LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

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_G\METHODS\8270-BG040615.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	2.750	5	10	20	rBV	221429	427688	20.50%	2.185%
2	2.832	20	24	29	rVV	98426	131532	6.30%	0.672%
3	2.879	29	32	38	rVB2	19496	27115	1.30%	0.139%
4	4.771	349	354	365	rVB	116752	168714	8.09%	0.862%
5	5.253	429	436	444	rBV	875697	1233563	59.12%	6.302%
6	6.851	701	708	718	rBV	884586	1335344	64.00%	6.822%
7	7.198	759	767	780	rBV	907279	1383771	66.32%	7.069%
8	7.662	837	846	852	rBV	273964	430274	20.62%	2.198%
9	7.979	892	900	907	rBV	631052	971252	46.55%	4.962%
10	8.813	1035	1042	1052	rBV	462947	768089	36.81%	3.924%
11	10.447	1312	1320	1326	rBV	390551	655256	31.40%	3.348%
12	12.920	1735	1741	1750	rBV	1095712	1551520	74.36%	7.926%
13	13.761	1878	1884	1893	rBV	97365	140258	6.72%	0.717%
14	14.301	1970	1976	1983	rVV2	614825	907903	43.51%	4.638%
15	14.900	2068	2078	2079	rBV3	11802	27737	1.33%	0.142%
16	15.094	2105	2111	2118	rVV5	9069	21308	1.02%	0.109%
17	15.159	2118	2122	2126	rVB	17663	21987	1.05%	0.112%
18	15.658	2201	2207	2213	rBV	15910	25897	1.24%	0.132%
19	15.793	2223	2230	2238	rBV	907359	1242179	59.53%	6.346%
20	16.017	2263	2268	2278	rBV	22019	43455	2.08%	0.222%
21	16.804	2398	2402	2408	rBV2	25496	37229	1.78%	0.190%
22	17.045	2437	2443	2447	rBV2	813109	1135865	54.44%	5.803%
23	17.086	2447	2450	2456	rVB	137105	177530	8.51%	0.907%
24	17.174	2461	2465	2471	rVB2	29498	45696	2.19%	0.233%
25	17.544	2524	2528	2533	rBV3	30477	37353	1.79%	0.191%
26	17.944	2592	2596	2611	rVB2	122247	259846	12.45%	1.328%
27	18.114	2620	2625	2627	rVV3	23634	40917	1.96%	0.209%
28	18.150	2627	2631	2636	rVB2	56771	80682	3.87%	0.412%
29	18.238	2642	2646	2650	rBV3	24084	31762	1.52%	0.162%
30	18.514	2689	2693	2696	rBV2	33365	40797	1.96%	0.208%
31	18.667	2715	2719	2724	rVB2	48880	59788	2.87%	0.305%
32	18.937	2762	2765	2769	rVB2	32268	42264	2.03%	0.216%
33	19.043	2780	2783	2787	rVB	18603	23201	1.11%	0.119%
34	19.107	2788	2794	2799	rBV	92975	131015	6.28%	0.669%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

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_G\METHODS\8270-BG040615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.160	2799	2803	2807	rVB	50285	63917	3.06%	0.327%
36	19.231	2811	2815	2823	rVV4	35736	66373	3.18%	0.339%
37	19.360	2833	2837	2847	rVB6	14756	31881	1.53%	0.163%
38	19.466	2847	2855	2863	rBV	102945	168096	8.06%	0.859%
39	19.548	2866	2869	2875	rVB2	24202	33413	1.60%	0.171%
40	19.630	2879	2883	2885	rBV5	15505	22726	1.09%	0.116%
41	19.671	2885	2890	2900	rVB	1704792	2086540	100.00%	10.660%
42	19.883	2922	2926	2930	rBV	123975	150118	7.19%	0.767%
43	19.959	2936	2939	2947	rVB4	21893	42949	2.06%	0.219%
44	20.935	3101	3105	3116	rBV	257886	352712	16.90%	1.802%
45	21.140	3136	3140	3144	rVB	94437	98962	4.74%	0.506%
46	21.222	3148	3154	3158	rVV	1010982	1252687	60.04%	6.400%
47	21.258	3158	3160	3166	rVB	56523	67551	3.24%	0.345%
48	21.375	3177	3180	3185	rBV3	17423	24628	1.18%	0.126%
49	23.449	3526	3533	3541	rBV2	588830	1174779	56.30%	6.002%
50	26.346	4019	4026	4037	rVB2	102959	277783	13.31%	1.419%

