LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

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-BF122116.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	4.721	245	248	257	rBV	934115	1373309	35.16%	3.919%
2	5.190	287	289	304	rBV	3458431	3574788	91.51%	10.201%
3	6.264	380	383	385	rBV	2661950	3353662	85.85%	9.570%
4	6.367	390	392	394	rBV	3676129	3249147	83.17%	9.272%
5	6.596	410	412	414	rBV	945166	969046	24.81%	2.765%
6	6.744	423	425	428	rBV	1963943	2378730	60.89%	6.788%
7	7.167	459	462	464	rBV	1943744	2052824	52.55%	5.858%
8	7.876	522	524	527	rBV	1343059	1571707	40.23%	4.485%
9	8.962	616	619	621	rBV	4065518	3906420	100.00%	11.148%
10	9.362	652	654	656	rBV	798564	689696	17.66%	1.968%
11	9.625	675	677	680	rBV	1362537	1390704	35.60%	3.969%
12	10.082	715	717	718	rVB	60396	66521	1.70%	0.190%
13	10.299	732	736	739	rBV	25228	45370	1.16%	0.129%
14	10.413	744	746	749	rBV2	1814992	2125414	54.41%	6.065%
15	10.550	755	758	762	rBV	100798	124972	3.20%	0.357%
16	10.996	795	797	798	rBV	57471	56818	1.45%	0.162%
17	11.111	804	807	809	rBV	997179	1370599	35.09%	3.911%
18	11.659	853	855	859	rBV2	198801	190072	4.87%	0.542%
19	12.311	910	912	914	rBV	45718	40030	1.02%	0.114%
20	12.436	921	923	929	rBV	29945	42846	1.10%	0.122%
21	12.539	929	932	934	rVB	39705	46669	1.19%	0.133%
22	12.688	943	945	948	rBV	2674360	2901991	74.29%	8.281%
23	12.939	963	967	969	rBV2	36265	54329	1.39%	0.155%
24	13.602	1022	1025	1034	rBV	192432	319119	8.17%	0.911%
25	13.728	1034	1036	1039	rBV	875054	942603	24.13%	2.690%
26	14.231	1077	1080	1086	rBV3	40231	100100	2.56%	0.286%
27	14.517	1101	1105	1109	rBV	24437	42661	1.09%	0.122%
28	14.585	1109	1111	1113	rVV	73634	80679	2.07%	0.230%
29	14.642	1114	1116	1119	rVB	59008	60308	1.54%	0.172%
30	14.814	1128	1131	1132	rBV	44872	57802	1.48%	0.165%
31	14.837	1132	1133	1138	rVB3	27299	58313	1.49%	0.166%
32	15.088	1153	1155	1158	rBV	701282	863145	22.10%	2.463%
33	15.500	1188	1191	1193	rBV	59465	82827	2.12%	0.236%
34	15.557	1193	1196	1199	rBV4	20414	53753	1.38%	0.153%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.162	1246	1249	1252	rVB2	29287	55747	1.43%	0.159%
36	16.345	1262	1265	1267	rBV2	22009	45267	1.16%	0.129%
37	16.403	1267	1270	1272	rBV	35509	64003	1.64%	0.183%
38	16.551	1280	1283	1284	rBV	67962	125282	3.21%	0.358%
39	16.585	1284	1286	1292	rVB	146096	290000	7.42%	0.828%
40	16.814	1302	1306	1313	rVB3	59830	144298	3.69%	0.412%
41	17.648	1375	1379	1384	rBV4	24532	81141	2.08%	0.232%

