LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

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-BF080416.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	4.661	266	269	287	rBV	141347	379579	24.07%	3.110%
2	5.336	326	328	358	rBV	747788	1388000	88.03%	11.373%
3	6.982	469	472	479	rBV	797468	1327008	84.16%	10.874%
4	7.096	479	482	494	rVB	1036262	1554590	98.60%	12.739%
5	7.439	510	512	523	rBV	125201	221040	14.02%	1.811%
6	7.679	530	533	548	rBV	883771	1178620	74.75%	9.658%
7	8.353	589	592	618	rBV	557134	909778	57.70%	7.455%
8	9.473	687	690	696	rBV	170826	296087	18.78%	2.426%
9	11.256	842	846	848	rBV	1059505	1576693	100.00%	12.920%
10	11.942	903	906	916	rBV	120619	198496	12.59%	1.627%
11	12.296	934	937	940	rBV	187371	303180	19.23%	2.484%
12	13.154	1009	1012	1014	rBB	14882	18989	1.20%	0.156%
13	13.577	1047	1049	1058	rBV	445563	661071	41.93%	5.417%
14	13.919	1076	1079	1084	rBV	21496	34169	2.17%	0.280%
15	14.685	1144	1146	1149	rBV	161678	215028	13.64%	1.762%
16	15.691	1231	1234	1240	rBV2	23925	33716	2.14%	0.276%
17	16.491	1301	1304	1310	rBB	20668	28136	1.78%	0.231%
18	16.788	1328	1330	1338	rBV	23373	42929	2.72%	0.352%
19	17.051	1350	1353	1356	rBV	815194	951841	60.37%	7.800%
20	18.308	1461	1463	1467	rBV	44065	85755	5.44%	0.703%
21	18.388	1467	1470	1475	rVB	142980	243252	15.43%	1.993%
22	19.120	1531	1534	1541	rBV	42872	93009	5.90%	0.762%
23	19.543	1568	1571	1573	rVB	18760	20898	1.33%	0.171%
24	19.646	1576	1580	1587	rVB	10942	30490	1.93%	0.250%
25	19.829	1593	1596	1597	rBV	16728	20102	1.27%	0.165%
26	20.046	1613	1615	1622	rVB	168296	205262	13.02%	1.682%
27	20.331	1637	1640	1643	rBV2	10176	18693	1.19%	0.153%
28	20.514	1654	1656	1658	rBV	12681	16245	1.03%	0.133%
29	20.560	1658	1660	1662	rBV2	12799	25269	1.60%	0.207%
30	21.120	1706	1709	1712	rVB	9326	16288	1.03%	0.133%
31	21.417	1732	1735	1739	rBV3	15531	30650	1.94%	0.251%
32	21.680	1755	1758	1762	rVB3	10645	23126	1.47%	0.189%
33	22.229	1803	1806	1811	rBV4	6930	19180	1.22%	0.157%
34	23.155	1883	1887	1892	rBV4	12532	36642	2.32%	0.300%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMA-FL-01

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-BF080416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 12203811

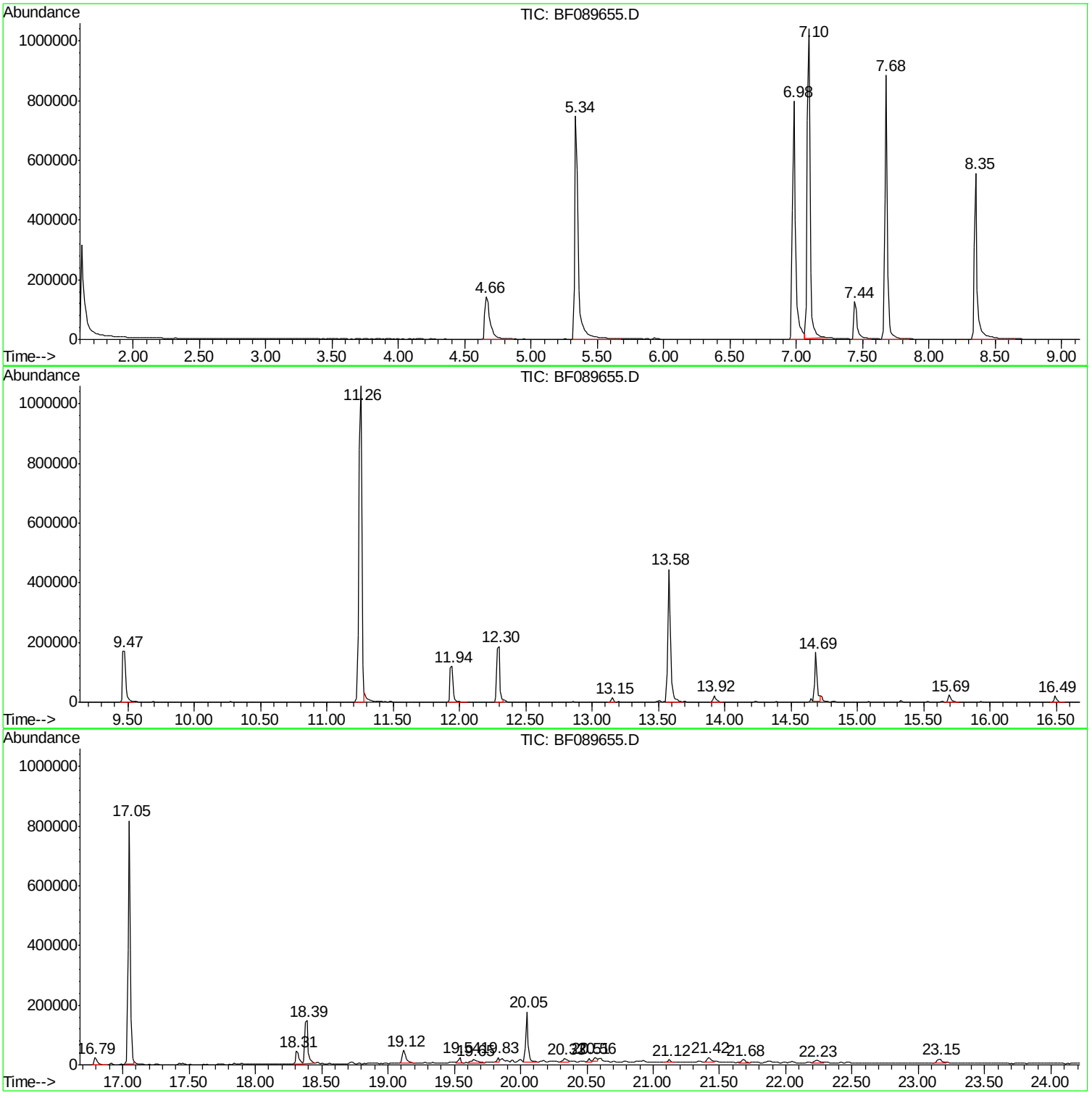
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

