LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

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-BF103015.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	5.070	257	261	263	rBV	1850403	3068294	49.03%	5.670%
2	5.481	294	297	300	rBV	4851714	5180153	82.78%	9.573%
3	6.510	383	387	389	rBV	5558503	5986477	95.66%	11.063%
4	6.647	396	399	401	rBV	6273459	6257907	100.00%	11.565%
5	6.876	417	419	421	rBV	1471136	1180566	18.87%	2.182%
6	7.036	430	433	435	rBV	4682438	4121599	65.86%	7.617%
7	7.436	465	468	471	rBV	3250157	3597795	57.49%	6.649%
8	8.167	529	532	534	rBV	1219888	1463281	23.38%	2.704%
9	9.242	623	626	628	rBV	5577606	4867325	77.78%	8.995%
10	9.630	658	660	663	rBV	720970	704459	11.26%	1.302%
11	9.916	683	685	688	rBV	1791439	1655874	26.46%	3.060%
12	10.705	751	754	757	rBV	4411064	4298400	68.69%	7.944%
13	10.831	764	765	770	rBV2	55397	125839	2.01%	0.233%
14	11.288	803	805	806	rBV2	89162	82558	1.32%	0.153%
15	11.402	812	815	817	rBV	1902702	1667621	26.65%	3.082%
16	11.471	817	821	823	rVB4	32135	65916	1.05%	0.122%
17	11.711	840	842	844	rBV	79136	69735	1.11%	0.129%
18	11.939	860	862	867	rBV	729107	792286	12.66%	1.464%
19	12.728	929	931	938	rVB	225920	308005	4.92%	0.569%
20	12.991	952	954	957	rVB	4616586	5087938	81.30%	9.403%
21	13.894	1031	1033	1043	rBV	500985	869158	13.89%	1.606%
22	14.042	1043	1046	1048	rBV	1085193	1236772	19.76%	2.286%
23	14.534	1087	1089	1097	rVB3	40196	99513	1.59%	0.184%
24	14.911	1120	1122	1125	rVB	76049	84842	1.36%	0.157%
25	15.482	1169	1172	1175	rBV	832337	1062889	16.98%	1.964%
26	16.020	1217	1219	1223	rBV2	81534	175359	2.80%	0.324%

