LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100149.D
Acq On : 3 Nov 2017 21:53
Operator : SJ/JU
Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

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-BF102317.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	4.993	491	494	512	rBV	186299	337810	15.28%	1.784%
2	5.398	559	563	591	rBV	1703780	2022338	91.47%	10.679%
3	6.422	733	737	754	rBV	1788073	2082803	94.21%	10.998%
4	6.545	754	758	770	rVB	2237619	2103596	95.15%	11.108%
5	6.769	793	796	806	rBV	523339	476359	21.55%	2.515%
6	6.922	818	822	844	rVB	1743246	1632381	73.84%	8.620%
7	7.339	890	893	915	rBV	1178575	1286331	58.18%	6.793%
8	8.051	1010	1014	1032	rBV	730489	668827	30.25%	3.532%
9	8.616	1107	1110	1119	rBB	29409	30568	1.38%	0.161%
10	9.122	1192	1196	1200	rBV	2297822	2210813	100.00%	11.674%
11	9.522	1261	1264	1277	rBV	310256	249112	11.27%	1.315%
12	9.804	1308	1312	1324	rVB	830496	713244	32.26%	3.766%
13	10.522	1431	1434	1441	rBB	100348	86204	3.90%	0.455%
14	10.604	1444	1448	1460	rBV	1152039	1157662	52.36%	6.113%
15	11.298	1562	1566	1575	rBV	718333	621345	28.10%	3.281%
16	11.810	1650	1653	1665	rBV	41043	44490	2.01%	0.235%
17	12.880	1830	1835	1838	rBV	1751129	1598710	72.31%	8.442%
18	13.757	1980	1984	1991	rBV	67061	87418	3.95%	0.462%
19	13.951	2013	2017	2026	rBV	406667	380700	17.22%	2.010%
20	14.486	2100	2108	2120	rBV7	11199	40464	1.83%	0.214%
21	14.668	2135	2139	2147	rVB	418231	390059	17.64%	2.060%
22	15.362	2253	2257	2260	rBV	28645	32755	1.48%	0.173%
23	15.410	2260	2265	2273	rVV	307239	401529	18.16%	2.120%
24	15.774	2322	2327	2333	rBV	32760	48488	2.19%	0.256%
25	16.251	2404	2408	2415	rVB2	36329	60244	2.72%	0.318%
26	16.809	2499	2503	2513	rVB	30102	60881	2.75%	0.321%
27	17.468	2609	2615	2626	rVB2	27061	63503	2.87%	0.335%
28	18.262	2742	2750	2757	rBV7	16649	48695	2.20%	0.257%

Sum of corrected areas: 18937329

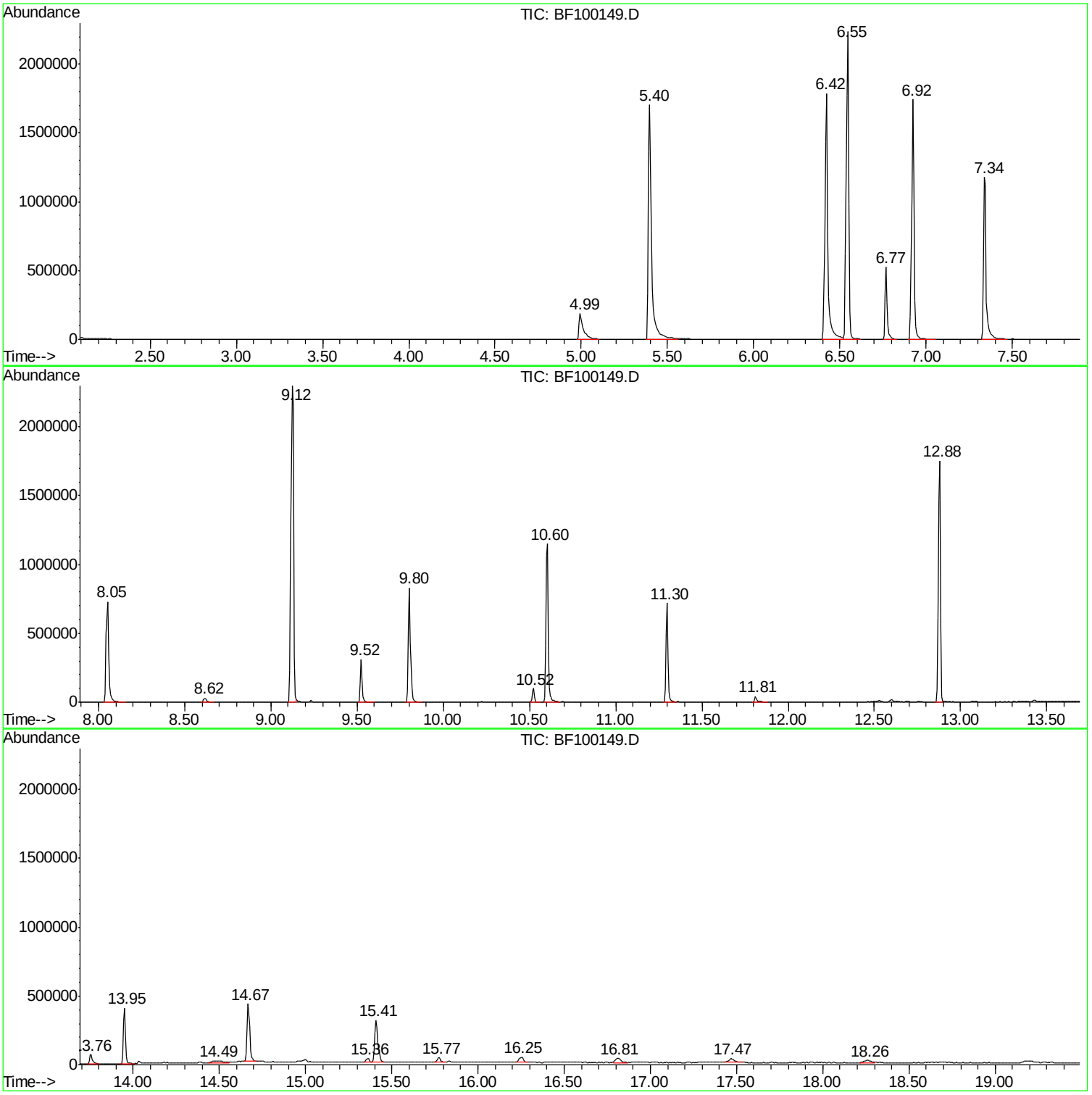
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100149.D
Acq On : 3 Nov 2017 21:53
Operator : SJ/JU
Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

