LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

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-BG120215.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	2.994	21	26	46	rVV	1018173	1358048	44.55%	7.813%
2	3.135	46	50	60	rVV2	37351	77546	2.54%	0.446%
3	3.217	60	64	74	rVB	75115	106693	3.50%	0.614%
4	5.191	394	400	410	rVB	128359	196788	6.46%	1.132%
5	5.661	473	480	490	rBV	610213	953253	31.27%	5.485%
6	7.265	745	753	764	rBV	663830	1119170	36.71%	6.439%
7	7.647	811	818	827	rBV	636556	1053901	34.57%	6.064%
8	8.117	891	898	905	rBV	114998	197437	6.48%	1.136%
9	8.446	947	954	963	rVB	446616	763999	25.06%	4.396%
10	9.286	1089	1097	1106	rVB	393361	696101	22.83%	4.005%
11	9.386	1106	1114	1123	rBV2	18458	32441	1.06%	0.187%
12	10.937	1369	1378	1386	rVB	173450	304185	9.98%	1.750%
13	13.376	1782	1793	1802	rBV	1182547	1801471	59.09%	10.365%
14	14.198	1925	1933	1942	rBV	318096	443948	14.56%	2.554%
15	14.751	2015	2027	2035	rBV2	304739	481219	15.79%	2.769%
16	16.231	2271	2279	2290	rBV	1074513	1582899	51.92%	9.107%
17	16.449	2312	2316	2319	rBV	25185	33316	1.09%	0.192%
18	17.489	2487	2493	2502	rBV2	422556	638288	20.94%	3.672%
19	18.370	2634	2643	2650	rBV	65941	104500	3.43%	0.601%
20	19.633	2855	2858	2865	rBV5	26702	44632	1.46%	0.257%
21	20.097	2931	2937	2942	rBV	2322212	3048445	100.00%	17.539%
22	20.303	2968	2972	2977	rBV	25697	34630	1.14%	0.199%
23	20.779	3050	3053	3060	rVB2	57789	76256	2.50%	0.439%
24	20.855	3060	3066	3073	rBV6	28157	61983	2.03%	0.357%
25	20.996	3086	3090	3094	rBV	38767	57392	1.88%	0.330%
26	21.043	3095	3098	3102	rVB	74423	86860	2.85%	0.500%
27	21.114	3107	3110	3115	rVB	34996	47438	1.56%	0.273%
28	21.402	3156	3159	3169	rVB4	39822	60138	1.97%	0.346%
29	21.560	3179	3186	3193	rVB	59498	93455	3.07%	0.538%
30	21.631	3195	3198	3203	rBV2	24276	40218	1.32%	0.231%
31	21.766	3214	3221	3230	rVB	511077	825957	27.09%	4.752%
32	22.113	3276	3280	3285	rVB2	26582	40043	1.31%	0.230%
33	23.511	3512	3518	3528	rVB	84023	167974	5.51%	0.966%
34	25.056	3771	3781	3795	rVB	263595	750207	24.61%	4.316%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

