LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

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-BF092415.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	5.120	259	261	264	rVB	356485	485025	14.86%	1.952%
2	5.532	294	297	299	rBV	1526772	1388025	42.52%	5.586%
3	6.560	384	387	388	rBV	600676	822913	25.21%	3.312%
4	6.697	397	399	402	rBV	1780447	2377083	72.82%	9.567%
5	6.937	418	420	422	rBV	878343	714506	21.89%	2.876%
6	7.097	431	434	436	rVB	2651228	2413483	73.93%	9.714%
7	7.509	467	470	472	rBV	1811560	2008874	61.54%	8.085%
8	8.229	530	533	535	rVB	816947	883287	27.06%	3.555%
9	9.303	624	627	629	rBV	3742899	3264433	100.00%	13.138%
10	9.978	684	686	689	rBV	842131	935008	28.64%	3.763%
11	10.766	753	755	758	rBV2	1467359	1785047	54.68%	7.184%
12	11.464	814	816	819	rBV2	712488	832892	25.51%	3.352%
13	12.869	937	939	942	rBV	118647	111358	3.41%	0.448%
14	13.052	953	955	958	rBV	2043692	2715121	83.17%	10.928%
15	13.578	999	1001	1003	rBV	81528	72371	2.22%	0.291%
16	13.852	1021	1025	1031	rVB7	11761	48387	1.48%	0.195%
17	14.104	1045	1047	1050	rBV	530754	752748	23.06%	3.030%
18	14.367	1067	1070	1074	rBV5	15837	47968	1.47%	0.193%
19	14.881	1113	1115	1118	rVB2	33398	42389	1.30%	0.171%
20	15.578	1173	1176	1184	rBV	469996	792515	24.28%	3.190%
21	16.458	1245	1253	1265	rBV2	59061	361109	11.06%	1.453%
22	17.133	1308	1312	1317	rVB	47761	112883	3.46%	0.454%
23	18.253	1398	1410	1411	rBV	109759	587493	18.00%	2.364%
24	19.670	1530	1534	1542	rVB2	41391	156880	4.81%	0.631%
25	21.476	1684	1692	1698	rBV	236854	1134645	34.76%	4.567%

Sum of corrected areas: 24846443

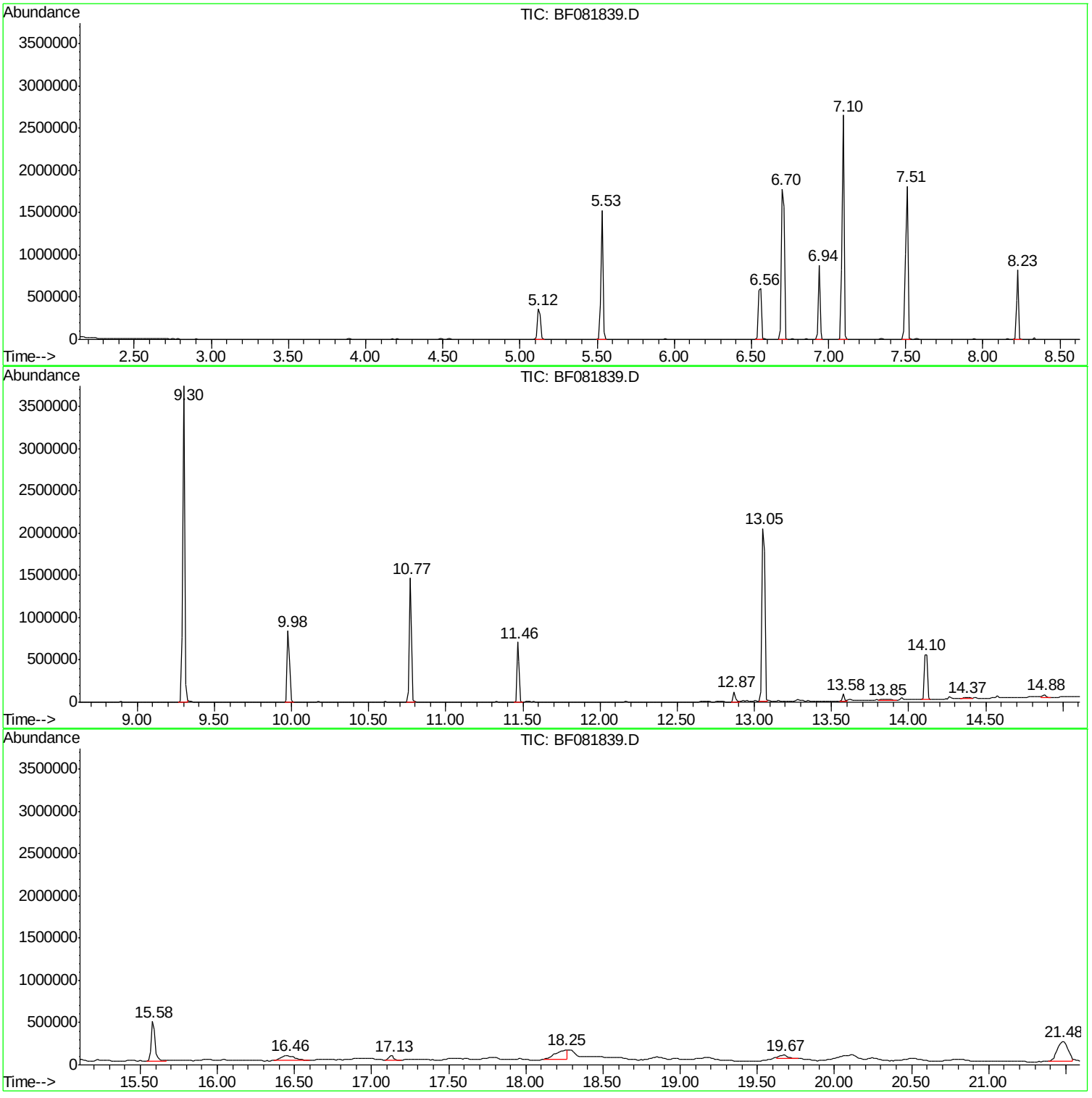
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