Sum of corrected areas: 35042712

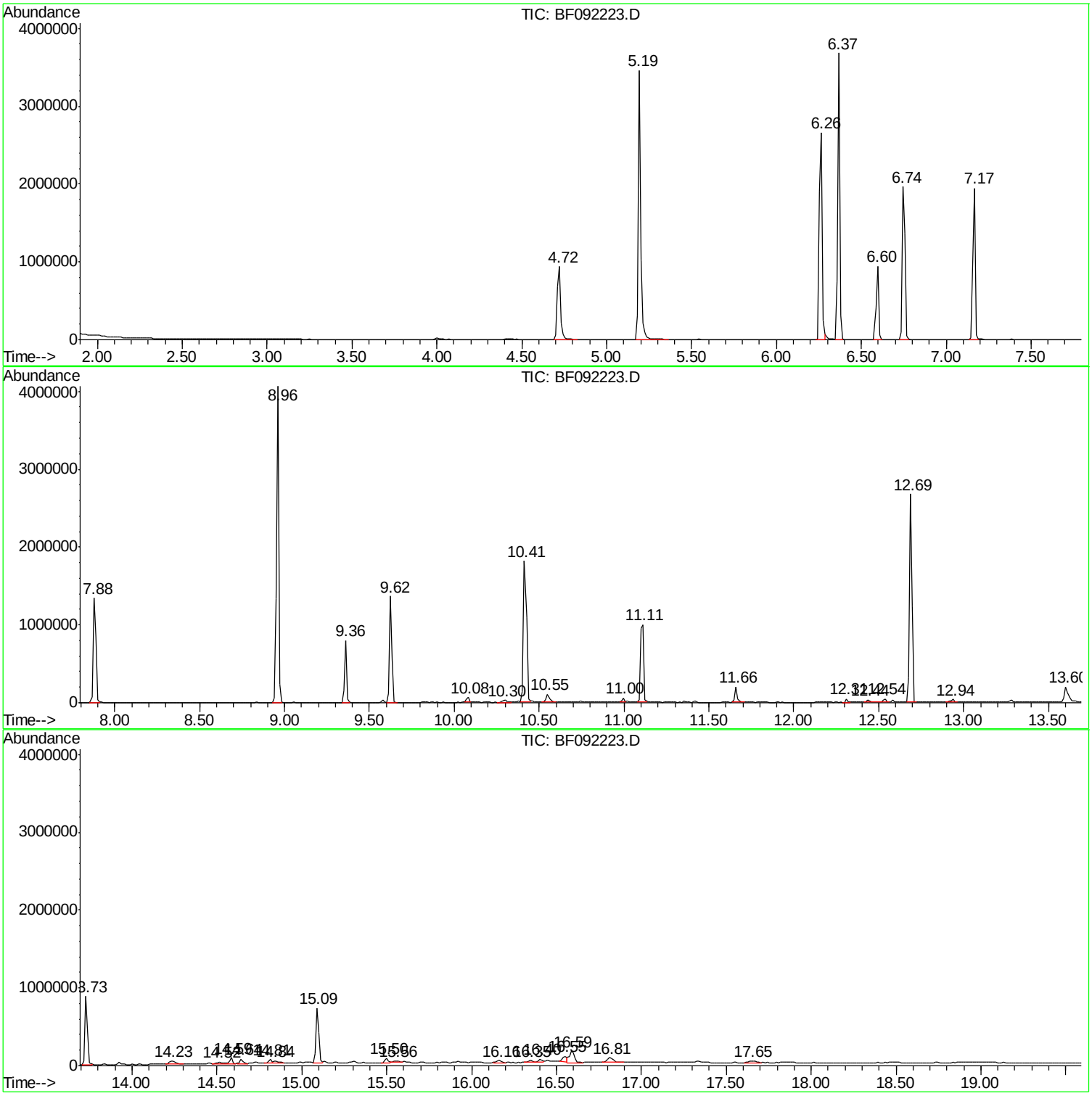
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

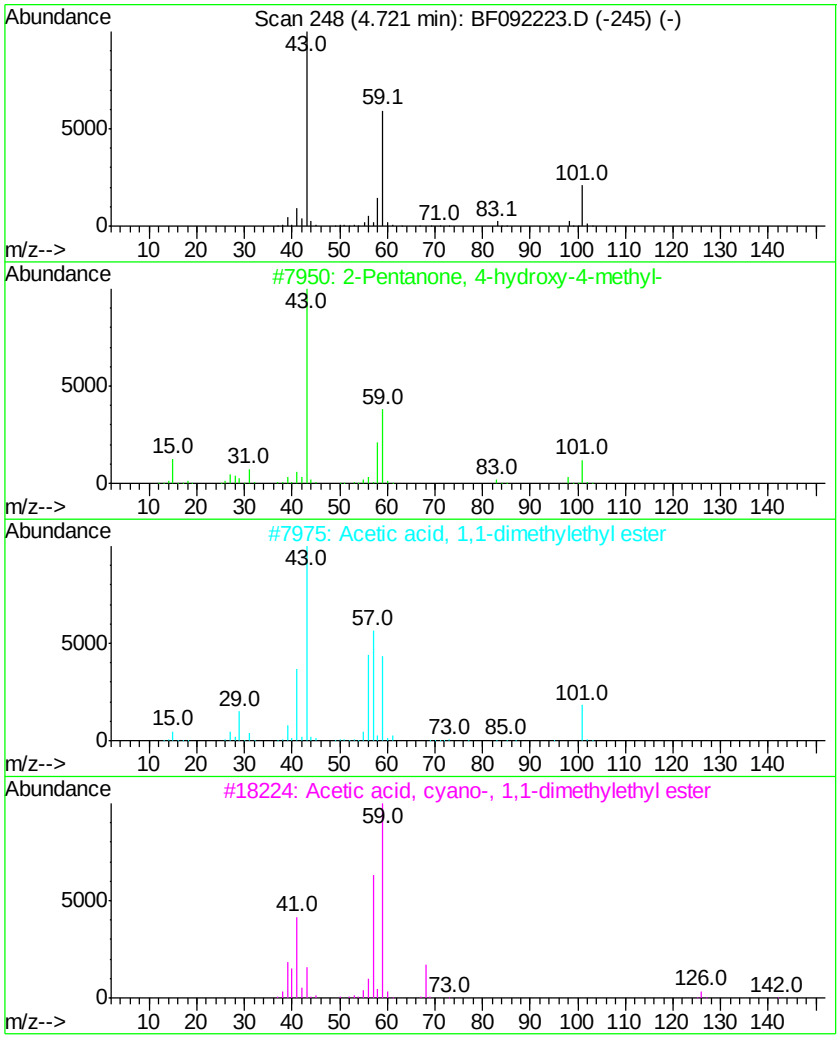
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

