LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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	2.213	9	11	22	rVB	437266	651224	9.81%	1.133%
2	3.230	98	100	111	rBV3	18106	67513	1.02%	0.117%
3	5.070	257	261	263	rBV	1645525	2909318	43.83%	5.061%
4	5.481	294	297	300	rBV	4934620	5073973	76.44%	8.827%
5	6.510	384	387	389	rBV	5564880	5904421	88.95%	10.272%
6	6.647	396	399	401	rBV	6084737	6017636	90.65%	10.469%
7	6.876	417	419	421	rBV	1490075	1199836	18.08%	2.087%
8	7.036	430	433	435	rBV	5076201	4351287	65.55%	7.570%
9	7.436	465	468	471	rBV	3186401	3342894	50.36%	5.816%
10	8.167	529	532	534	rBV	1357697	1499295	22.59%	2.608%
11	9.242	623	626	629	rBV	5537608	5939550	89.48%	10.333%
12	9.630	658	660	663	rBV	695108	910446	13.72%	1.584%
13	9.916	683	685	688	rBV	1756833	1714965	25.84%	2.984%
14	10.339	720	722	723	rBV	144478	115279	1.74%	0.201%
15	10.705	751	754	757	rBV	4350124	4320272	65.08%	7.516%
16	10.842	764	766	770	rVB2	33756	67332	1.01%	0.117%
17	11.288	803	805	806	rBV	64425	66665	1.00%	0.116%
18	11.402	812	815	817	rBV	2205663	1838291	27.69%	3.198%
19	11.939	860	862	873	rBV	621734	762095	11.48%	1.326%
20	12.728	929	931	936	rBV	219000	235158	3.54%	0.409%
21	12.991	951	954	957	rBV	5285361	6638010	100.00%	11.548%
22	13.894	1031	1033	1043	rBV	473095	669043	10.08%	1.164%
23	14.042	1043	1046	1048	rBV	1768883	1725481	25.99%	3.002%
24	14.545	1088	1090	1096	rBV2	33107	68954	1.04%	0.120%
25	14.922	1121	1123	1125	rBV	79054	97095	1.46%	0.169%
26	15.482	1169	1172	1175	rBV	843223	1211369	18.25%	2.107%
27	16.031	1217	1220	1223	rBV2	36487	82911	1.25%	0.144%

