LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

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-BF112916.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	5.053	238	242	247	rBV	1010233	1679032	36.98%	3.725%
2	5.464	275	278	280	rBV	4110837	4098891	90.27%	9.092%
3	6.493	365	368	371	rBV	3922631	4540481	100.00%	10.072%
4	6.630	377	380	382	rBV	4363309	4352060	95.85%	9.654%
5	6.859	398	400	402	rBV	1276507	1035972	22.82%	2.298%
6	7.019	411	414	416	rBV	3727041	3297656	72.63%	7.315%
7	7.419	446	449	452	rBV	2091719	2506740	55.21%	5.561%
8	8.150	510	513	515	rBV	910925	1274297	28.07%	2.827%
9	9.225	604	607	609	rBV	5009561	4446817	97.94%	9.864%
10	9.613	639	641	644	rBV	449131	373933	8.24%	0.829%
11	9.899	663	666	668	rBV	1661258	1422965	31.34%	3.157%
12	10.333	703	704	706	rVB	88687	82113	1.81%	0.182%
13	10.562	720	724	726	rBV2	32282	54084	1.19%	0.120%
14	10.688	732	735	737	rBV	2270238	2499994	55.06%	5.546%
15	10.813	744	746	750	rBV	104178	153777	3.39%	0.341%
16	11.259	781	785	786	rBV	111524	122570	2.70%	0.272%
17	11.385	793	796	799	rBV	1014881	1511858	33.30%	3.354%
18	11.454	799	802	804	rVB	103725	95714	2.11%	0.212%
19	11.682	820	822	824	rBV	57555	53774	1.18%	0.119%
20	11.842	833	836	838	rBV	59812	98626	2.17%	0.219%
21	11.911	840	842	845	rVV2	506219	624496	13.75%	1.385%
22	11.991	847	849	854	rVB2	110104	161410	3.55%	0.358%
23	12.174	863	865	869	rVB3	44938	76882	1.69%	0.171%
24	12.425	885	887	889	rBV	40011	51038	1.12%	0.113%
25	12.585	899	901	903	rBV	549011	581243	12.80%	1.289%
26	12.619	903	904	909	rVV3	56293	89920	1.98%	0.199%
27	12.699	909	911	918	rVV2	307628	357921	7.88%	0.794%
28	12.814	918	921	924	rBV	542847	607131	13.37%	1.347%
29	12.974	932	935	937	rVB	2427654	3377016	74.38%	7.491%
30	13.042	937	941	944	rVV3	39447	72741	1.60%	0.161%
31	13.145	944	950	952	rVB2	71856	119651	2.64%	0.265%
32	13.248	957	959	960	rBV	71772	66626	1.47%	0.148%
33	13.442	972	976	981	rVB7	15803	50687	1.12%	0.112%
34	13.545	981	985	989	rBV4	27112	85262	1.88%	0.189%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

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-BF112916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.648	992	994	997	rVB	47363	55914	1.23%	0.124%
36	13.762	1001	1004	1005	rBV2	48885	78029	1.72%	0.173%
37	13.808	1005	1008	1011	rVV2	31681	109512	2.41%	0.243%
38	13.865	1011	1013	1017	rVB2	271021	283809	6.25%	0.630%
39	14.014	1023	1026	1027	rBV2	1309716	1405842	30.96%	3.119%
40	14.117	1033	1035	1039	rBV2	51602	72912	1.61%	0.162%
41	14.402	1055	1060	1061	rBV	55799	91075	2.01%	0.202%
42	14.494	1066	1068	1074	rVB6	46480	164606	3.63%	0.365%
43	14.871	1098	1101	1104	rBV	460790	457701	10.08%	1.015%
44	15.031	1112	1115	1120	rBV	211449	434353	9.57%	0.964%
45	15.134	1122	1124	1127	rVB2	59696	87617	1.93%	0.194%
46	15.328	1138	1141	1143	rVB	116089	167269	3.68%	0.371%
47	15.385	1143	1146	1149	rBV	165199	209402	4.61%	0.465%
48	15.443	1149	1151	1154	rBV	584946	858006	18.90%	1.903%
49	15.957	1194	1196	1204	rVB7	38300	106678	2.35%	0.237%
50	16.140	1209	1212	1217	rVB7	23354	59011	1.30%	0.131%
51	16.300	1223	1226	1231	rVB6	28817	71629	1.58%	0.159%
52	16.677	1257	1259	1263	rVB3	29337	60595	1.33%	0.134%
53	16.837	1270	1273	1278	rVB2	67270	147365	3.25%	0.327%
54	17.260	1306	1310	1317	rVB	49468	135373	2.98%	0.300%

