LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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	5.613	553	557	565	rBV	1513614	1710086	4.86%	1.786%
2	6.613	723	727	736	rVB	1029783	1265119	3.60%	1.321%
3	6.748	746	750	753	rBV	3029890	2747935	7.81%	2.870%
4	6.966	783	787	790	rBV	1125566	922685	2.62%	0.964%
5	7.125	809	814	817	rBV	2798607	2621889	7.45%	2.738%
6	7.531	877	883	886	rBV	2393506	2339287	6.65%	2.443%
7	8.248	1001	1005	1008	rBV	1508342	1186814	3.37%	1.239%
8	8.948	1117	1124	1127	rBV	410814	512180	1.46%	0.535%
9	9.325	1183	1188	1191	rVB	4063390	3853006	10.95%	4.024%
10	10.007	1300	1304	1307	rVB	1591946	1309067	3.72%	1.367%
11	10.801	1434	1439	1442	rBV	2634269	2482629	7.06%	2.593%
12	11.183	1495	1504	1521	rBV	2678127	4677005	13.29%	4.884%
13	11.495	1554	1557	1561	rVB	1414412	1250581	3.55%	1.306%
14	11.595	1570	1574	1582	rBV	519156	523099	1.49%	0.546%
15	12.130	1630	1665	1681	rBV5	5429599	35179279	100.00%	36.736%
16	12.336	1697	1700	1703	rVV	569019	476087	1.35%	0.497%
17	12.436	1714	1717	1732	rVB	1024827	953479	2.71%	0.996%
18	12.777	1763	1775	1776	rBV	4094858	10467881	29.76%	10.931%
19	12.854	1782	1788	1797	rVB	4398326	9300777	26.44%	9.712%
20	13.089	1824	1828	1831	rBV	3317362	3142117	8.93%	3.281%
21	13.471	1888	1893	1899	rBV	398584	587873	1.67%	0.614%
22	13.560	1900	1908	1921	rVB	2959205	4945840	14.06%	5.165%
23	14.148	2004	2008	2012	rBV	1211595	1052082	2.99%	1.099%
24	15.671	2262	2267	2273	rVB	766199	1029561	2.93%	1.075%
25	16.595	2418	2424	2434	rBV4	261543	559912	1.59%	0.585%
26	17.806	2622	2630	2643	rVB4	219753	665056	1.89%	0.694%

Sum of corrected areas: 95761326

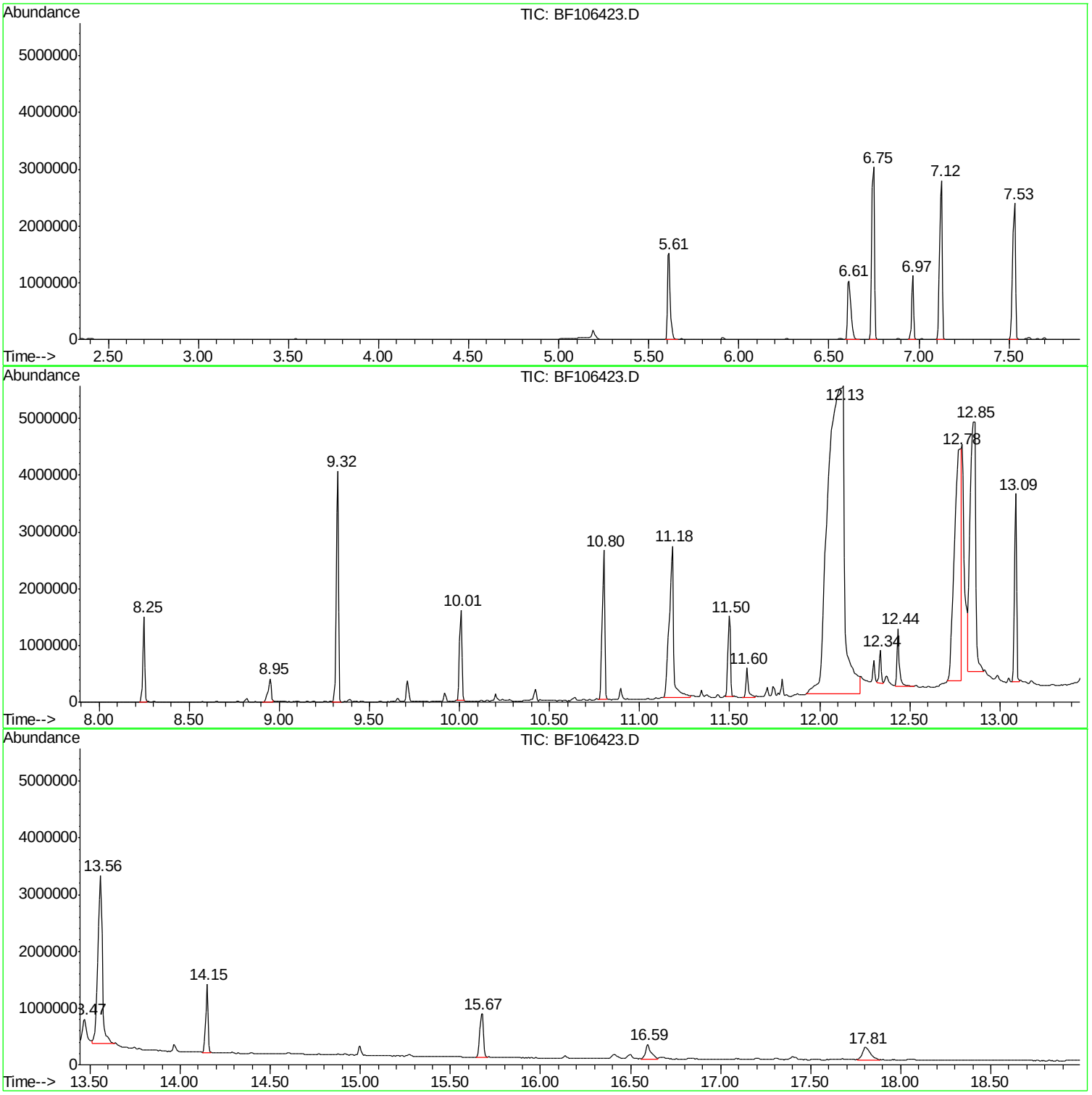
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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Data File : BF106423.D
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Misc :
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Instrument : BNA_F
ClientSampleId : W-27

