883	1619	1623	1626	rBV	3251485	2518675	31.87%	5.660%
16	12.577	1736	1741	1743	rBV	5385433	7017455	88.79%	15.770%
17	12.601	1743	1745	1751	rVV2	6188416	7903500	100.00%	17.761%
18	12.677	1755	1758	1761	rVV	1846124	1457214	18.44%	3.275%
19	12.754	1766	1771	1775	rBV4	45647	89987	1.14%	0.202%
20	12.913	1793	1798	1802	rBV	204078	197364	2.50%	0.444%
21	13.089	1824	1828	1831	rBV	2804357	2597930	32.87%	5.838%
22	13.277	1858	1860	1862	rVB2	145308	113408	1.43%	0.255%
23	13.324	1862	1868	1874	rVB	407750	436928	5.53%	0.982%
24	13.401	1878	1881	1883	rBV	313779	251956	3.19%	0.566%
25	13.513	1897	1900	1905	rBV2	111718	130728	1.65%	0.294%
26	13.836	1950	1955	1961	rVB2	222876	325497	4.12%	0.731%
27	13.971	1975	1978	1982	rBV	285384	259721	3.29%	0.584%
28	14.077	1992	1996	1999	rBV	231217	216140	2.73%	0.486%
29	14.154	2005	2009	2013	rBV	1375114	1206271	15.26%	2.711%
30	15.701	2267	2272	2278	rVB	666868	903782	11.44%	2.031%

Sum of corrected areas: 44499886

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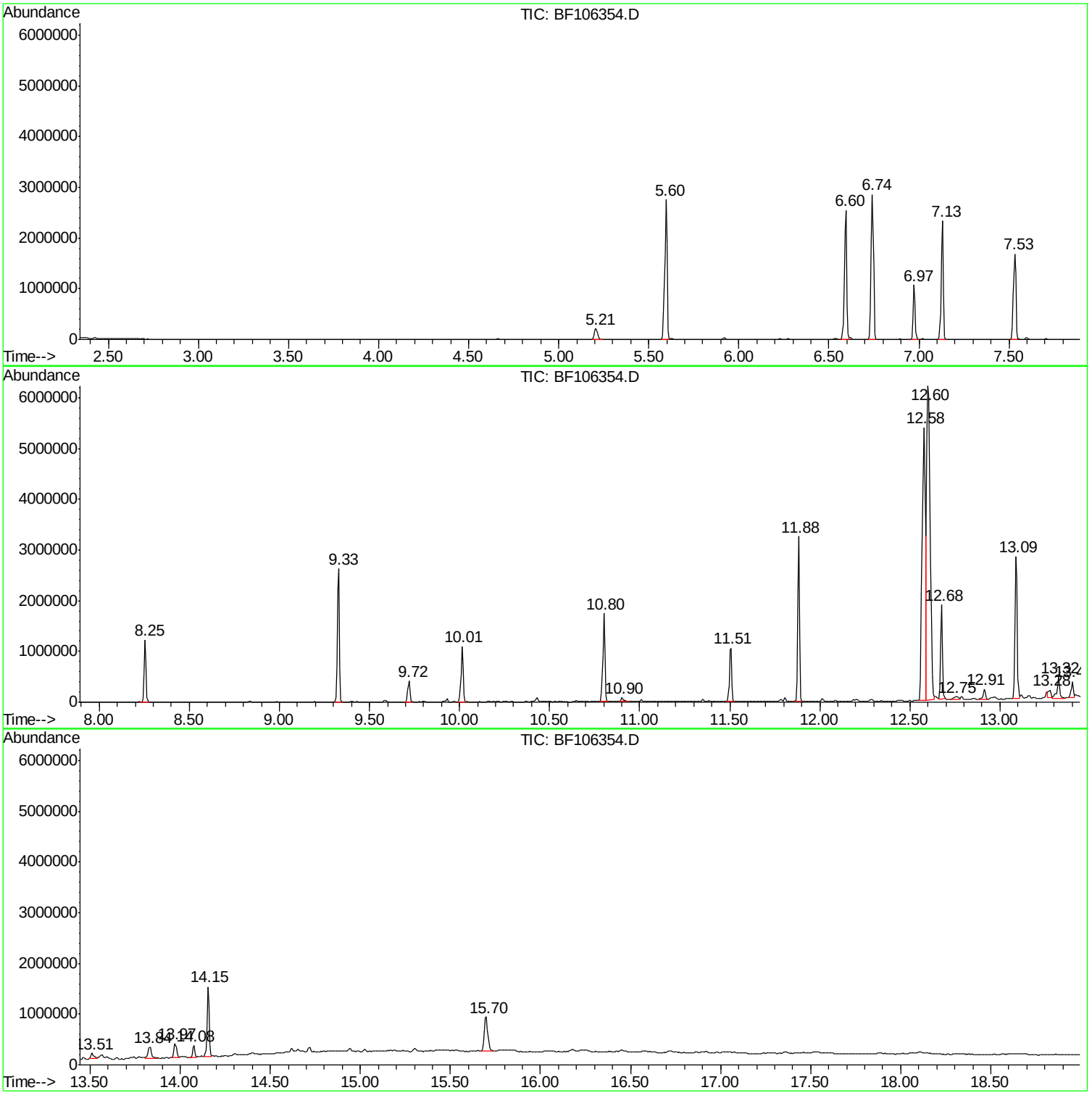
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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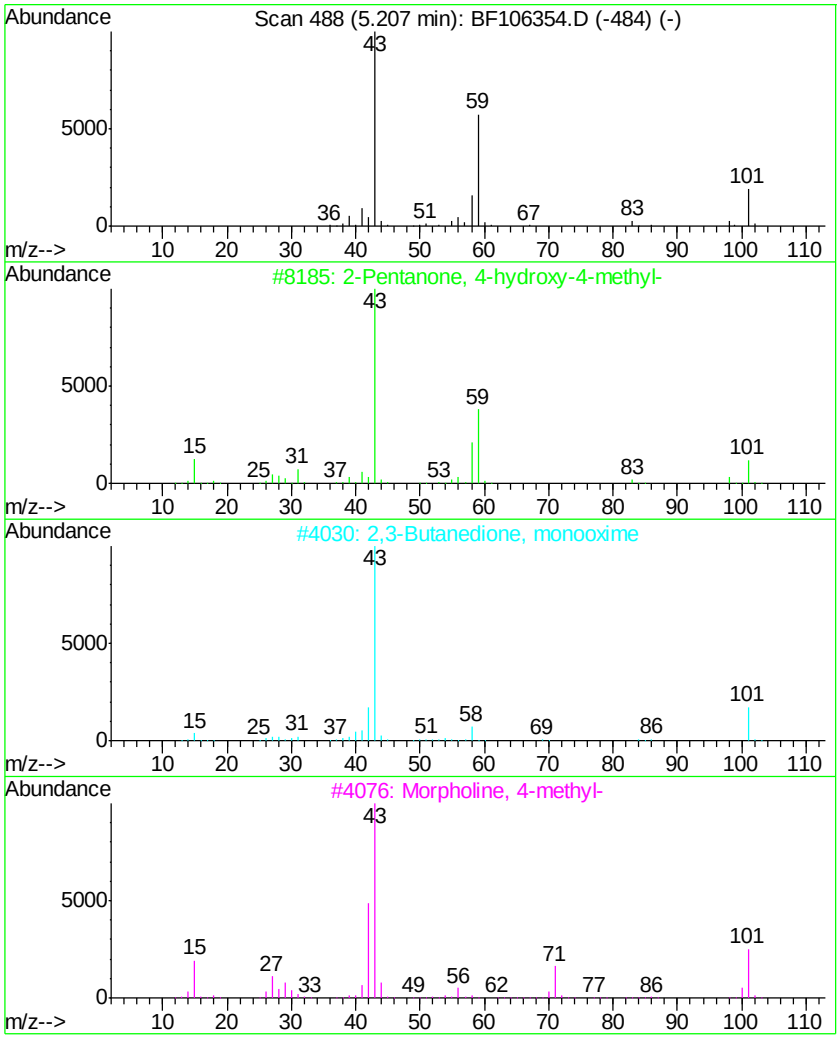
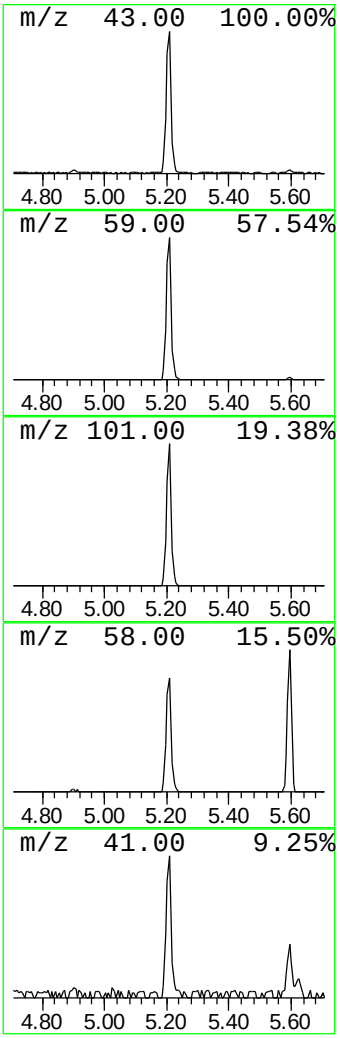
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	5.46 ng	236623	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





