LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

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-BF051716.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	1.701	8	10	55	rVB	2883317	6201649	100.00%	13.634%
2	4.684	269	271	294	rBV	266603	612054	9.87%	1.346%
3	5.142	308	311	332	rBV	3792812	4370415	70.47%	9.608%
4	6.227	403	406	408	rBV	4056337	4544437	73.28%	9.991%
5	6.330	413	415	417	rBV	4532104	4641651	74.85%	10.205%
6	6.559	433	435	441	rVB	657780	861340	13.89%	1.894%
7	6.707	446	448	451	rBV	3229598	2952545	47.61%	6.491%
8	7.130	483	485	488	rBV	2550048	2659598	42.89%	5.847%
9	7.839	545	547	550	rBV	1050584	1158300	18.68%	2.547%
10	8.925	639	642	644	rBV	4357204	4647531	74.94%	10.218%
11	9.325	675	677	679	rBV	562136	494873	7.98%	1.088%
12	9.531	693	695	697	rBV	133892	134598	2.17%	0.296%
13	9.588	697	700	702	rBV	1511771	1372223	22.13%	3.017%
14	10.033	736	739	740	rBV	222435	200786	3.24%	0.441%
15	10.251	755	758	761	rBV	69906	111209	1.79%	0.244%
16	10.376	766	769	772	rBV	2642754	2657496	42.85%	5.842%
17	10.502	777	780	787	rVB	225215	286906	4.63%	0.631%
18	11.062	827	829	832	rBV	1412515	1338274	21.58%	2.942%
19	12.651	965	968	970	rBV	3939422	4046730	65.25%	8.897%
20	13.611	1048	1052	1057	rBV2	58775	227860	3.67%	0.501%
21	13.691	1057	1059	1066	rVB	1168806	1151568	18.57%	2.532%
22	15.040	1175	1177	1186	rBV	671595	813773	13.12%	1.789%

