LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-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-BF050416.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	4.887	242	245	252	rBV	138993	188991	9.15%	0.748%
2	5.322	280	283	286	rBV	2187581	2066002	100.00%	8.181%
3	5.539	300	302	308	rVB	24513	48234	2.33%	0.191%
4	5.733	316	319	326	rVB	23007	37929	1.84%	0.150%
5	6.373	373	375	378	rBV	1673964	1910550	92.48%	7.565%
6	6.499	384	386	389	rBV	1645920	2050983	99.27%	8.121%
7	6.567	389	392	395	rVB	23330	37356	1.81%	0.148%
8	6.613	395	396	405	rVB2	25017	49853	2.41%	0.197%
9	6.739	405	407	409	rBV	1138195	1081150	52.33%	4.281%
10	6.887	418	420	423	rBV	1256873	1550841	75.06%	6.141%
11	7.002	428	430	436	rVB	30237	54883	2.66%	0.217%
12	7.299	454	456	459	rBV	1017453	1139176	55.14%	4.511%
13	7.596	480	482	487	rVB	96862	148485	7.19%	0.588%
14	8.019	517	519	522	rBV	853270	1245341	60.28%	4.931%
15	8.248	537	539	541	rBV	70294	66201	3.20%	0.262%
16	8.305	542	544	547	rBV	90026	87761	4.25%	0.348%
17	8.728	579	581	586	rVB3	25118	41983	2.03%	0.166%
18	9.105	611	614	616	rBV	1970115	1867455	90.39%	7.395%
19	9.231	623	625	626	rBV	38006	47477	2.30%	0.188%
20	9.493	646	648	651	rBV	77831	102513	4.96%	0.406%
21	9.642	659	661	664	rVB	15414	24684	1.19%	0.098%
22	9.722	664	668	670	rBV	50896	64663	3.13%	0.256%
23	9.779	670	673	675	rBV	1070090	1141613	55.26%	4.521%
24	10.213	709	711	715	rVB	59447	68303	3.31%	0.270%
25	10.316	719	720	723	rVB2	17248	22925	1.11%	0.091%
26	10.431	728	730	733	rVB	17224	25083	1.21%	0.099%
27	10.556	739	741	744	rBV2	775967	943904	45.69%	3.738%
28	10.694	751	753	756	rBV	49957	78534	3.80%	0.311%
29	11.139	788	792	797	rBV4	28787	74253	3.59%	0.294%
30	11.254	800	802	807	rBV2	996315	1203537	58.25%	4.766%
31	11.334	807	809	811	rVB	52509	62700	3.03%	0.248%
32	11.494	821	823	827	rBV	14031	27612	1.34%	0.109%
33	11.756	844	846	847	rBV	32340	37445	1.81%	0.148%
34	11.791	847	849	851	rVV	61462	86319	4.18%	0.342%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-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-BF050416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.871	854	856	860	rVB2	50396	94216	4.56%	0.373%
36	12.054	870	872	876	rBV2	24431	53735	2.60%	0.213%
37	12.305	892	894	896	rBV	27235	43245	2.09%	0.171%
38	12.385	900	901	903	rBV	18570	31336	1.52%	0.124%
39	12.465	906	908	910	rBV	554849	505055	24.45%	2.000%
40	12.694	925	928	930	rBV	407180	504201	24.40%	1.997%
41	12.728	930	931	936	rVB3	27761	44892	2.17%	0.178%
42	12.808	936	938	939	rBV	28151	37424	1.81%	0.148%
43	12.842	939	941	943	rVV	1546044	1501168	72.66%	5.944%
44	12.911	943	947	951	rVV4	32669	92755	4.49%	0.367%
45	13.014	954	956	958	rVB	46743	76417	3.70%	0.303%
46	13.082	961	962	964	rVV	53930	54323	2.63%	0.215%
47	13.128	964	966	969	rVV2	38390	70491	3.41%	0.279%
48	13.745	1018	1020	1024	rBV3	72601	131780	6.38%	0.522%
49	13.882	1029	1032	1039	rBV	853283	1537266	74.41%	6.087%
50	14.888	1118	1120	1124	rBV	210792	486781	23.56%	1.928%
51	15.163	1142	1144	1146	rBV2	157505	240307	11.63%	0.952%
52	15.277	1153	1154	1160	rVB	452183	807647	39.09%	3.198%
53	15.917	1208	1210	1217	rVB	251520	641196	31.04%	2.539%
54	16.305	1241	1244	1249	rVB	321806	615081	29.77%	2.436%

