LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

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-BF081715.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	3.244	105	110	114	rBV	1327886	2661227	100.00%	17.061%
2	4.719	236	239	249	rBV	554358	741603	27.87%	4.755%
3	5.176	276	279	281	rBV	1087446	1163661	43.73%	7.460%
4	6.250	370	373	375	rBV	1330676	1292313	48.56%	8.285%
5	6.365	381	383	386	rBV	1021038	1100785	41.36%	7.057%
6	6.605	401	404	406	rBV	502289	412496	15.50%	2.645%
7	6.765	415	418	420	rBV	620803	777671	29.22%	4.986%
8	7.176	451	454	456	rBV	785452	828338	31.13%	5.311%
9	7.896	514	517	519	rBV	366253	505307	18.99%	3.240%
10	8.970	608	611	613	rBV	1481498	1282745	48.20%	8.224%
11	9.371	644	646	648	rBV	184920	205278	7.71%	1.316%
12	9.633	667	669	672	rBB	683572	579469	21.77%	3.715%
13	10.422	735	738	740	rBV2	552062	766134	28.79%	4.912%
14	11.108	795	798	800	rBV	678487	607353	22.82%	3.894%
15	12.537	920	923	924	rBV	108675	115838	4.35%	0.743%
16	12.582	924	927	932	rVV2	118820	203120	7.63%	1.302%
17	12.685	934	936	939	rBV	908953	970102	36.45%	6.219%
18	13.234	982	984	986	rBV	105706	91989	3.46%	0.590%
19	13.279	986	988	989	rBV	32826	28409	1.07%	0.182%
20	13.611	1015	1017	1024	rBV	65437	141390	5.31%	0.906%
21	13.725	1024	1027	1029	rVV	386903	416613	15.65%	2.671%
22	13.920	1042	1044	1051	rVB	35956	36746	1.38%	0.236%
23	14.228	1069	1071	1072	rBV	27403	30793	1.16%	0.197%
24	14.251	1072	1073	1078	rVB2	13152	29539	1.11%	0.189%
25	14.514	1094	1096	1098	rVB	24689	26859	1.01%	0.172%
26	14.811	1120	1122	1124	rBV	31307	37393	1.41%	0.240%
27	15.063	1142	1144	1147	rVV	267972	349868	13.15%	2.243%
28	15.485	1179	1181	1185	rVB	27336	40271	1.51%	0.258%
29	15.600	1185	1191	1193	rVV4	13260	40775	1.53%	0.261%
30	16.811	1293	1297	1307	rVV6	12092	50178	1.89%	0.322%
31	17.611	1364	1367	1374	rVB5	10262	33803	1.27%	0.217%
32	18.434	1435	1439	1445	rVB7	8332	29817	1.12%	0.191%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2A(0-2)-1

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-BF081715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