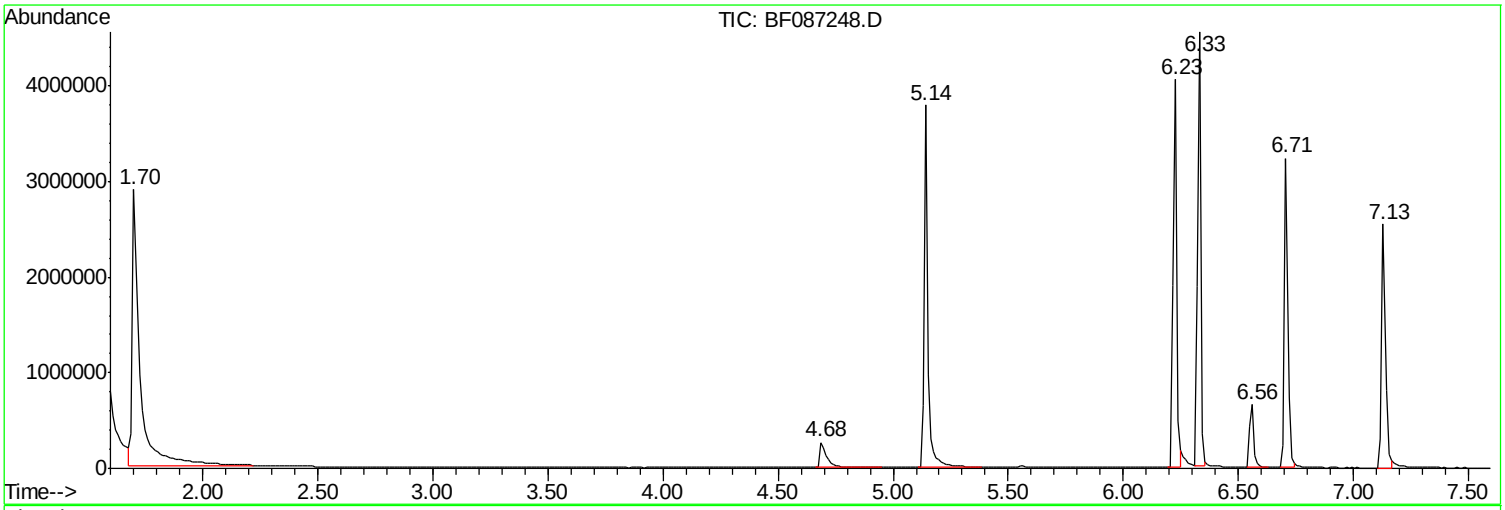
Sum of corrected areas: 45485816

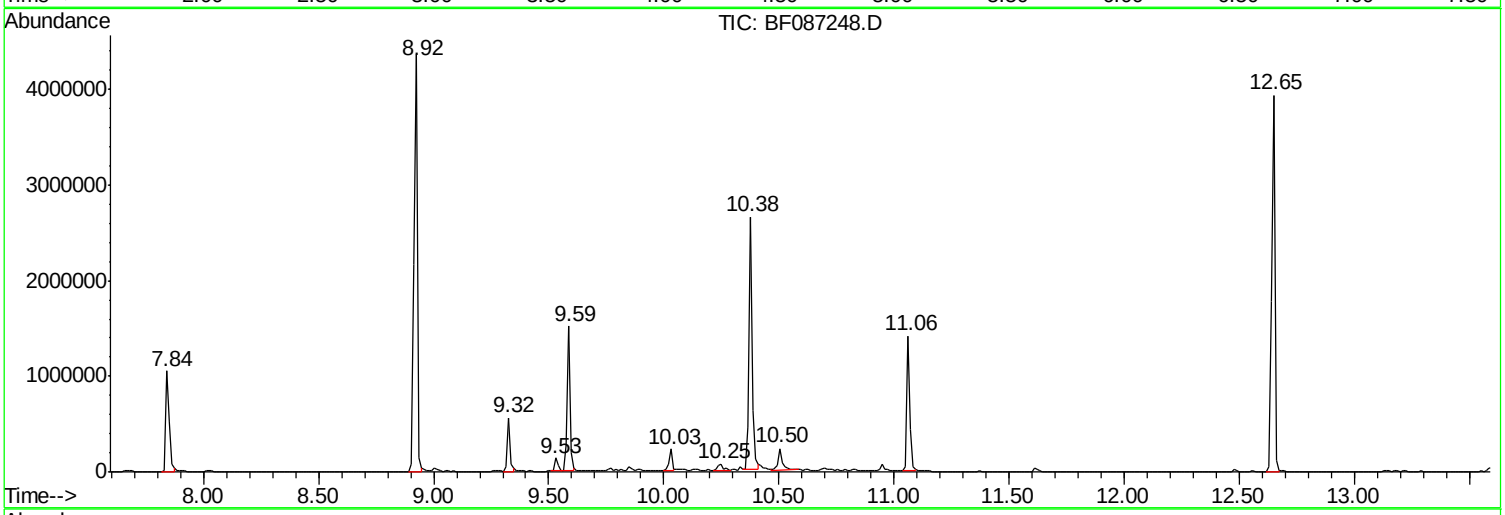
Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