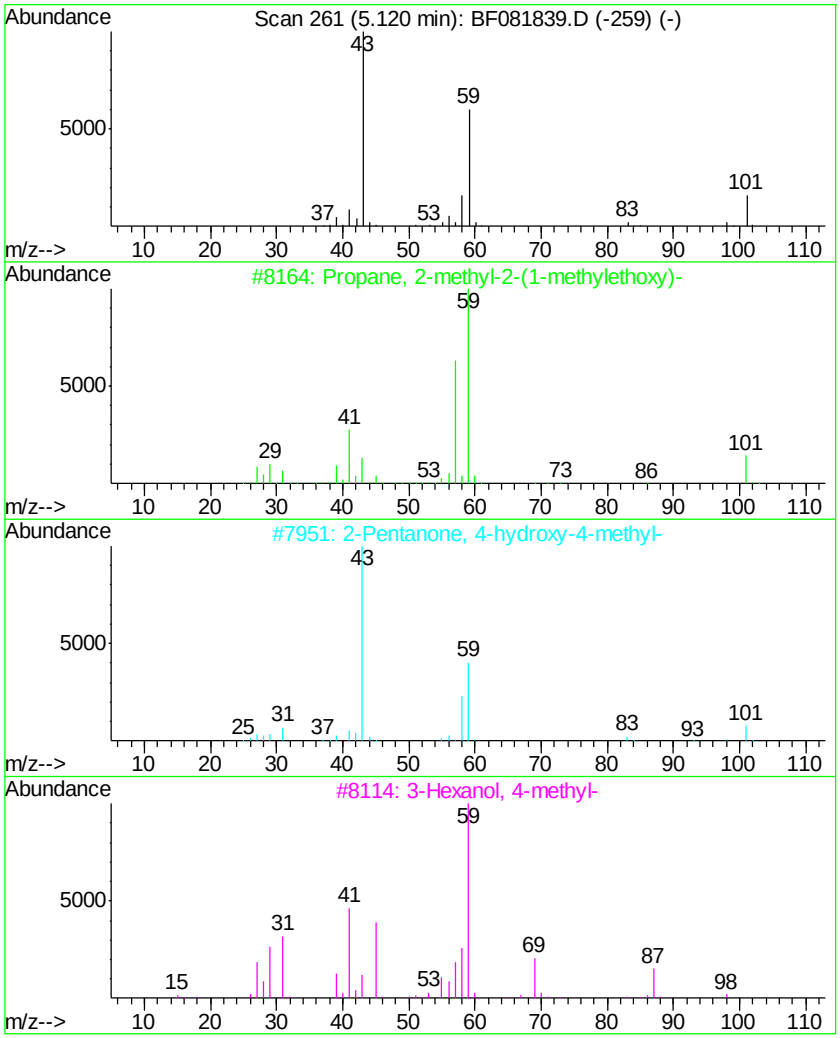
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