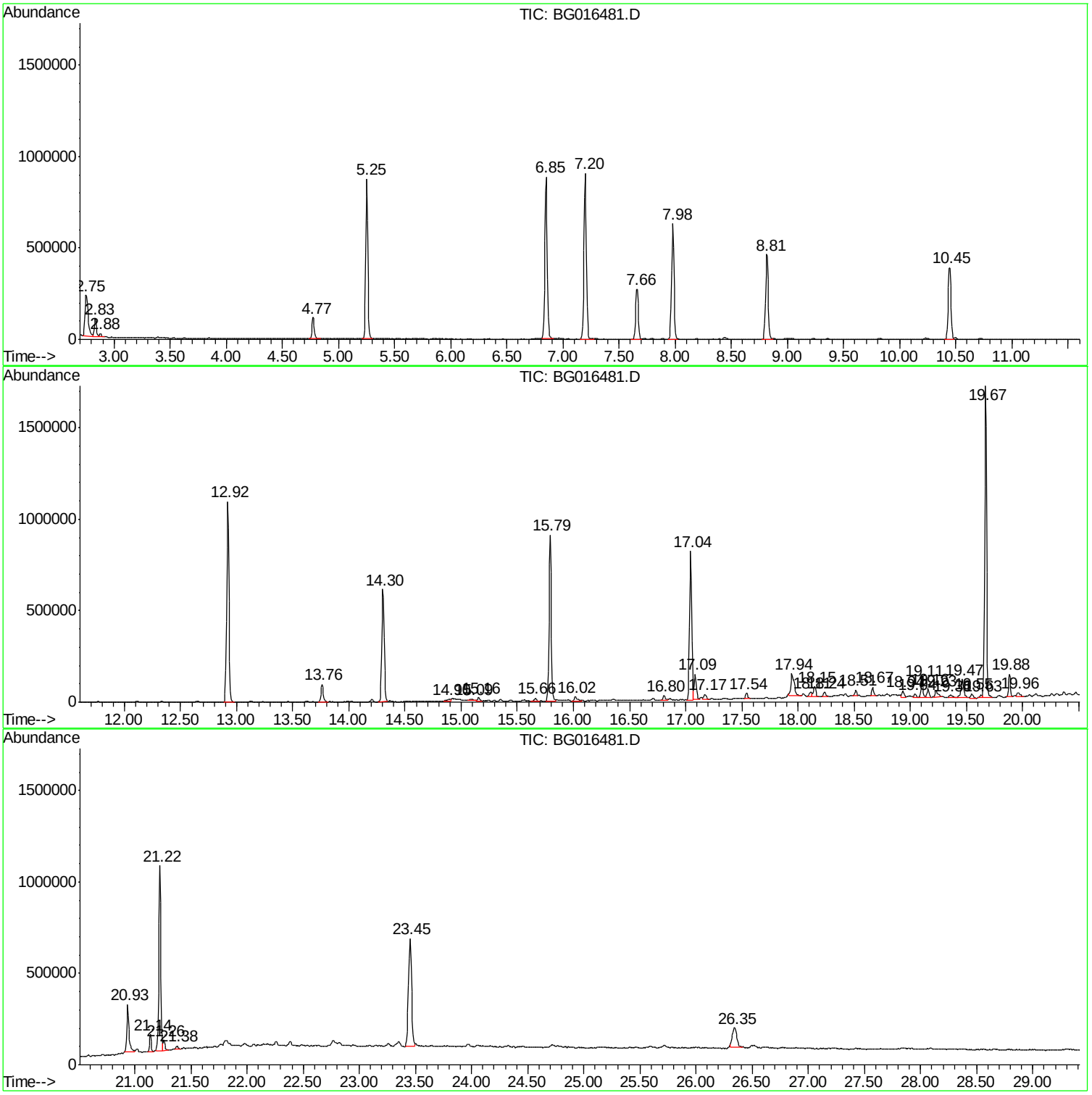
Sum of corrected areas: 19573902

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

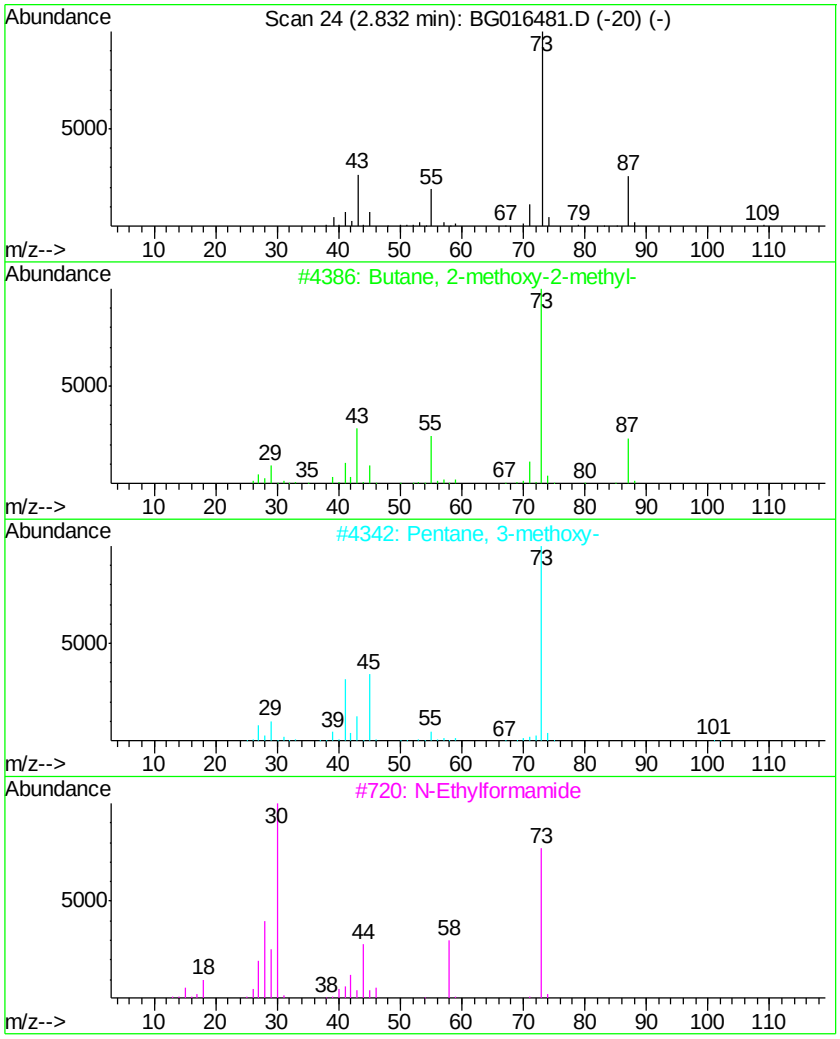
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