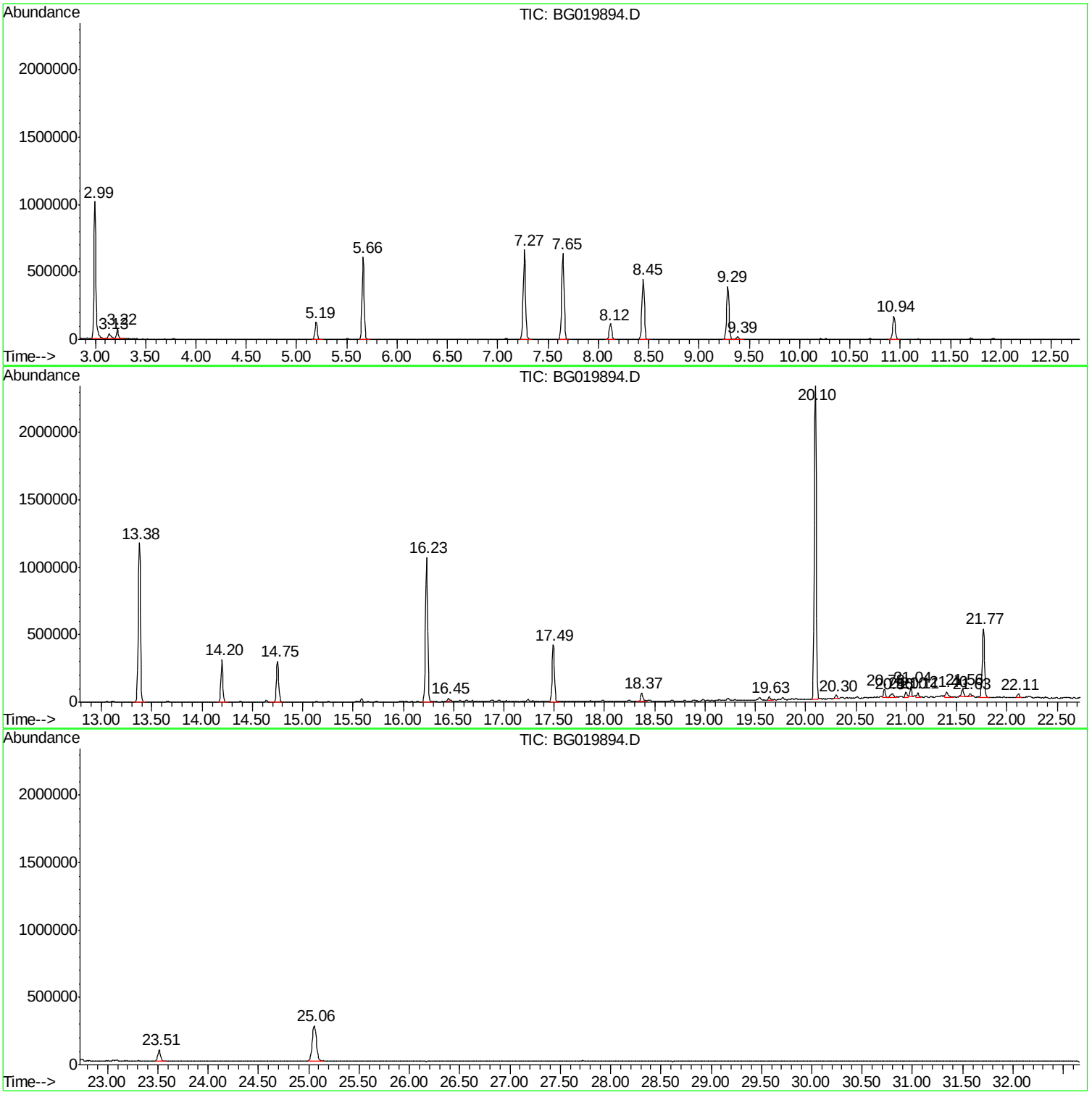
Sum of corrected areas: 17380831

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
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Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

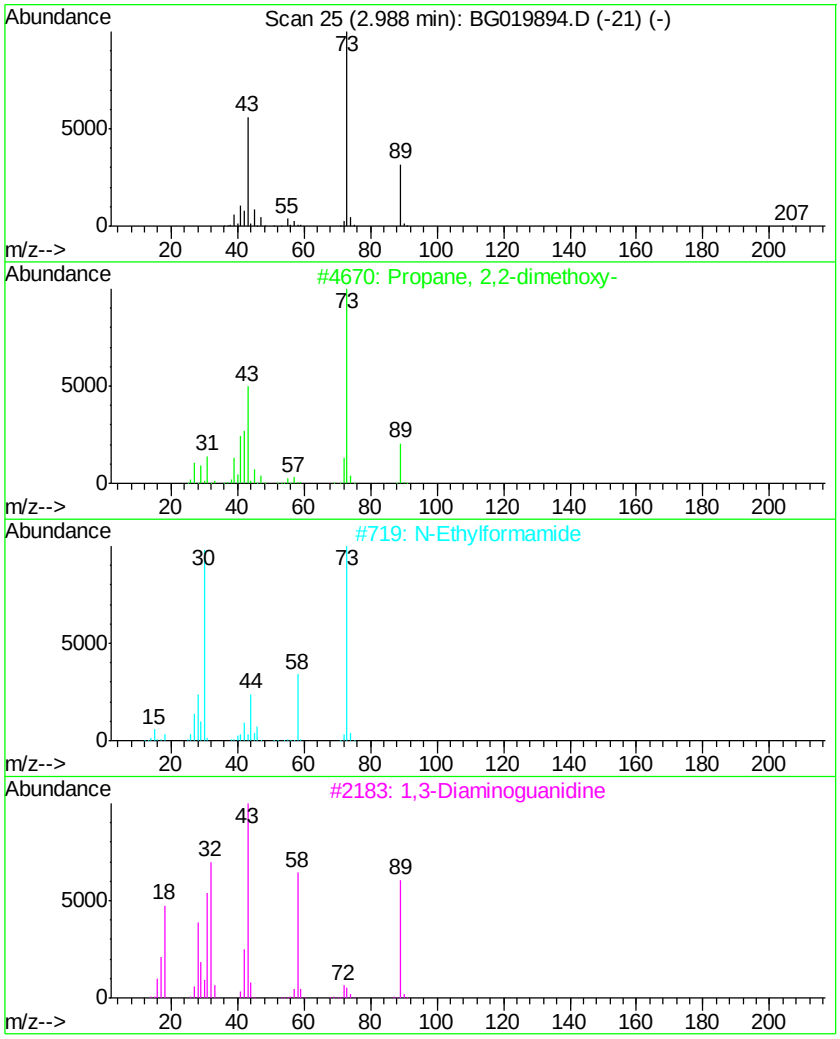
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

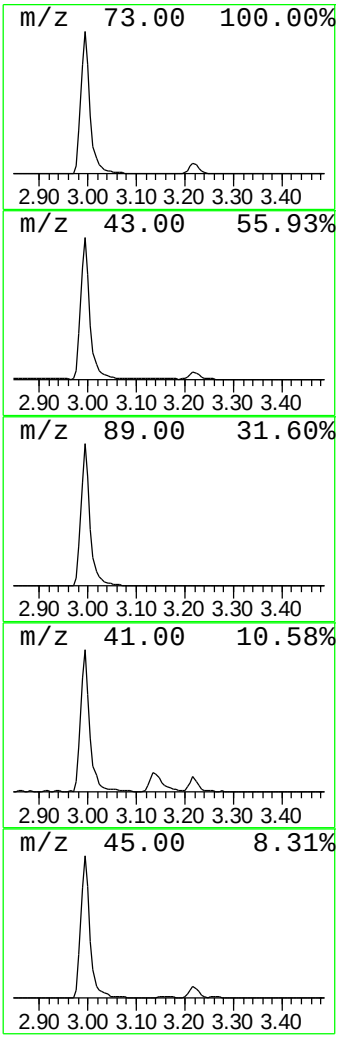
****

Peak Number 1 unknown2.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	137.57 ng	1358050	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