Sum of corrected areas: 25254055

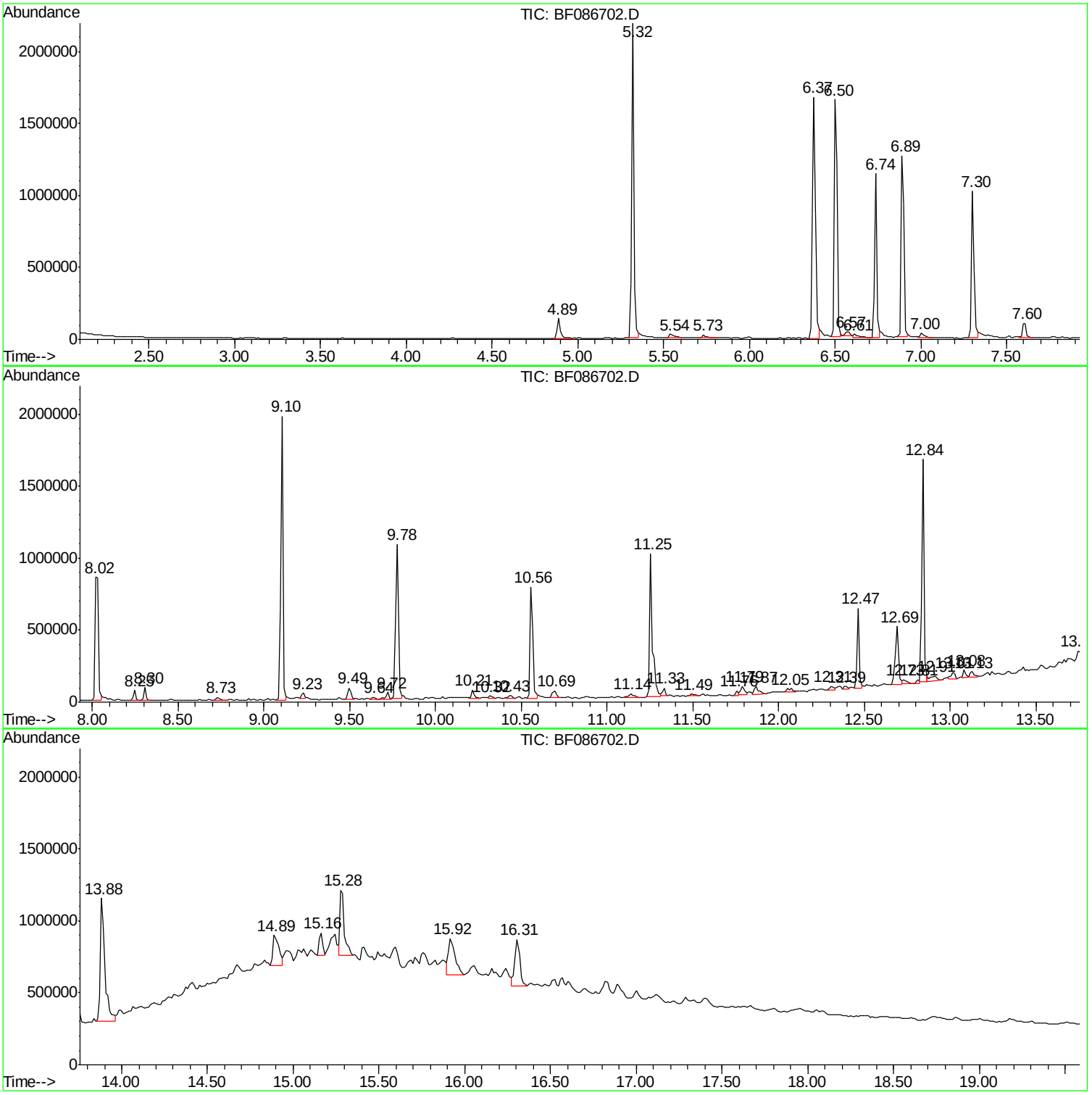
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
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Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