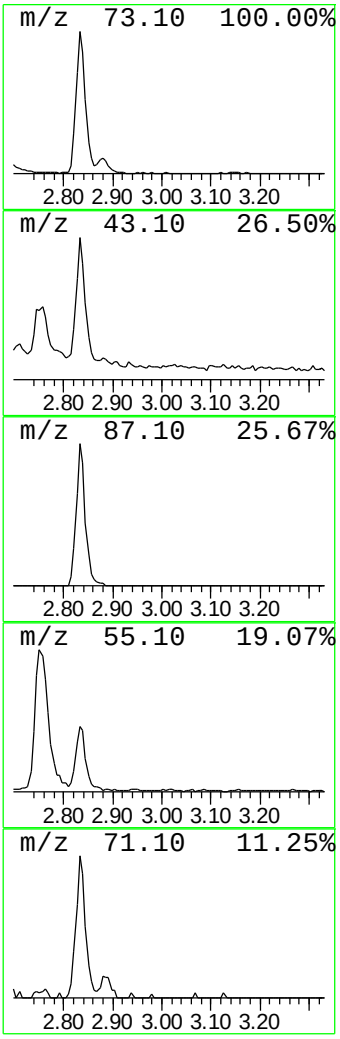
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	6.11 ng	131532	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

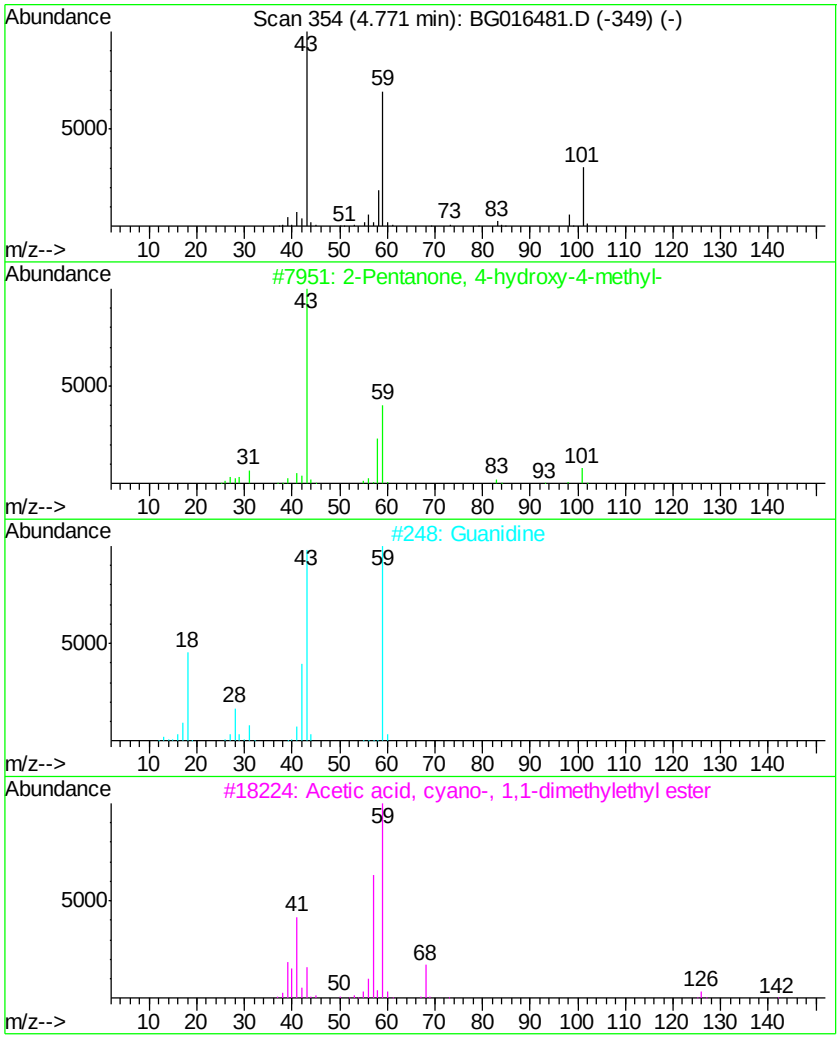
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