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Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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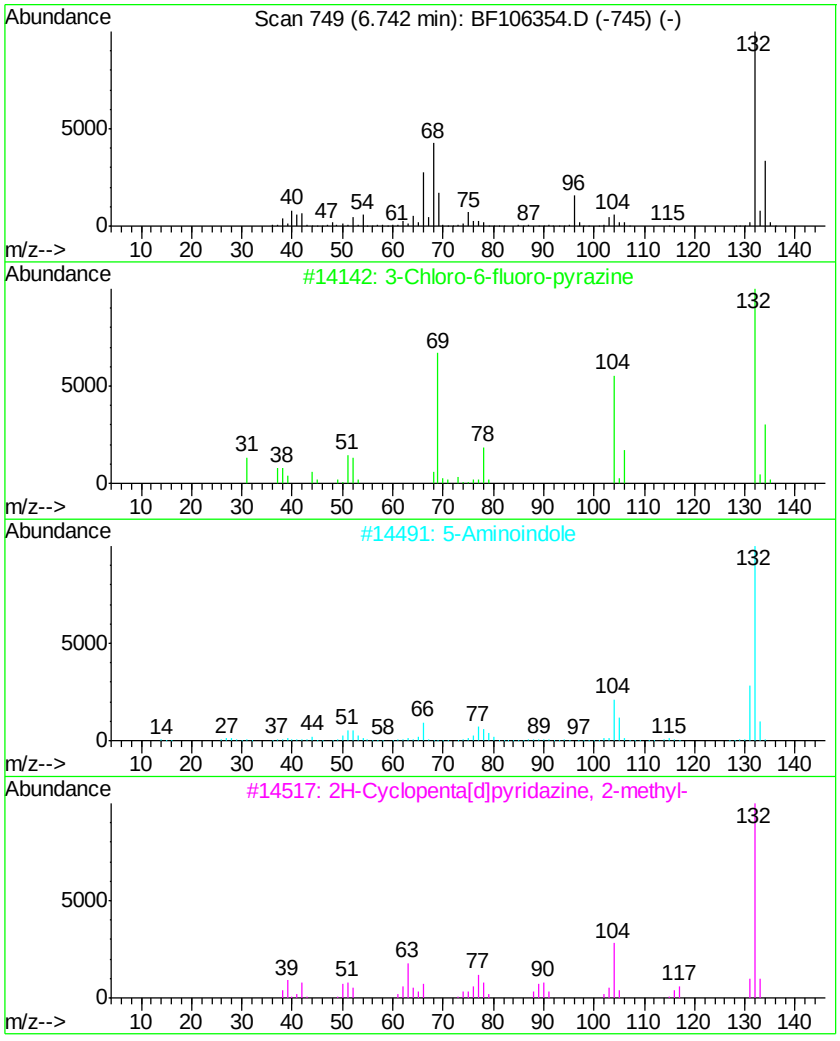
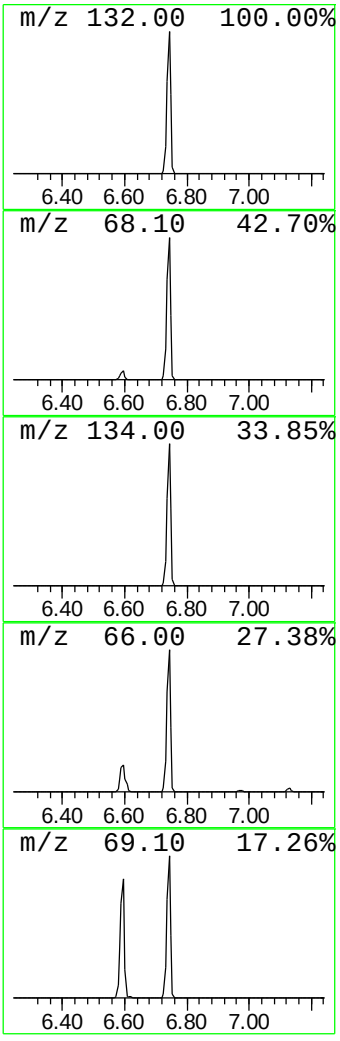
Peak Number 2 unknown6.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	56.70 ng	2457930	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