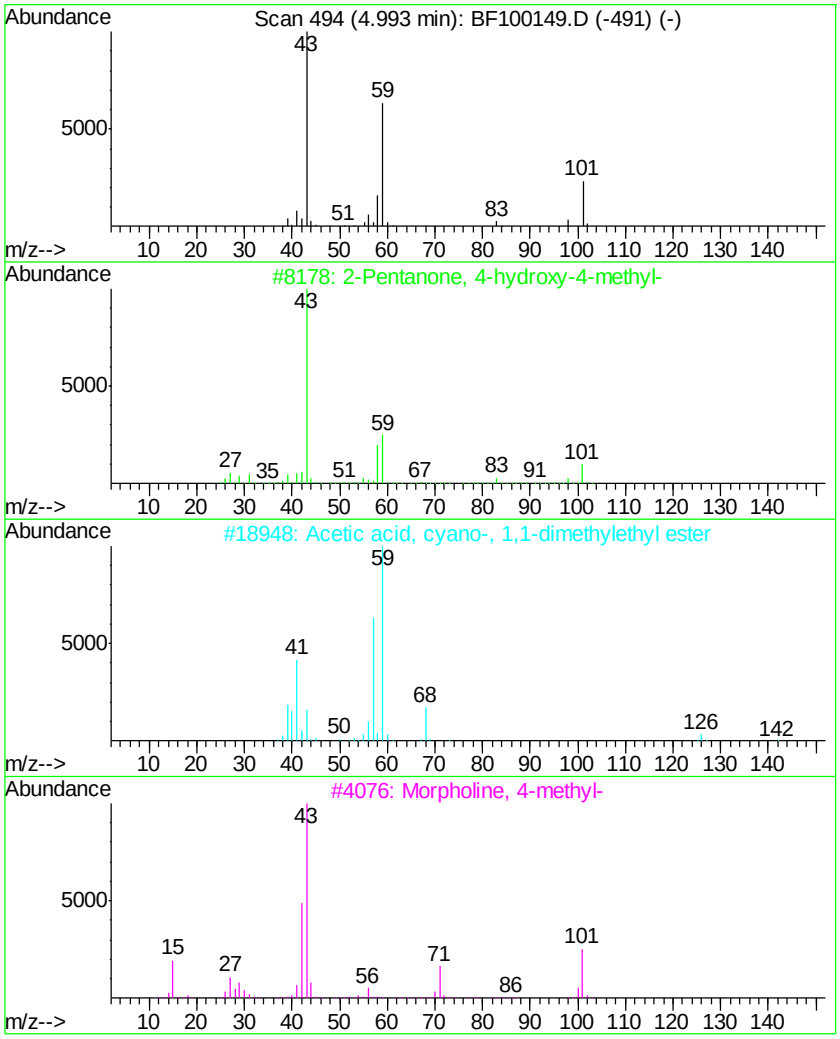
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

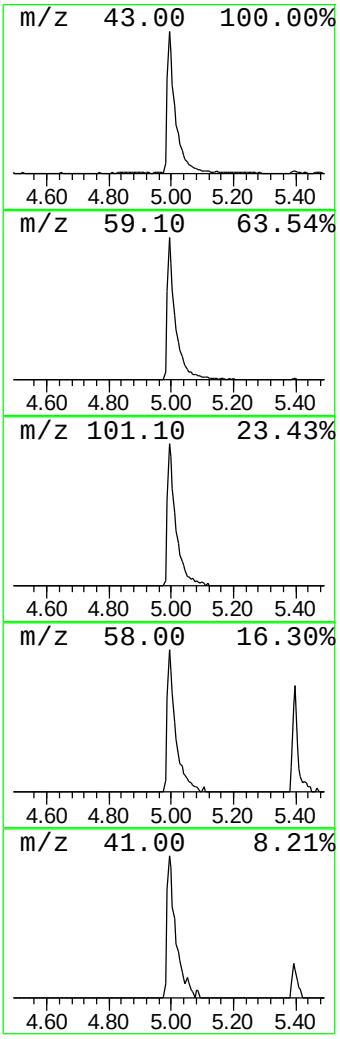
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	14.18 ng	337810	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