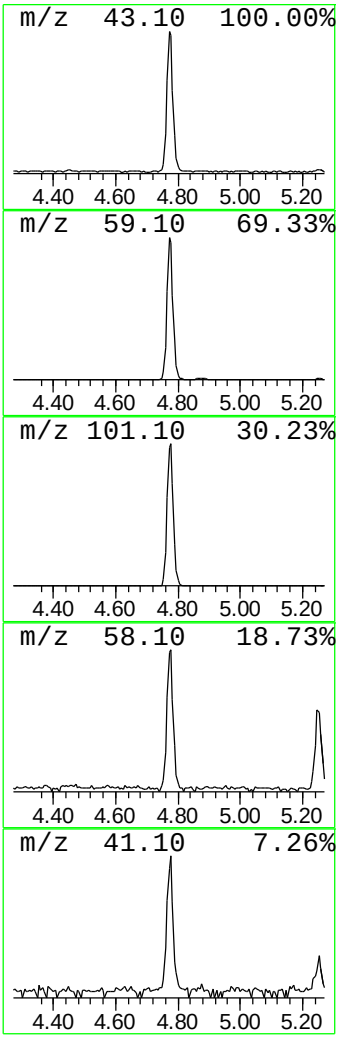
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	7.84 ng	168714	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

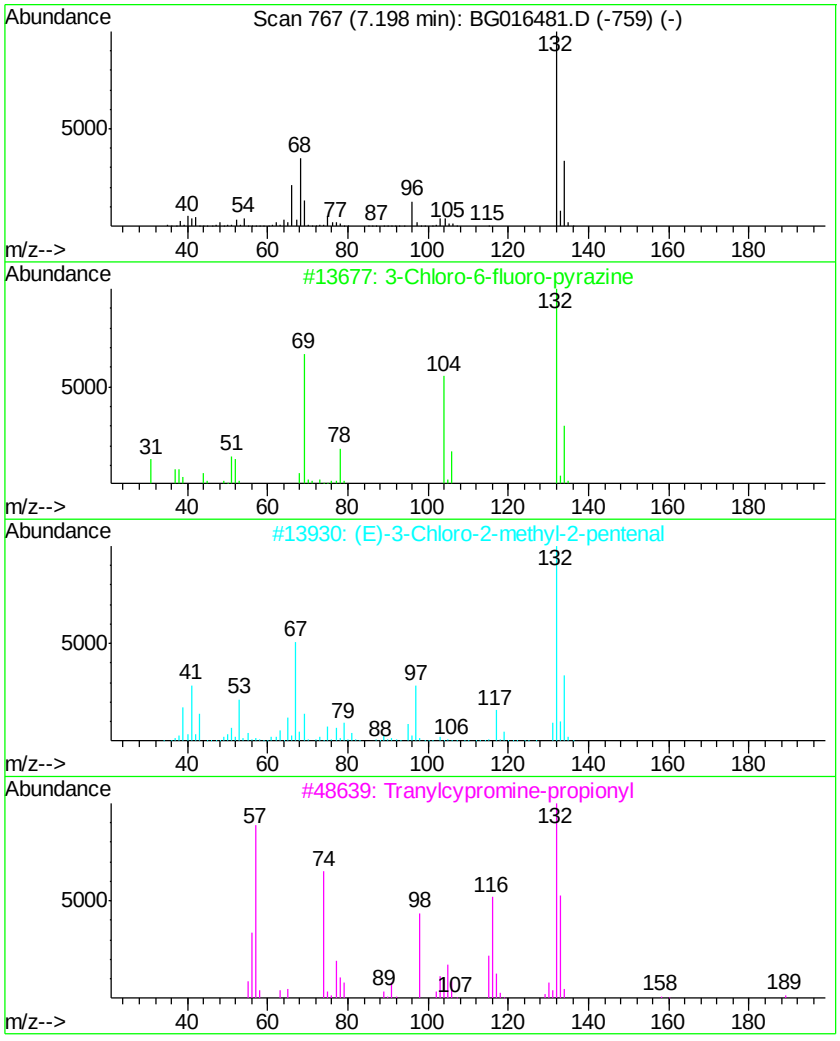
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

