LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

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-BF052316.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	1.644	4	5	53	rVB	2563479	4937505	100.00%	15.275%
2	4.776	277	279	298	rBV	138371	384037	7.78%	1.188%
3	5.439	334	337	359	rBV	2042574	3231501	65.45%	9.997%
4	7.085	478	481	483	rBV	2231471	3117276	63.13%	9.644%
5	7.176	487	489	505	rVB	2262464	3312467	67.09%	10.248%
6	7.519	516	519	524	rBV	562679	719040	14.56%	2.224%
7	7.759	537	540	546	rBV	1836811	2439188	49.40%	7.546%
8	8.433	596	599	617	rBV	1559472	2094731	42.42%	6.480%
9	9.553	694	697	706	rBV	591684	846614	17.15%	2.619%
10	11.325	849	852	855	rBV	2118255	3018355	61.13%	9.338%
11	12.022	910	913	918	rBV	199171	258084	5.23%	0.798%
12	12.376	941	944	947	rBV	611257	801829	16.24%	2.481%
13	13.211	1015	1017	1020	rVB	57353	77657	1.57%	0.240%
14	13.668	1054	1057	1064	rBV	1091017	1508588	30.55%	4.667%
15	13.988	1083	1085	1090	rBV	74031	120339	2.44%	0.372%
16	14.777	1151	1154	1156	rVV	510450	640709	12.98%	1.982%
17	16.571	1309	1311	1315	rVB	109590	143862	2.91%	0.445%
18	16.880	1335	1338	1341	rBV	142887	166319	3.37%	0.515%
19	16.983	1344	1347	1349	rBV	71731	102675	2.08%	0.318%
20	17.131	1357	1360	1362	rBV	1850850	2162914	43.81%	6.691%
21	17.908	1425	1428	1430	rBV	53551	66306	1.34%	0.205%
22	18.389	1467	1470	1474	rBV	42160	101313	2.05%	0.313%
23	18.468	1474	1477	1479	rVV2	580058	726351	14.71%	2.247%
24	18.503	1479	1480	1482	rVV	76139	119931	2.43%	0.371%
25	18.537	1482	1483	1486	rVB	105554	90647	1.84%	0.280%
26	19.131	1527	1535	1536	rBV5	14024	51418	1.04%	0.159%
27	19.509	1565	1568	1569	rBV	92253	140504	2.85%	0.435%
28	19.600	1573	1576	1578	rVV2	26309	51846	1.05%	0.160%
29	19.737	1586	1588	1596	rBV	92341	200829	4.07%	0.621%
30	20.034	1611	1614	1616	rBV	43481	71355	1.45%	0.221%
31	20.092	1616	1619	1621	rVV	65472	88019	1.78%	0.272%
32	20.137	1621	1623	1630	rVV	368792	476680	9.65%	1.475%
33	21.383	1729	1732	1735	rBV	27093	55409	1.12%	0.171%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

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-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 32324298

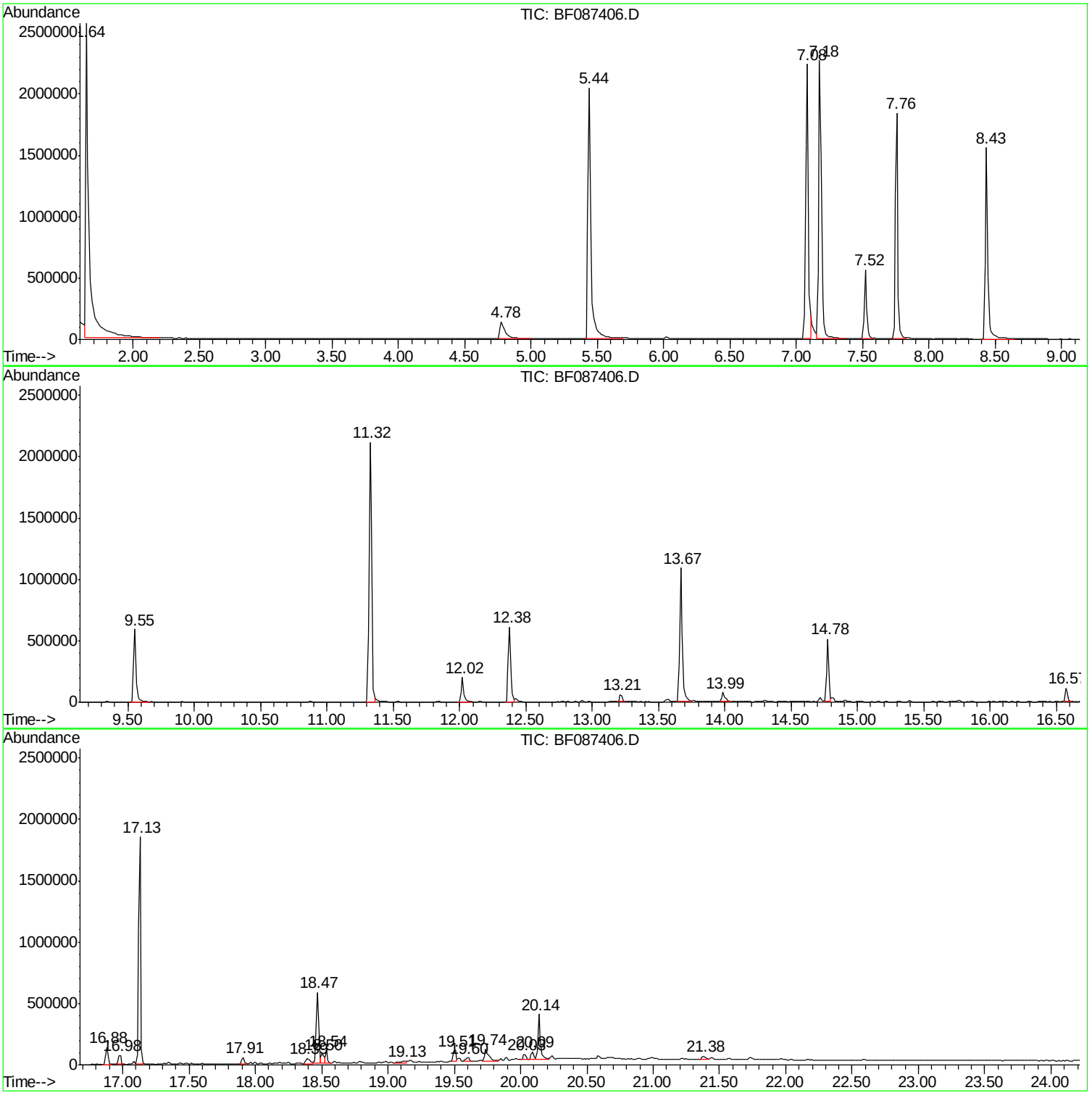
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
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Operator : UM/SJ
Sample : H3220-22
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Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