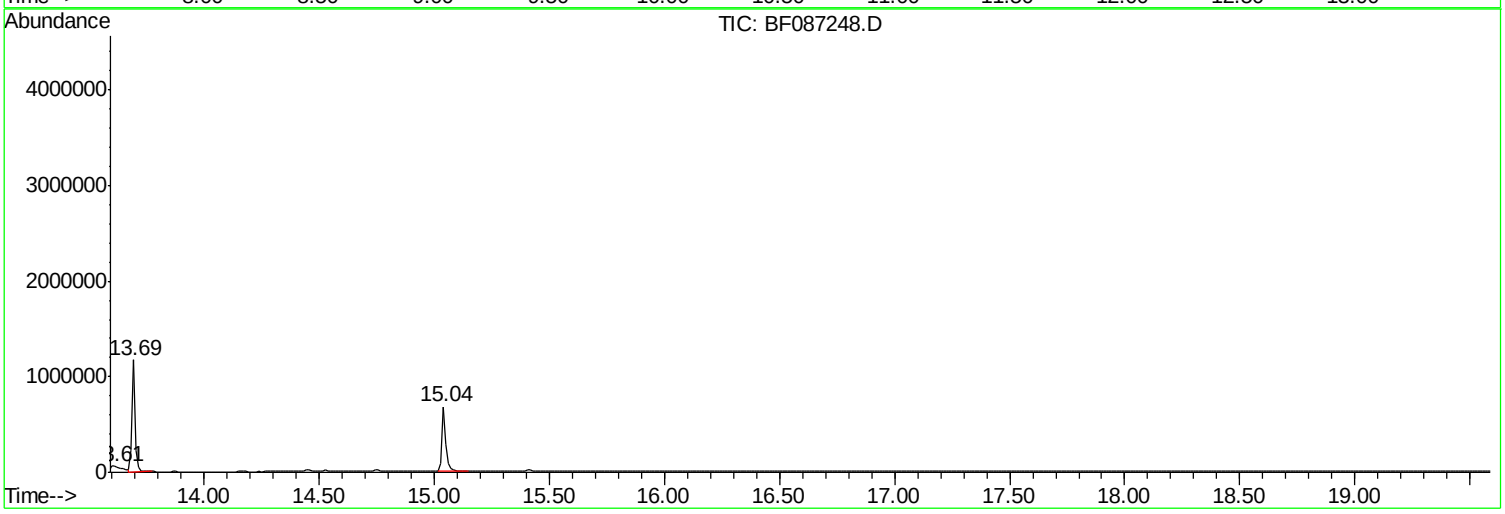
Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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 F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

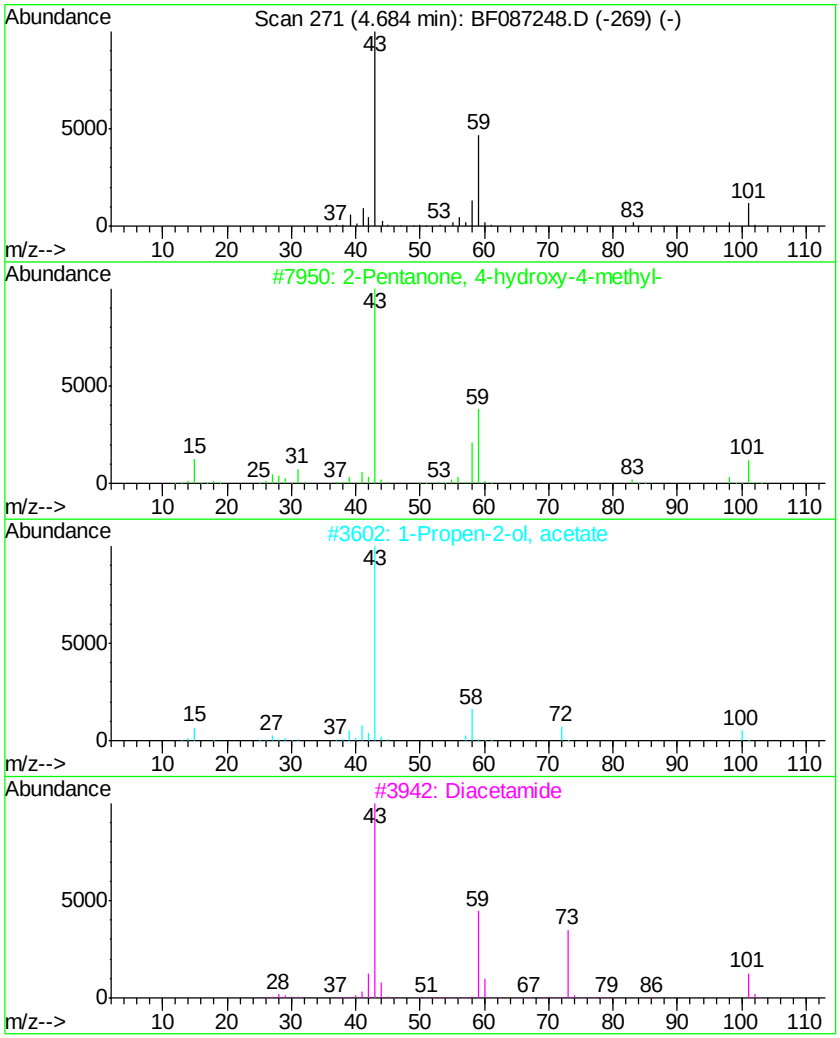
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