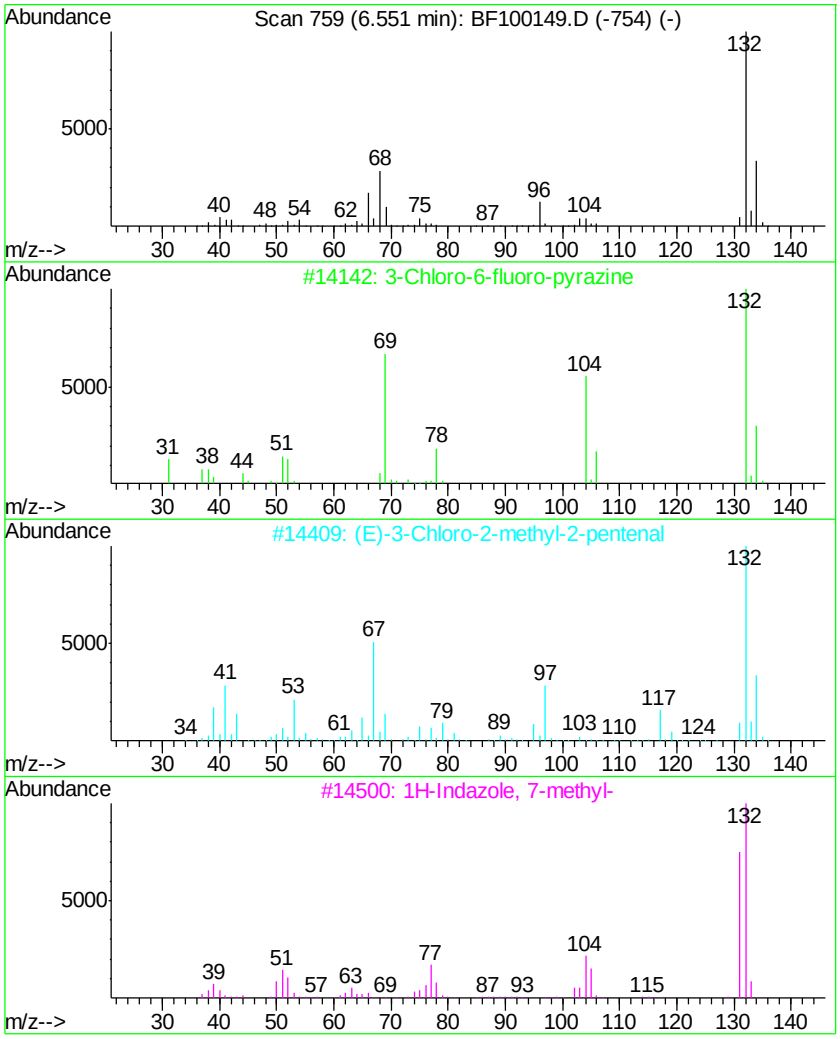
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

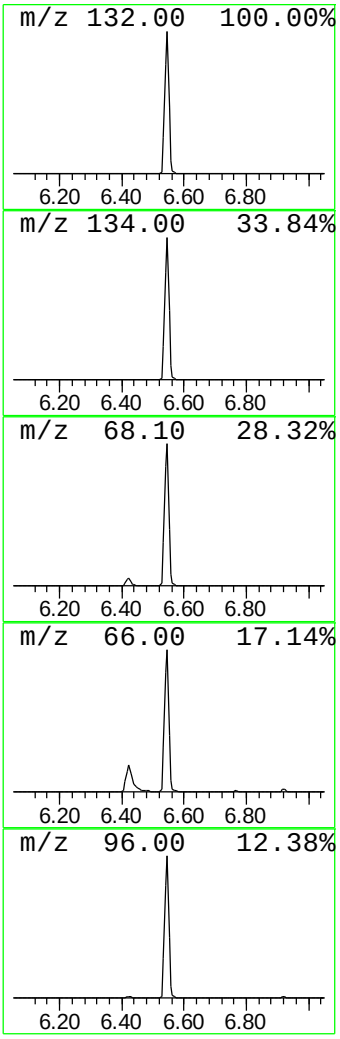
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	88.32 ng	2103600	1,4-Dichlorobenzene-d4	6.77

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	17
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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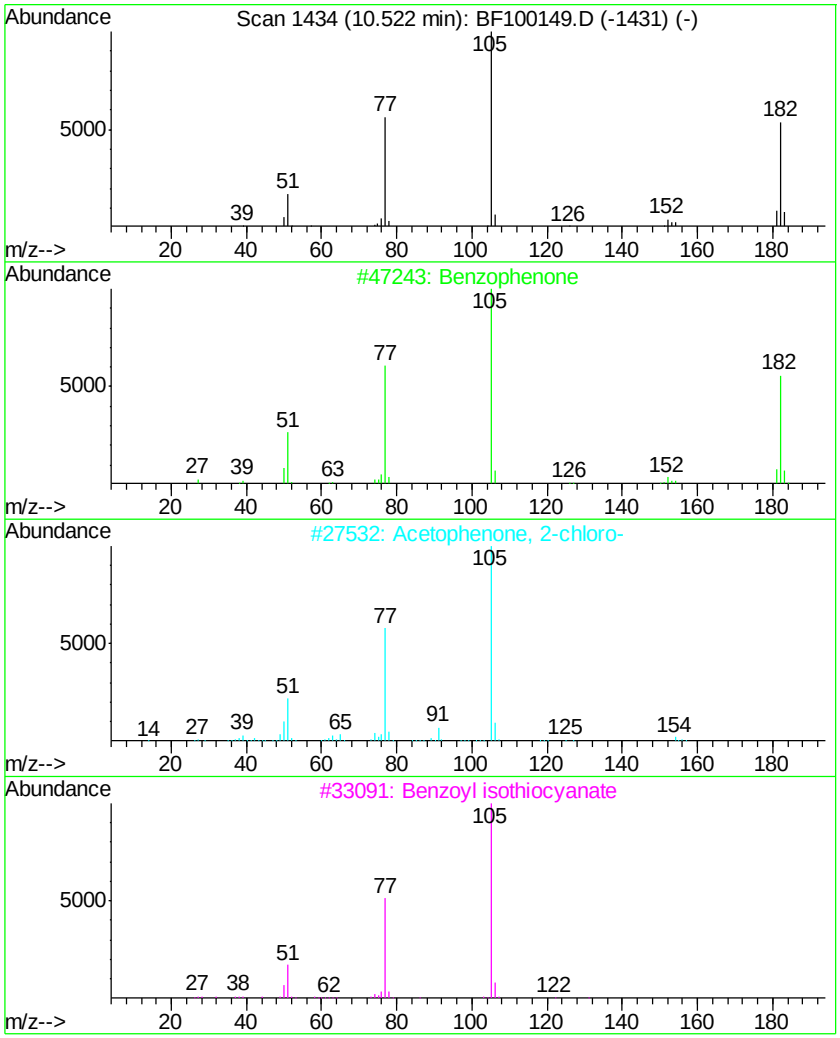
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