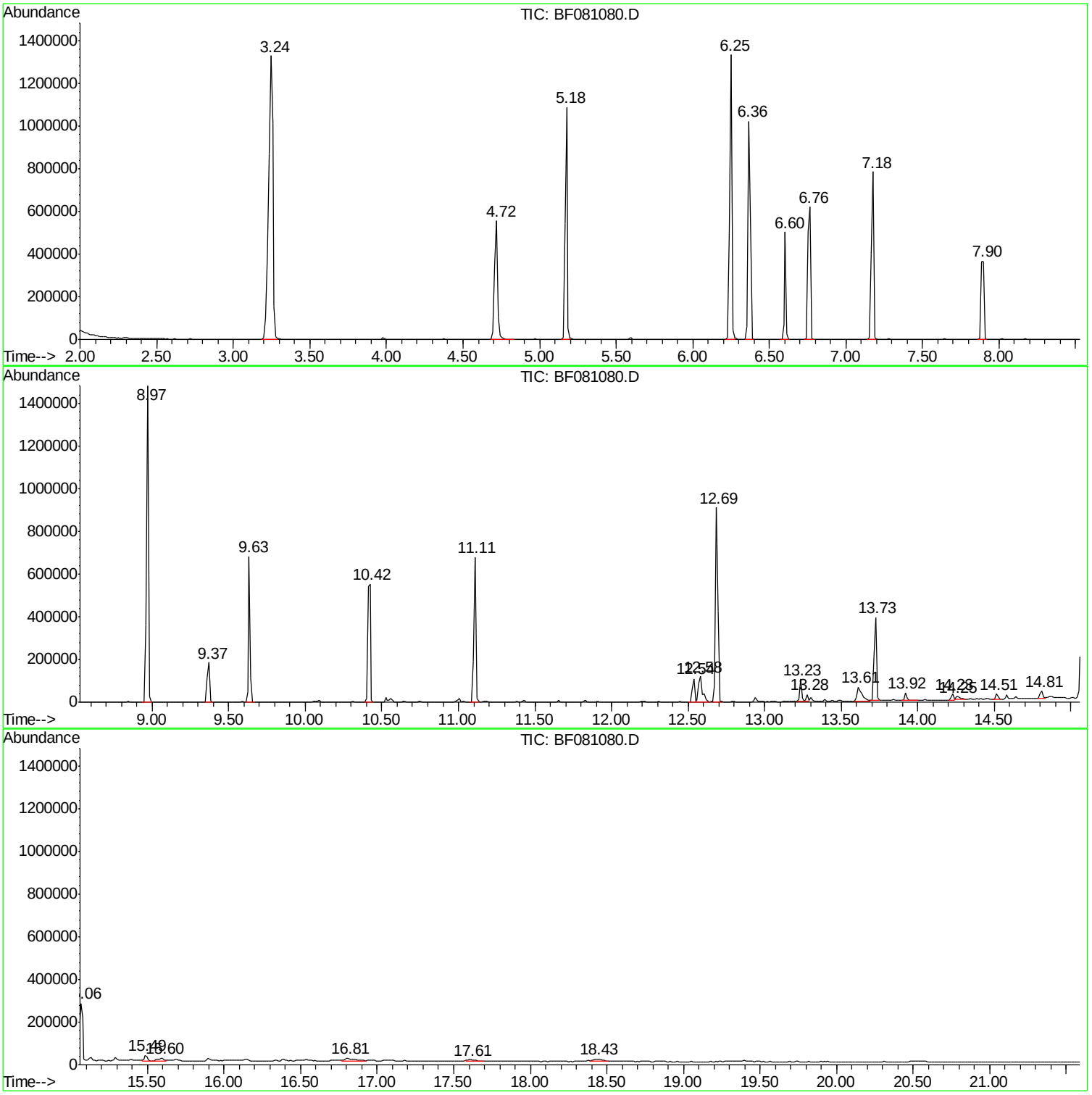
Sum of corrected areas: 15597883

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

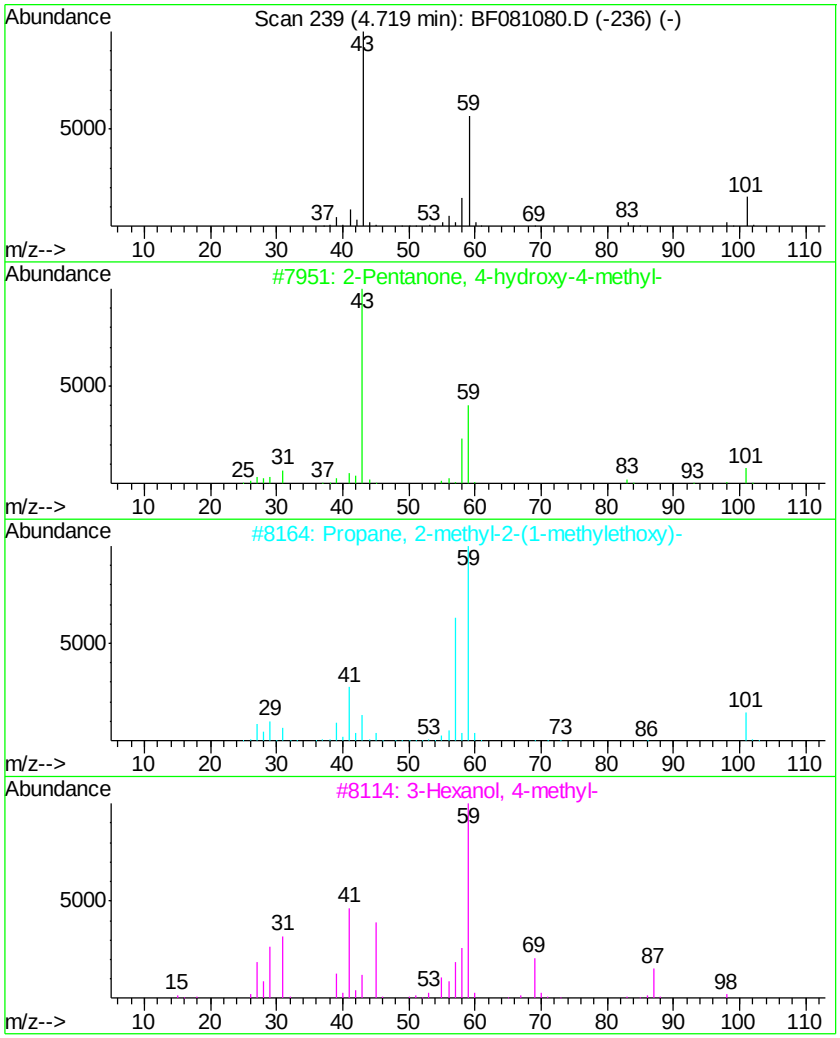
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

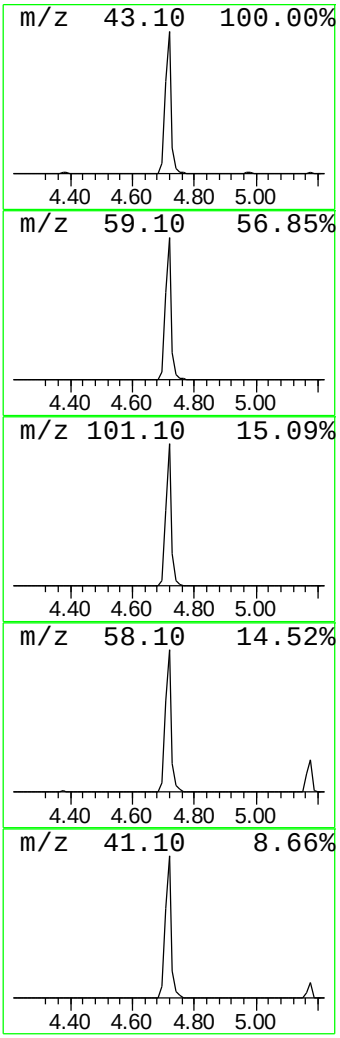
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	35.96 ng	741603	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