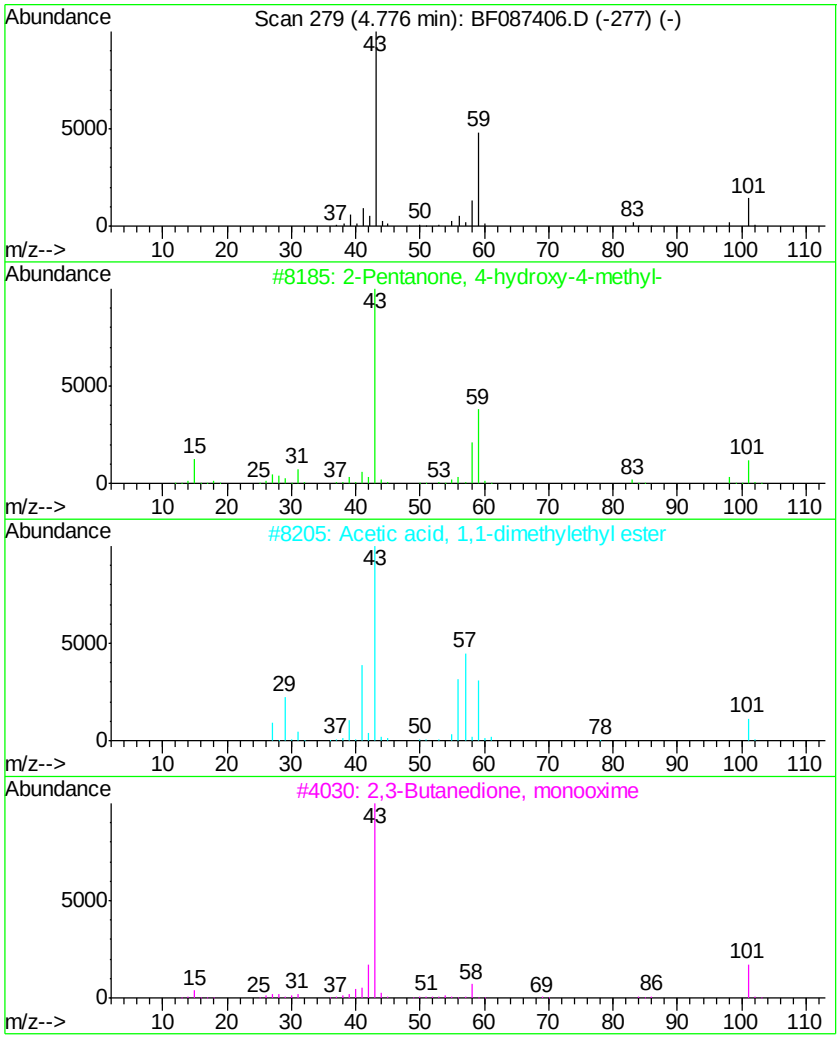
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

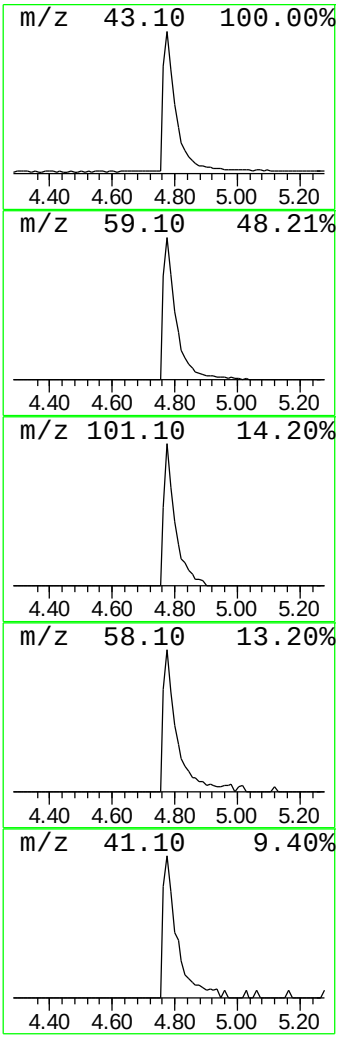
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	10.68 ng	384037	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

