LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

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-BF101015.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	4.297	187	189	196	rBV	14911	24435	1.00%	0.102%
2	4.972	245	248	258	rVB	917516	1333911	54.69%	5.567%
3	5.394	283	285	288	rBV	1387499	1823566	74.76%	7.610%
4	5.794	318	320	323	rVB	32992	32385	1.33%	0.135%
5	6.446	374	377	379	rBV	1937572	1996471	81.85%	8.331%
6	6.572	385	388	390	rBV	2215558	2175211	89.18%	9.077%
7	6.800	406	408	413	rBV	618692	544408	22.32%	2.272%
8	6.960	419	422	424	rBV	1474117	1690476	69.30%	7.054%
9	7.372	456	458	461	rBV	1216463	1195126	49.00%	4.987%
10	8.092	518	521	523	rBV	780033	714939	29.31%	2.983%
11	9.178	613	616	618	rBV	1706475	2439195	100.00%	10.179%
12	9.566	648	650	653	rBV	424978	412563	16.91%	1.722%
13	9.852	672	675	677	rBV	809092	837323	34.33%	3.494%
14	10.183	701	704	706	rBV3	16771	30447	1.25%	0.127%
15	10.275	711	712	716	rVV	63336	56288	2.31%	0.235%
16	10.401	720	723	726	rVV	19311	32364	1.33%	0.135%
17	10.492	729	731	735	rVB	25755	43528	1.78%	0.182%
18	10.641	741	744	747	rBV	1454108	1451786	59.52%	6.058%
19	10.755	751	754	758	rVB	74187	121557	4.98%	0.507%
20	10.846	758	762	764	rBV5	10332	27068	1.11%	0.113%
21	11.075	780	782	786	rBV4	11236	25174	1.03%	0.105%
22	11.201	790	793	794	rBV	79876	73202	3.00%	0.305%
23	11.224	794	795	799	rVB2	40200	53652	2.20%	0.224%
24	11.338	803	805	806	rBV	908030	838692	34.38%	3.500%
25	11.418	809	812	813	rVB2	35472	54464	2.23%	0.227%
26	11.578	822	826	829	rBV5	31298	63152	2.59%	0.264%
27	11.624	829	830	832	rVB2	29810	30257	1.24%	0.126%
28	11.841	847	849	850	rBV	30907	33834	1.39%	0.141%
29	11.875	850	852	854	rVV	96519	156474	6.41%	0.653%
30	11.955	857	859	864	rVB2	51004	94470	3.87%	0.394%
31	12.115	871	873	876	rBV2	40327	58791	2.41%	0.245%
32	12.287	884	888	889	rBV3	11882	28496	1.17%	0.119%
33	12.389	895	897	899	rBV	27050	39156	1.61%	0.163%
34	12.424	899	900	903	rVB3	21258	24437	1.00%	0.102%

LSC Area Percent Report

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Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.549	909	911	914	rBV	265825	258119	10.58%	1.077%
36	12.652	918	920	922	rBV3	23468	34212	1.40%	0.143%
37	12.778	928	931	934	rBV	237492	305443	12.52%	1.275%
38	12.835	934	936	939	rVB2	21044	31803	1.30%	0.133%
39	12.927	942	944	947	rBV	2053918	2282106	93.56%	9.523%
40	13.109	957	960	962	rVB	37249	64556	2.65%	0.269%
41	13.178	962	966	968	rBV3	38776	74747	3.06%	0.312%
42	13.224	968	970	973	rVB3	25784	48248	1.98%	0.201%
43	13.852	1023	1025	1029	rBV2	90011	179997	7.38%	0.751%
44	14.001	1035	1038	1040	rBV	536162	826162	33.87%	3.448%
45	15.087	1131	1133	1137	rBV	64160	110580	4.53%	0.461%
46	15.441	1162	1164	1167	rBV	71307	114650	4.70%	0.478%
47	15.510	1167	1170	1175	rVV	379399	650004	26.65%	2.713%
48	15.624	1178	1180	1183	rVB3	50443	81372	3.34%	0.340%
49	16.161	1225	1227	1233	rVB	77742	169902	6.97%	0.709%
50	16.573	1261	1263	1268	rVB	55650	115400	4.73%	0.482%
51	17.121	1309	1311	1315	rVB2	30569	58536	2.40%	0.244%