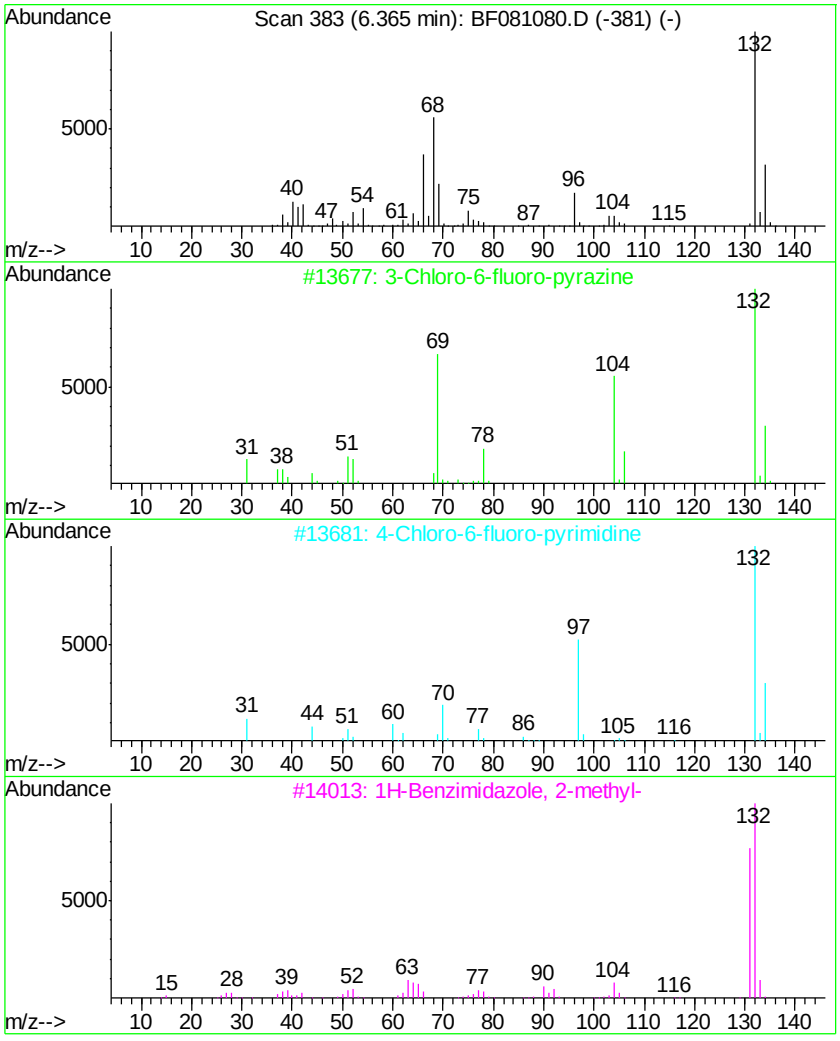
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

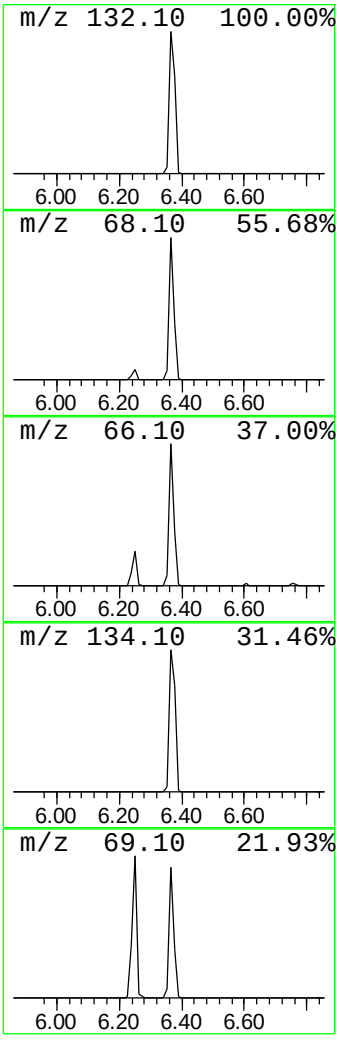
****

Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	53.37 ng	1100790	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