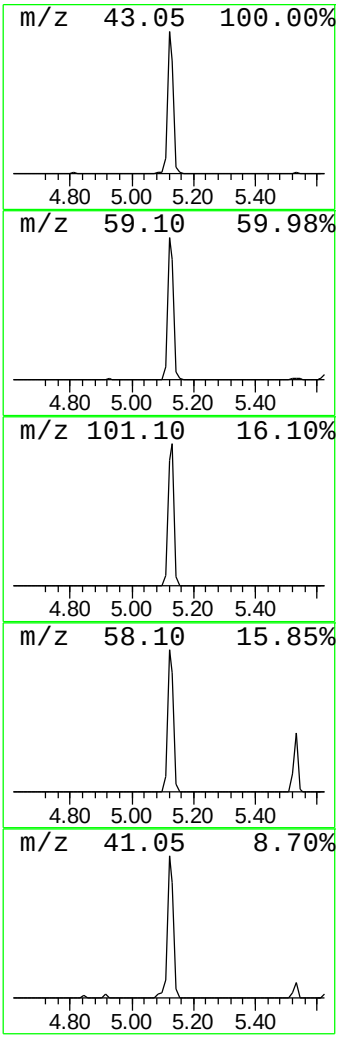
****

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	13.58 ng	485025	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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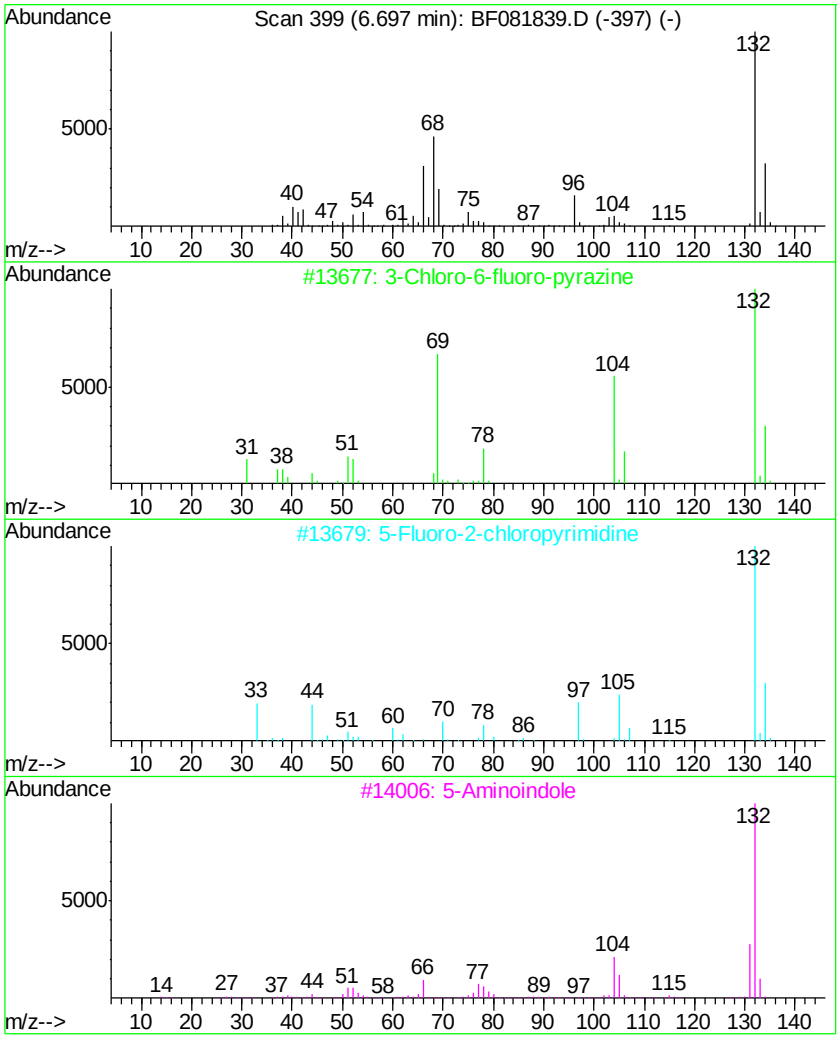
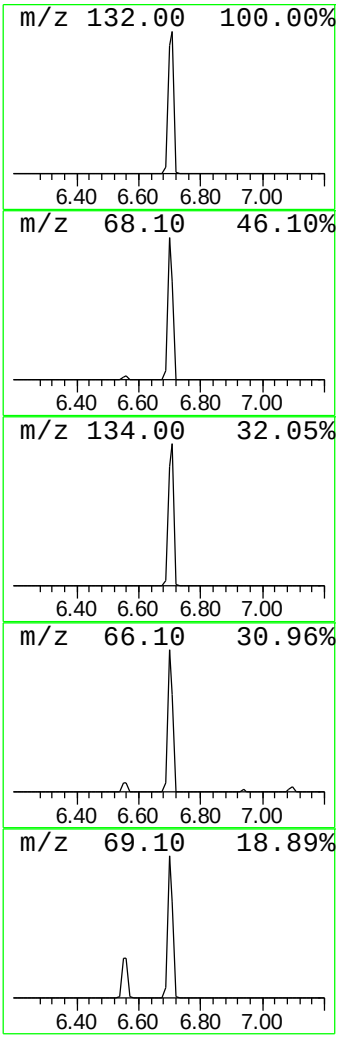
Peak Number 2 unknown6.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	66.54 ng	2377080	1,4-Dichlorobenzene-d4	6.94