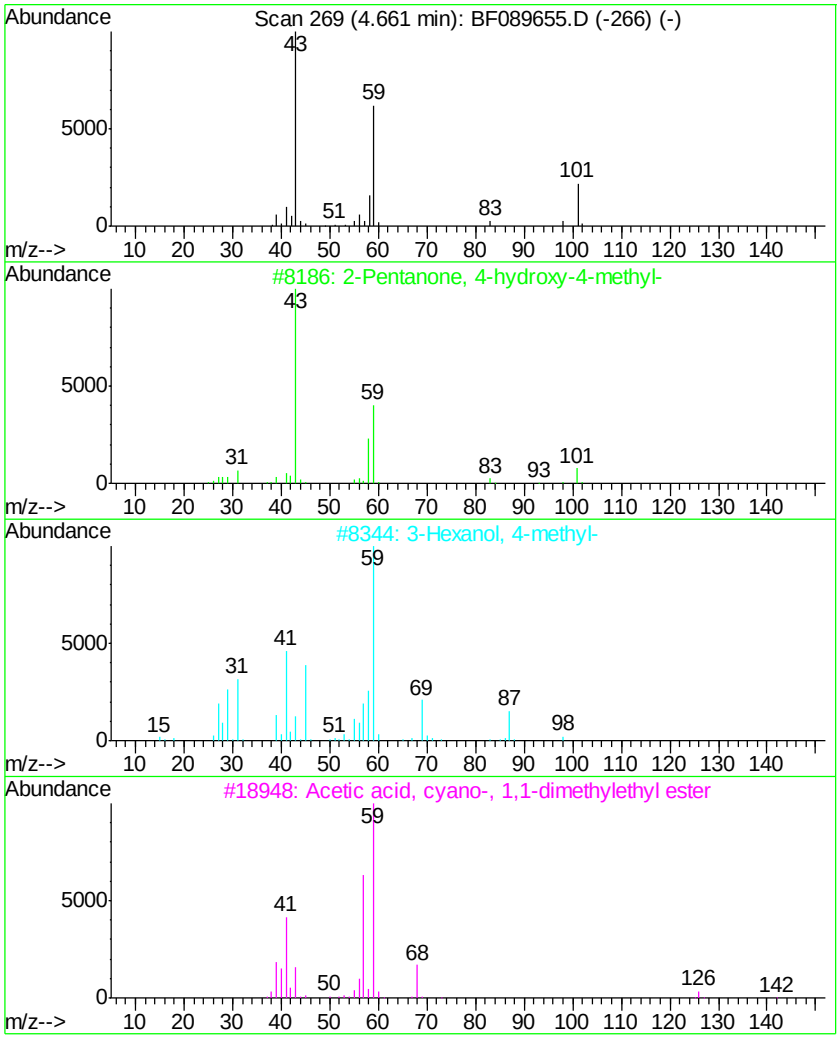
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

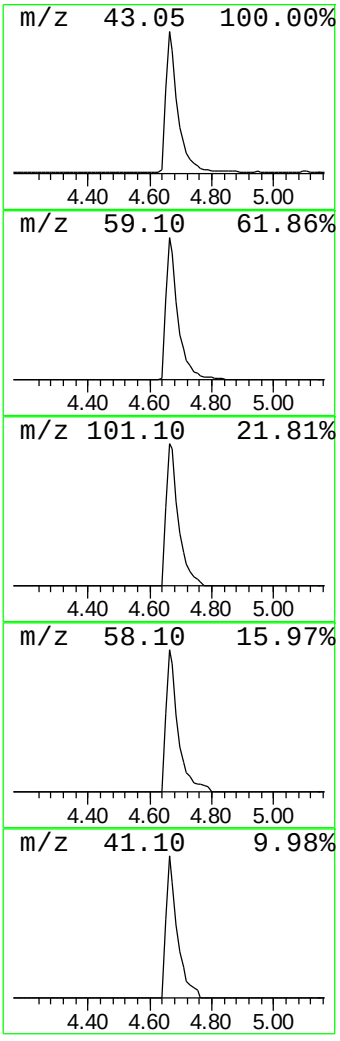
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	34.34 ng	379579	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

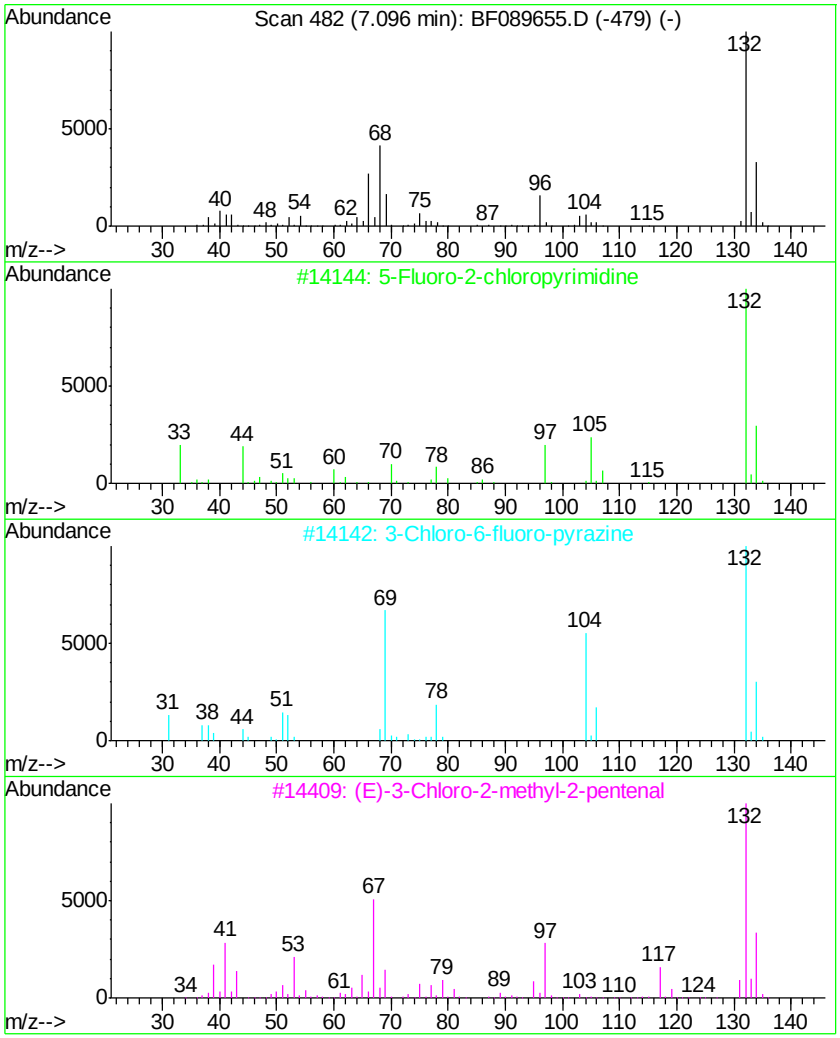
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

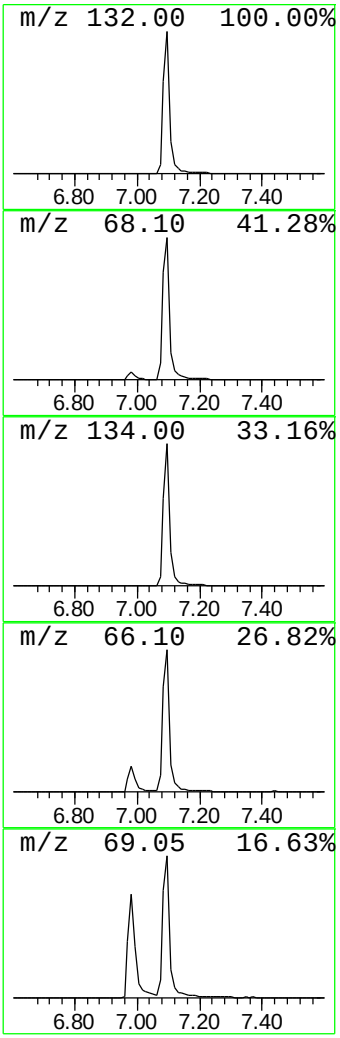
****

Peak Number 2 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	140.66 ng	1554590	1,4-Dichlorobenzene-d4	7.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

