LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)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_G\METHODS\8270-BG070816.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	3.038	29	34	53	rBV	4994182	7424280	100.00%	13.227%
2	5.218	401	405	411	rVB	124767	186203	2.51%	0.332%
3	5.694	478	486	497	rBV	2041541	3387255	45.62%	6.035%
4	7.304	752	760	770	rBV	2372603	4165311	56.10%	7.421%
5	7.680	816	824	836	rBV	2223240	3767647	50.75%	6.713%
6	8.150	896	904	914	rVB2	375611	660295	8.89%	1.176%
7	8.479	952	960	967	rBV	1455945	2556794	34.44%	4.555%
8	9.325	1095	1104	1115	rBV	1476246	2655411	35.77%	4.731%
9	10.976	1377	1385	1393	rBV	588805	1064954	14.34%	1.897%
10	13.414	1792	1800	1809	rBV	3591662	5572499	75.06%	9.928%
11	14.237	1933	1940	1946	rBV	588473	832654	11.22%	1.484%
12	14.795	2028	2035	2045	rVB2	1033472	1720268	23.17%	3.065%
13	15.617	2170	2175	2180	rVB2	89949	109524	1.48%	0.195%
14	16.287	2283	2289	2300	rBV	3832901	5905480	79.54%	10.522%
15	16.481	2317	2322	2326	rBV2	98302	152418	2.05%	0.272%
16	17.280	2454	2458	2462	rBV	74012	92740	1.25%	0.165%
17	17.556	2498	2505	2510	rBV2	1306123	2108737	28.40%	3.757%
18	18.308	2627	2633	2638	rBV5	62596	122652	1.65%	0.219%
19	18.420	2647	2652	2660	rBV	305070	452557	6.10%	0.806%
20	19.601	2850	2853	2859	rVB	56992	83141	1.12%	0.148%
21	19.683	2864	2867	2875	rBV3	98584	144822	1.95%	0.258%
22	20.153	2941	2947	2953	rBV	5505544	7397996	99.65%	13.181%
23	21.281	3135	3139	3143	rVB5	77860	96138	1.29%	0.171%
24	21.458	3164	3169	3175	rBV4	152158	272706	3.67%	0.486%
25	21.675	3201	3206	3210	rBV7	61795	87477	1.18%	0.156%
26	21.845	3229	3235	3242	rBV2	1341718	2410556	32.47%	4.295%
27	23.044	3433	3439	3445	rVB6	84111	149723	2.02%	0.267%
28	25.206	3798	3807	3823	rVB2	789813	2318351	31.23%	4.130%
29	25.888	3915	3923	3930	rVB5	77821	229080	3.09%	0.408%

