LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

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-BF040216.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	4.921	246	248	259	rBV	67637	114932	4.17%	0.453%
2	5.344	282	285	287	rBV	2445634	2719558	98.58%	10.727%
3	6.396	374	377	379	rBV	2388829	2758664	100.00%	10.881%
4	6.510	385	387	390	rBV	2436086	2484472	90.06%	9.800%
5	6.739	405	407	410	rBV	619027	615121	22.30%	2.426%
6	6.899	419	421	423	rBV	2410209	2158079	78.23%	8.512%
7	7.310	454	457	460	rBV	1526876	1589051	57.60%	6.268%
8	7.425	465	467	474	rVB	21130	31580	1.14%	0.125%
9	8.030	518	520	522	rBV	793677	737174	26.72%	2.908%
10	9.105	612	614	617	rBV	2667228	2475415	89.73%	9.764%
11	9.505	647	649	651	rBV	401451	339320	12.30%	1.338%
12	9.722	666	668	671	rBV2	22136	34184	1.24%	0.135%
13	9.779	671	673	675	rVV	801606	681983	24.72%	2.690%
14	9.813	675	676	679	rVB	66473	59555	2.16%	0.235%
15	9.882	679	682	683	rBV2	20982	36762	1.33%	0.145%
16	10.008	689	693	698	rBV7	33129	138144	5.01%	0.545%
17	10.076	698	699	702	rVB2	23558	29111	1.06%	0.115%
18	10.213	709	711	713	rVB	48336	39210	1.42%	0.155%
19	10.271	715	716	719	rVV2	34092	46264	1.68%	0.182%
20	10.328	719	721	724	rVB3	46774	50877	1.84%	0.201%
21	10.568	740	742	745	rBV	1304592	1255244	45.50%	4.951%
22	10.682	751	752	759	rVB	38579	56833	2.06%	0.224%
23	11.265	801	803	804	rBV	533756	548541	19.88%	2.164%
24	11.288	804	805	807	rVB	74944	58168	2.11%	0.229%
25	11.802	848	850	855	rBV2	62712	133635	4.84%	0.527%
26	11.871	855	856	861	rVB4	21681	37707	1.37%	0.149%
27	12.476	906	909	911	rBV	124761	140288	5.09%	0.553%
28	12.579	916	918	921	rBV	49073	63254	2.29%	0.249%
29	12.705	925	929	931	rVV	94217	142869	5.18%	0.564%
30	12.842	939	941	944	rBV	1729604	1849784	67.05%	7.296%
31	13.094	959	963	965	rBV3	11574	28455	1.03%	0.112%
32	13.539	999	1002	1004	rBV4	20748	51937	1.88%	0.205%
33	13.699	1013	1016	1019	rBV	75892	106293	3.85%	0.419%
34	13.757	1019	1021	1024	rVB	43468	70115	2.54%	0.277%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

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-BF040216.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.894	1029	1033	1040	rBV	641614	905825	32.84%	3.573%
36	14.248	1061	1064	1065	rBV3	25074	60358	2.19%	0.238%
37	14.431	1076	1080	1084	rBV7	23191	95656	3.47%	0.377%
38	14.911	1120	1122	1126	rVB	47436	91211	3.31%	0.360%
39	15.185	1142	1146	1149	rBV	65132	161896	5.87%	0.639%
40	15.242	1149	1151	1153	rVB	59255	72670	2.63%	0.287%
41	15.300	1153	1156	1162	rBV	485001	700623	25.40%	2.763%
42	16.648	1271	1274	1277	rBV2	23782	68223	2.47%	0.269%
43	16.923	1296	1298	1299	rBV2	21713	42007	1.52%	0.166%
44	17.128	1314	1316	1320	rVB5	16936	34837	1.26%	0.137%
45	18.671	1448	1451	1456	rVB7	101050	278570	10.10%	1.099%
46	18.751	1456	1458	1462	rBV4	58677	136148	4.94%	0.537%
47	18.854	1465	1467	1468	rBV	20307	27961	1.01%	0.110%
48	18.900	1468	1471	1477	rVB7	51145	182878	6.63%	0.721%
49	18.991	1477	1479	1482	rBV4	25863	50829	1.84%	0.200%
50	19.060	1482	1485	1486	rVV3	140419	322767	11.70%	1.273%
51	19.094	1486	1488	1492	rVB3	152228	315629	11.44%	1.245%
52	19.163	1492	1494	1496	rBV3	21549	42736	1.55%	0.169%
53	19.346	1508	1510	1513	rBV4	15871	31026	1.12%	0.122%
54	19.471	1519	1521	1522	rBV2	26859	48342	1.75%	0.191%