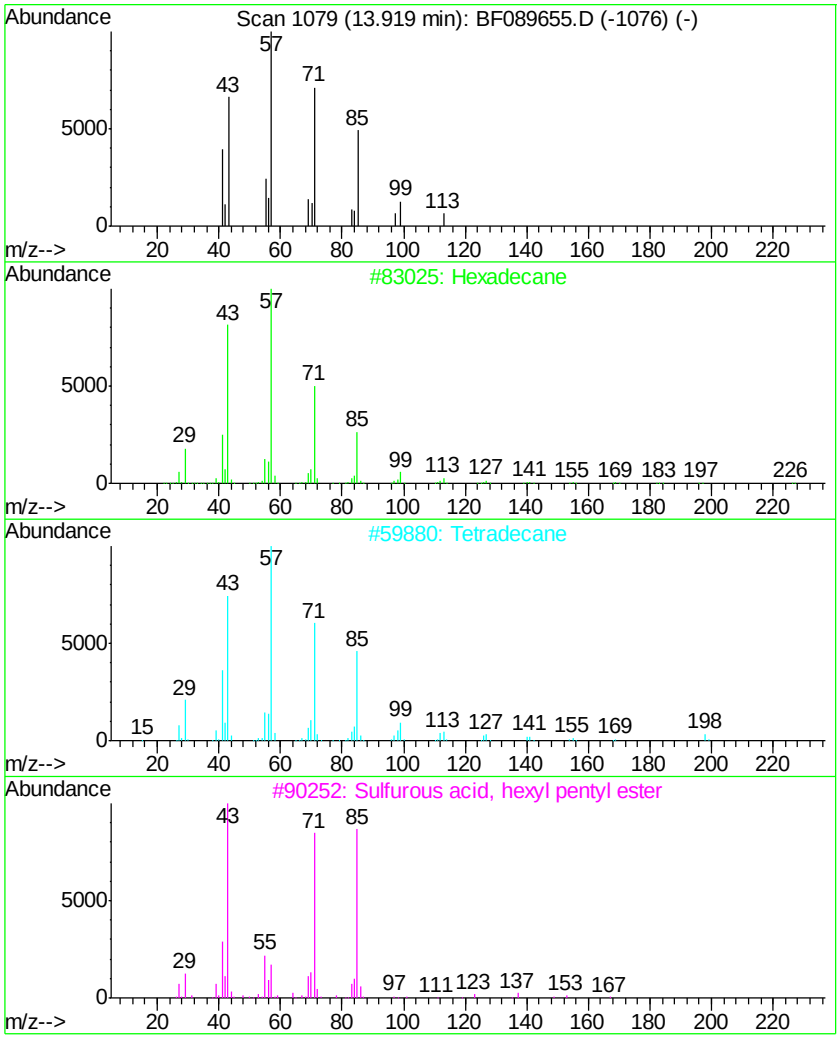
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

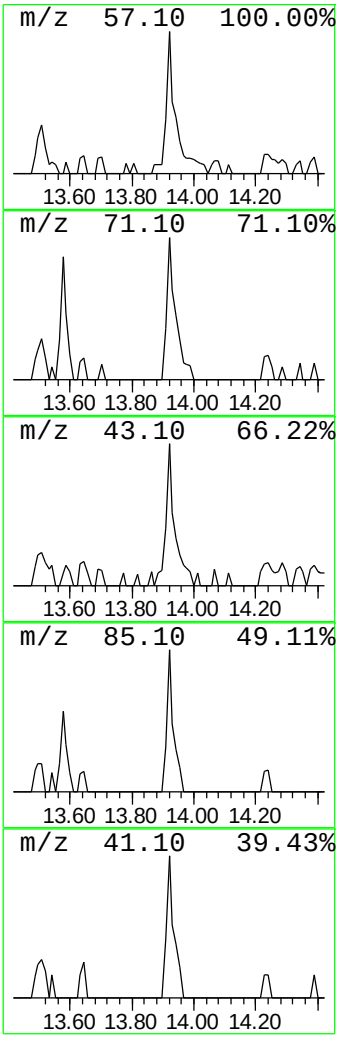
****

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.18 ng	34169	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tetradecane	198	C14H30	000629-59-4	78
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	72
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5	Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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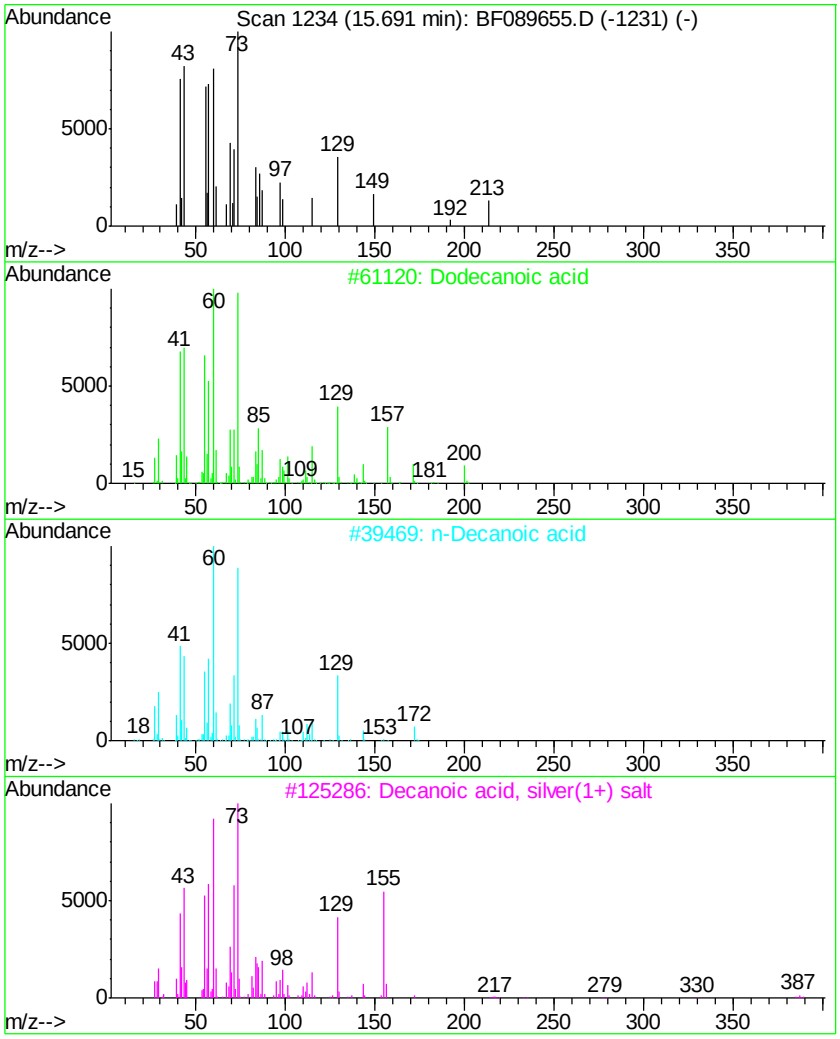
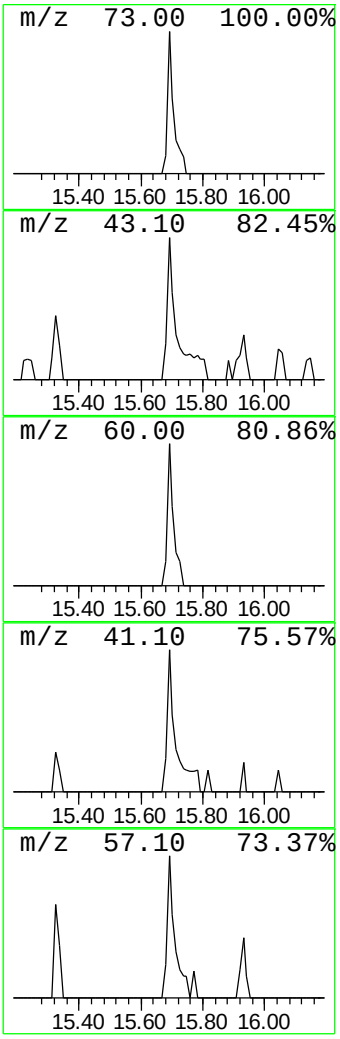
Peak Number 5 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.14 ng	33716	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47
4	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	27
5	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