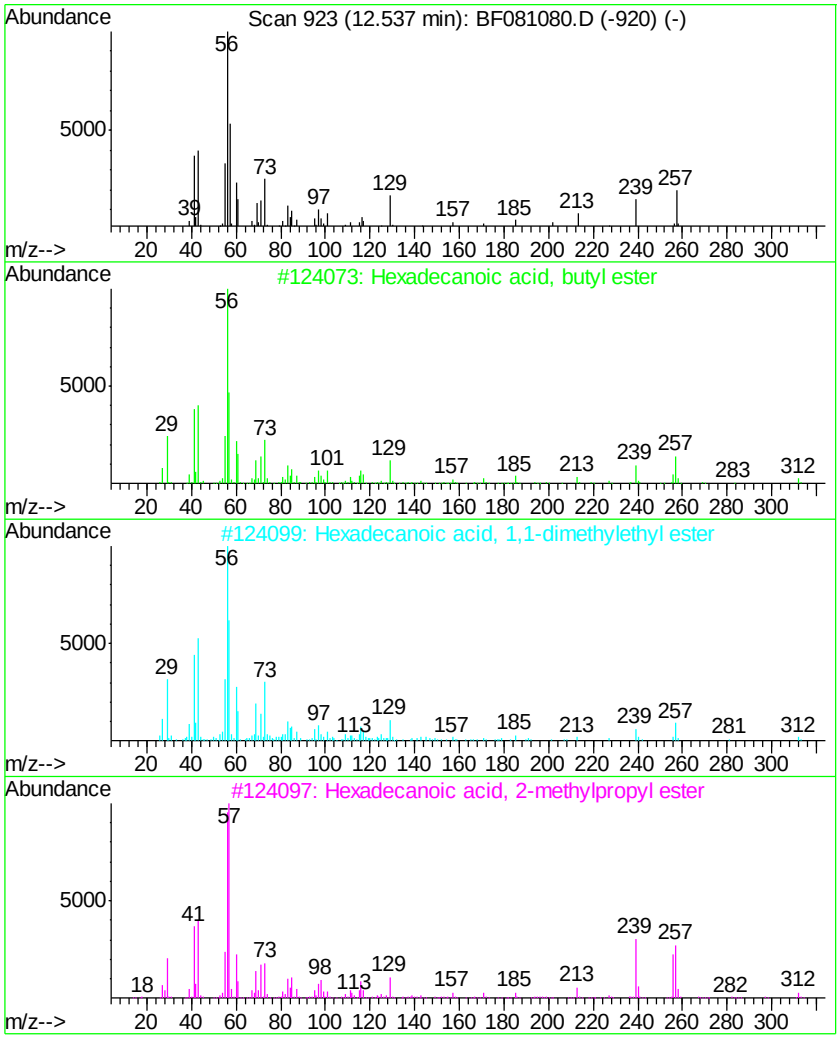
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

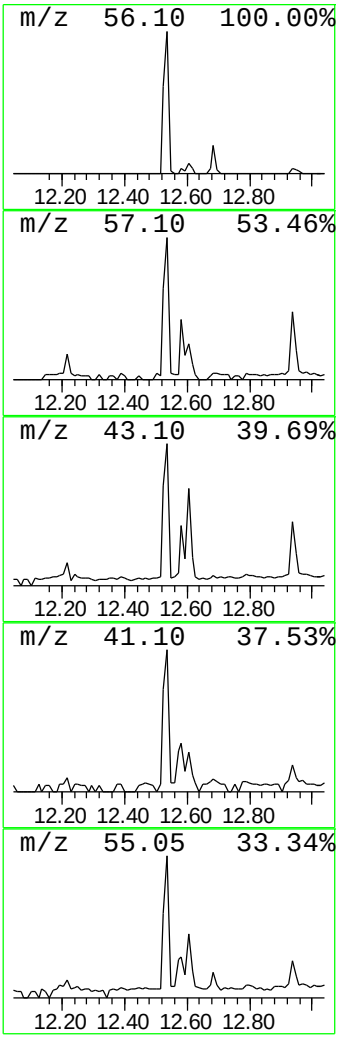
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	5.56 ng	115838	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	37
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

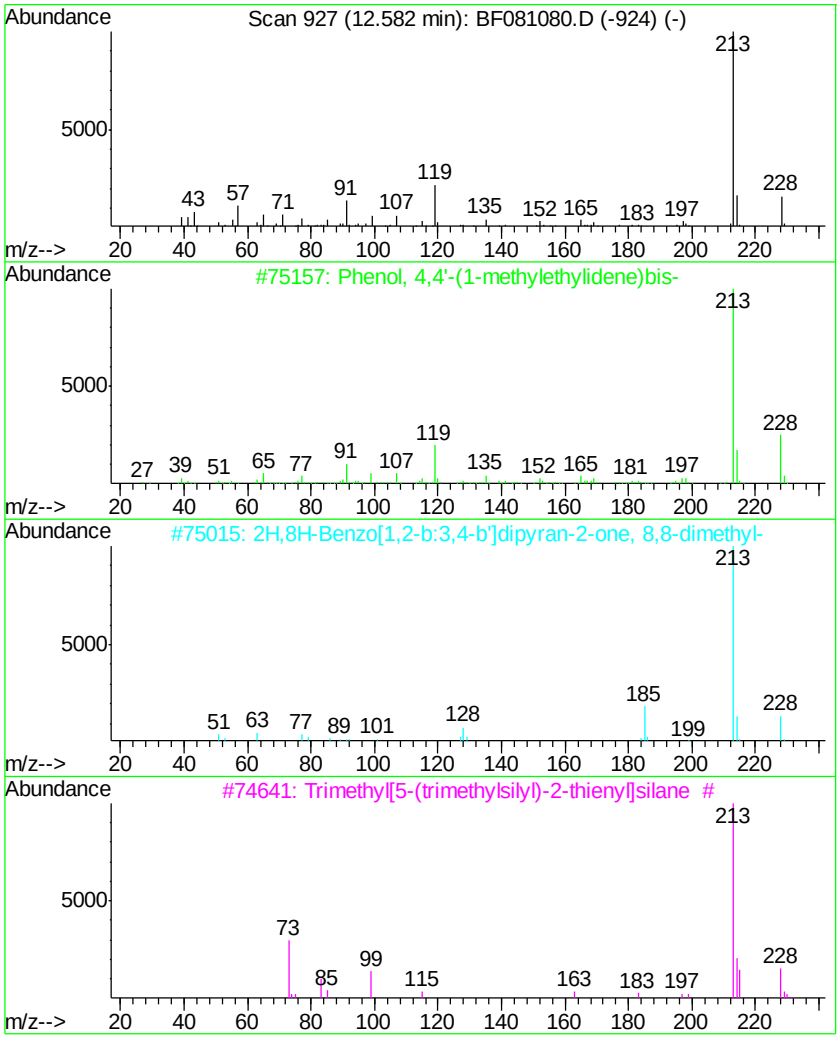
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