Sum of corrected areas: 25352771

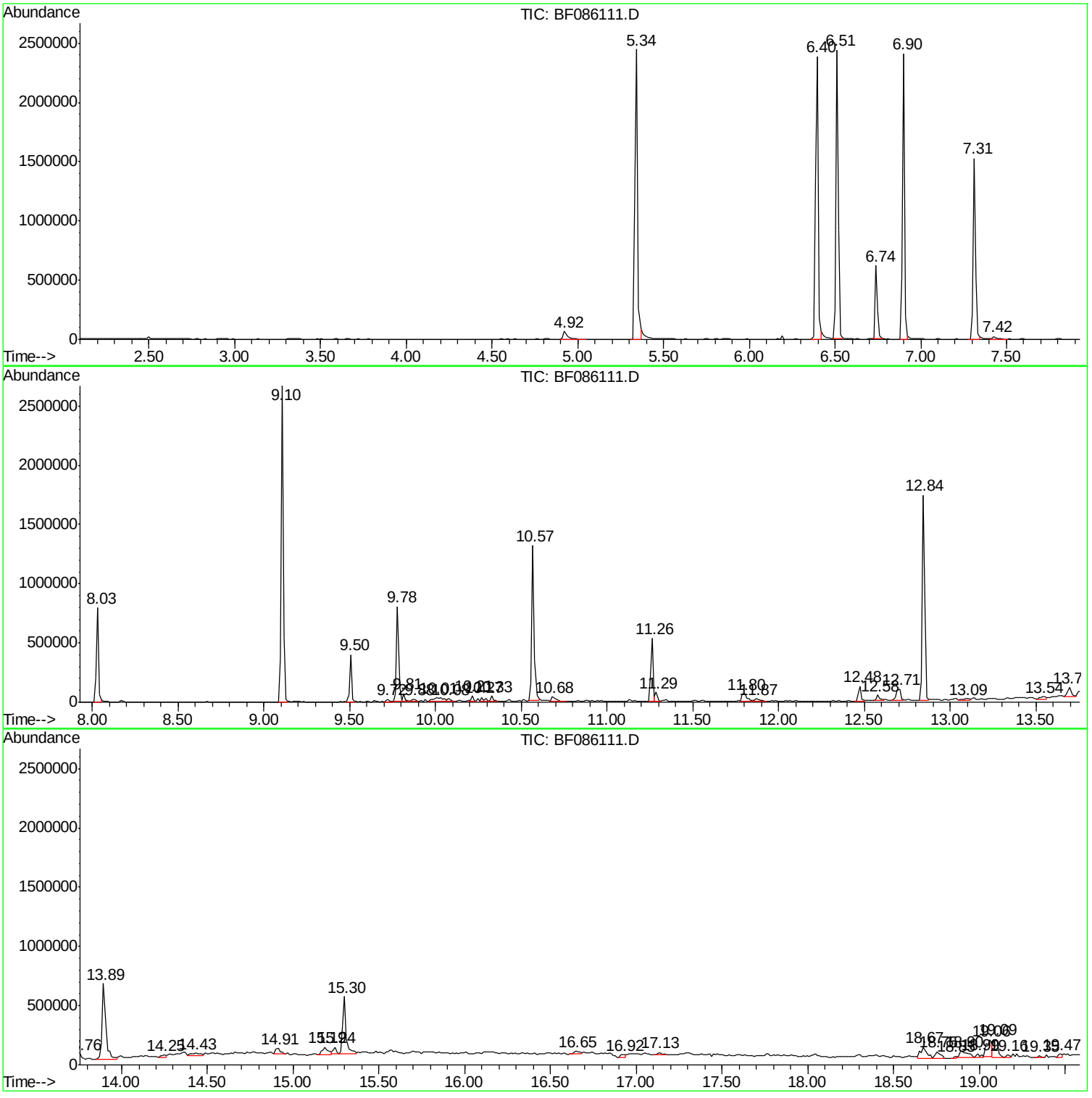
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