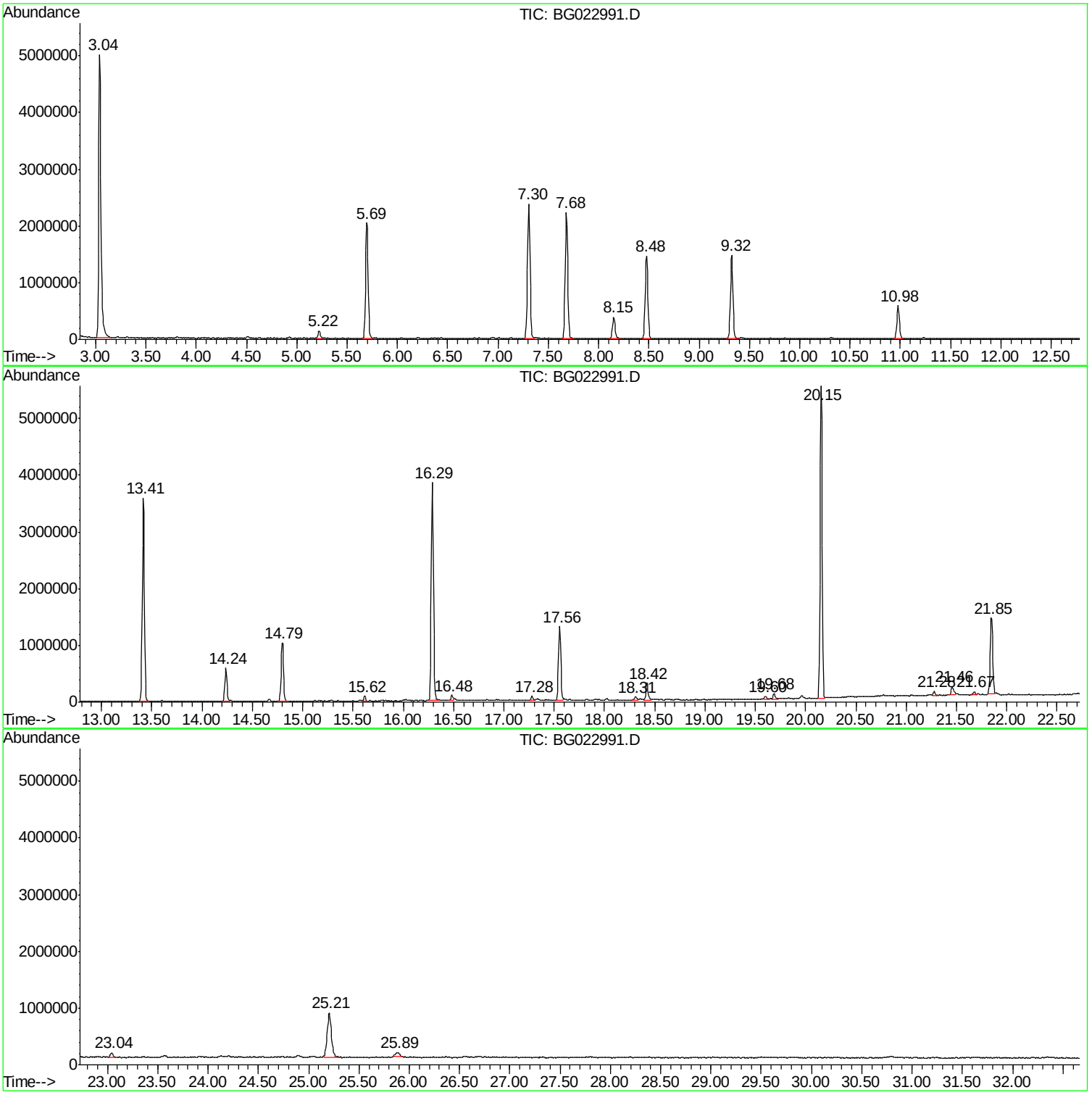
Sum of corrected areas: 56127669

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

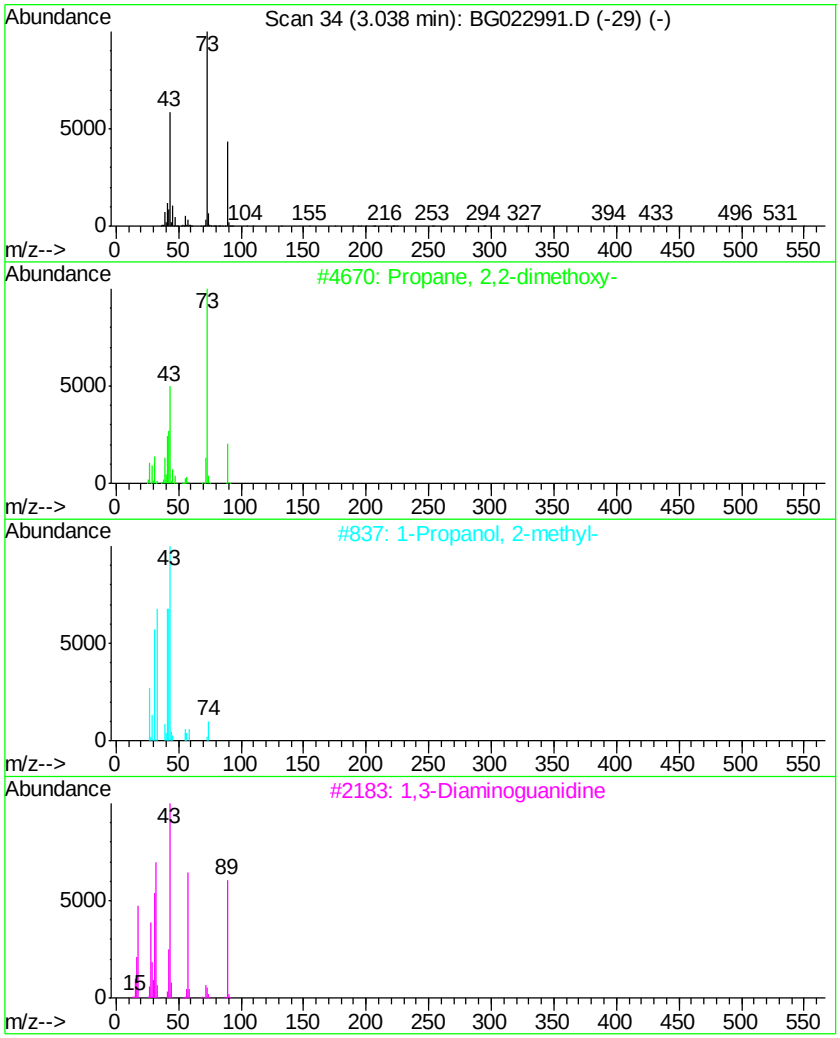
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