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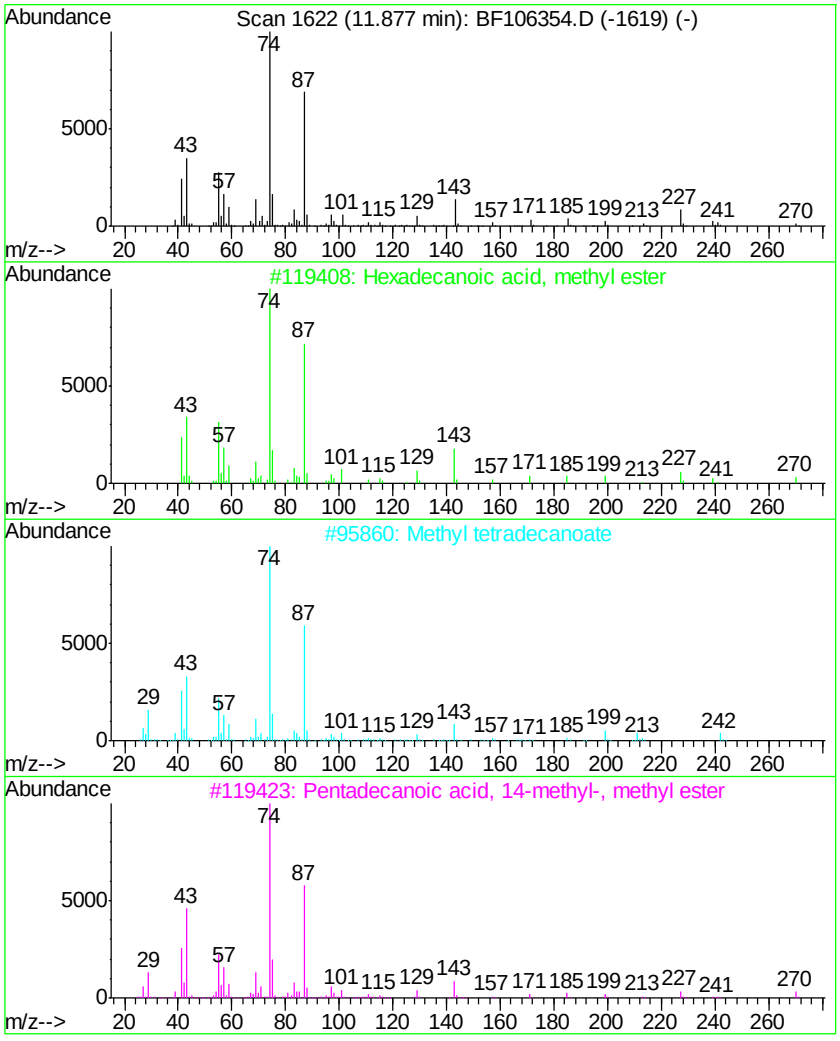
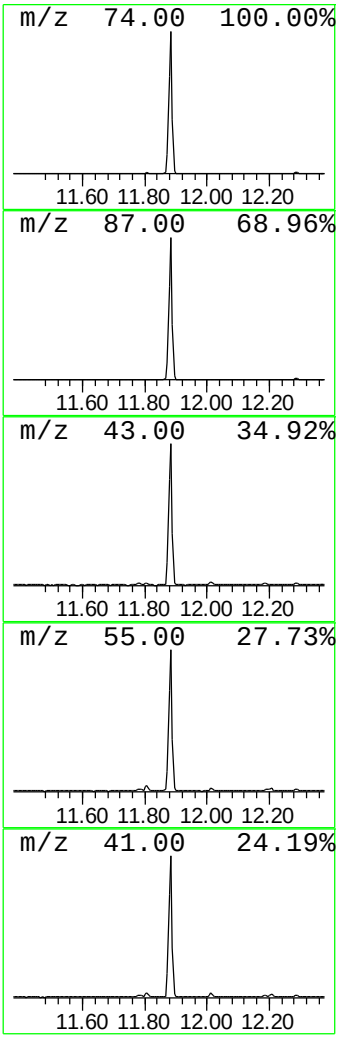
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	51.57 ng	2518680	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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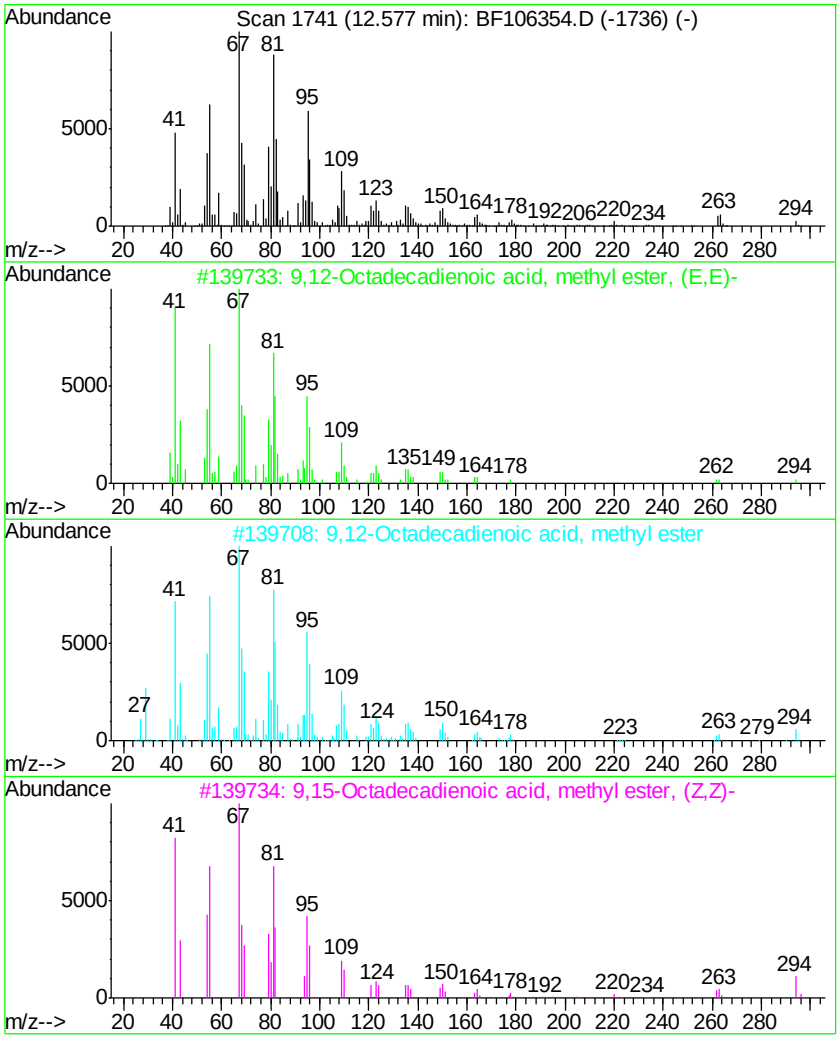
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

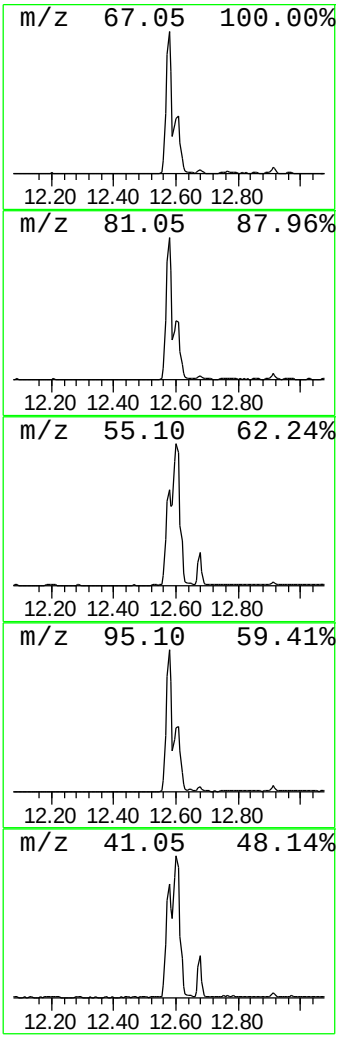
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	143.68 ng	7017460	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	97