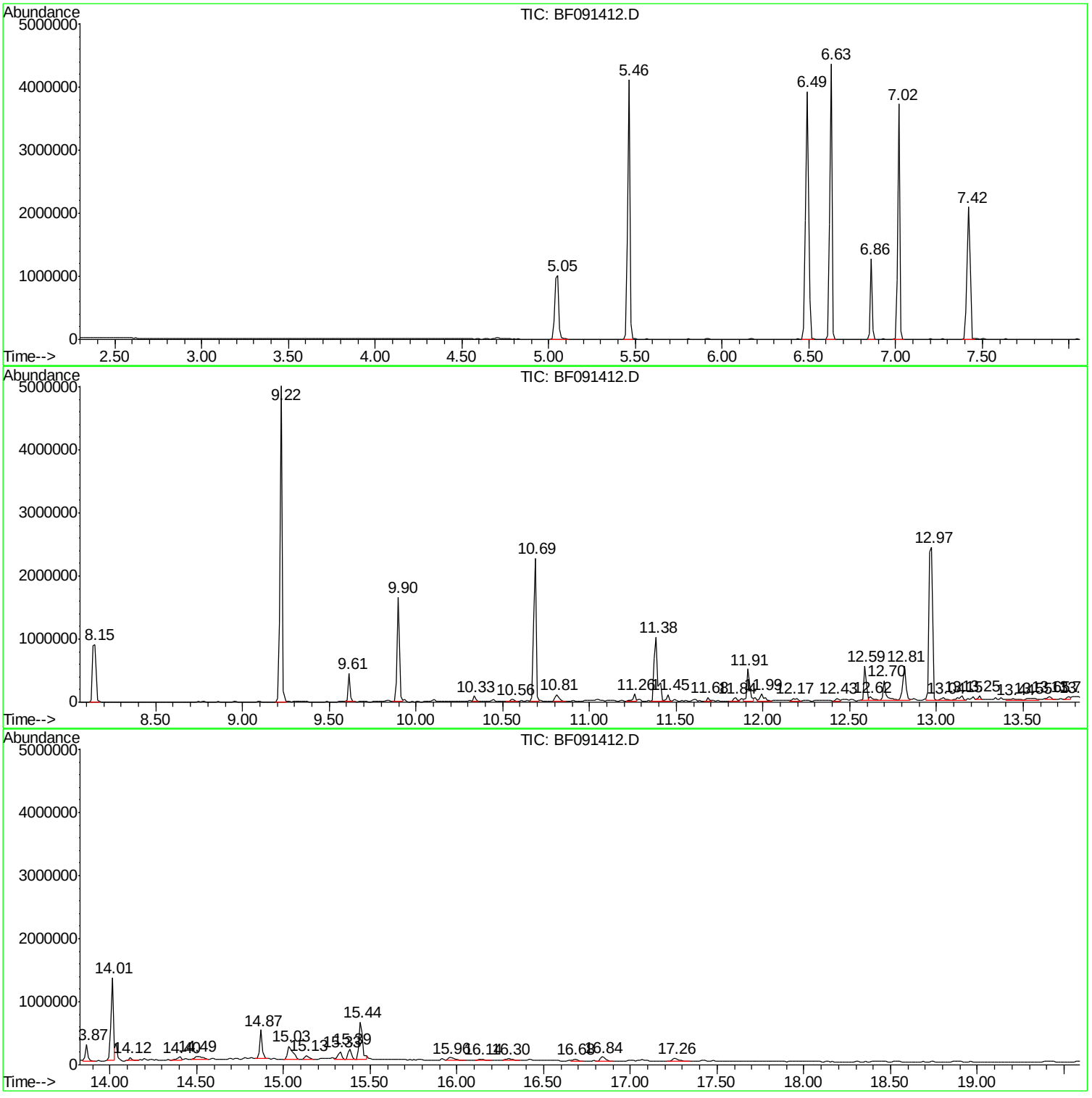
Sum of corrected areas: 45080076

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
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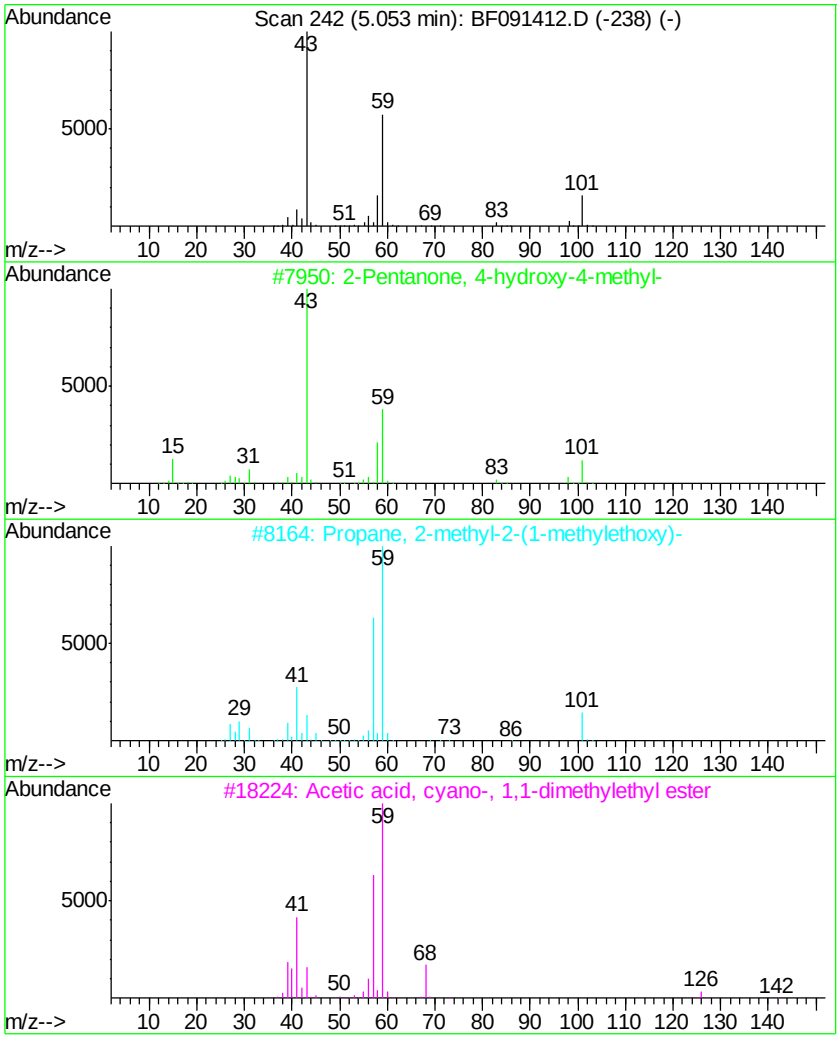
TIC Integration Parameters: LSCINT.P

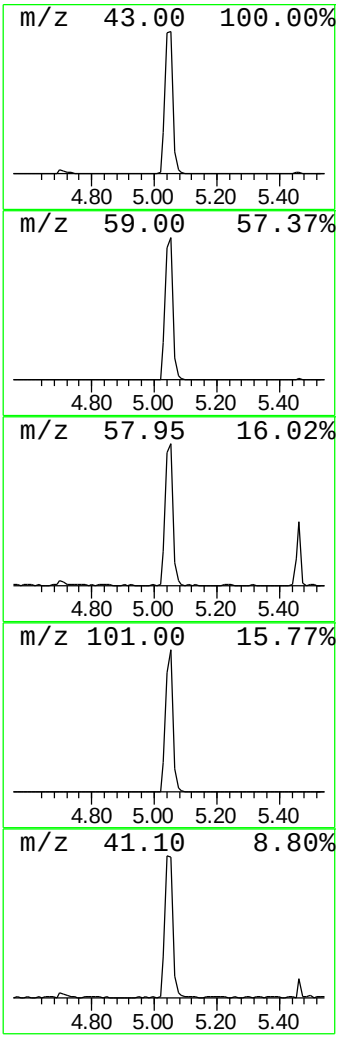
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	32.41 ng	1679030	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





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Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