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

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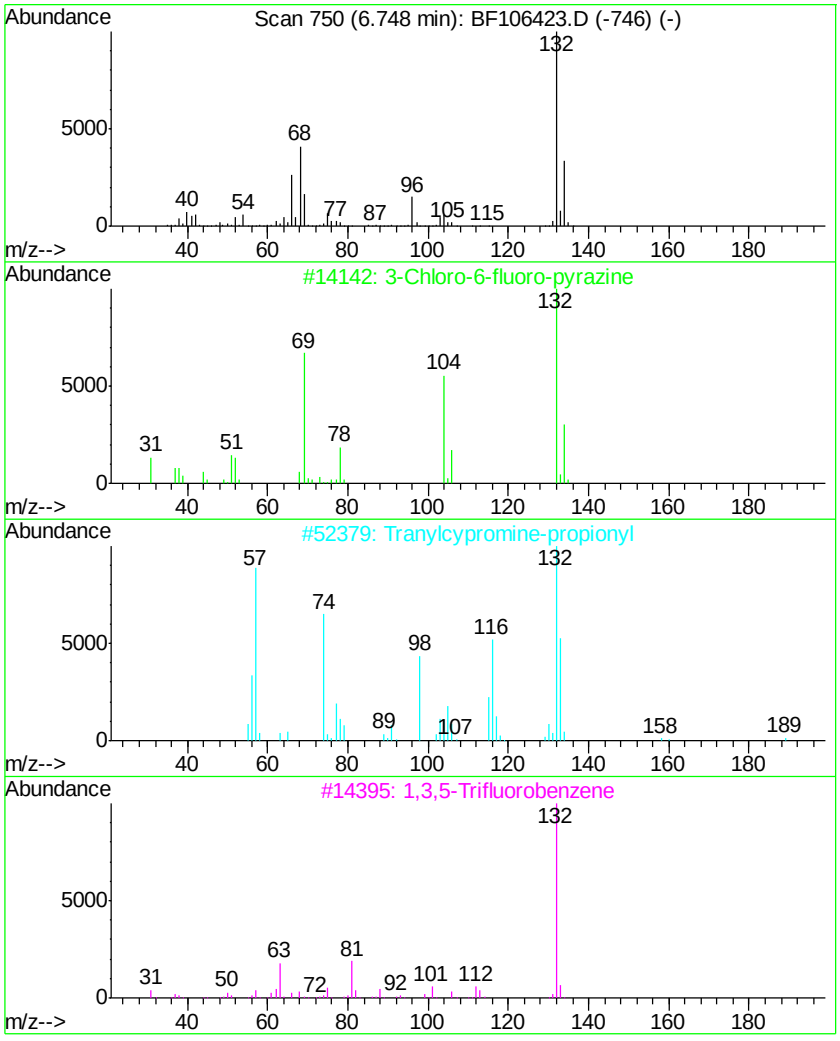
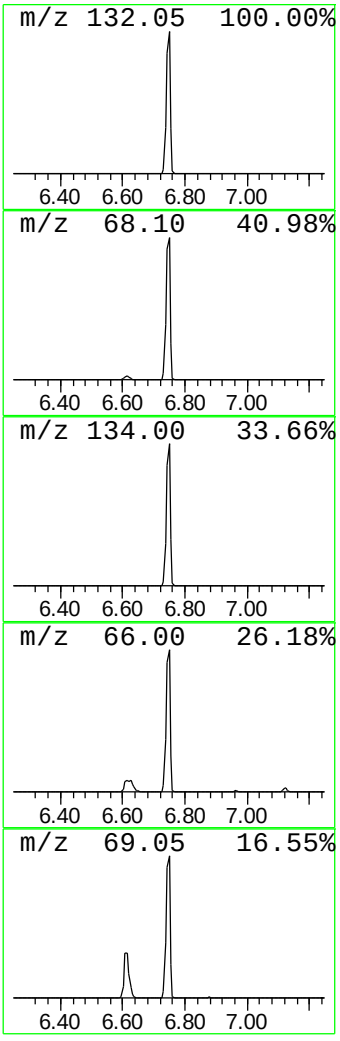
Peak Number 1 unknown6.75 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	59.56 ng	2747940	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	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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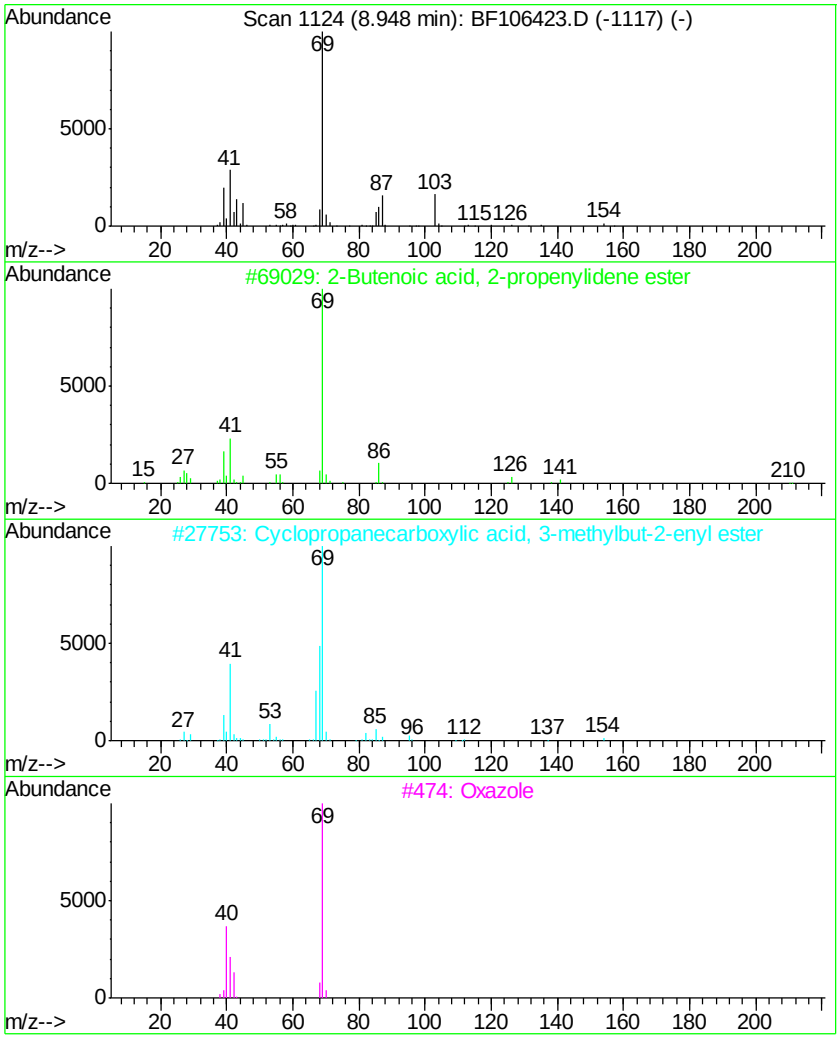
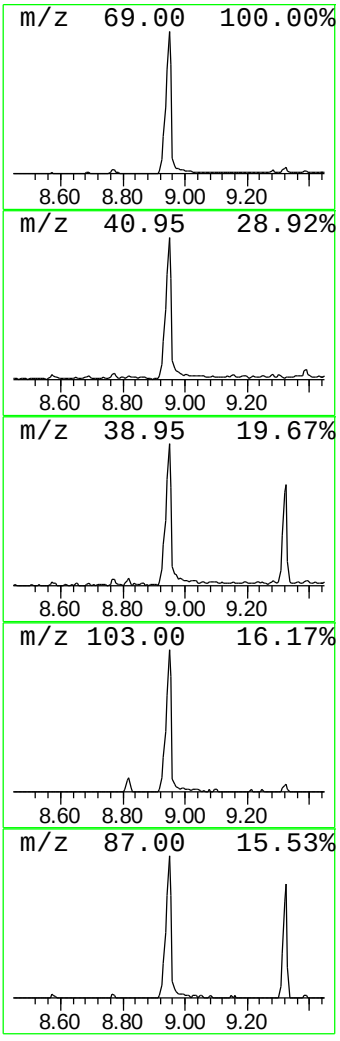
Peak Number 3 unknown8.95 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	8.63 ng	512180	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	38
2	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	33
3	Oxazole	69	C3H3NO	000288-42-6	9
4	1,6-Hexanediamine	116	C6H16N2	000124-09-4	9
5	meso-5,6-Decanediol	174	C10H22O2	003266-25-9	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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
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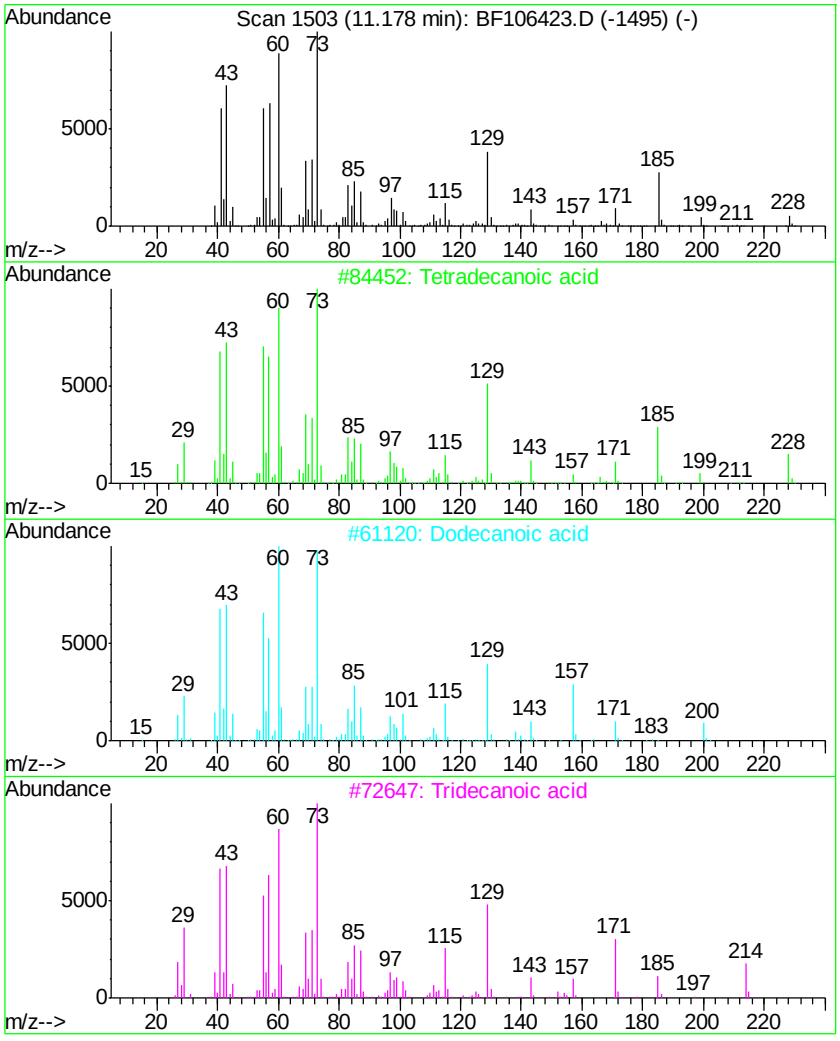
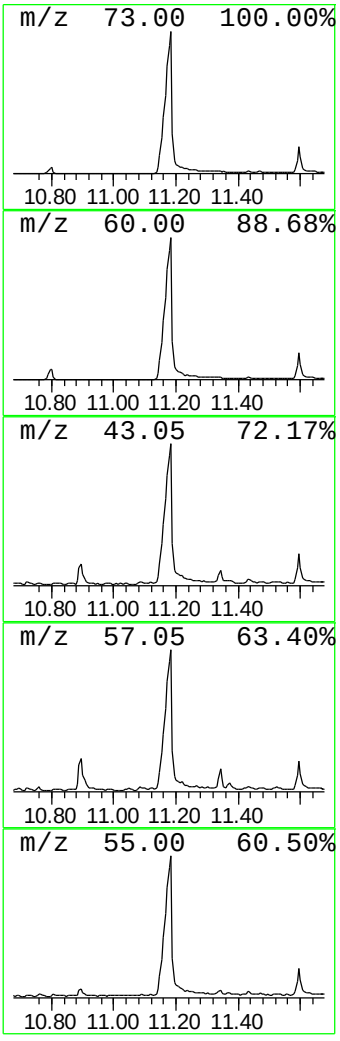
Peak Number 4 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	74.80 ng	4677010	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	Dodecanoic acid	200	C12H24O2	000143-07-7	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Library Search Compound Report