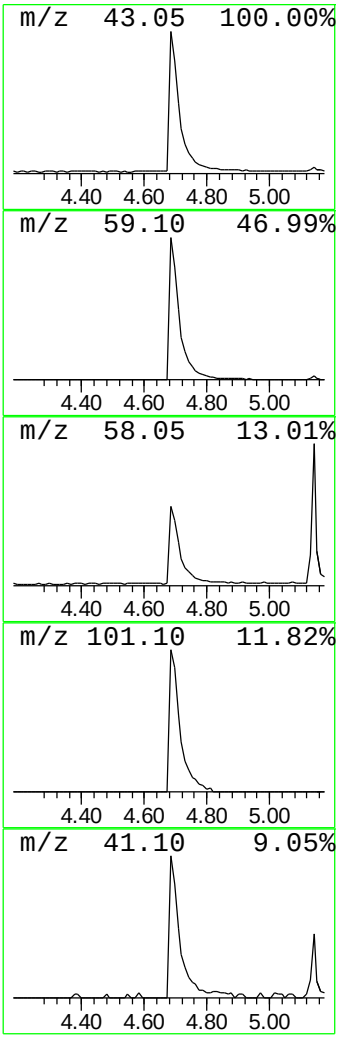
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	14.21 ng	612054	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

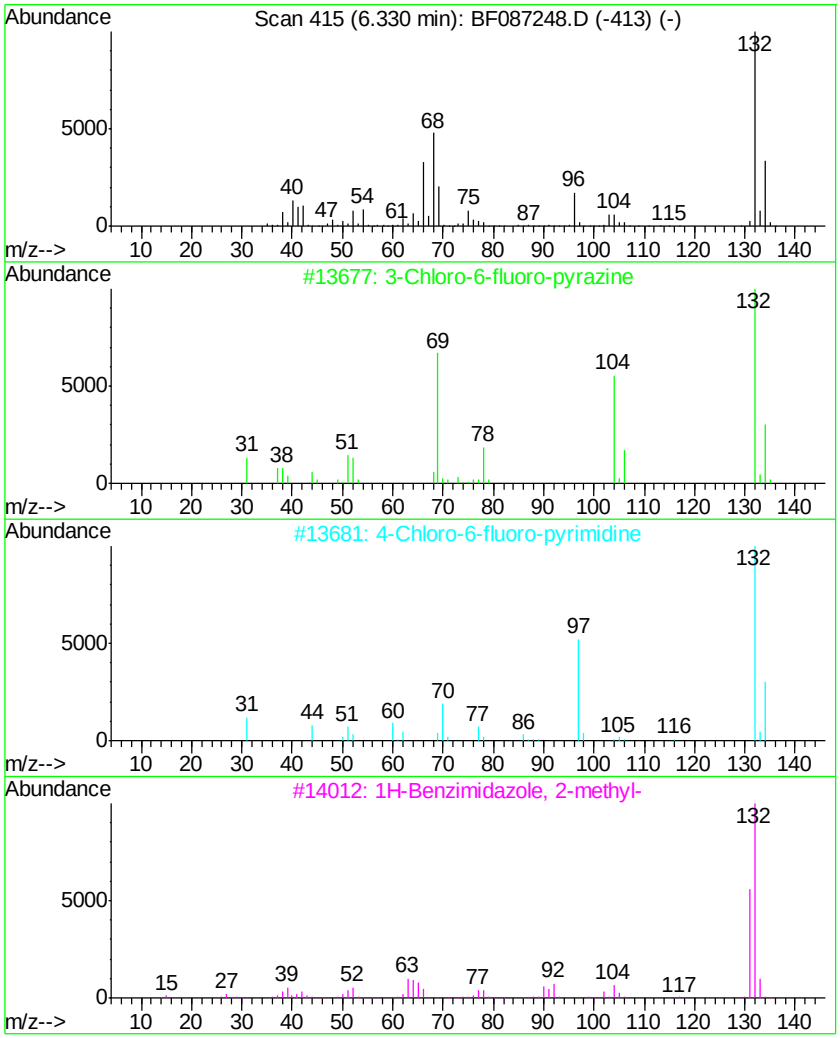
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

