LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

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-BF063016.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	1.678	7	8	17	rVB	147755	235204	9.40%	1.247%
2	1.804	17	19	62	rVB	1060146	2502959	100.00%	13.274%
3	2.867	110	112	122	rBV	16835	30165	1.21%	0.160%
4	4.170	223	226	230	rVB	16623	25327	1.01%	0.134%
5	4.867	285	287	291	rVB	105281	141828	5.67%	0.752%
6	5.301	322	325	328	rBV	1313224	1662260	66.41%	8.816%
7	6.353	414	417	420	rVB	1371810	1604998	64.12%	8.512%
8	6.479	425	428	431	rBV	1717454	1665108	66.53%	8.831%
9	6.707	446	448	450	rBB	415672	390370	15.60%	2.070%
10	6.867	459	462	464	rBB	1563159	1331208	53.19%	7.060%
11	7.279	495	498	500	rBV	1201573	1180836	47.18%	6.262%
12	7.999	558	561	563	rBV	555338	526491	21.03%	2.792%
13	9.073	652	655	657	rBV	2064292	1801128	71.96%	9.552%
14	9.473	687	690	692	rVB	275579	324235	12.95%	1.720%
15	9.748	711	714	716	rBV	478973	506646	20.24%	2.687%
16	10.525	780	782	785	rBV2	910937	973248	38.88%	5.162%
17	10.662	790	794	799	rBV	29132	38874	1.55%	0.206%
18	11.222	840	843	844	rBV	438209	449223	17.95%	2.382%
19	12.422	946	948	950	rVB	76900	62019	2.48%	0.329%
20	12.685	968	971	979	rVB	537293	715354	28.58%	3.794%
21	12.799	979	981	984	rVB	1157640	1332697	53.24%	7.068%
22	13.702	1058	1060	1067	rBV3	76189	112967	4.51%	0.599%
23	13.839	1069	1072	1076	rBV	507615	530277	21.19%	2.812%
24	14.342	1114	1116	1120	rBV5	16413	31987	1.28%	0.170%
25	14.834	1157	1159	1163	rBV	37175	72546	2.90%	0.385%
26	15.097	1180	1182	1185	rVB	29528	37854	1.51%	0.201%
27	15.154	1185	1187	1189	rBV	23068	27260	1.09%	0.145%
28	15.211	1190	1192	1195	rBV	248900	347804	13.90%	1.845%
29	15.657	1228	1231	1232	rBV	18467	36203	1.45%	0.192%
30	15.691	1232	1234	1241	rVB7	27695	64137	2.56%	0.340%
31	16.342	1289	1291	1296	rVB6	14551	31320	1.25%	0.166%
32	16.685	1317	1321	1327	rVB7	17651	63272	2.53%	0.336%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 18855805

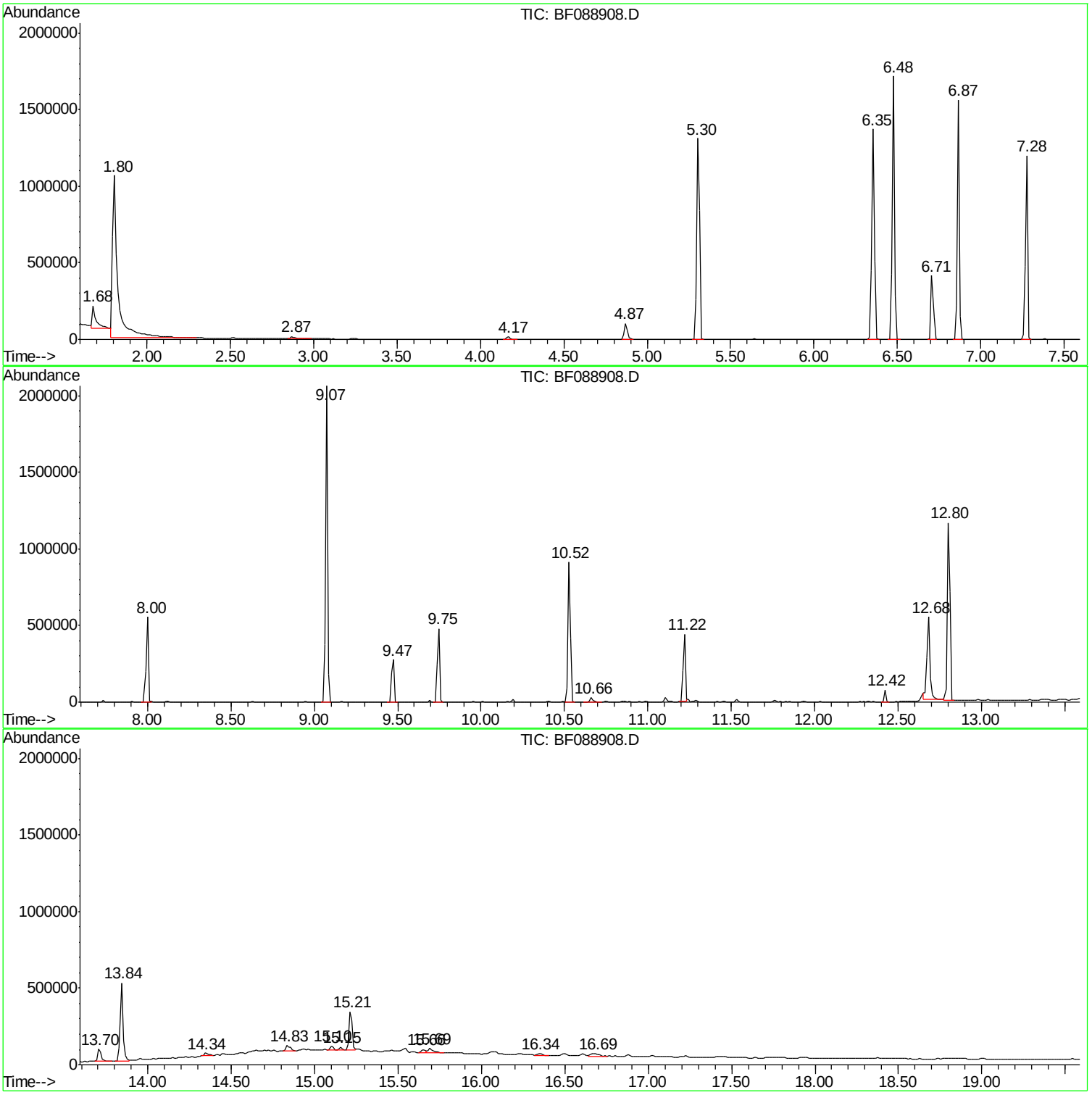
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

