LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102859.D
Acq On : 8 Feb 2018 16:39
Operator : SJ/JU
Sample : J1470-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

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-BF020318.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	2.163	7	13	20	rVB	417218	533337	2.07%	0.679%
2	5.504	576	581	584	rBV	4172246	3961618	15.35%	5.043%
3	6.510	747	752	758	rBV	3552827	3881701	15.04%	4.942%
4	6.657	772	777	780	rBV	3972021	3780625	14.65%	4.813%
5	6.887	812	816	819	rBV	1466789	1207984	4.68%	1.538%
6	7.040	838	842	846	rBV	2938008	2759330	10.69%	3.513%
7	7.445	906	911	914	rBV	2579688	2458821	9.53%	3.130%
8	7.928	988	993	1000	rBV	244977	280734	1.09%	0.357%
9	8.169	1030	1034	1037	rBV	1871281	1511598	5.86%	1.924%
10	9.239	1212	1216	1220	rBV	3273635	3007362	11.65%	3.828%
11	9.634	1279	1283	1286	rBV	306135	268520	1.04%	0.342%
12	9.922	1329	1332	1336	rBV	1455417	1367292	5.30%	1.741%
13	10.333	1398	1402	1407	rVB2	740494	719218	2.79%	0.916%
14	10.710	1460	1466	1476	rBV	1587101	1649421	6.39%	2.100%
15	11.410	1582	1585	1588	rBV	1094063	1041419	4.03%	1.326%
16	12.992	1850	1854	1858	rBV	1866894	1758808	6.81%	2.239%
17	13.880	2002	2005	2013	rBV	386597	381812	1.48%	0.486%
18	14.051	2030	2034	2038	rBV	1054361	983332	3.81%	1.252%
19	15.539	2282	2287	2294	rBV	662297	914592	3.54%	1.164%
20	17.633	2639	2643	2651	rVB5	138658	325670	1.26%	0.415%
21	17.868	2677	2683	2693	rVB3	342840	849901	3.29%	1.082%
22	18.039	2705	2712	2719	rBV3	260516	723683	2.80%	0.921%
23	18.127	2720	2727	2736	rVV4	399507	1179146	4.57%	1.501%
24	18.245	2737	2747	2756	rVV5	1438271	5015493	19.43%	6.385%
25	18.327	2756	2761	2776	rVB2	599630	1629993	6.32%	2.075%
26	18.504	2779	2791	2806	rVB3	1713738	6817721	26.41%	8.679%
27	18.768	2825	2836	2843	rBV	1266004	3732812	14.46%	4.752%
28	19.262	2897	2920	2932	rBV6	4357135	25810477	100.00%	32.858%

Sum of corrected areas: 78552420

LSC Report - Integrated Chromatogram

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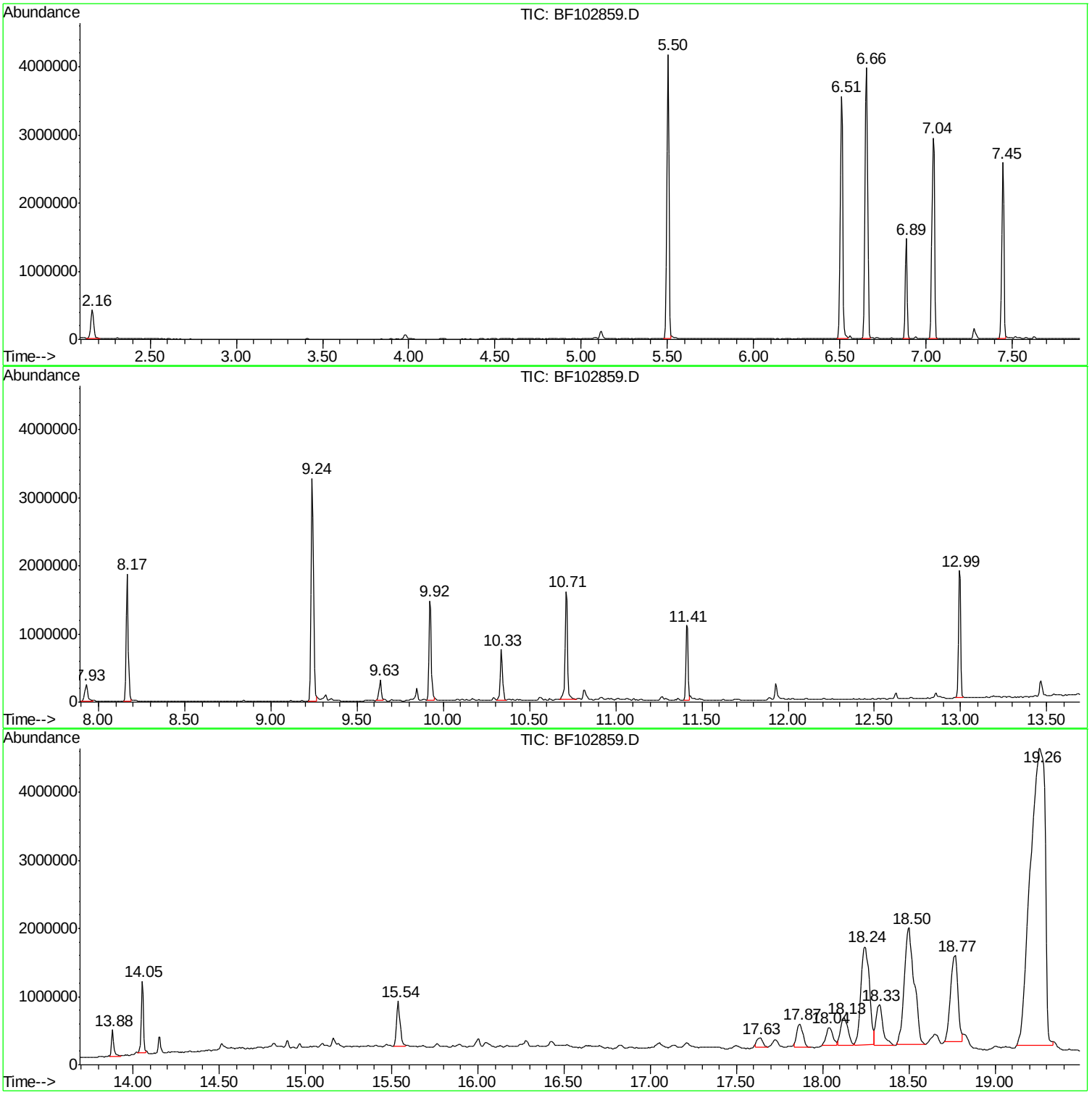
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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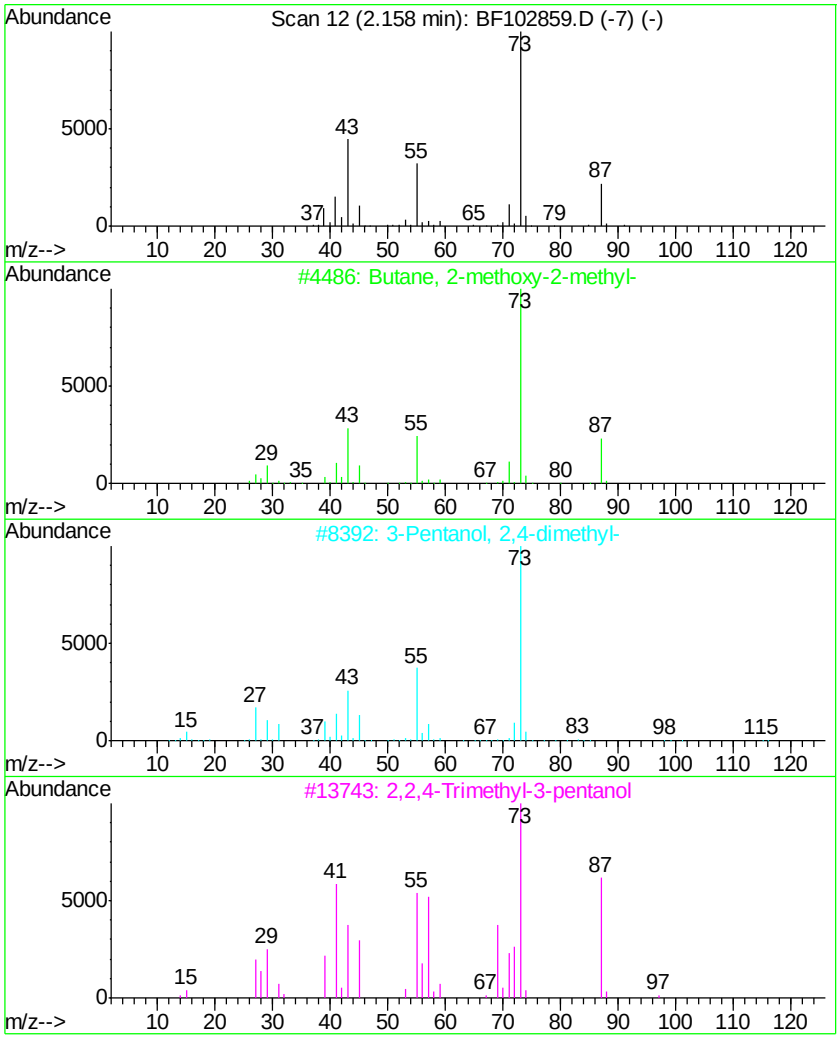
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