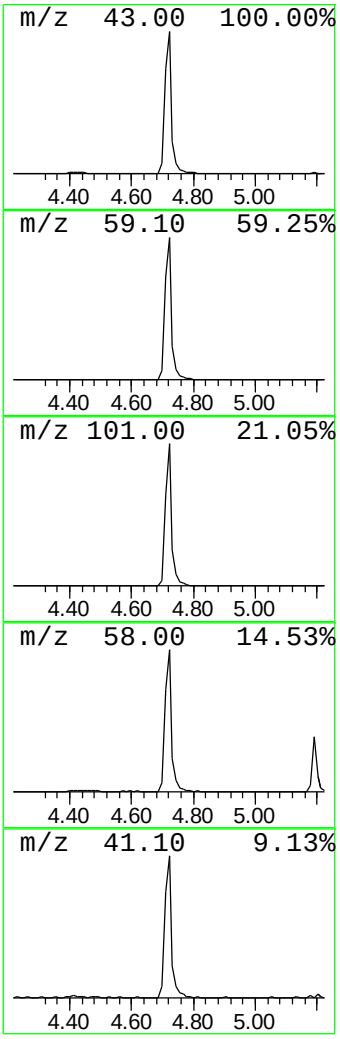
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	28.34 ng	1373310	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

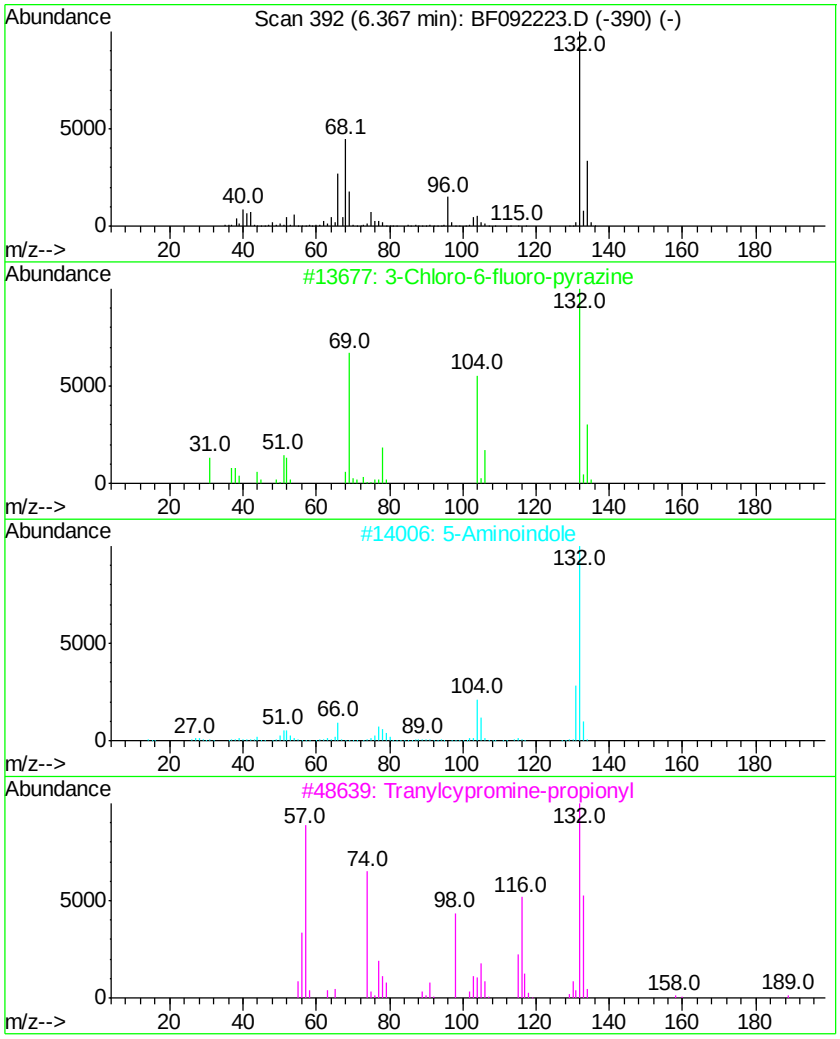
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

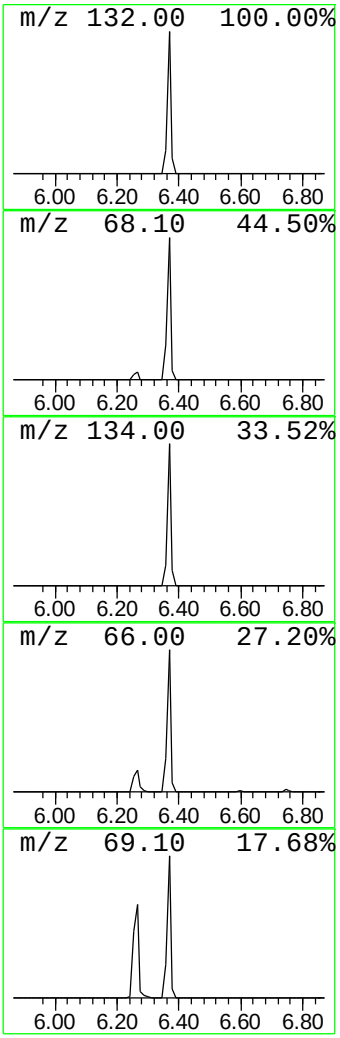
****

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	67.06 ng	3249150	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