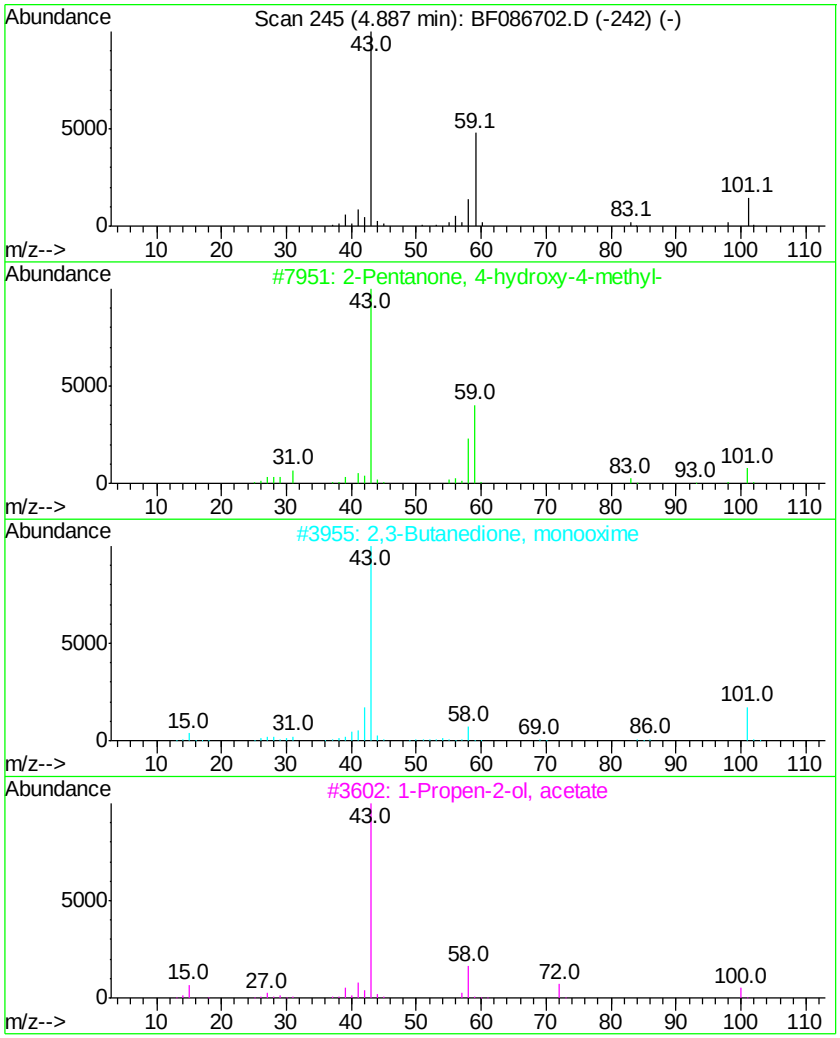
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

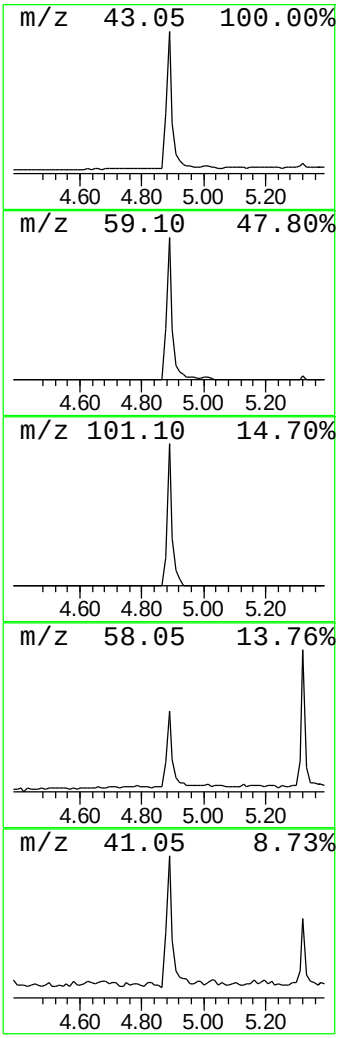
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	6.99 ng	188991	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

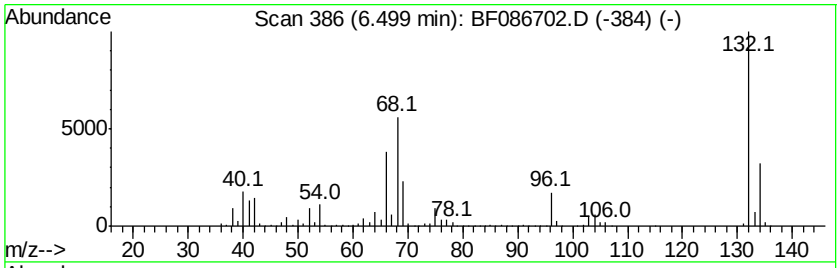
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