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Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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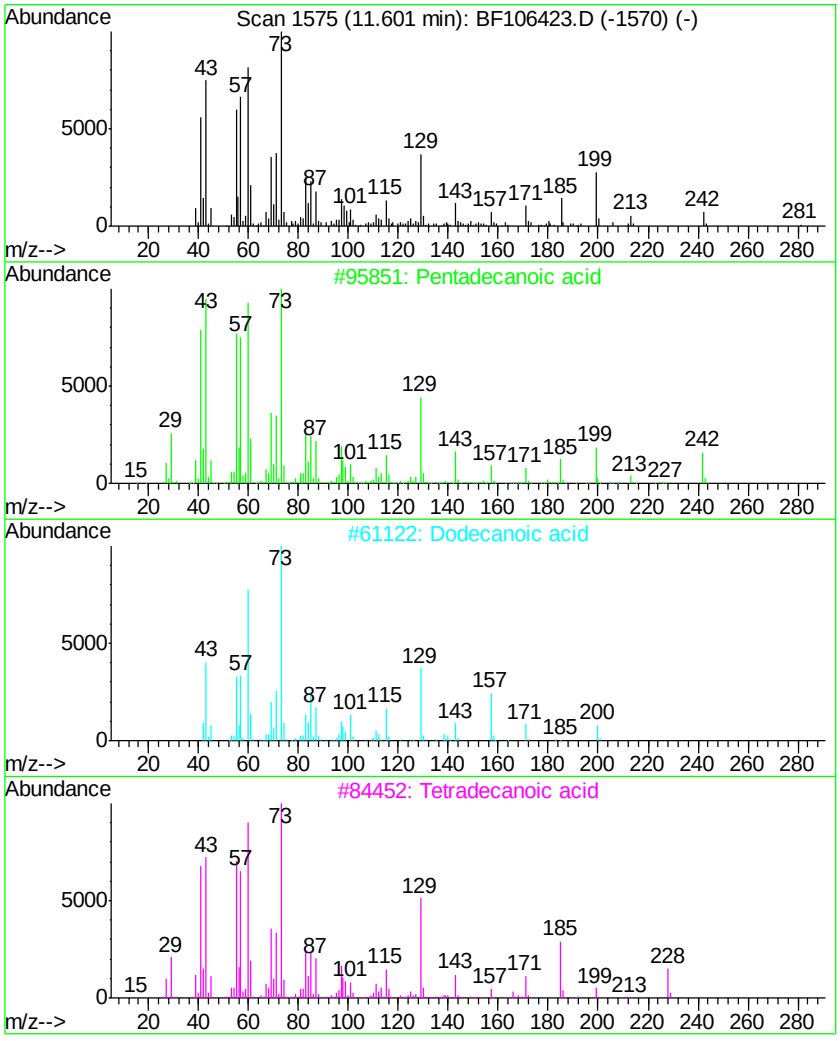
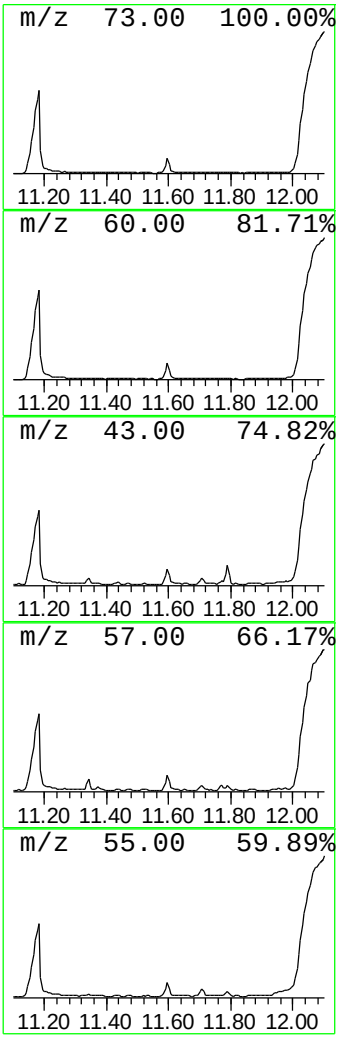
Peak Number 5 Pentadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	8.37 ng	523099	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	11





