LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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	5.187	395	400	406	rBV	54921	82967	2.38%	0.528%
2	5.657	473	480	489	rVB	342276	547153	15.66%	3.484%
3	7.255	745	752	761	rBV	233628	403900	11.56%	2.572%
4	7.643	810	818	826	rBV	634374	1087680	31.14%	6.925%
5	8.113	890	898	904	rBV	134293	225886	6.47%	1.438%
6	8.436	943	953	962	rBV	546151	954378	27.32%	6.076%
7	9.282	1088	1097	1105	rBV	511388	904070	25.88%	5.756%
8	10.933	1369	1378	1385	rVB	188314	339660	9.72%	2.163%
9	13.366	1782	1792	1801	rBV	1476418	2294935	65.70%	14.611%
10	14.741	2020	2026	2033	rBV2	318583	518502	14.84%	3.301%
11	16.227	2270	2279	2287	rBV	1231128	1897108	54.31%	12.079%
12	17.485	2484	2493	2499	rBV	414066	639008	18.29%	4.068%
13	18.354	2636	2641	2646	rBV	71479	94709	2.71%	0.603%
14	19.623	2852	2857	2865	rBV2	74449	112144	3.21%	0.714%
15	19.770	2877	2882	2887	rVB3	40770	68879	1.97%	0.439%
16	20.087	2929	2936	2948	rBV	2608094	3492992	100.00%	22.239%
17	20.763	3047	3051	3055	rVB	53430	66356	1.90%	0.422%
18	20.816	3056	3060	3062	rBV3	32373	44957	1.29%	0.286%
19	20.980	3084	3088	3092	rBV	39321	59901	1.71%	0.381%
20	21.027	3092	3096	3100	rVB	66393	82378	2.36%	0.524%
21	21.092	3105	3107	3117	rVB2	33313	54305	1.55%	0.346%
22	21.386	3153	3157	3164	rVB4	36589	60838	1.74%	0.387%
23	21.539	3179	3183	3191	rVB	51748	86600	2.48%	0.551%
24	21.756	3213	3220	3228	rVB	477722	800461	22.92%	5.096%
25	25.035	3766	3778	3790	rBV2	266339	786651	22.52%	5.008%