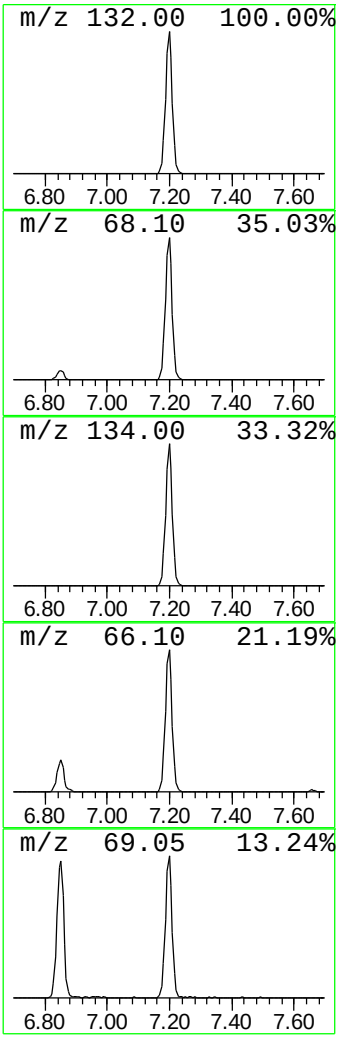
****

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	64.32 ng	1383770	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

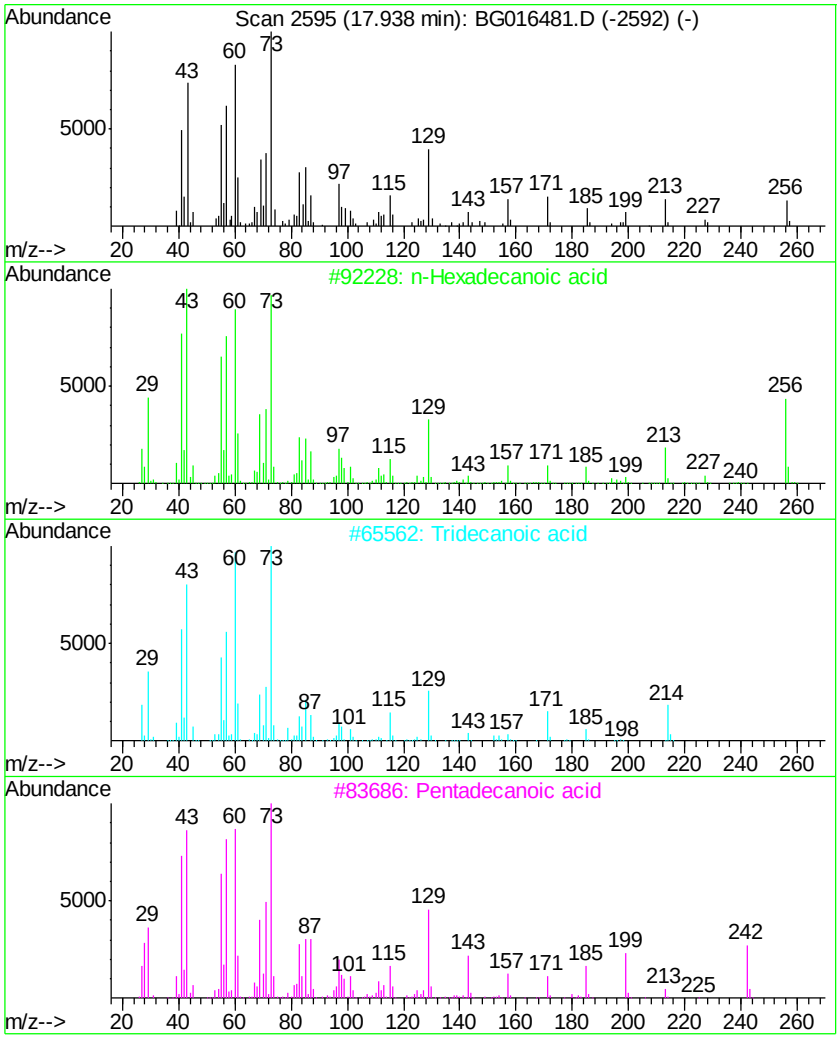
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

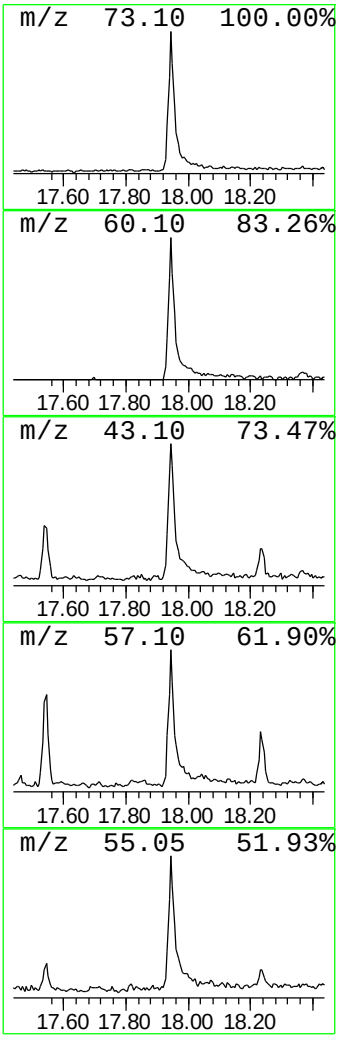
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	4.58 ng	259846	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