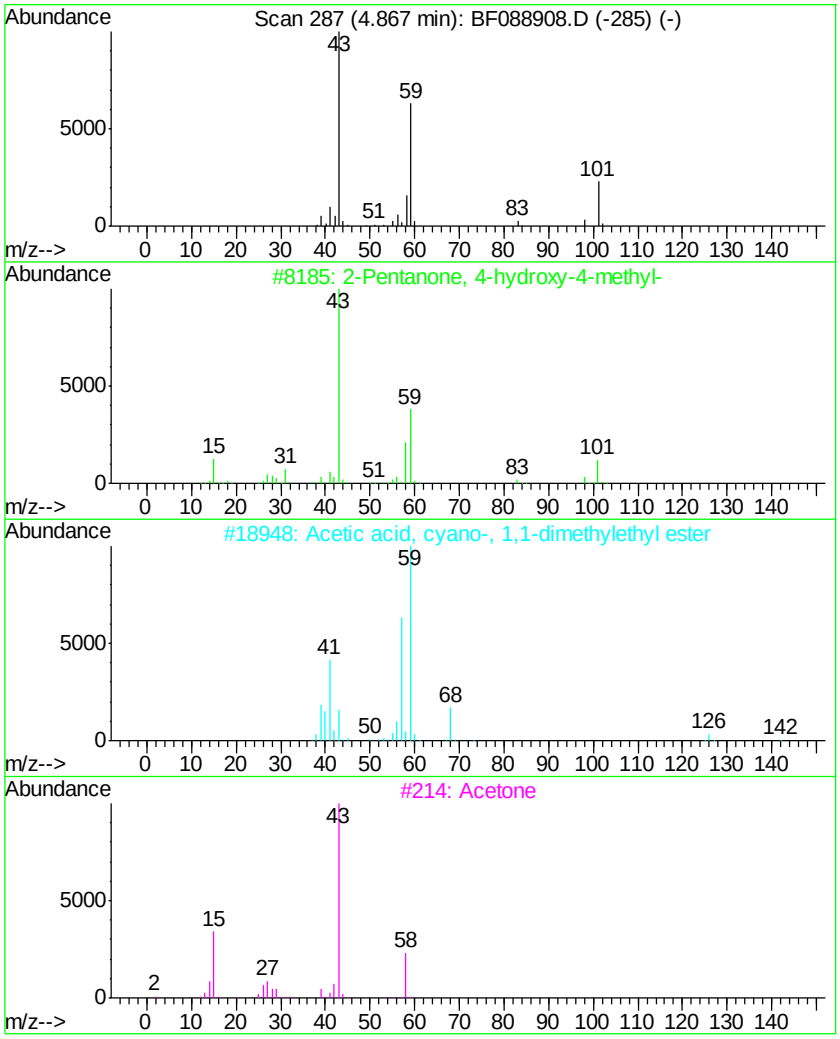
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

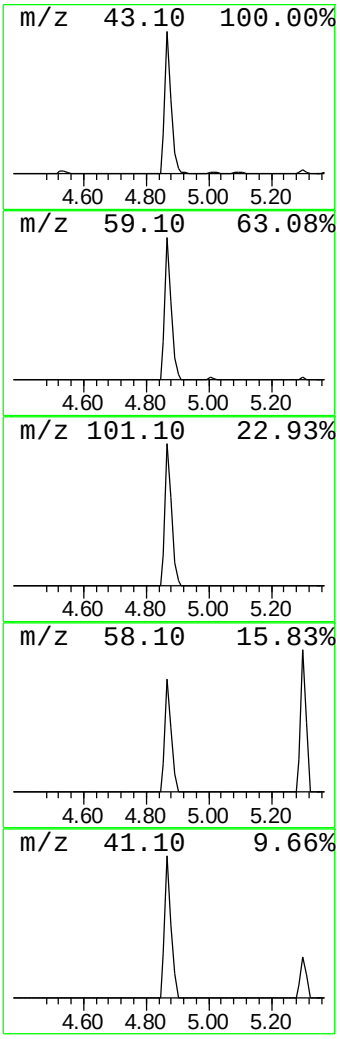
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	7.27 ng	141828	1,4-Dichlorobenzene-d4	6.71