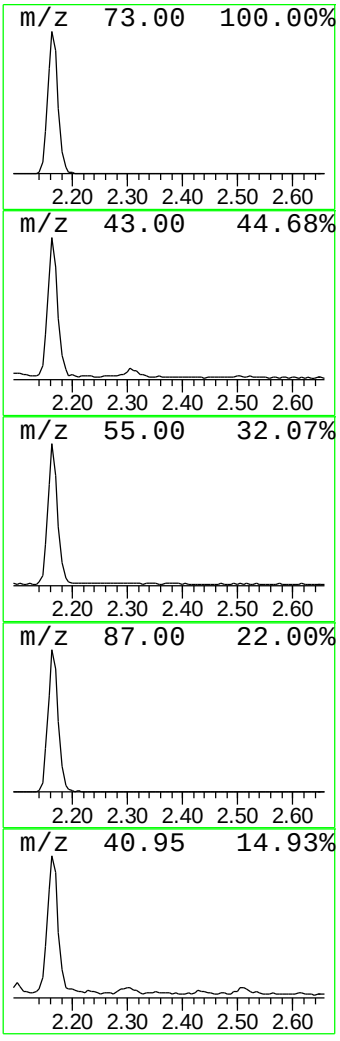
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	8.83 ng	533337	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28





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Operator : SJ/JU
Sample : J1470-03
Misc :
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Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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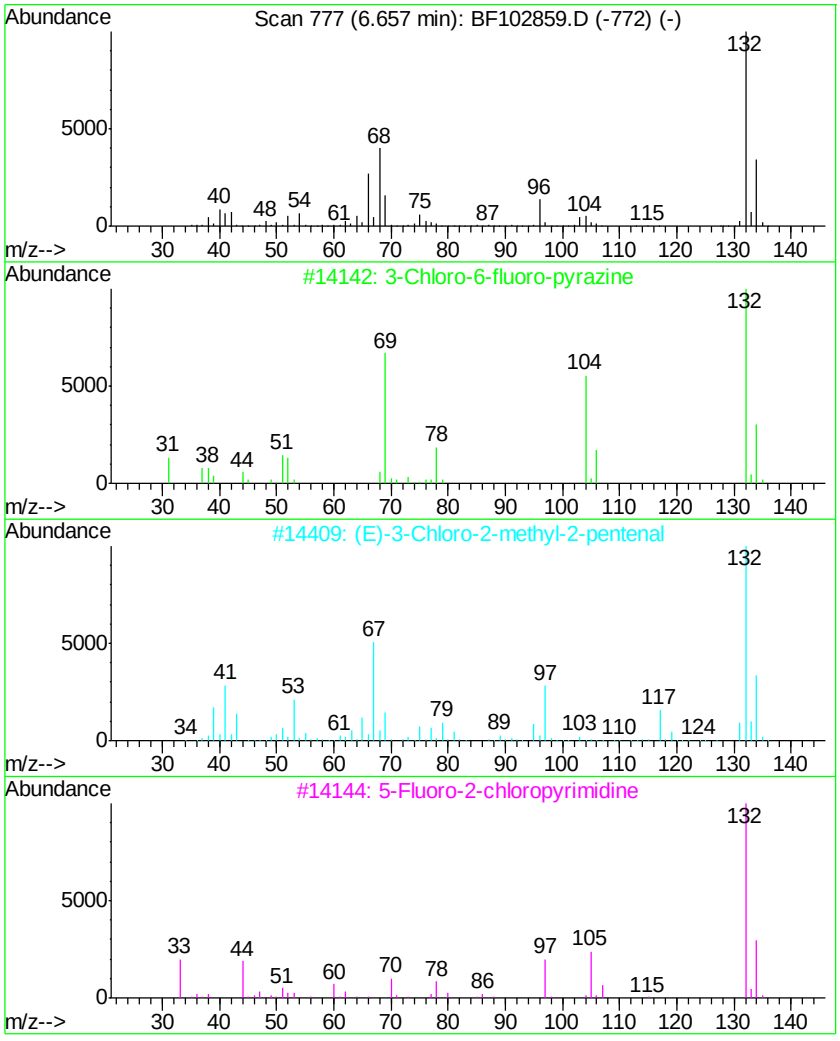
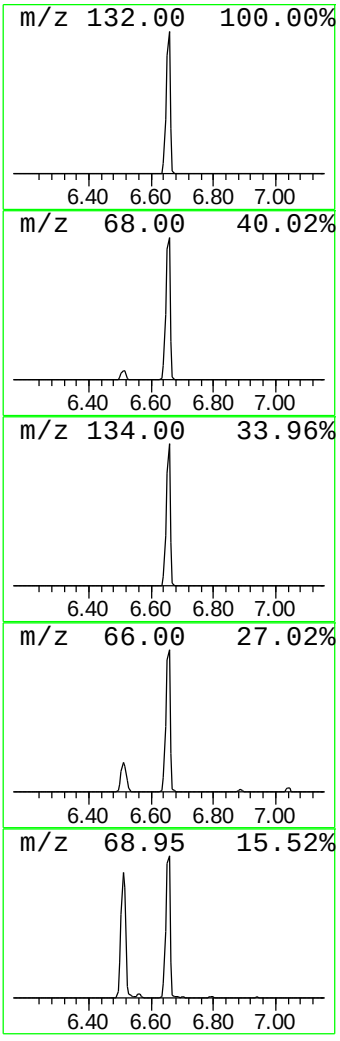
Peak Number 2 unknown6.66 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	62.59 ng	3780630	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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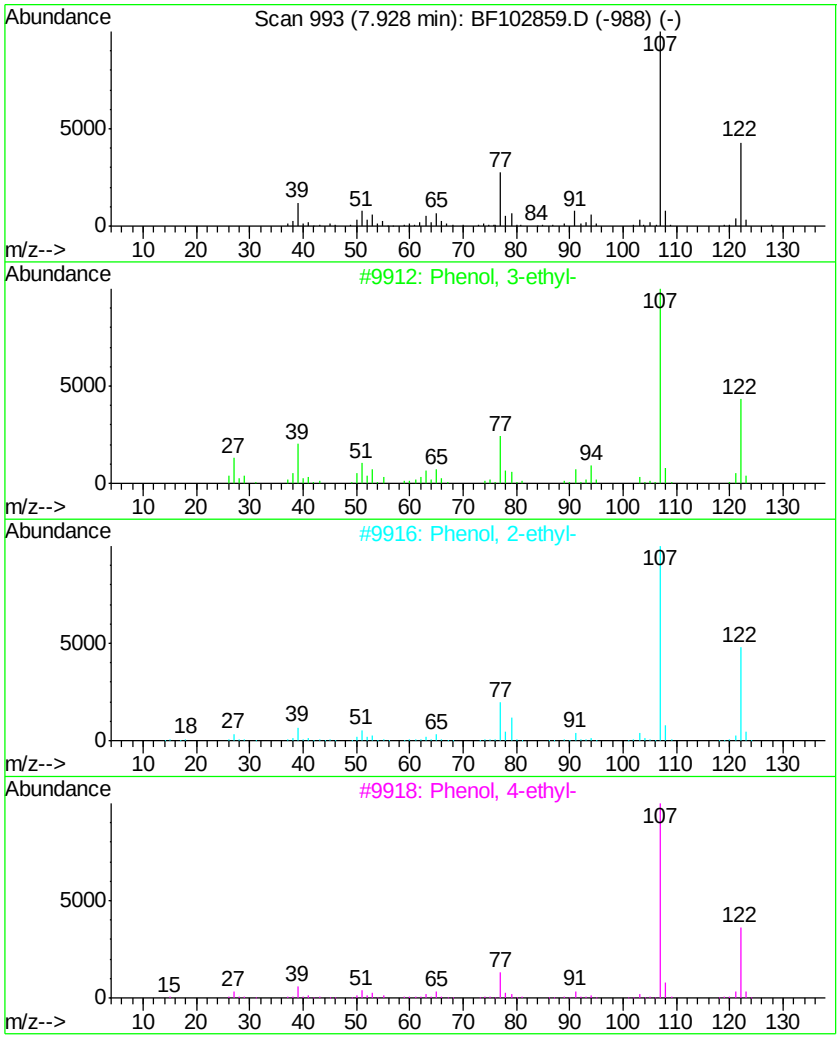
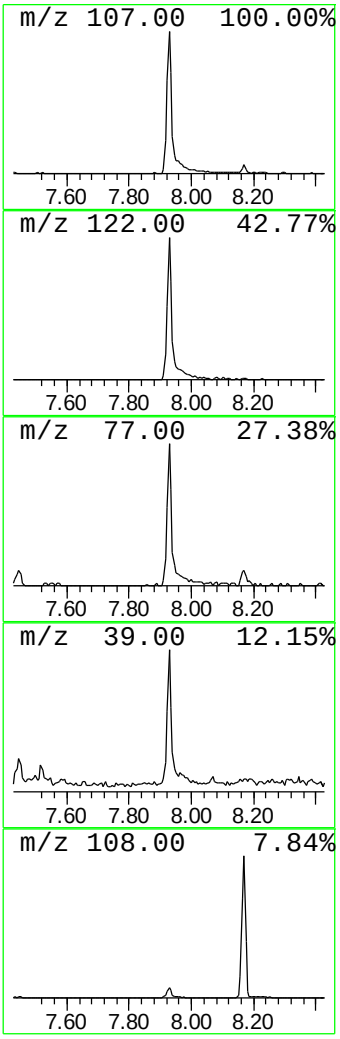
Peak Number 4 Phenol, 3-ethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	3.71 ng	280734	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	93
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	91
4	3,3-Dimethyl-6-methylenecyclohexene	122	C9H14	020185-16-4	78
5	2-Isopropylpyrazine	122	C7H10N2	029460-90-0	59