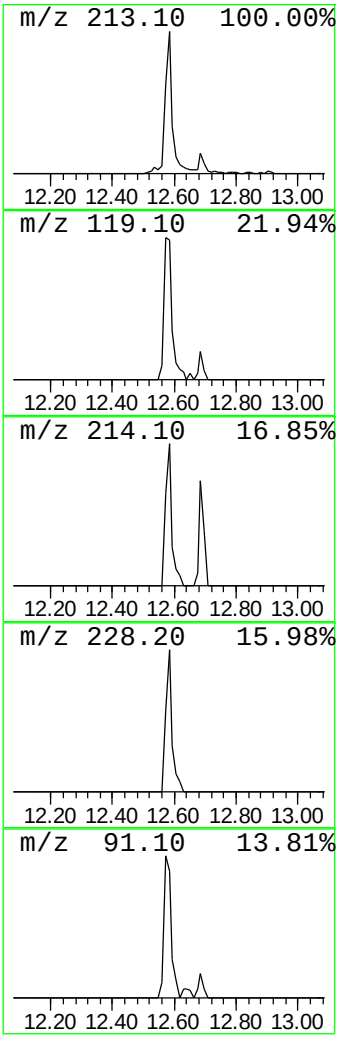
****

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	9.75 ng	203120	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	53
4	4-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-45-0	50
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	42





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

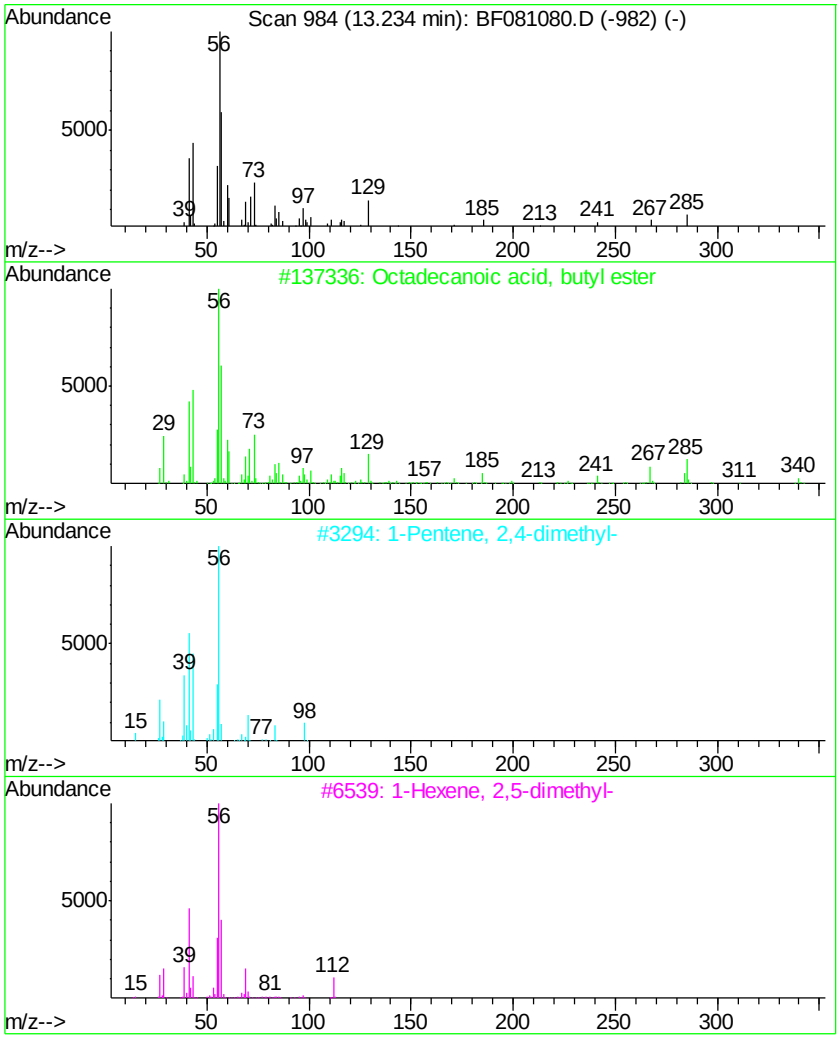
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