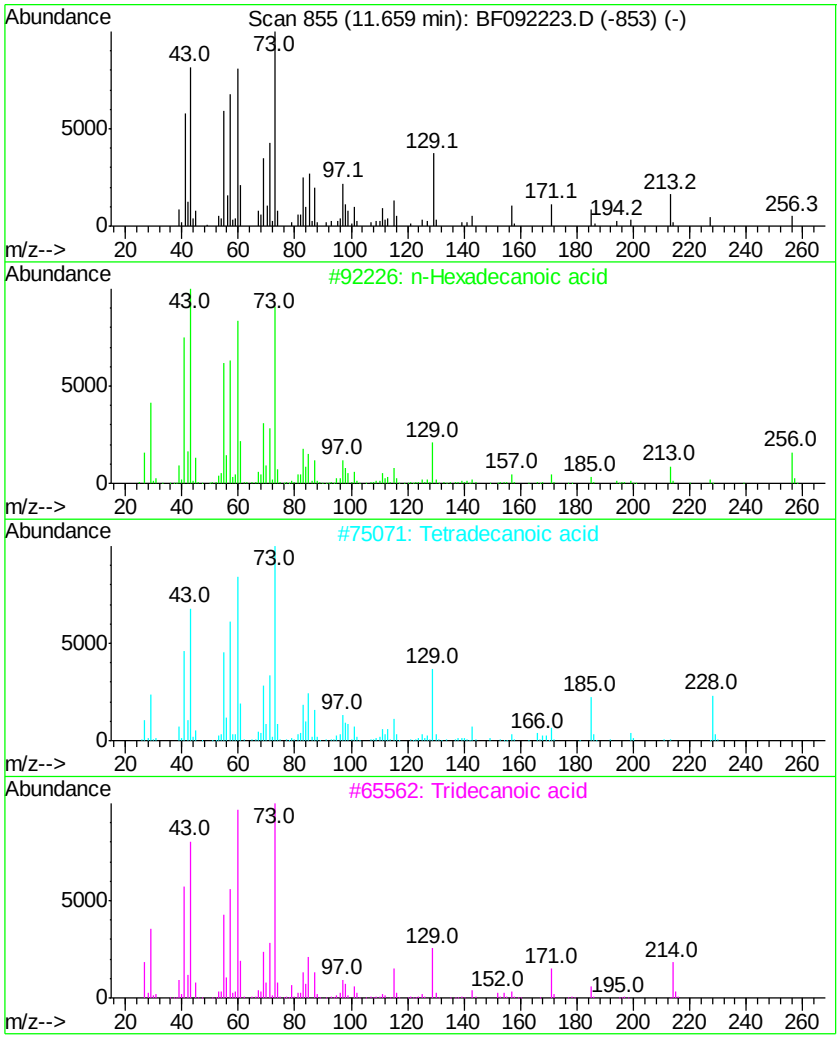
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

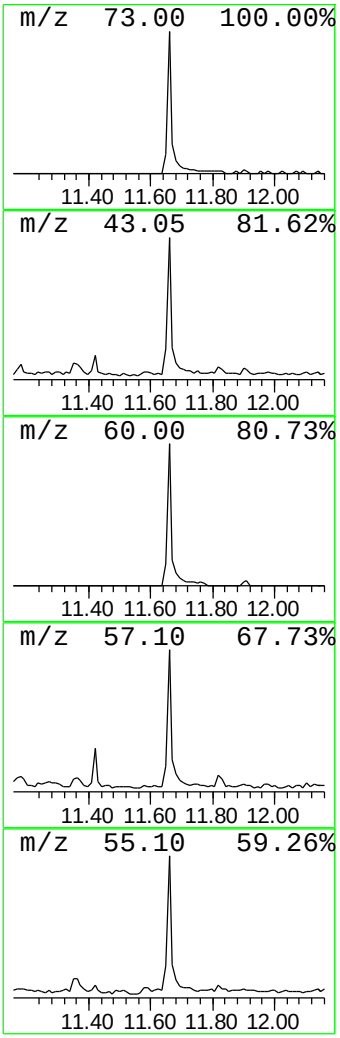
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	2.77 ng	190072	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