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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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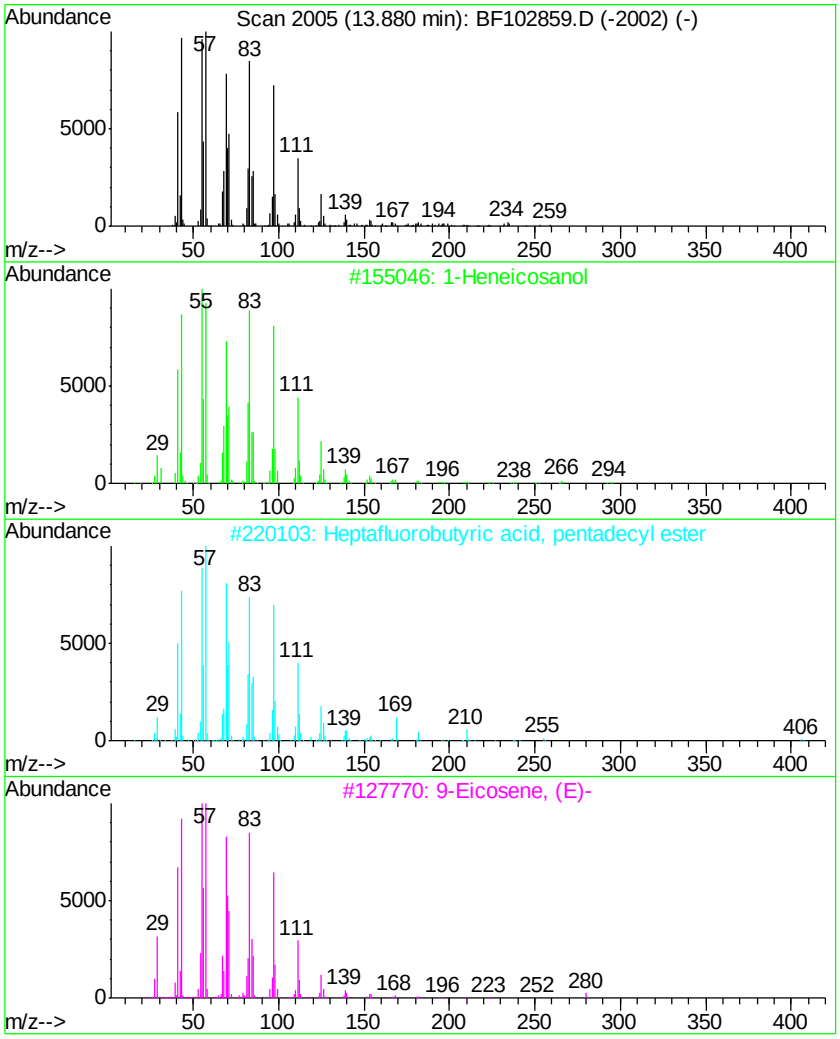
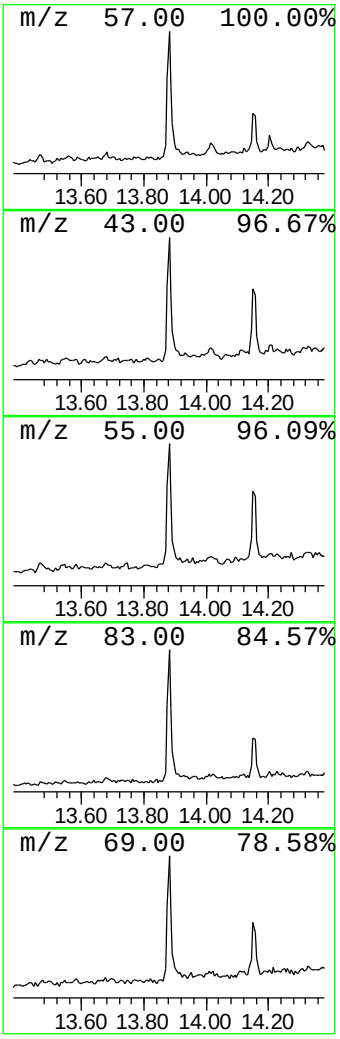
Peak Number 5 1-Heneicosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.77 ng	381812	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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Sample : J1470-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
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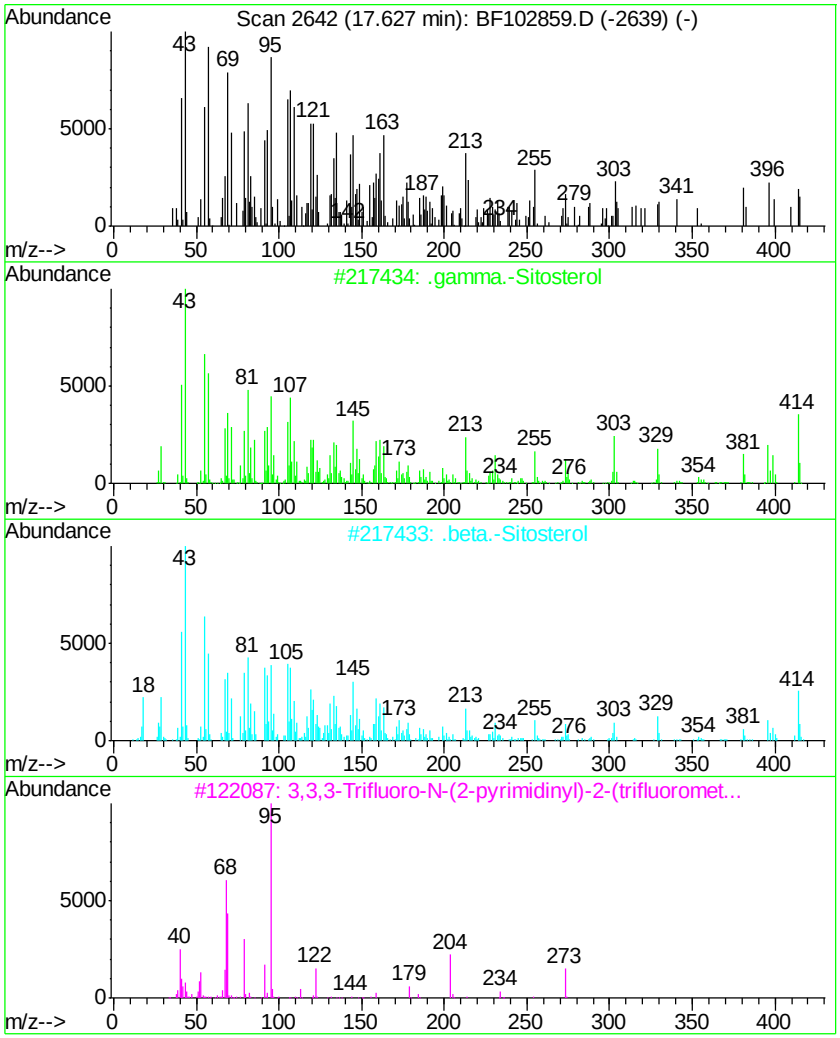
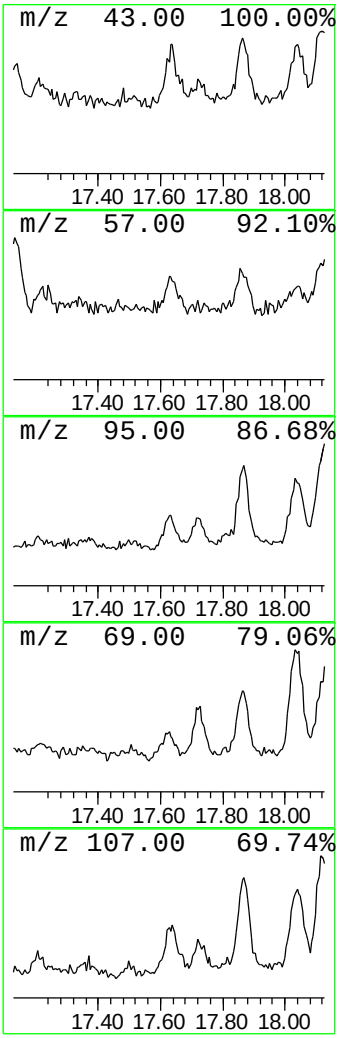
Peak Number 6 .gamma.-Sitosterol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	7.12 ng	325670	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	92
3	3,3,3-Trifluoro-N-(2-pyrimidinyl...	273	C8H5F6N3O	340137-97-5	14
4	N-Trichloroacetylimidazole	212	C5H3Cl3N2O	056739-51-6	12
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	11