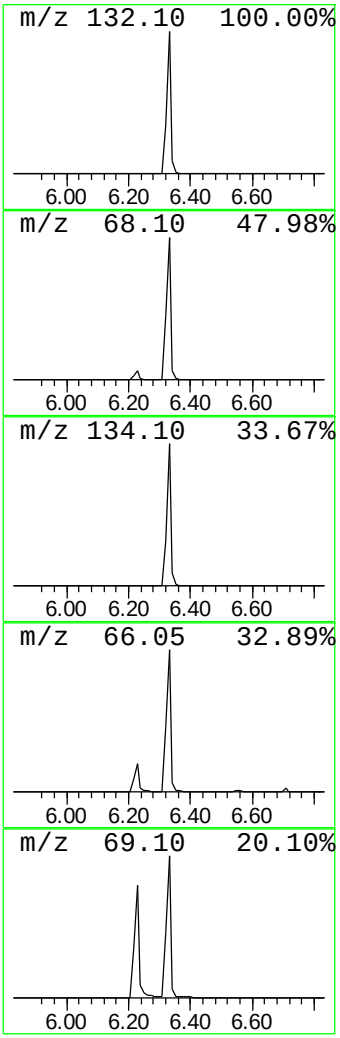
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	107.78 ng	4641650	1,4-Dichlorobenzene-d4	6.56

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	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

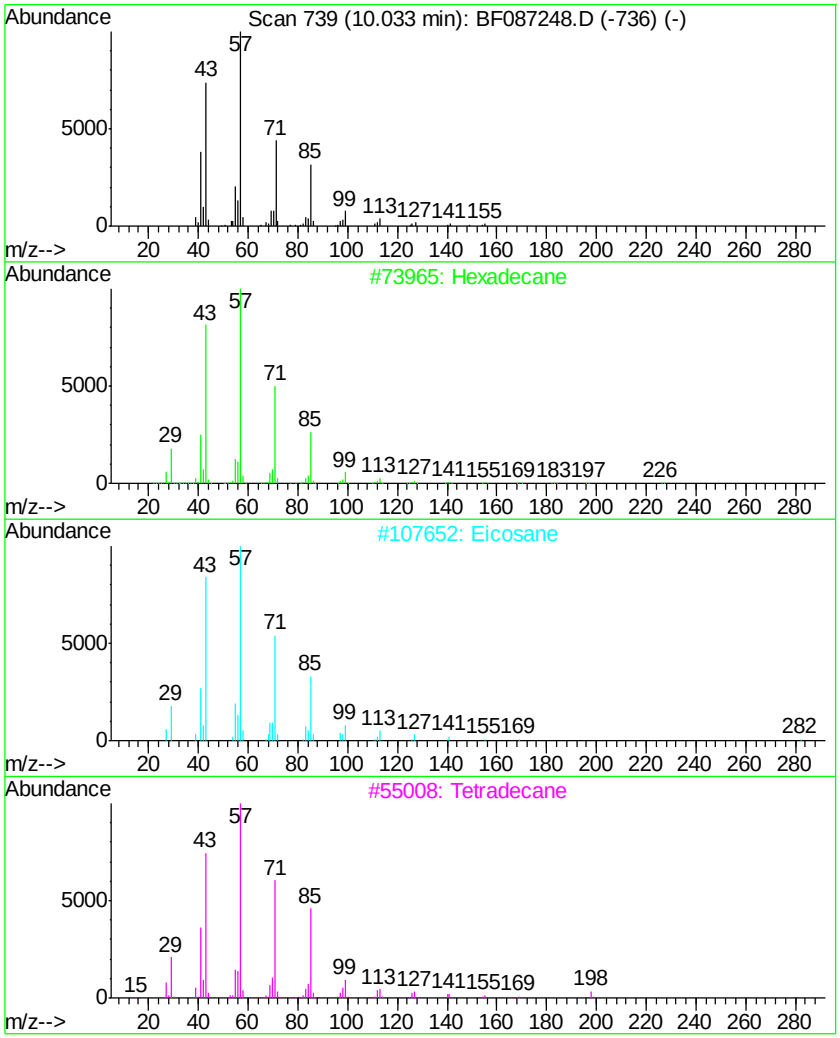
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