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	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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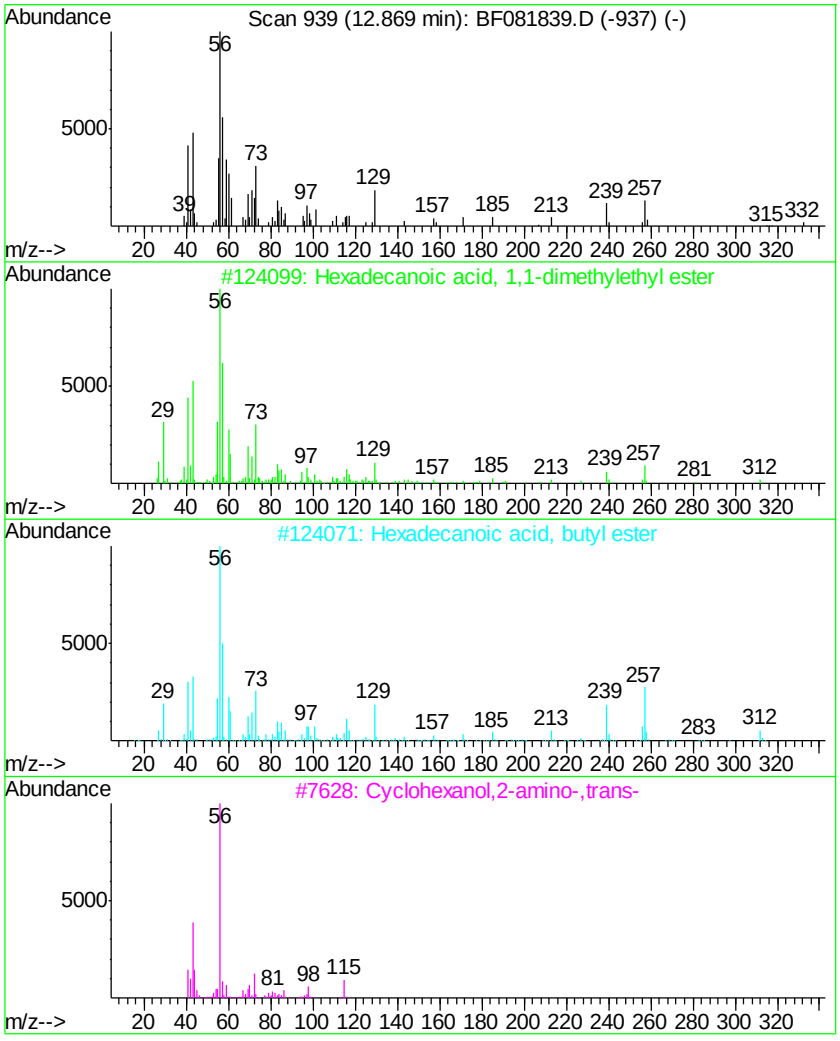
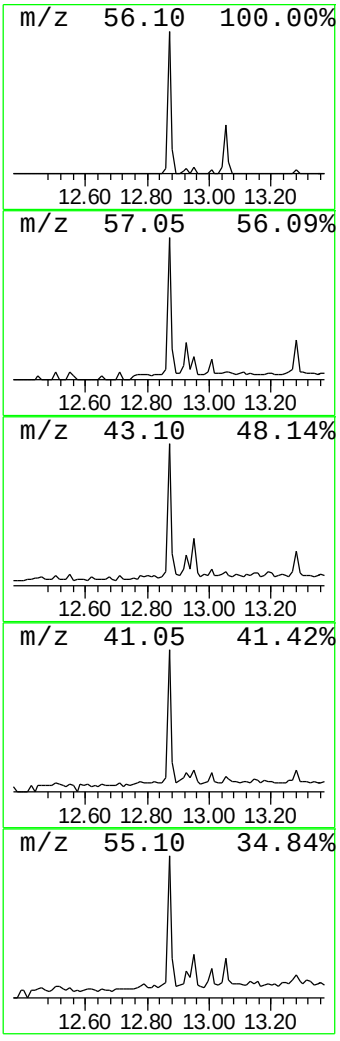
Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.96 ng	111358	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3	Cyclohexanol,2-amino-,trans-	115	C6H13NO	006982-39-4	38
4	5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	35
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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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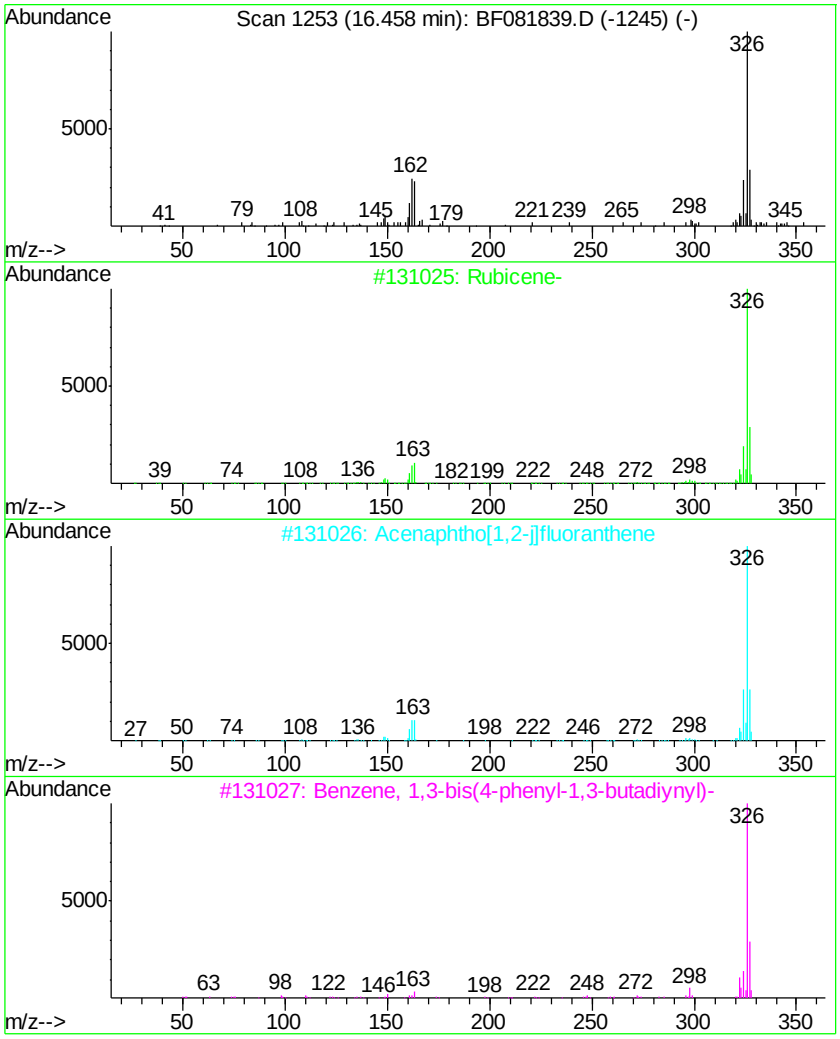
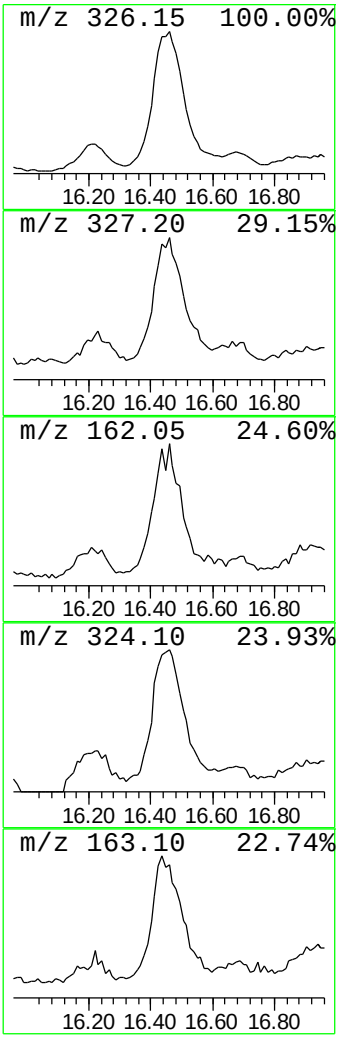
Peak Number 5 Rubicene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	9.11 ng	361109	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Rubicene-	326	C26H14	000197-61-5	90
2	Acenaphtho[1,2-j]fluoranthene	326	C26H14	000193-21-5	90
3	Benzene, 1,3-bis(4-phenyl-1,3-bu...	326	C26H14	037902-13-9	76
4	Bis(pentamethylcyclopentadienyl)...	326	C20H30Fe	012126-50-0	52
5	Benzenamine, N-(9-anthracenylmet...	326	C21H14N2O2	014607-12-6	43