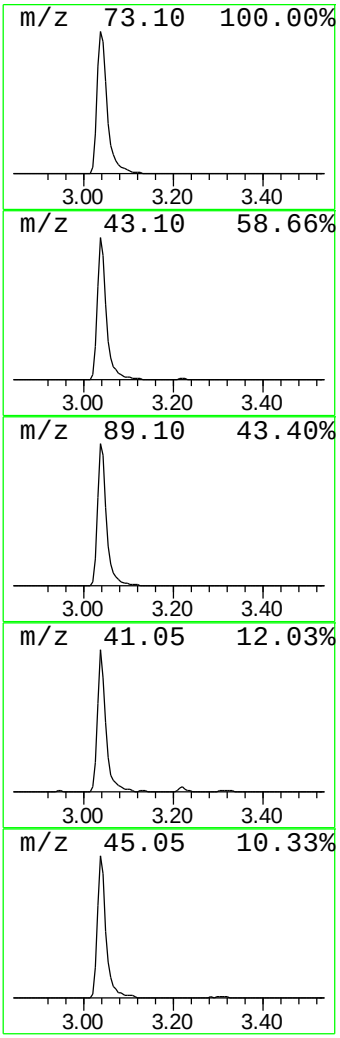
****

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	224.88 ng	7424280	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