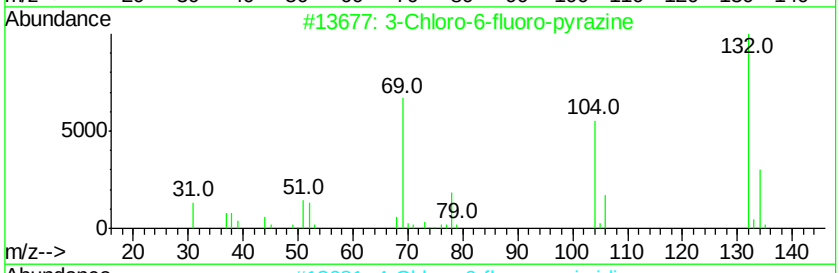
****

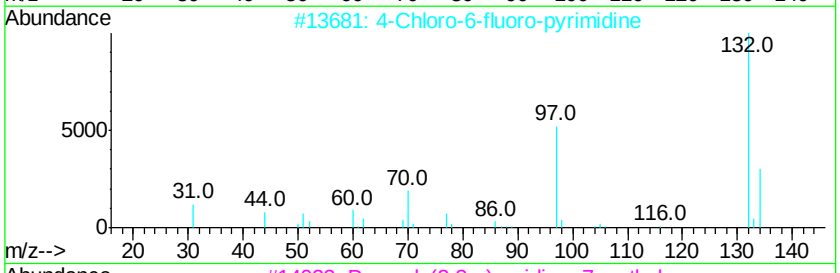
Peak Number 2 unknown6.50 Concentration Rank 1

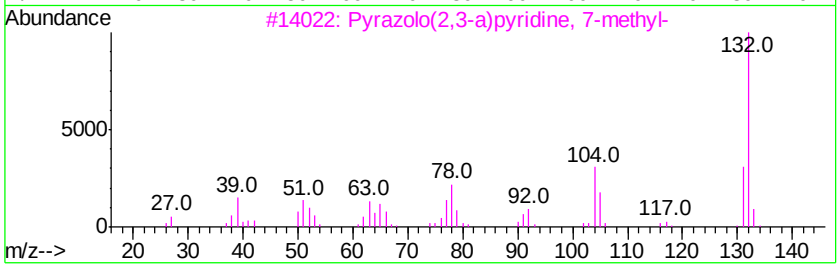
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	75.88 ng	2050980	1,4-Dichlorobenzene-d4	6.74

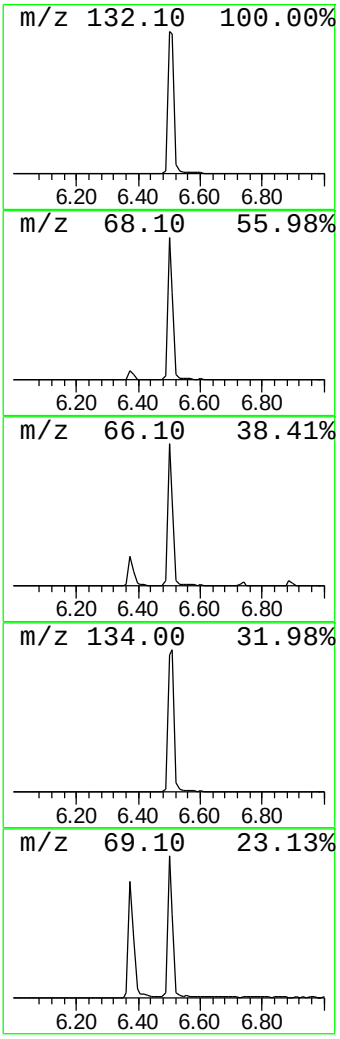
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10











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Acq On : 5 May 2016 3:19
Operator : UM/SJ
Sample : H2829-07 2X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

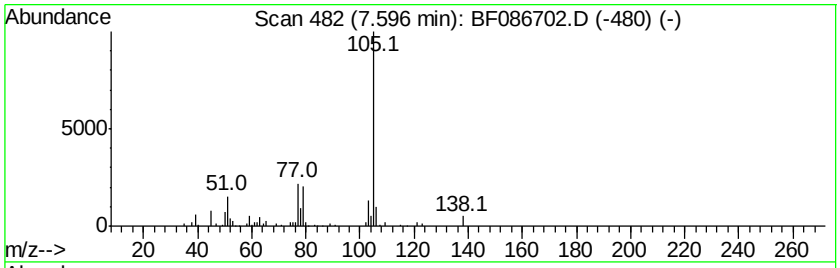
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