Sum of corrected areas: 23963135

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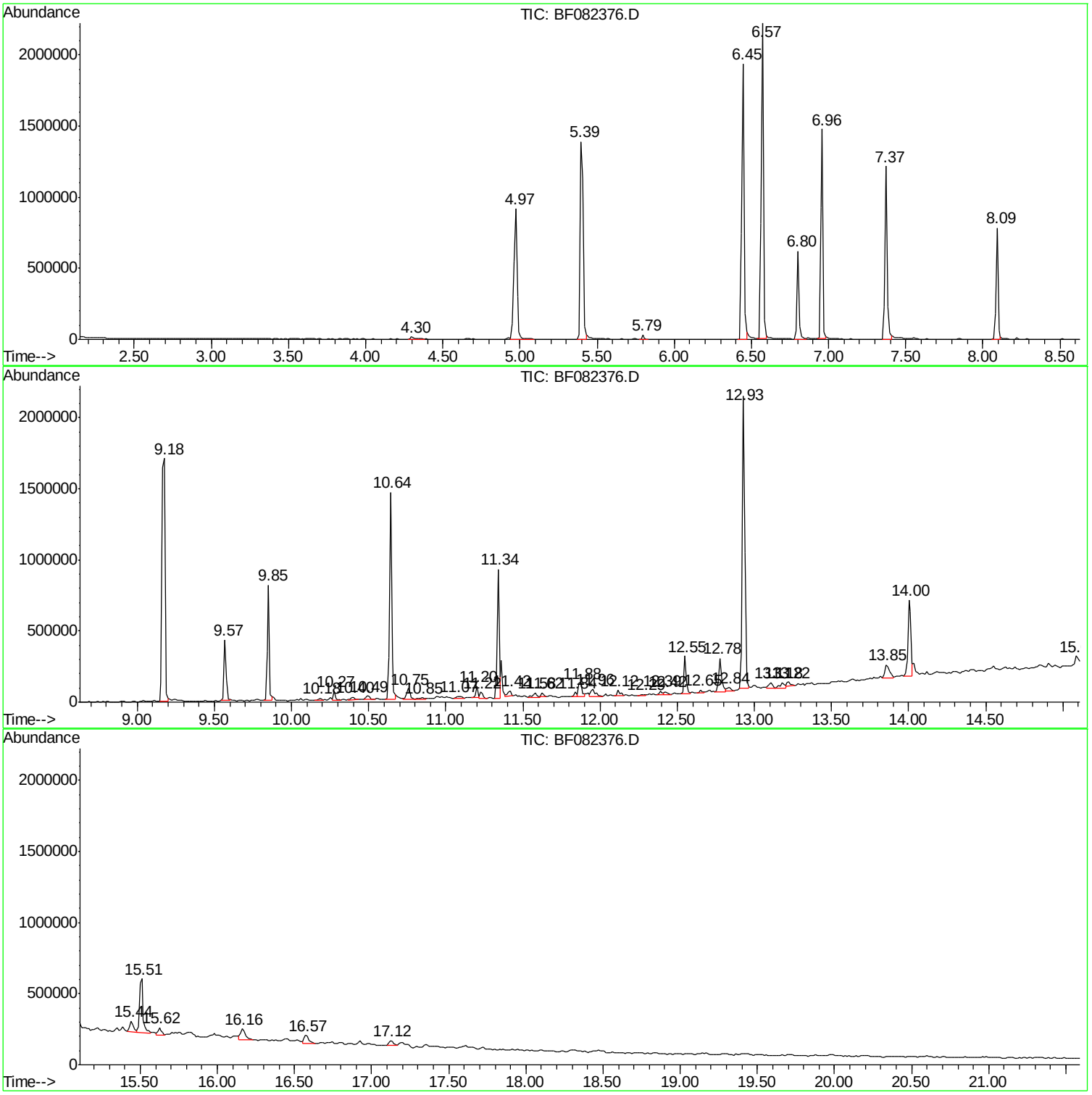
Instrument :
BNA_F
ClientSampleId :
IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

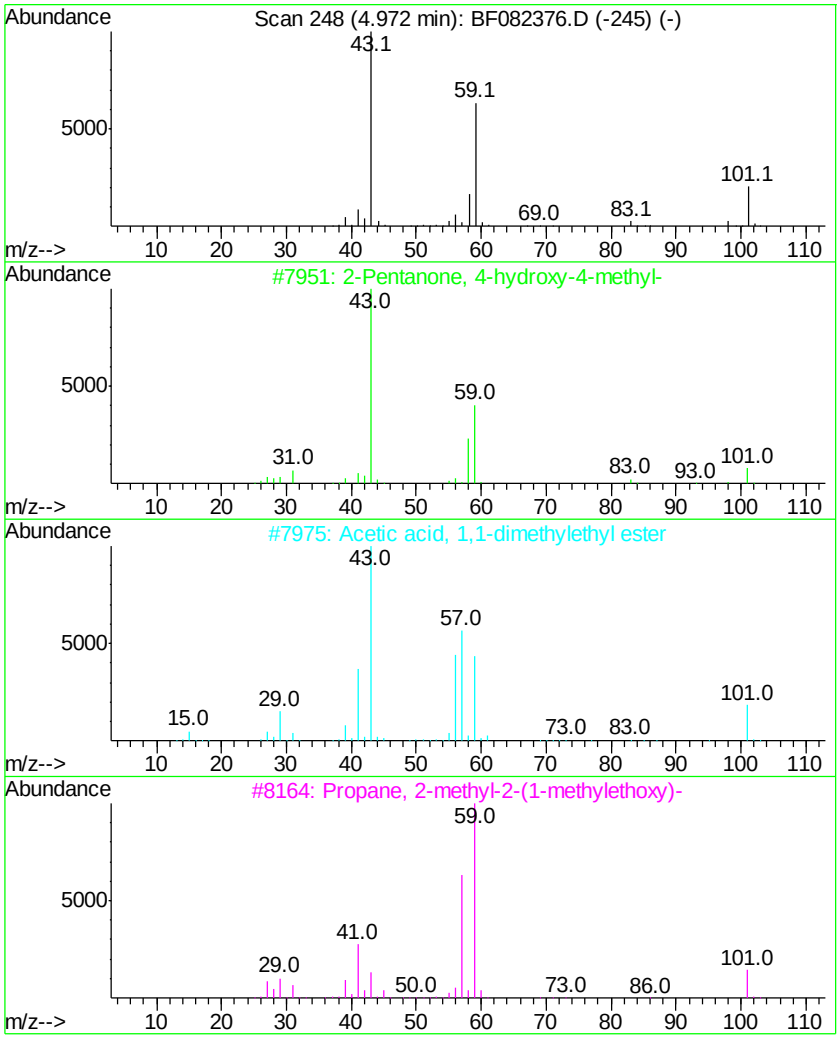
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