Sum of corrected areas: 15706418

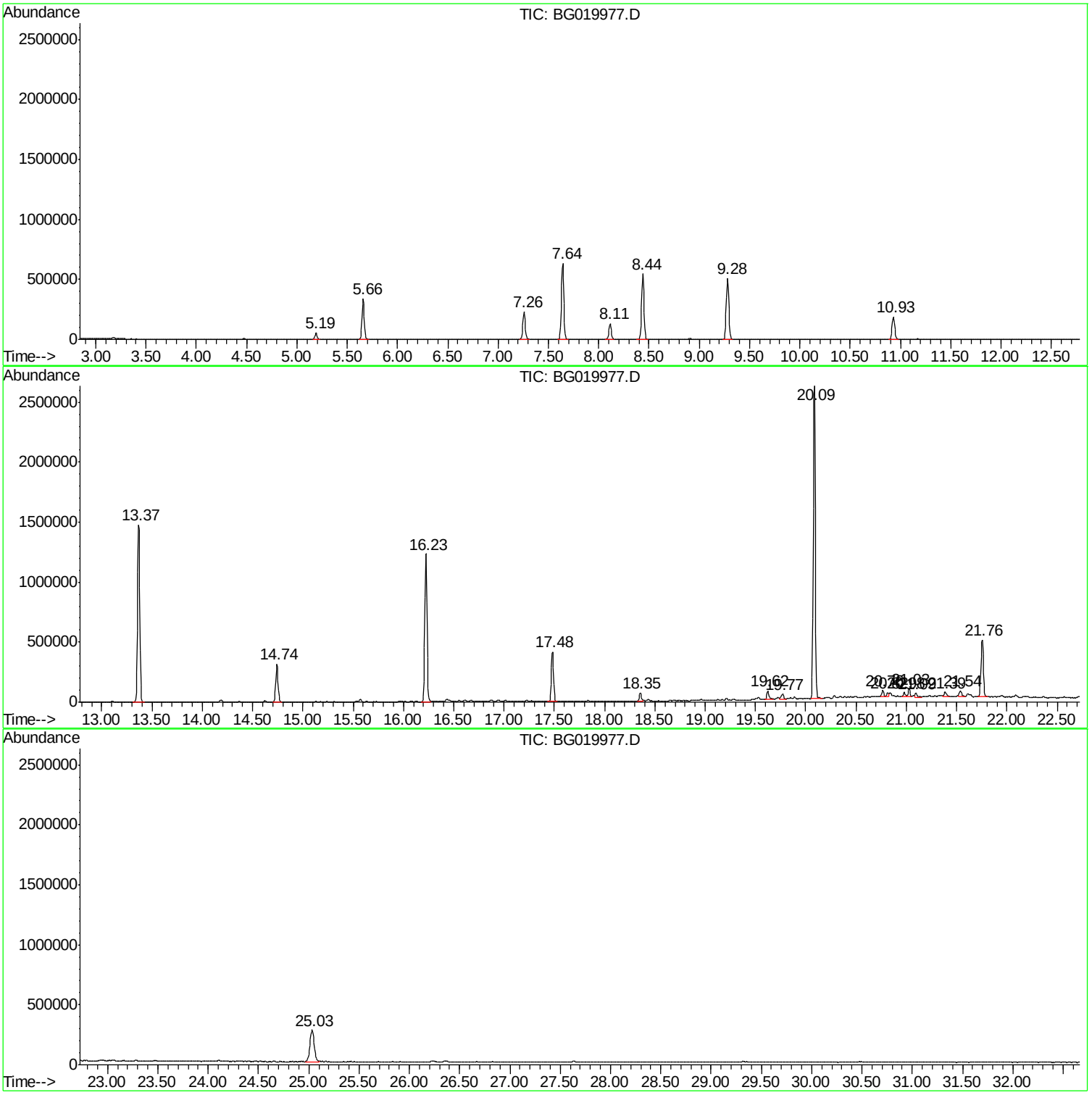
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

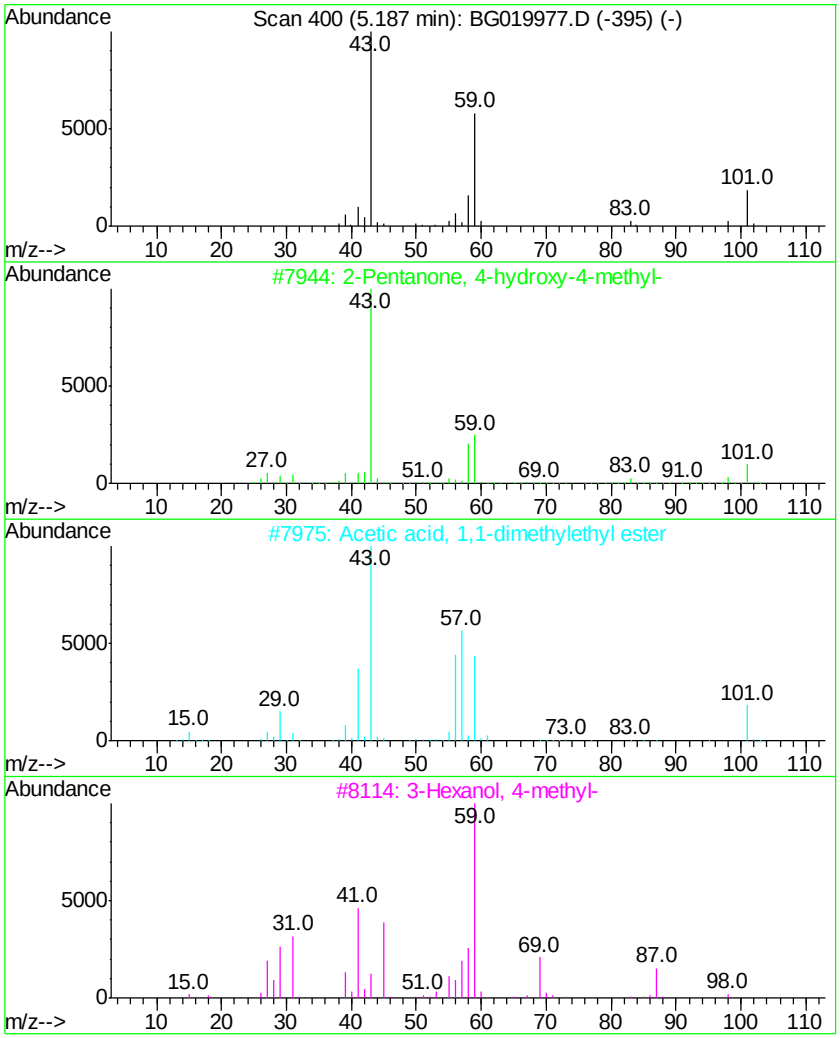
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