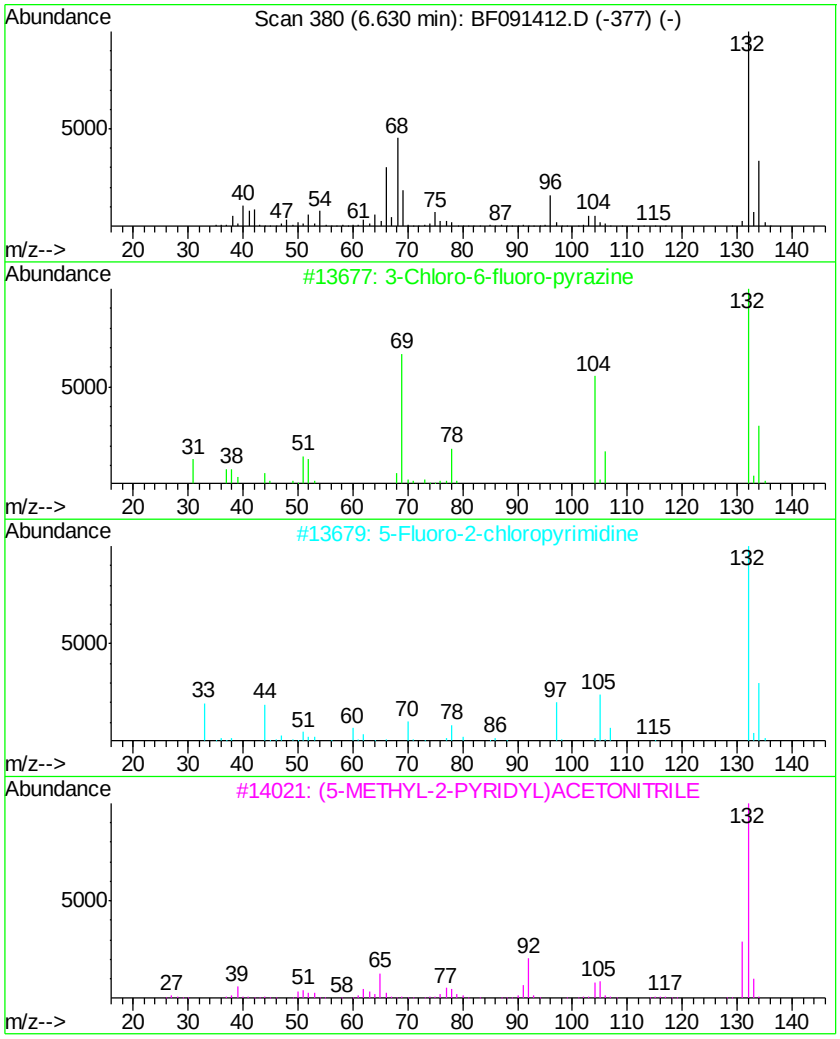
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

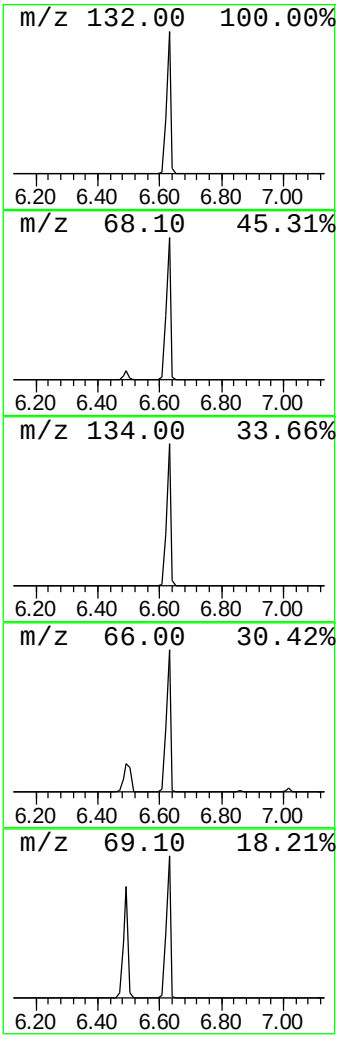
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.02 ng	4352060	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	9
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
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Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

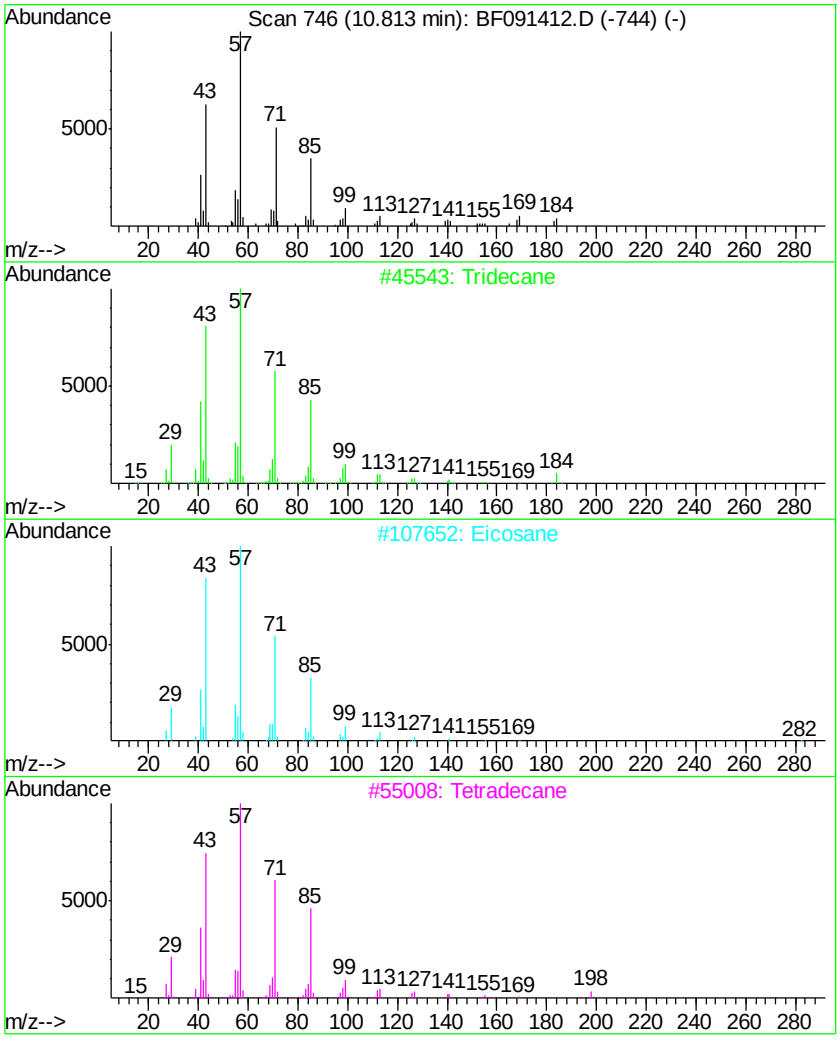
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