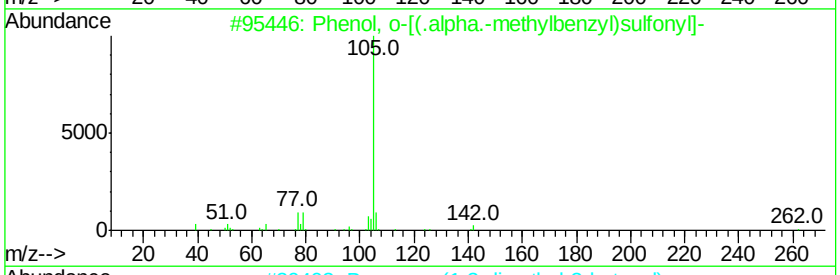
****

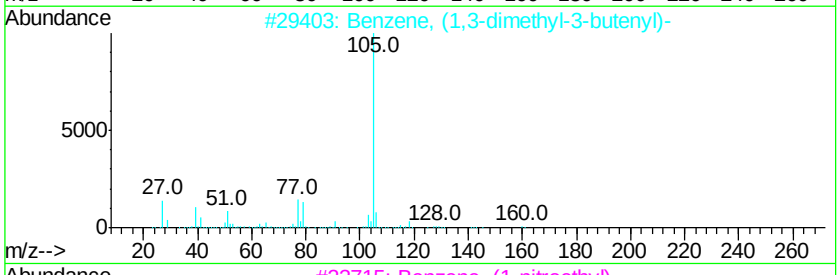
Peak Number 4 Phenol, o-[(.alpha.-methylb... Concentration Rank 7

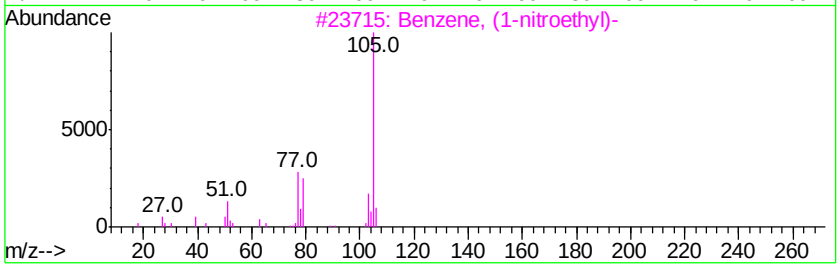
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	4.77 ng	148485	Naphthalene-d8	8.03

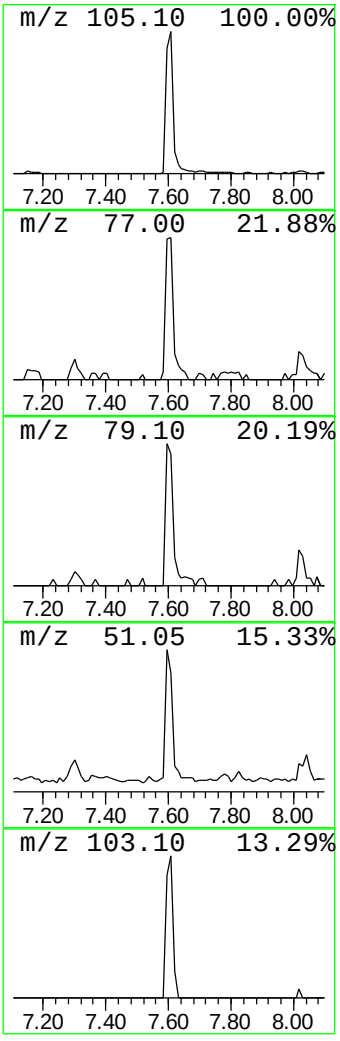
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, o-[(.alpha.-methylbenzyl...	262	C14H14O3S	029634-38-6	78
2	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	72
3	Benzene, (1-nitroethyl)-	151	C8H9NO2	007214-61-1	64
4	Benzene, (1-bromoethyl)-	184	C8H9Br	000585-71-7	64
5	Thiophene, 2-(4-methylbenzylsulf...	252	C12H12O2S2	153837-88-8	59











Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
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Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