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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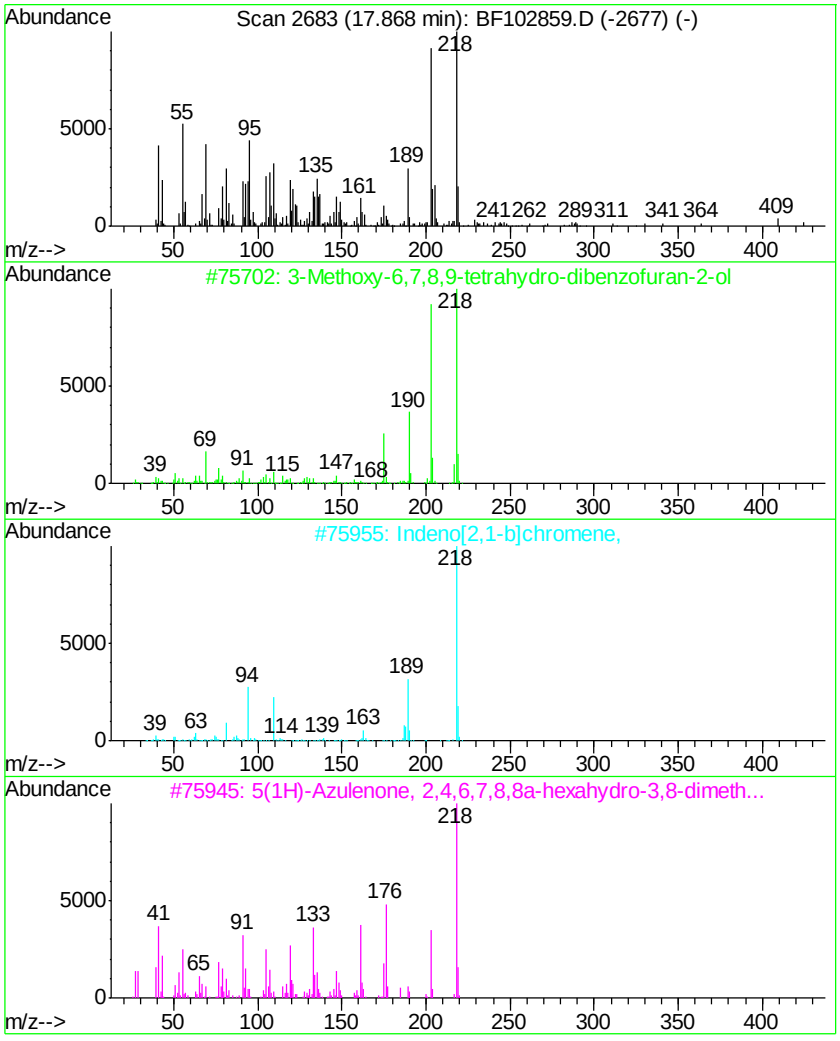
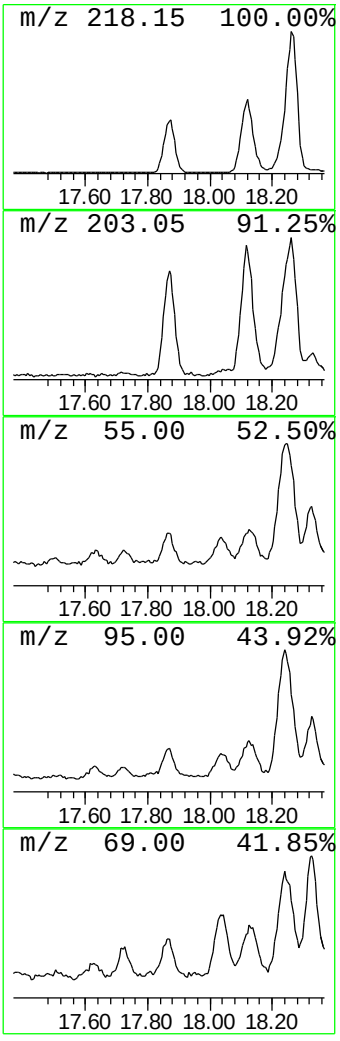
Peak Number 7 unknown17.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	18.59 ng	849901	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	49
2	Indeno[2,1-b]chromene,	218	C16H10O	000243-24-3	38
3	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	38
4	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	38
5	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	38