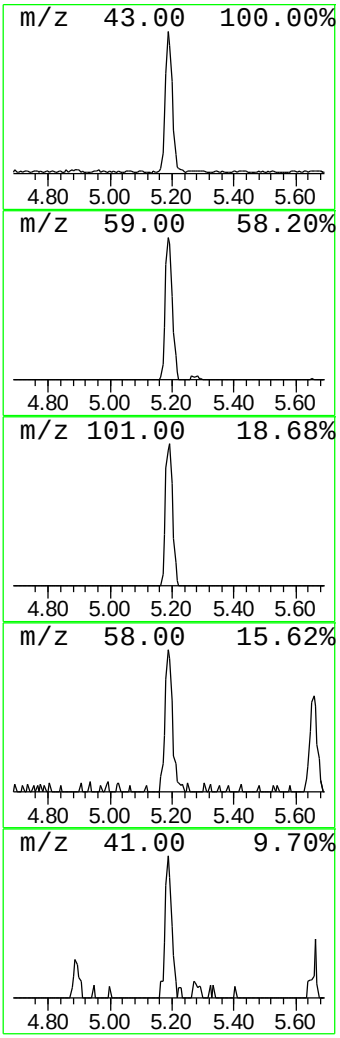
****

Peak Number 1 unknown5.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	7.35 ng	82967	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

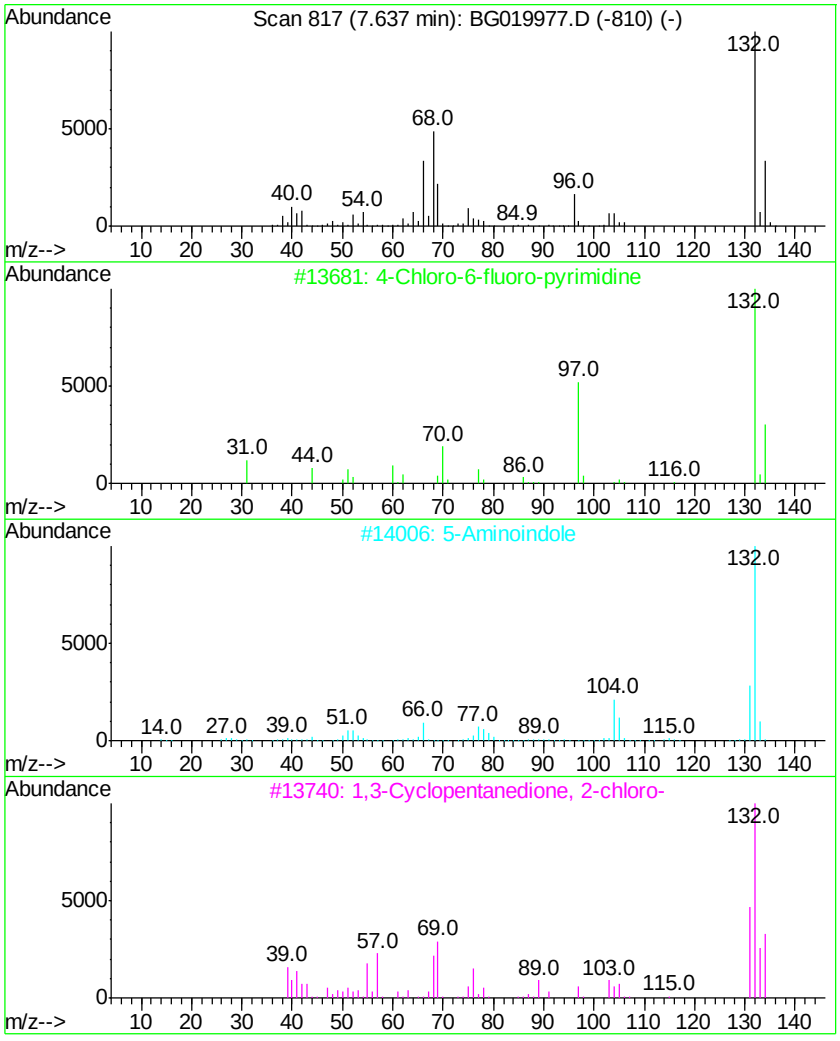
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