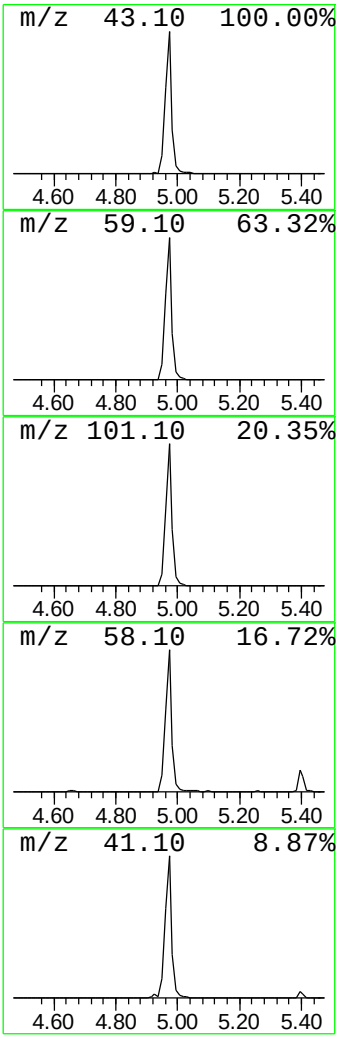
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	49.00 ng	1333910	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
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Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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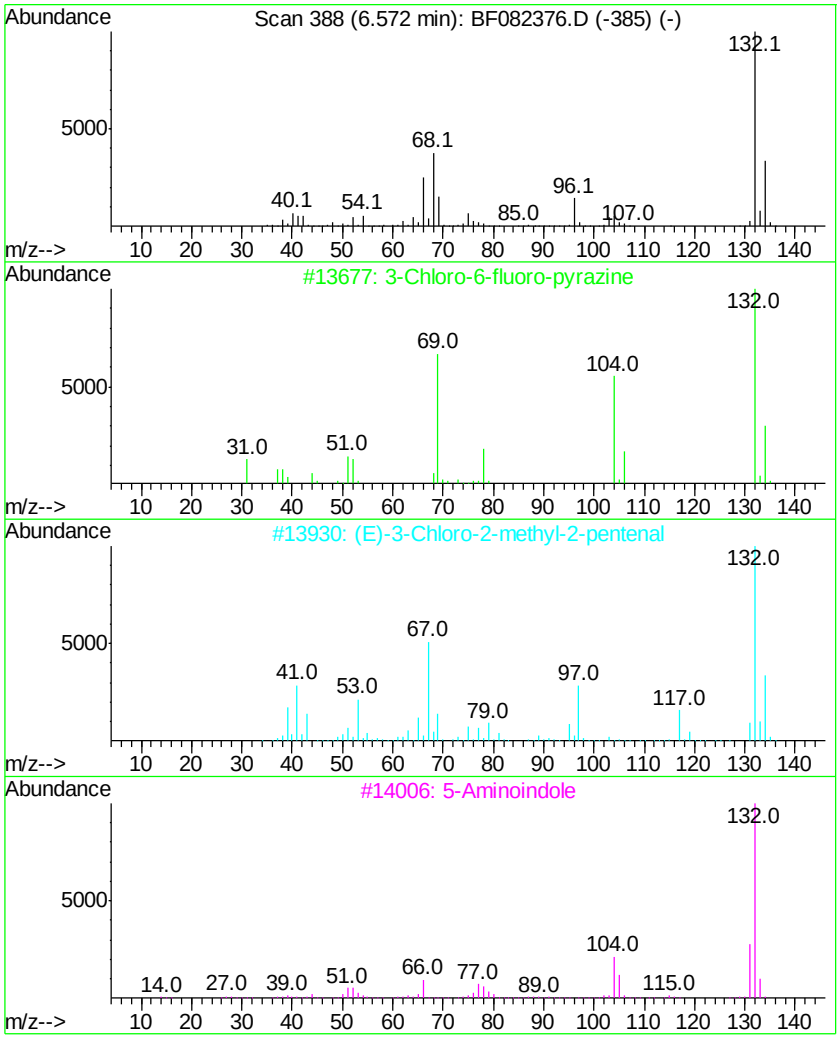
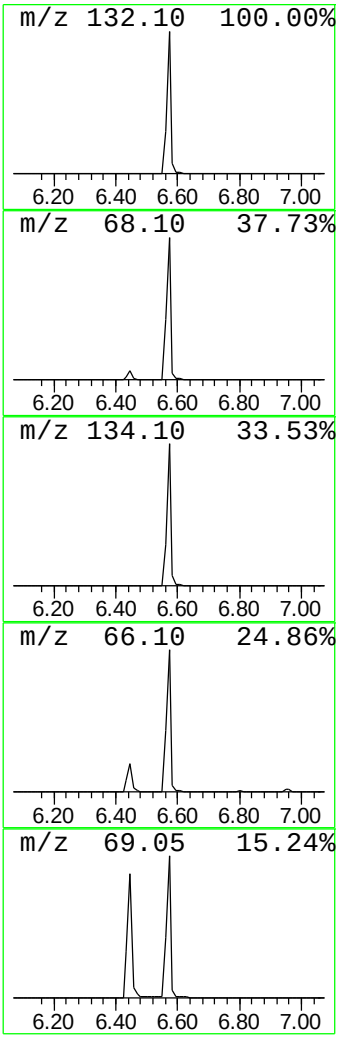
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	79.91 ng	2175210	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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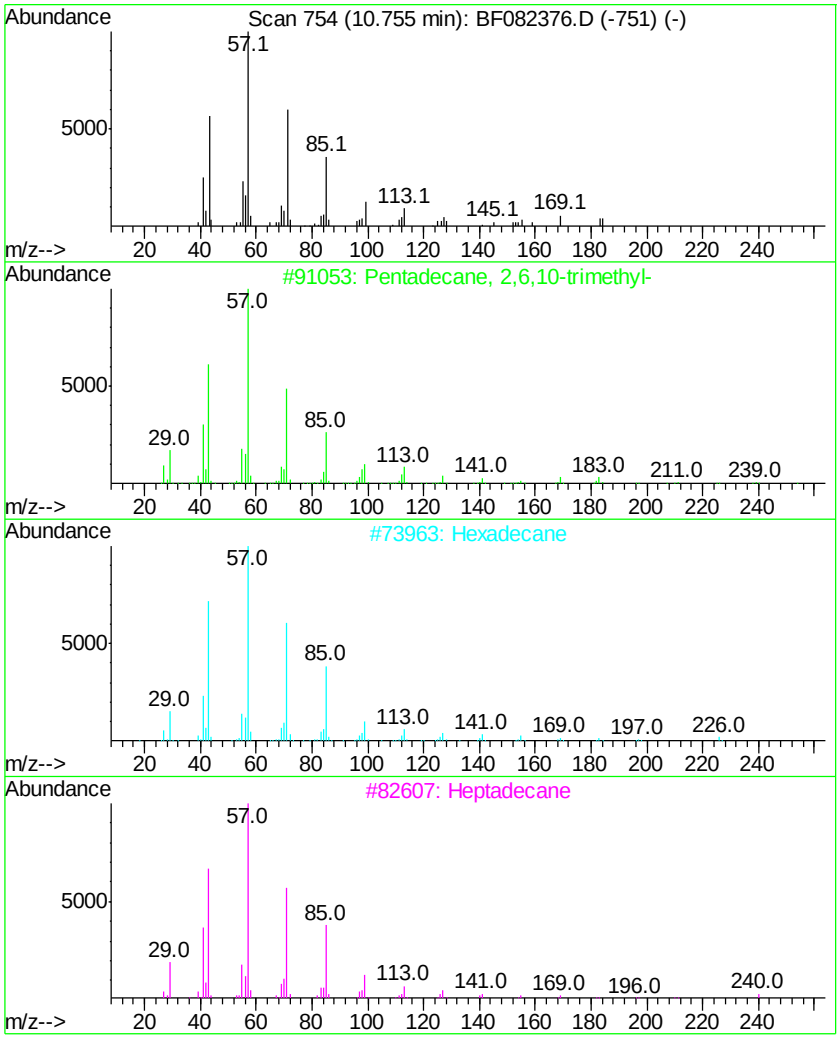
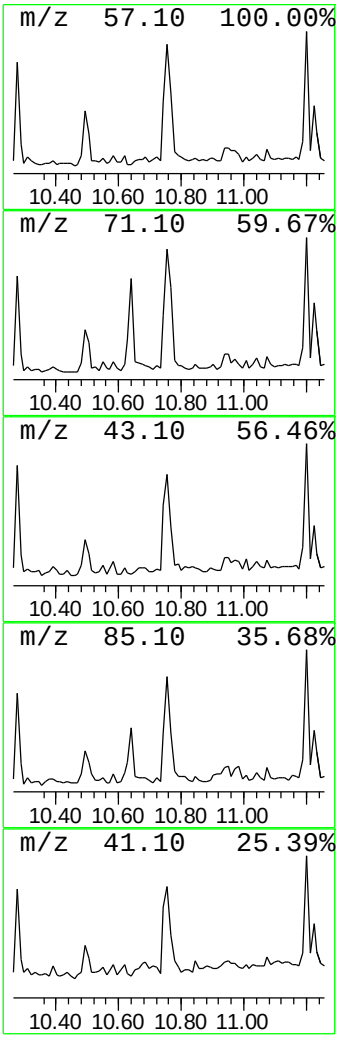