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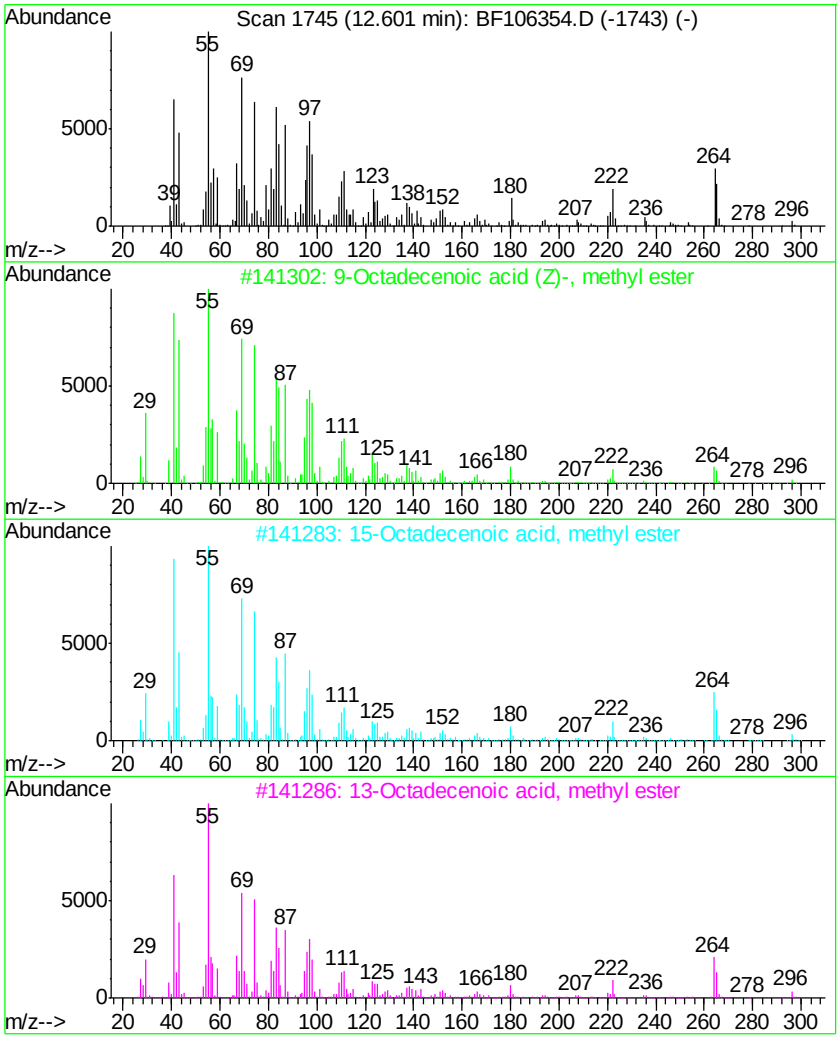
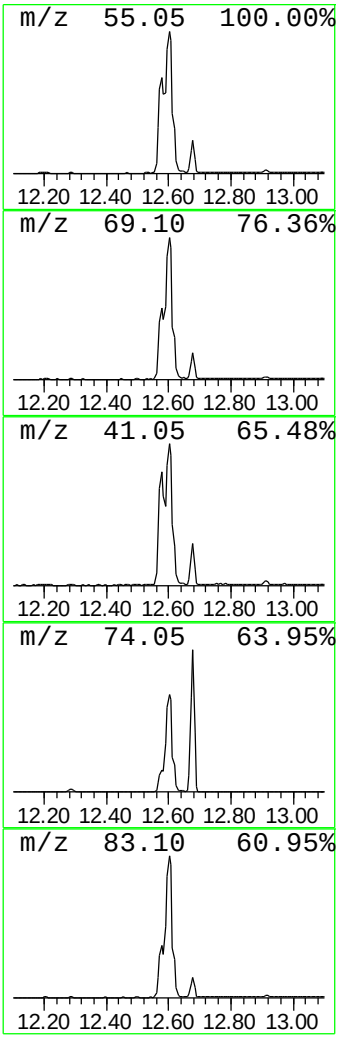
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	161.82 ng	7903500	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99





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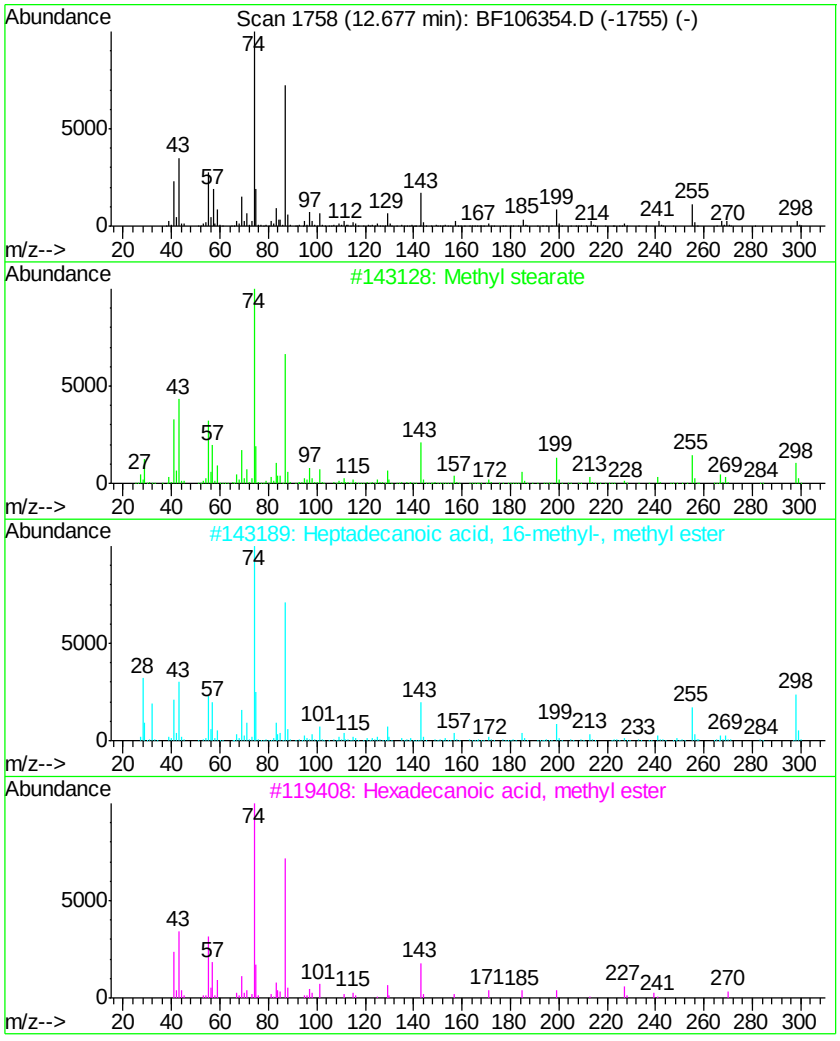
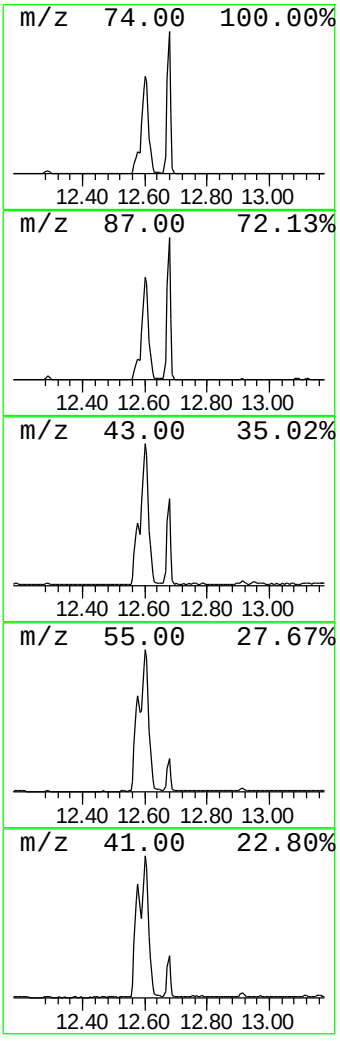
****