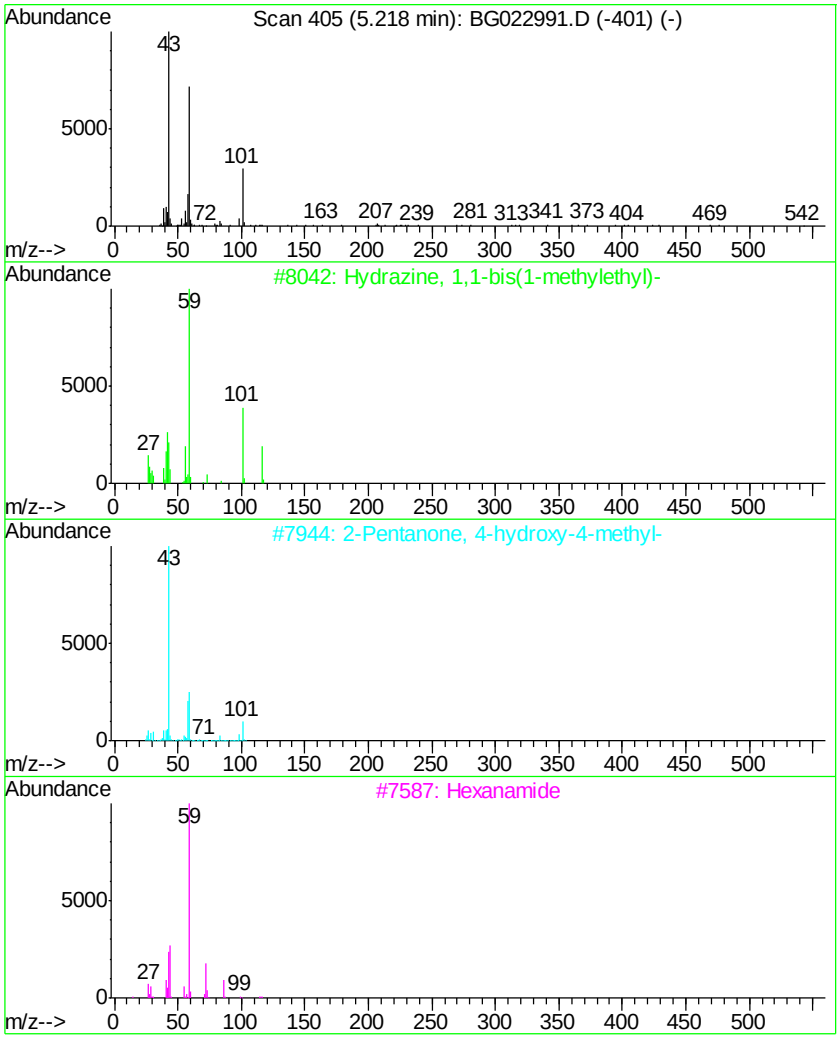
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

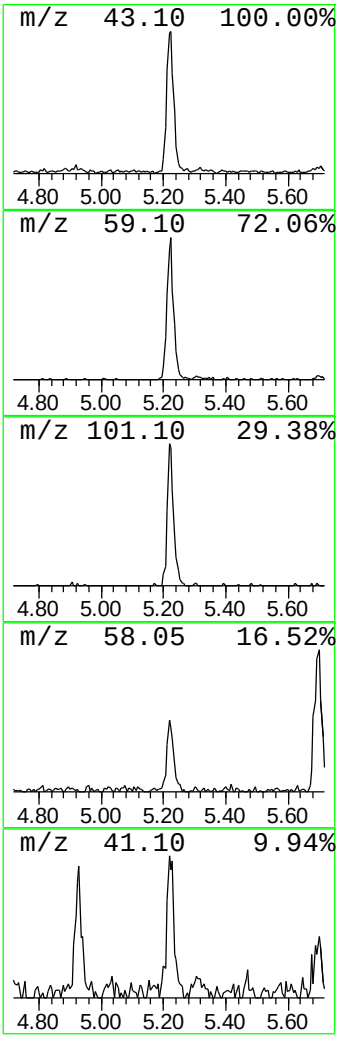
****

Peak Number 2 unknown5.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.64 ng	186203	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	42
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	Hexanamide	115	C6H13NO	000628-02-4	35
4	Guanidine	59	CH5N3	000113-00-8	35
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