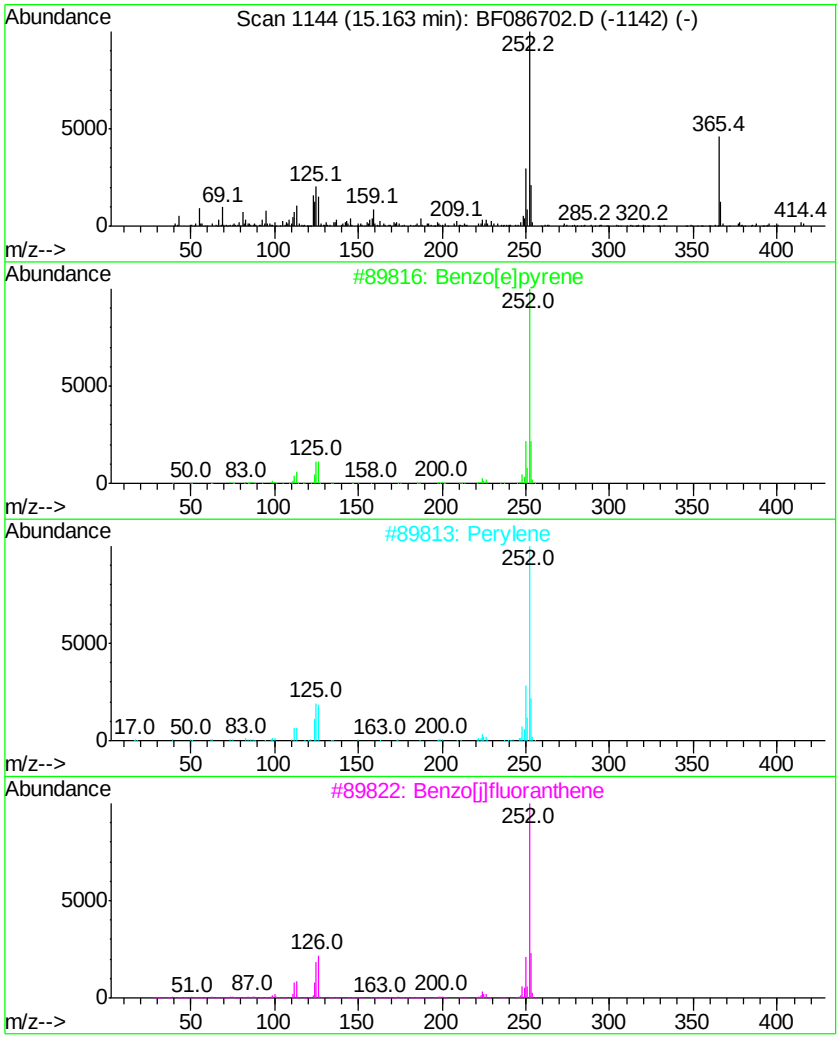
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

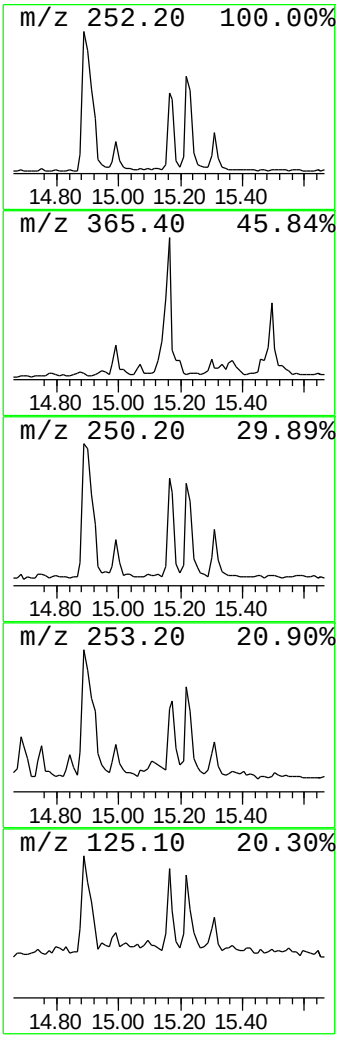
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	11.90 ng	240307	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	91
2	Perylene	252	C20H12	000198-55-0	91
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	87





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ClientSampleId : WPG-B2(0-9.5)-C