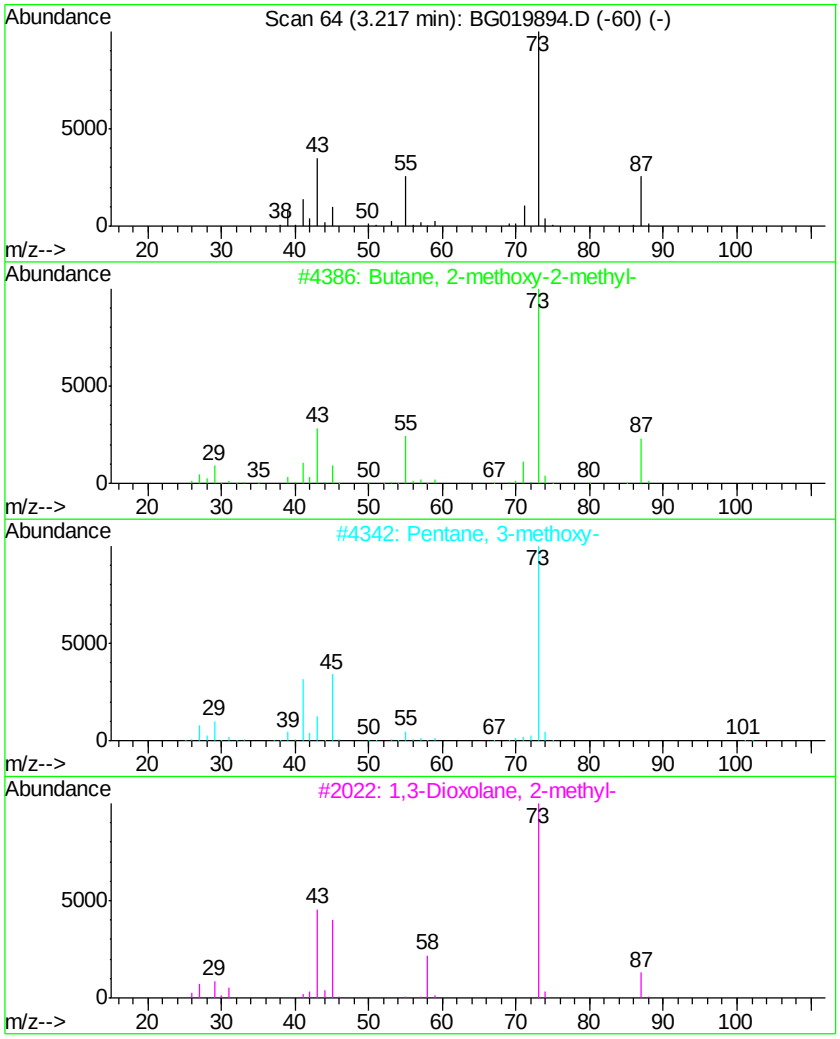
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

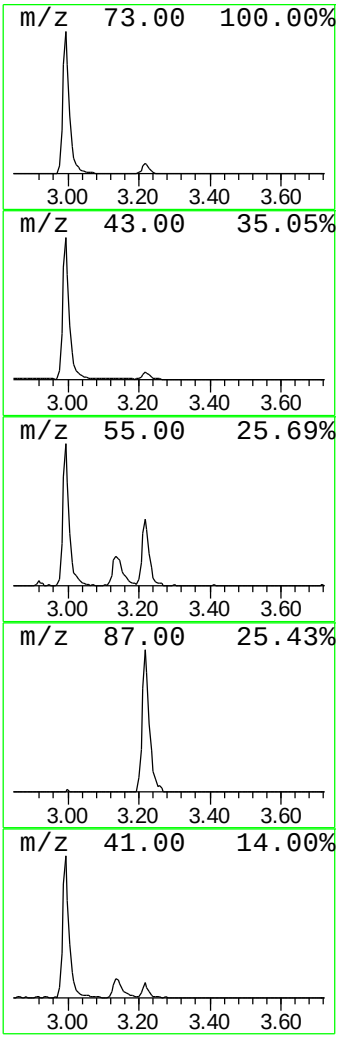
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	10.81 ng	106693	1,4-Dichlorobenzene-d4	8.12

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	17
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

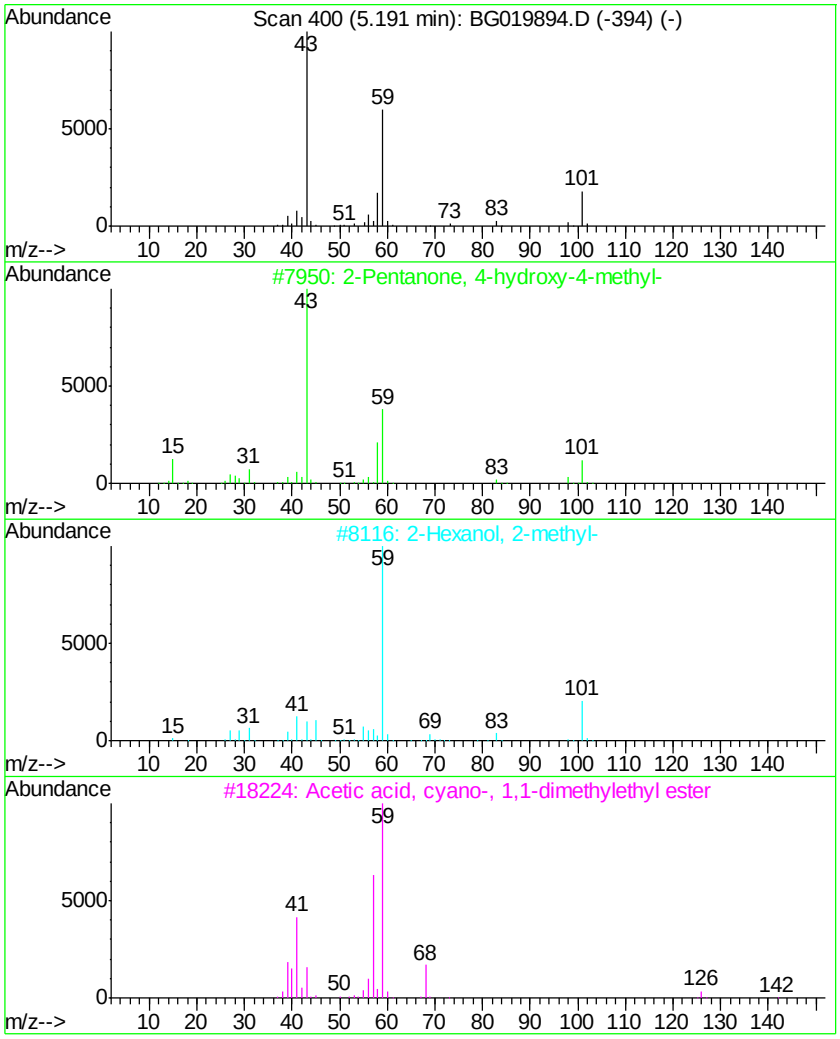
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