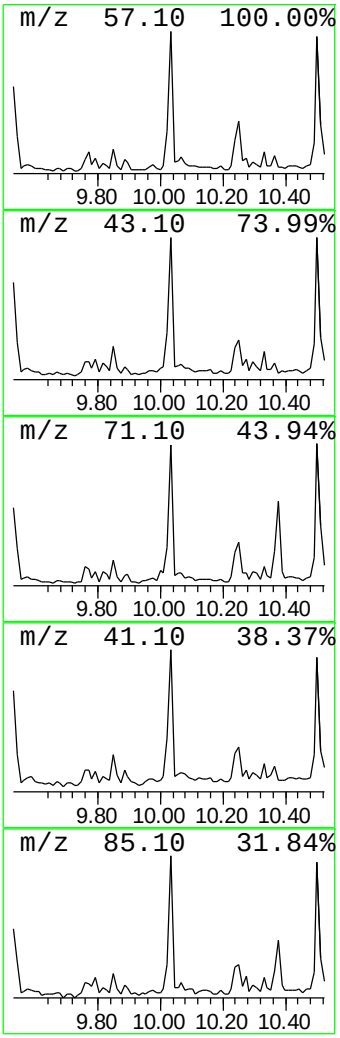
****

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.93 ng	200786	Acenaphthene-d10	9.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	87
3	Tetradecane	198	C14H30	000629-59-4	83
4	Decane, 3-bromo-	220	C10H21Br	030571-71-2	80
5	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