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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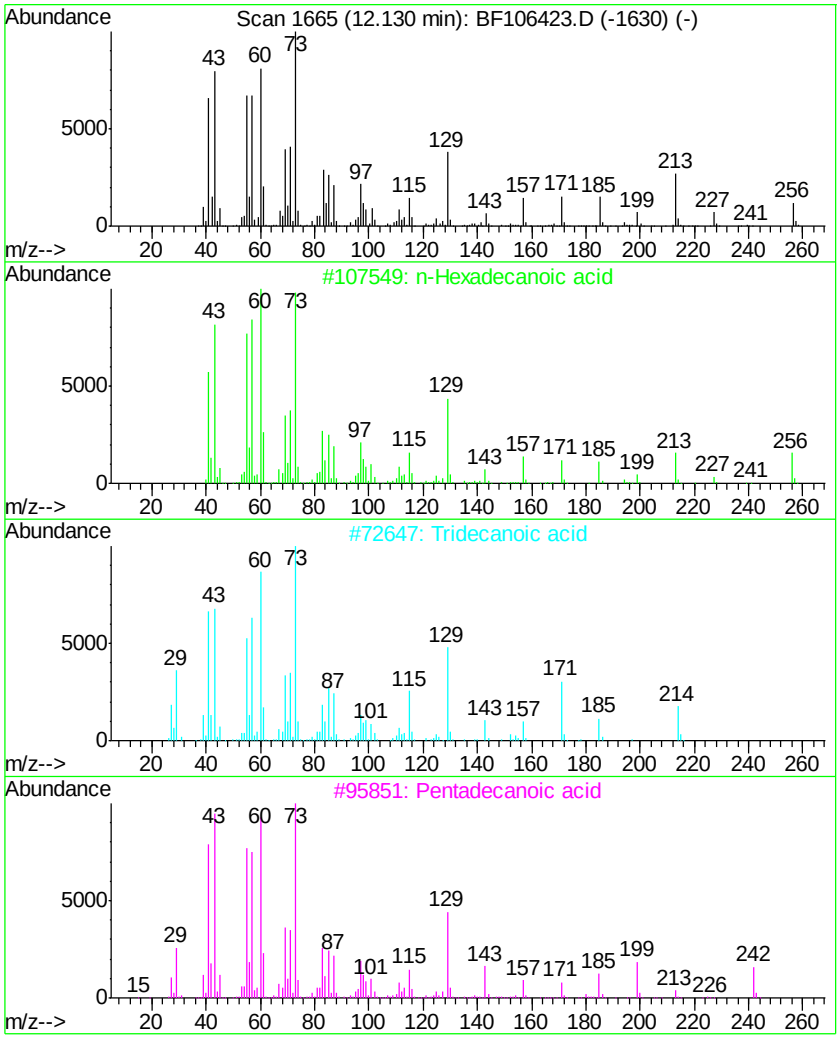
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

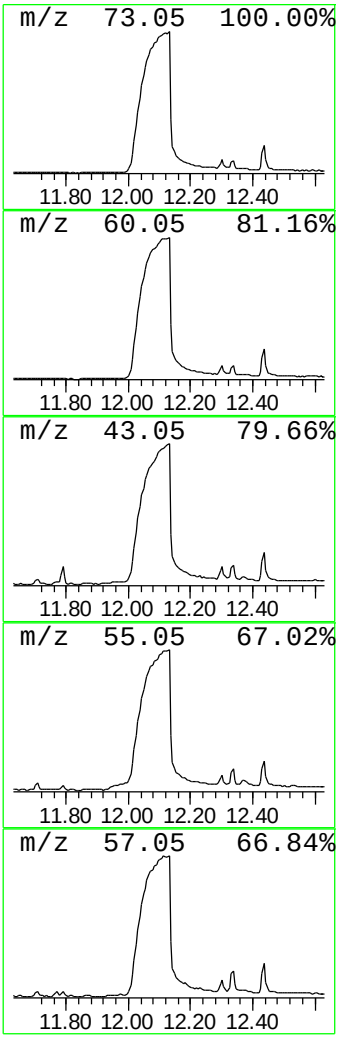
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	562.61 ng	35179300	Phenanthrene-d10	11.50

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Library Search Compound Report

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Data File : BF106423.D
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Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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

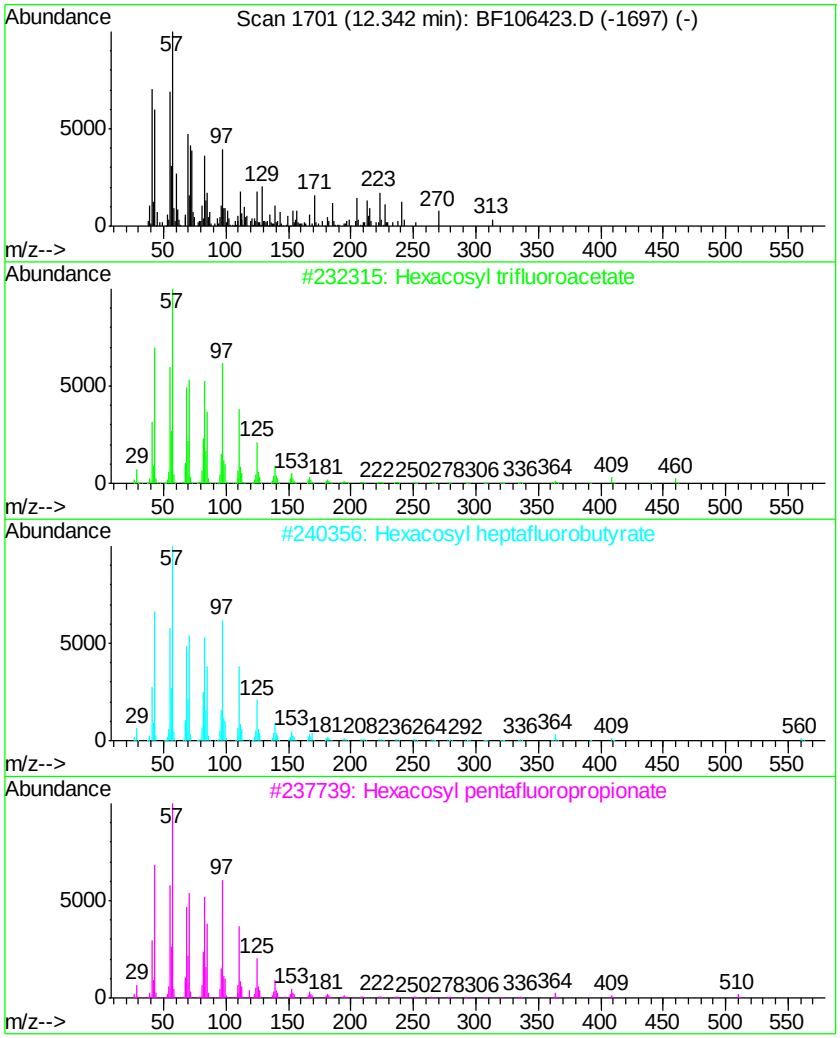
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