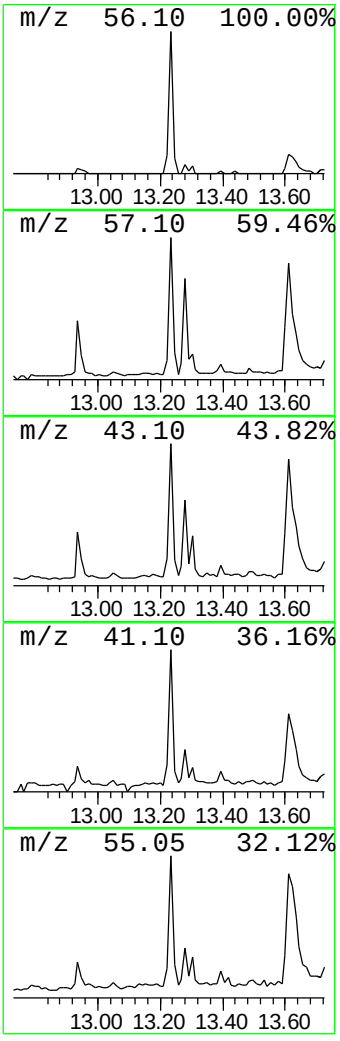
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	4.42 ng	91989	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
4	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
5	Undecane, 5-methylene-	168	C12H24	005698-48-6	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

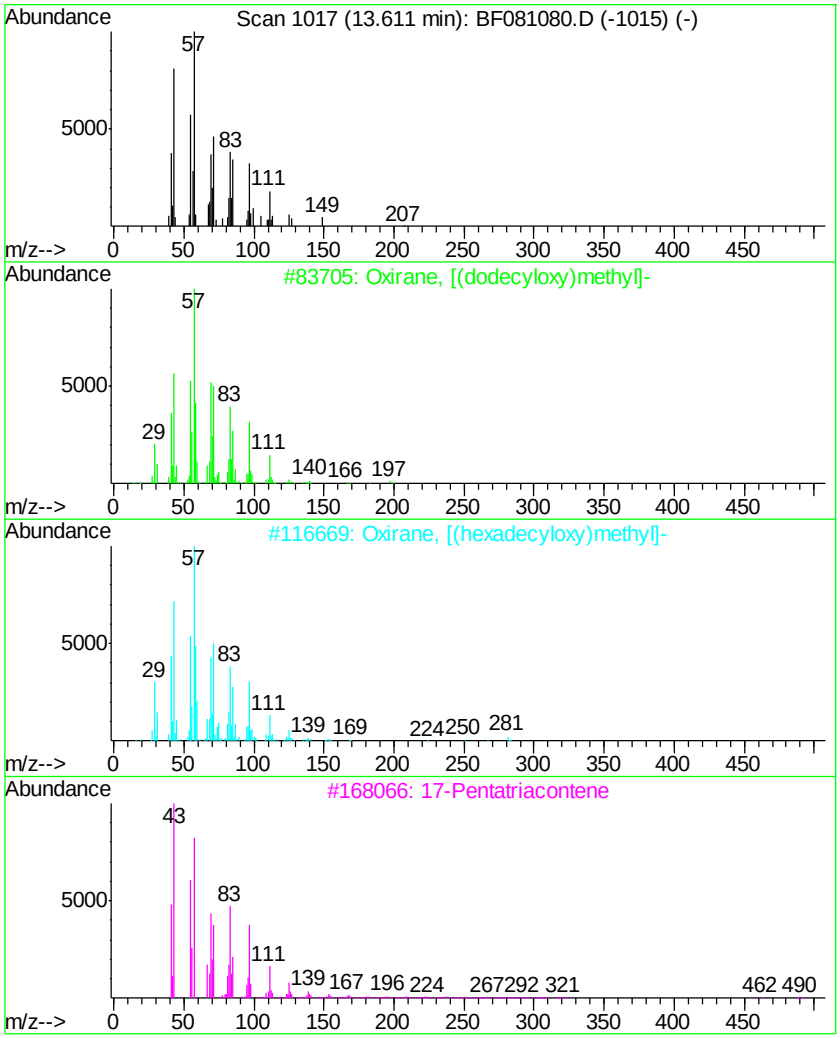
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