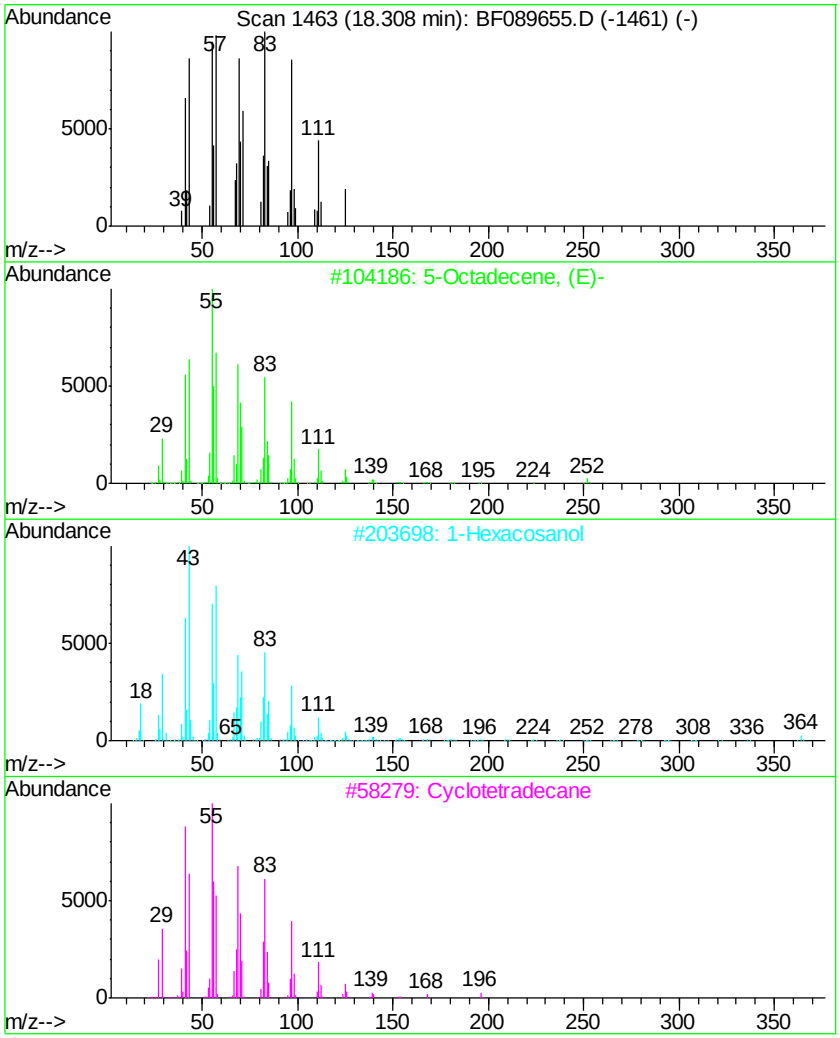
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