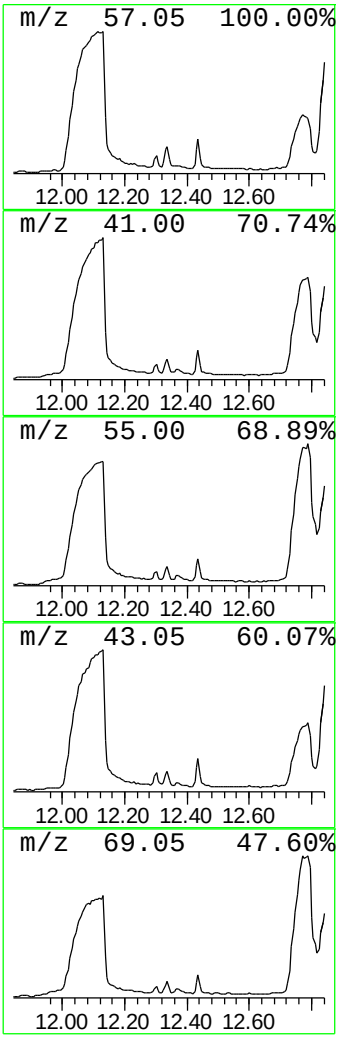
****

Peak Number 7 unknown12.34 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	7.61 ng	476087	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	49
2	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	46
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	46
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	46
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
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Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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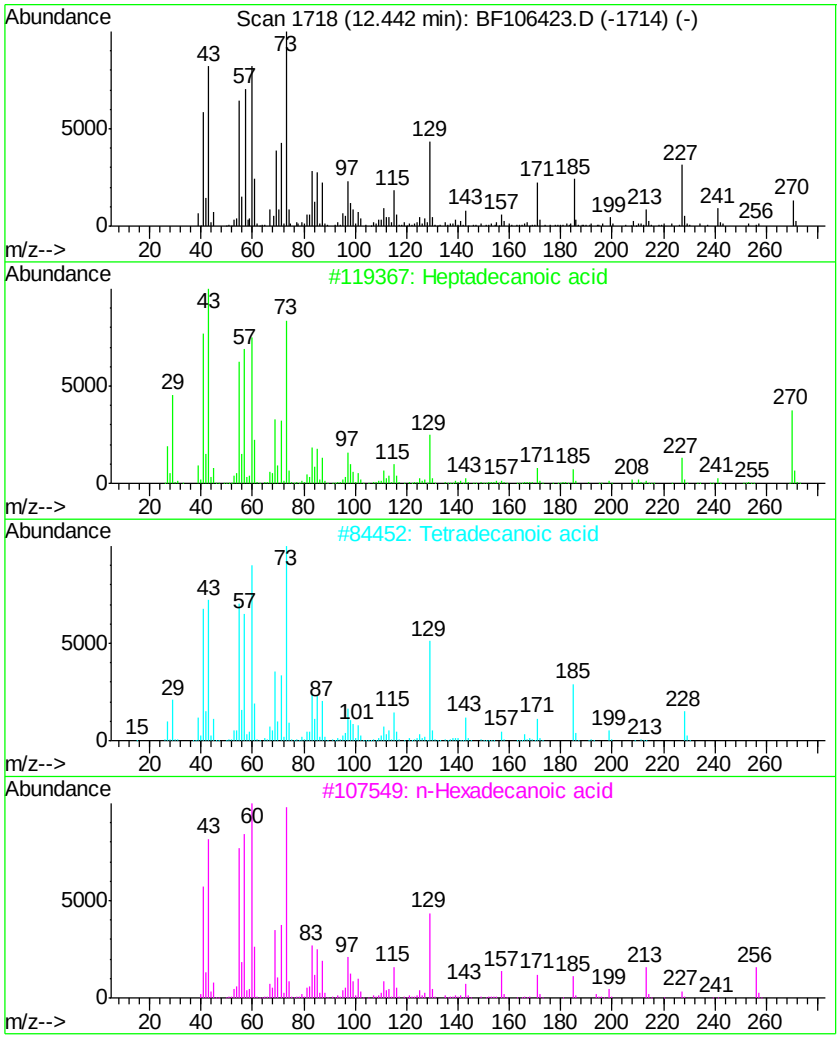
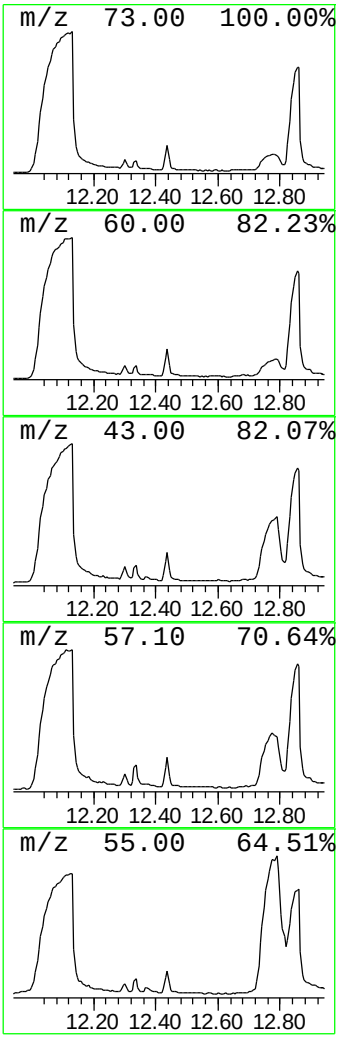
Peak Number 8 Heptadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	15.25 ng	953479	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Sample : J3447-01
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