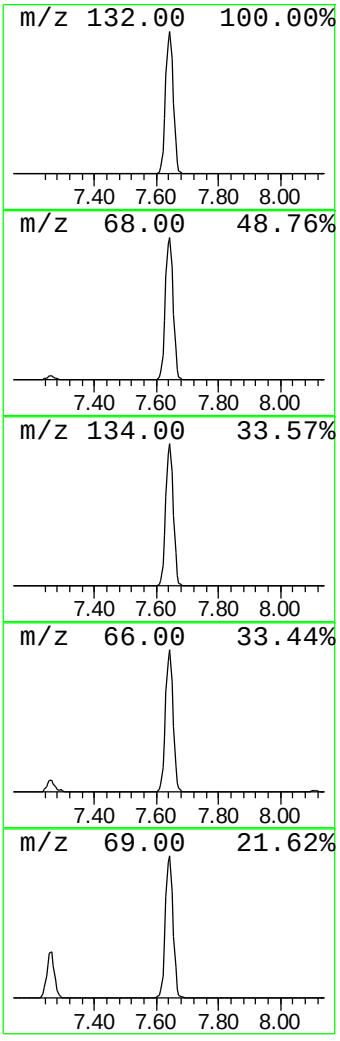
****

Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	96.30 ng	1087680	1,4-Dichlorobenzene-d4	8.11

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	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

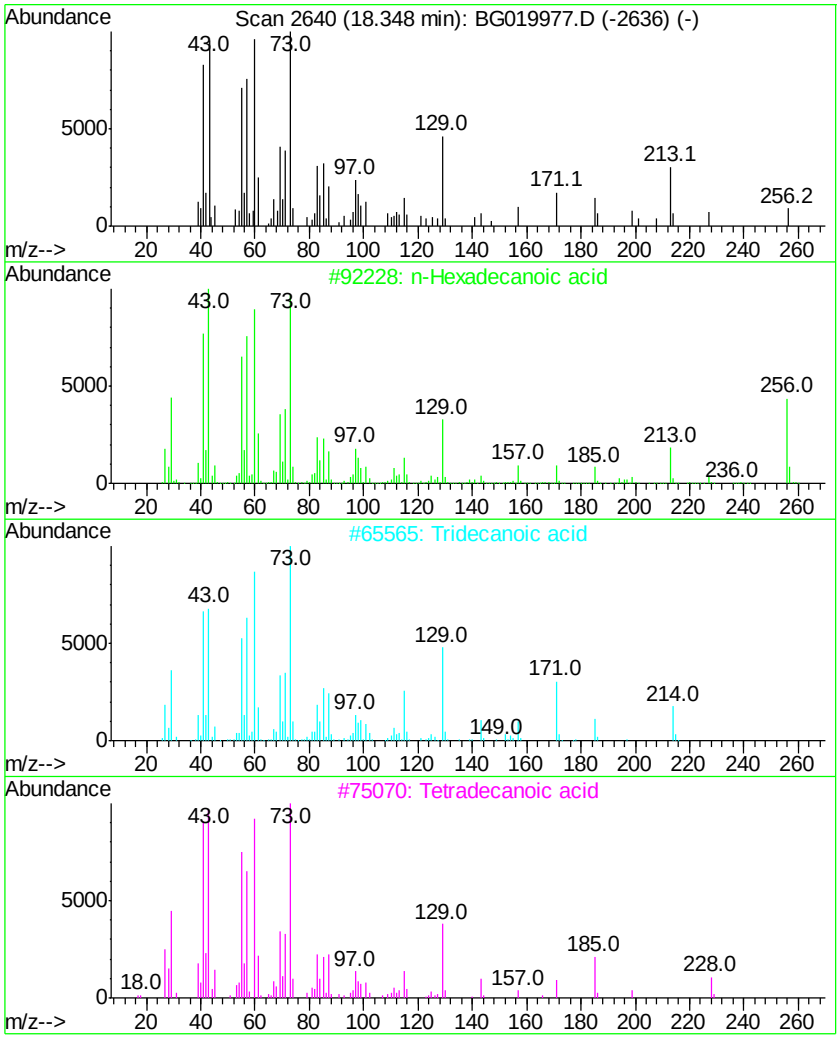
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