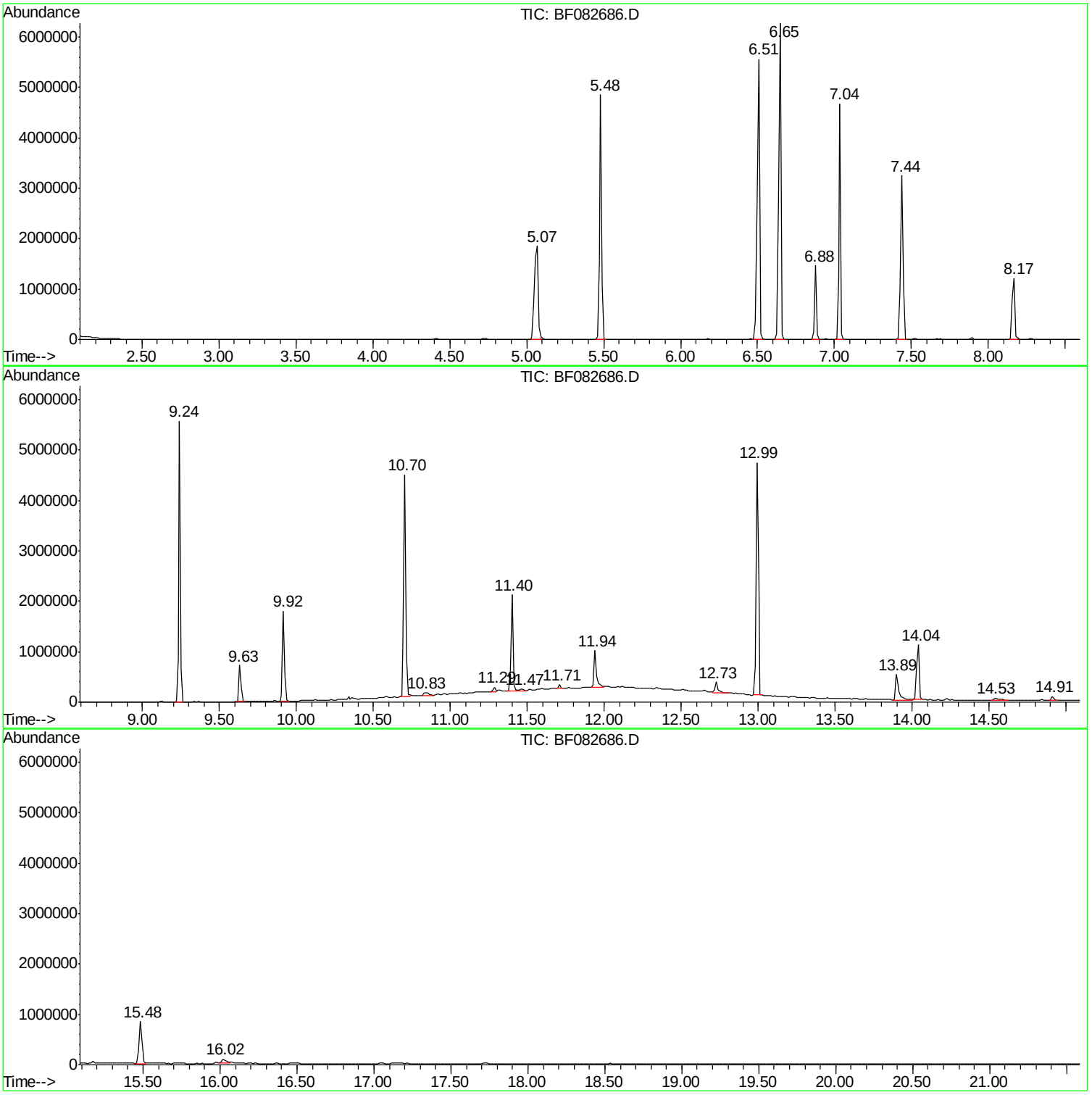
Sum of corrected areas: 54110561

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

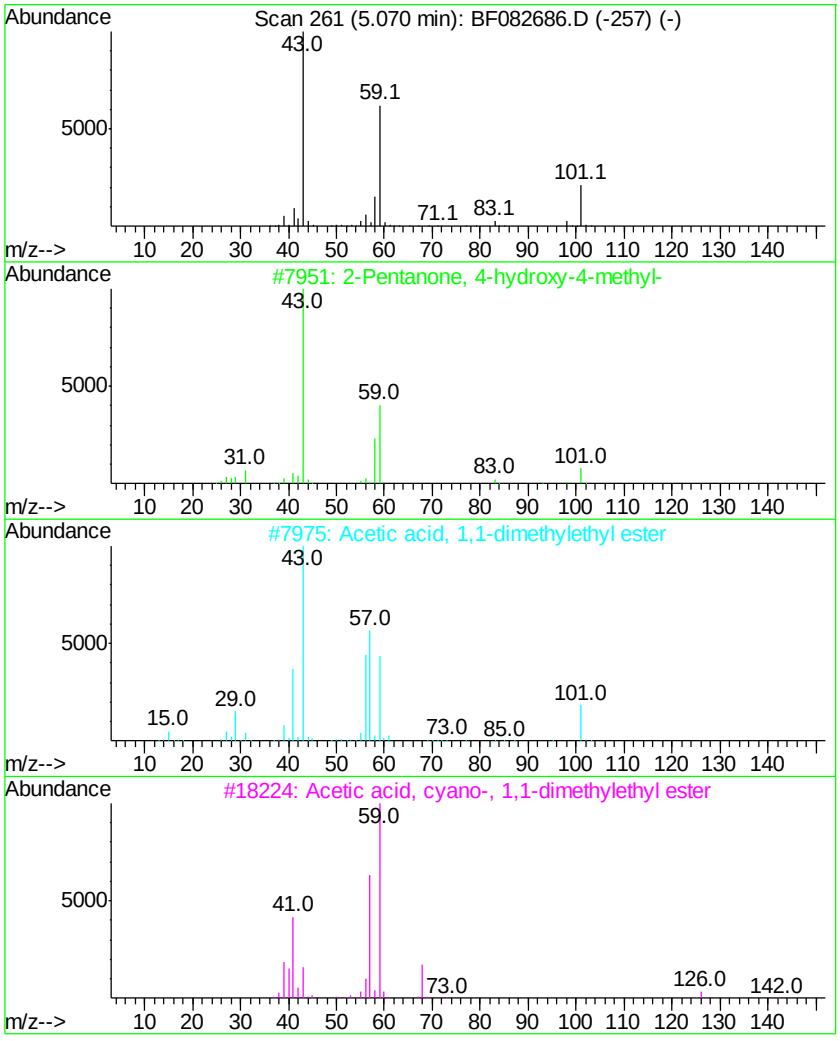
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