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TIC Library : C:\DATABASE\NIST11.L
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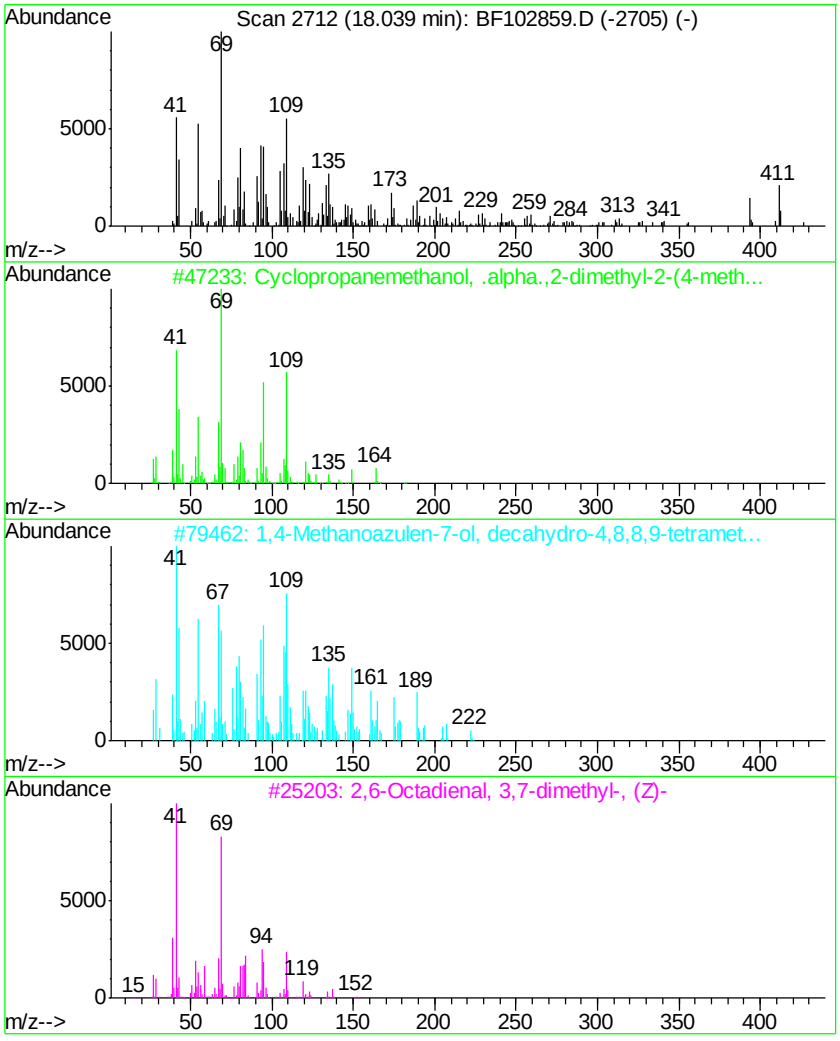
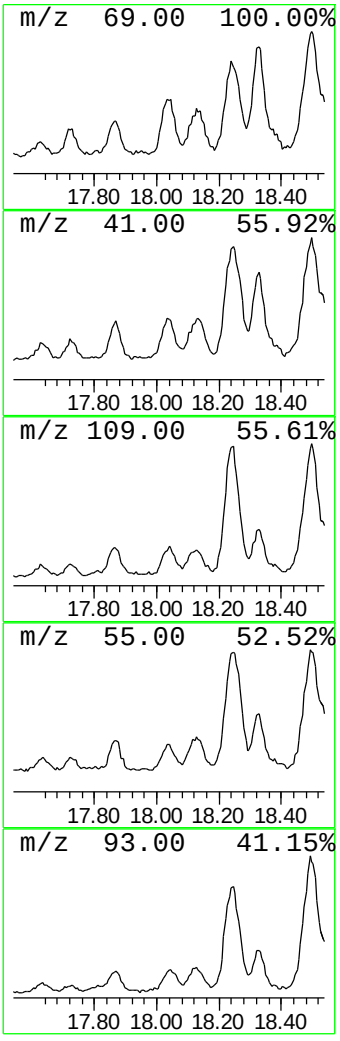
Peak Number 8 unknown18.04 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	15.83 ng	723683	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	47
2	1,4-Methanoazulen-7-ol, decahydr...	222	C15H26O	018319-27-2	38
3	2,6-Octadienal, 3,7-dimethyl-, (Z)-	152	C10H16O	000106-26-3	25
4	Diethylmalonic acid, monochlorid...	332	C13H14BrClO3	1000369-83-6	14
5	Methoxy(methyl)chlorosilane	110	C2H7ClOSi	018151-27-4	14