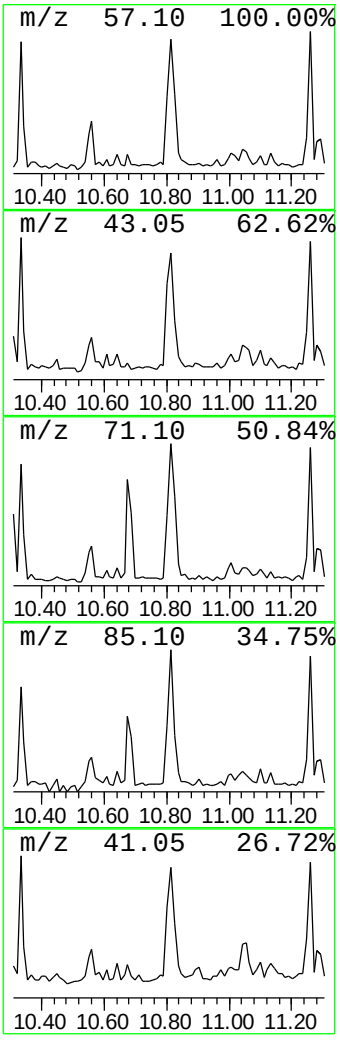
****

Peak Number 4 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.03 ng	153777	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Tetradecane	198	C14H30	000629-59-4	86
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

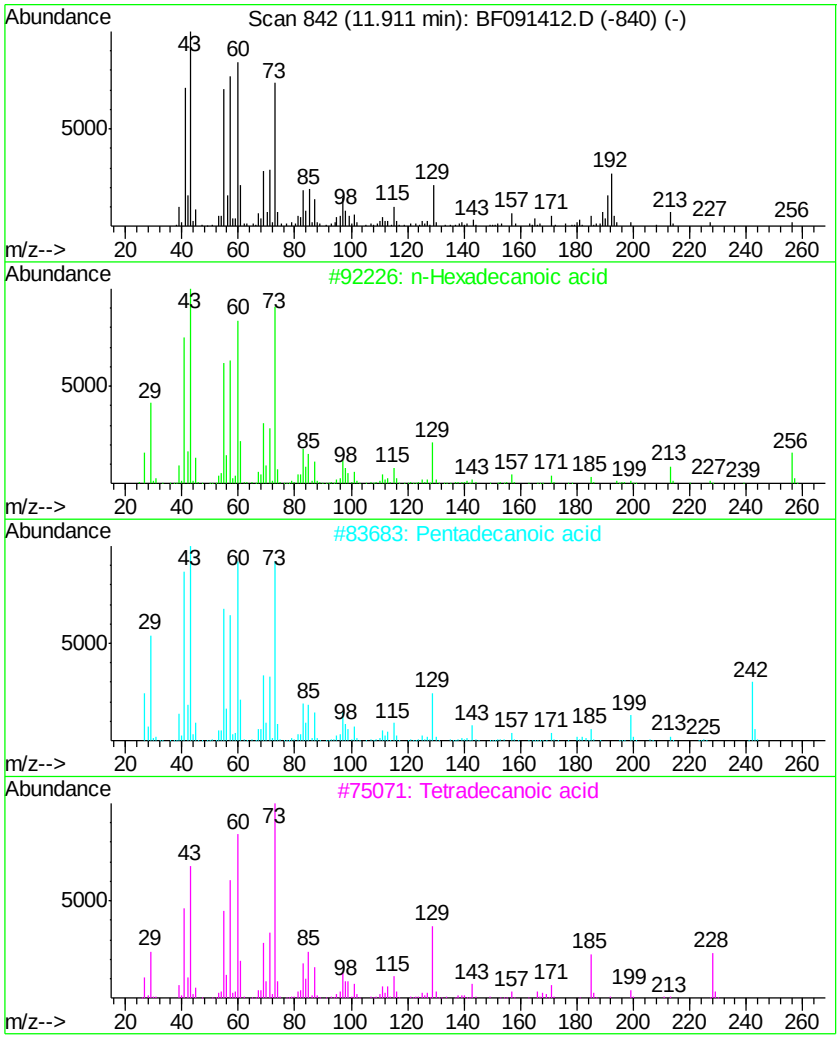
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