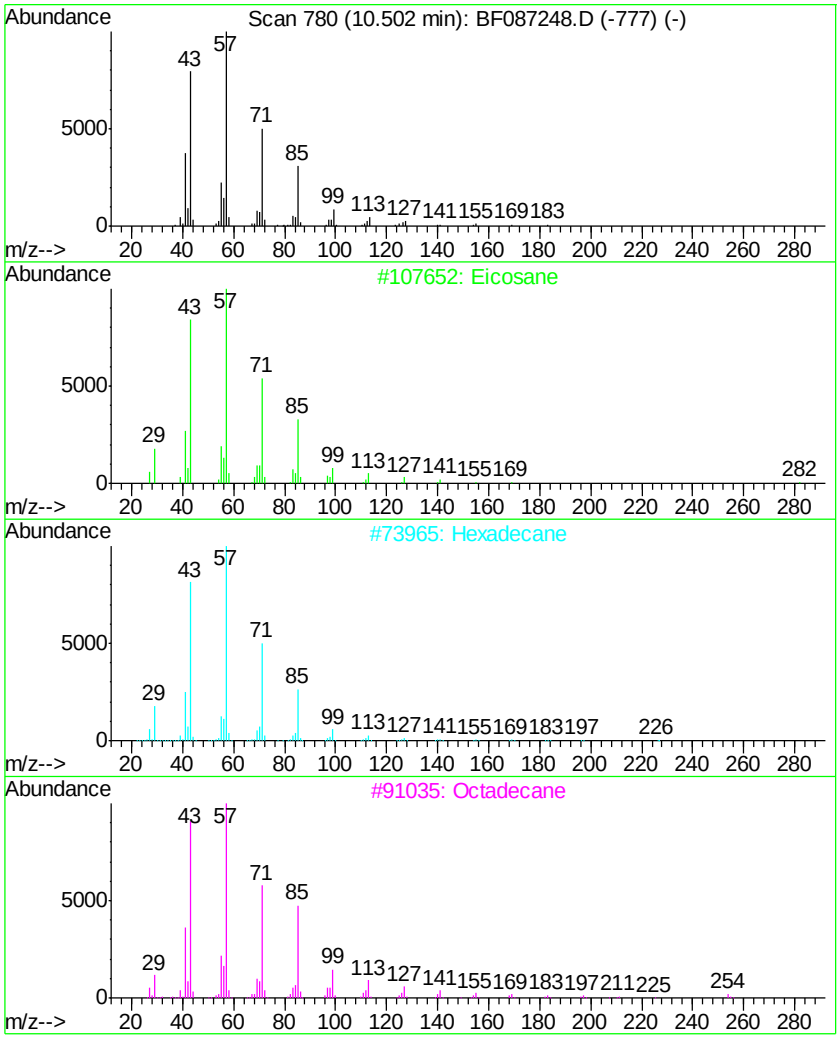
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

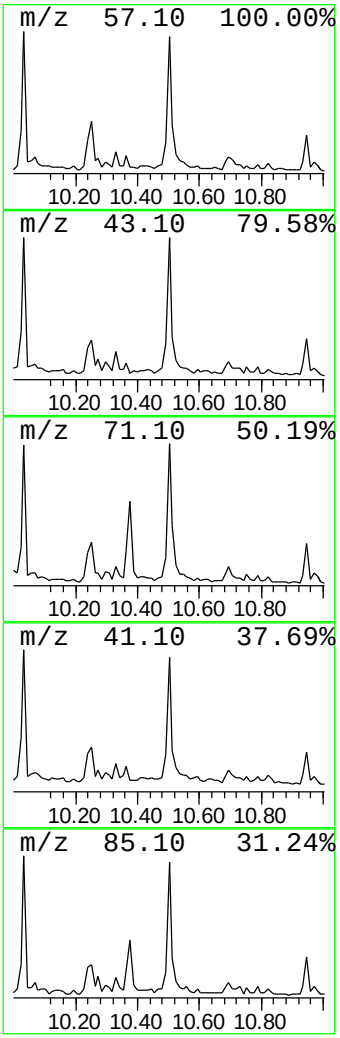
****

Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	4.29 ng	286906	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Octadecane	254	C18H38	000593-45-3	86
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