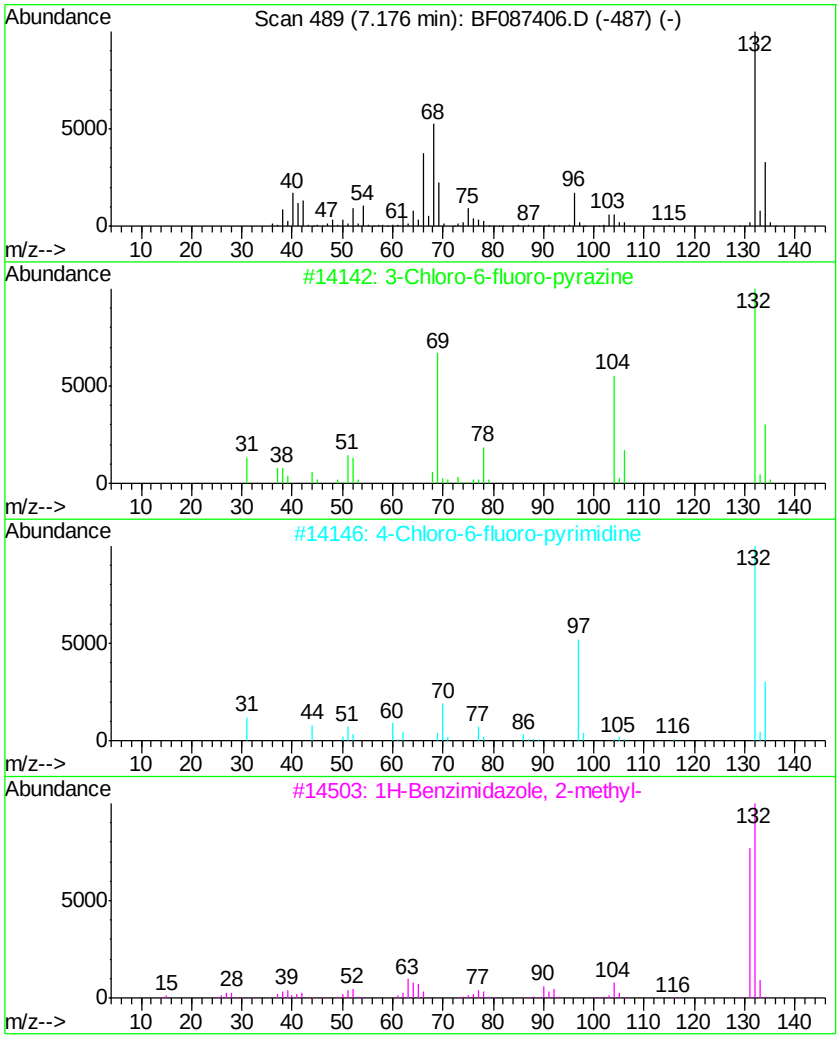
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