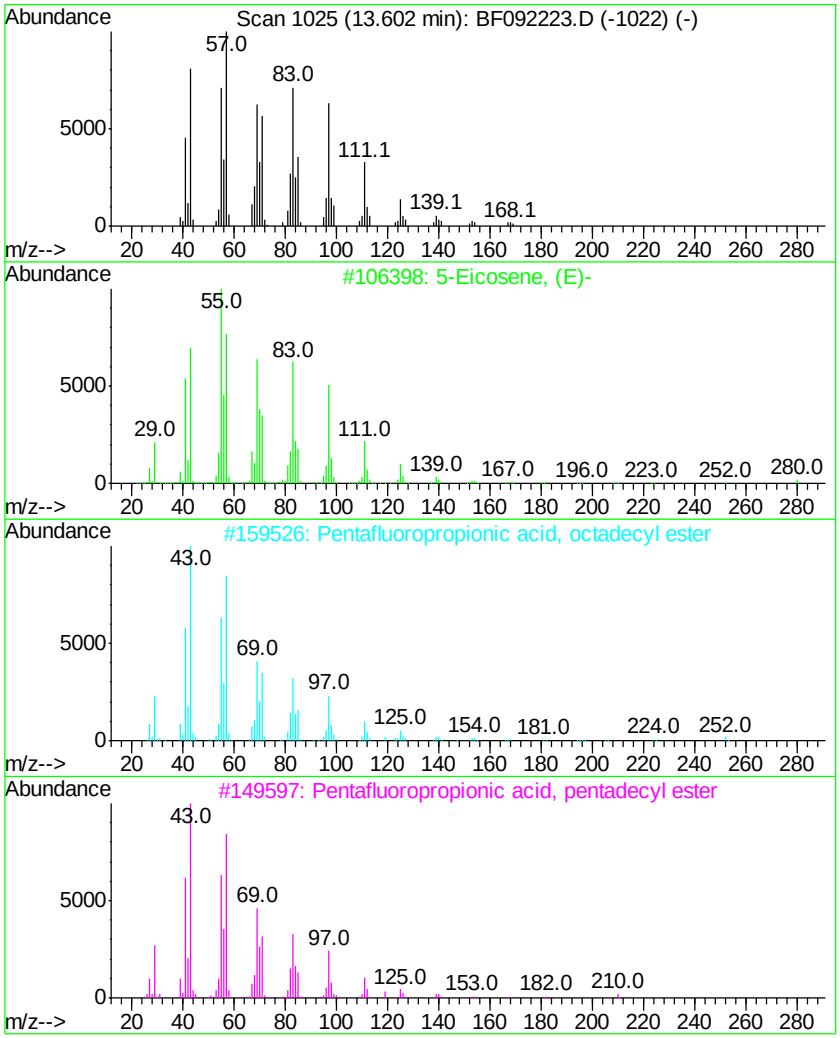
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

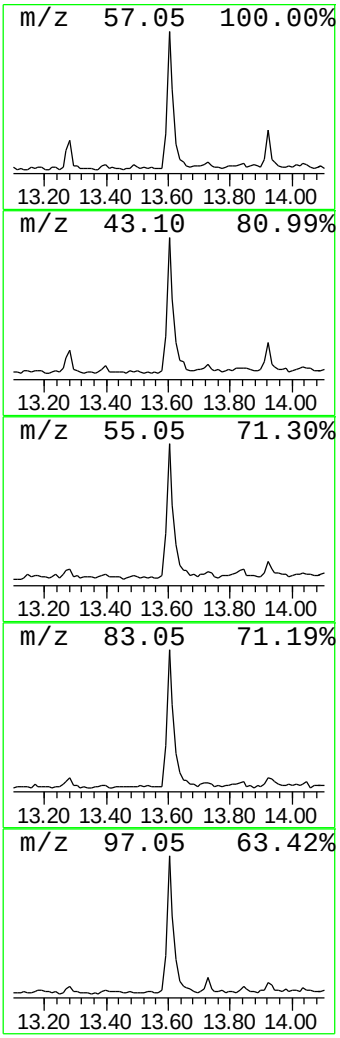
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	6.77 ng	319119	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
4	1-Docosene	308	C22H44	001599-67-3	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

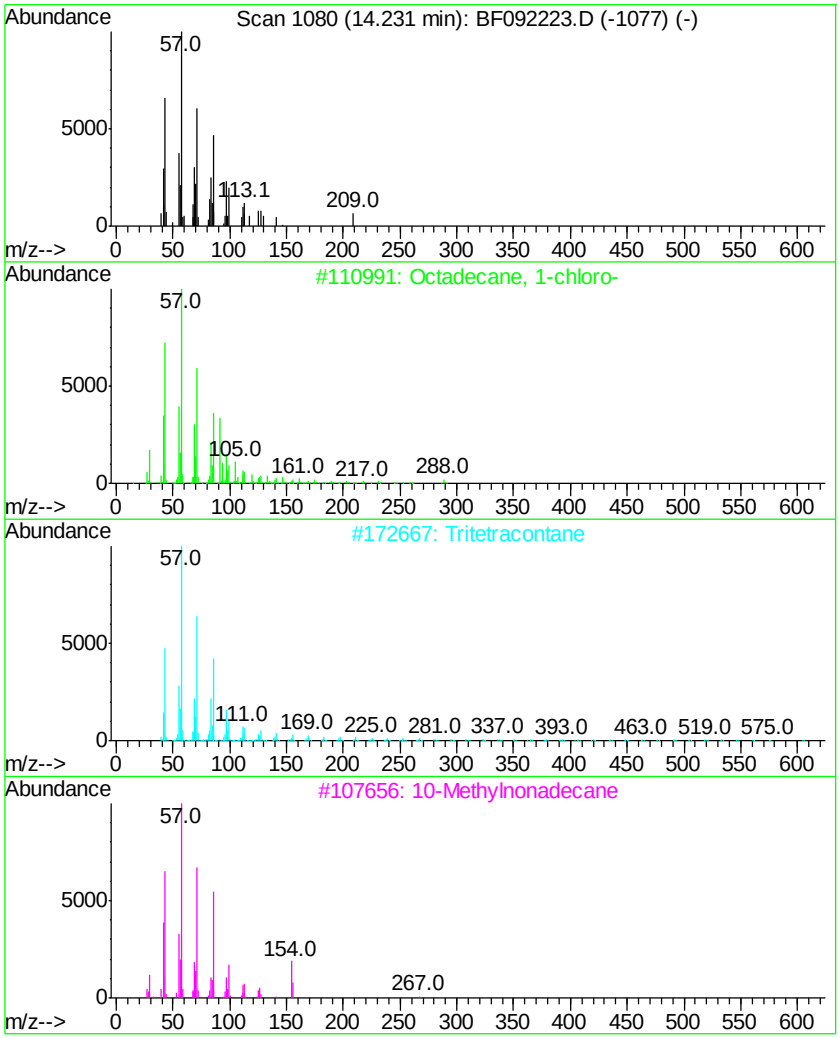
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