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Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

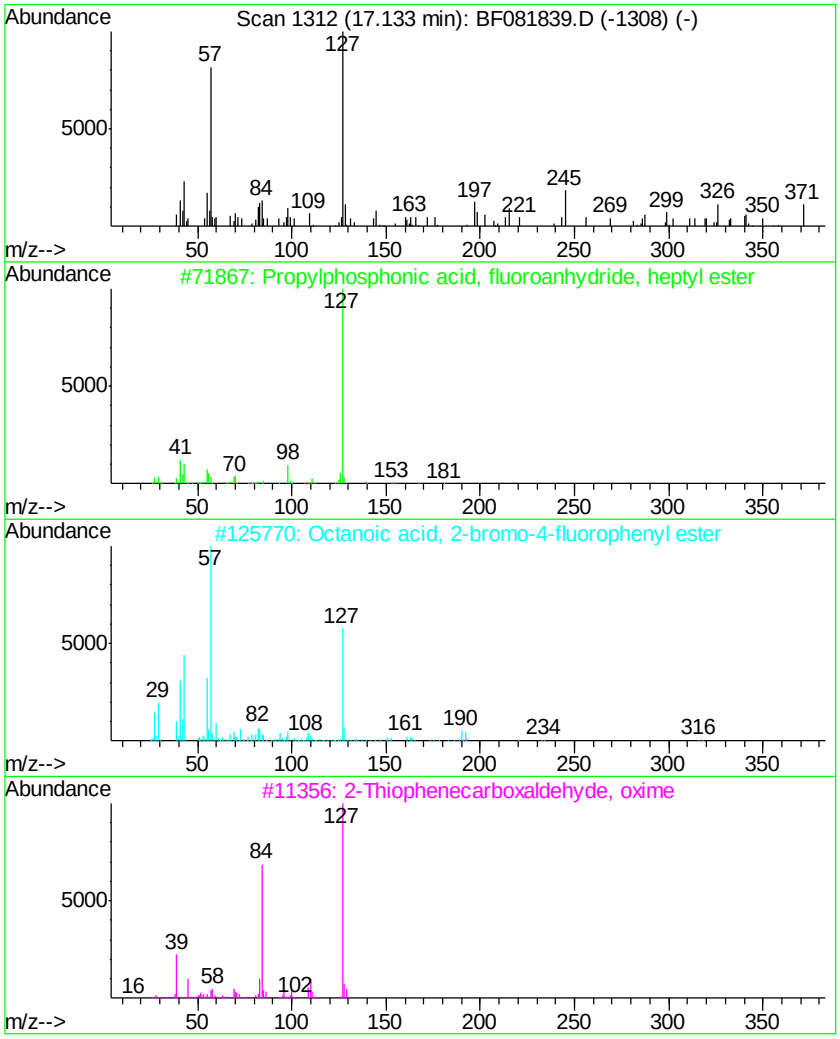
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