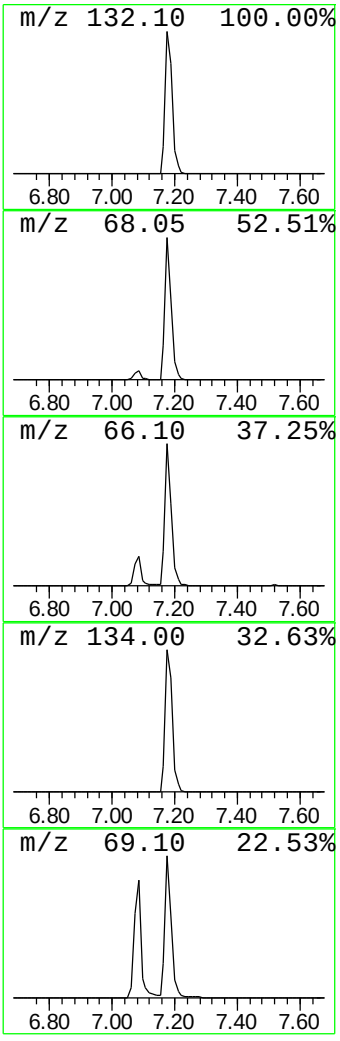
****

Peak Number 3 unknown7.18 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	92.14 ng	3312470	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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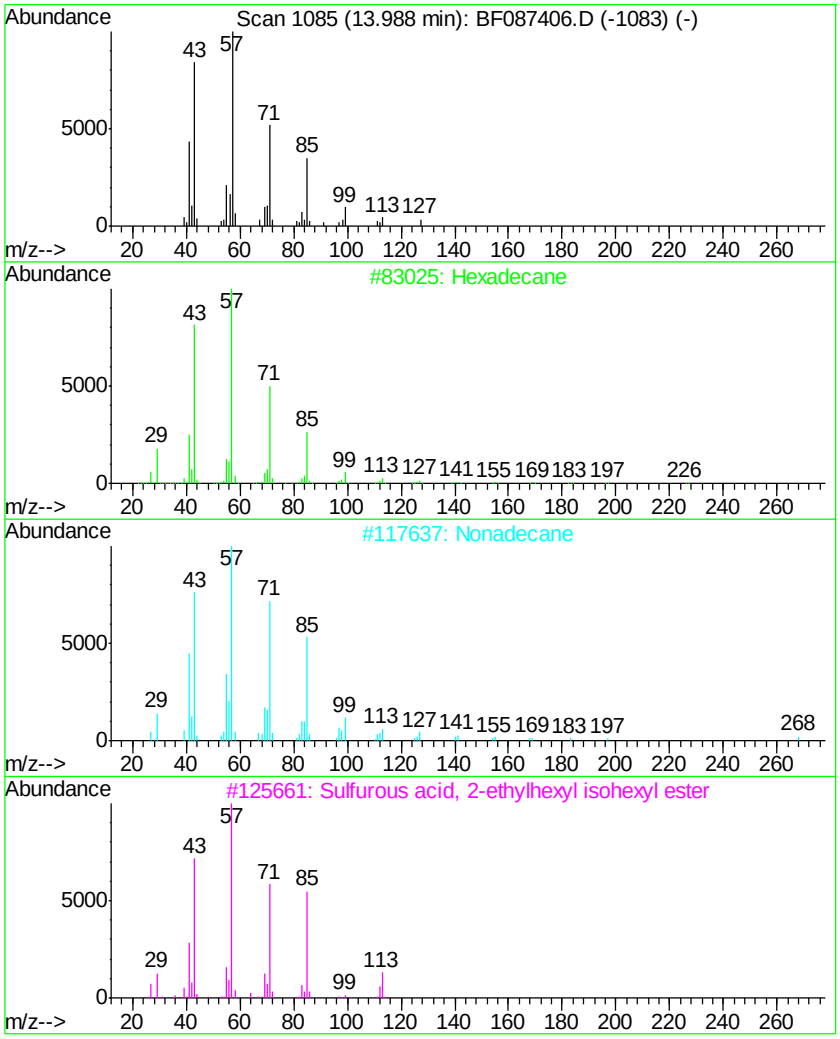
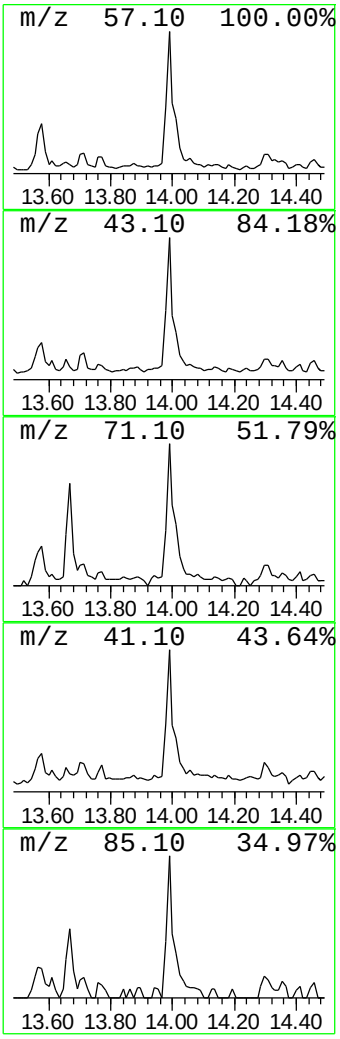
Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	3.76 ng	120339	Phenanthrene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Nonadecane	268	C19H40	000629-92-5	80
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	80
4	Eicosane	282	C20H42	000112-95-8	72
5	Heptacosane	380	C27H56	000593-49-7	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