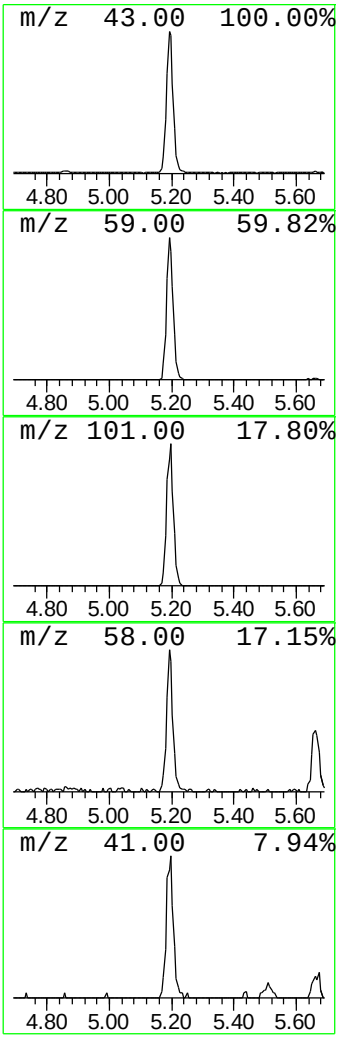
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	19.93 ng	196788	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

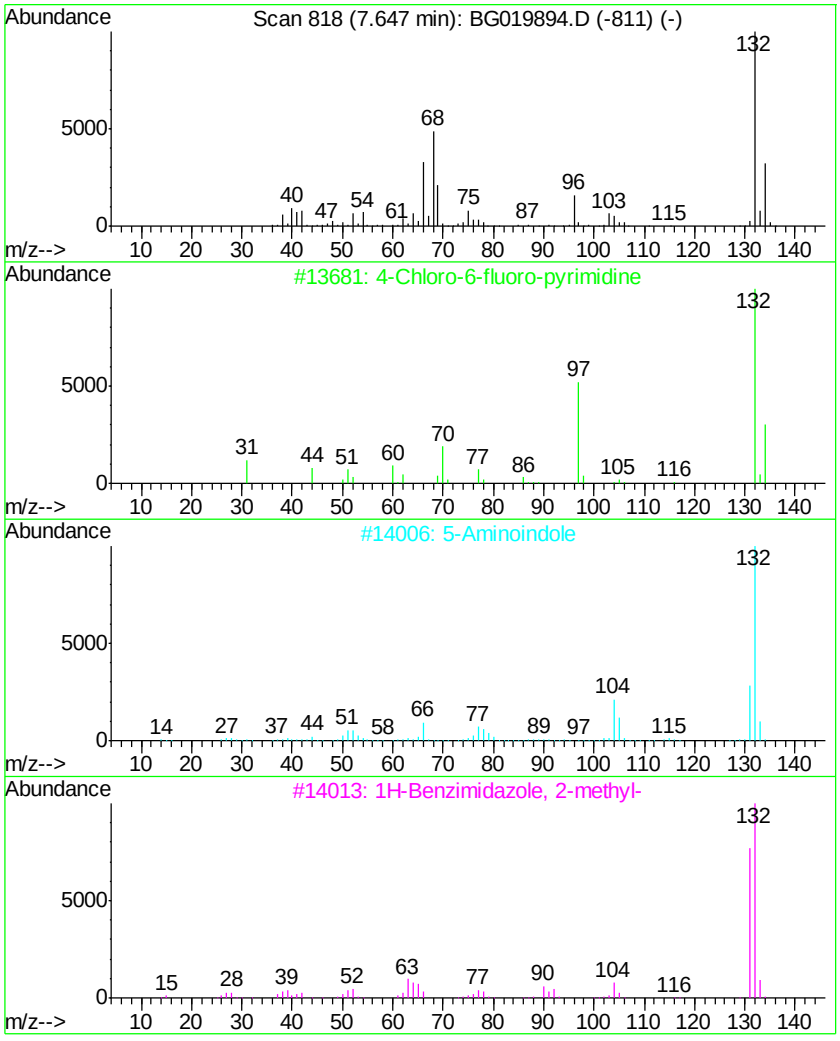
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

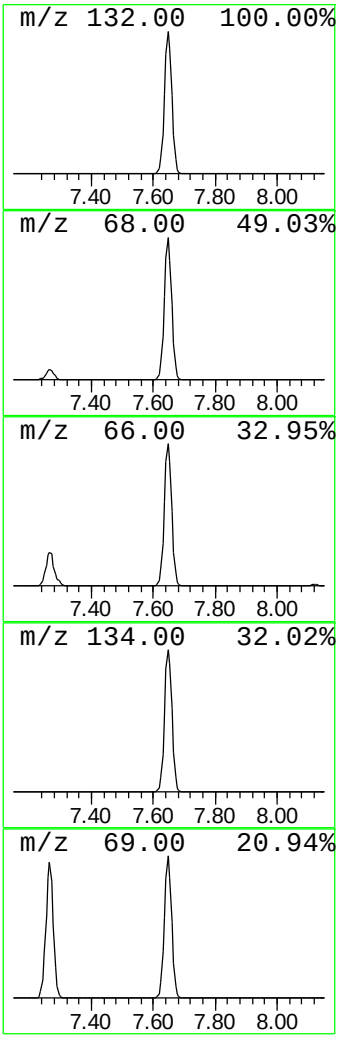
****

Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	106.76 ng	1053900	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