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

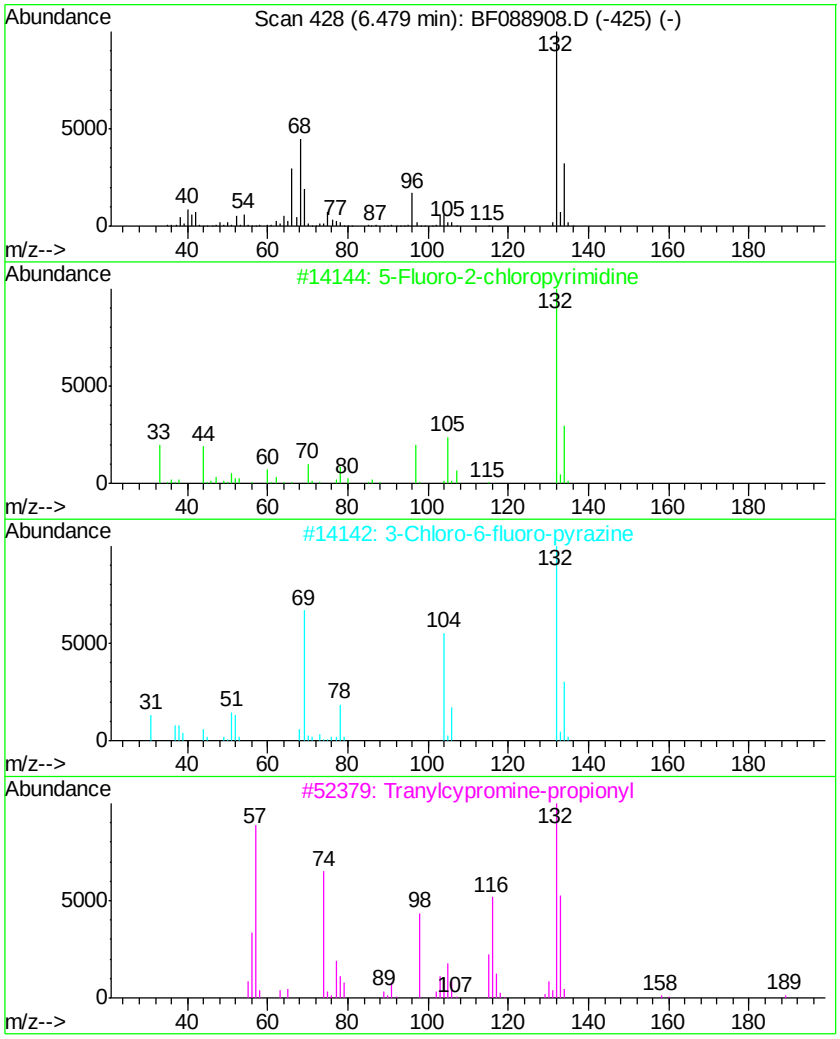
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

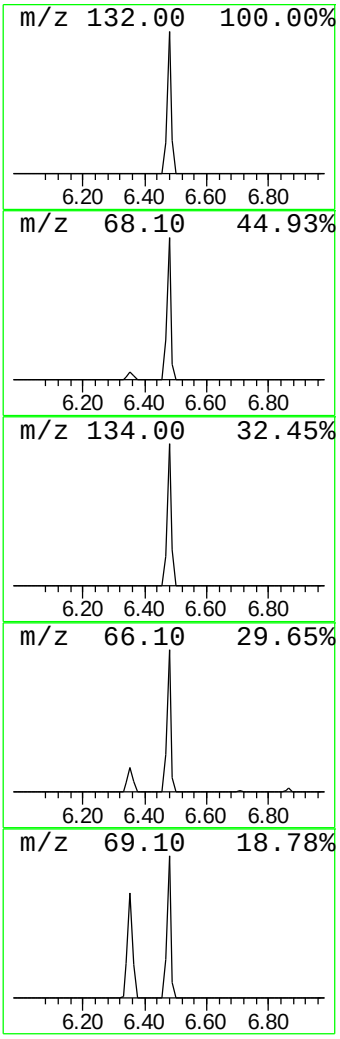
****

Peak Number 4 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	85.31 ng	1665110	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