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	29.84 ng	1457210	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	96
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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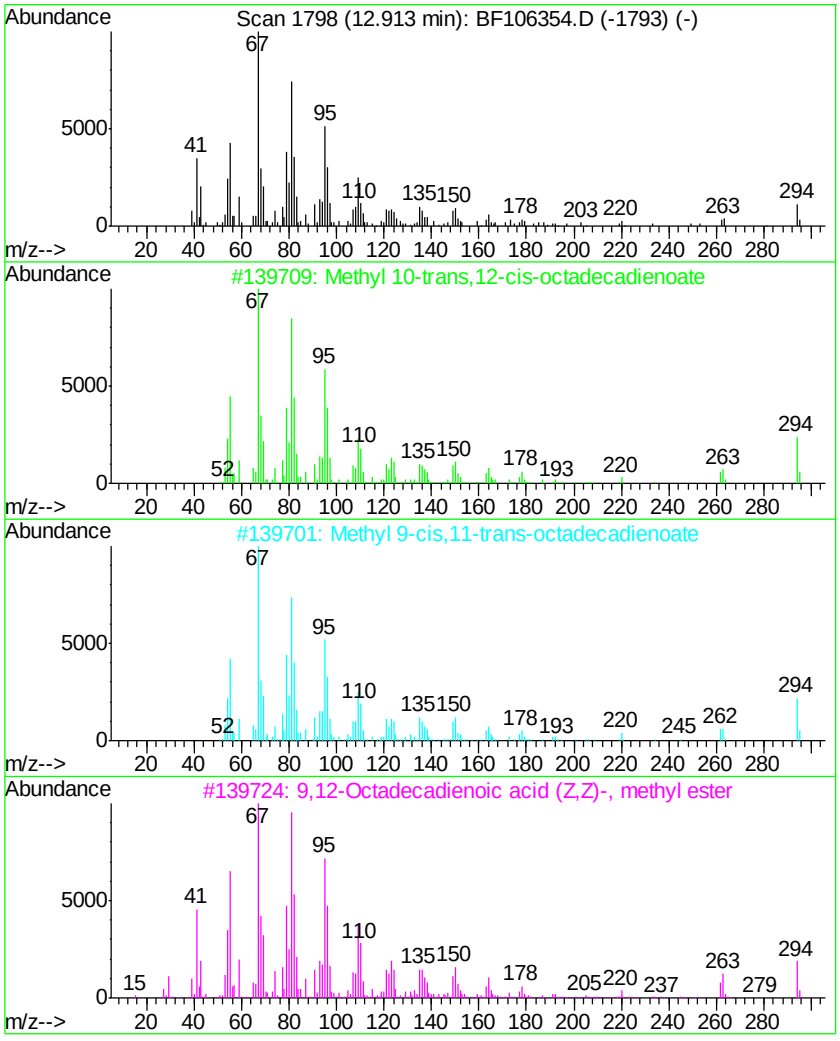
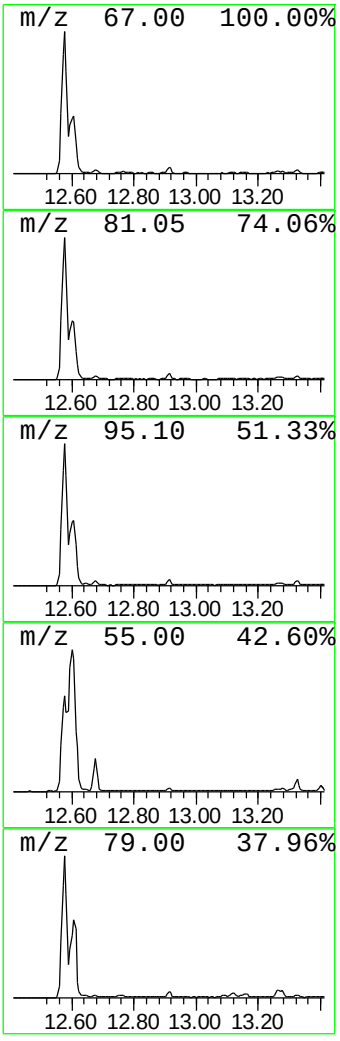
Peak Number 8 Methyl 10-trans,12-cis-octa... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	3.27 ng	197364	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	96
4	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	95
5	7,10-Octadecadienoic acid, methy...	294	C19H34O2	056554-24-6	93





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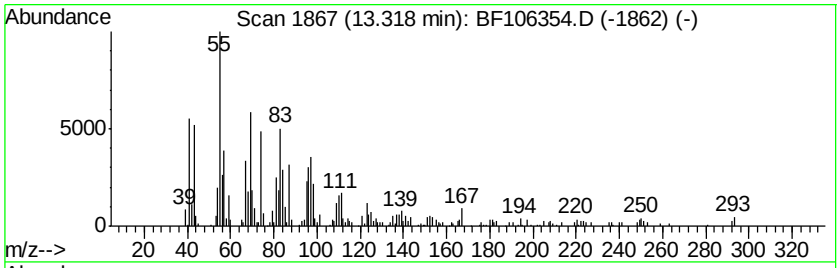
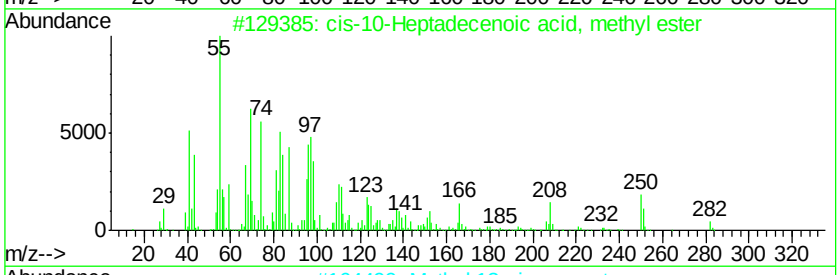
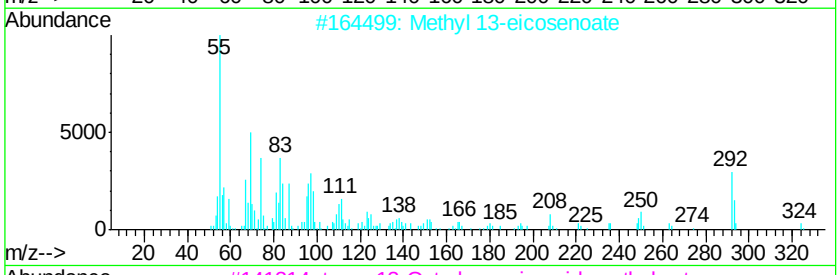
Peak Number 9 cis-10-Heptadecenoic acid, ... Concentration Rank 7

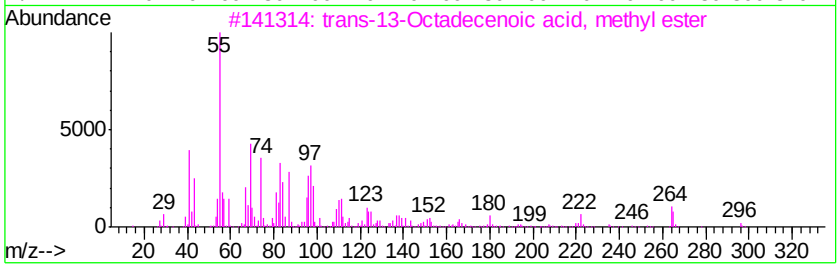
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	7.24 ng	436928	Chrysene-d12	14.15

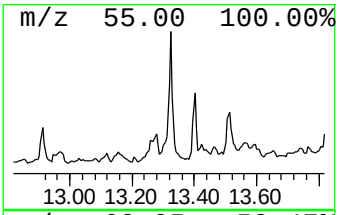
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
2	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	91
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	81
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	81

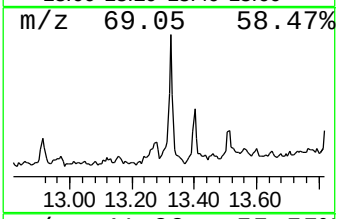


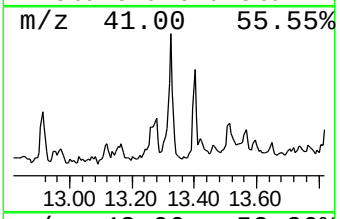


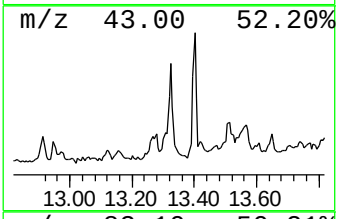


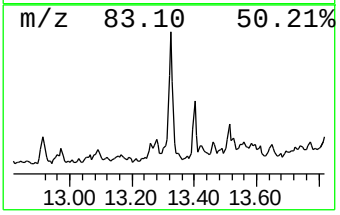












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106354.D
Acq On : 12 Jun 2018 19:36
Operator : JU/SJ
Sample : J3415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