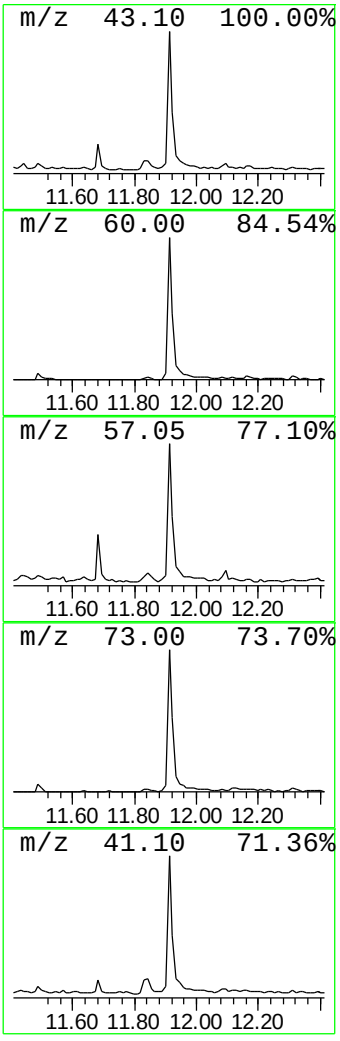
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	8.26 ng	624496	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
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Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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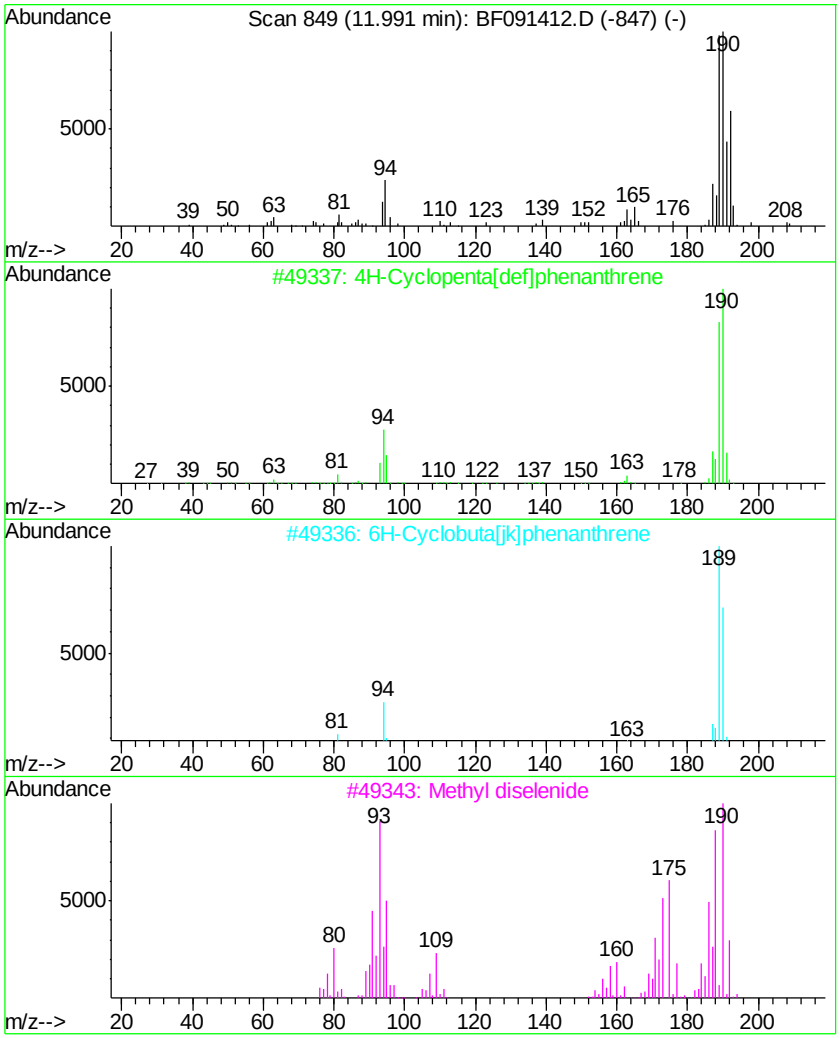
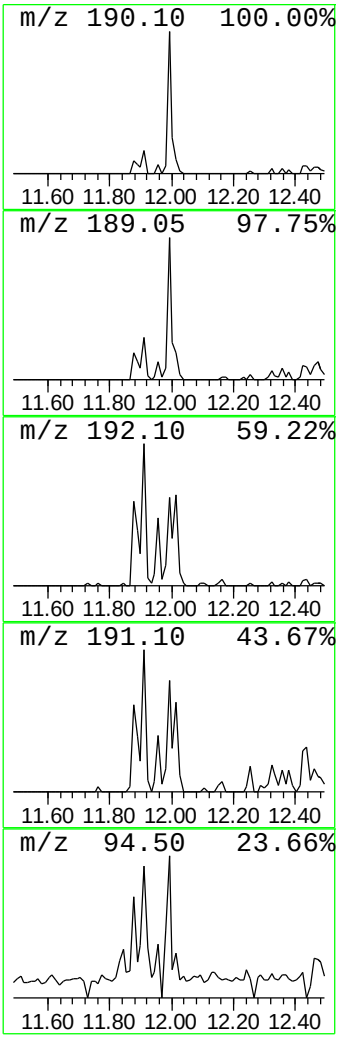
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.14 ng	161410	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	45
4	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	35
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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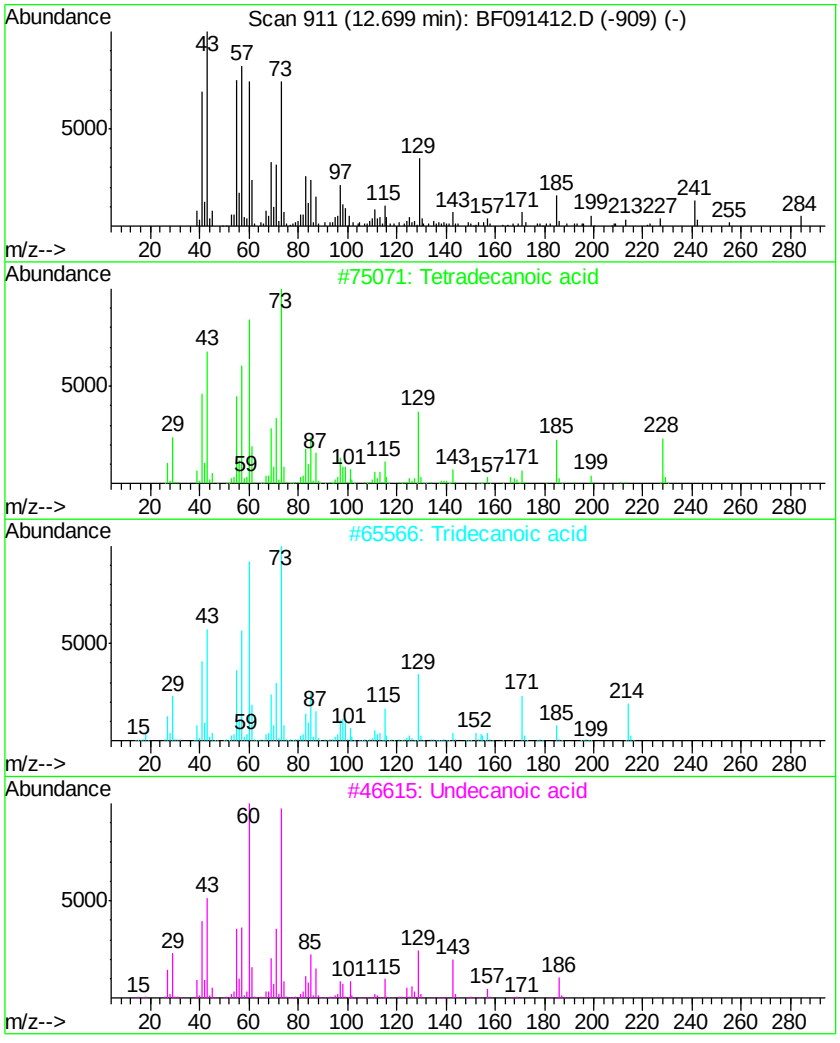