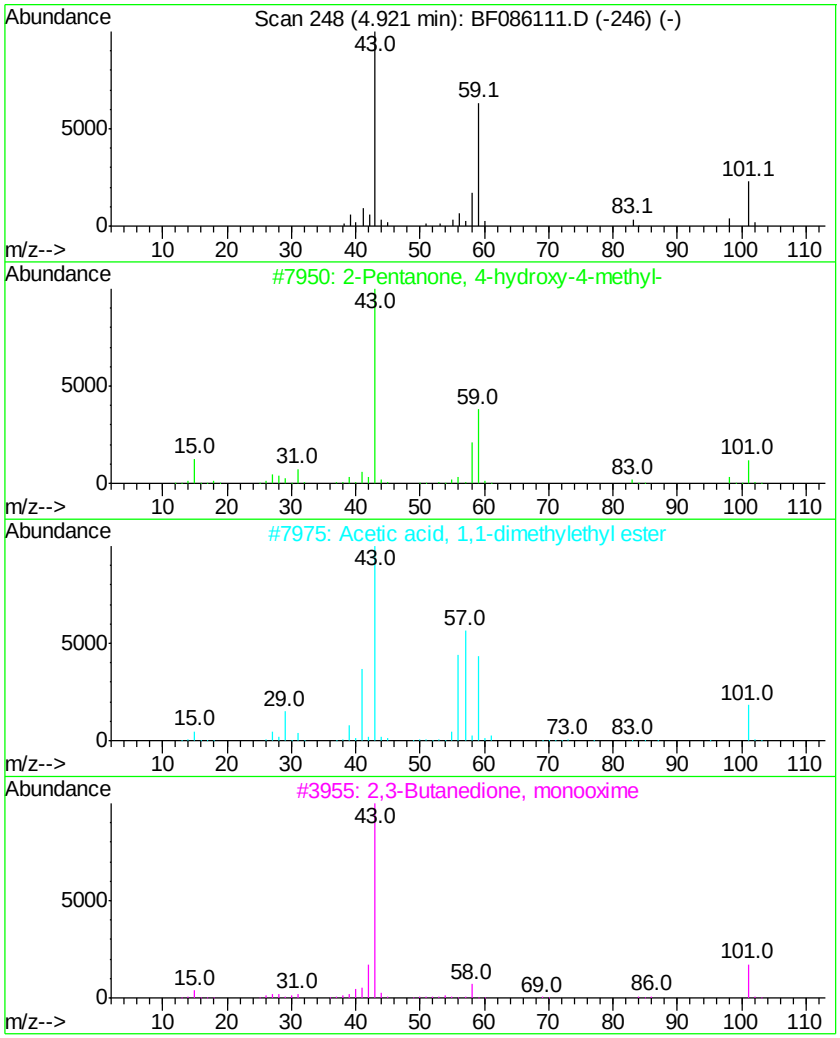
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

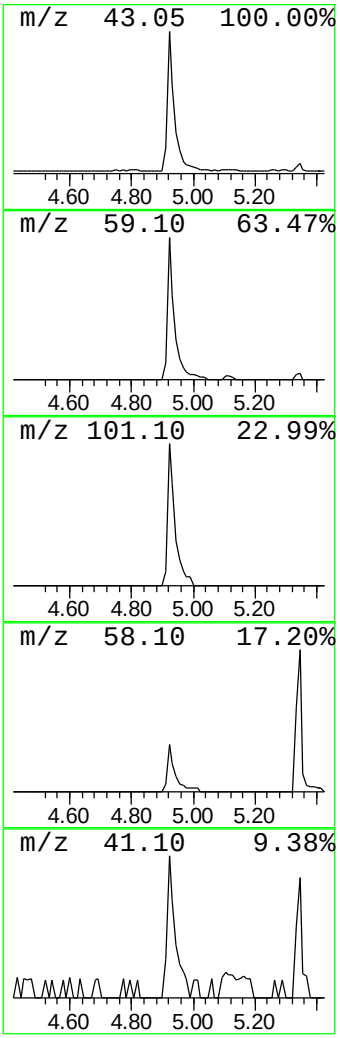
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.74 ng	114932	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	t-Butyl ethyl ether	102	C6H14O	1000118-18-4	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