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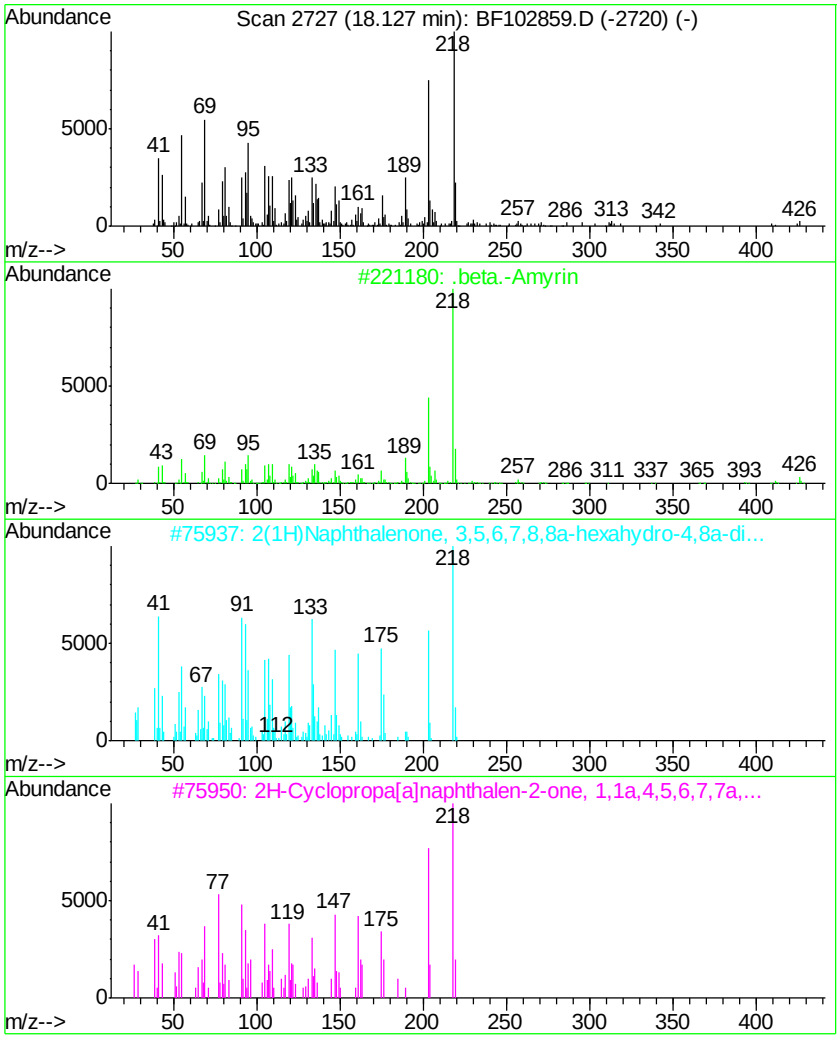
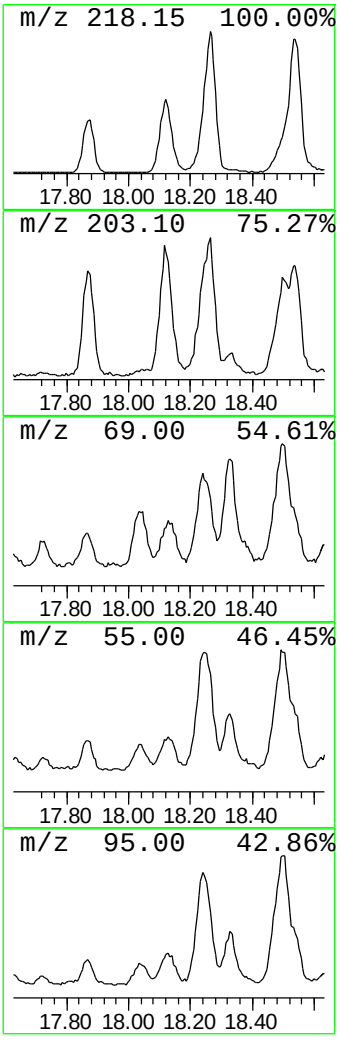
Peak Number 9 .beta.-Amyrin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	25.79 ng	1179150	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	87
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	58
3	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	52
4	.alpha.-Amyrin	426	C30H50O	000638-95-9	49
5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	46





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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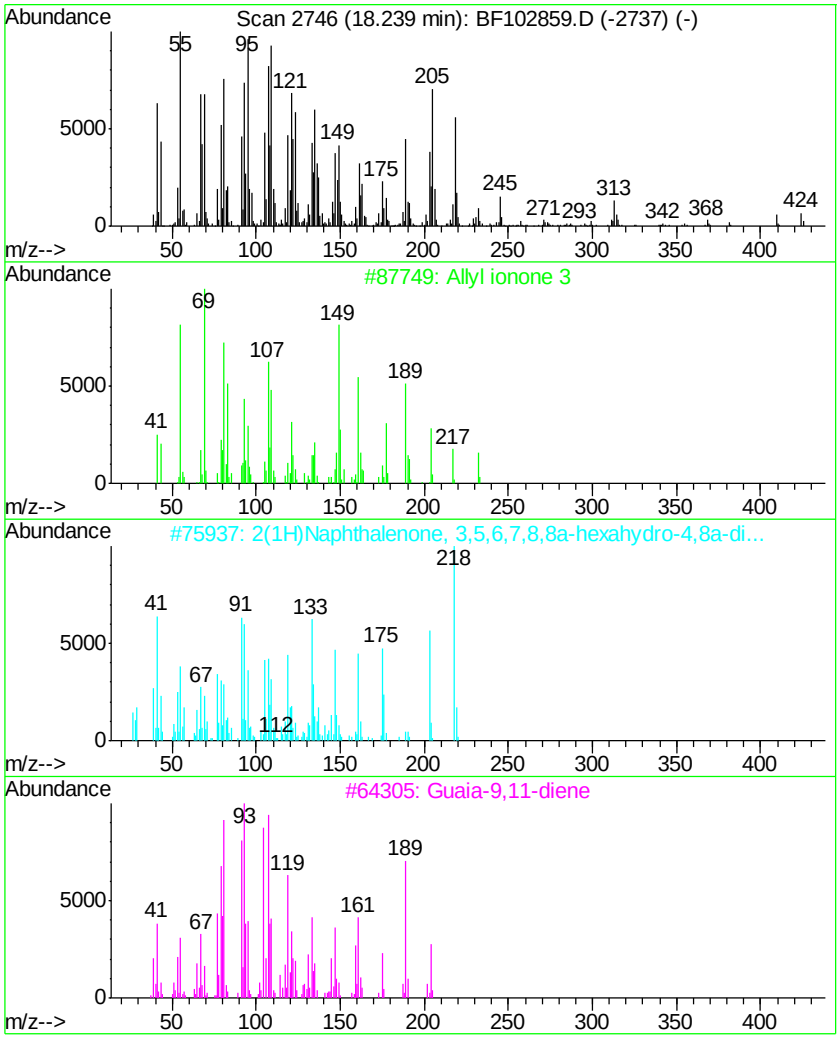
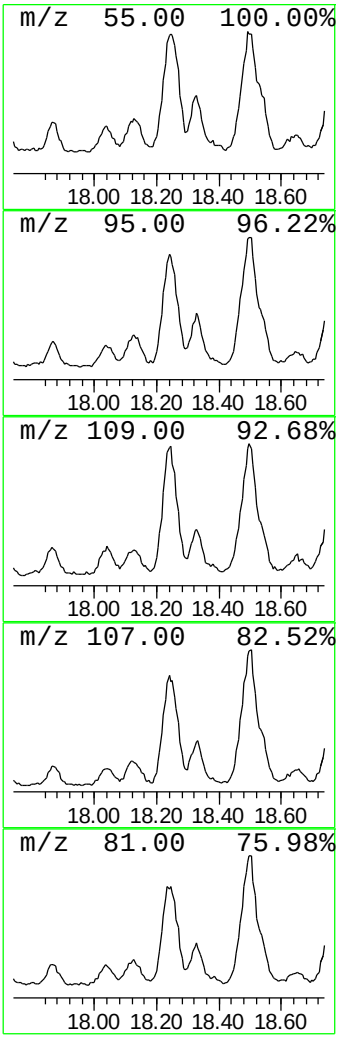
Peak Number 10 Allyl ionone 3 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	109.68 ng	5015490	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl ionone 3	232	C16H24O	1000284-92-9	53
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	52
3	Guaia-9,11-diene	204	C15H24	1000374-19-8	50
4	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	42
5	4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	38





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TIC Integration Parameters: LSCINT.P