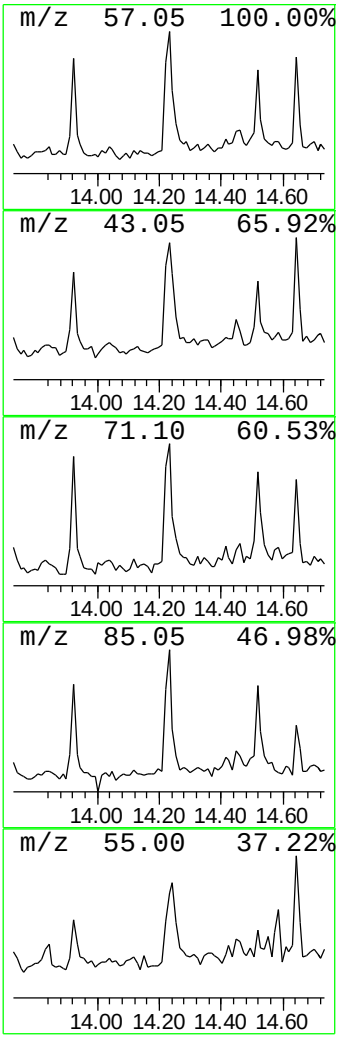
****

Peak Number 6 Octadecane, 1-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.12 ng	100100	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
2	Tritetracontane	605	C43H88	007098-21-7	80
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Heneicosane	296	C21H44	000629-94-7	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

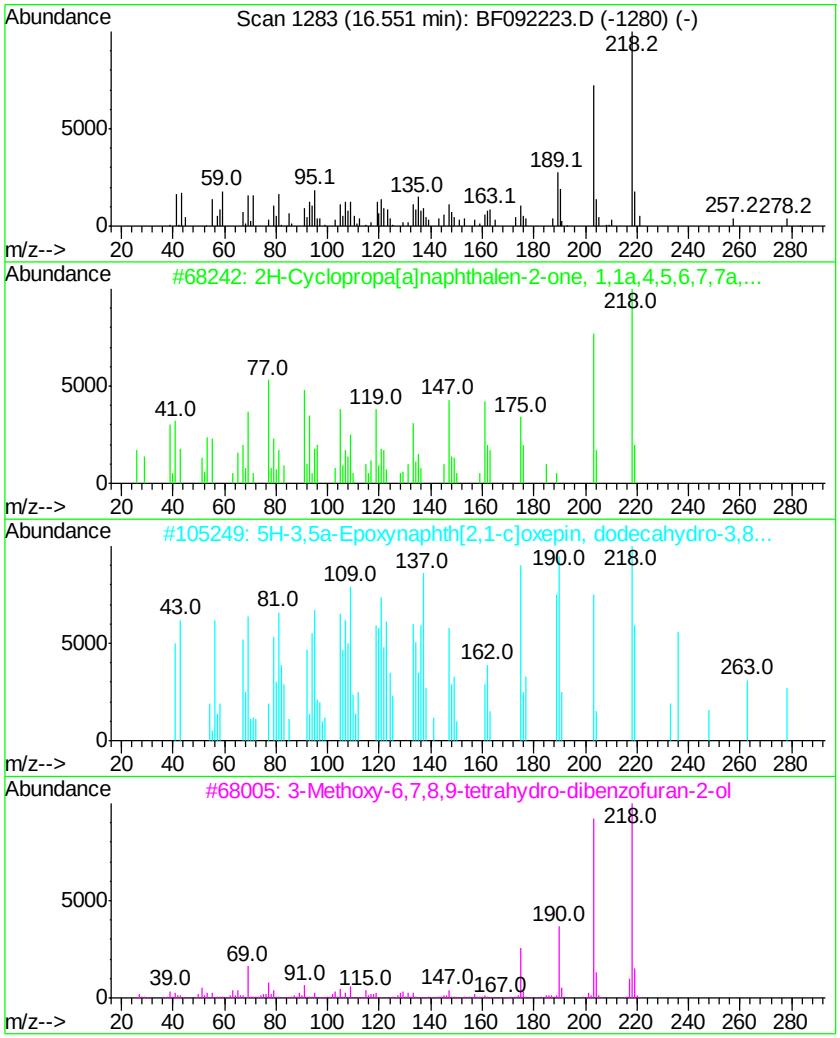
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