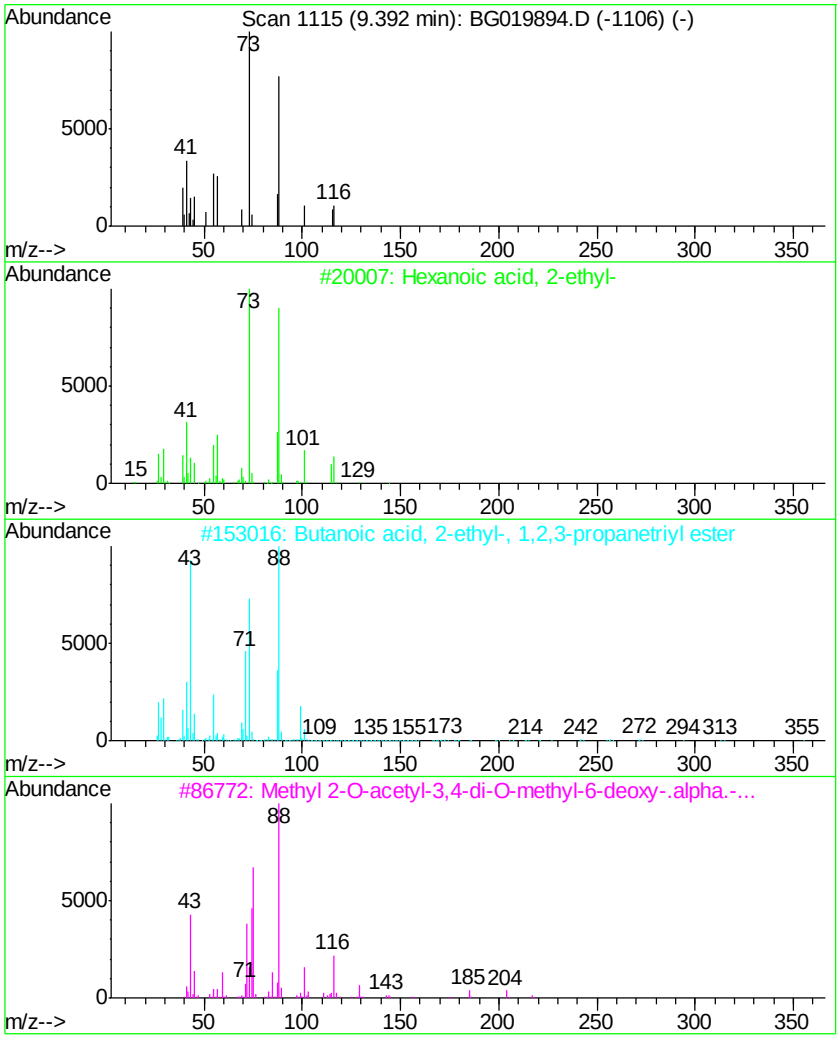
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

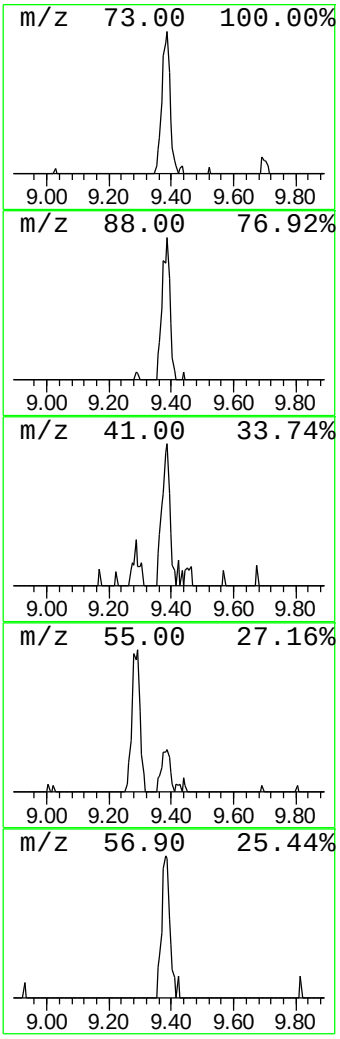
****

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	3.29 ng	32441	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
3	Methyl 2-O-acetyl-3,4-di-O-methy...	248	C11H20O6	072922-26-0	42
4	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	33





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Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