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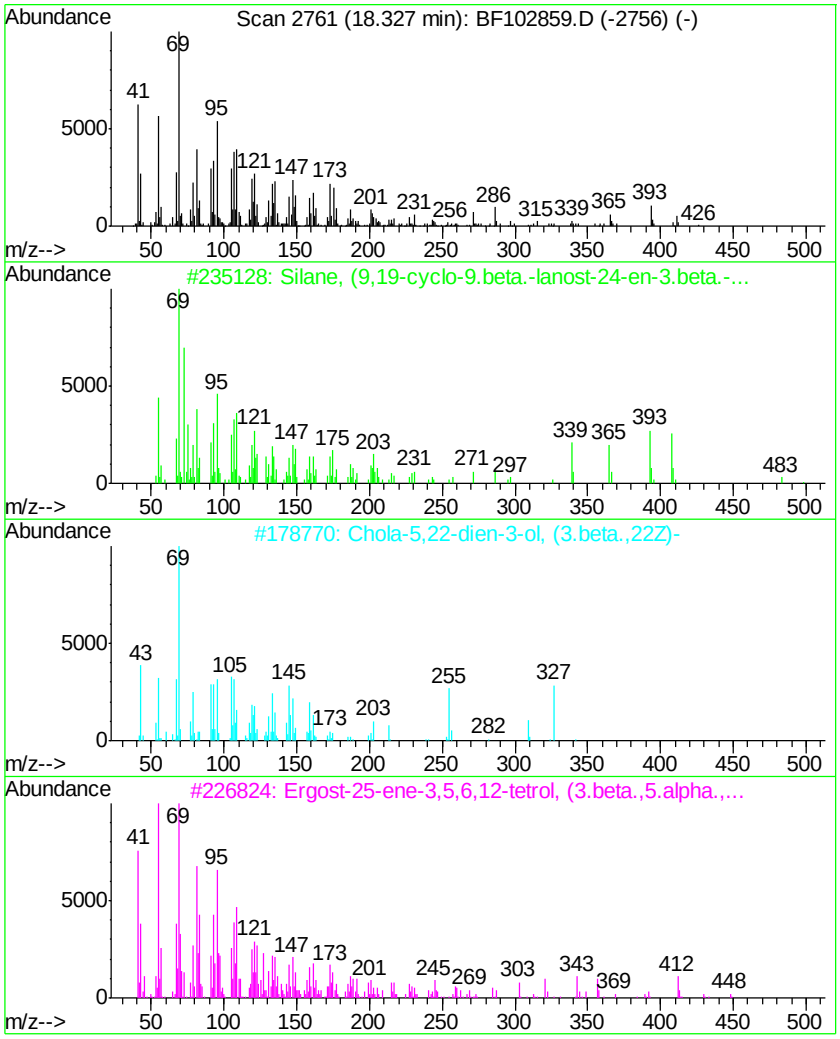
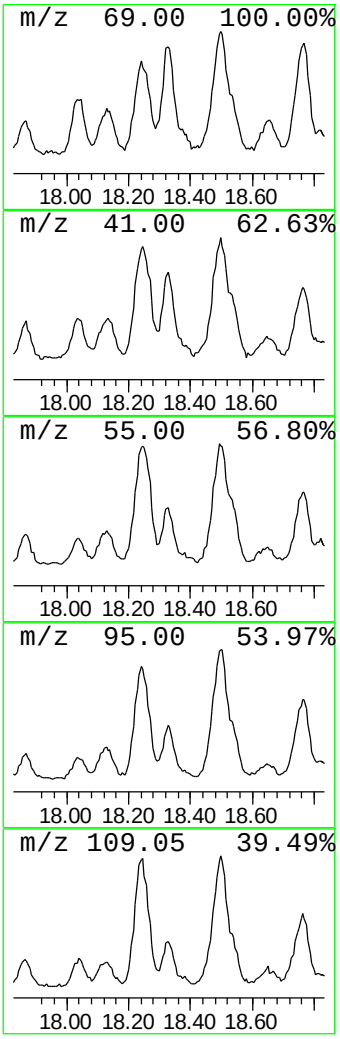
Peak Number 11 Silane, (9,19-cyclo-9.beta.... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	35.64 ng	1629990	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, (9,19-cyclo-9.beta.-lano...	498	C33H58OSi	017608-55-8	78
2	Chola-5,22-dien-3-ol, (3.beta.,2...	342	C24H38O	057597-14-5	70
3	Ergost-25-ene-3,5,6,12-tetrol, (...	448	C28H48O4	056052-97-2	42
4	Acetic acid, 1,3,7-trimethylocta...	210	C13H22O2	091418-25-6	35
5	Cyclopropanemethanol, 2-methyl-2...	168	C11H20O	098678-70-7	32





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Acq On : 8 Feb 2018 16:39
Operator : SJ/JU
Sample : J1470-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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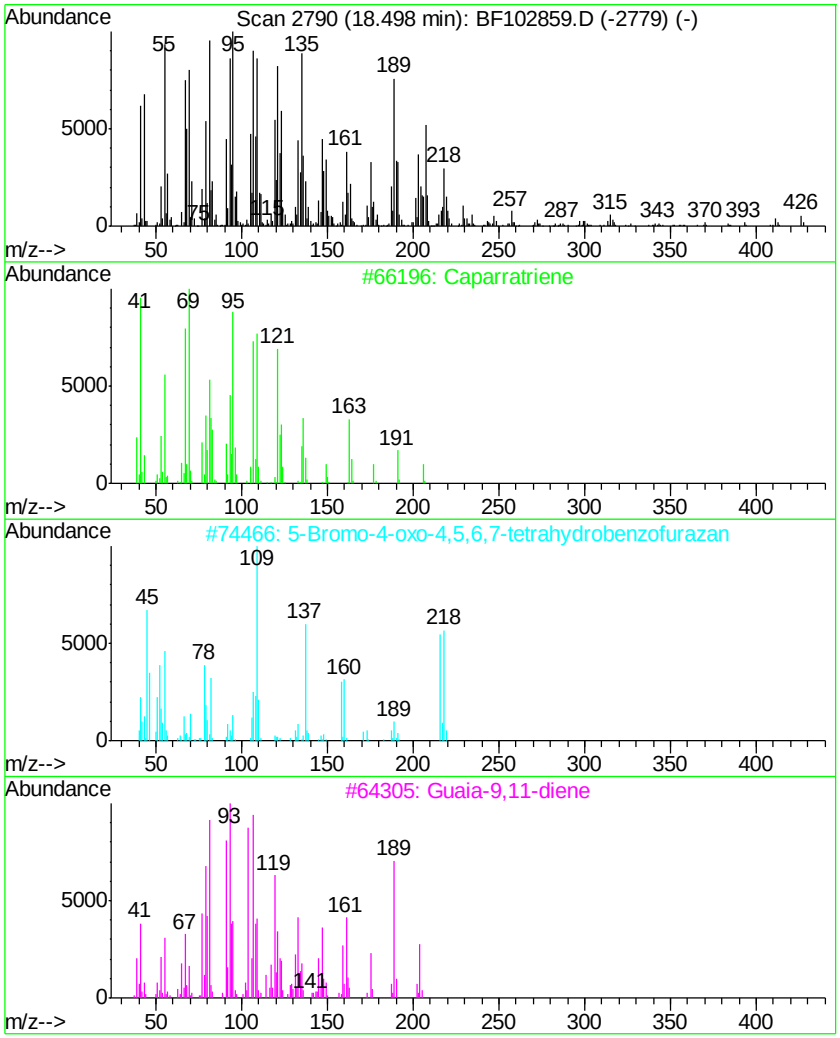
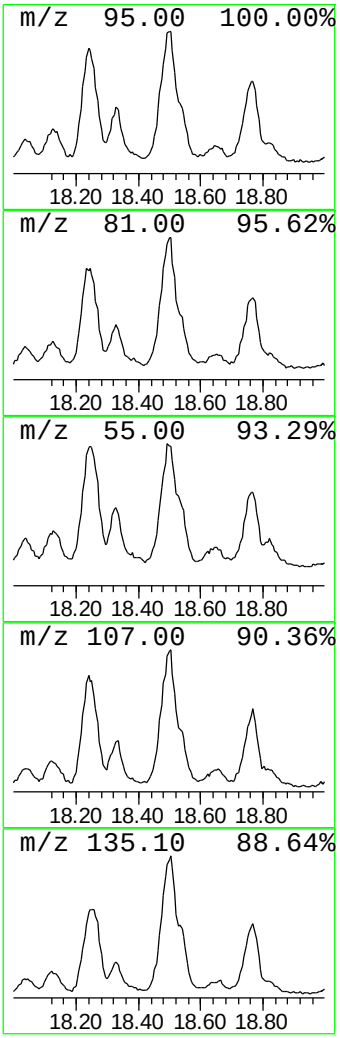
Peak Number 12 Caparratriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	149.09 ng	6817720	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	64
2	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
3	Guaia-9,11-diene	204	C15H24	1000374-19-8	51
4	(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	50
5	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	003242-08-8	46