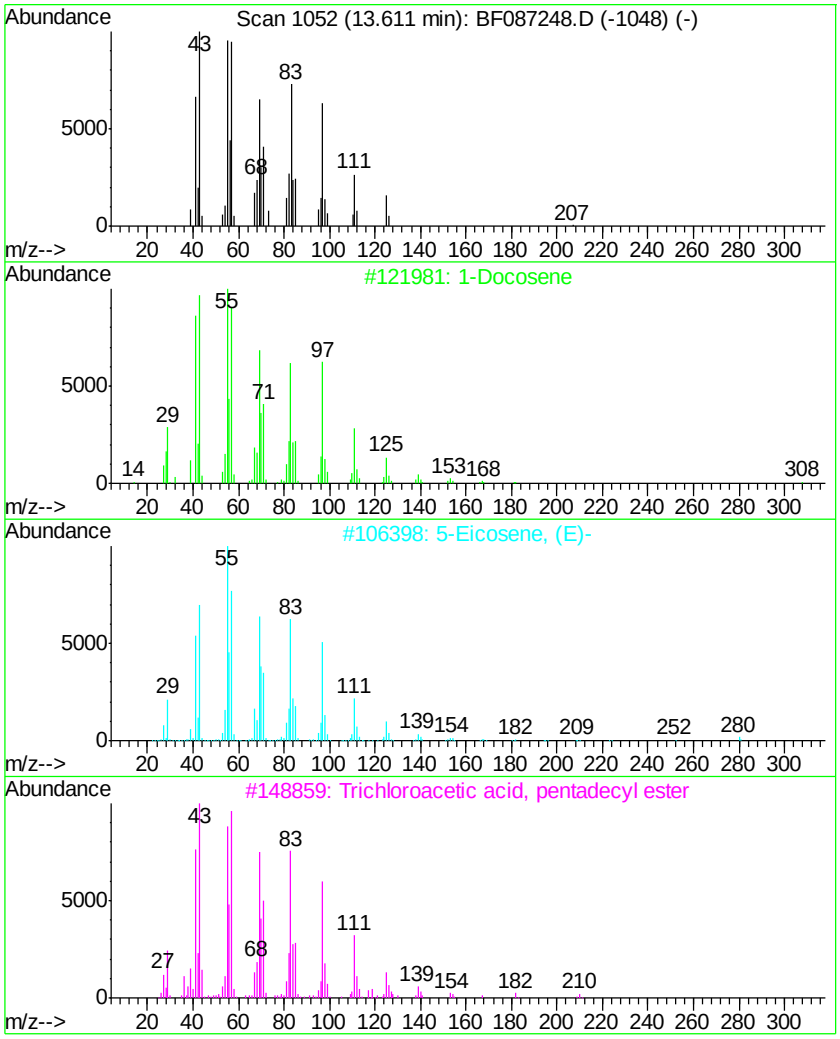
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

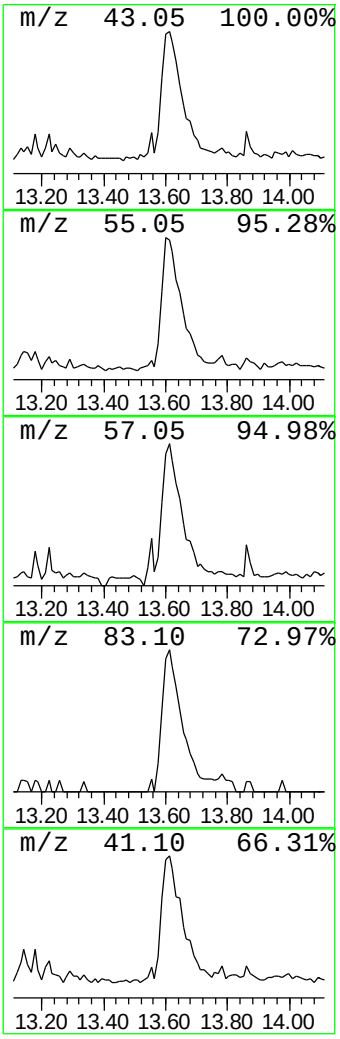
****

Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	3.96 ng	227860	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	1-Tetracosanol	354	C24H50O	000506-51-4	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087248.D
Acq On : 21 May 2016 2:48
Operator : UM/SJ
Sample : H3144-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
9-AB-AC(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	14.2	ng	612054	1	6.56	861340	20.0
unknown6.33	6.33	107.8	ng	4641650	1	6.56	861340	20.0
Hexadecane	10.03	2.9	ng	200786	3	9.59	1372220	20.0
Eicosane	10.50	4.3	ng	286906	4	11.06	1338270	20.0
1-Docosene	13.61	4.0	ng	227860	5	13.69	1151570	20.0