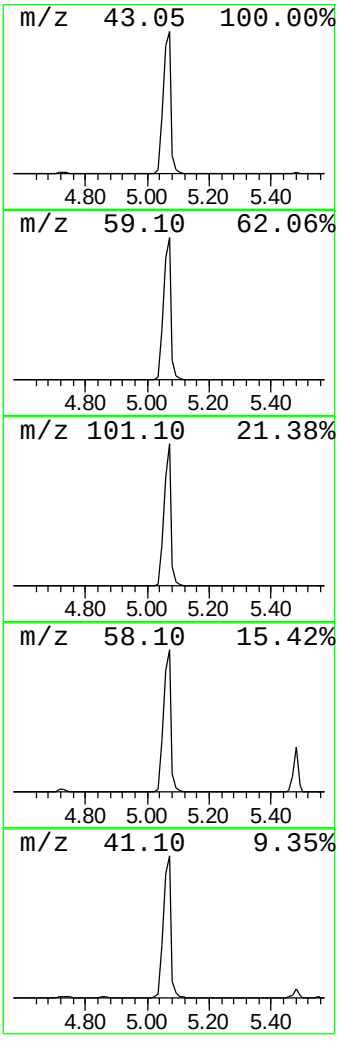
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	51.98 ng	3068290	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

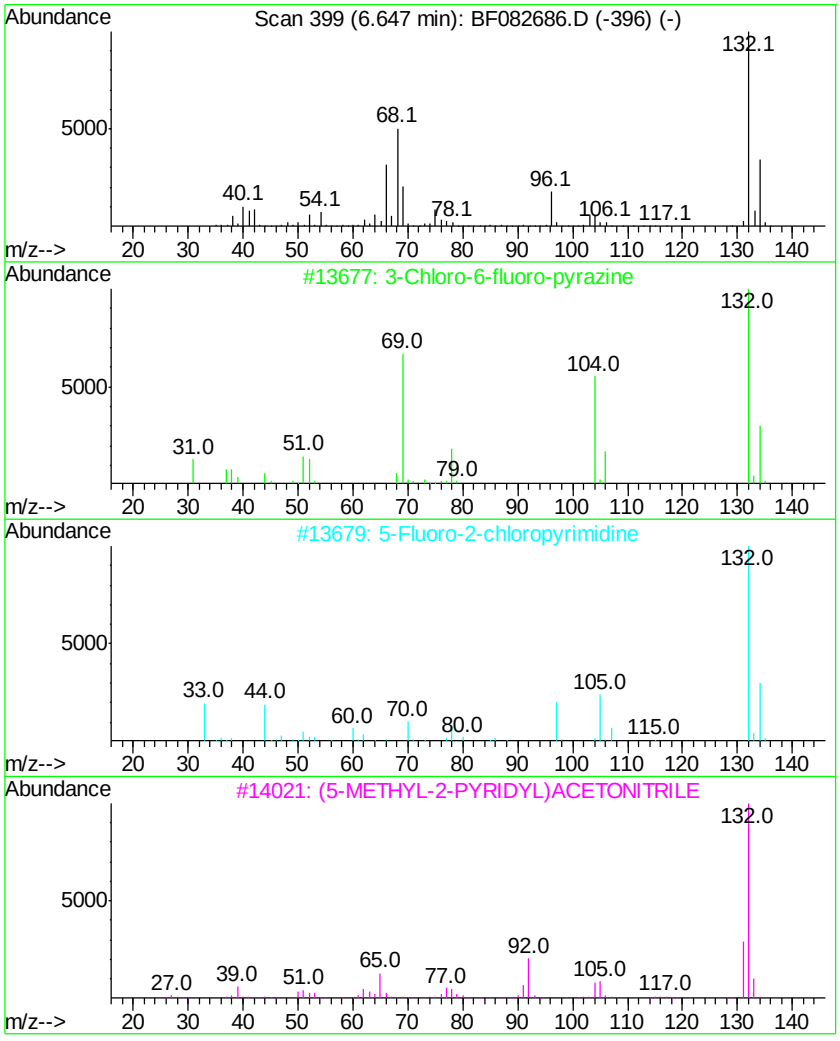
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