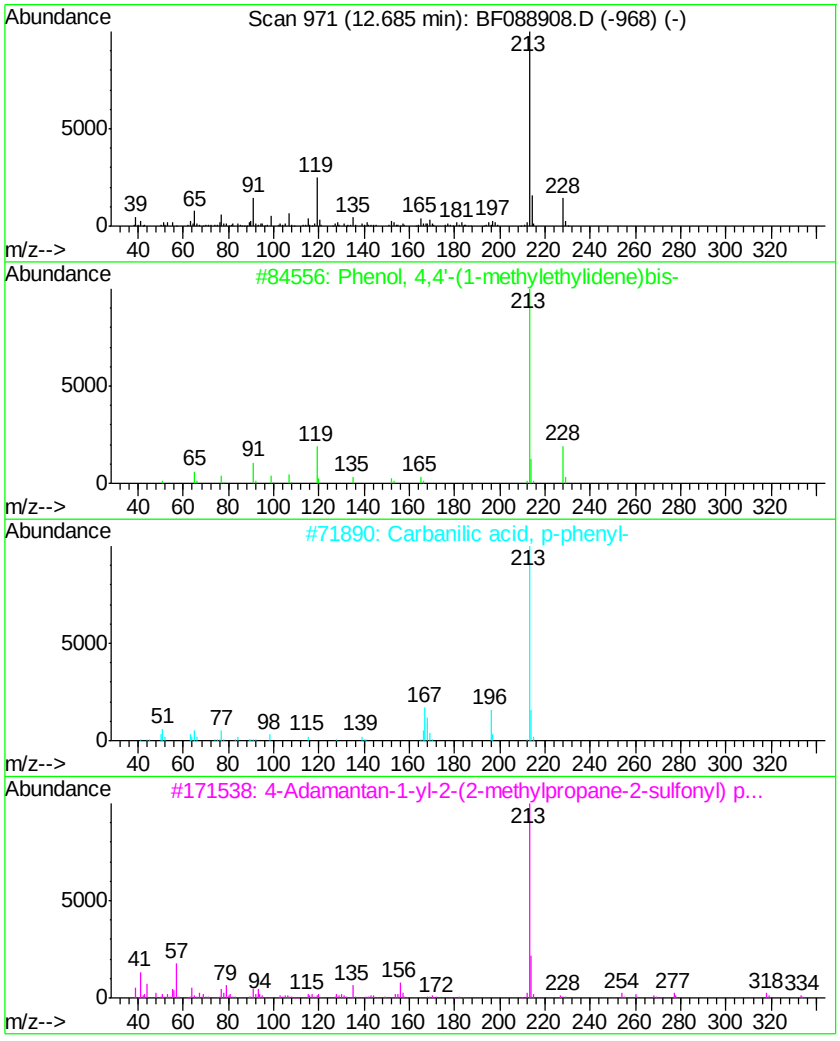
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

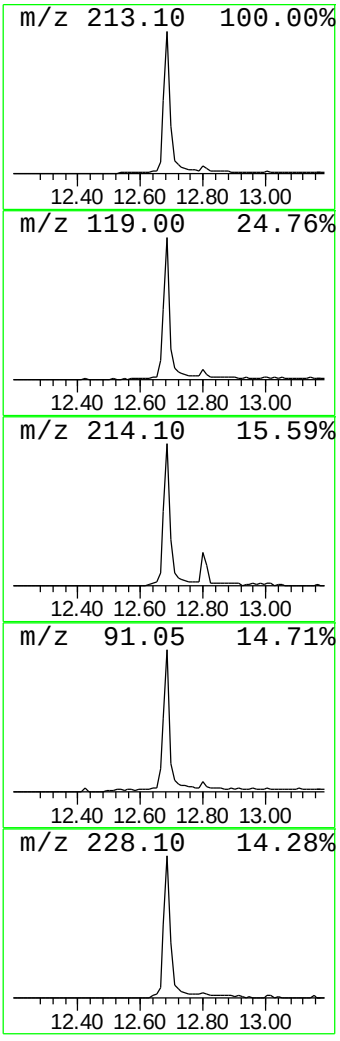
****

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	26.98 ng	715354	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49
3	4-Adamantan-1-yl-2-(2-methylprop...	333	C19H27NO2S	1000311-66-6	42
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	42
5	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

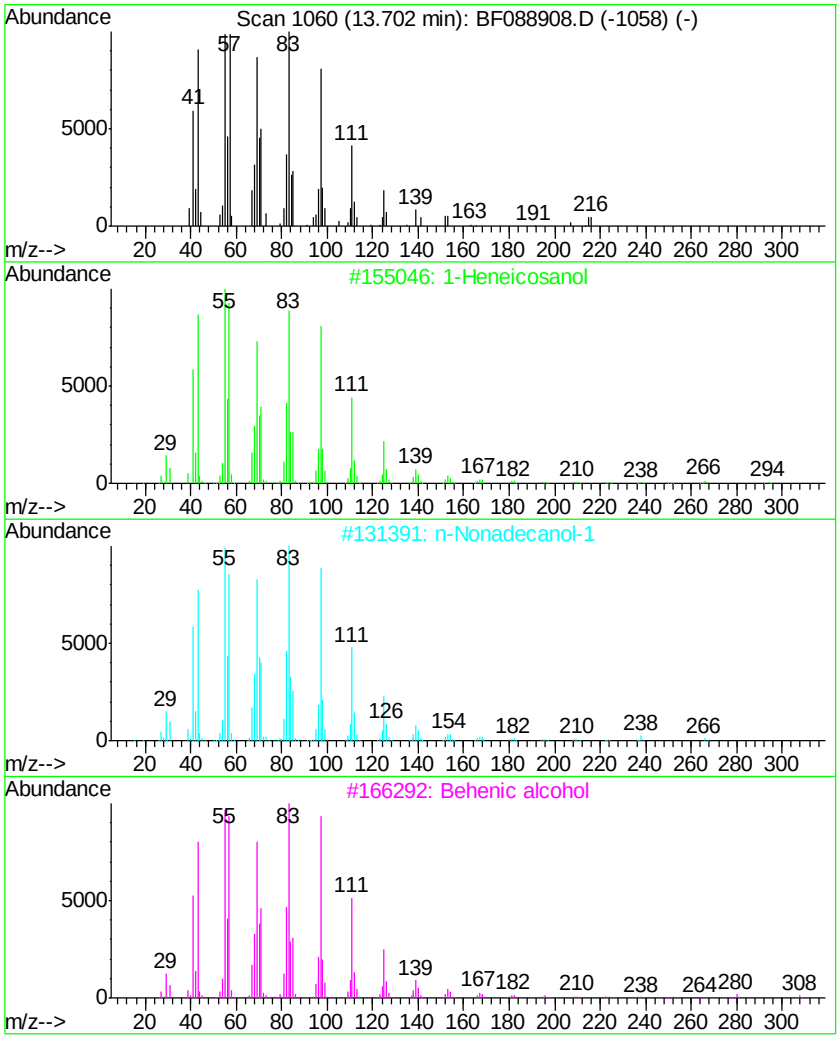
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