Peak Number 4 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.90 ng	121557	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
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Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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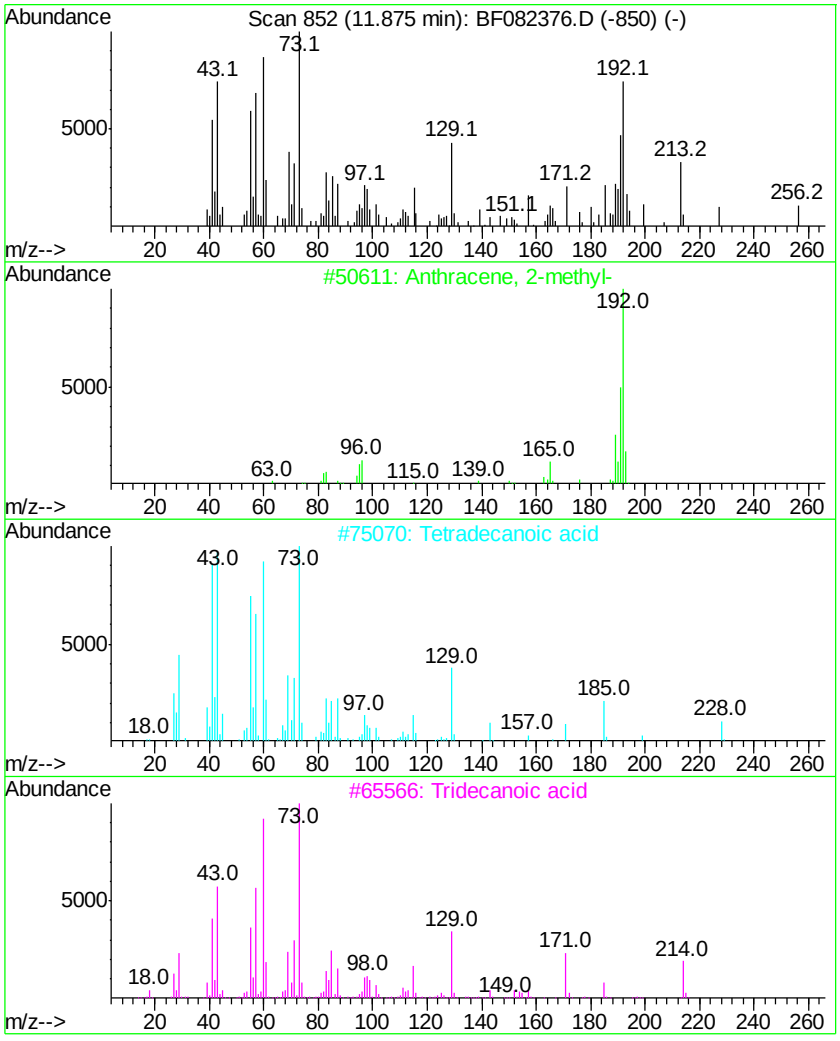
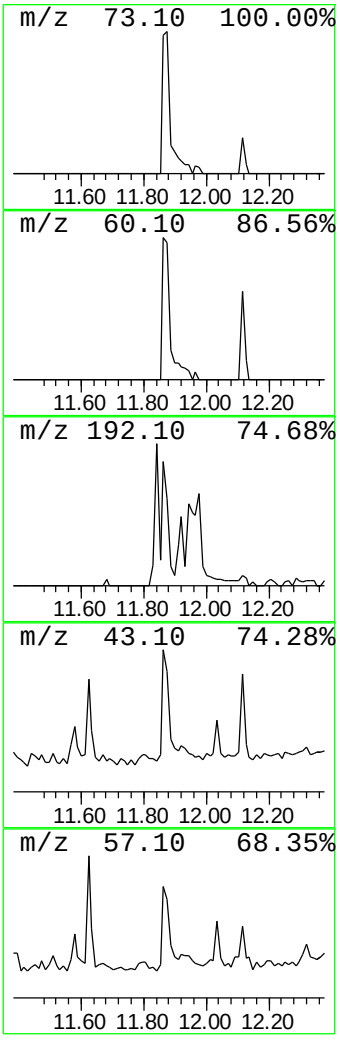
Peak Number 5 unknown11.88 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.73 ng	156474	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	30
3	Tridecanoic acid	214	C13H26O2	000638-53-9	30
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	25