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TIC Library : C:\DATABASE\NIST02.L
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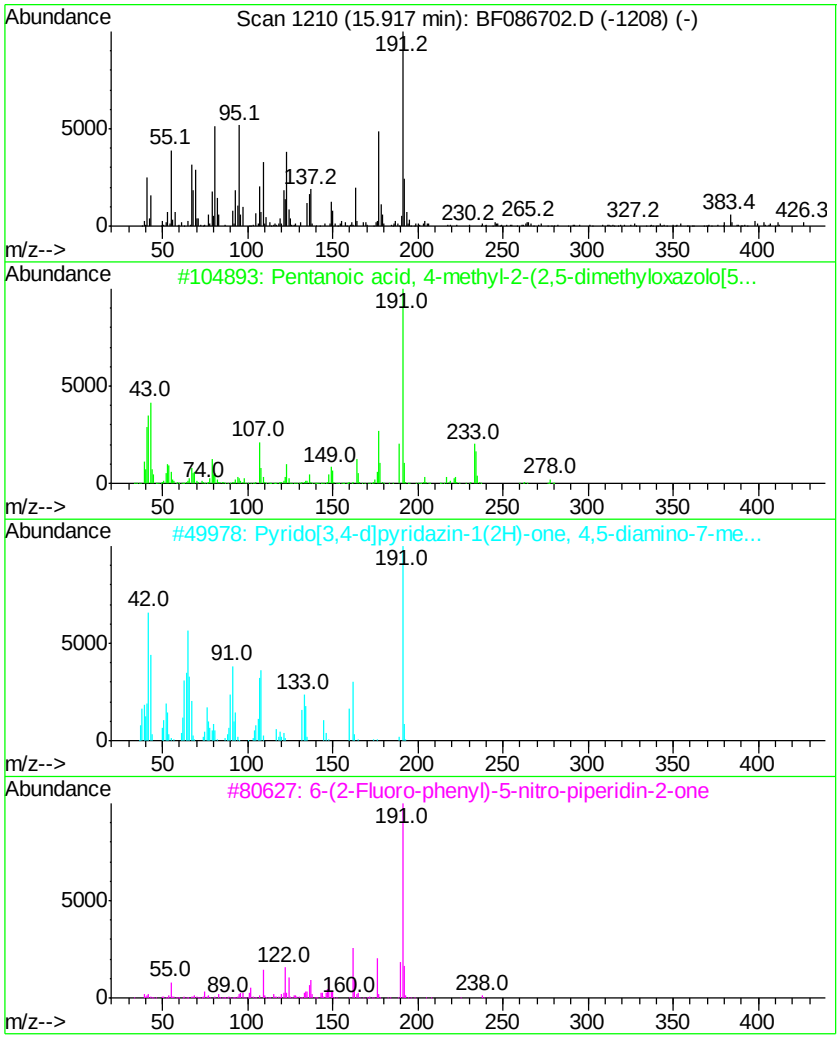
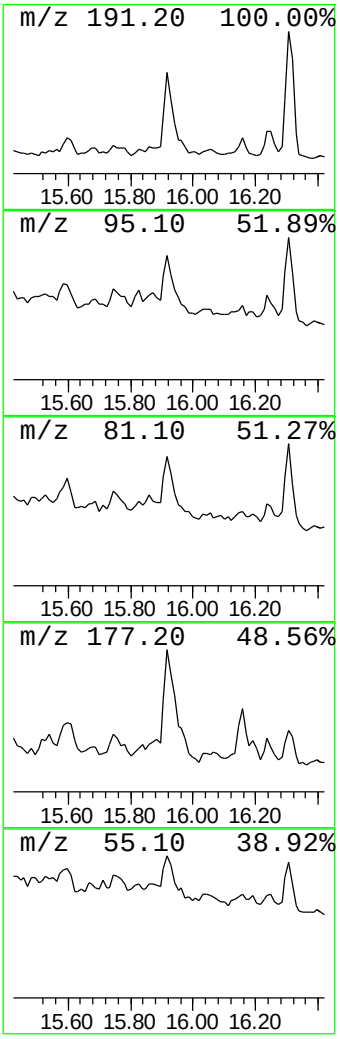
****

Peak Number 6 unknown15.92 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	31.76 ng	641196	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-2-(2,5-...	278	C13H18N4O3	1000294-63-5	32
2	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	22
3	6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	22
4	Anthracene, 9-butyl-	234	C18H18	001498-69-7	22
5	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	22





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Sample : H2829-07 2X
Misc :
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Instrument : BNA_F
ClientSampleId : WPG-B2(0-9.5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