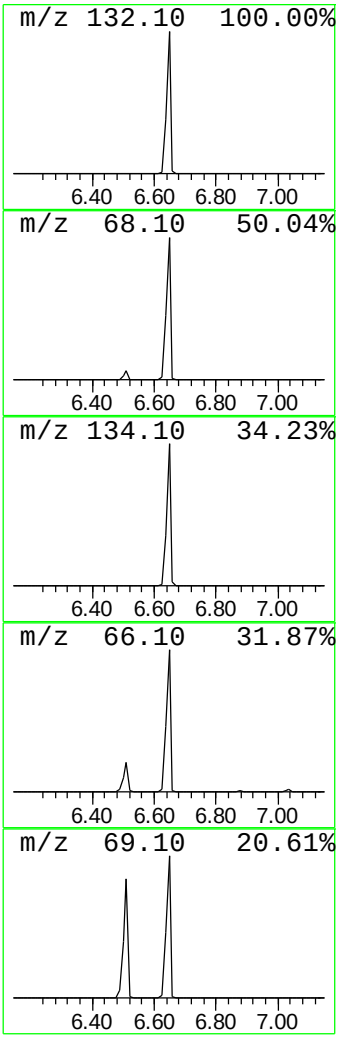
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	106.02 ng	6257910	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