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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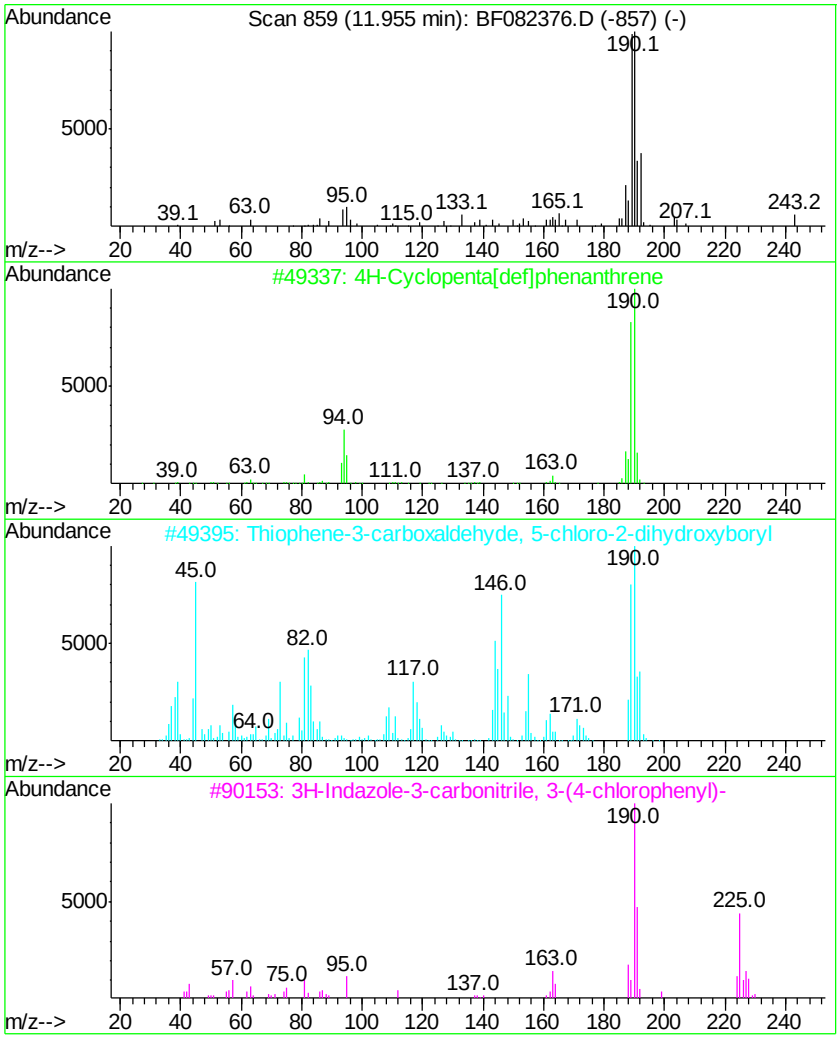
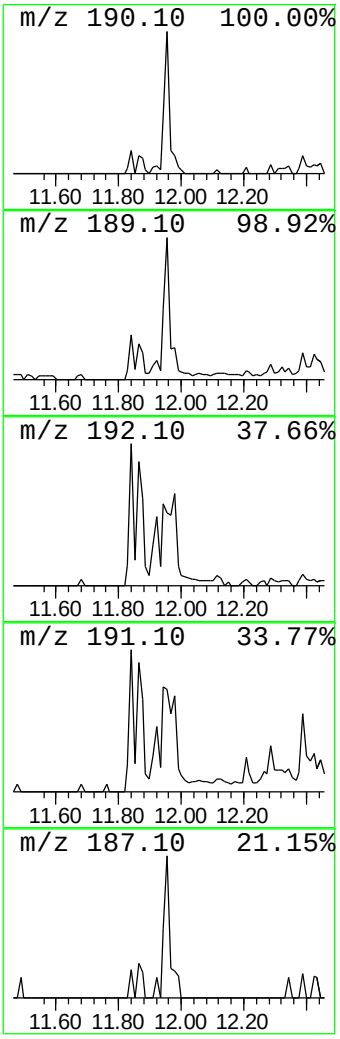
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.25 ng	94470	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
3	3H-Indazole-3-carbonitrile, 3-(4...	253	C14H8ClN3	056630-97-8	32
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	27
5	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	25