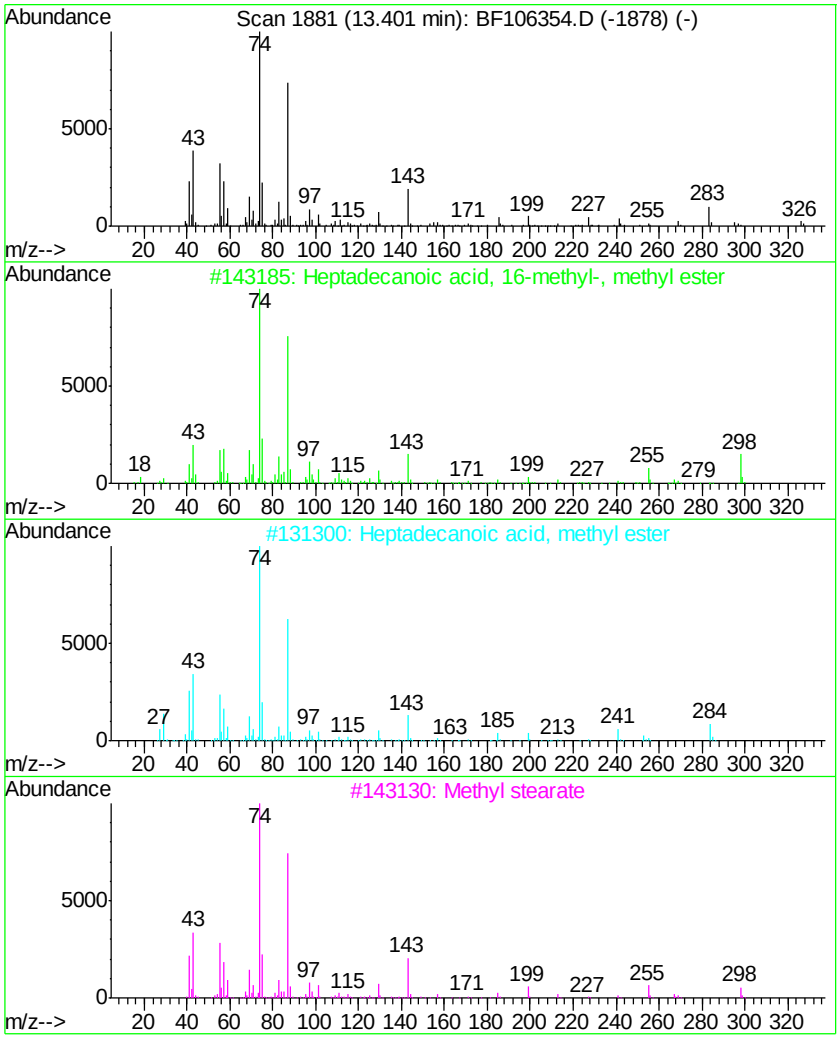
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

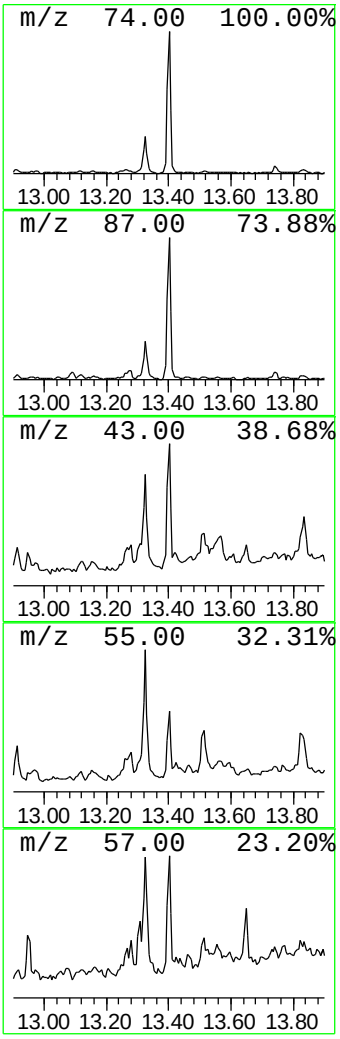
****

Peak Number 10 Heptadecanoic acid, 16-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	4.18 ng	251956	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	97
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	95
3	Methyl stearate	298	C19H38O2	000112-61-8	95
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061218\
Data File : BF106354.D
Acq On : 12 Jun 2018 19:36
Operator : JU/SJ
Sample : J3415-06
Misc :
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Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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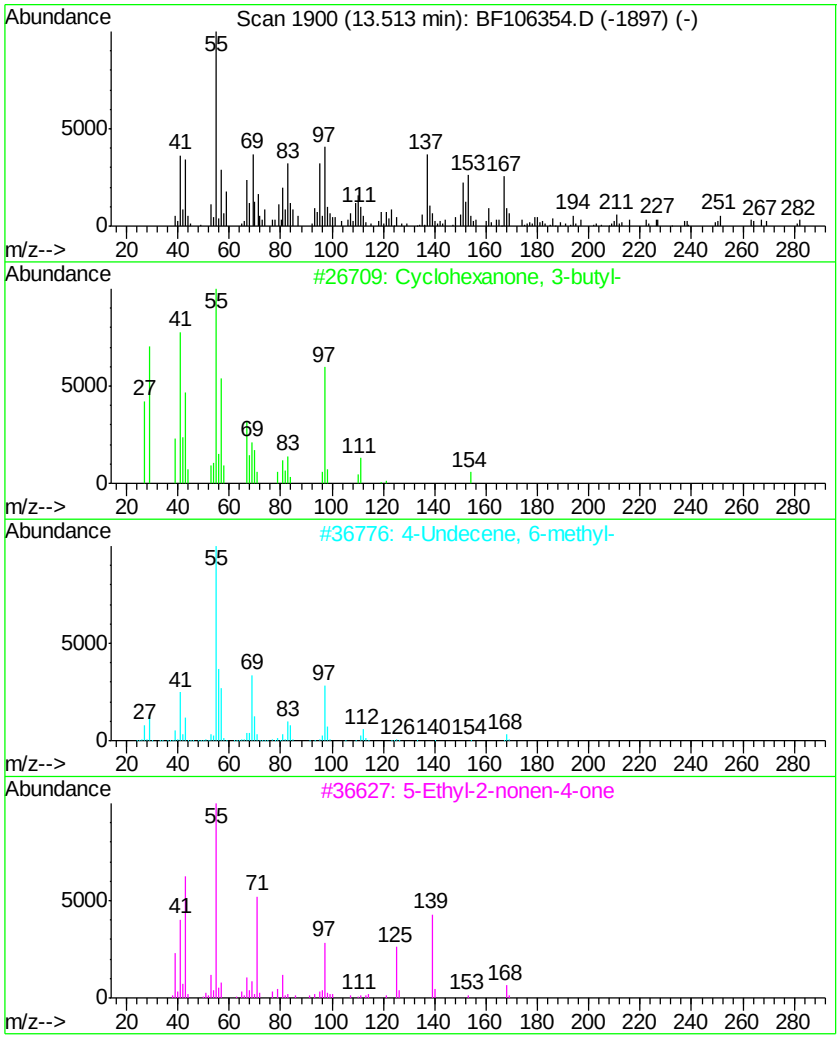
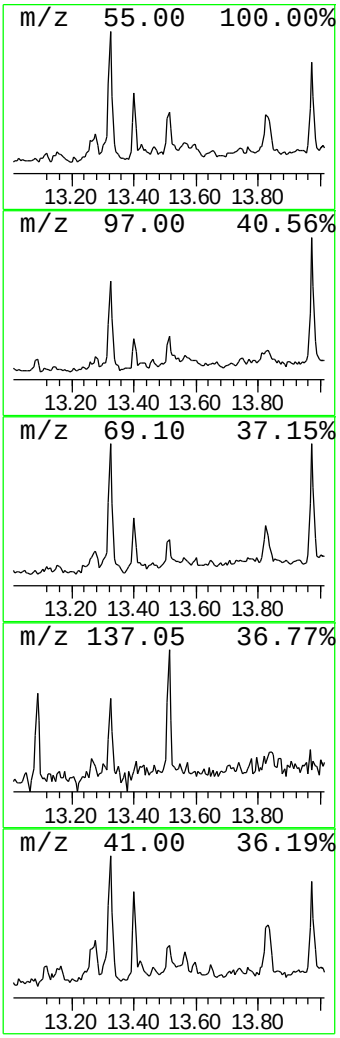
Peak Number 11 unknown13.51 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	2.17 ng	130728	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	25
2	4-Undecene, 6-methyl-	168	C12H24	1000061-85-4	14
3	5-Ethyl-2-nonen-4-one	168	C11H20O	1000374-06-8	14
4	10-Methyldodec-2-en-4-olide	210	C13H22O2	1000370-41-0	14
5	Fumaric acid, di(2-methylallyl) ...	224	C12H16O4	1000330-55-8	12