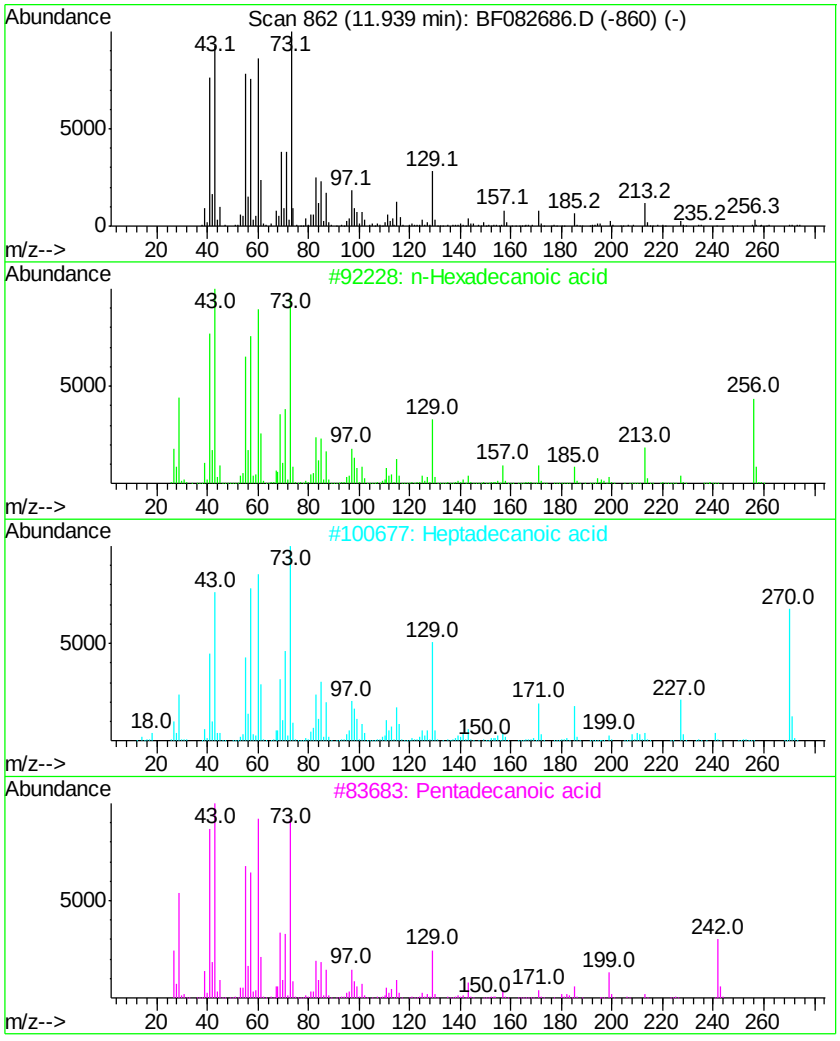
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

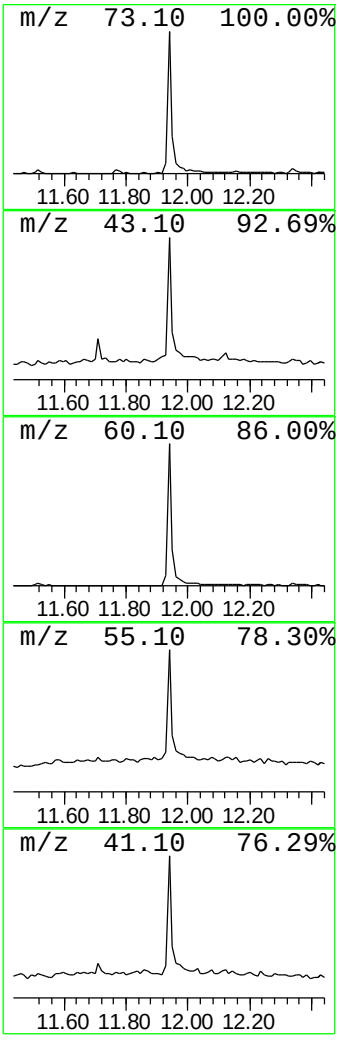
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	9.50 ng	792286	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