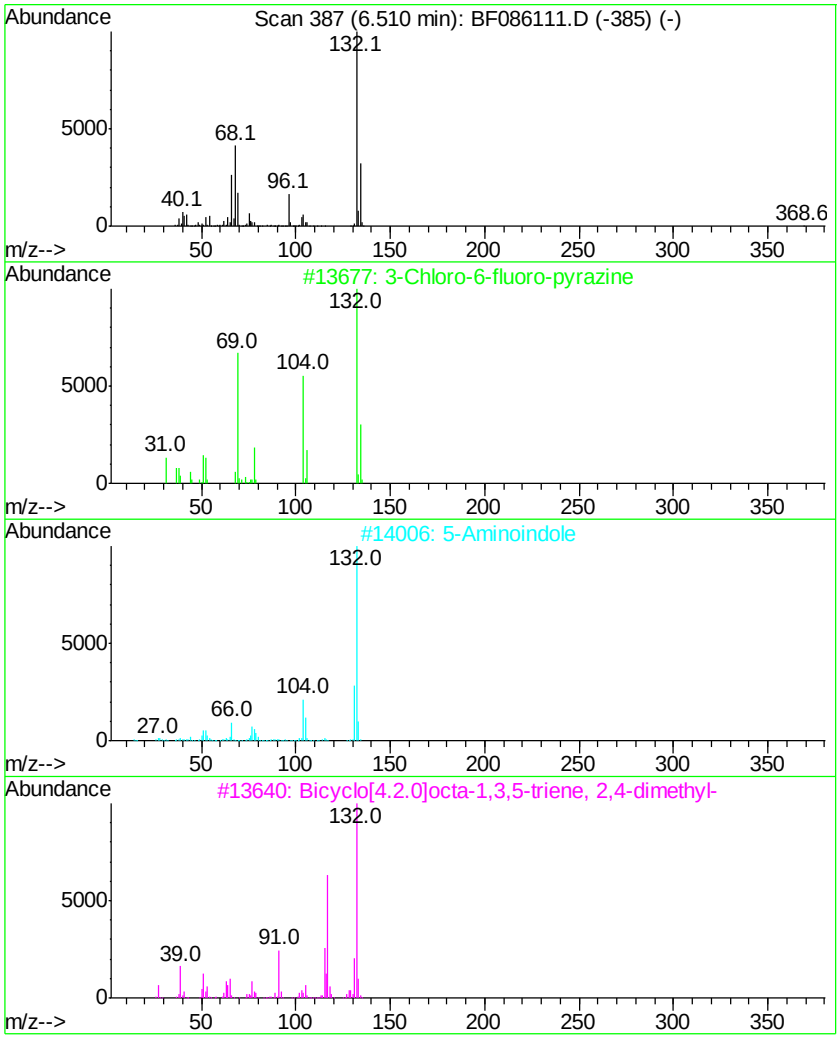
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

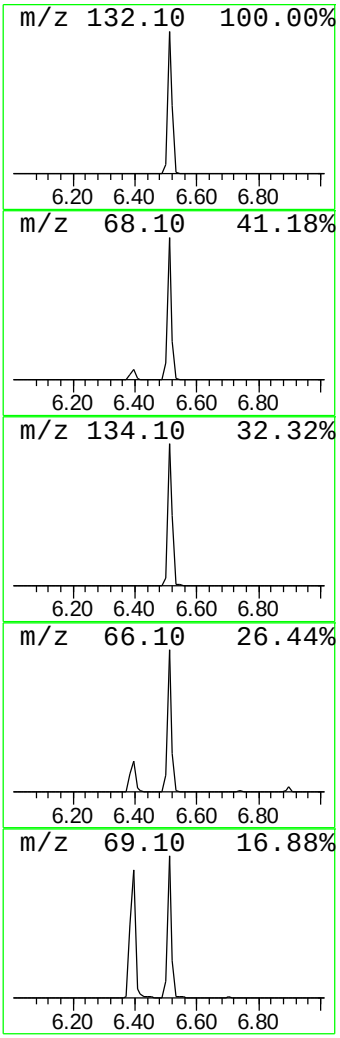
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	80.78 ng	2484470	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