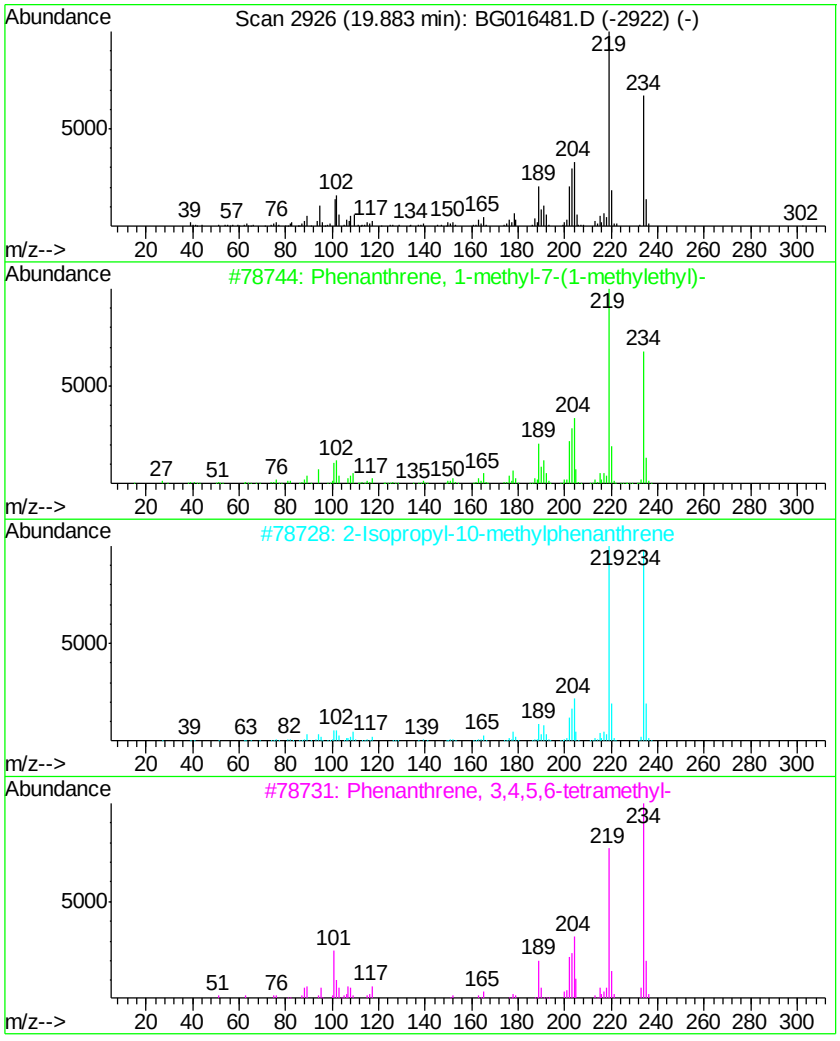
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

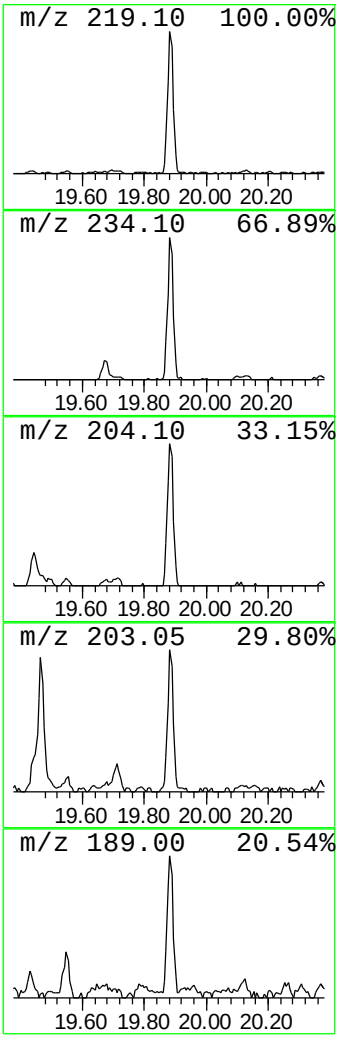
****

Peak Number 8 Phenanthrene, 1-methyl-7-(1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.88	2.40 ng	150118	Chrysene-d12	21.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-7-(1-meth...	234	C18H18	000483-65-8	99
2	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3	Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	89
4	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	89
5	1-Phenyl-4-(3,5-dimethylphenyl)b...	234	C18H18	1000202-15-0	80