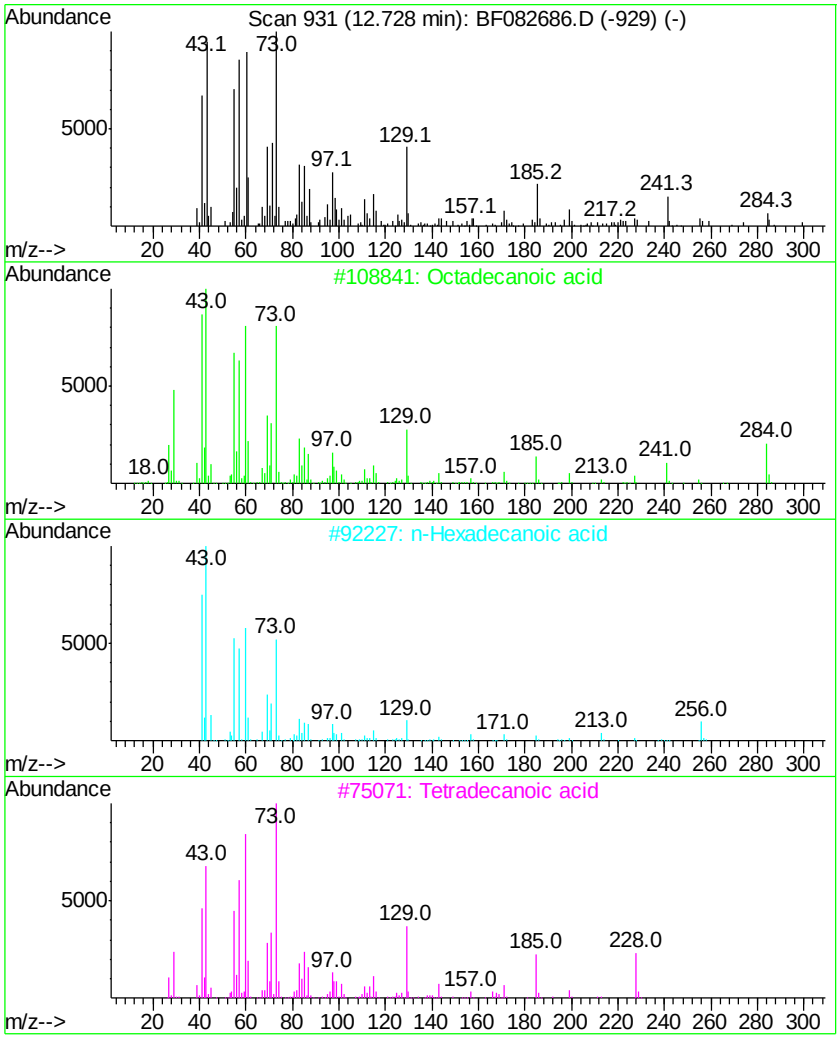
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

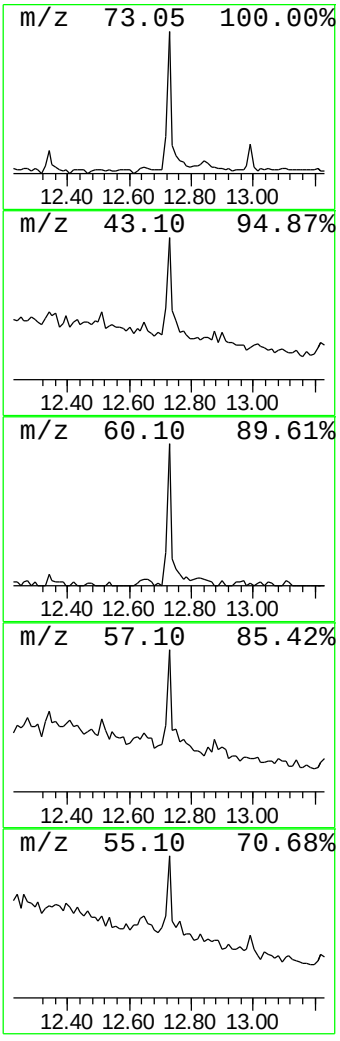
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	4.98 ng	308005	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