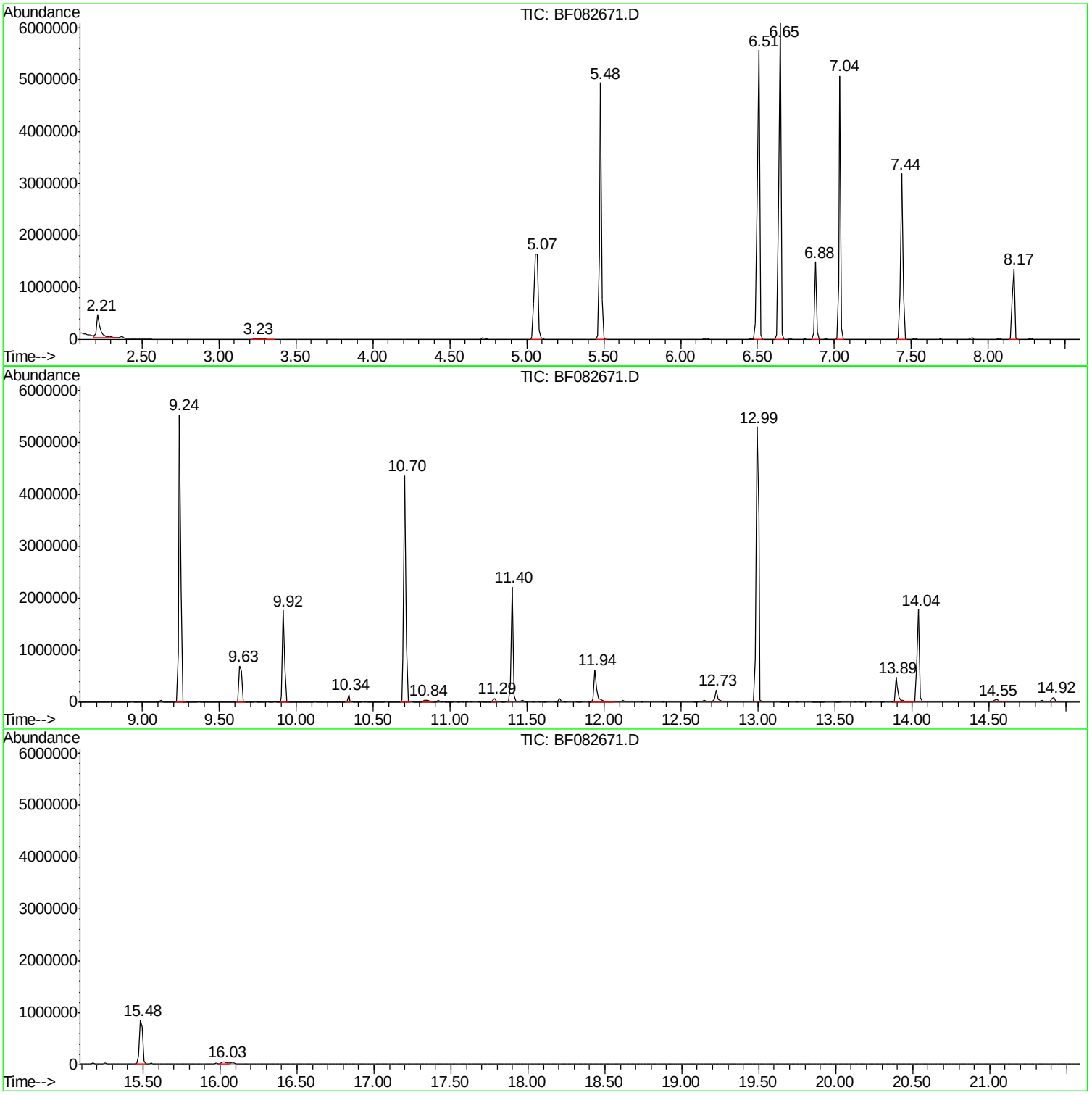
Sum of corrected areas: 57480313

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05(16-18)

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

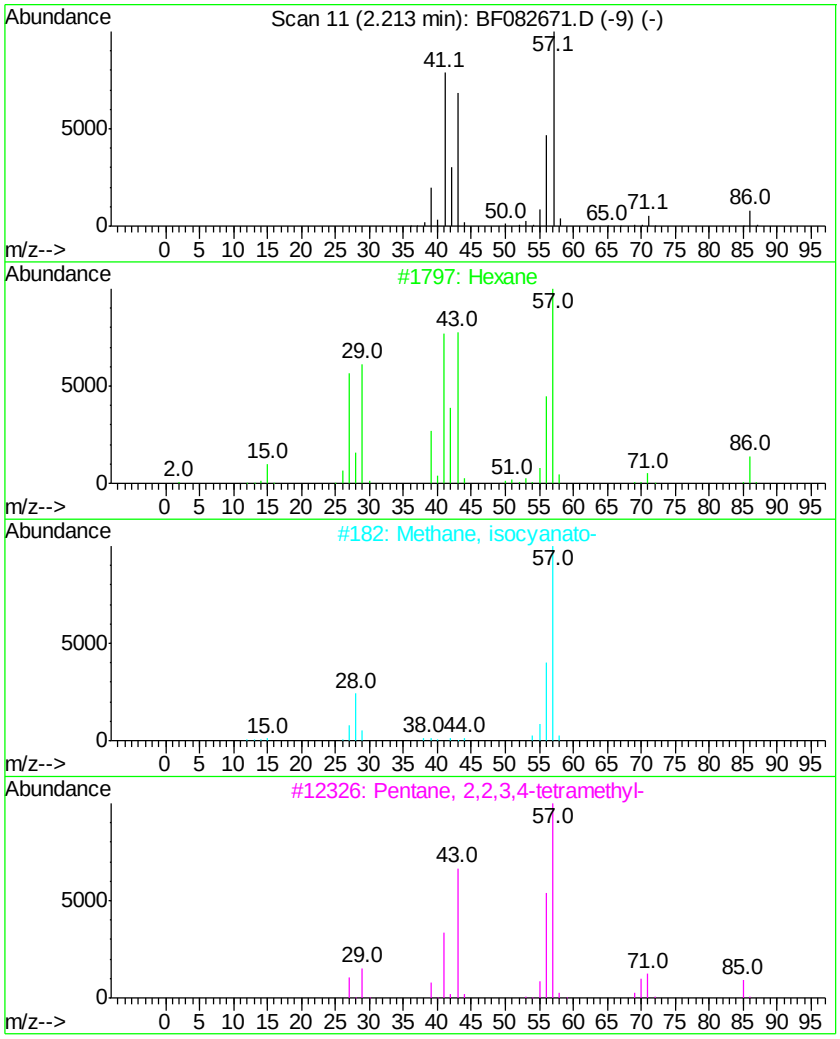
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