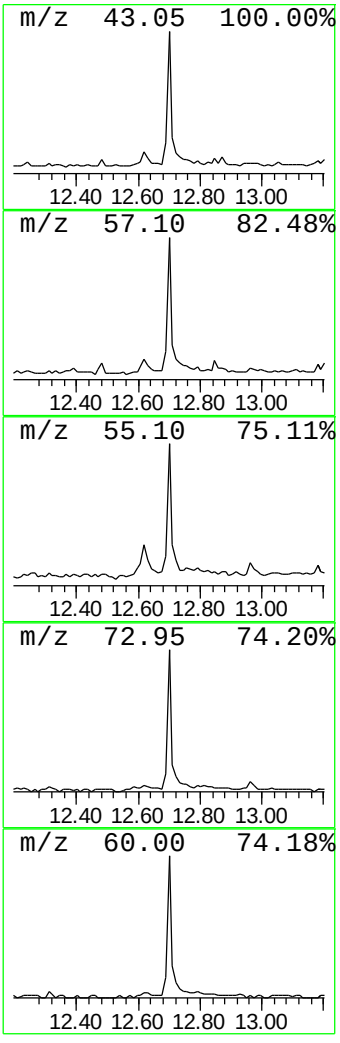
Peak Number 7 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	5.09 ng	357921	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Undecanoic acid	186	C11H22O2	000112-37-8	68
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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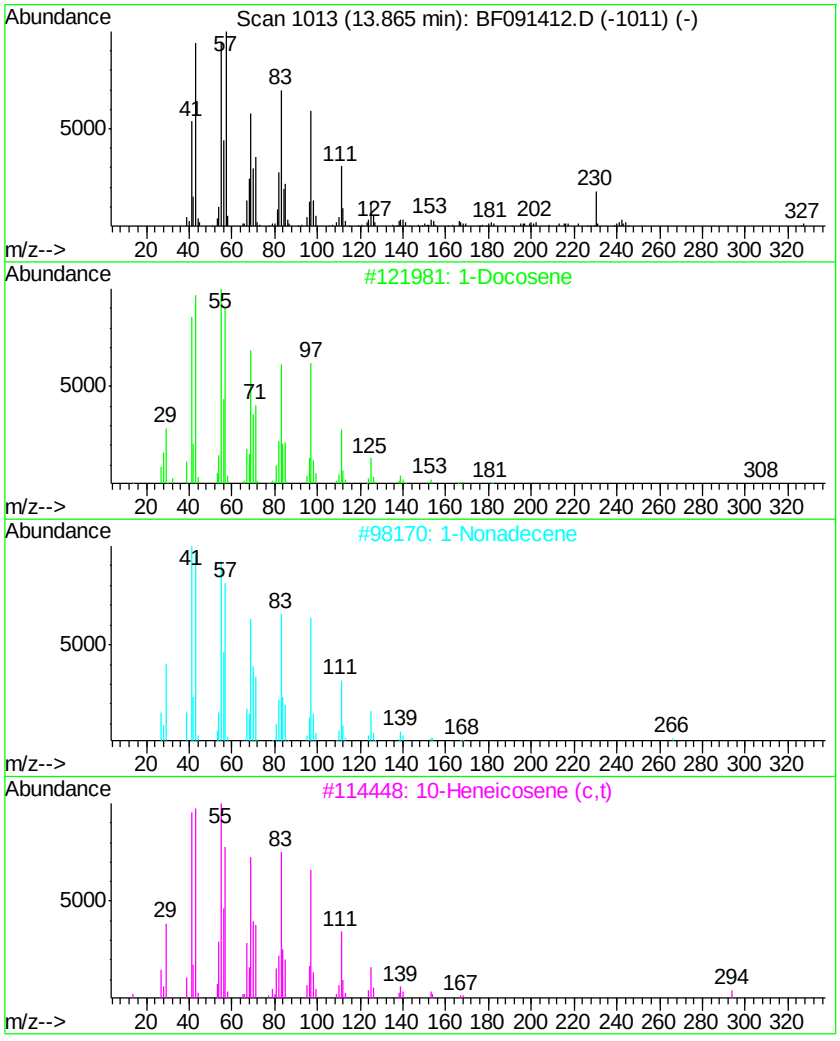
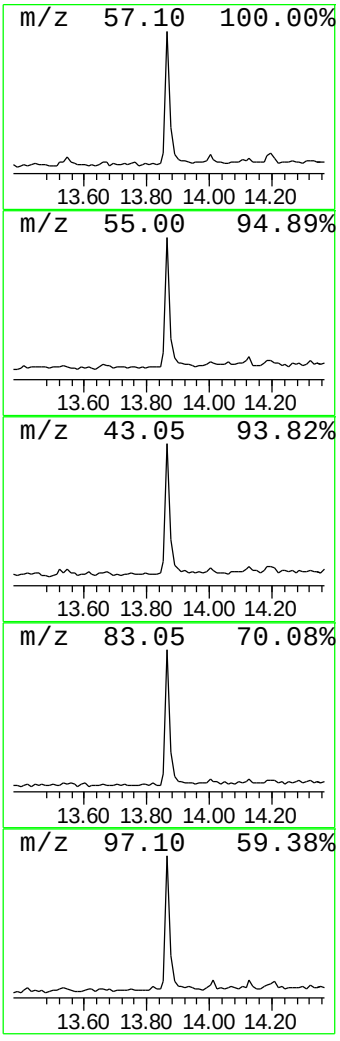
Peak Number 8 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.04 ng	283809	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	91
4	1-Nonadecanol	284	C19H40O	001454-84-8	87