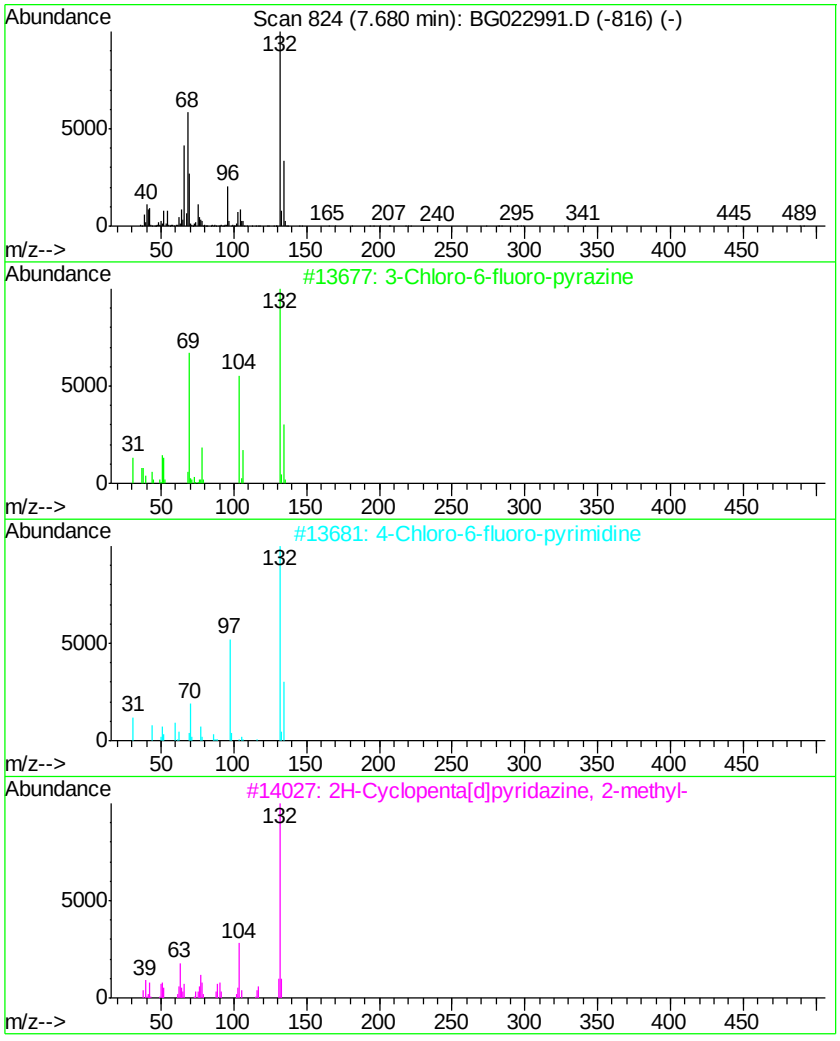
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

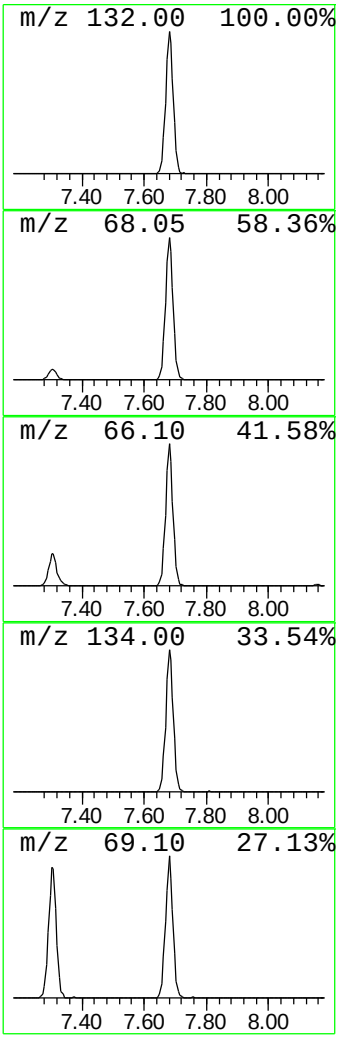
****

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	114.12 ng	3767650	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