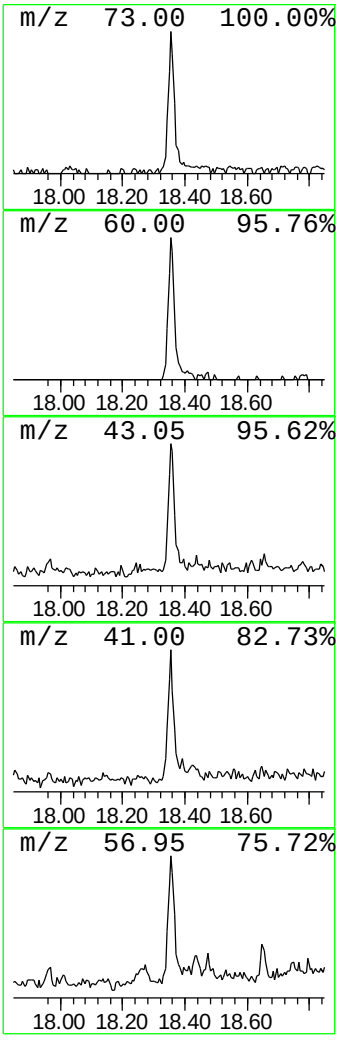
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	2.96 ng	94709	Phenanthrene-d10	17.48

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

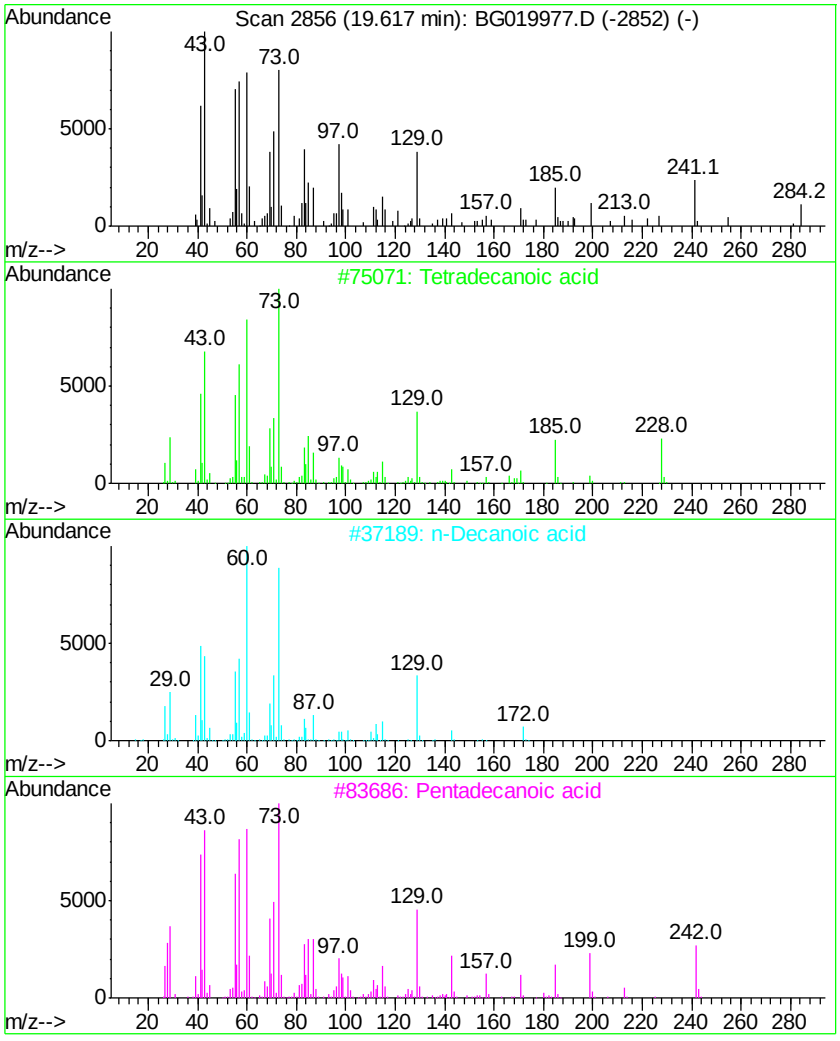
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