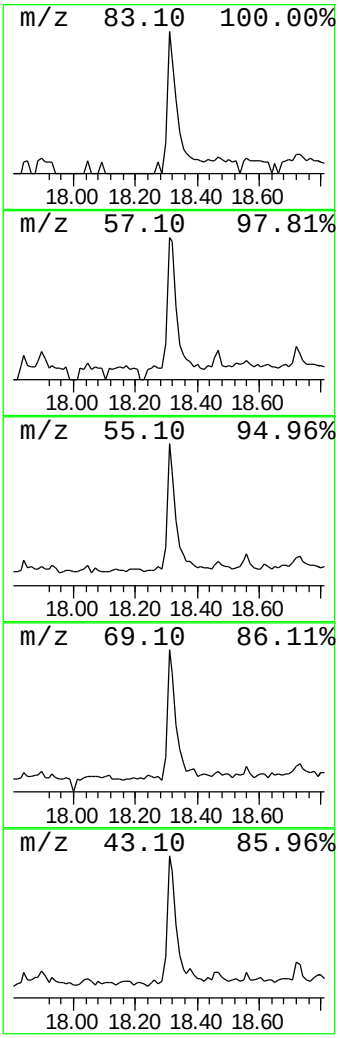
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	7.05 ng	85755	Chrysene-d12	18.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	78
2	1-Hexacosanol	382	C26H54O	000506-52-5	64
3	Cyclotetradecane	196	C14H28	000295-17-0	58
4	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	58
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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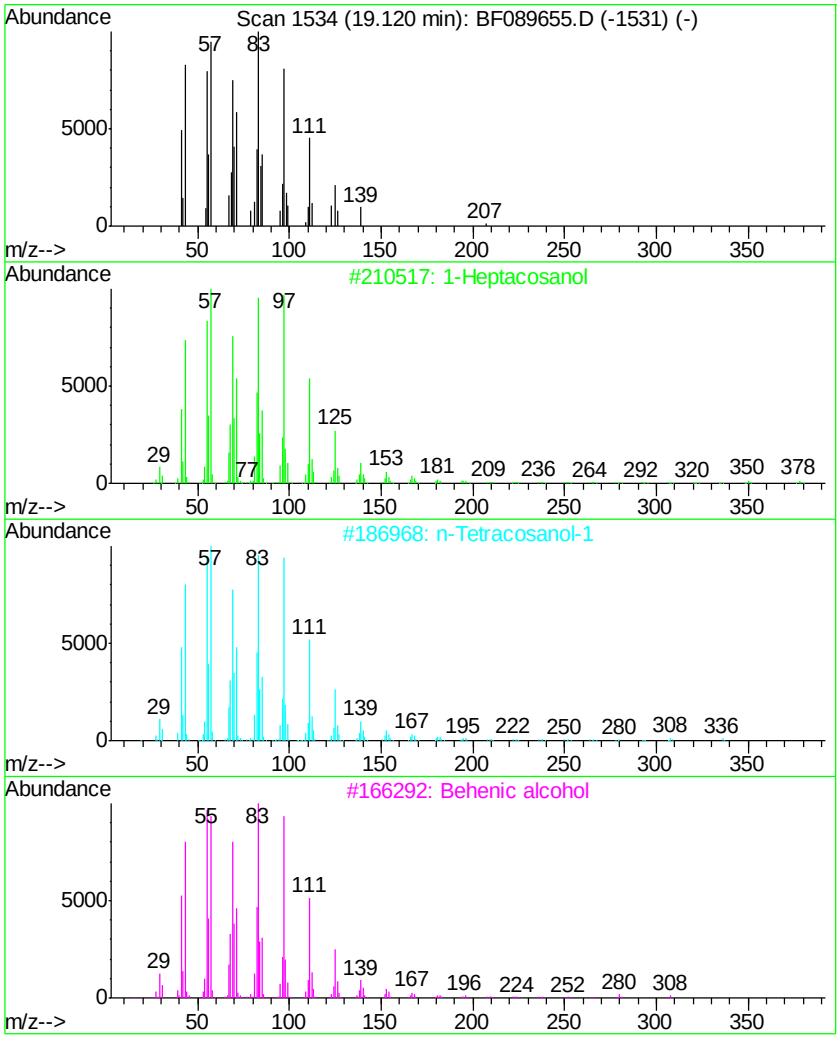
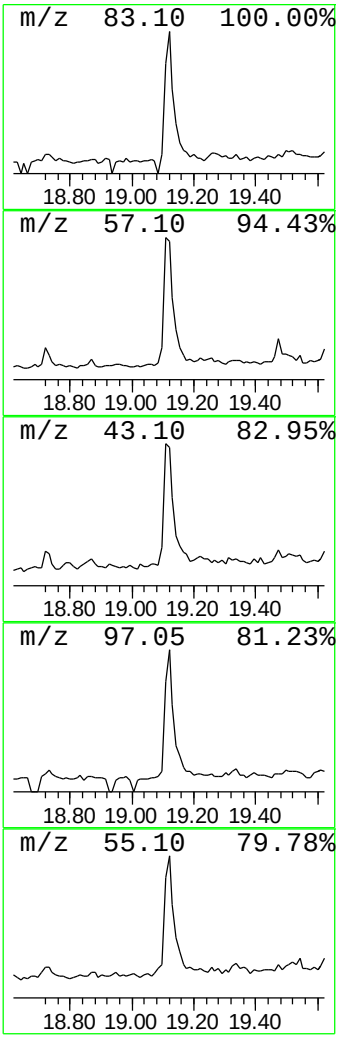
Peak Number 8 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	7.65 ng	93009	Chrysene-d12	18.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Octacosyl acetate	452	C30H60O2	018206-97-8	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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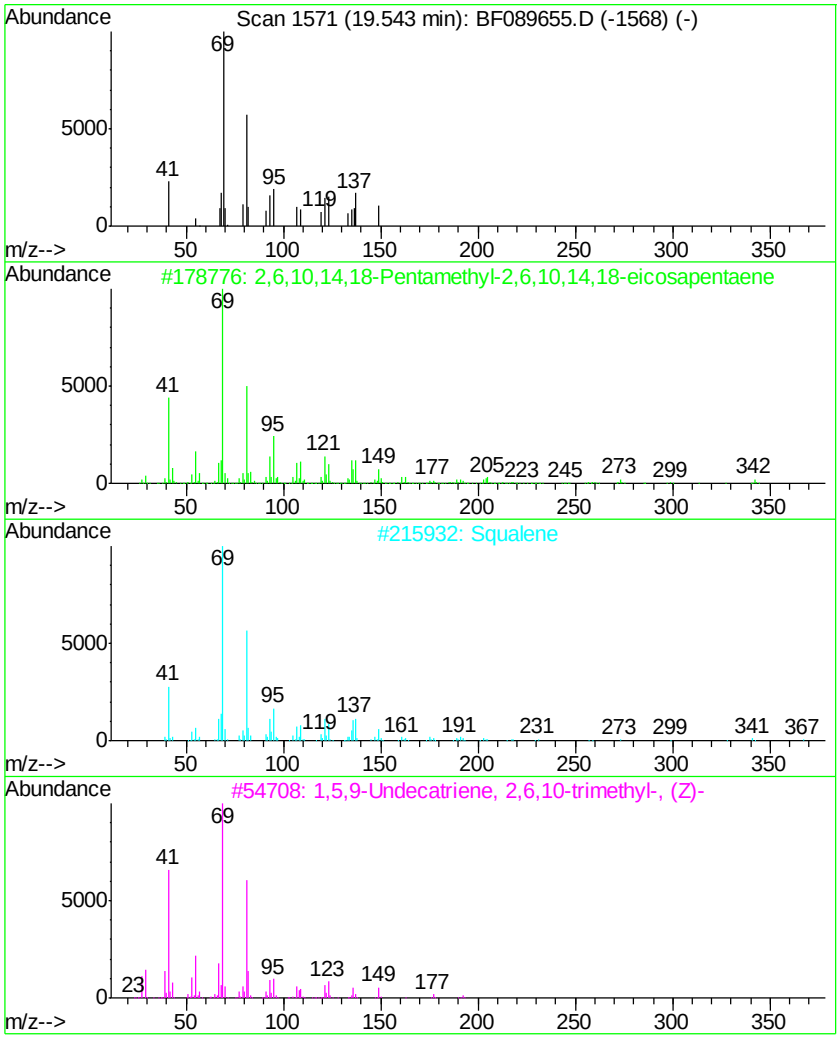
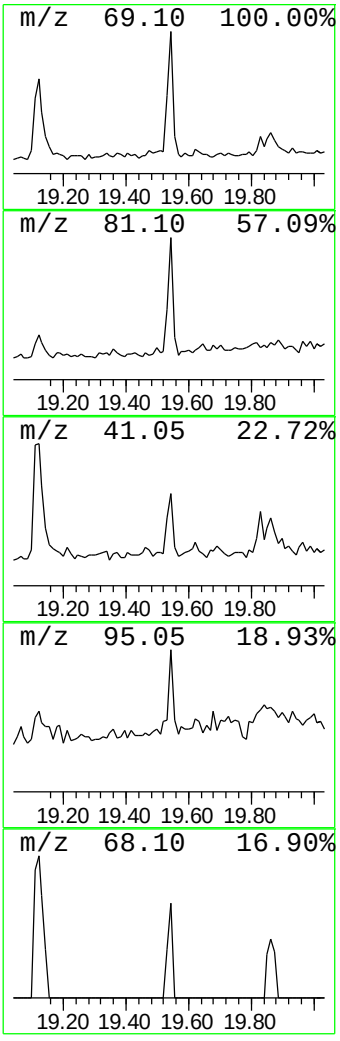
Peak Number 9 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	2.04 ng	20898	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	90
2	Squalene	410	C30H50	000111-02-4	78
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56
5	trans-Farnesol	222	C15H26O	000106-28-5	56