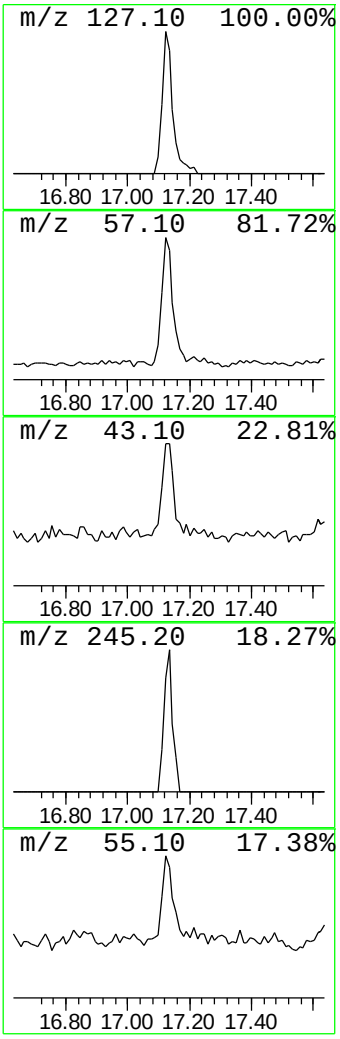
****

Peak Number 6 unknown17.13 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.85 ng	112883	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylphosphonic acid, fluoroanh...	224	C10H22FO2P	333416-19-6	43
2	Octanoic acid, 2-bromo-4-fluorop...	316	C14H18BrFO2	002923-78-6	43
3	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	43
4	2,4-Imidazolidinedione, 1,5,5-tr...	142	C6H10N2O2	006851-81-6	43
5	Phosphonofluoridic acid, propyl-...	252	C12H26FO2P	333416-21-0	43





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Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

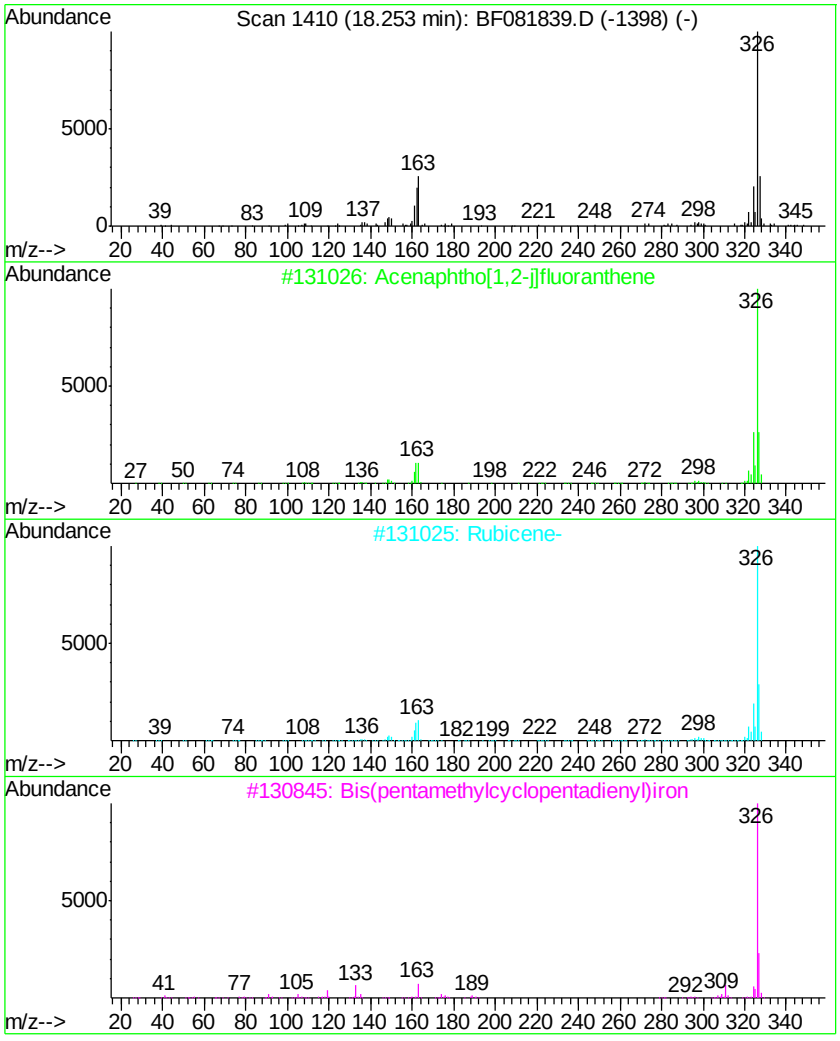
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

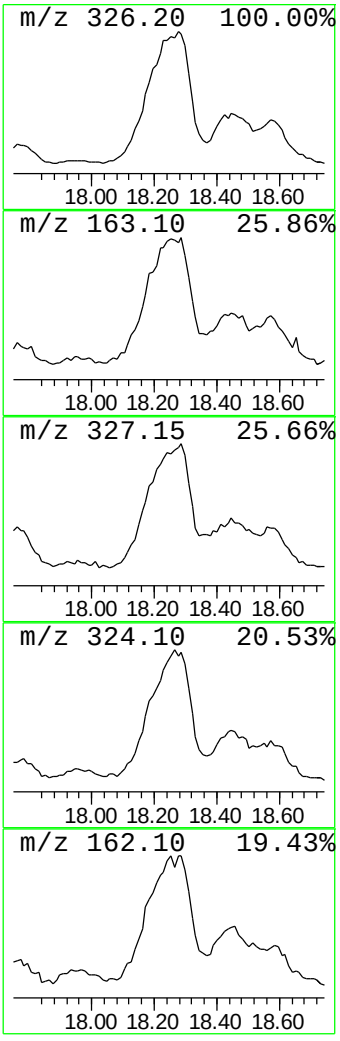
****

Peak Number 7 Acenaphtho[1,2-j]fluoranthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	14.83 ng	587493	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphtho[1,2-j]fluoranthene	326	C26H14	000193-21-5	93
2	Rubicene-	326	C26H14	000197-61-5	86
3	Bis(pentamethylcyclopentadienyl)...	326	C20H30Fe	012126-50-0	52
4	9-Anthracenamine, N-[(4-nitrophe...	326	C21H14N2O2	127387-74-0	43
5	4-Hydroxy-4'-phenoxydiphenylsulfone	326	C18H14O4S	018995-10-3	38