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Operator : JU/SJ
Sample : J3415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Integration Parameters: LSCINT.P

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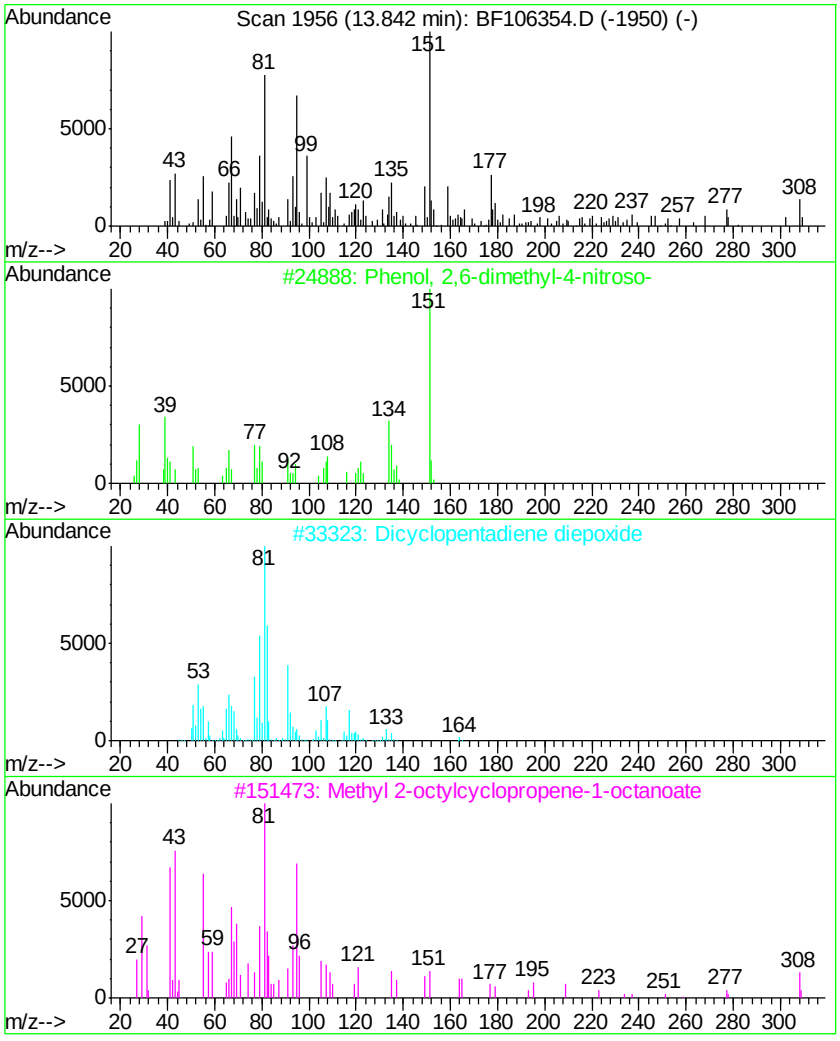
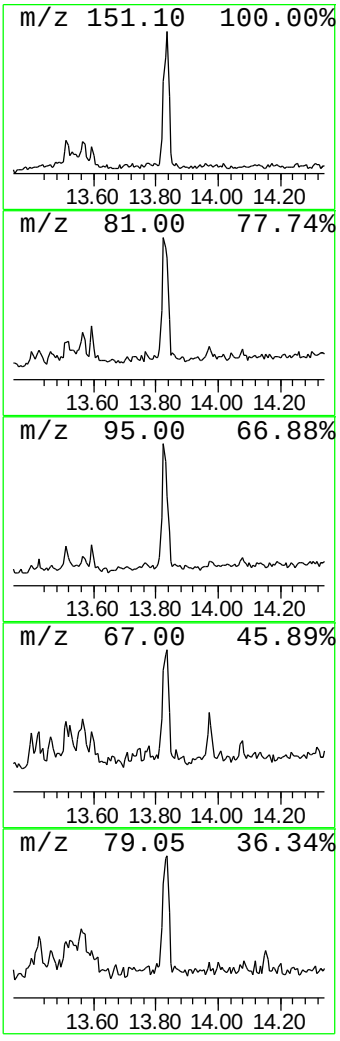
Peak Number 12 unknown13.84 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.40 ng	325497	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethyl-4-nitroso-	151	C8H9NO2	013331-93-6	45
2	Dicyclopentadiene diepoxide	164	C10H12O2	000081-21-0	41
3	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	38
4	4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	27
5	Butyric acid, 2-(3-oxo-3H-benzo[...	237	C11H11NO3S	1000316-00-8	25