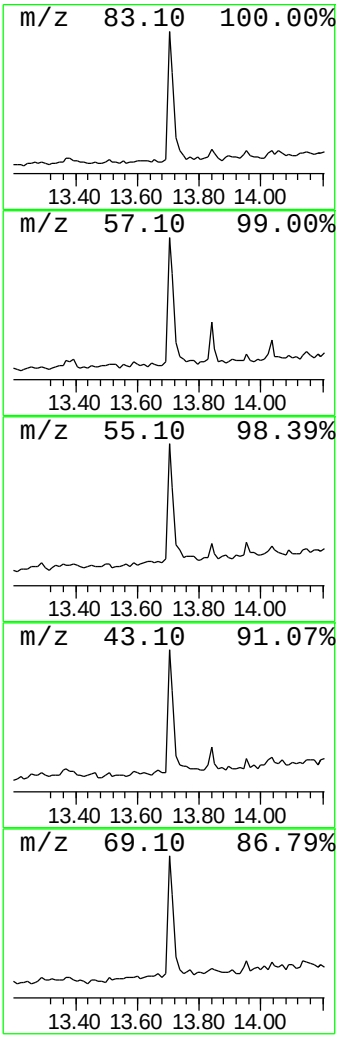
****

Peak Number 7 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.26 ng	112967	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

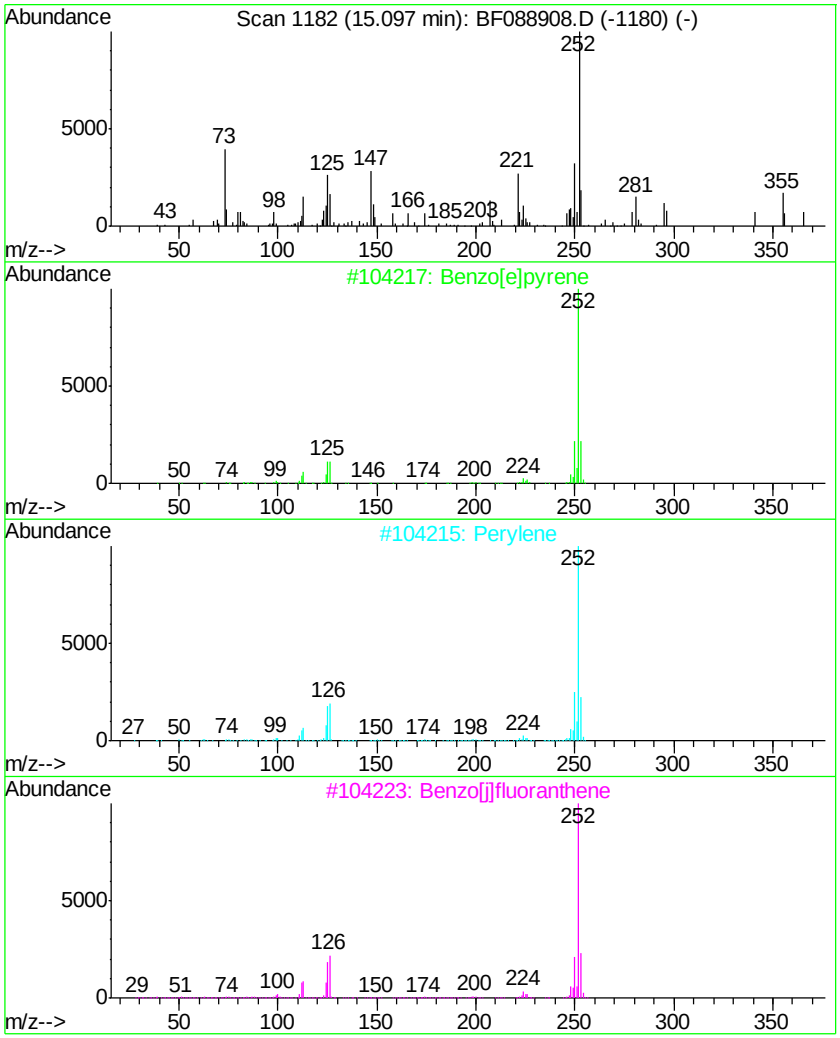
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