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

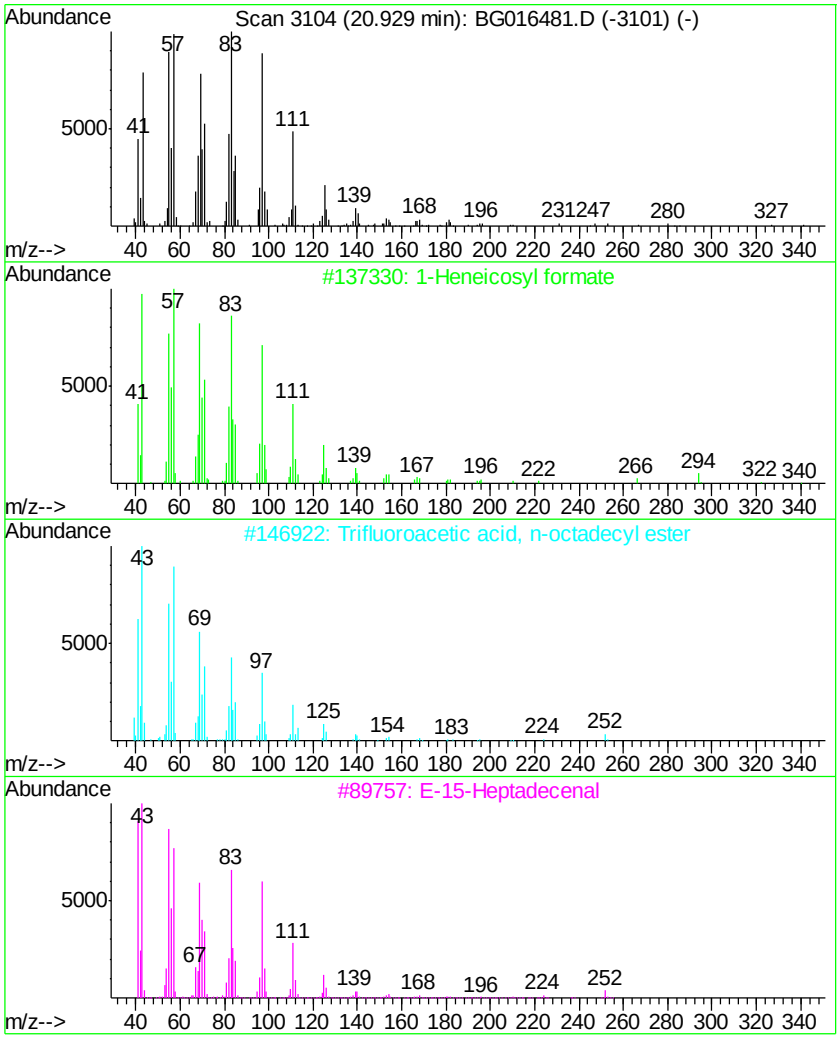
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

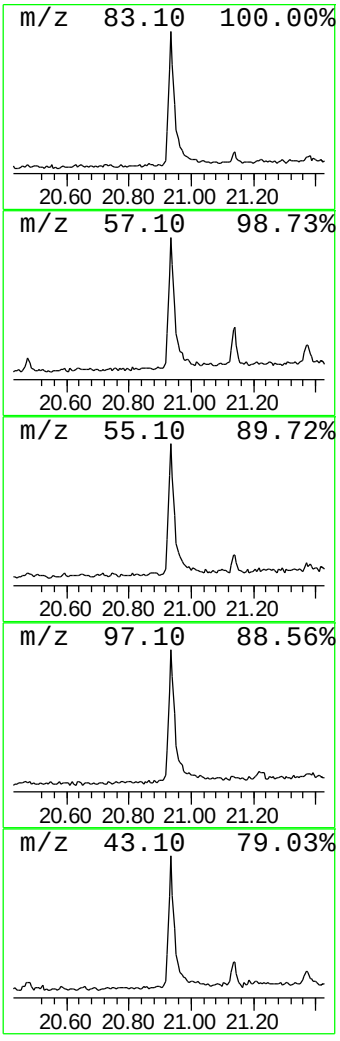
****

Peak Number 9 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	5.63 ng	352712	Chrysene-d12	21.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	1-Heptadecanol	256	C17H36O	001454-85-9	87