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Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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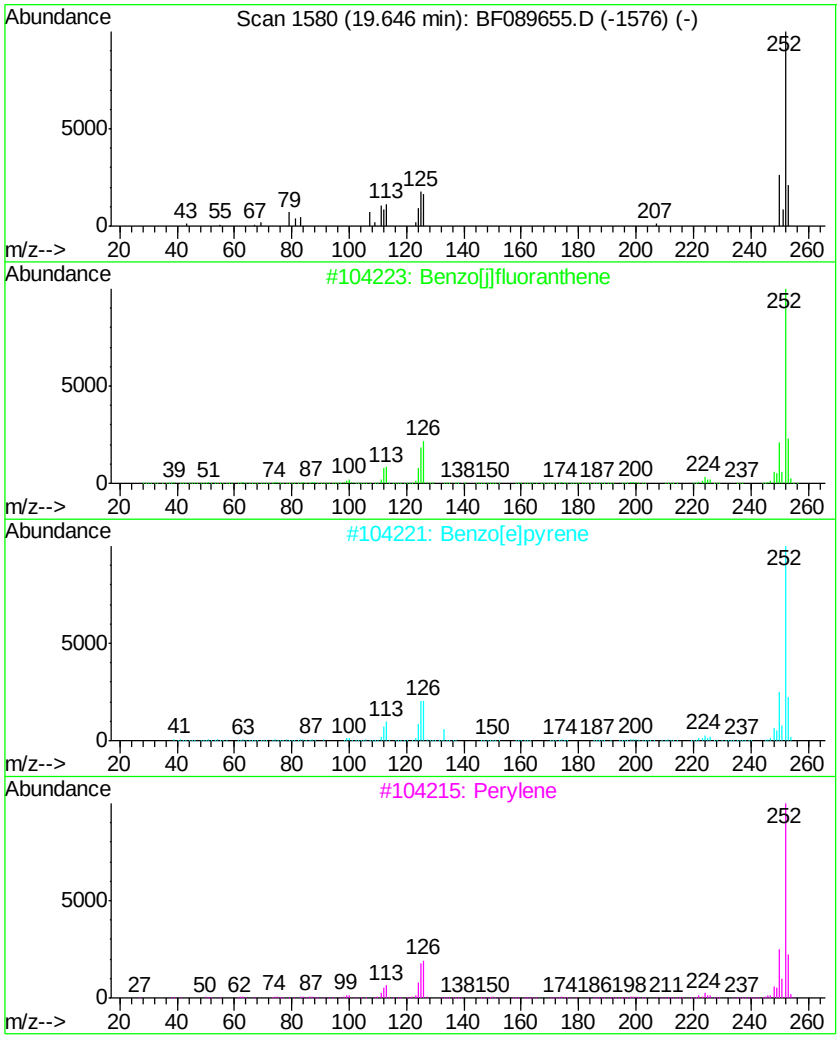
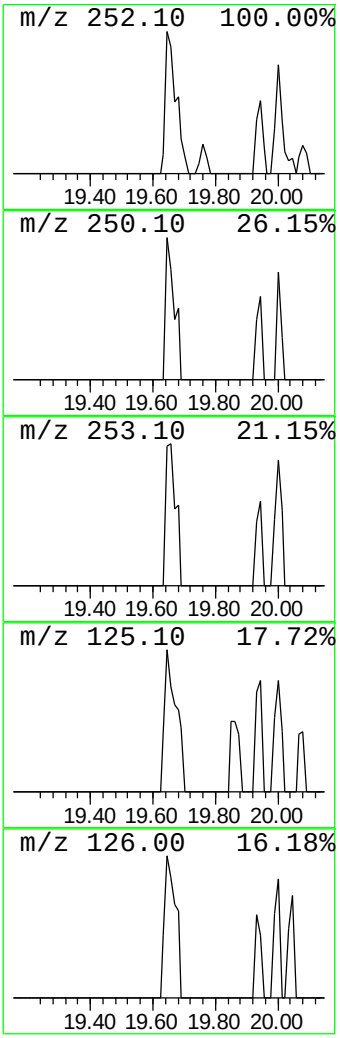
Peak Number 10 Benzo[j]fluoranthene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.65	2.97 ng	30490	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	87
2	Benzo[e]pyrene	252	C20H12	000192-97-2	87
3	Perylene	252	C20H12	000198-55-0	87
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	83
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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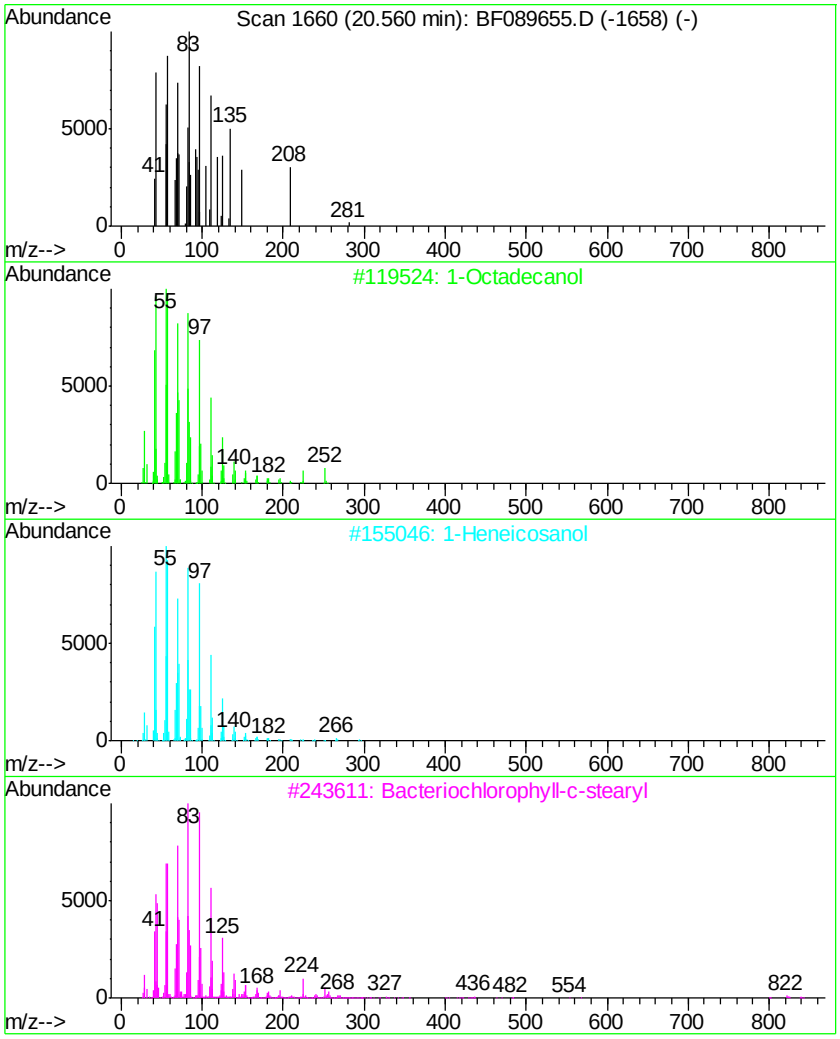
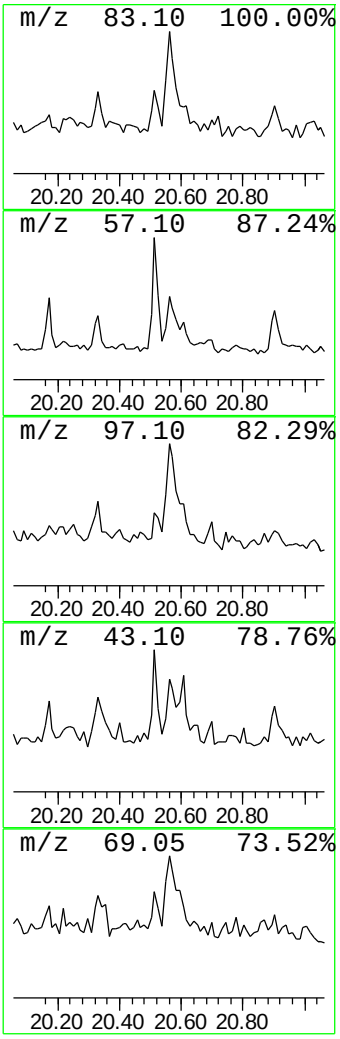
Peak Number 11 1-Octadecanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	2.46 ng	25269	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	58
2	1-Heneicosanol	312	C21H44O	015594-90-8	58
3	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	58
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	52
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	52