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Sample : J1470-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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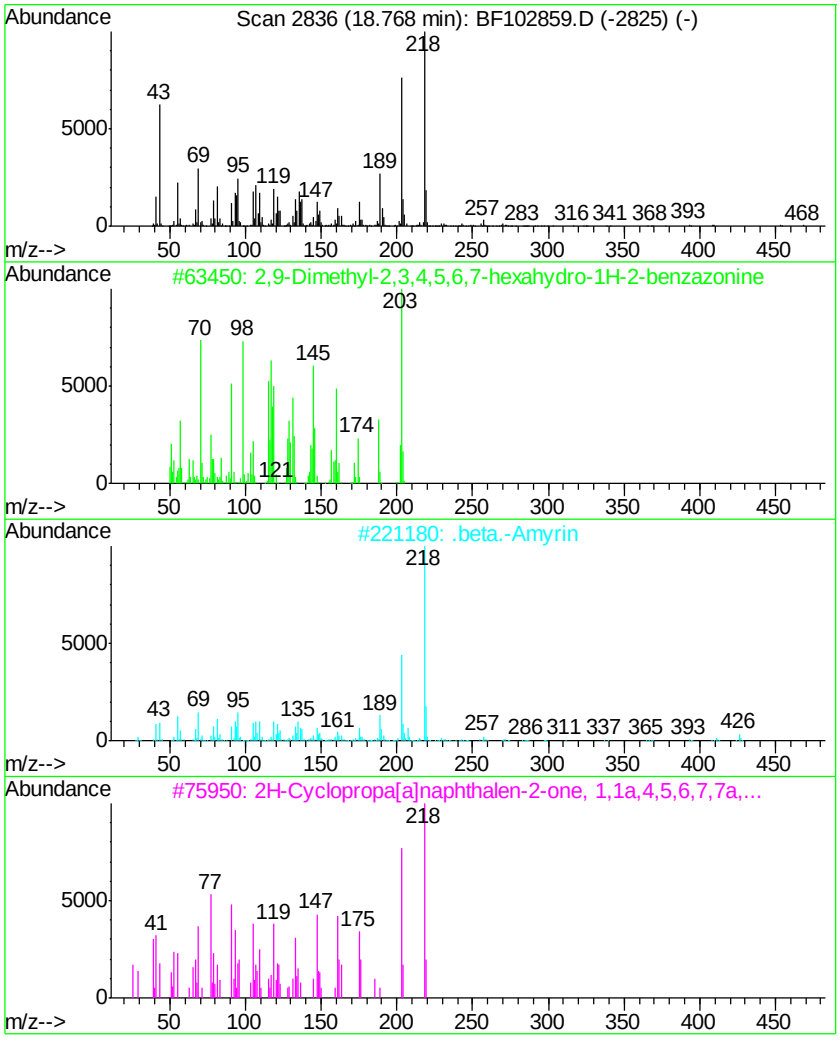
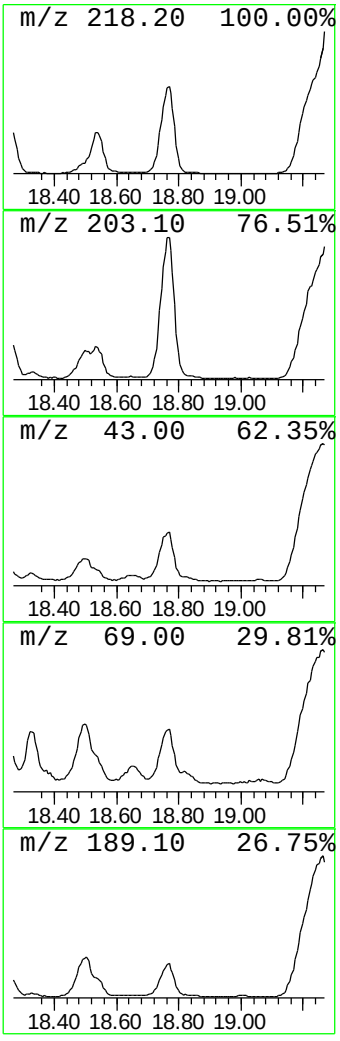
Peak Number 13 2,9-Dimethyl-2,3,4,5,6,7-he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	81.63 ng	3732810	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,9-Dimethyl-2,3,4,5,6,7-hexahyd...	203	C14H21N	077581-11-4	78
2	.beta.-Amyrin	426	C30H50O	000559-70-6	74
3	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	58
4	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	58
5	2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	53





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Data File : BF102859.D
Acq On : 8 Feb 2018 16:39
Operator : SJ/JU
Sample : J1470-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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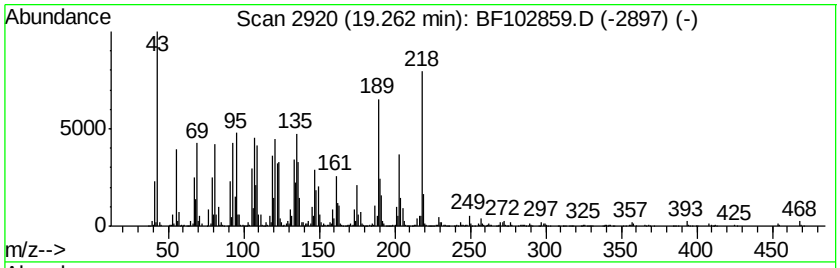
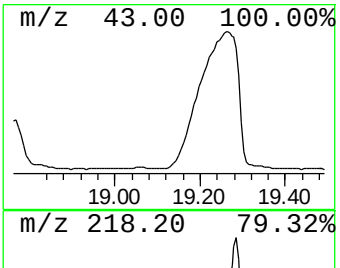
Peak Number 14 Urs-12-en-3-ol, acetate, (3... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	564.42 ng	25810500	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urs-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	000863-76-3	86
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	70
3	Urs-12-en-24-oic acid, 3-oxo-, m...	468	C31H48O3	020475-86-9	52
4	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	49
5	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	8.8	ng	533337	1	6.89	1207980	20.0
unknown6.66	6.66	62.6	ng	3780630	1	6.89	1207980	20.0
Phenol, 3-ethyl-	7.93	3.7	ng	280734	2	8.17	1511600	20.0
1-Heneicosanol	13.88	7.8	ng	381812	5	14.05	983332	20.0
.gamma.-Sitosterol	17.63	7.1	ng	325670	6	15.54	914592	20.0
unknown17.87	17.87	18.6	ng	849901	6	15.54	914592	20.0
unknown18.04	18.04	15.8	ng	723683	6	15.54	914592	20.0
.beta.-Amyrin	18.13	25.8	ng	1179150	6	15.54	914592	20.0
Allyl ionone 3	18.24	109.7	ng	5015490	6	15.54	914592	20.0
Silane, (9,19-cyc...	18.33	35.6	ng	1629990	6	15.54	914592	20.0
Caparratriene	18.50	149.1	ng	6817720	6	15.54	914592	20.0
2,9-Dimethyl-2,3,...	18.77	81.6	ng	3732810	6	15.54	914592	20.0
Urs-12-en-3-ol, a...	19.26	564.4	ng	25810500	6	15.54	914592	20.0