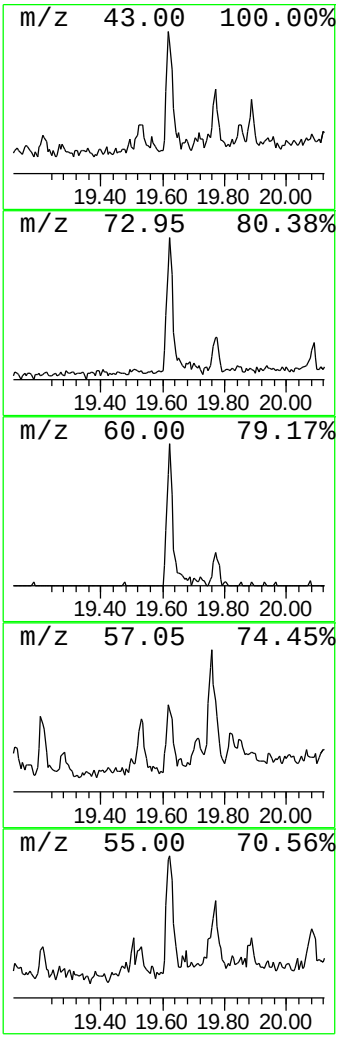
****

Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.80 ng	112144	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2	n-Decanoic acid	172	C10H20O2	000334-48-5	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

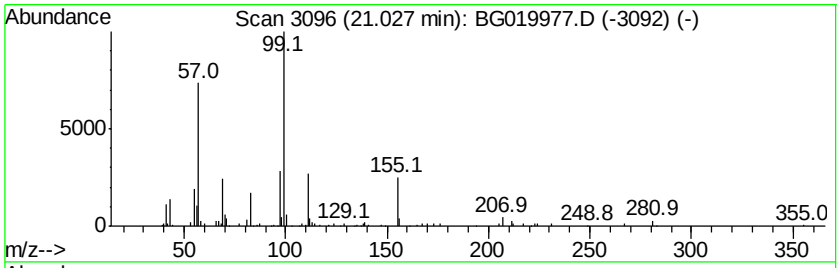
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

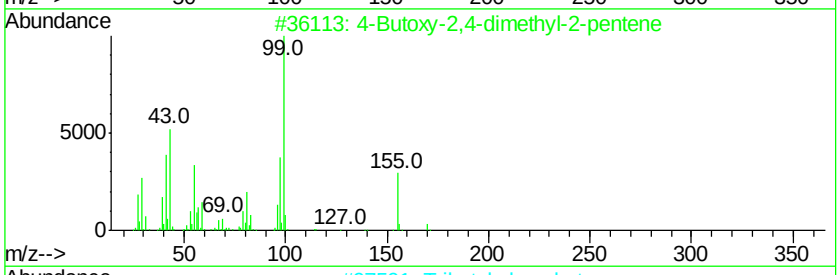
****

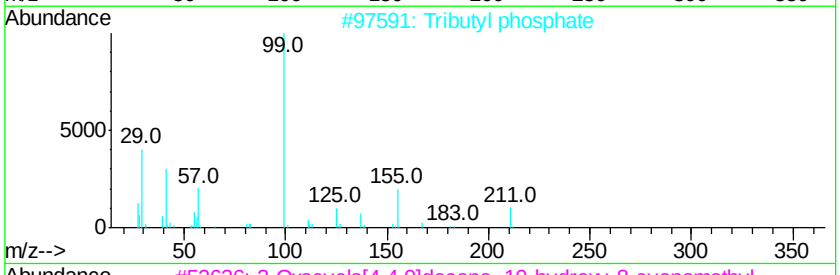
Peak Number 6 unknown21.03 Concentration Rank 7