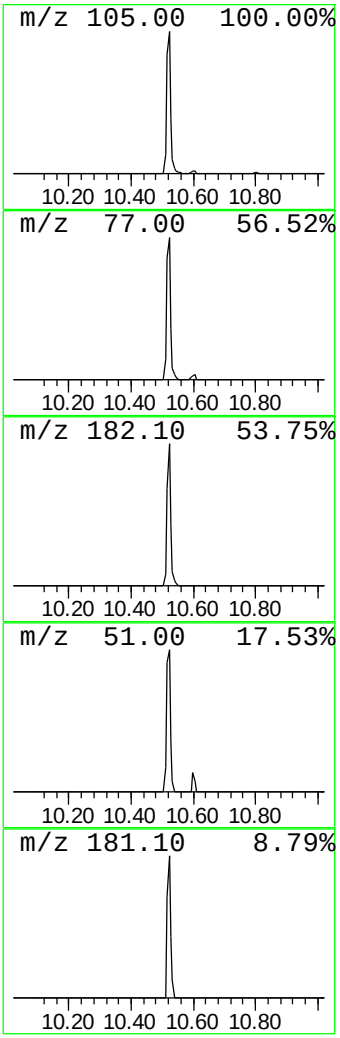
****

Peak Number 4 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.42 ng	86204	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	93
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	43





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Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

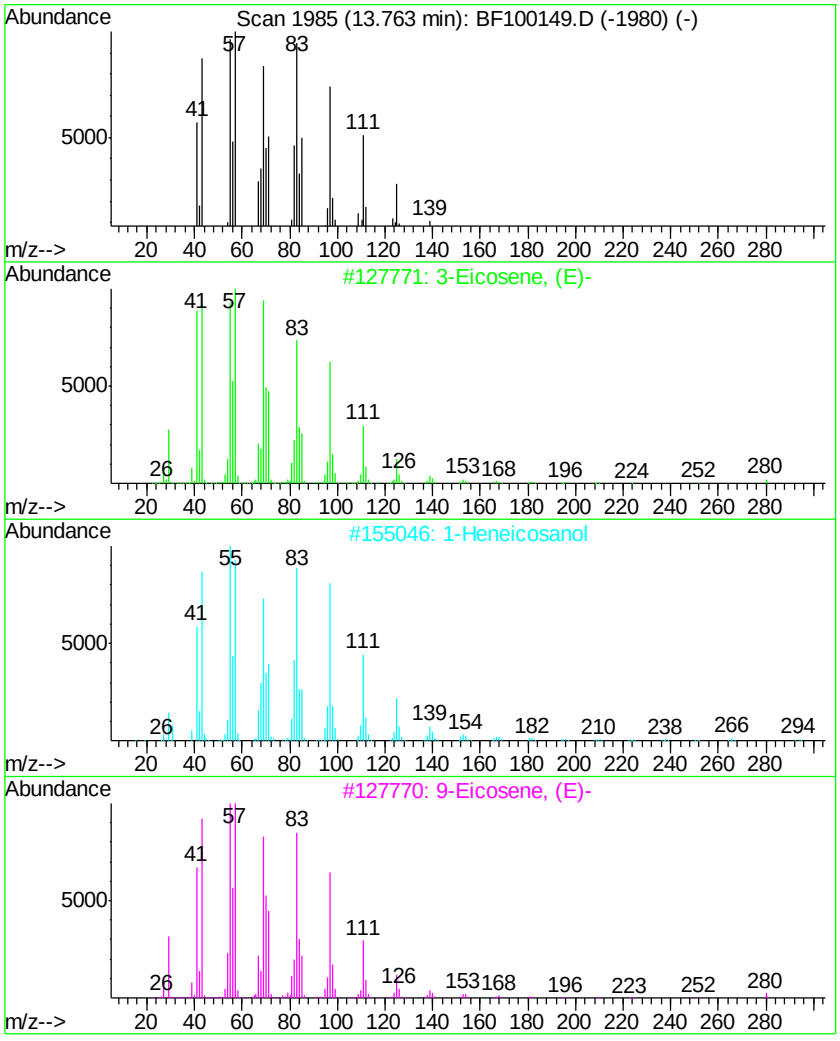
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

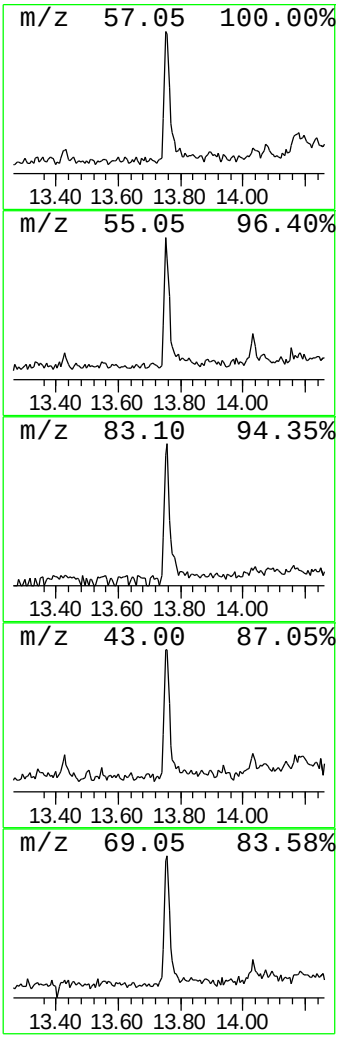
****

Peak Number 5 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.59 ng	87418	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
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Acq On : 3 Nov 2017 21:53
Operator : SJ/JU
Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