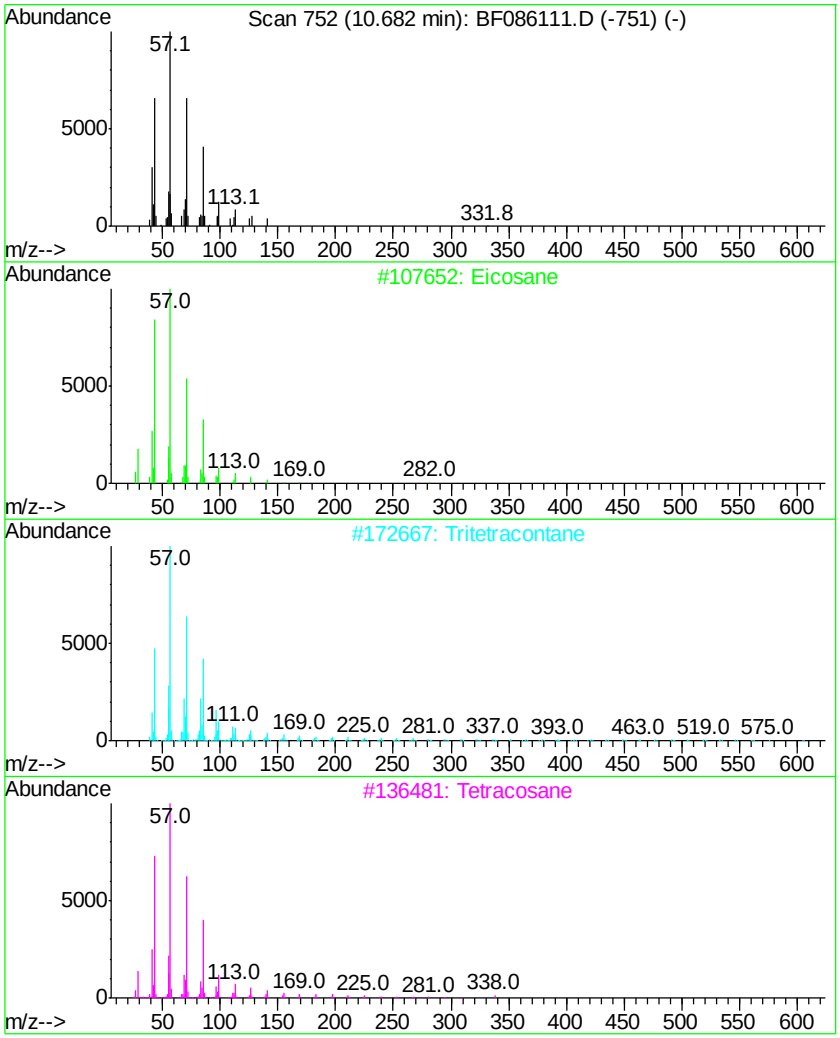
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

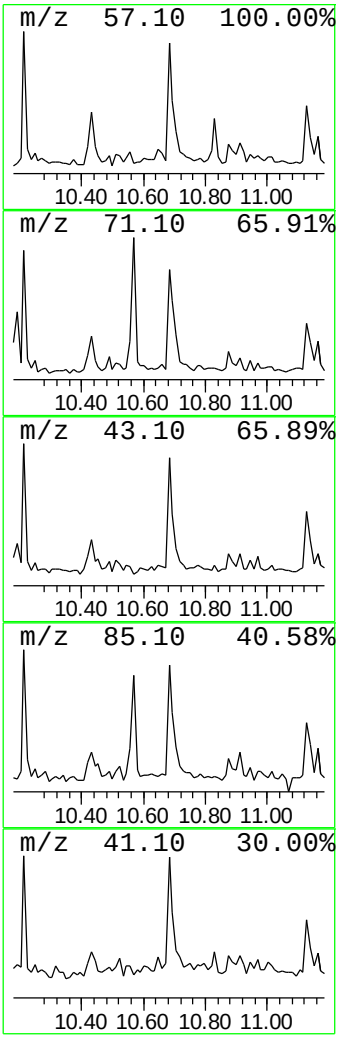
****

Peak Number 5 Eicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.07 ng	56833	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Tritetracontane	605	C43H88	007098-21-7	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Tetradecane	198	C14H30	000629-59-4	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