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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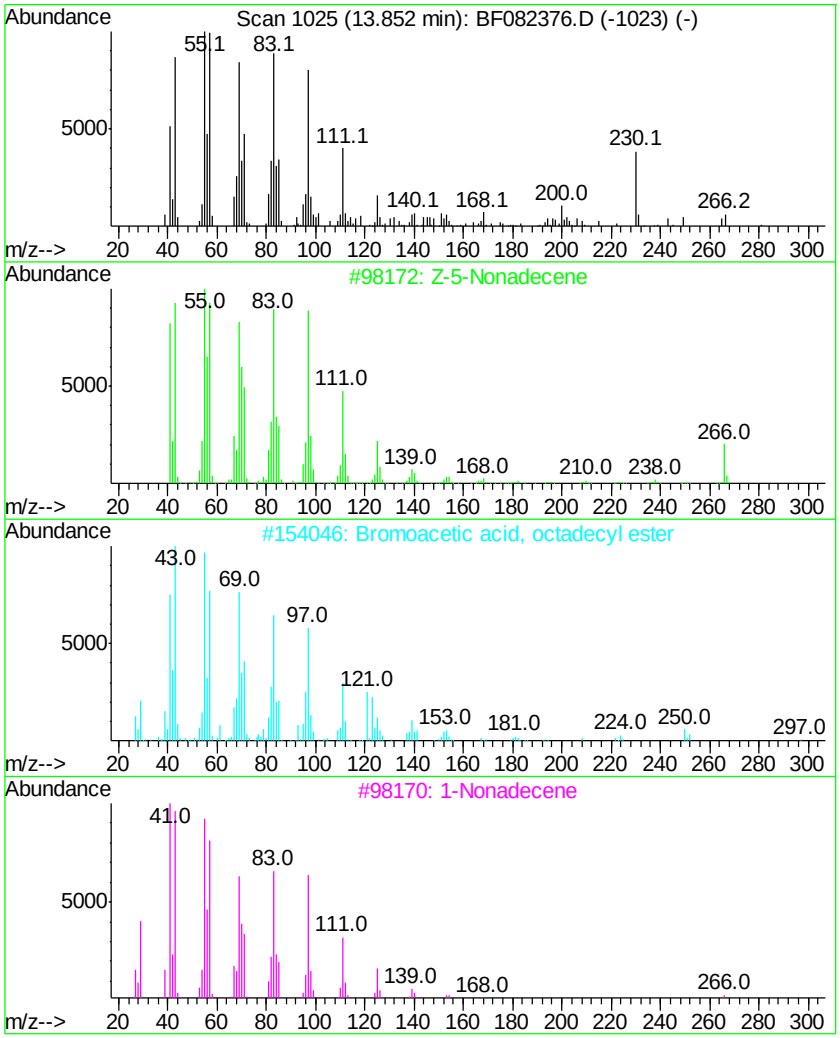
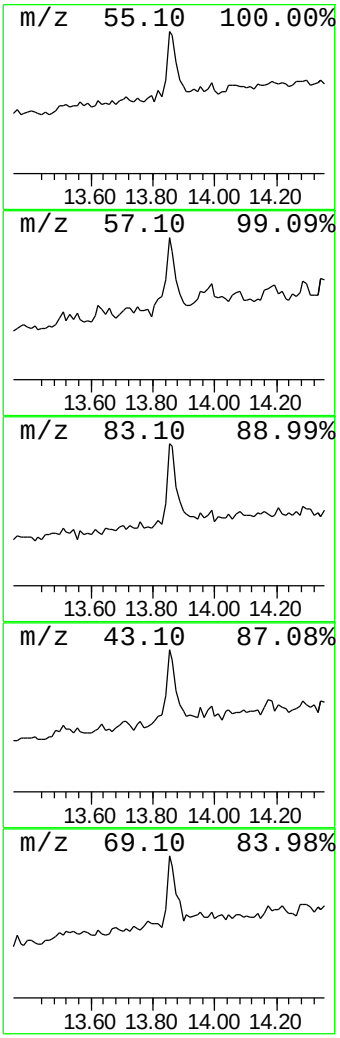
Peak Number 7 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.36 ng	179997	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	90
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
3	1-Nonadecene	266	C19H38	018435-45-5	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	1000280-07-3	64