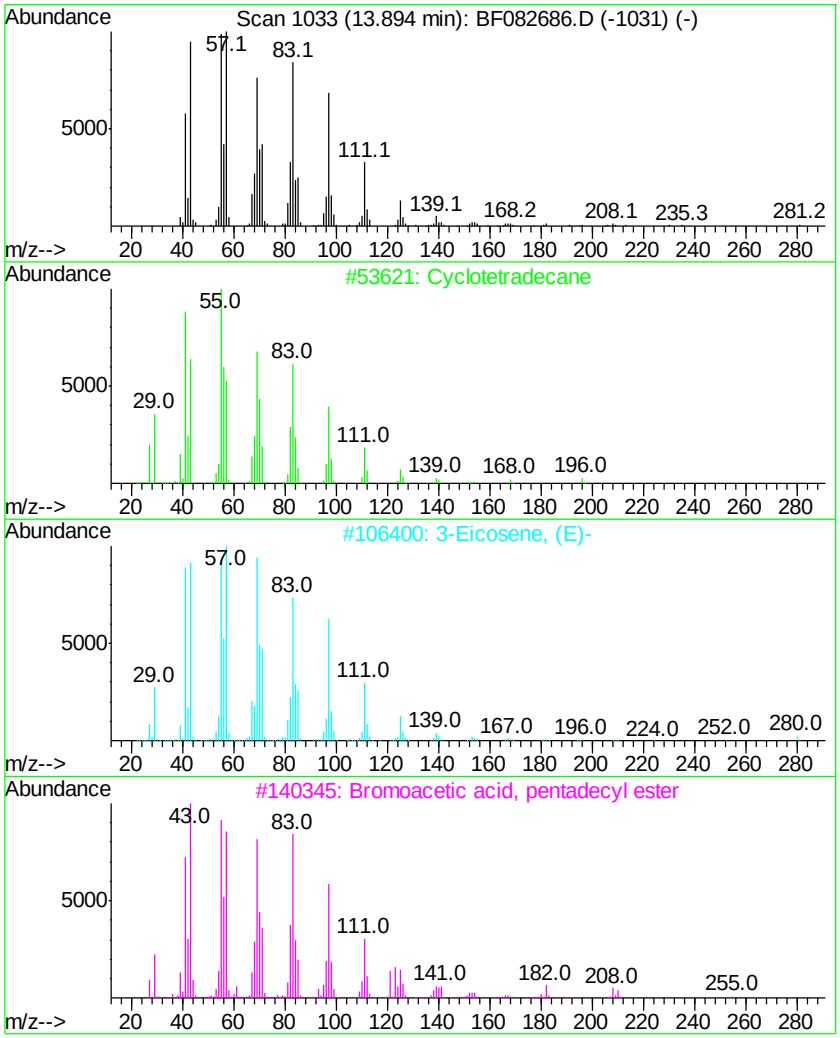
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

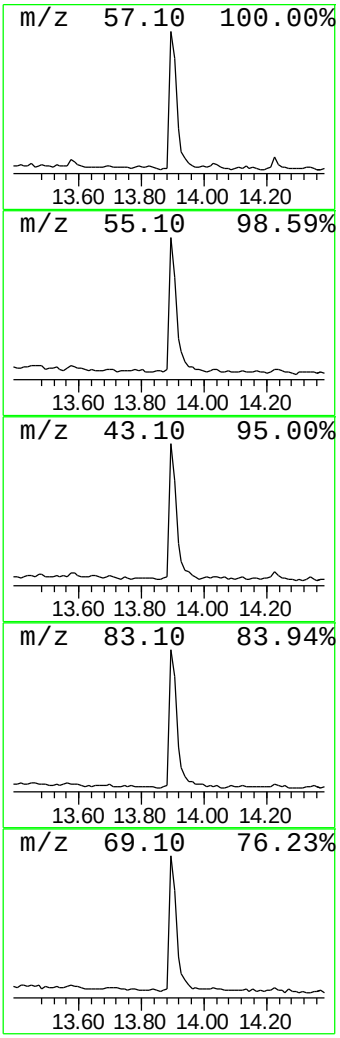
****

Peak Number 6 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	14.06 ng	869158	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