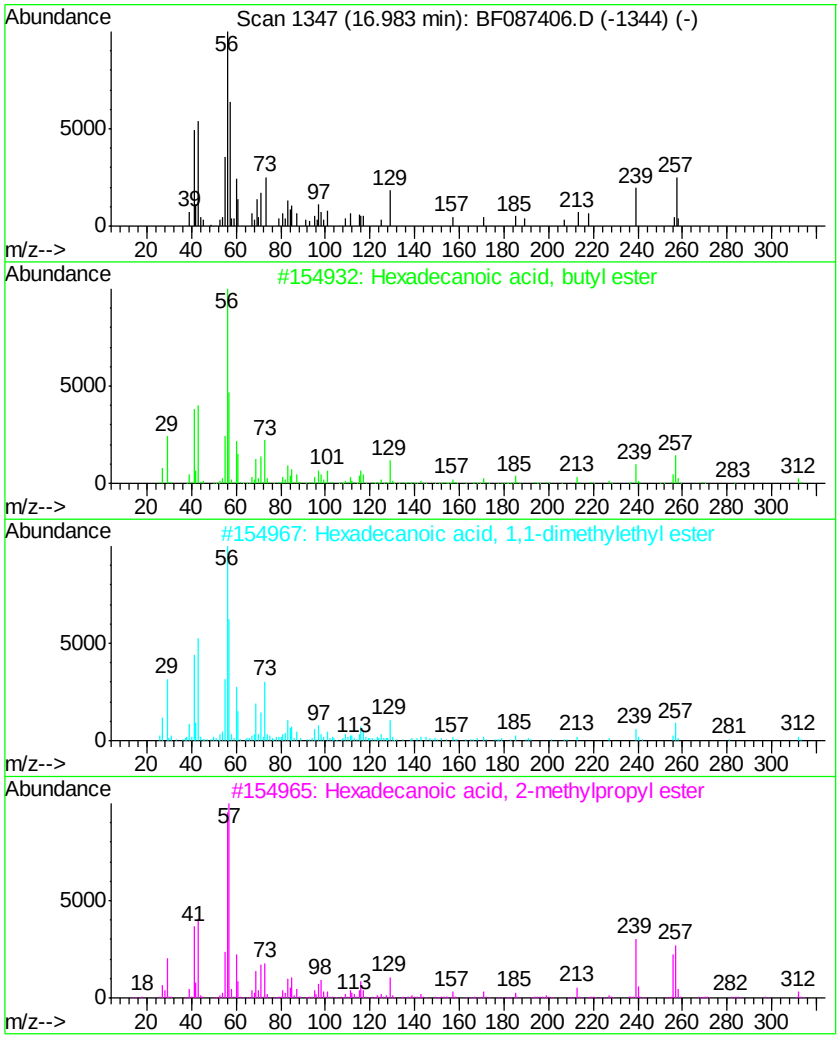
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

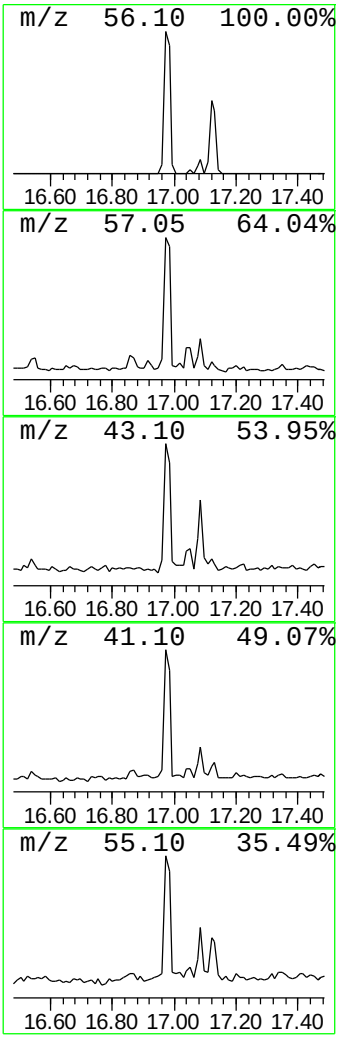
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	2.83 ng	102675	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	37
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
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Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

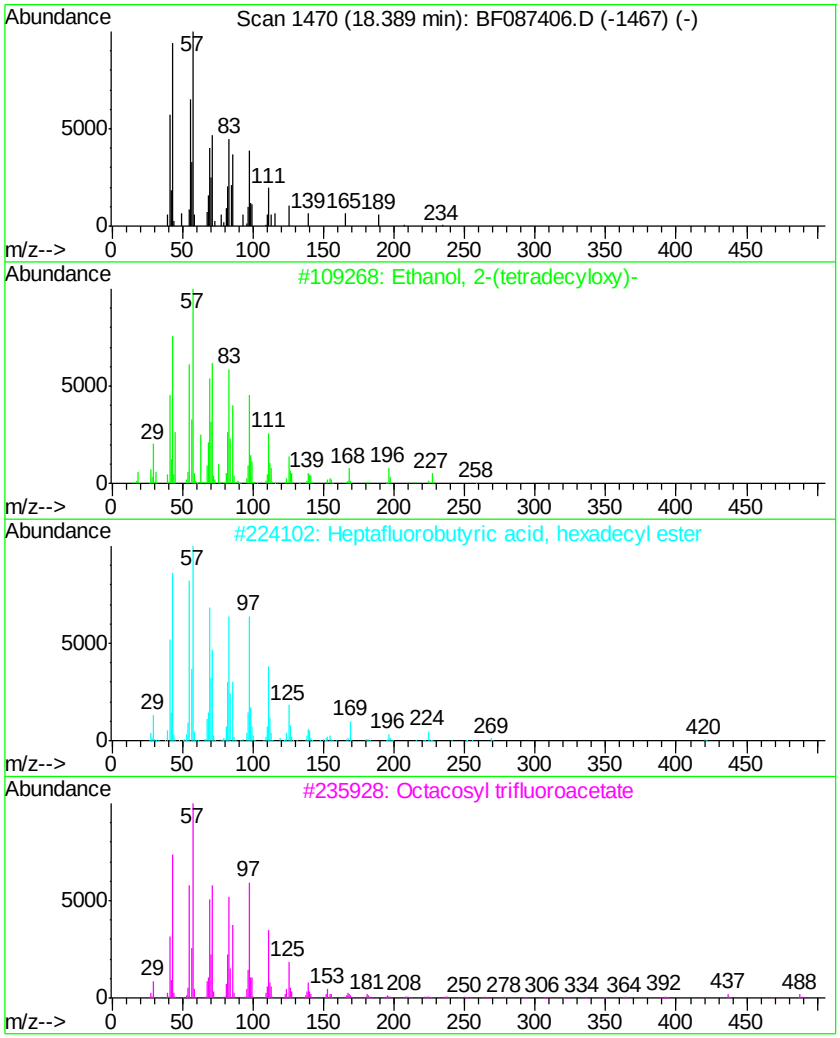
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