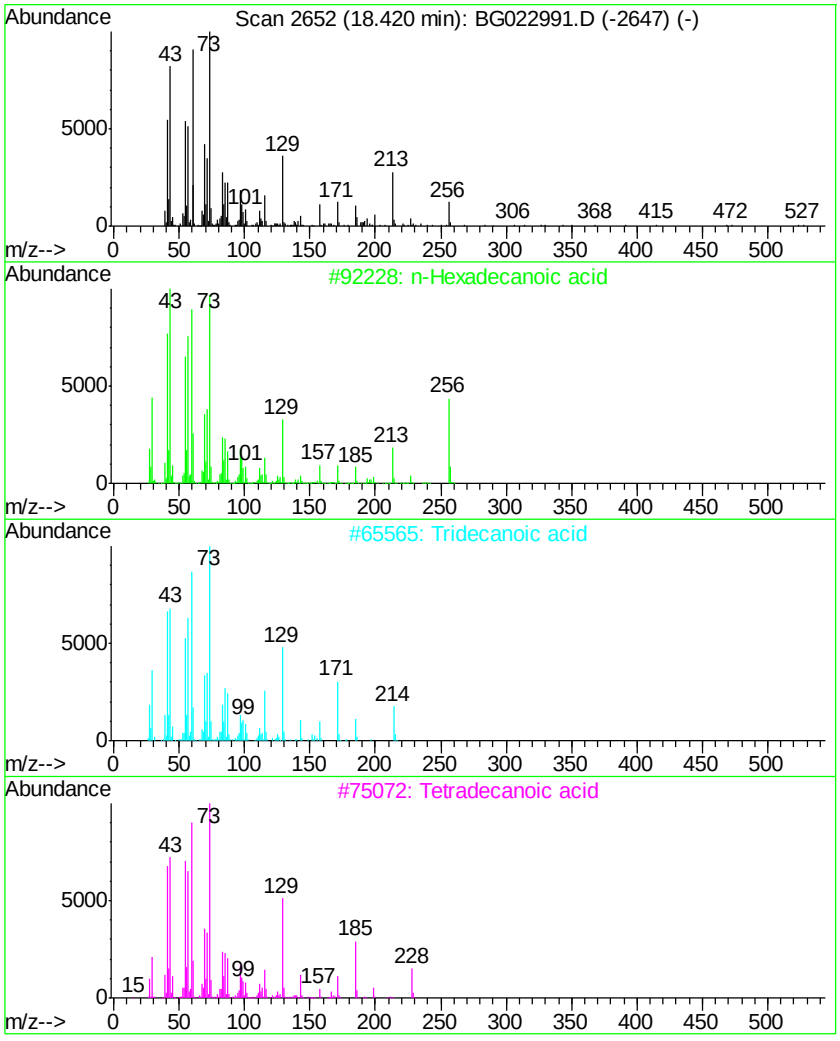
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

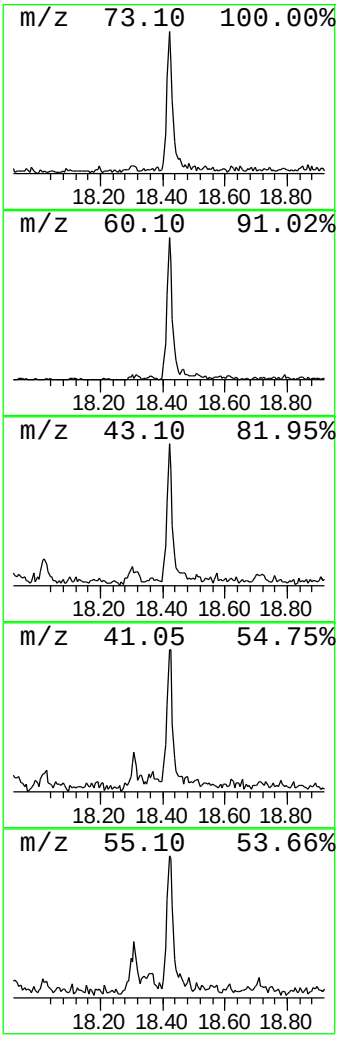
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.29 ng	452557	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