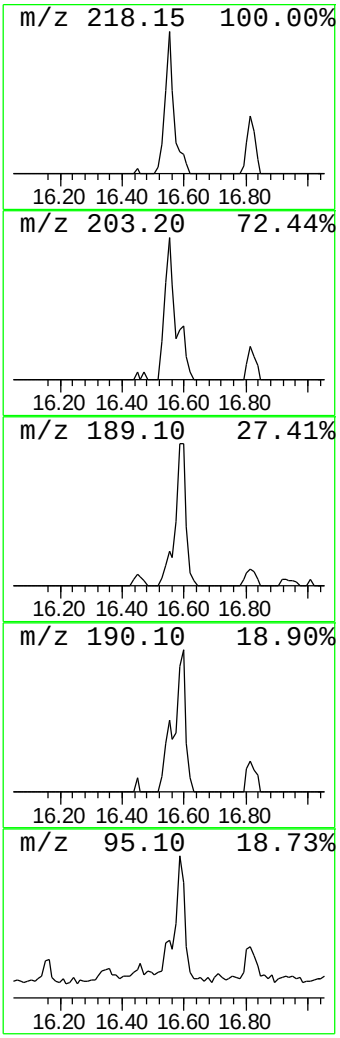
****

Peak Number 7 2H-Cyclopropa[a]naphthalen-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.90 ng	125282	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	76
2	5H-3,5a-Epoxynaphth[2,1-c]oxepin...	278	C18H30O2	001153-35-1	64
3	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64
4	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	64
5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

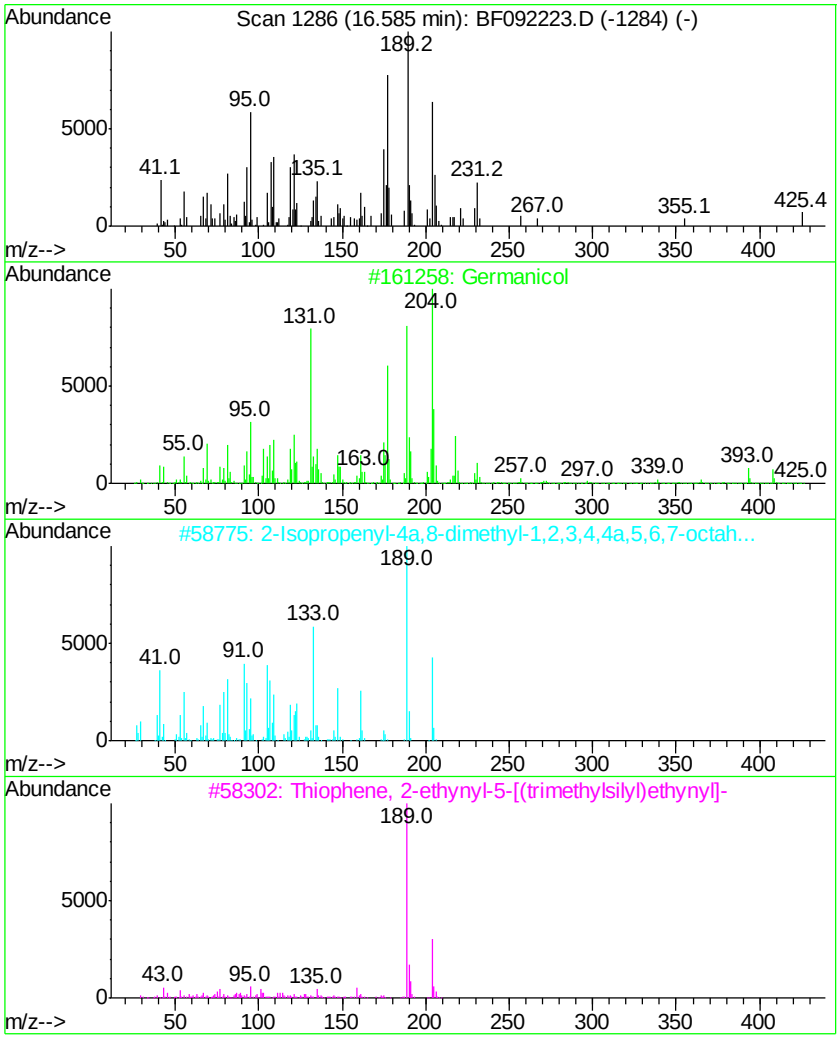
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

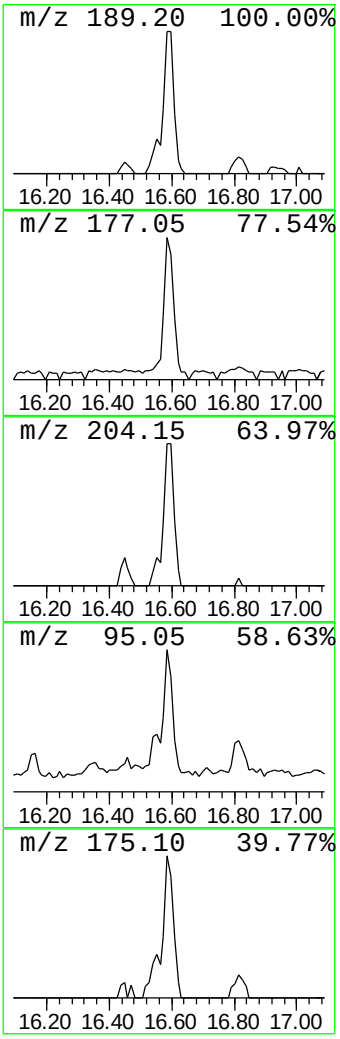
****

Peak Number 8 unknown16.59 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	6.72 ng	290000	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Germanicol	426	C30H50O	000465-02-1	43
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	38
3	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	38
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	35
5	3H-1,2-Dithiole-3-thione, 5-tert...	204	C8H12S3	013120-76-8	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