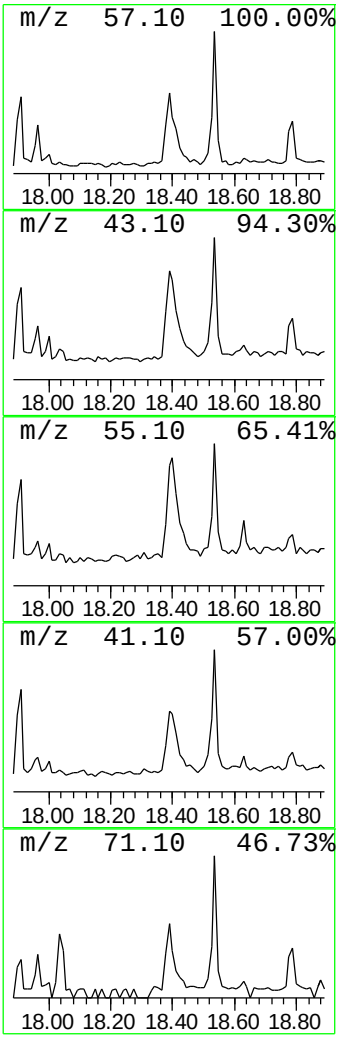
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.79 ng	101313	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87





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Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

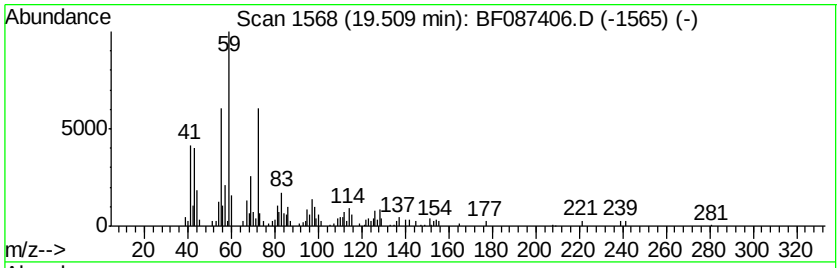
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

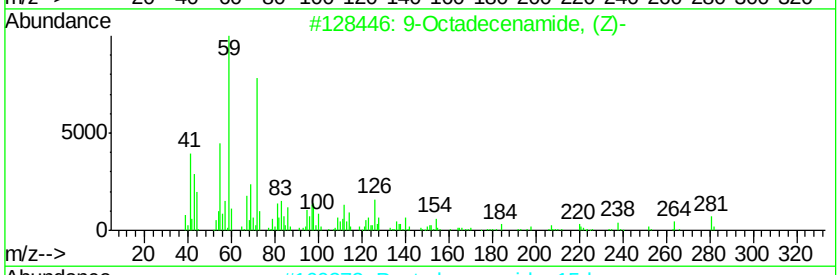
****

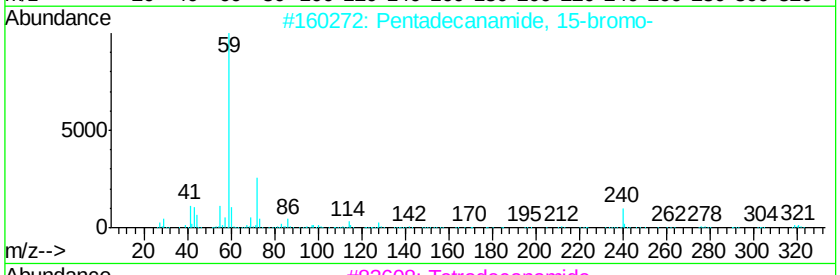
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

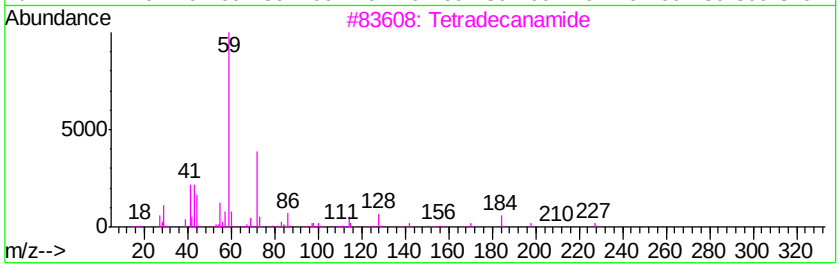
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.51	5.90 ng	140504	Perylene-d12	20.14

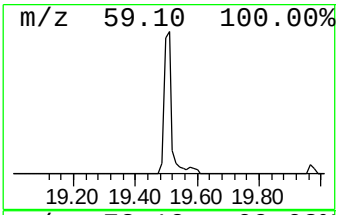
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Decanamide-	171	C10H21NO	002319-29-1	53
5	d-Glucosamine	179	C6H13NO5	000090-77-7	53