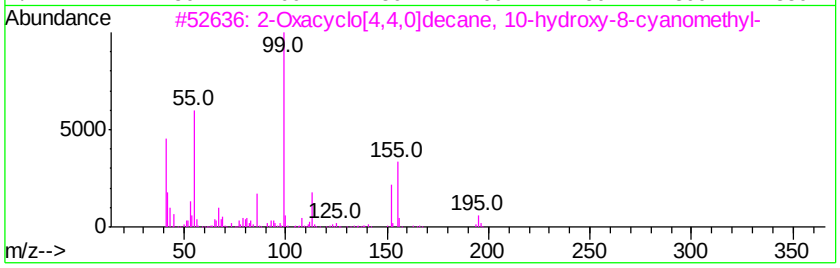
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	2.06 ng	82378	Chrysene-d12	21.76

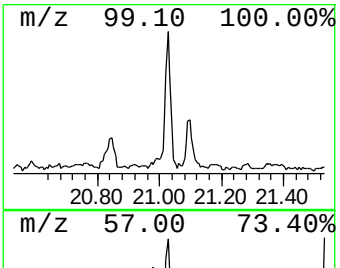
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42
2	Tributyl phosphate	266	C12H27O4P	000126-73-8	40
3	2-Oxacyclo[4,4,0]decane, 10-hydr...	195	C11H17NO2	1000130-46-5	38
4	2-Propylthiazole	127	C6H9NS	017626-75-4	35
5	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	28

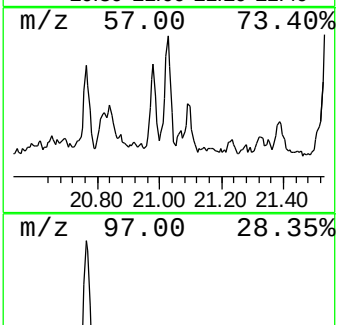


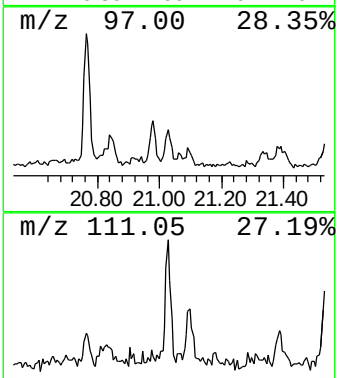


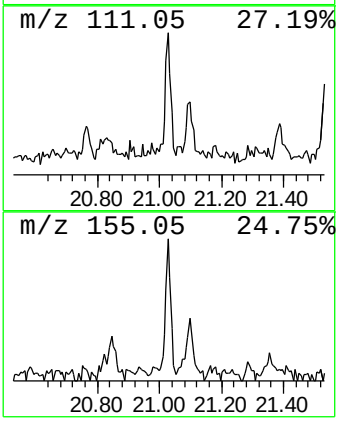












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Data File : BG019977.D
Acq On : 6 Dec 2015 21:33
Operator : UM/NP
Sample : G4630-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-32