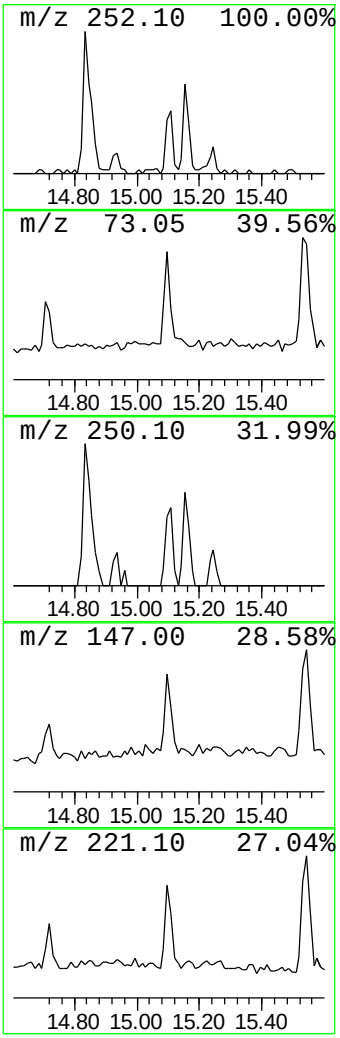
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	2.18 ng	37854	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	70
2	Perylene	252	C20H12	000198-55-0	46
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	46
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	41
5	Benzo[a]pyrene	252	C20H12	000050-32-8	41





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

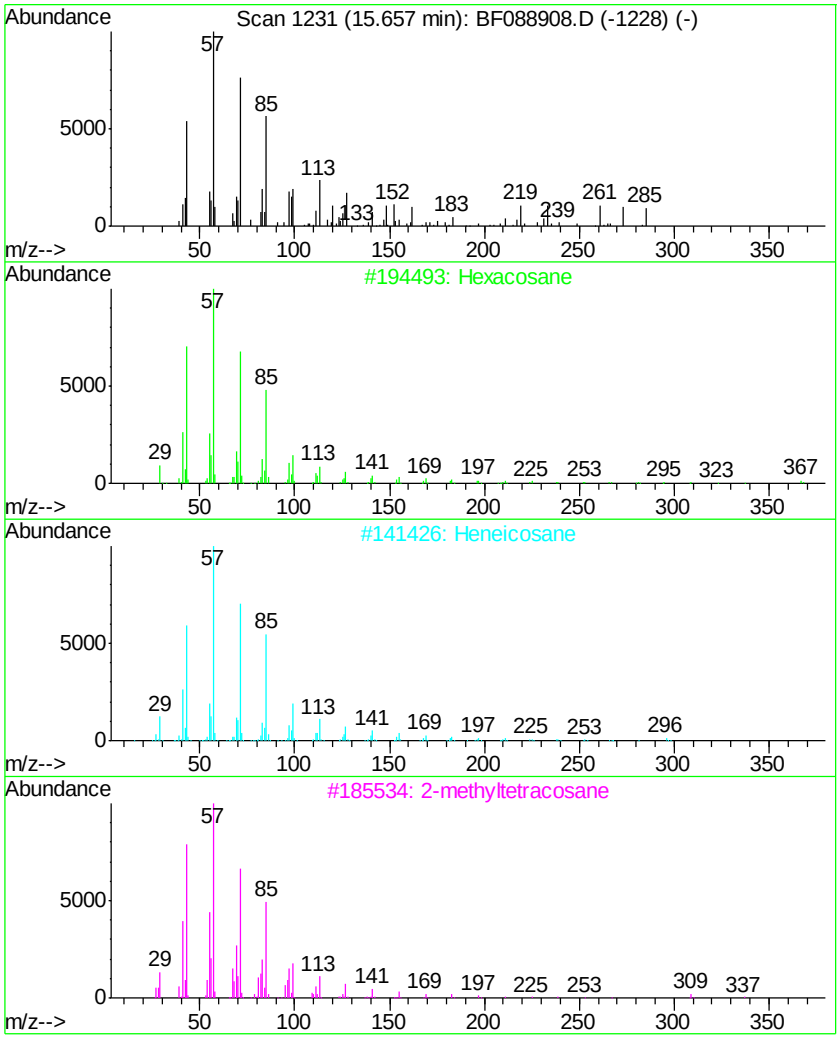
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

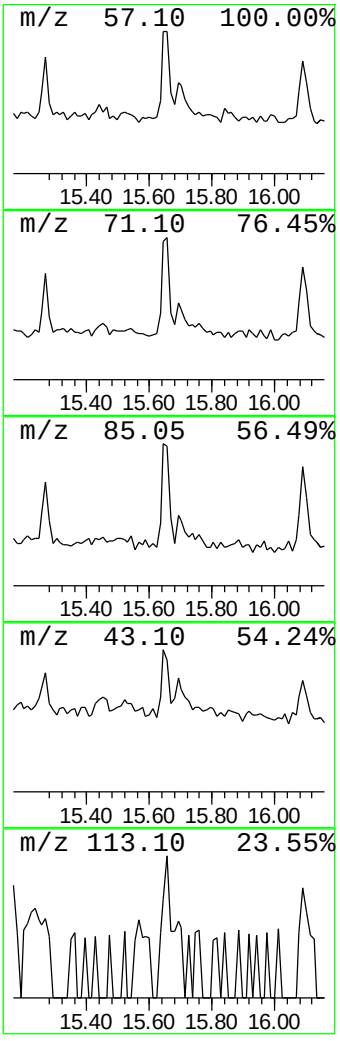
****

Peak Number 9 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.08 ng	36203	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	52
2	Heneicosane	296	C21H44	000629-94-7	52
3	2-methyltetracosane	352	C25H52	1000376-72-6	52
4	Hentriacontane	437	C31H64	000630-04-6	52
5	Heptadecane	240	C17H36	000629-78-7	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