5	Cyclohexadecane	224	C16H32	000295-65-8	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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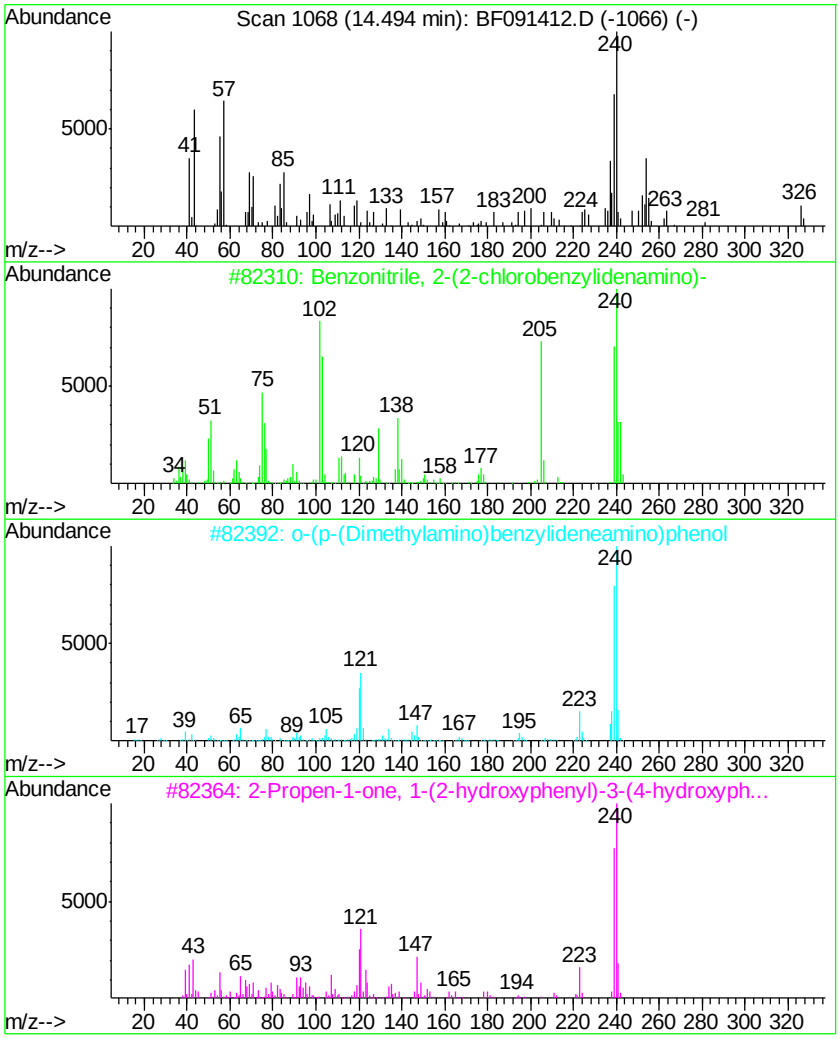
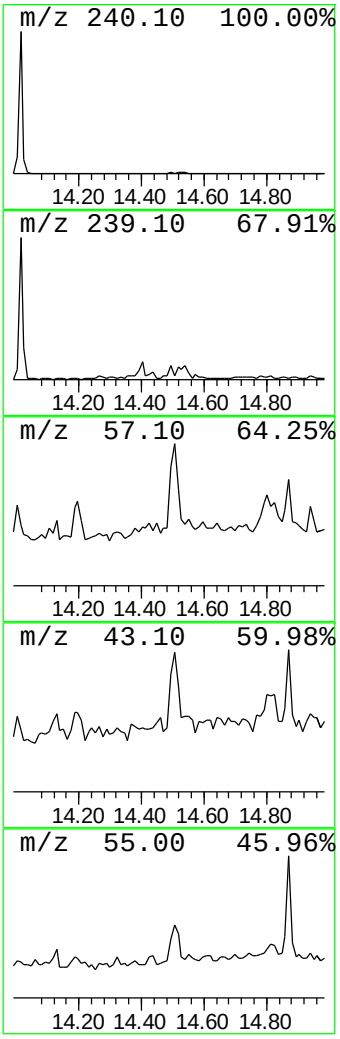
Peak Number 9 unknown14.49 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.34 ng	164606	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 2-(2-chlorobenzyli...	240	C14H9ClN2	104830-19-5	38
2	o-(p-(Dimethylamino)benzylidenea...	240	C15H16N2O	023837-35-6	38
3	2-Propen-1-one, 1-(2-hydroxyphen...	240	C15H12O3	013323-66-5	37
4	5,6-Dimethyl-4-phenyl-3-cyanopyr...	240	C14H12N2S	094639-18-6	32
5	Ferrocene, 1,1'-(1,4-butanediyl)-	240	C14H16Fe	033039-65-5	27