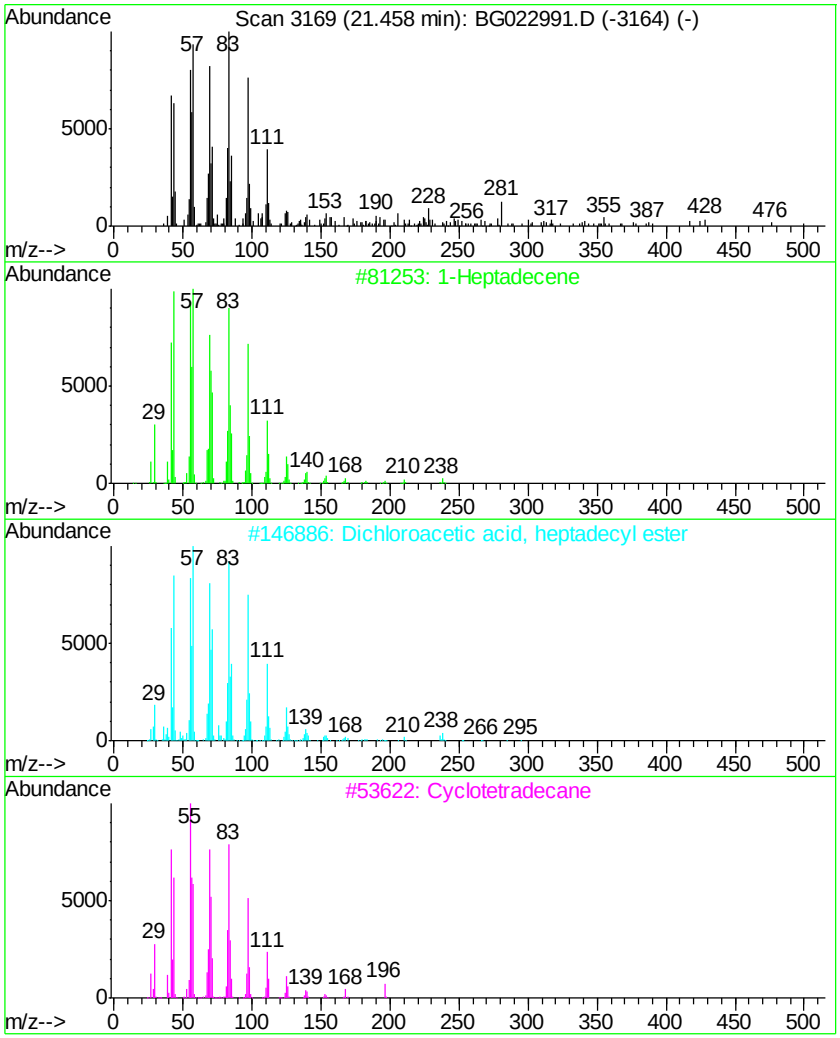
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

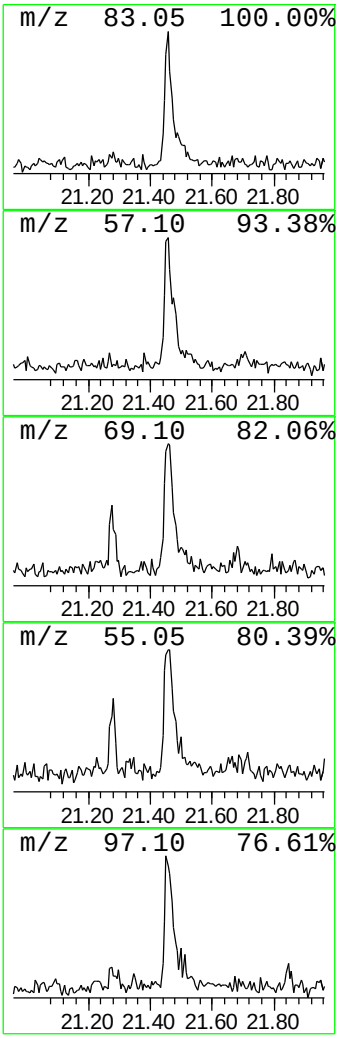
****

Peak Number 6 1-Heptadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	2.26 ng	272706	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	83
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
3	Cyclotetradecane	196	C14H28	000295-17-0	81
4	1-Pentadecene	210	C15H30	013360-61-7	81
5	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022991.D
Acq On : 10 Jul 2016 8:49
Operator : UM/SJ
Sample : H3921-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 07-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
unknown3.04	3.04	224.9	ng	7424280	1	8.15	660295	20.0
unknown5.22	5.22	5.6	ng	186203	1	8.15	660295	20.0
unknown7.68	7.68	114.1	ng	3767650	1	8.15	660295	20.0
n-Hexadecanoic acid	18.42	4.3	ng	452557	4	17.56	2108740	20.0
1-Heptadecene	21.46	2.3	ng	272706	5	21.85	2410560	20.0