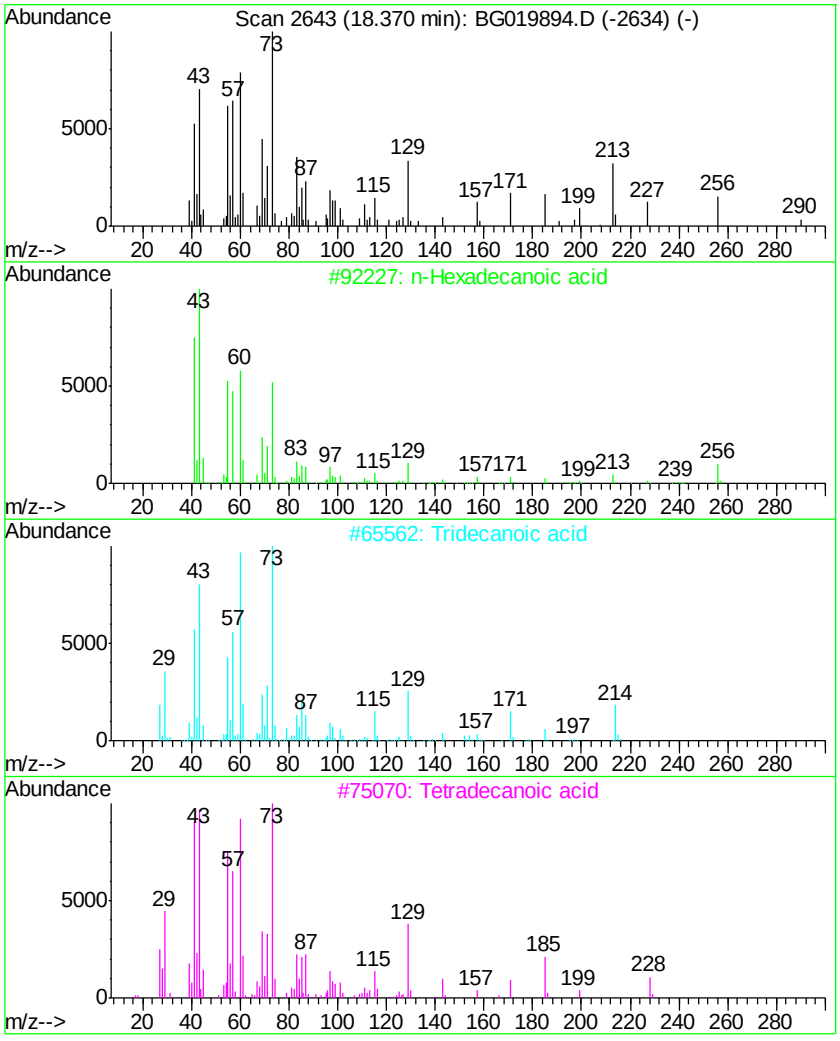
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

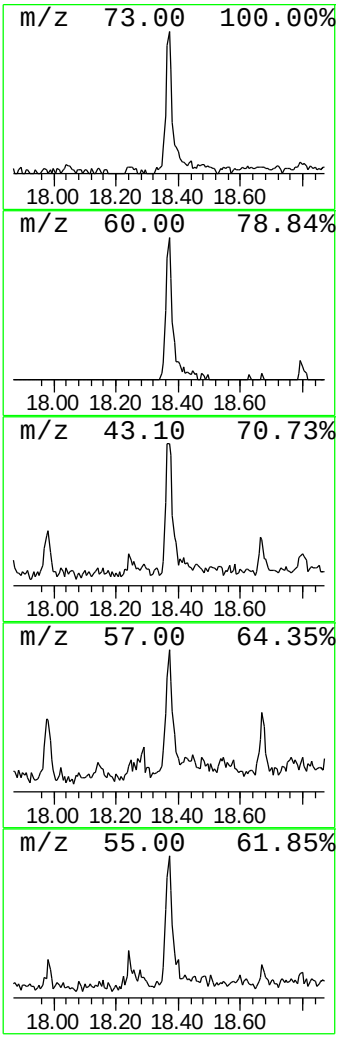
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	3.27 ng	104500	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

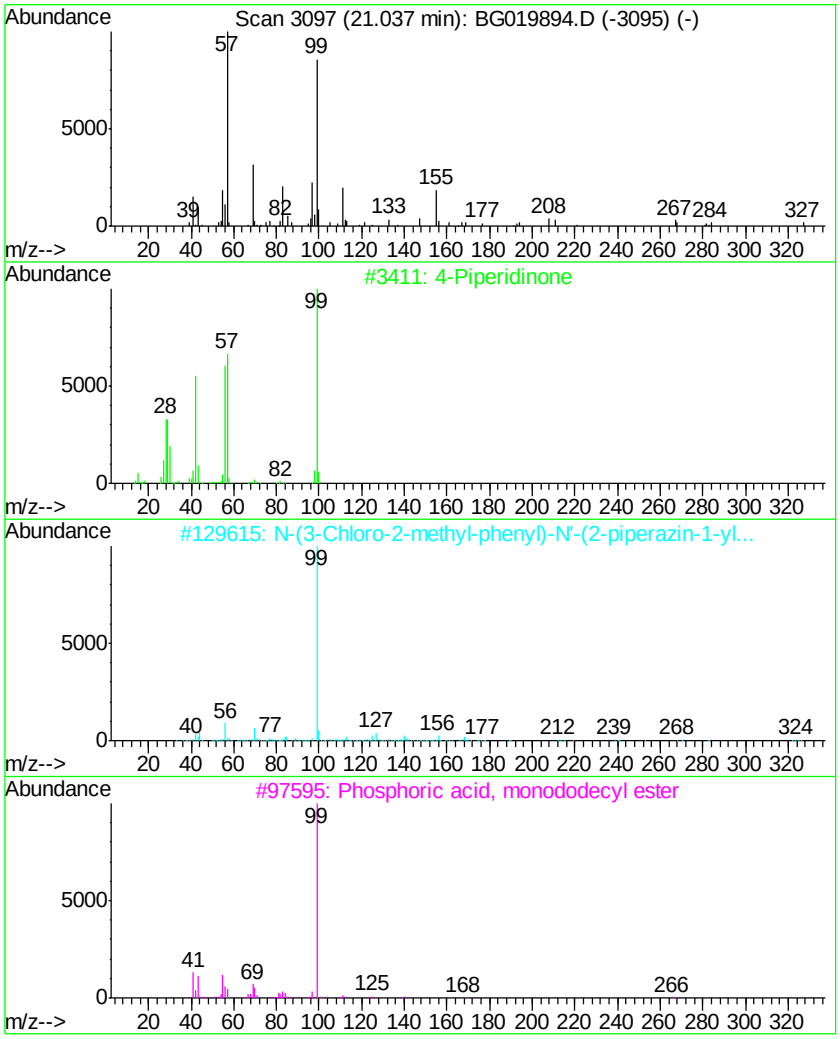
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