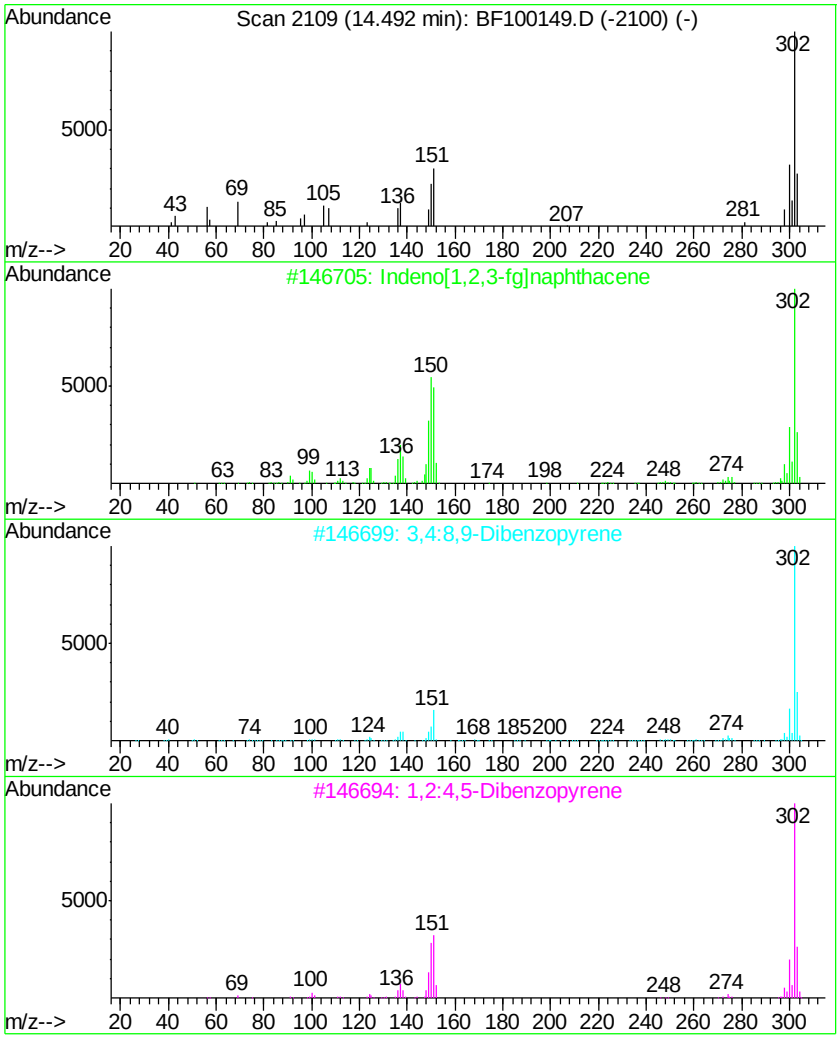
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

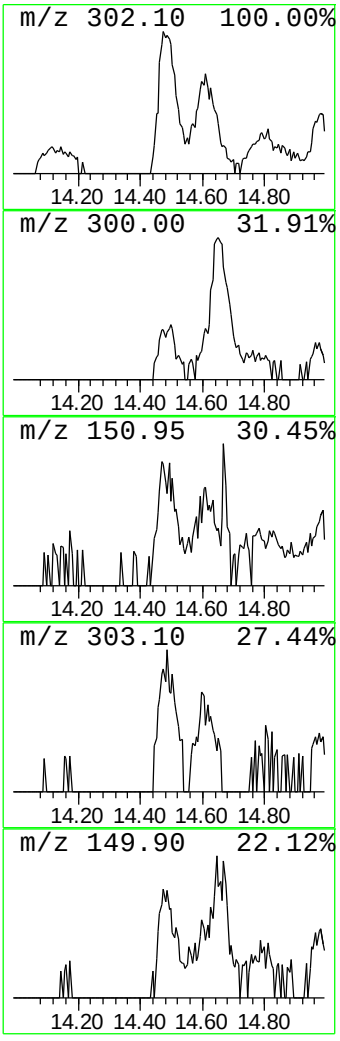
****

Peak Number 6 Indeno[1,2,3-fg]naphthacene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.13 ng	40464	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	53
2	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	47
3	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	42
4	Androst-4-ene-3,17-dione, 11-hyd...	302	C19H26O3	000382-44-5	12
5	Norethandrolone	302	C20H30O2	000052-78-8	9