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Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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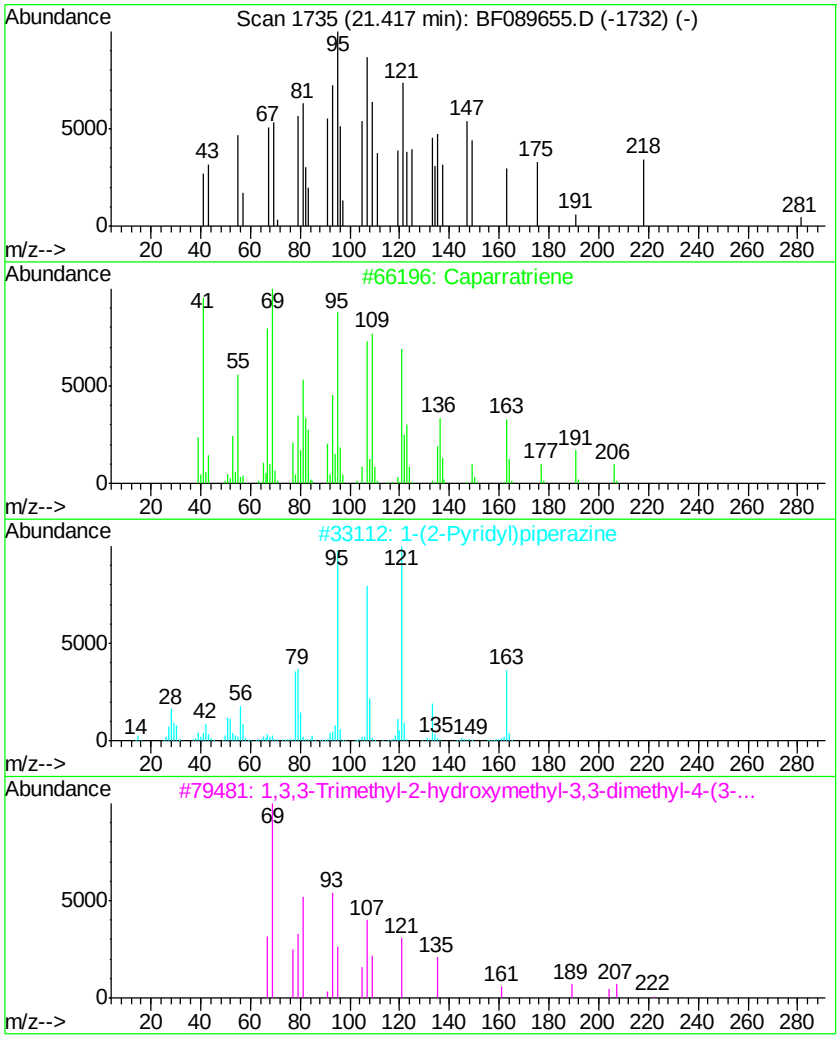
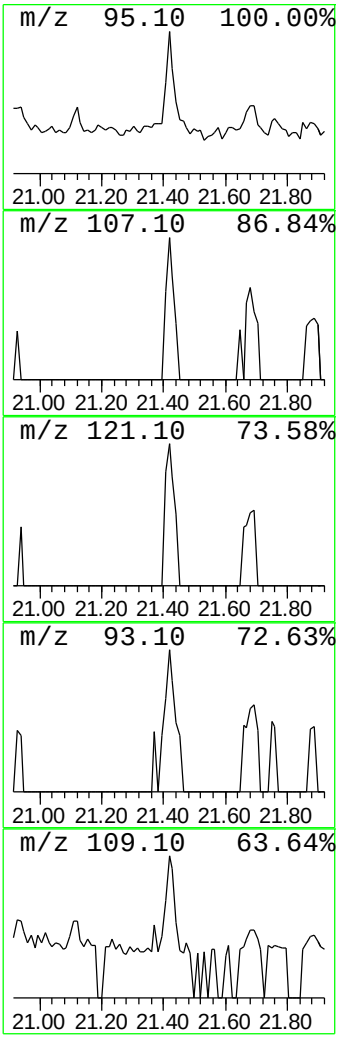
Peak Number 12 unknown21.42 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.99 ng	30650	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	43
2	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	38
3	1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	35
4	Methyl 3-cis,9-cis,12-cis-octade...	292	C19H32O2	1000336-38-4	32
5	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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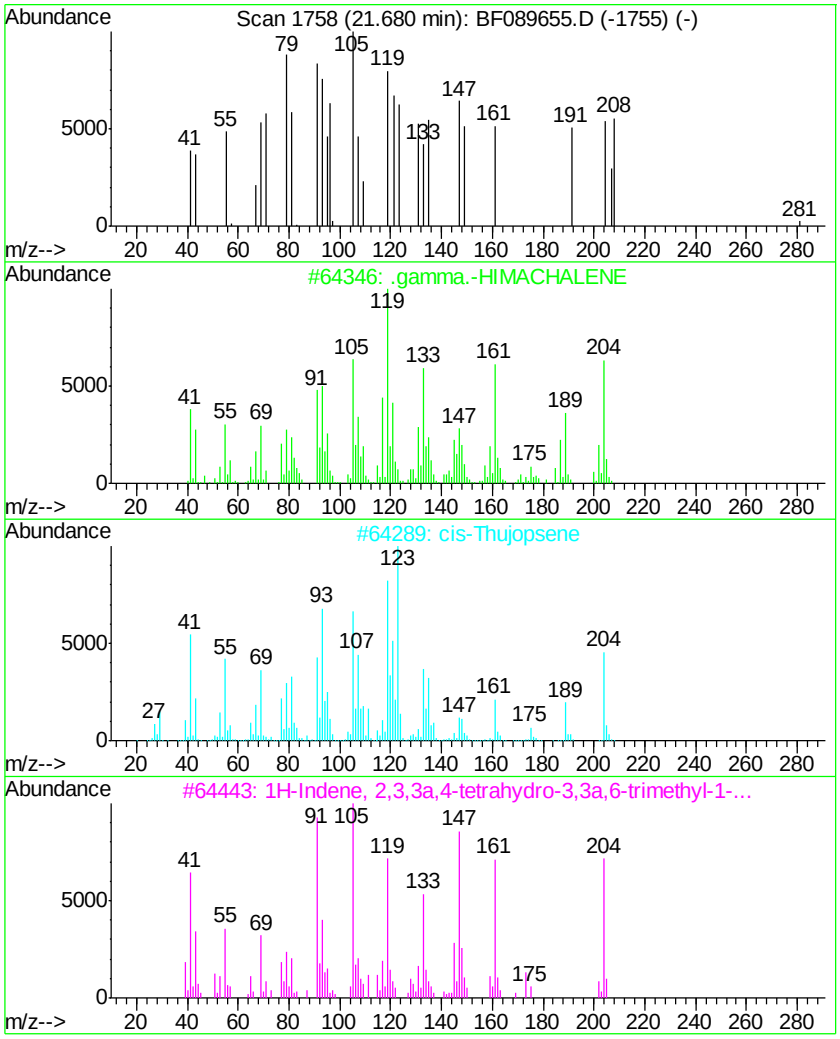
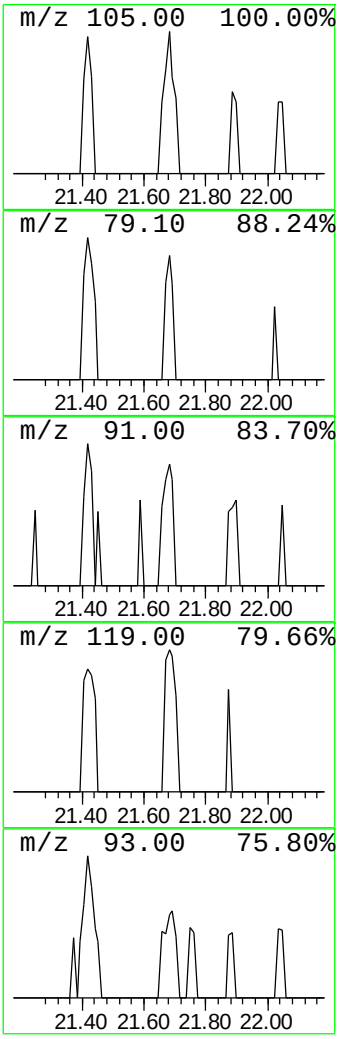
Peak Number 13 unknown21.68 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.68	2.25 ng	23126	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-HIMACHALENE	204	C15H24	1000140-08-0	38
2	cis-Thujopsene	204	C15H24	000470-40-6	38
3	1H-Indene, 2,3,3a,4-tetrahydro-3...	204	C15H24	059742-39-1	38
4	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	35
5	4,7-Methanoazulene, 1,2,3,4,5,6,...	204	C15H24	000514-51-2	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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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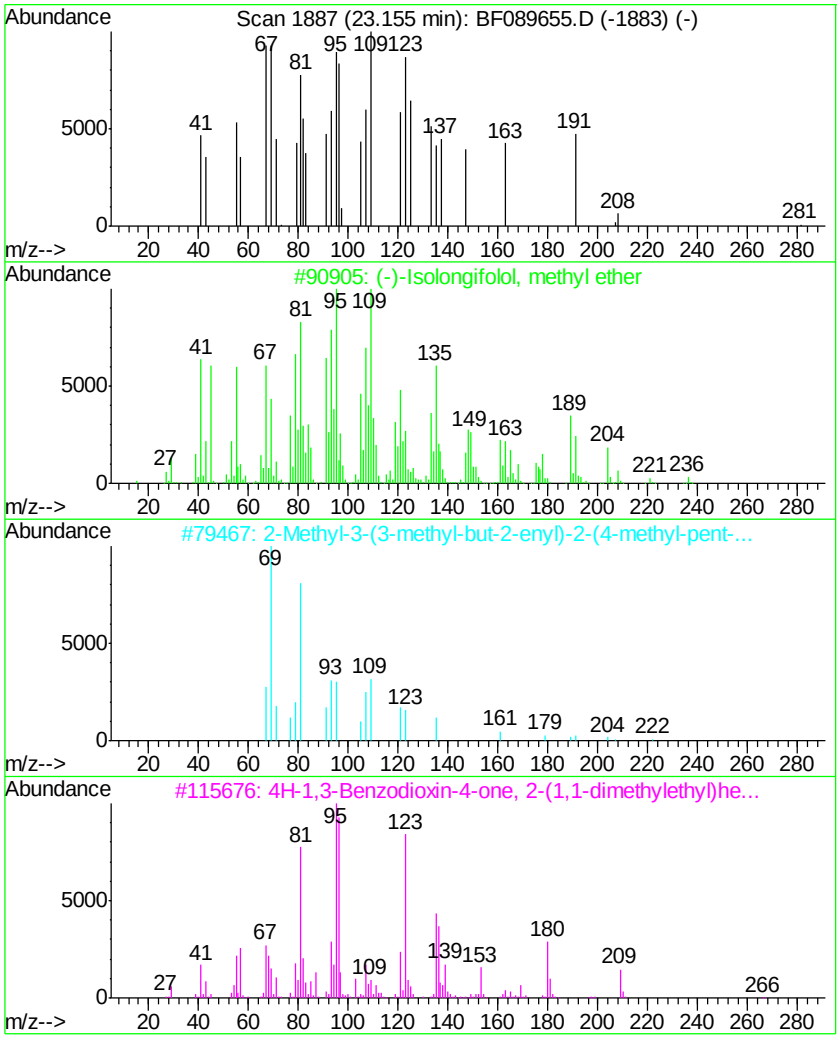