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Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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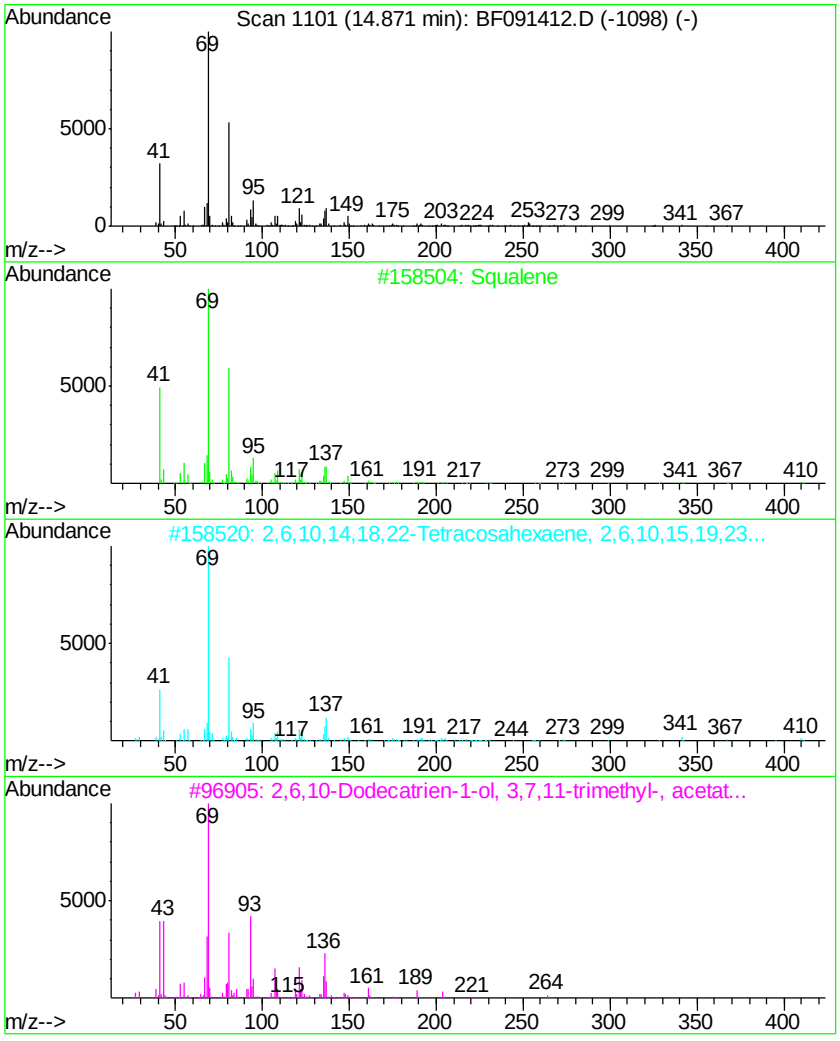
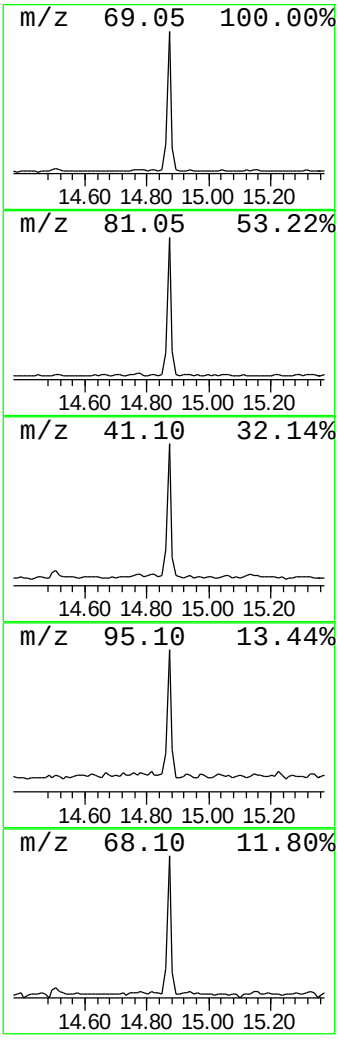
Peak Number 10 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	10.67 ng	457701	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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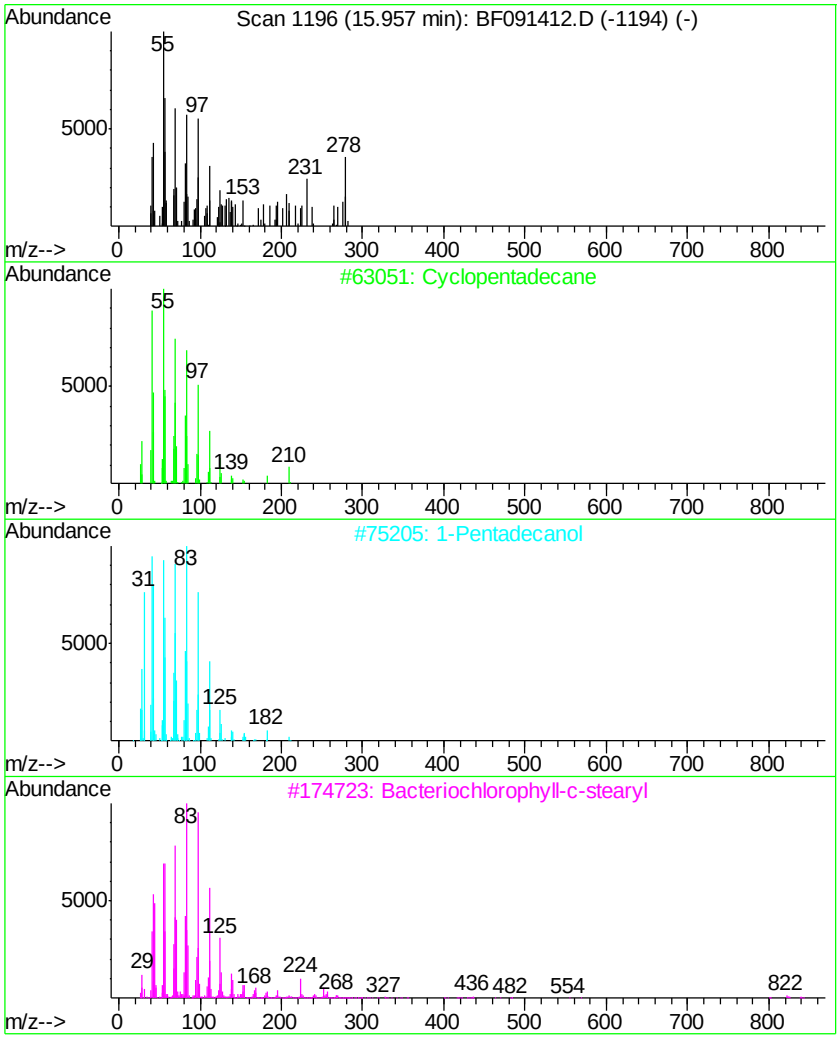
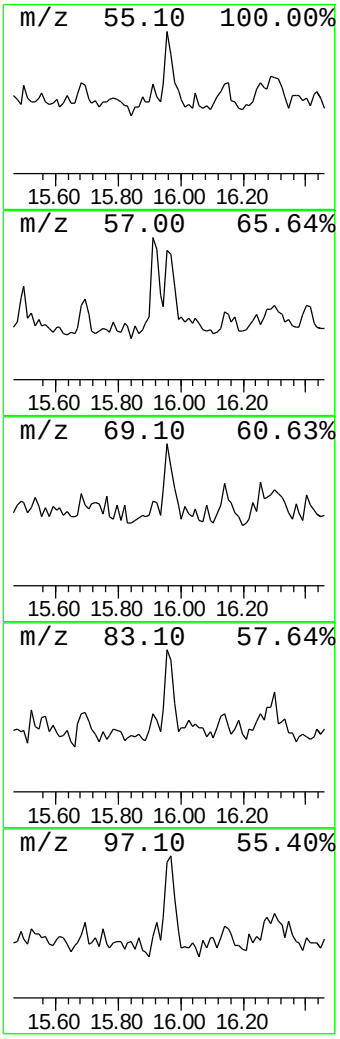
Peak Number 13 Cyclopentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.49 ng	106678	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	55
2	1-Pentadecanol	228	C15H32O	000629-76-5	30
3	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	25
4	1-Octadecanol	270	C18H38O	000112-92-5	22
5	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	22





Tentatively Identified Compound (LSC) summary

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Data File : BF091412.D
Acq On : 3 Dec 2016 1:52
Operator : UM/SJ
Sample : H5825-04
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12016SF-S-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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...	5.05	32.4	ng	1679030	1	6.86	1035970	20.0
unknown6.63	6.63	84.0	ng	4352060	1	6.86	1035970	20.0
Tridecane	10.81	2.0	ng	153777	4	11.39	1511860	20.0
n-Hexadecanoic acid	11.91	8.3	ng	624496	4	11.39	1511860	20.0
4H-Cyclopenta[def...	11.99	2.1	ng	161410	4	11.39	1511860	20.0
Tetradecanoic acid	12.70	5.1	ng	357921	5	14.01	1405840	20.0
1-Docosene	13.87	4.0	ng	283809	5	14.01	1405840	20.0
unknown14.49	14.49	2.3	ng	164606	5	14.01	1405840	20.0
Squalene	14.87	10.7	ng	457701	6	15.44	858006	20.0
Cyclopentadecane	15.96	2.5	ng	106678	6	15.44	858006	20.0