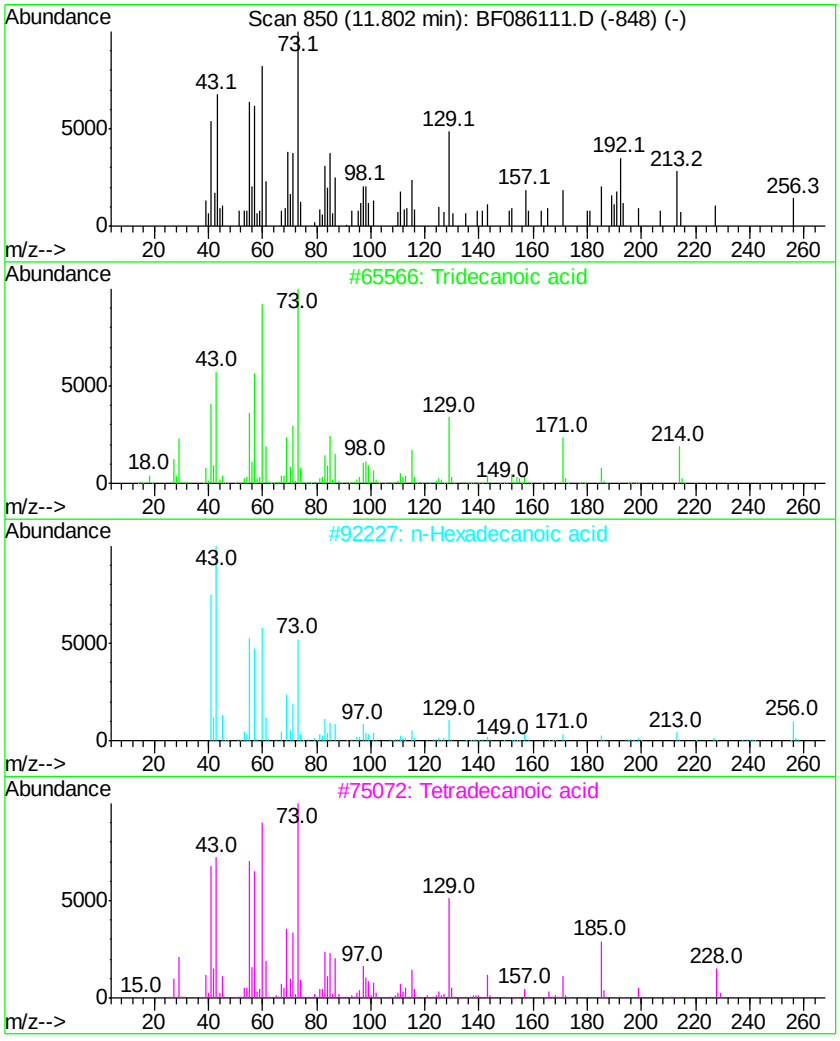
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

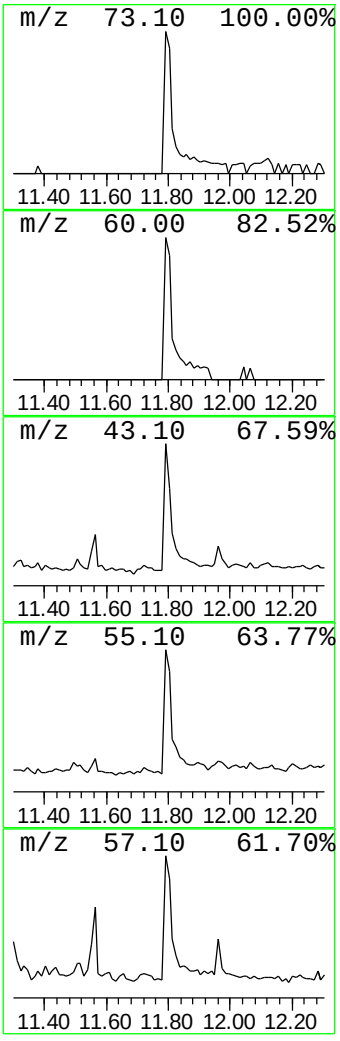
****

Peak Number 6 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	4.87 ng	133635	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