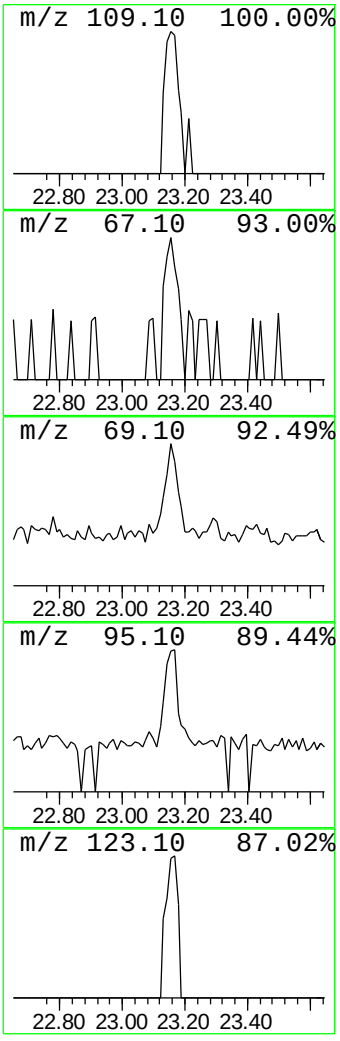
Peak Number 14 unknown23.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	3.57 ng	36642	Perylene-d12	20.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	35
2	2-Methyl-3-(3-methyl-but-2-enyl)...	222	C15H26O	1000144-10-2	27
3	4H-1,3-Benzodioxin-4-one, 2-(1,1...	266	C16H26O3	124899-18-9	27
4	5-Eicosyne	278	C20H38	074685-31-7	25
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089655.D
Acq On : 6 Aug 2016 7:32
Operator : UM/SJ
Sample : H4364-01
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMA-FL-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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...	4.66	34.3	ng	379579	1	7.44	221040	20.0
unknown7.10	7.10	140.7	ng	1554590	1	7.44	221040	20.0
Hexadecane	13.92	3.2	ng	34169	4	14.69	215028	20.0
Dodecanoic acid	15.69	3.1	ng	33716	4	14.69	215028	20.0
5-Octadecene, (E)-	18.31	7.0	ng	85755	5	18.39	243252	20.0
1-Heptacosanol	19.12	7.7	ng	93009	5	18.39	243252	20.0
2,6,10,14,18-Pent...	19.54	2.0	ng	20898	6	20.05	205262	20.0
Benzo[j]fluoranthene	19.65	3.0	ng	30490	6	20.05	205262	20.0
1-Octadecanol	20.56	2.5	ng	25269	6	20.05	205262	20.0
unknown21.42	21.42	3.0	ng	30650	6	20.05	205262	20.0
unknown21.68	21.68	2.3	ng	23126	6	20.05	205262	20.0
unknown23.15	23.15	3.6	ng	36642	6	20.05	205262	20.0