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

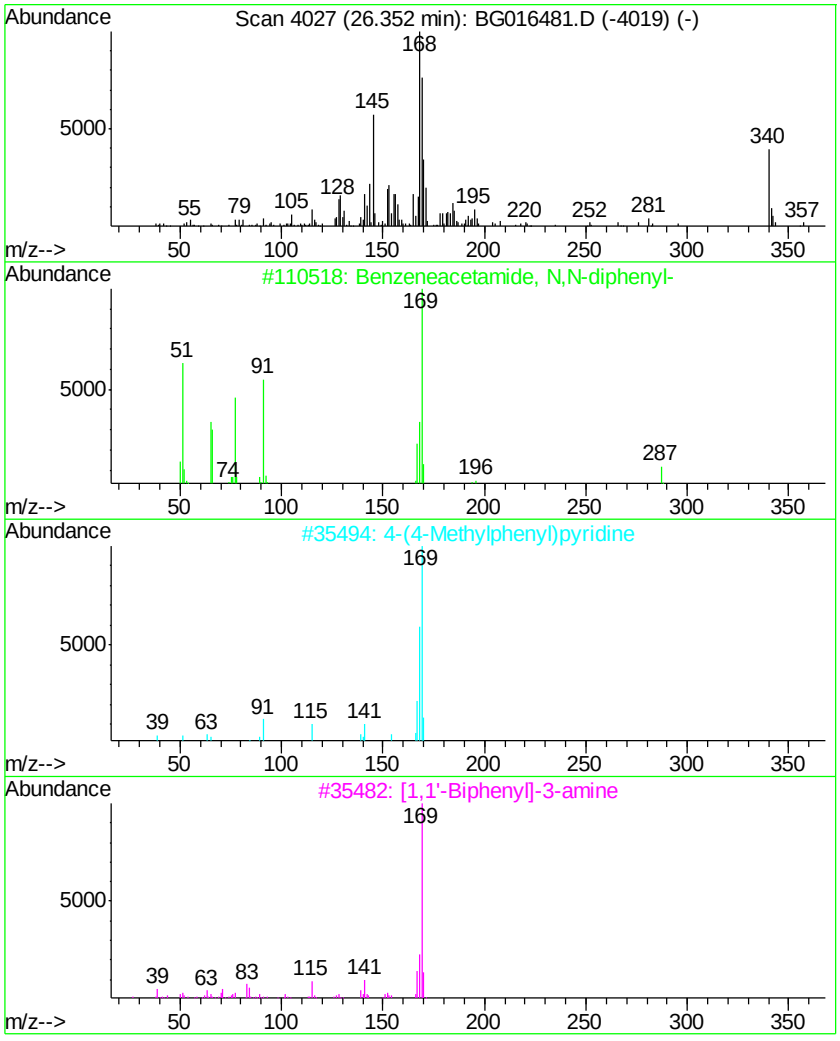
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

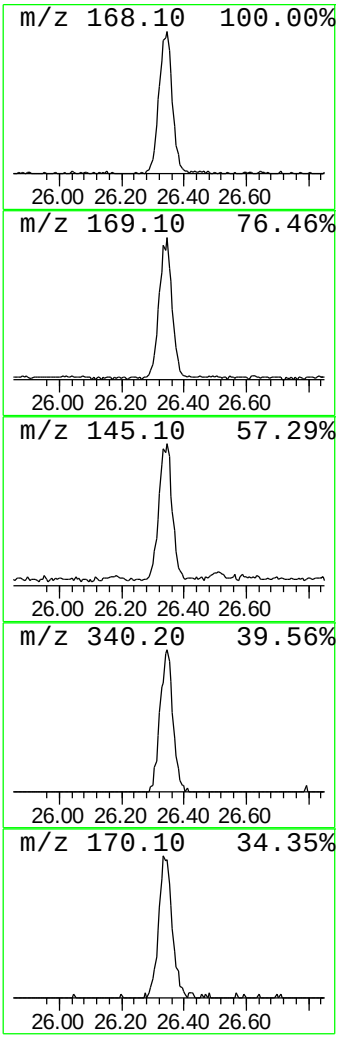
****

Peak Number 10 unknown26.35 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.35	4.73 ng	277783	Perylene-d12	23.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetamide, N,N-diphenyl-	287	C20H17NO	033675-70-6	47
2	4-(4-Methylphenyl)pyridine	169	C12H11N	004423-10-3	35
3	[1,1'-Biphenyl]-3-amine	169	C12H11N	002243-47-2	27
4	Nickel,bis(1,2,3-.eta.)-2-methyl...	168	C8H14Ni	012261-14-2	25
5	3-Methyl-5-phenylpyridine	169	C12H11N	010477-94-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041615\
Data File : BG016481.D
Acq On : 17 Apr 2015 7:58
Operator : TP/IZ
Sample : G1891-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-81D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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
Butane, 2-methoxy...	2.83	6.1	ng	131532	1	7.66	430274	20.0
2-Pentanone, 4-hy...	4.77	7.8	ng	168714	1	7.66	430274	20.0
unknown7.20	7.20	64.3	ng	1383770	1	7.66	430274	20.0
n-Hexadecanoic acid	17.94	4.6	ng	259846	4	17.05	1135870	20.0
Phenanthrene, 1-m...	19.88	2.4	ng	150118	5	21.22	1252690	20.0
1-Heneicosyl formate	20.93	5.6	ng	352712	5	21.22	1252690	20.0
unknown26.35	26.35	4.7	ng	277783	6	23.46	1174780	20.0