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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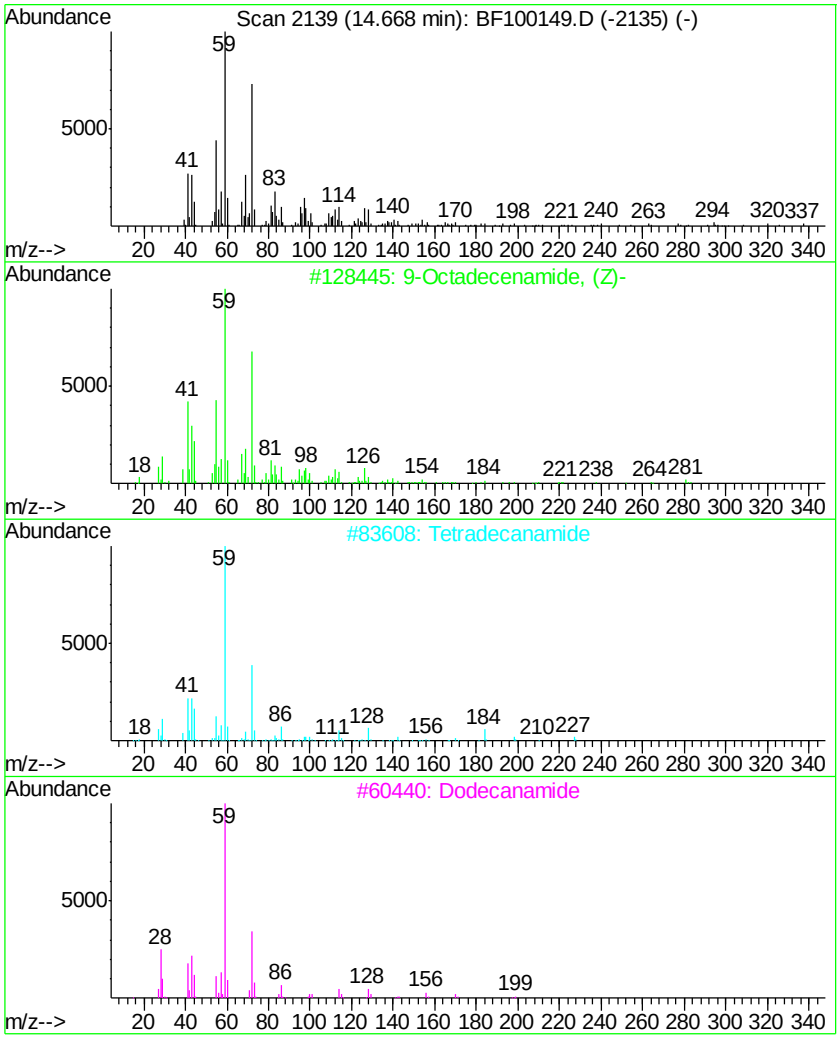
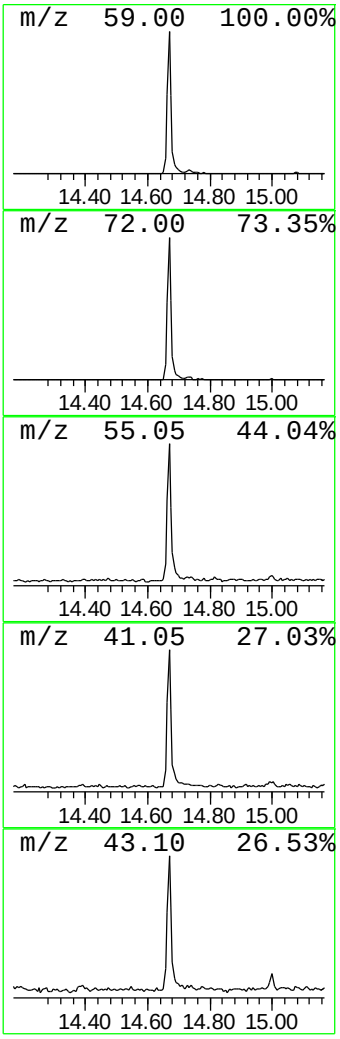
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	20.49 ng	390059	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Dodecanamide	199	C12H25NO	001120-16-7	43
4	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43
5	Hexadecanamide	255	C16H33NO	000629-54-9	43





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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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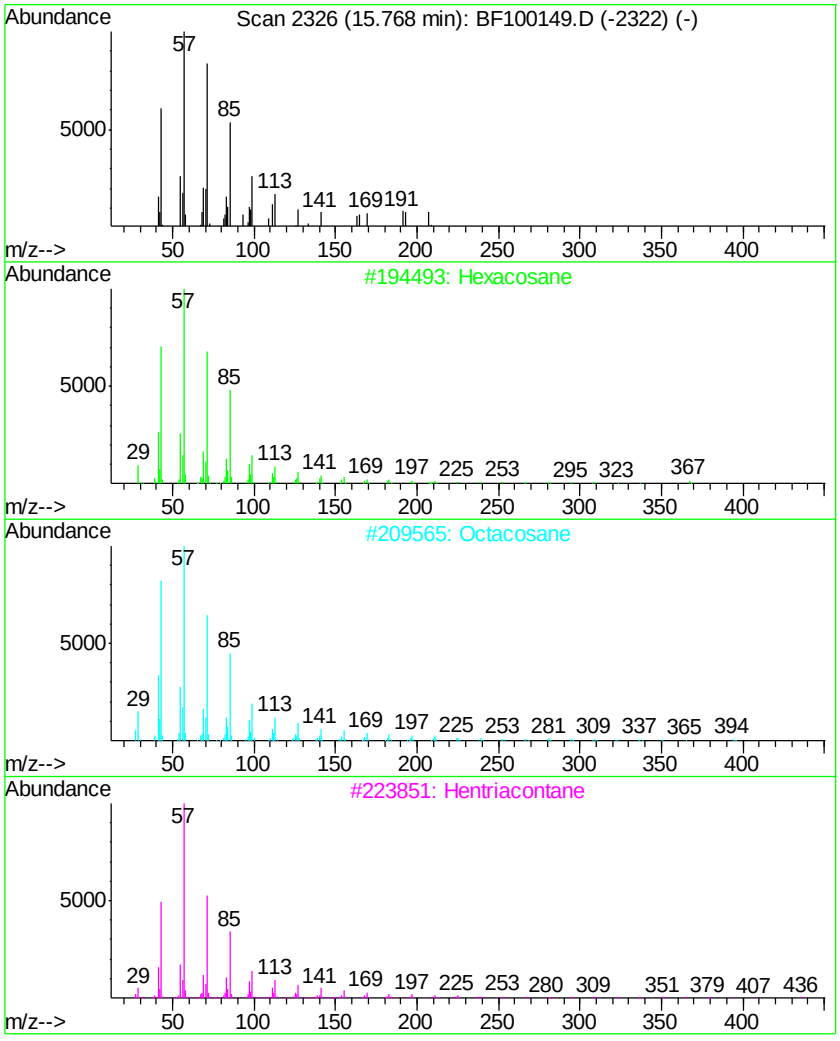
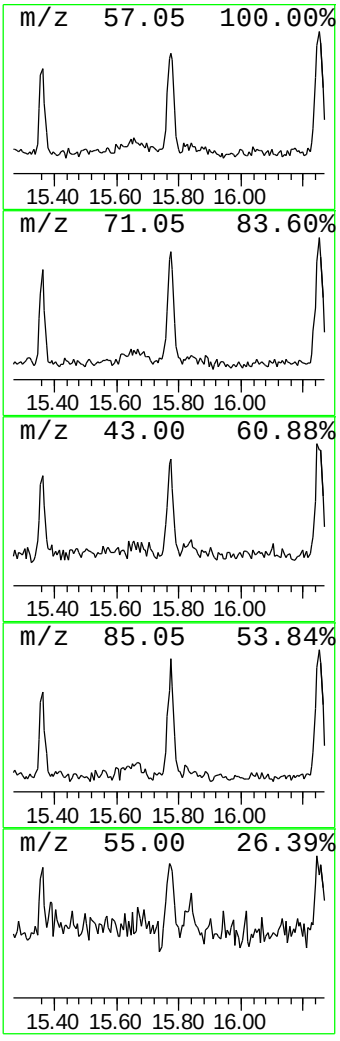
Peak Number 8 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.42 ng	48488	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Hexatriacontane	507	C36H74	000630-06-8	90
5	Heptacosane	380	C27H56	000593-49-7	90