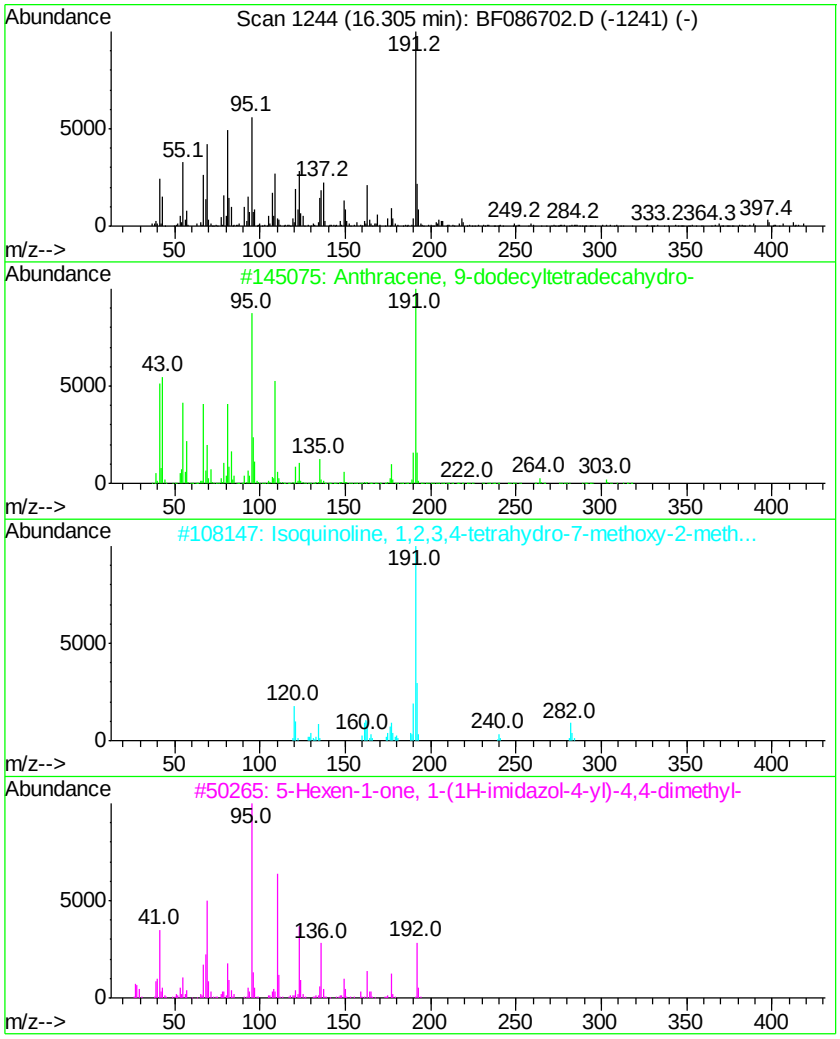
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

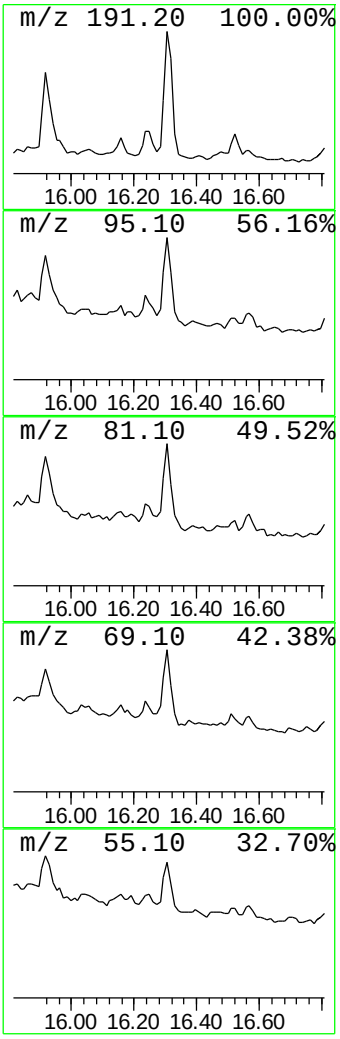
****

Peak Number 7 unknown16.31 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.31	30.46 ng	615081	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	40
2	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	38
3	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	38
4	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086702.D
Acq On : 5 May 2016 3:19
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
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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...	4.89	7.0	ng	188991	1	6.74	1081150	40.0
unknown6.50	6.50	75.9	ng	2050980	1	6.74	1081150	40.0
Phenol, o-[(.alph...	7.60	4.8	ng	148485	2	8.03	1245340	40.0
Benzo[e]pyrene	15.16	11.9	ng	240307	6	15.29	807647	40.0
unknown15.92	15.92	31.8	ng	641196	6	15.29	807647	40.0
unknown16.31	16.31	30.5	ng	615081	6	15.29	807647	40.0