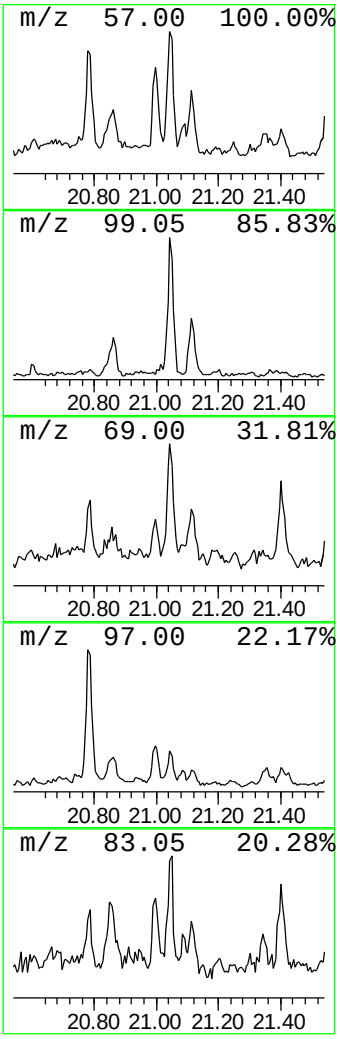
****

Peak Number 9 unknown21.04 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.10 ng	86860	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Piperidinone	99	C5H9NO	041661-47-6	38
2	N-(3-Chloro-2-methyl-phenyl)-N'-...	324	C15H21ClN4O2	1000294-79-6	35
3	Phosphoric acid, monododecyl ester	266	C12H27O4P	002627-35-2	32
4	Tributyl phosphate	266	C12H27O4P	000126-73-8	28
5	Tetrahydrofuran-2-one, 3-[2-pent...	168	C10H16O2	1000132-08-6	25





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Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

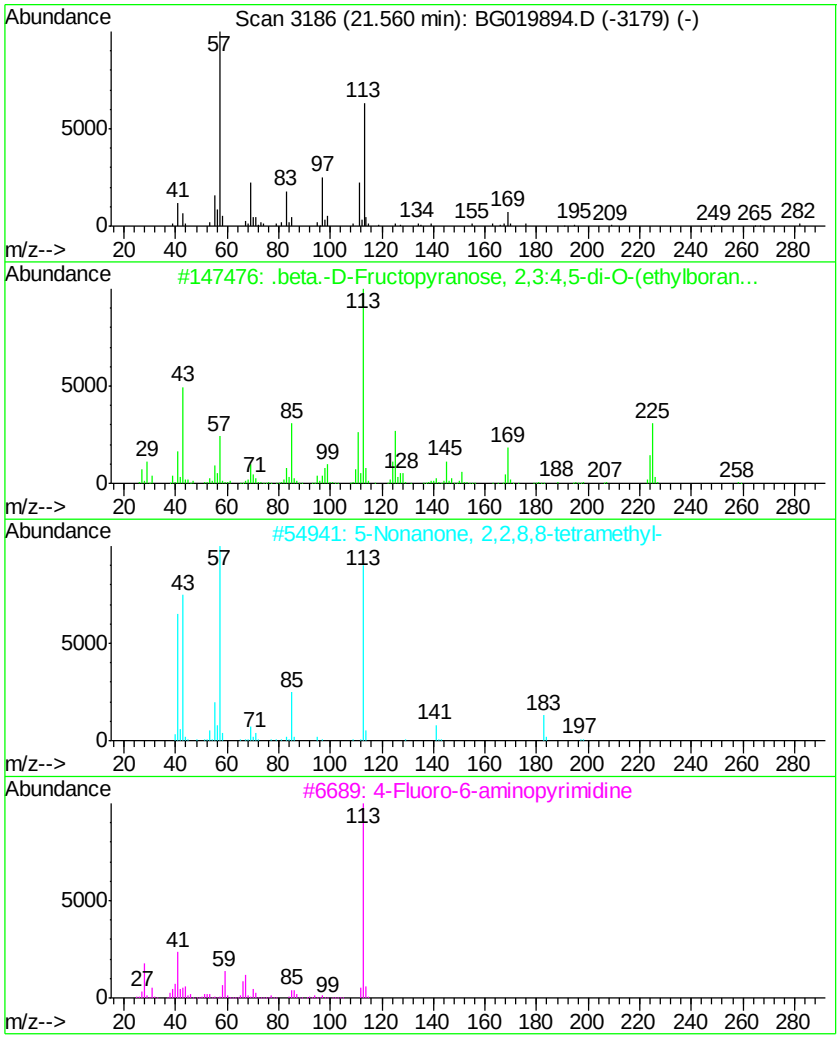
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

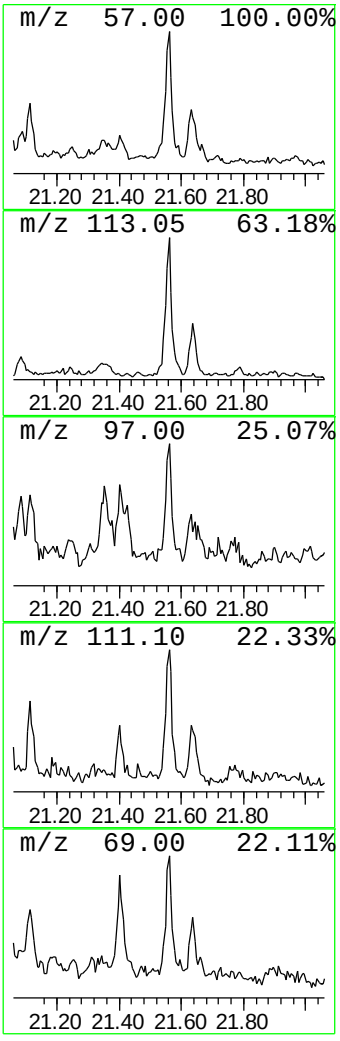
****

Peak Number 10 unknown21.56 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.56	2.26 ng	93455	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	32
2	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32
3	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	27
4	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	25
5	1-Isopropyl-2-methylpropyl ethyl...	210	C9H20FO2P	1000298-33-2	17