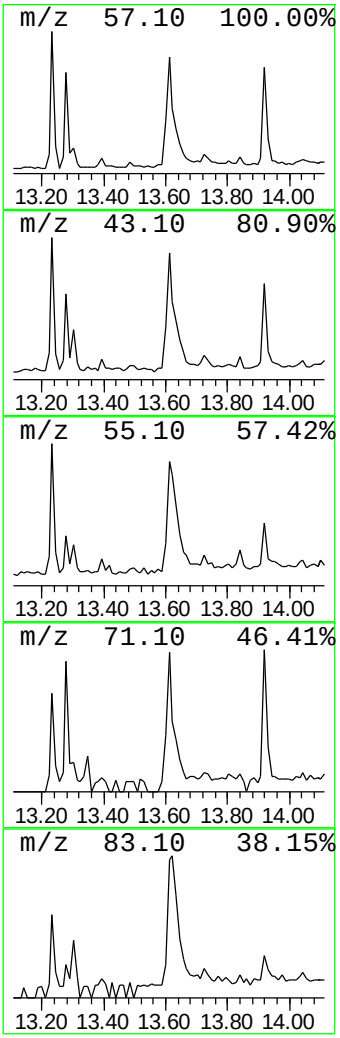
****

Peak Number 8 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	6.79 ng	141390	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	86
2	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	80
3	17-Pentatriacontene	491	C35H70	006971-40-0	64
4	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	64
5	1-Tetracosanol	354	C24H50O	000506-51-4	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

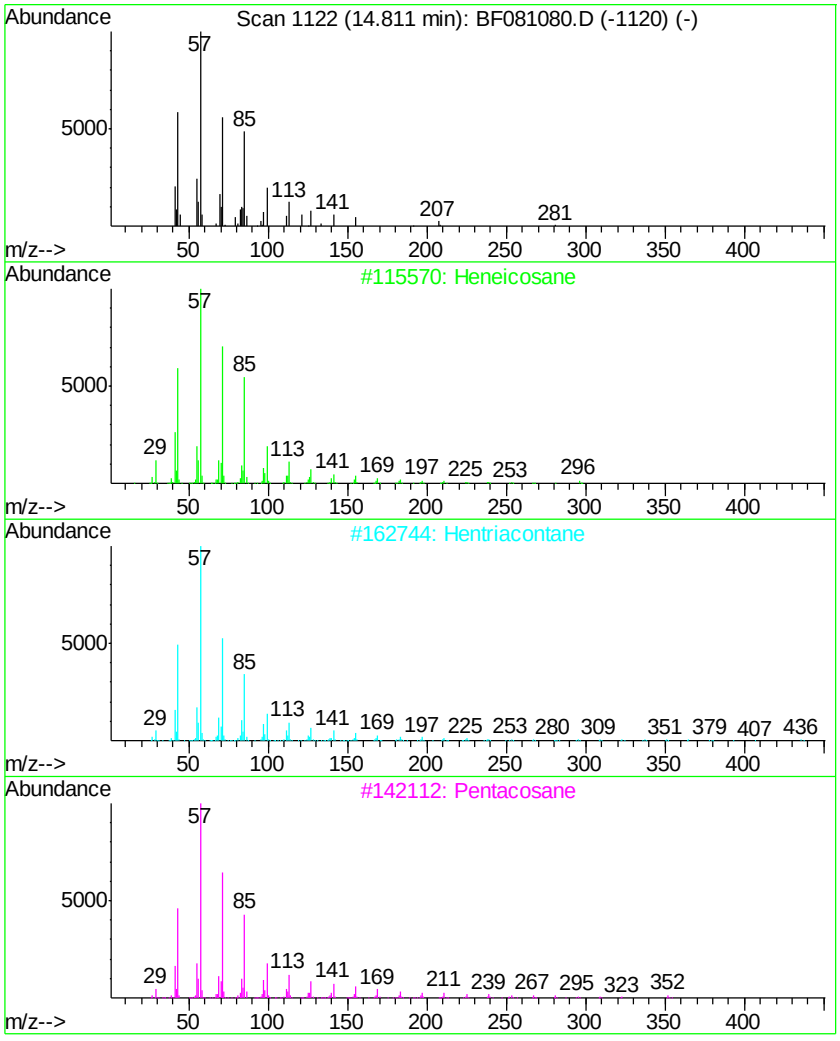
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

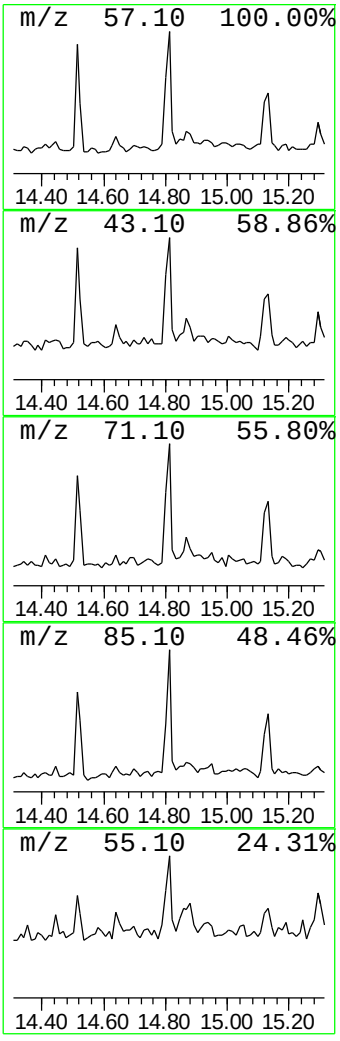
****

Peak Number 9 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.14 ng	37393	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Pentacosane	352	C25H52	000629-99-2	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Hexacosane	366	C26H54	000630-01-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