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Misc :
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Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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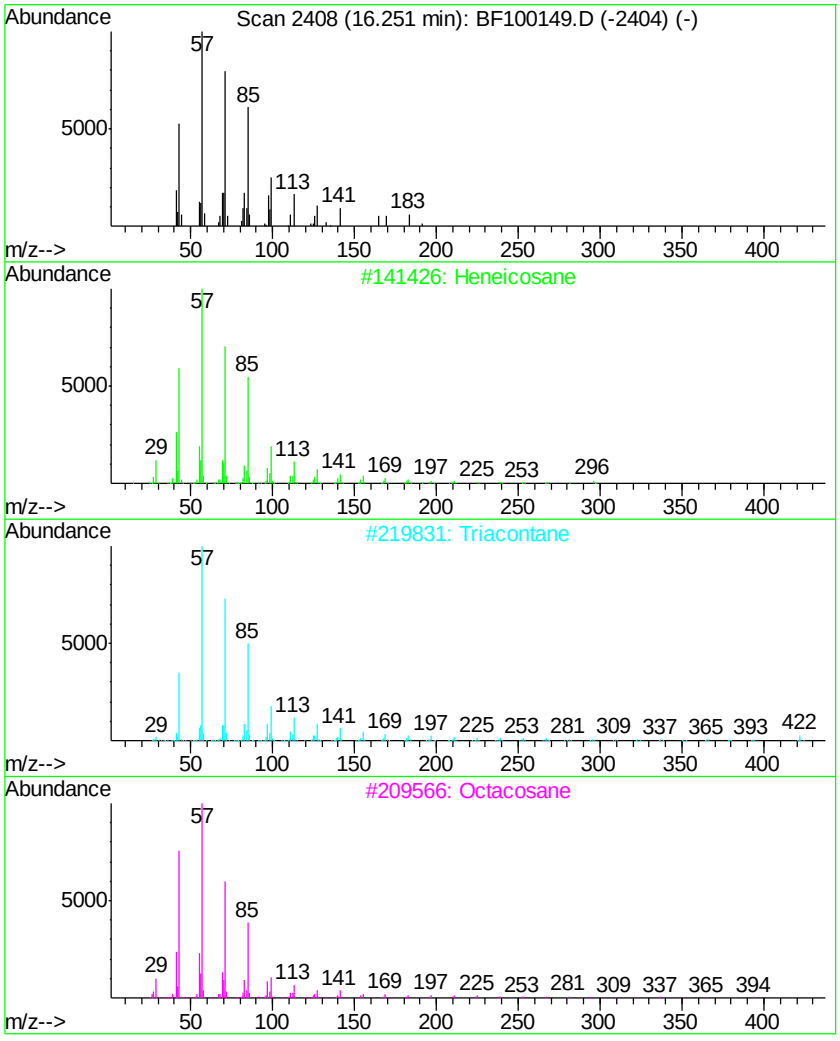
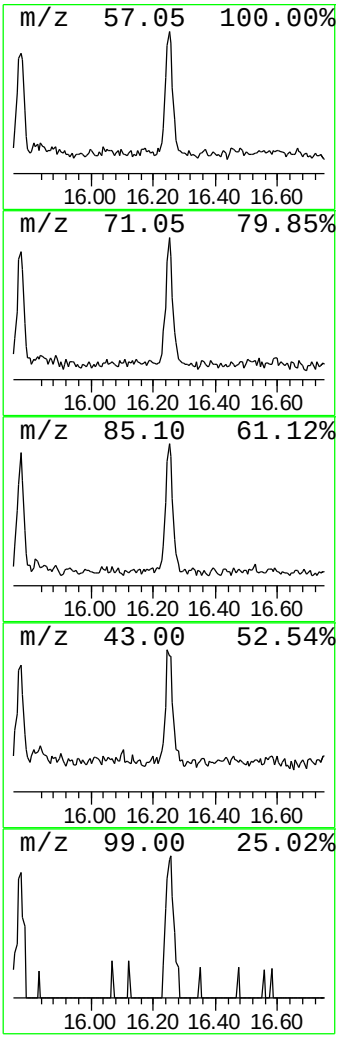
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.00 ng	60244	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Hexacosane	366	C26H54	000630-01-3	90