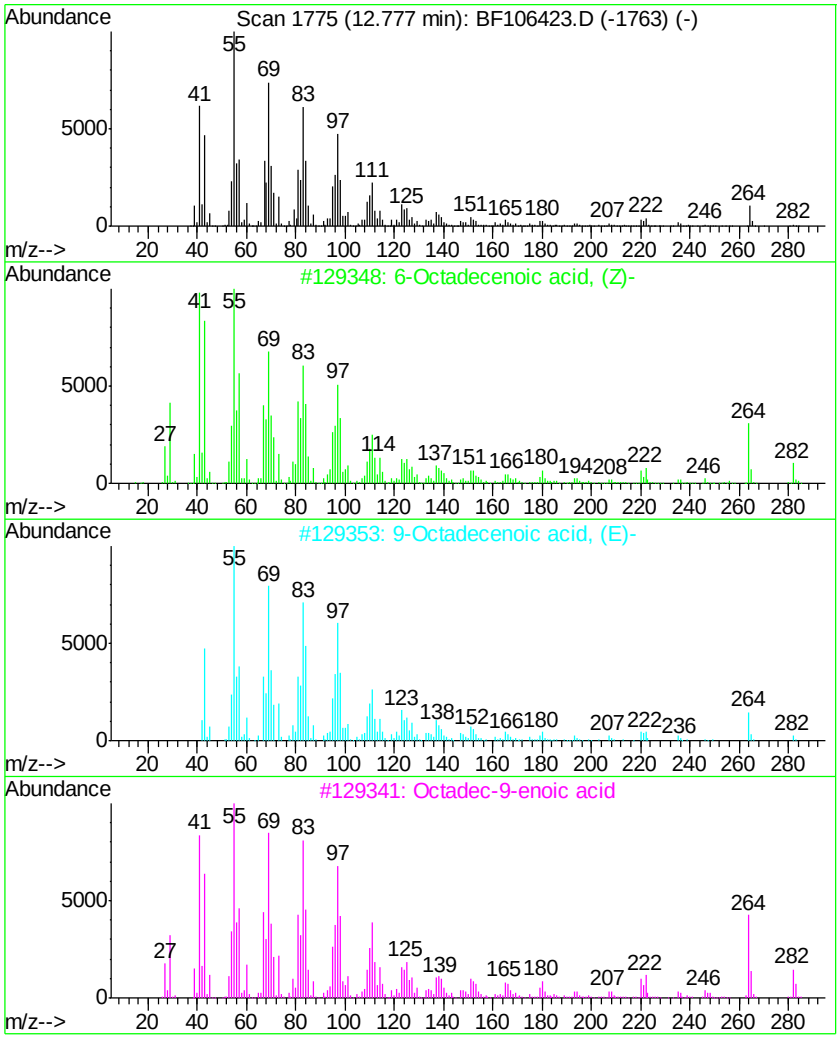
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

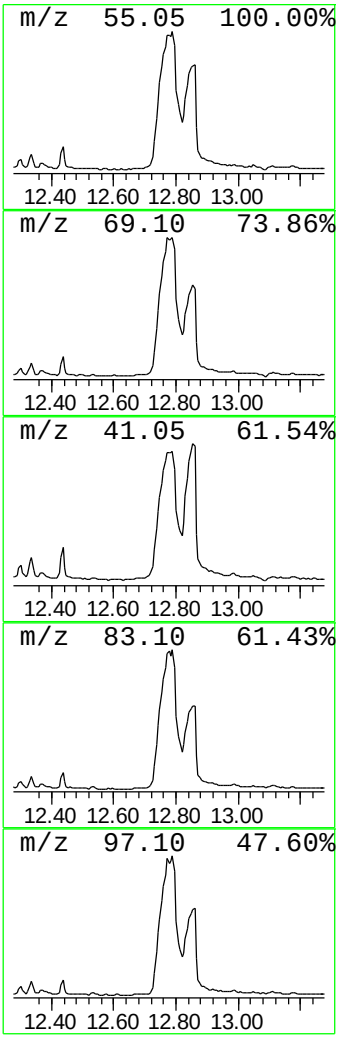
****

Peak Number 9 6-Octadecenoic acid, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	167.41 ng	10467900	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	98
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94
3	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	91
4	Oleic Acid	282	C18H34O2	000112-80-1	91
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	86





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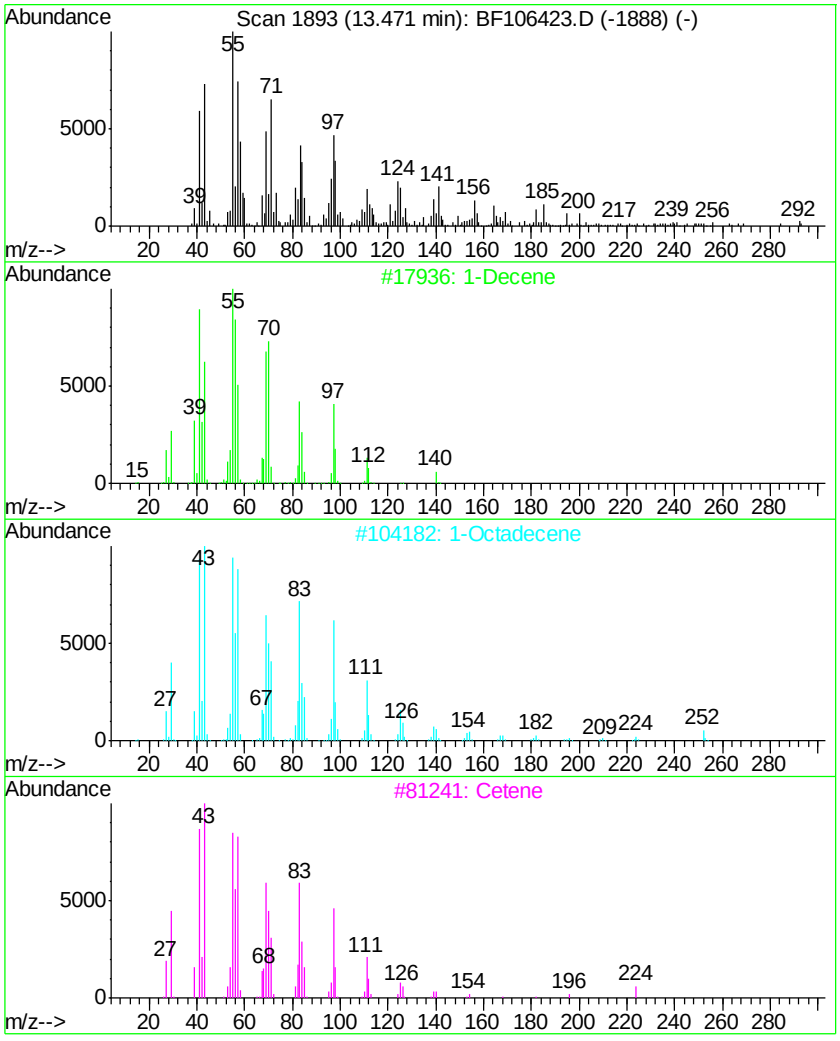
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

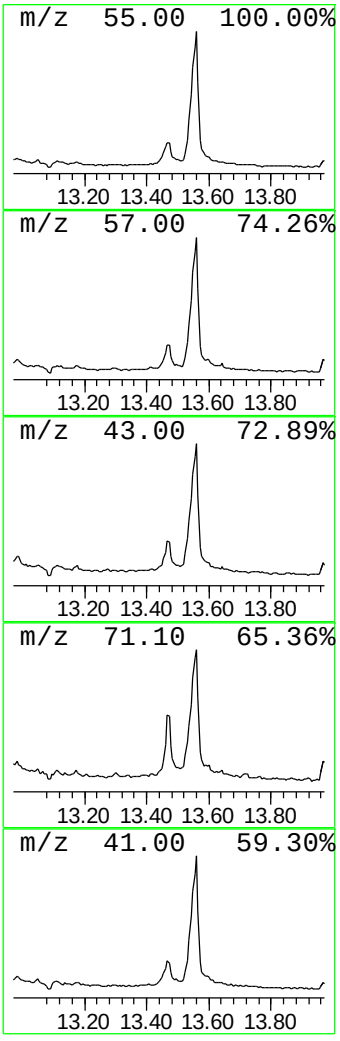
****

Peak Number 11 unknown13.47 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	11.18 ng	587873	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene	140	C10H20	000872-05-9	49
2	1-Octadecene	252	C18H36	000112-88-9	49
3	Cetene	224	C16H32	000629-73-2	49
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	46
5	Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	46