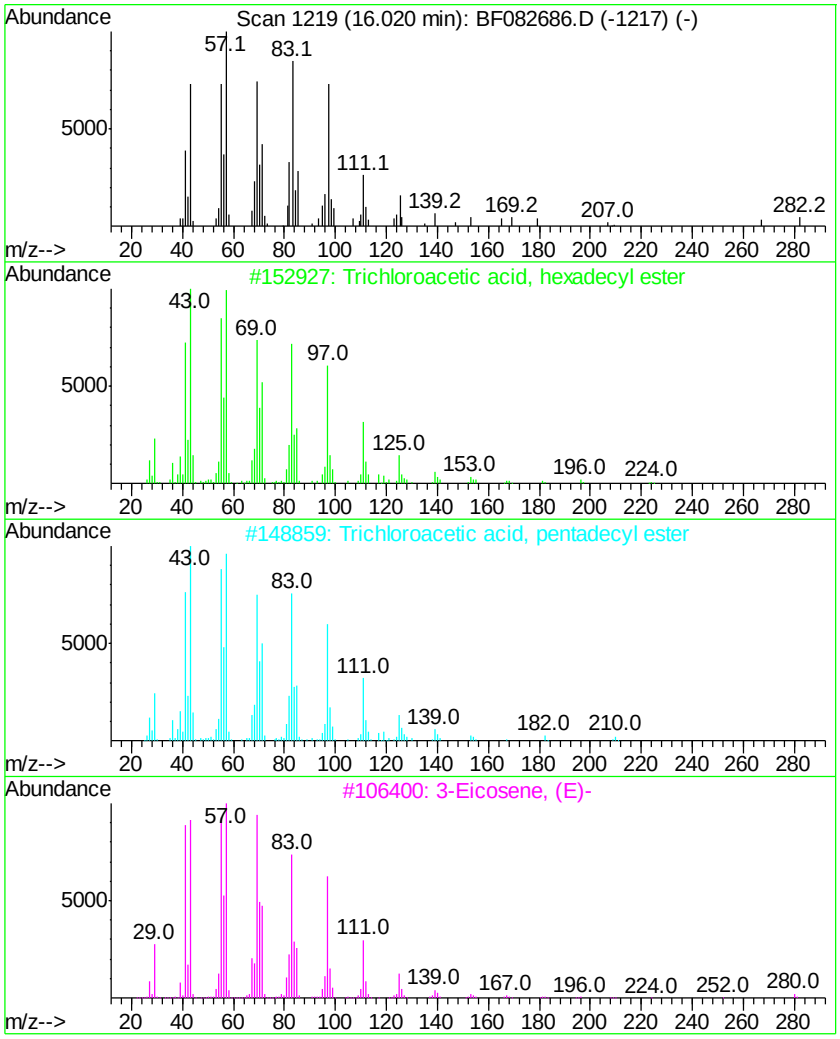
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

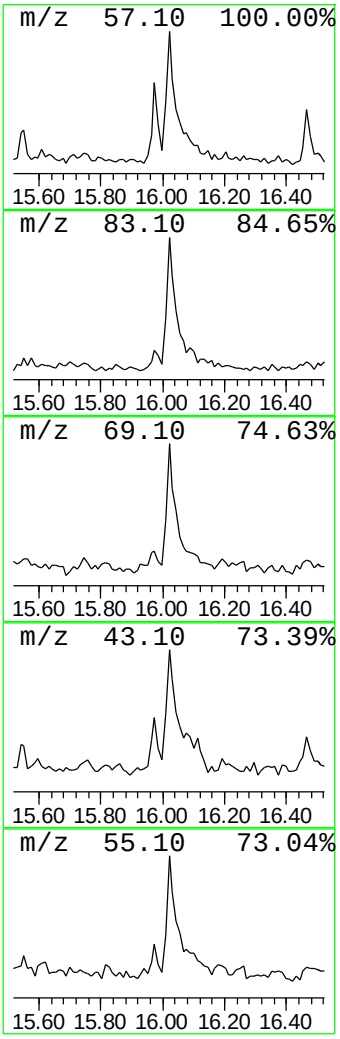
****

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	3.30 ng	175359	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	72
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	68
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110415\
Data File : BF082686.D
Acq On : 4 Nov 2015 6:16
Operator : UM/IZ
Sample : G4240-14
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04(2-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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...	5.07	52.0	ng	3068290	1	6.88	1180570	20.0
unknown6.65	6.65	106.0	ng	6257910	1	6.88	1180570	20.0
n-Hexadecanoic acid	11.94	9.5	ng	792286	4	11.40	1667620	20.0
Octadecanoic acid	12.73	5.0	ng	308005	5	14.04	1236770	20.0
Cyclotetradecane	13.89	14.1	ng	869158	5	14.04	1236770	20.0
Trichloroacetic a...	16.02	3.3	ng	175359	6	15.48	1062890	20.0