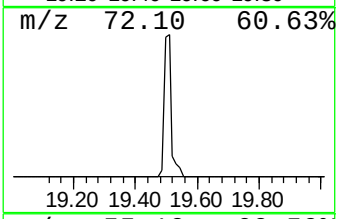


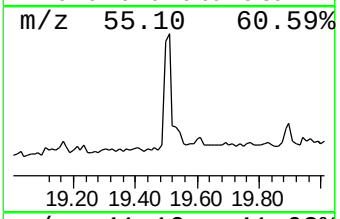


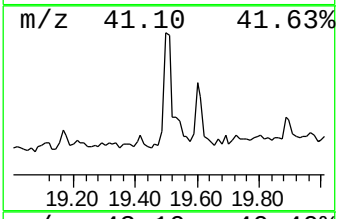


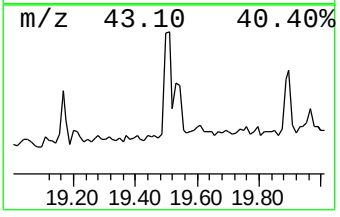












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Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

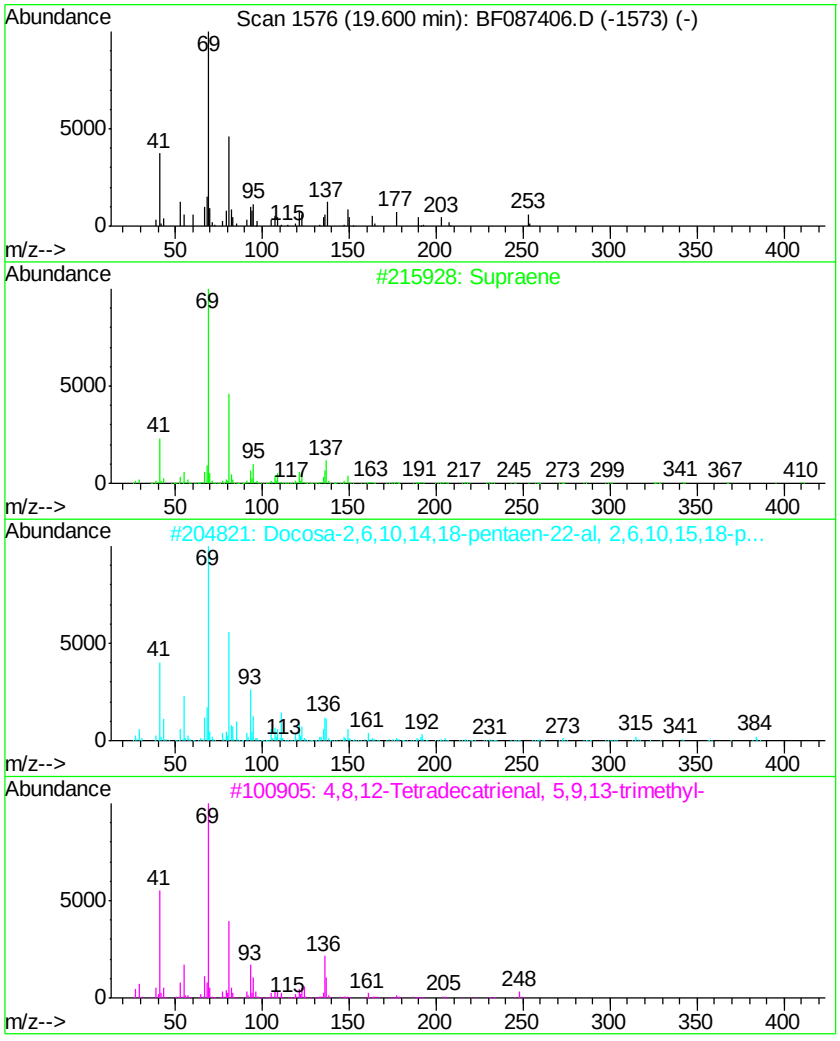
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