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Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
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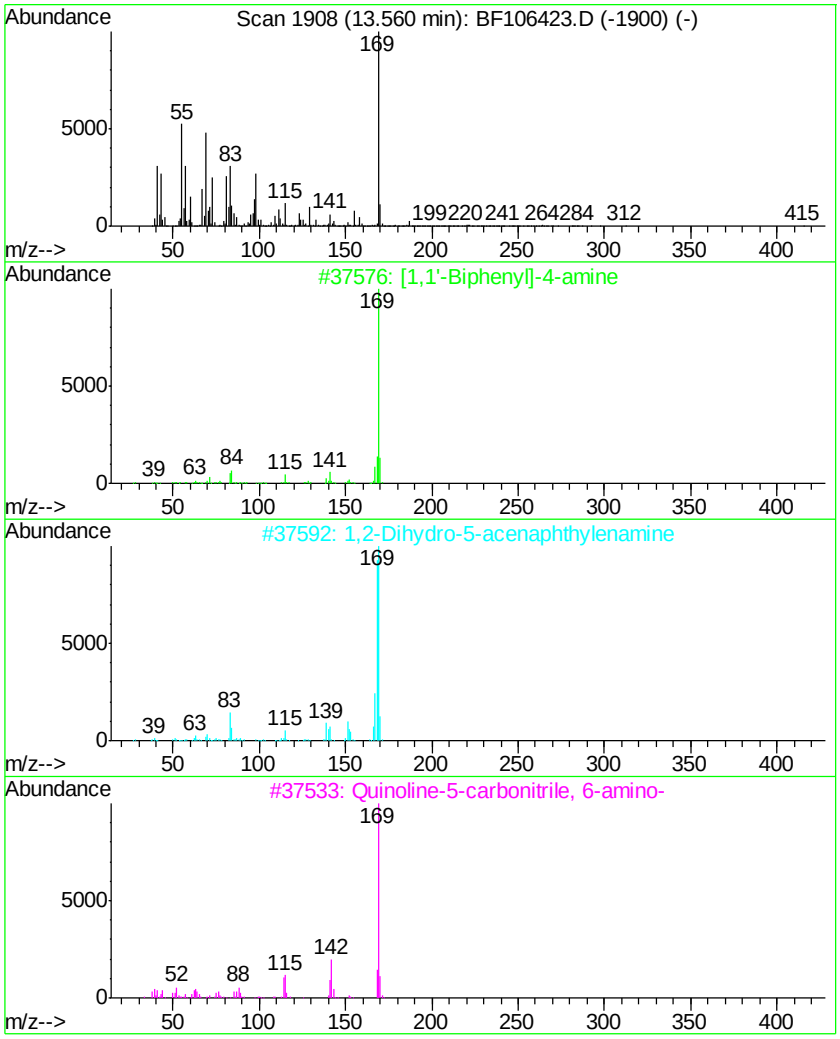
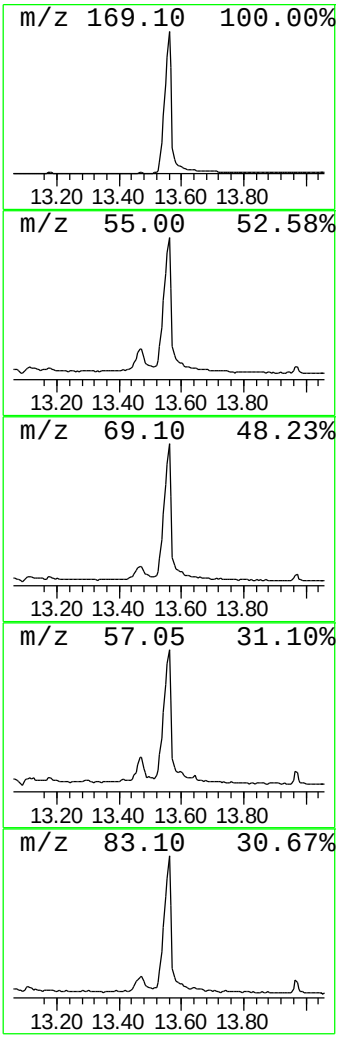
Peak Number 12 unknown13.56 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	94.02 ng	4945840	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	43
2	1,2-Dihydro-5-acenaphthylenamine	169	C12H11N	004657-93-6	38
3	Quinoline-5-carbonitrile, 6-amino-	169	C10H7N3	1000317-01-9	27
4	Phenol, 4-methoxy-2-nitro-	169	C7H7NO4	001568-70-3	27
5	10-Undecenoyl chloride	202	C11H19ClO	038460-95-6	20





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Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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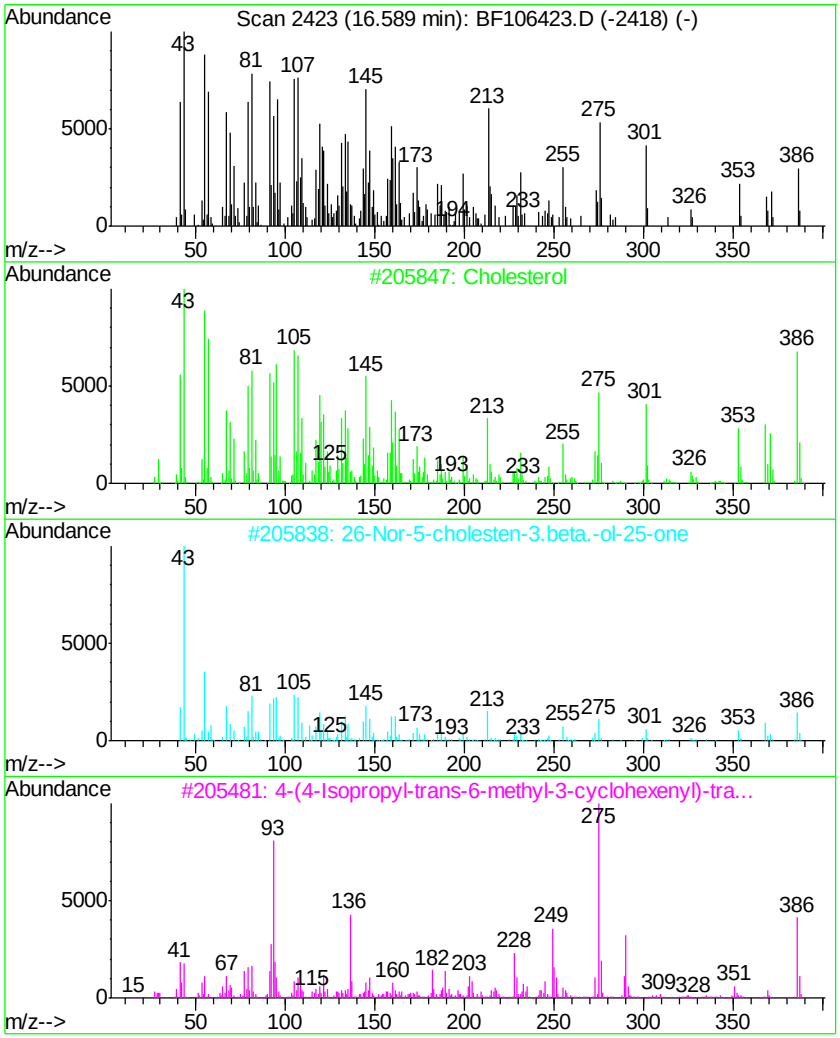
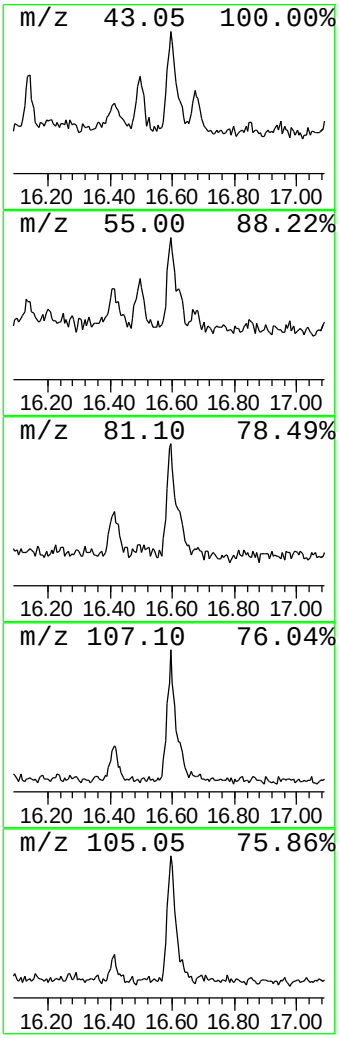
Peak Number 13 Cholesterol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	10.88 ng	559912	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	4-(4-Isopropyl-trans-6-methyl-3-...	386	C20H26N4O4	1000243-17-3	45
4	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	44
5	Cholesta-3,5-diene	368	C27H44	000747-90-0	41