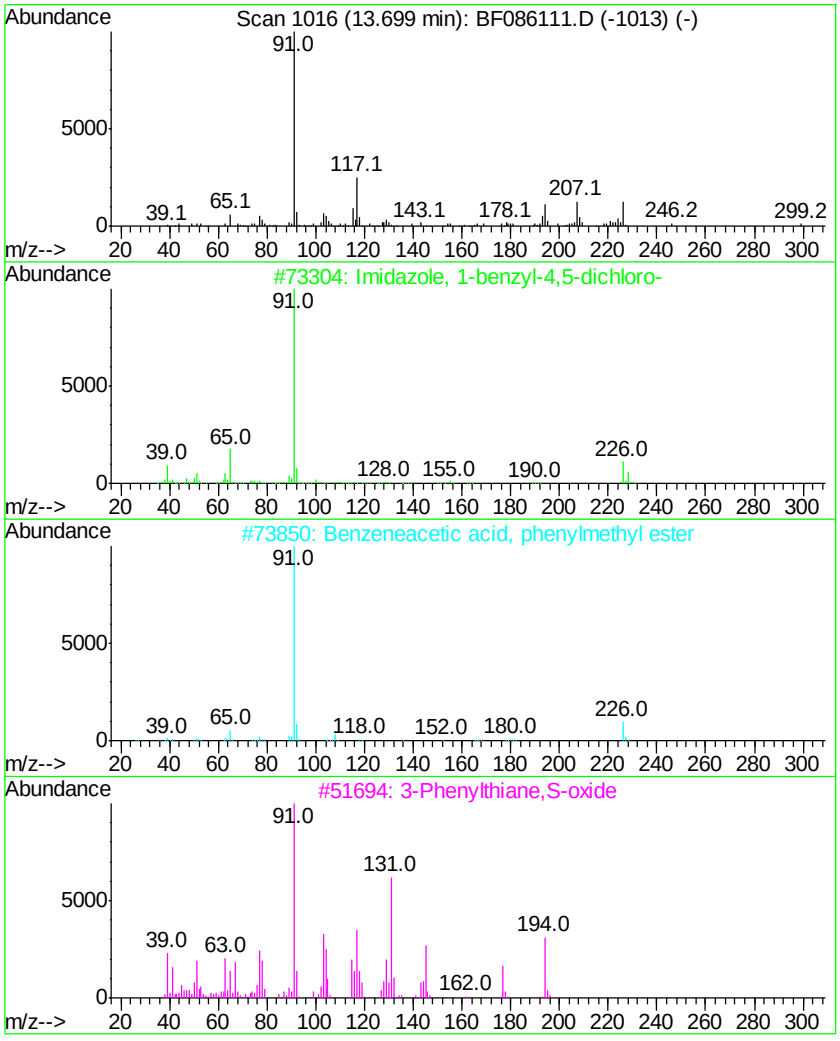
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

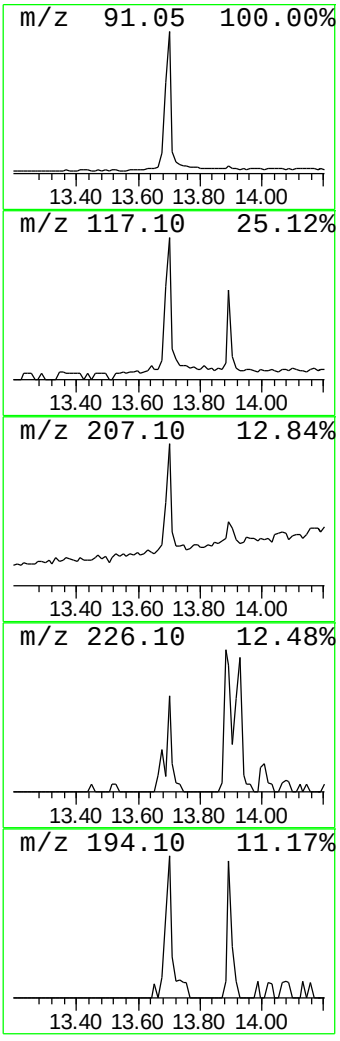
****

Peak Number 7 unknown13.70 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.35 ng	106293	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 1-benzyl-4,5-dichloro-	226	C10H8Cl2N2	107108-24-7	22
2	Benzeneacetic acid, phenylmethyl...	226	C15H14O2	000102-16-9	22
3	3-Phenylthiane,S-oxide	194	C11H14OS	058121-26-9	17
4	1-Heptafluorobutyryloxy-3-phenyl...	332	C13H11F7O2	1000215-96-2	12
5	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