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

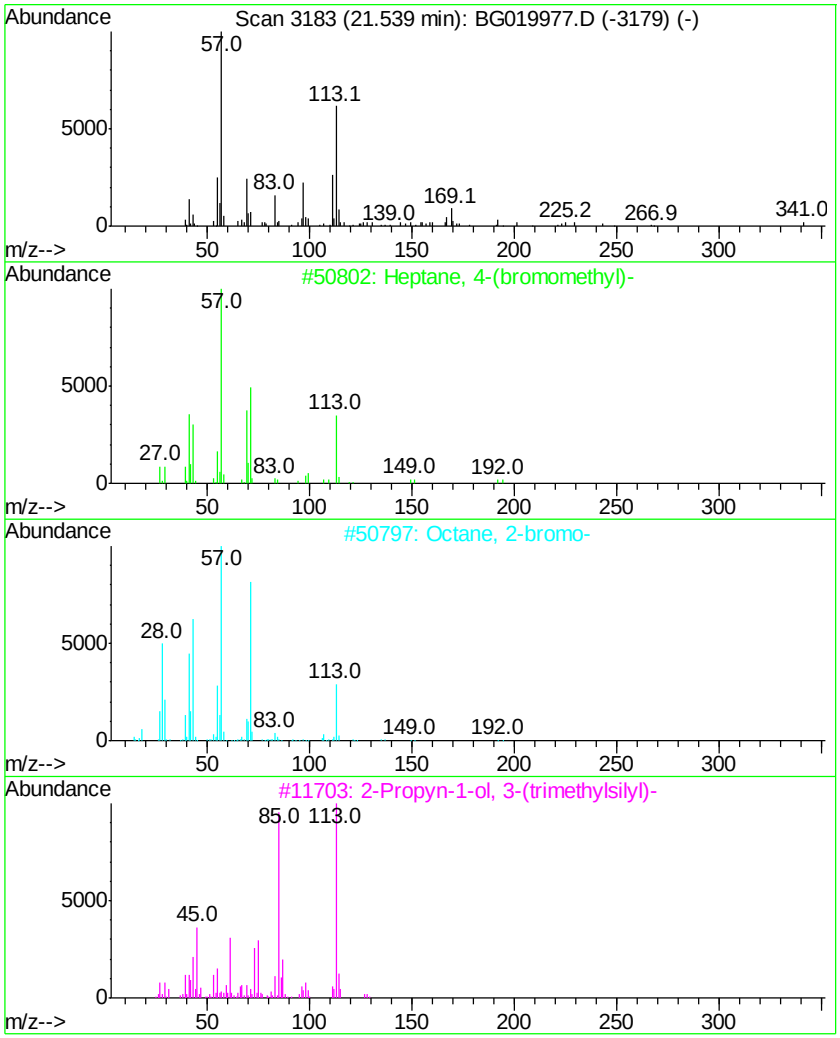
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

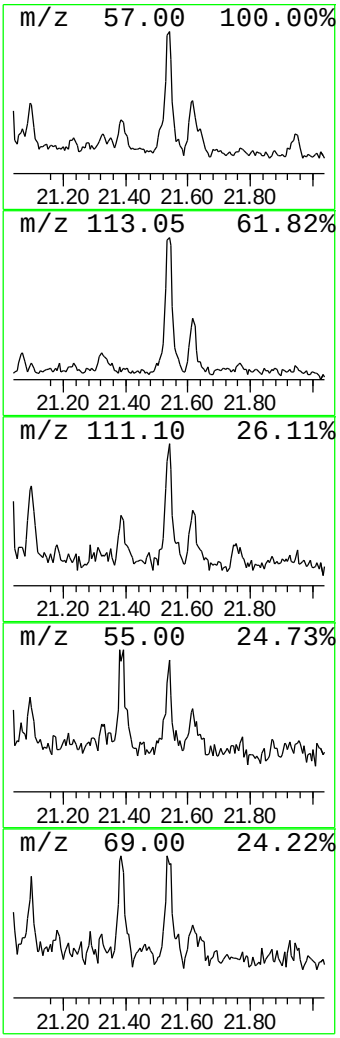
****

Peak Number 7 unknown21.54 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.54	2.16 ng	86600	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	38
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
3	2-Propyn-1-ol, 3-(trimethylsilyl)-	128	C6H12OSi	005272-36-6	27
4	Acetamide, 2-(4-methyl-1-piperaz...	267	C13H18ClN3O	296245-55-1	27
5	6,9-Epoxy-2H,6H-pyrimido[2,1-b][...	226	C9H10N2O5	022329-20-0	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019977.D
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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
unknown5.19	5.19	7.3	ng	82967	1	8.11	225886	20.0
unknown7.64	7.64	96.3	ng	1087680	1	8.11	225886	20.0
n-Hexadecanoic acid	18.35	3.0	ng	94709	4	17.48	639008	20.0
Tetradecanoic acid	19.62	2.8	ng	112144	5	21.76	800461	20.0
unknown21.03	21.03	2.1	ng	82378	5	21.76	800461	20.0
unknown21.54	21.54	2.2	ng	86600	5	21.76	800461	20.0