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Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

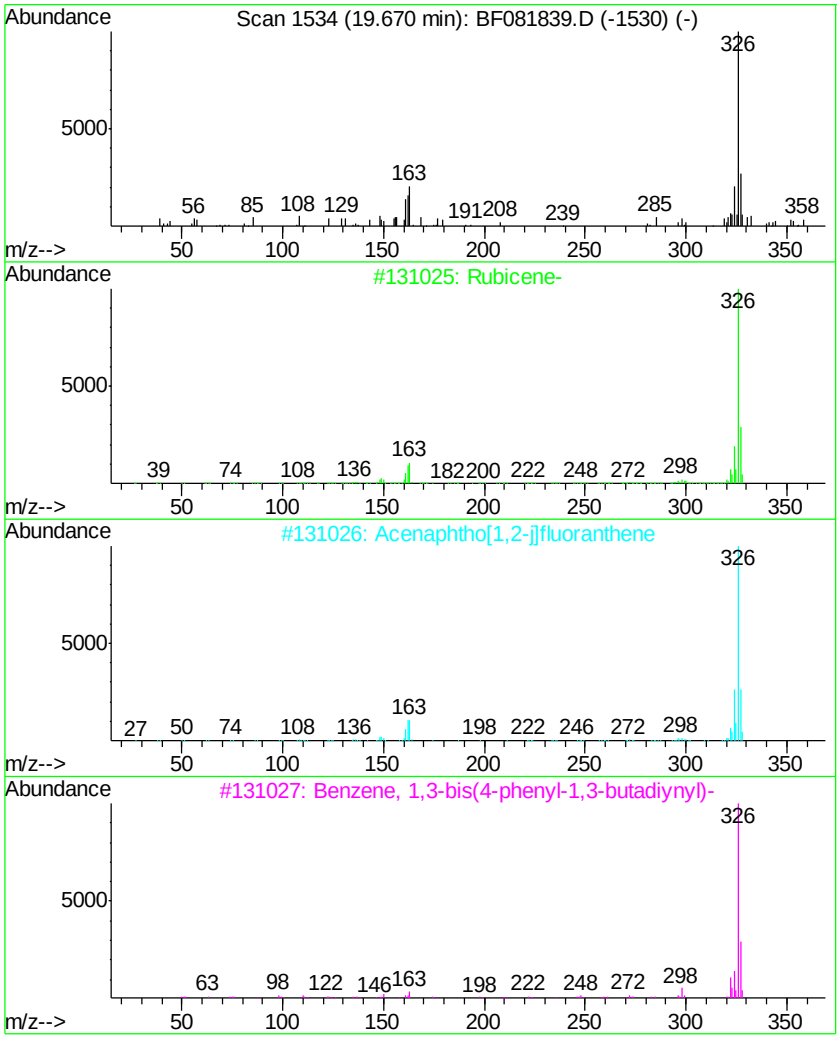
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

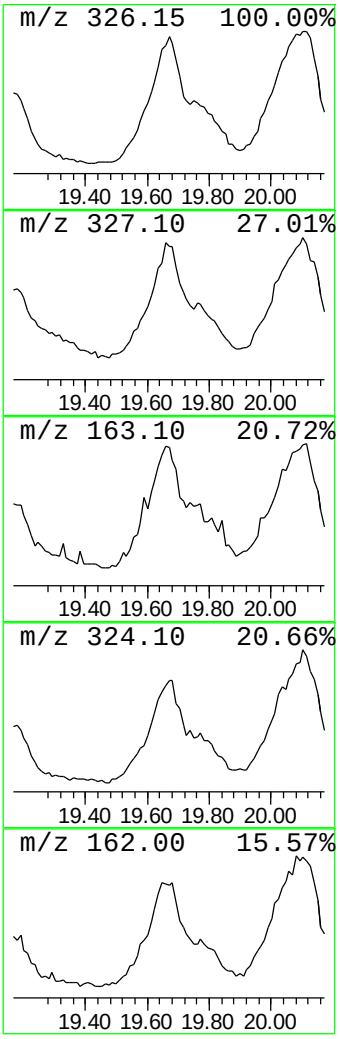
****

Peak Number 8 Benzene, 1,3-bis(4-phenyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.67	3.96 ng	156880	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Rubicene-	326	C26H14	000197-61-5	92
2	Acenaphtho[1,2-j]fluoranthene	326	C26H14	000193-21-5	89
3	Benzene, 1,3-bis(4-phenyl-1,3-bu...	326	C26H14	037902-13-9	81
4	Silane, (estra-1,3,5(10),16-tetr...	326	C21H30OSi	069688-27-3	50
5	4-(3-Nitroanilino)-5,6,7,8-tetra...	326	C16H14N4O2S	313952-58-8	47





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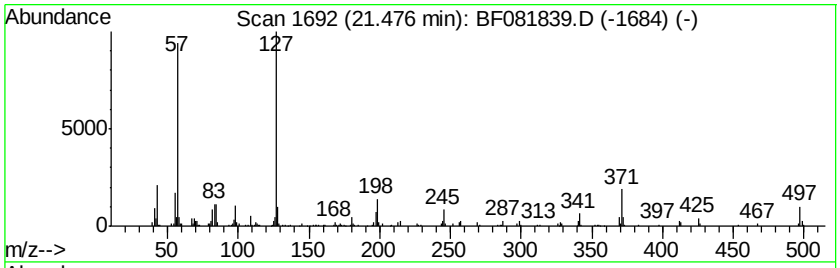
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