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
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TIC Library : C:\DATABASE\NIST02.L
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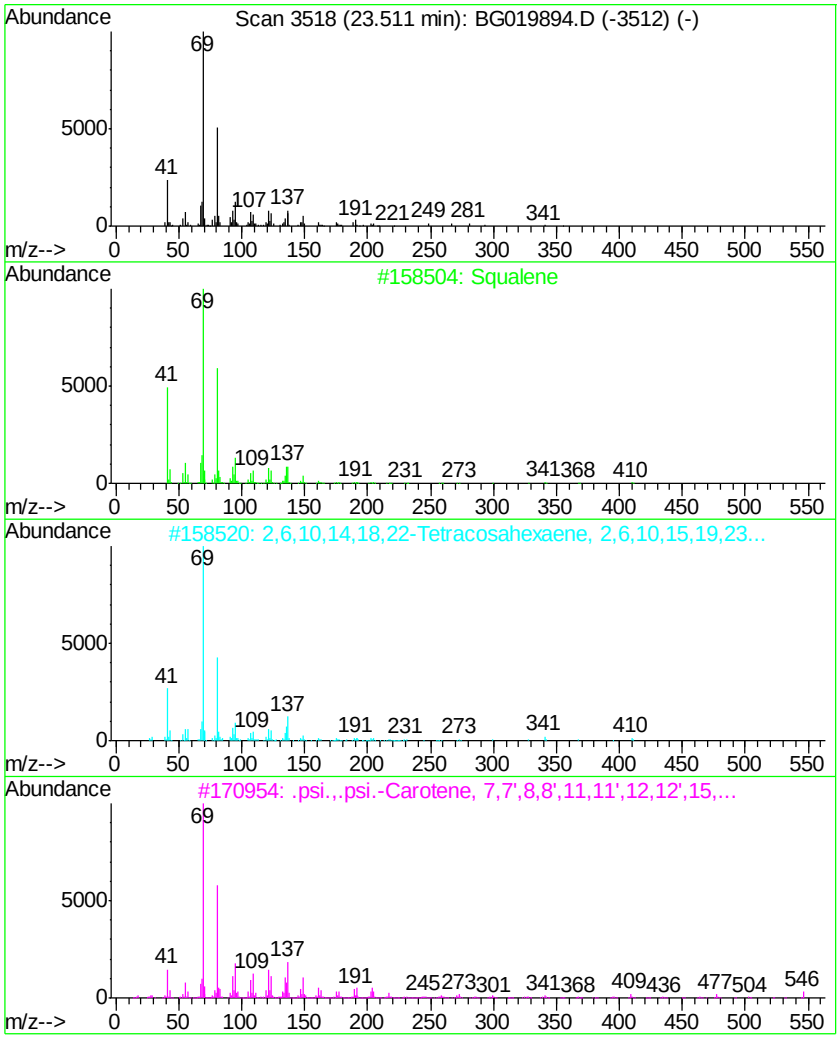
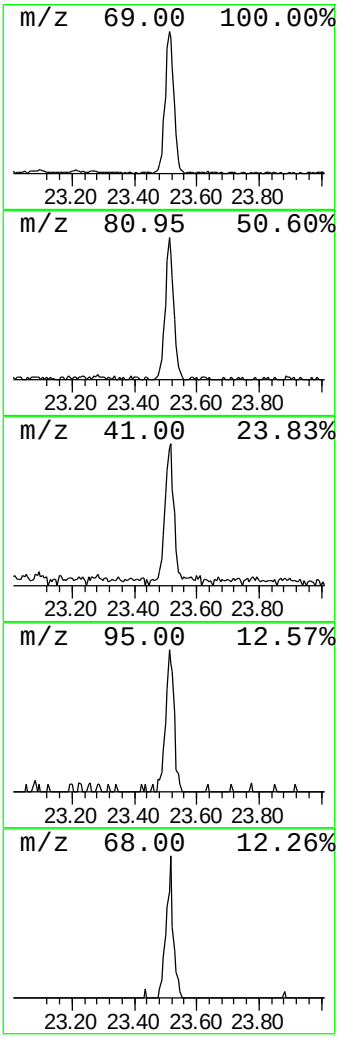
Peak Number 11 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	4.48 ng	167974	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
Data File : BG019894.D
Acq On : 4 Dec 2015 6:21
Operator : UM/NP
Sample : G4609-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-3-8.5-9.0-113015

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
unknown2.99	2.99	137.6	ng	1358050	1	8.12	197437	20.0
Butane, 2-methoxy...	3.22	10.8	ng	106693	1	8.12	197437	20.0
2-Pentanone, 4-hy...	5.19	19.9	ng	196788	1	8.12	197437	20.0
unknown7.65	7.65	106.8	ng	1053900	1	8.12	197437	20.0
Hexanoic acid, 2-...	9.39	3.3	ng	32441	1	8.12	197437	20.0
n-Hexadecanoic acid	18.37	3.3	ng	104500	4	17.49	638288	20.0
unknown21.04	21.04	2.1	ng	86860	5	21.77	825957	20.0
unknown21.56	21.56	2.3	ng	93455	5	21.77	825957	20.0
Squalene	23.51	4.5	ng	167974	6	25.05	750207	20.0