Library Search Compound Report

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Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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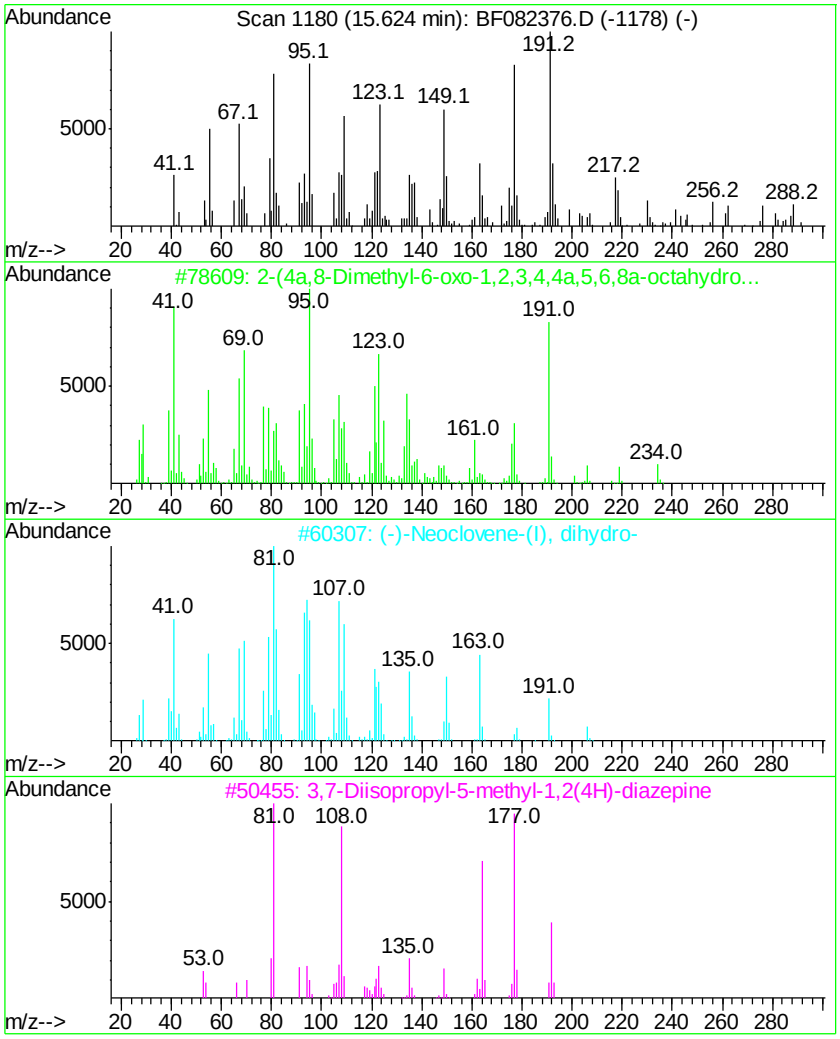
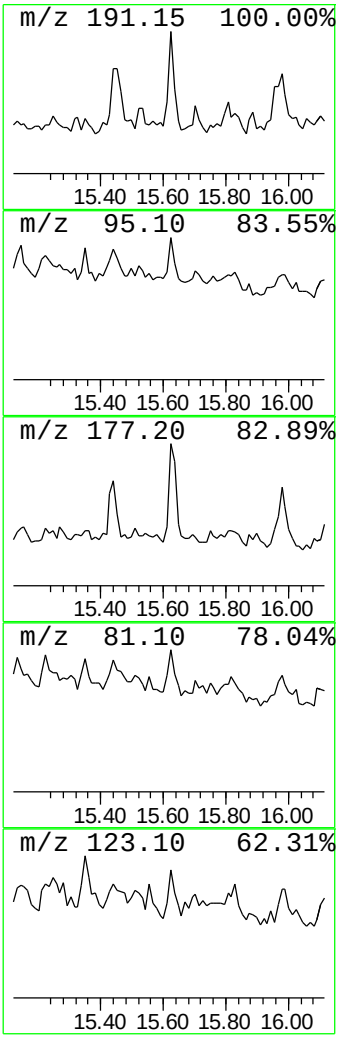
Peak Number 8 unknown15.62 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.50 ng	81372	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	38
2	(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	27
3	3,7-Diisopropyl-5-methyl-1,2(4H)...	192	C12H20N2	088829-71-4	27
4	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	14
5	Cyclodecene, 3-bromo-	216	C10H17Br	056325-56-5	14





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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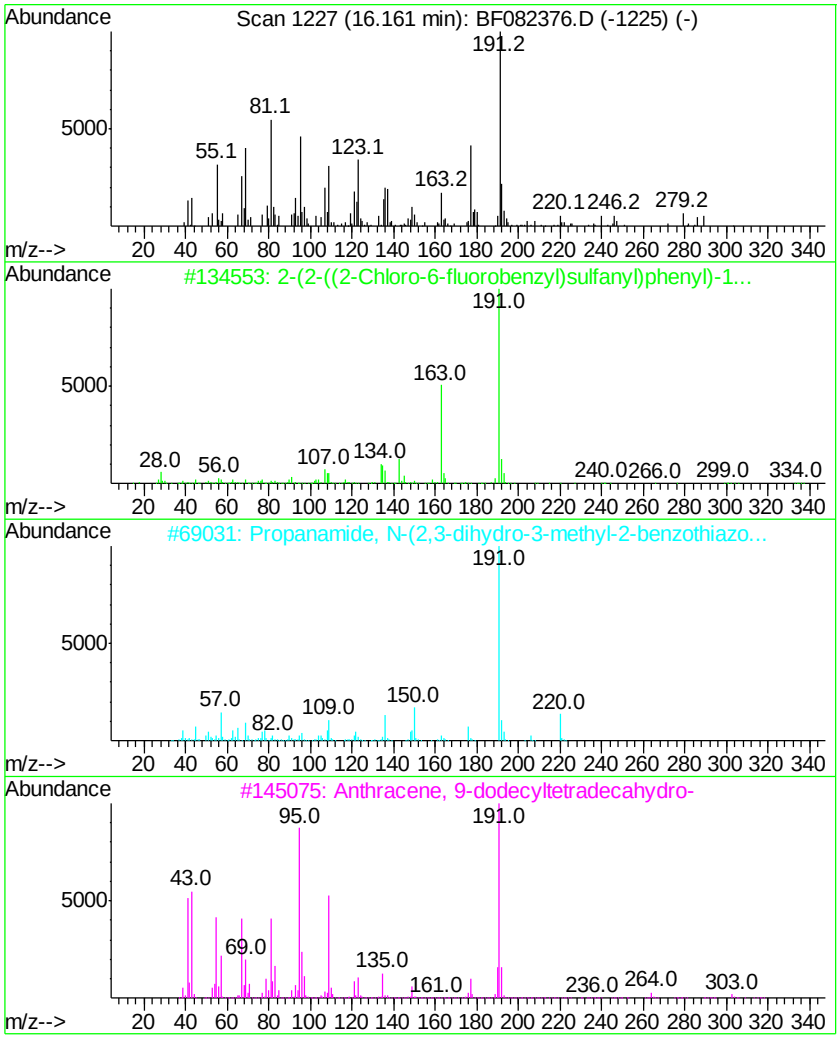
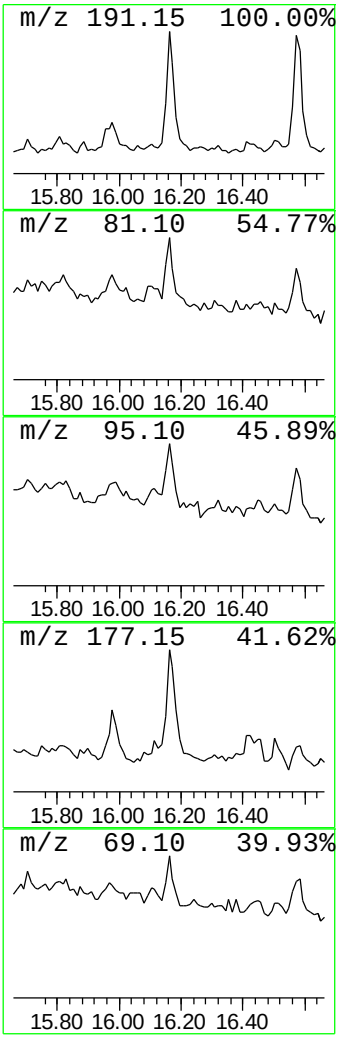
Peak Number 9 unknown16.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	5.23 ng	169902	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	35
2	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	27
3	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	25
4	N,N'-Ethylenebis(2-[2-hydroxyphe...	360	C18H20N2O6	001170-02-1	25
5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	22