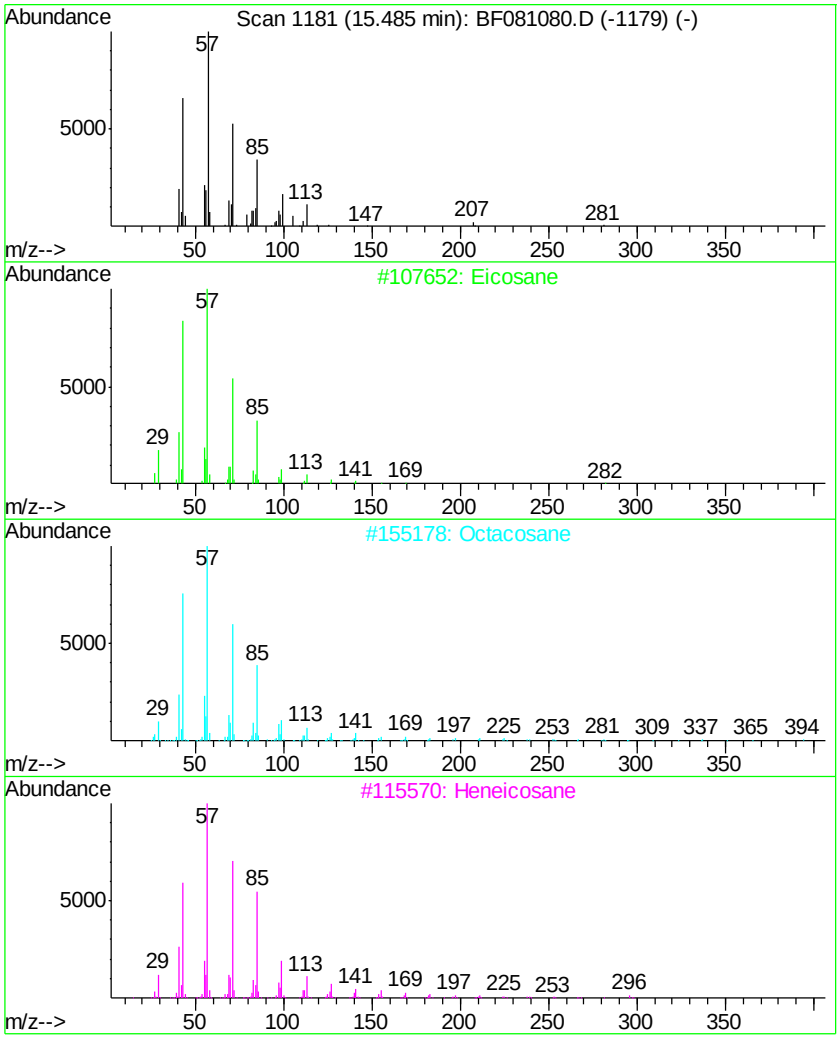
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

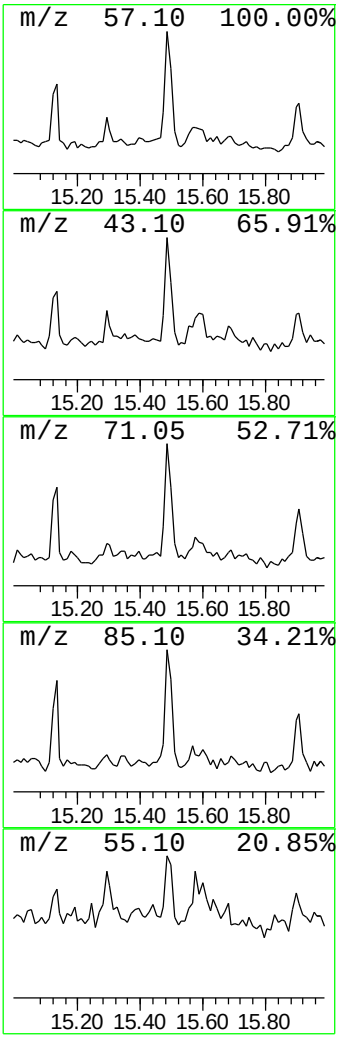
****

Peak Number 10 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	2.30 ng	40271	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Heptadecane	240	C17H36	000629-78-7	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081080.D
Acq On : 19 Aug 2015 12:12
Operator : UM/IZ
Sample : G3290-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2A(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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...	4.72	36.0	ng	741603	1	6.60	412496	20.0
unknown6.36	6.36	53.4	ng	1100790	1	6.60	412496	20.0
Hexadecanoic acid...	12.54	5.6	ng	115838	5	13.73	416613	20.0
Phenol, 4,4'-(1-m...	12.58	9.8	ng	203120	5	13.73	416613	20.0
Octadecanoic acid...	13.23	4.4	ng	91989	5	13.73	416613	20.0
Oxirane, [(dodecy...	13.61	6.8	ng	141390	5	13.73	416613	20.0
Heneicosane	14.81	2.1	ng	37393	6	15.06	349868	20.0
Eicosane	15.49	2.3	ng	40271	6	15.06	349868	20.0