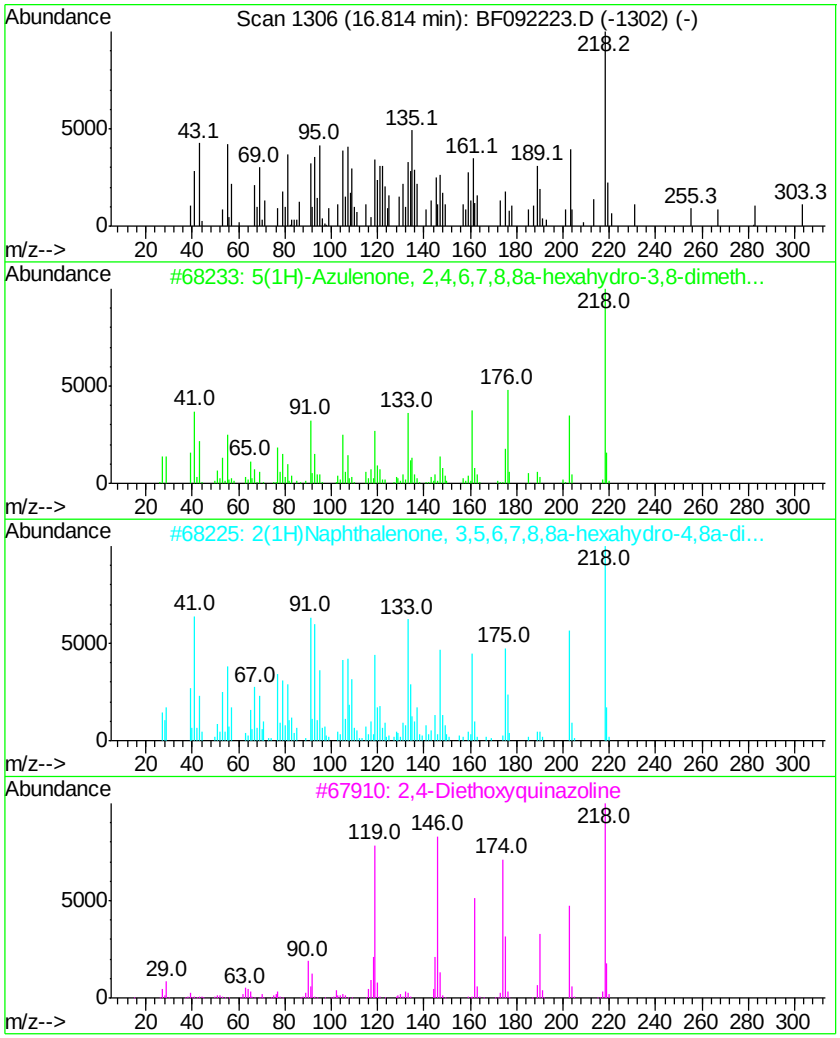
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

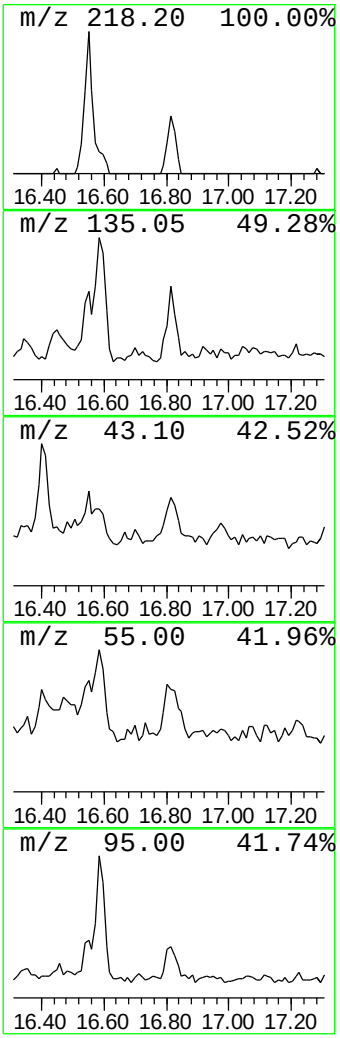
****

Peak Number 9 5(1H)-Azulenone, 2,4,6,7,8,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	3.34 ng	144298	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	50
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	49
3	2,4-Diethoxyquinazoline	218	C12H14N2O2	000611-65-4	38
4	9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	35
5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092223.D
Acq On : 12 Jan 2017 22:34
Operator : UM/SJ
Sample : I1030-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-0018

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	28.3	ng	1373310	1	6.60	969046	20.0
unknown6.37	6.37	67.1	ng	3249150	1	6.60	969046	20.0
n-Hexadecanoic acid	11.66	2.8	ng	190072	4	11.11	1370600	20.0
5-Eicosene, (E)-	13.60	6.8	ng	319119	5	13.73	942603	20.0
Octadecane, 1-chl...	14.23	2.1	ng	100100	5	13.73	942603	20.0
2H-Cyclopropa[a]n...	16.55	2.9	ng	125282	6	15.09	863145	20.0
unknown16.59	16.59	6.7	ng	290000	6	15.09	863145	20.0
5(1H)-Azulenone, ...	16.81	3.3	ng	144298	6	15.09	863145	20.0