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Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

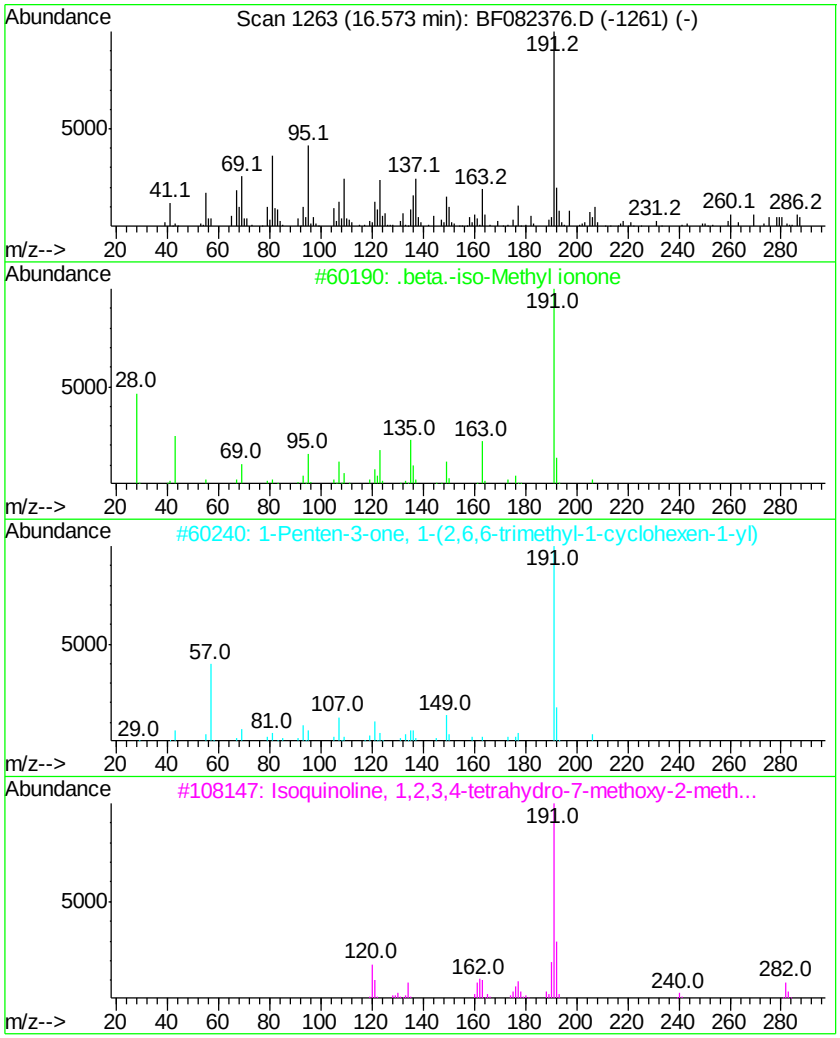
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

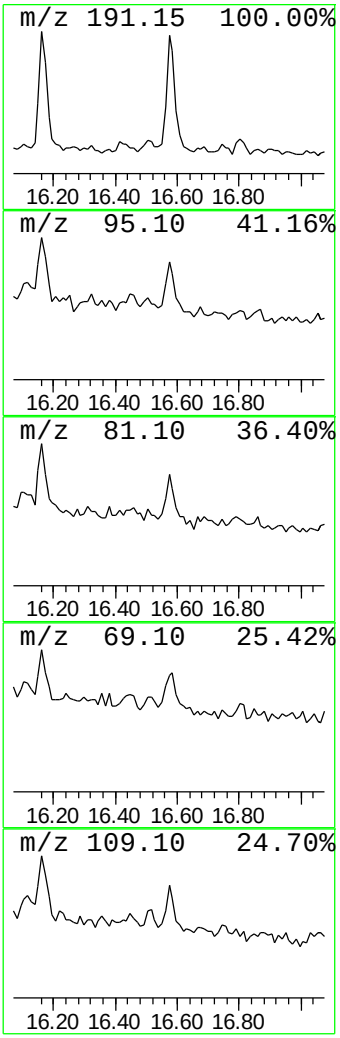
****

Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	3.55 ng	115400	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	64
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
3	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	38
4	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37
5	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	35





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF101915\
Data File : BF082376.D
Acq On : 20 Oct 2015 2:10
Operator : UM/IZ
Sample : G4040-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	49.0	ng	1333910	1	6.80	544408	20.0
unknown6.57	6.57	79.9	ng	2175210	1	6.80	544408	20.0
Pentadecane, 2,6,...	10.76	2.9	ng	121557	4	11.34	838692	20.0
unknown11.88	11.88	3.7	ng	156474	4	11.34	838692	20.0
4H-Cyclopenta[def...	11.96	2.3	ng	94470	4	11.34	838692	20.0
Z-5-Nonadecene	13.85	4.4	ng	179997	5	14.01	826162	20.0
unknown15.62	15.62	2.5	ng	81372	6	15.51	650004	20.0
unknown16.16	16.16	5.2	ng	169902	6	15.51	650004	20.0
.beta.-iso-Methyl...	16.57	3.5	ng	115400	6	15.51	650004	20.0