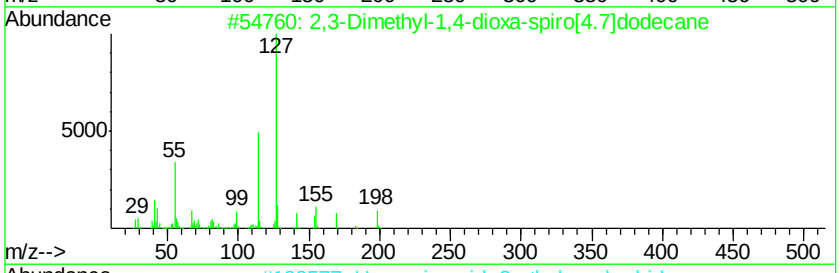
****

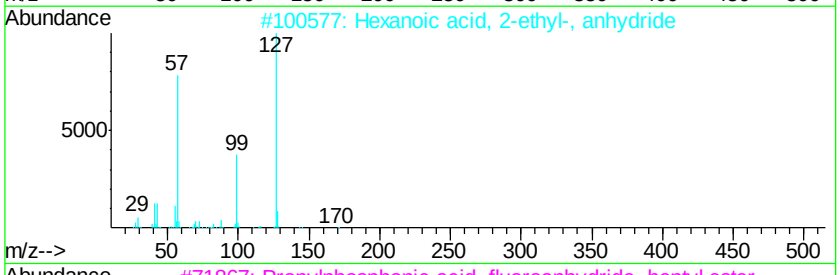
Peak Number 9 2,3-Dimethyl-1,4-dioxa-spir... Concentration Rank 3

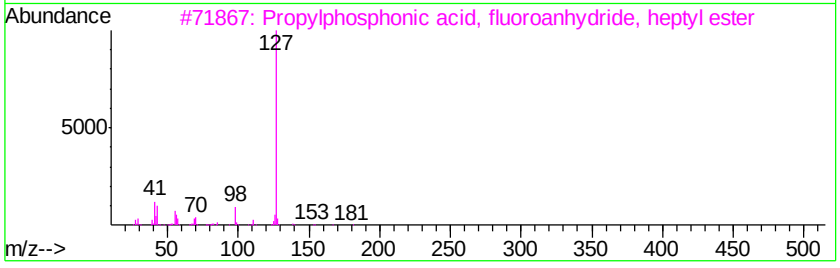
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.48	28.63 ng	1134650	Perylene-d12	15.58

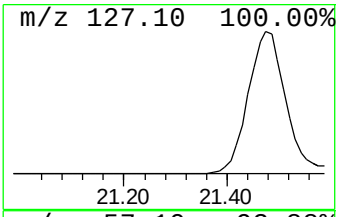
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-1,4-dioxa-spiro[4.7...	198	C12H22O2	062406-91-1	53
2	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	47
3	Propylphosphonic acid, fluoroanh...	224	C10H22FO2P	333416-19-6	47
4	Phosphonofluoridic acid, (1-meth...	210	C9H20FO2P	333416-32-3	47
5	2-Mercaptopyridine-N-oxide	127	C5H5NOS	001121-31-9	47

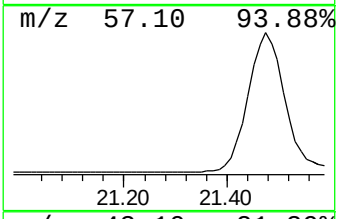


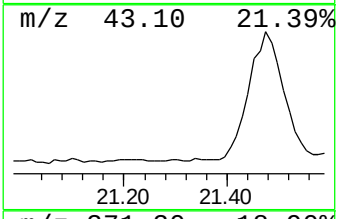


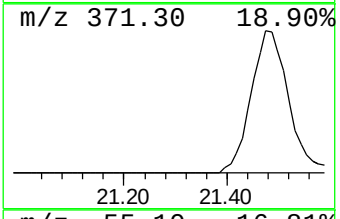


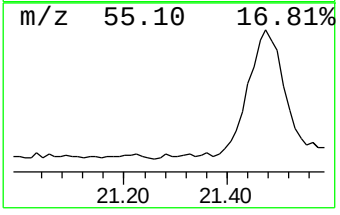












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092615\
Data File : BF081839.D
Acq On : 26 Sep 2015 20:58
Operator : UM/IZ
Sample : G3754-11
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EQUIPMENTBLANK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092415.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
Propane, 2-methyl...	5.12	13.6	ng	485025	1	6.94	714506	20.0
unknown6.70	6.70	66.5	ng	2377080	1	6.94	714506	20.0
Hexadecanoic acid...	12.87	3.0	ng	111358	5	14.12	752748	20.0
Rubicene-	16.46	9.1	ng	361109	6	15.58	792515	20.0
unknown17.13	17.13	2.9	ng	112883	6	15.58	792515	20.0
Acenaphtho[1,2-j]...	18.25	14.8	ng	587493	6	15.58	792515	20.0
Benzene, 1,3-bis(...	19.67	4.0	ng	156880	6	15.58	792515	20.0
2,3-Dimethyl-1,4-...	21.48	28.6	ng	1134650	6	15.58	792515	20.0