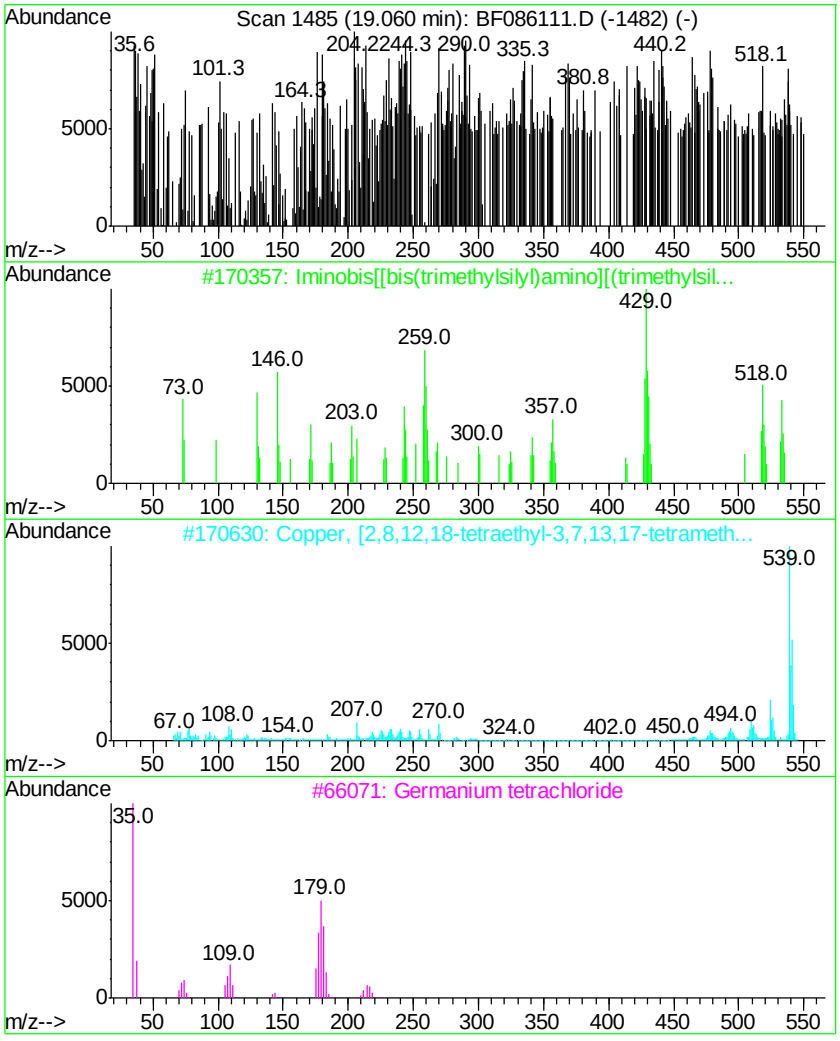
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

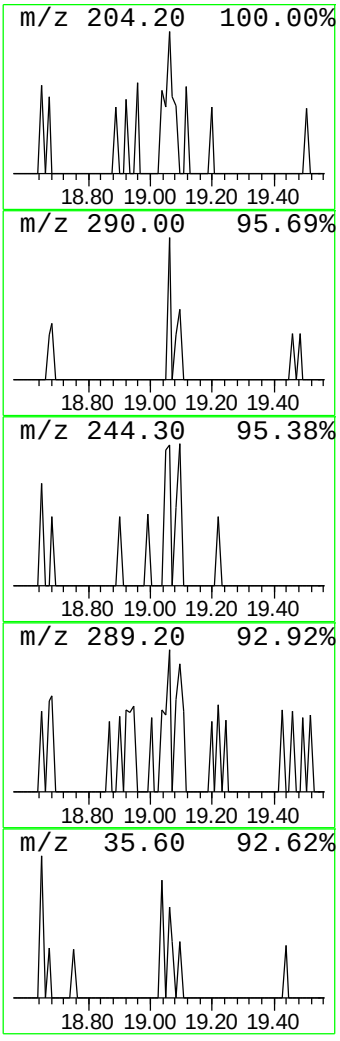
****

Peak Number 14 unknown19.06 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	9.21 ng	322767	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Iminobis[[bis(trimethylsilyl)ami...	533	C18H57B2N5Si6	113678-60-7	25
2	Copper, [2,8,12,18-tetraethyl-3,...	539	C32H36CuN4	014055-18-6	9
3	Germanium tetrachloride	214	Cl4Ge	010038-98-9	9
4	2-Hexenedioic acid, 2,4-dichloro...	226	C6H4Cl2O5	056771-78-9	9
5	4-(4-Hydroxyphenyl)pyrimidine	172	C10H8N2O	023380-78-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040616\
Data File : BF086111.D
Acq On : 6 Apr 2016 21:29
Operator : UM/SJ
Sample : H2074-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB01B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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...	4.92	3.7	ng	114932	1	6.74	615121	20.0
unknown6.51	6.51	80.8	ng	2484470	1	6.74	615121	20.0
Eicosane	10.68	2.1	ng	56833	4	11.26	548541	20.0
Tridecanoic acid	11.80	4.9	ng	133635	4	11.26	548541	20.0
unknown13.70	13.70	2.4	ng	106293	5	13.89	905825	20.0
unknown19.06	19.06	9.2	ng	322767	6	15.30	700623	20.0