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Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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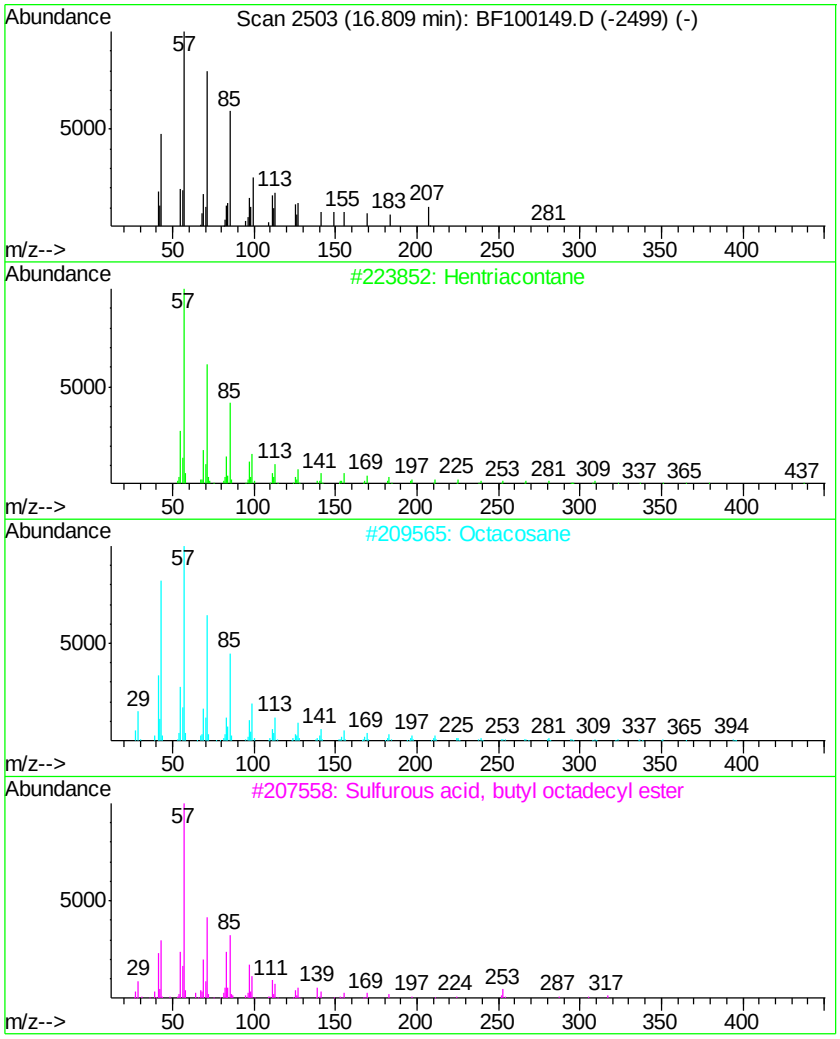
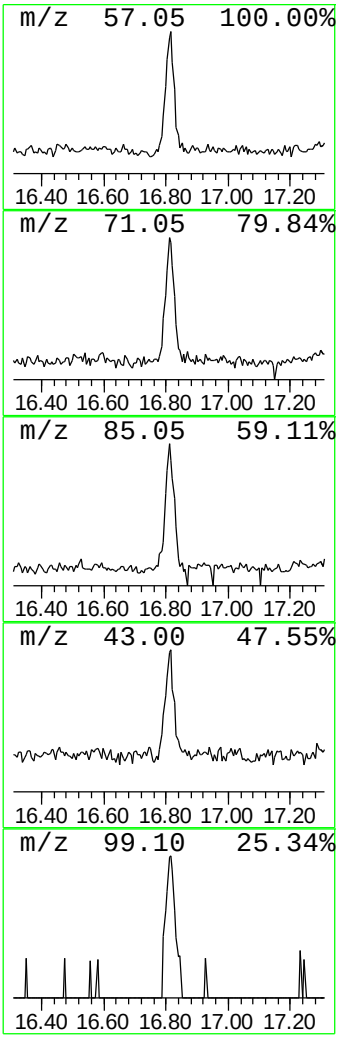
Peak Number 10 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	3.03 ng	60881	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	86
2	Octacosane	394	C28H58	000630-02-4	86
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	86
4	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	83
5	Heneicosane	296	C21H44	000629-94-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100149.D
Acq On : 3 Nov 2017 21:53
Operator : SJ/JU
Sample : I6081-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q5-COMP-NATIVE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	4.99	14.2	ng	337810	1	6.77	476359	20.0
unknown6.55	6.55	88.3	ng	2103600	1	6.77	476359	20.0
Benzophenone	10.52	2.4	ng	86204	3	9.80	713244	20.0
3-Eicosene, (E)-	13.76	4.6	ng	87418	5	13.95	380700	20.0
Indeno[1,2,3-fg]n...	14.49	2.1	ng	40464	5	13.95	380700	20.0
9-Octadecenamide,...	14.67	20.5	ng	390059	5	13.95	380700	20.0
Hexacosane	15.77	2.4	ng	48488	6	15.41	401529	20.0
Heneicosane	16.25	3.0	ng	60244	6	15.41	401529	20.0
Hentriacontane	16.81	3.0	ng	60881	6	15.41	401529	20.0