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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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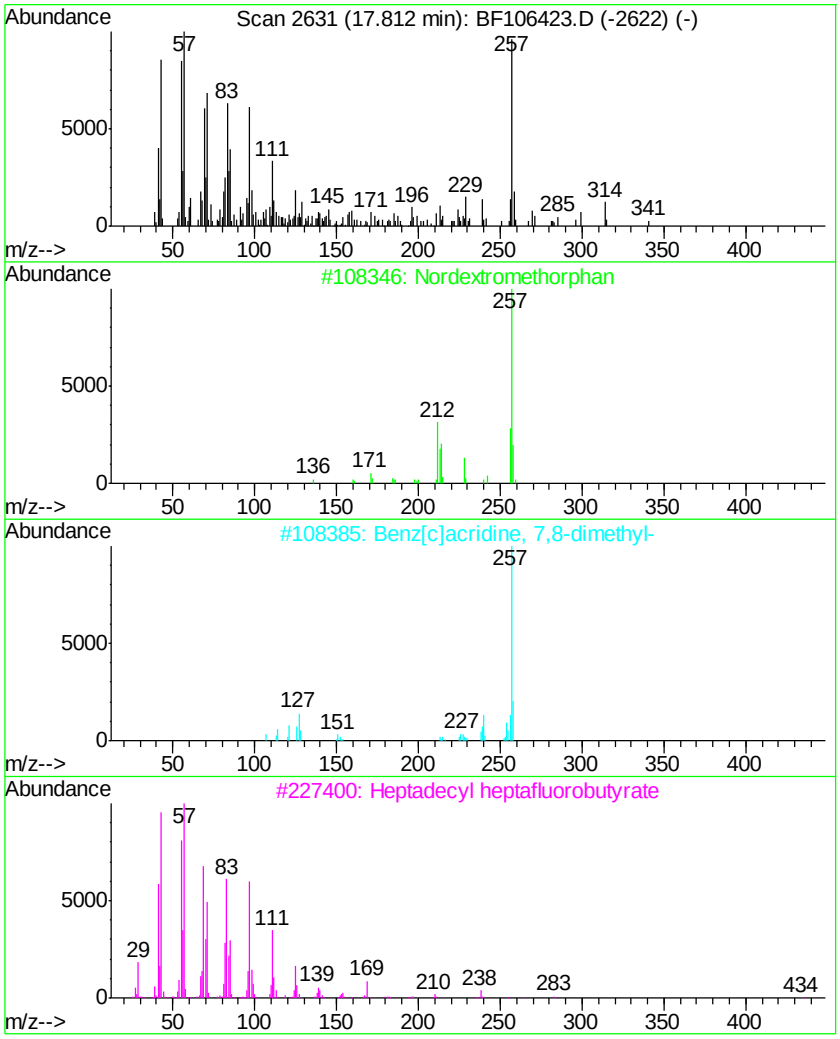
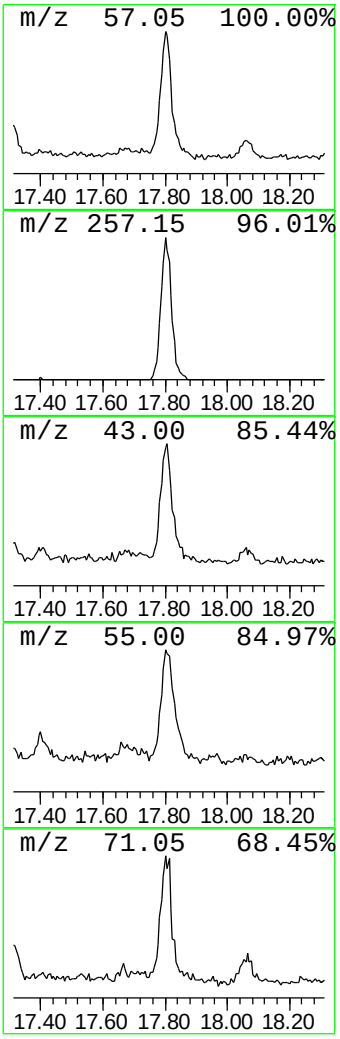
Peak Number 14 Nordextromethorphan Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	12.92 ng	665056	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nordextromethorphan	257	C17H23NO	051195-74-5	87
2	Benz[c]acridine, 7,8-dimethyl-	257	C19H15N	003518-01-2	62
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	60
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	60
5	Chloroacetic acid, 4-hexadecyl e...	318	C18H35ClO2	1000282-93-2	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061318\
Data File : BF106423.D
Acq On : 14 Jun 2018 6:10
Operator : JU/SJ
Sample : J3447-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.75	6.75	59.6	ng	2747940	1	6.97	922685	20.0
unknown8.95	8.95	8.6	ng	512180	2	8.25	1186810	20.0
Tetradecanoic acid	11.18	74.8	ng	4677010	4	11.50	1250580	20.0
Pentadecanoic acid	11.60	8.4	ng	523099	4	11.50	1250580	20.0
n-Hexadecanoic acid	12.13	562.6	ng	35179300	4	11.50	1250580	20.0
unknown12.34	12.34	7.6	ng	476087	4	11.50	1250580	20.0
Heptadecanoic acid	12.44	15.3	ng	953479	4	11.50	1250580	20.0
6-Octadecenoic ac...	12.78	167.4	ng	10467900	4	11.50	1250580	20.0
unknown13.47	13.47	11.2	ng	587873	5	14.15	1052080	20.0
unknown13.56	13.56	94.0	ng	4945840	5	14.15	1052080	20.0
Cholesterol	16.59	10.9	ng	559912	6	15.68	1029560	20.0
Nordextromethorphan	17.81	12.9	ng	665056	6	15.68	1029560	20.0