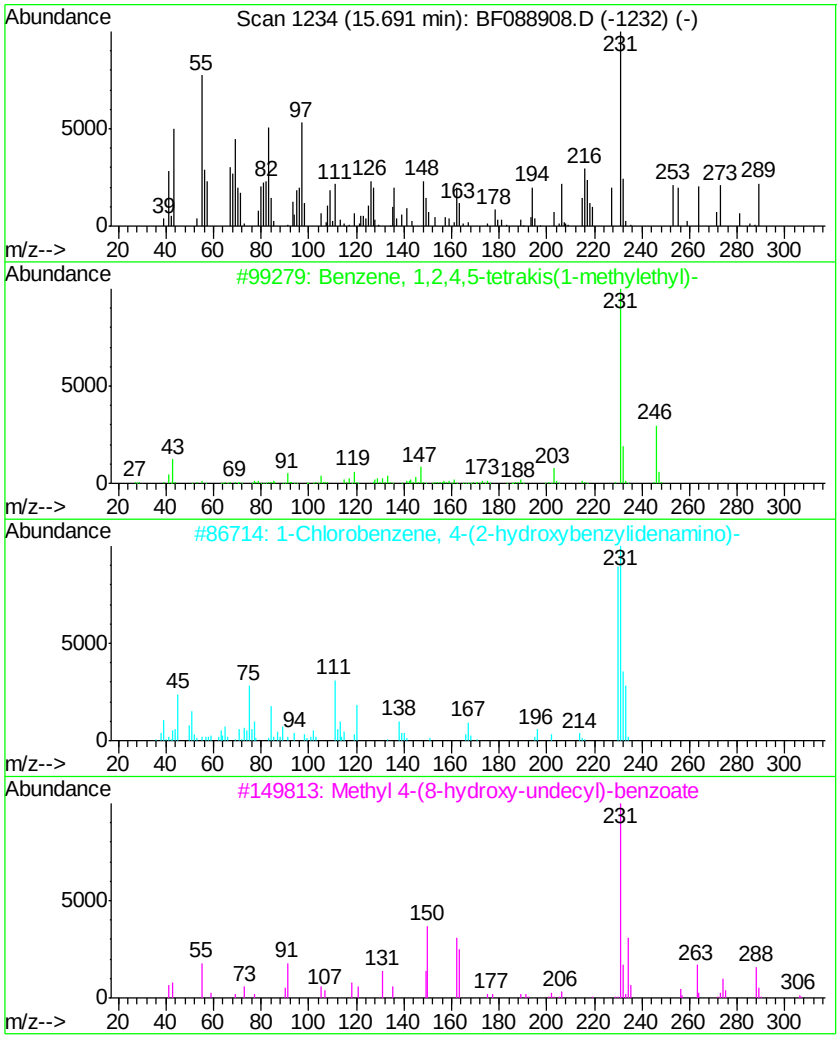
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

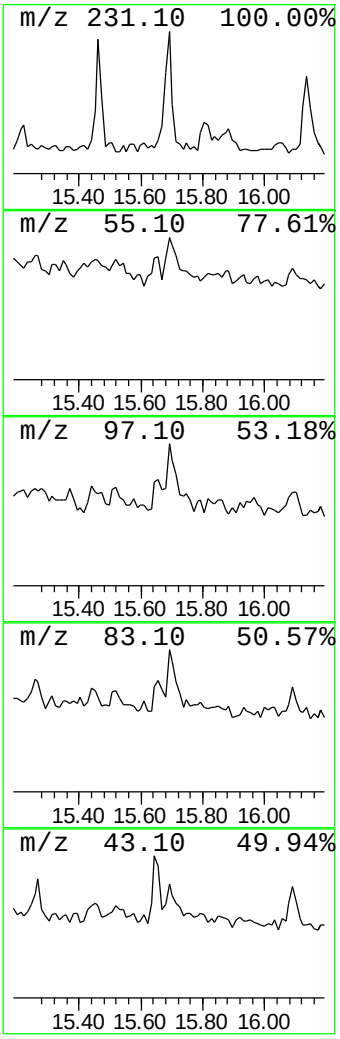
****

Peak Number 10 unknown15.69 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.69 ng	64137	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetrakis(1-meth...	246	C18H30	000635-11-0	22
2	1-Chlorobenzene, 4-(2-hydroxyben...	231	C13H10ClNO	1000221-93-4	22
3	Methyl 4-(8-hydroxy-undecyl)-ben...	306	C19H30O3	056306-72-0	12
4	2,6-Diphenylpyridine	231	C17H13N	003558-69-8	12
5	Cyclohexanamine, 2-[(phenylethyn...	231	C14H17NS	1000327-34-1	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