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Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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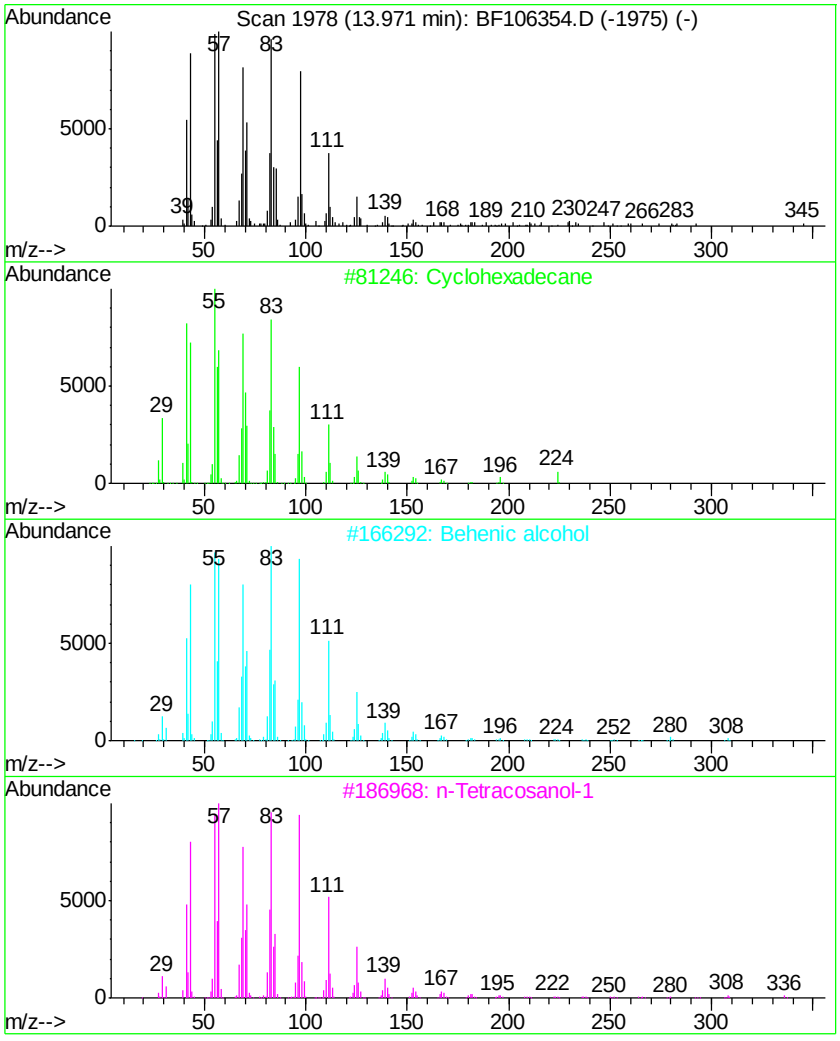
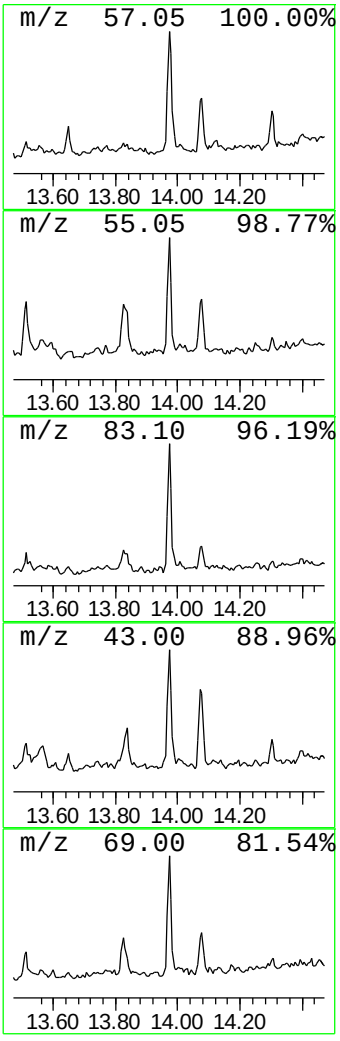
Peak Number 13 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.31 ng	259721	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Operator : JU/SJ
Sample : J3415-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-37COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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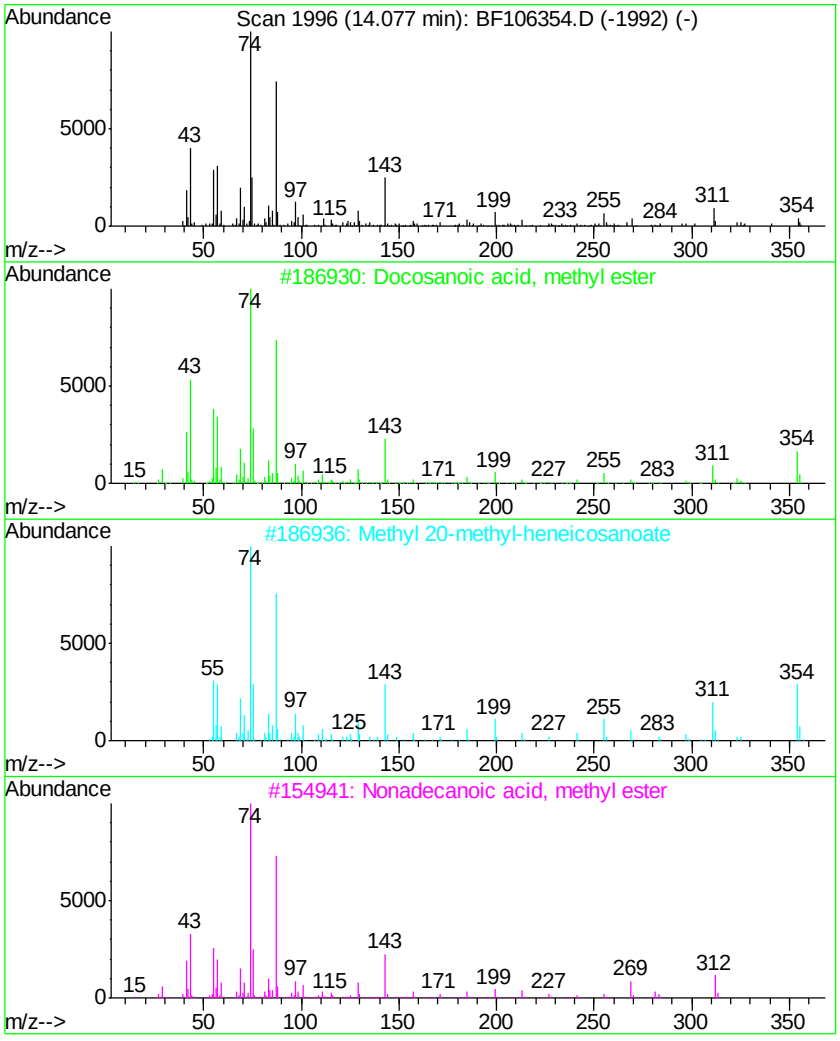
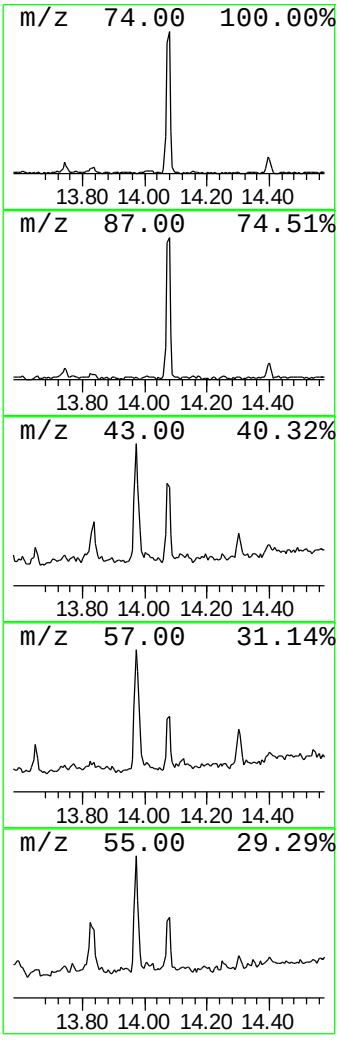
Peak Number 14 Docosanoic acid, methyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	3.58 ng	216140	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	95
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	5.5	ng	236623	1	6.97	867034	20.0
unknown6.74	6.74	56.7	ng	2457930	1	6.97	867034	20.0
Hexadecanoic acid...	11.88	51.6	ng	2518680	4	11.51	976826	20.0
9,12-Octadecadien...	12.58	143.7	ng	7017460	4	11.51	976826	20.0
9-Octadecenoic ac...	12.60	161.8	ng	7903500	4	11.51	976826	20.0
Methyl stearate	12.68	29.8	ng	1457210	4	11.51	976826	20.0
Methyl 10-trans,1...	12.91	3.3	ng	197364	5	14.15	1206270	20.0
cis-10-Heptadecen...	13.32	7.2	ng	436928	5	14.15	1206270	20.0
Heptadecanoic aci...	13.40	4.2	ng	251956	5	14.15	1206270	20.0
unknown13.51	13.51	2.2	ng	130728	5	14.15	1206270	20.0
unknown13.84	13.84	5.4	ng	325497	5	14.15	1206270	20.0
Cyclohexadecane	13.97	4.3	ng	259721	5	14.15	1206270	20.0
Docosanoic acid, ...	14.08	3.6	ng	216140	5	14.15	1206270	20.0