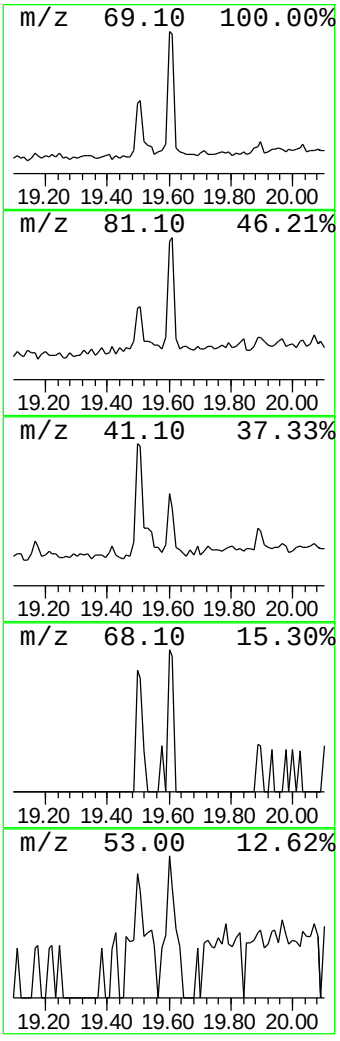
****

Peak Number 9 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.18 ng	51846	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	64
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
4	Squalene	410	C30H50	000111-02-4	59
5	Geranyl bromide	216	C10H17Br	006138-90-5	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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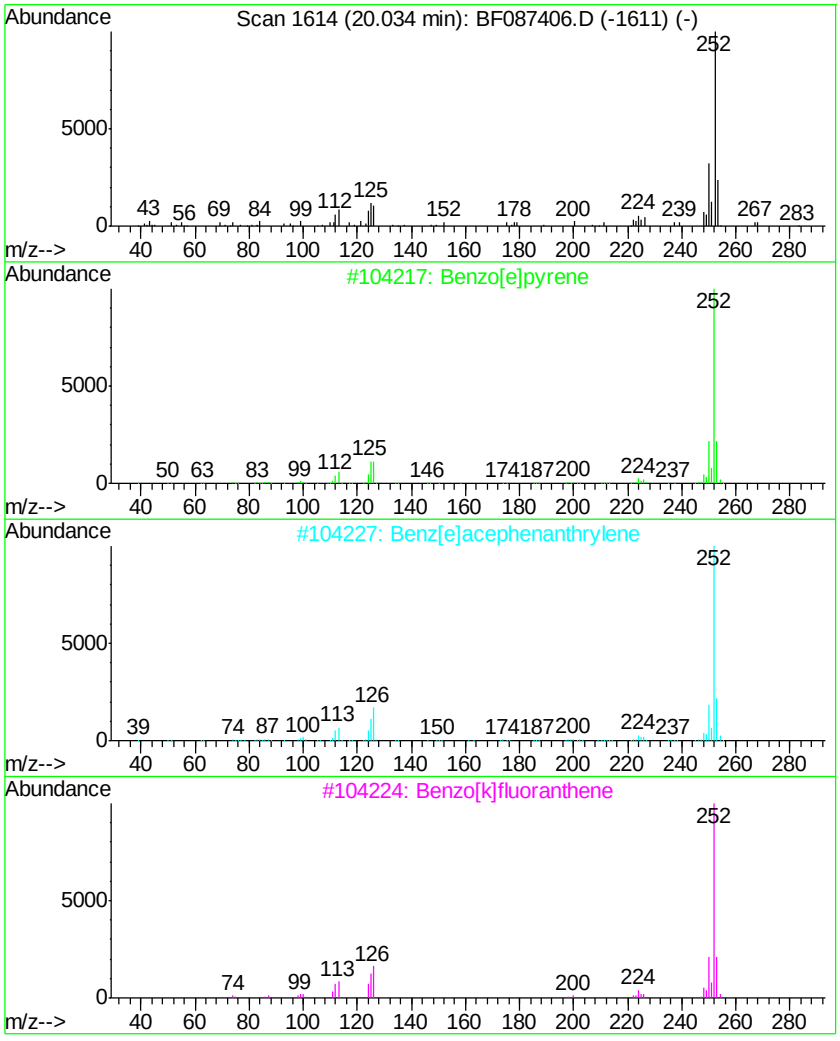
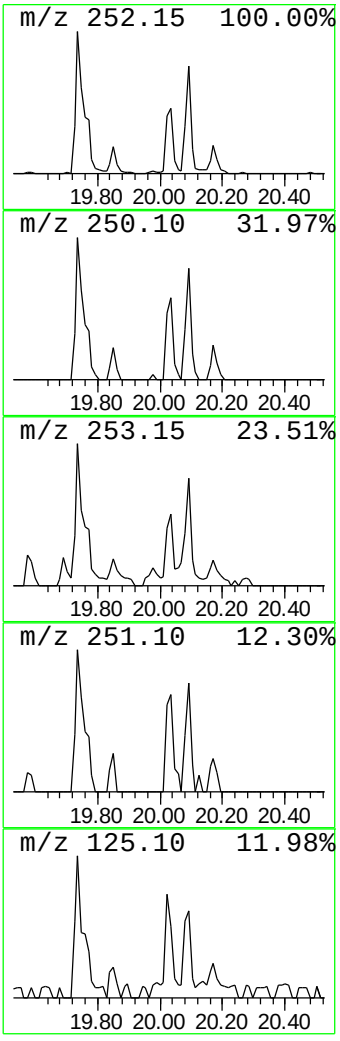
Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.03	2.99 ng	71355	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
4	Perylene	252	C20H12	000198-55-0	81
5	Benzo[a]pyrene	252	C20H12	000050-32-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052516\
Data File : BF087406.D
Acq On : 26 May 2016 10:58
Operator : UM/SJ
Sample : H3220-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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
2-Pentanone, 4-hy...	4.78	10.7	ng	384037	1	7.52	719040	20.0
unknown7.18	7.18	92.1	ng	3312470	1	7.52	719040	20.0
Hexadecane	13.99	3.8	ng	120339	4	14.78	640709	20.0
Hexadecanoic acid...	16.98	2.8	ng	102675	5	18.47	726351	20.0
Ethanol, 2-(tetra...	18.39	2.8	ng	101313	5	18.47	726351	20.0
9-Octadecenamide,...	19.51	5.9	ng	140504	6	20.14	476680	20.0
Supraene	19.60	2.2	ng	51846	6	20.14	476680	20.0
Benzo[e]pyrene	20.03	3.0	ng	71355	6	20.14	476680	20.0