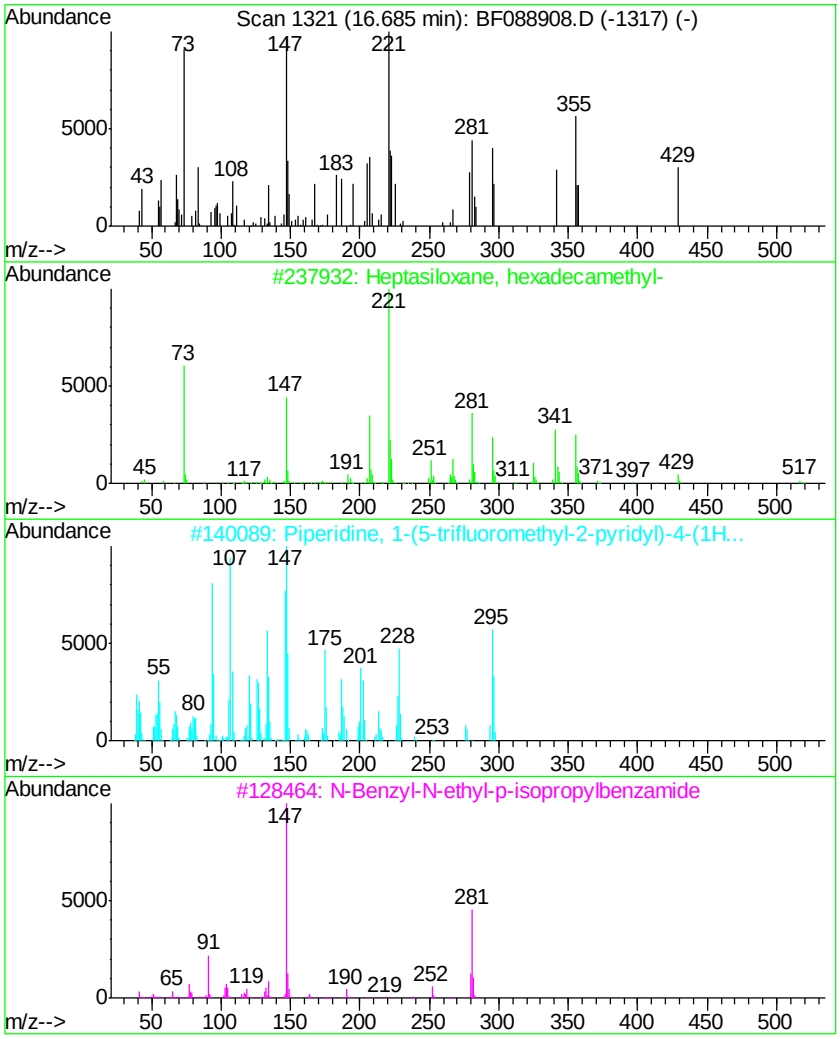
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

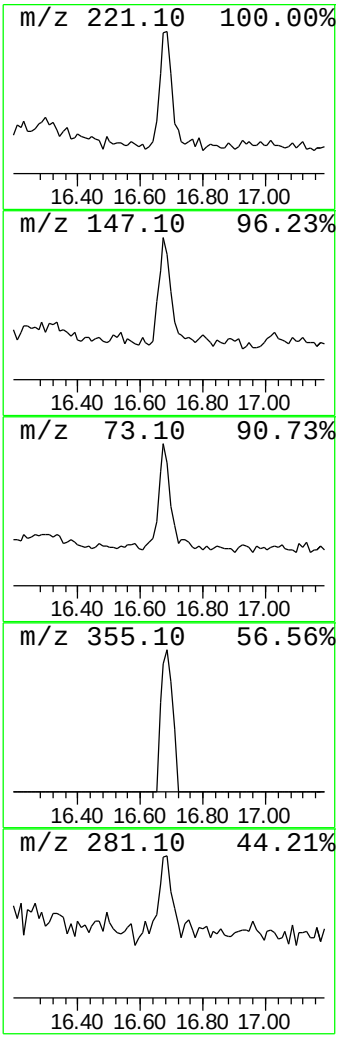
****

Peak Number 11 unknown16.69 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	3.64 ng	63272	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	37
2	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	35
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	18
4	4-Pyrimidinethiol, 5-(4-chlorph...	222	C10H7ClN2S	1000319-28-4	14
5	Silane, [[4-[1,2-bis[(trimethyls...	458	C20H42O4Si4	056114-62-6	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
Data File : BF088908.D
Acq On : 11 Jul 2016 19:25
Operator : UM/SJ
Sample : H3915-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P7-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.87	7.3	ng	141828	1	6.71	390370	20.0
unknown6.48	6.48	85.3	ng	1665110	1	6.71	390370	20.0
Phenol, 4,4'-(1-m...	12.69	27.0	ng	715354	5	13.84	530277	20.0
1-Heneicosanol	13.70	4.3	ng	112967	5	13.84	530277	20.0
Benzo[e]pyrene	15.10	2.2	ng	37854	6	15.21	347804	20.0
Hexacosane	15.66	2.1	ng	36203	6	15.21	347804	20.0
unknown15.69	15.69	3.7	ng	64137	6	15.21	347804	20.0
unknown16.69	16.69	3.6	ng	63272	6	15.21	347804	20.0