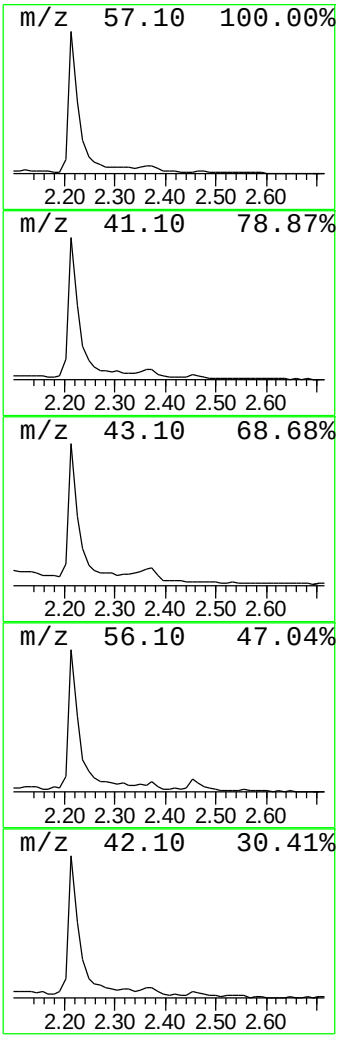
****

Peak Number 1 Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	10.86 ng	651224	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane	86	C6H14	000110-54-3	74
2	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	33
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	33
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

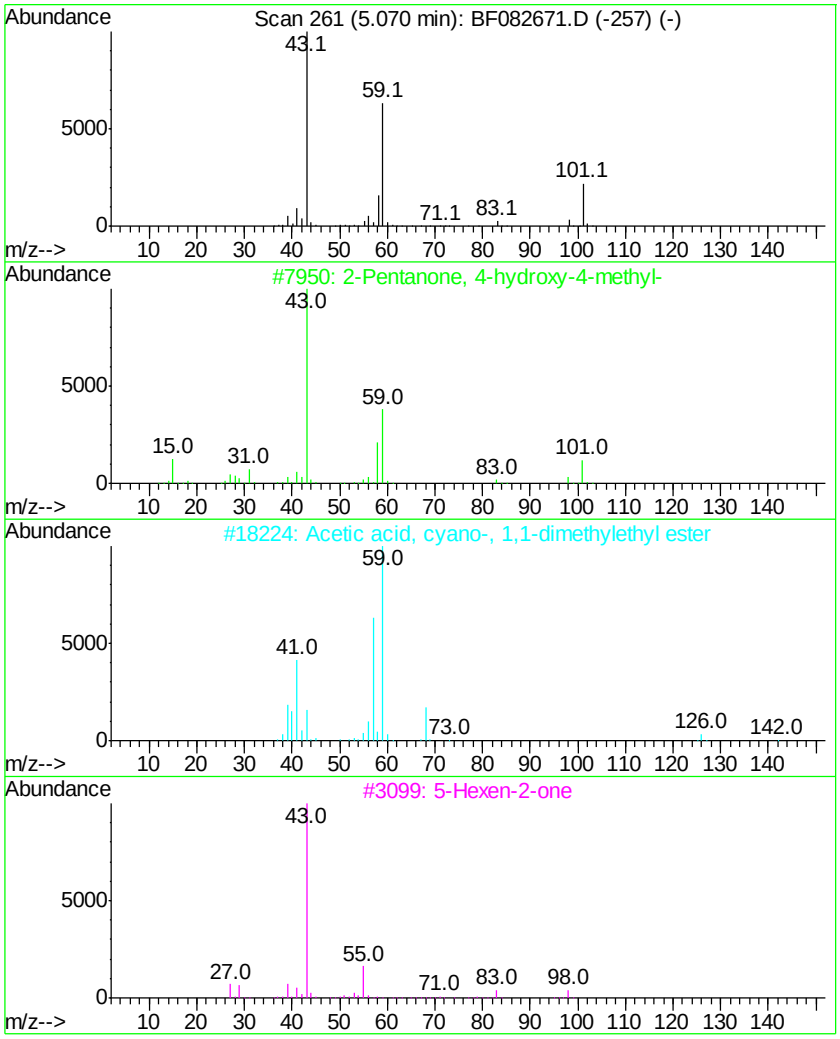
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

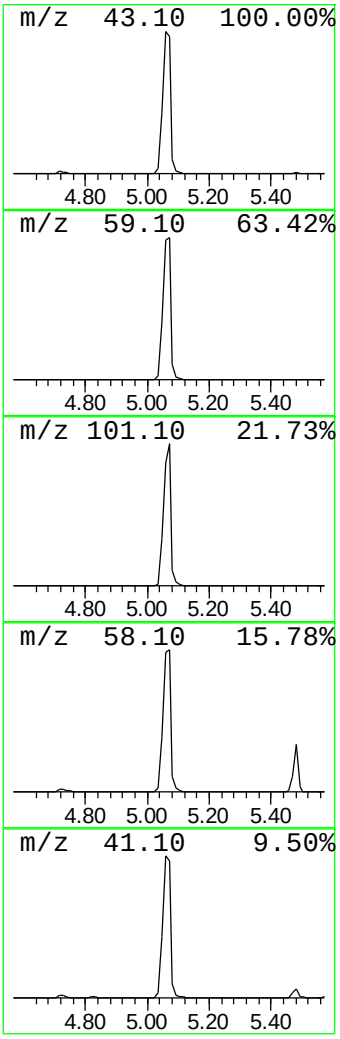
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	48.50 ng	2909320	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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

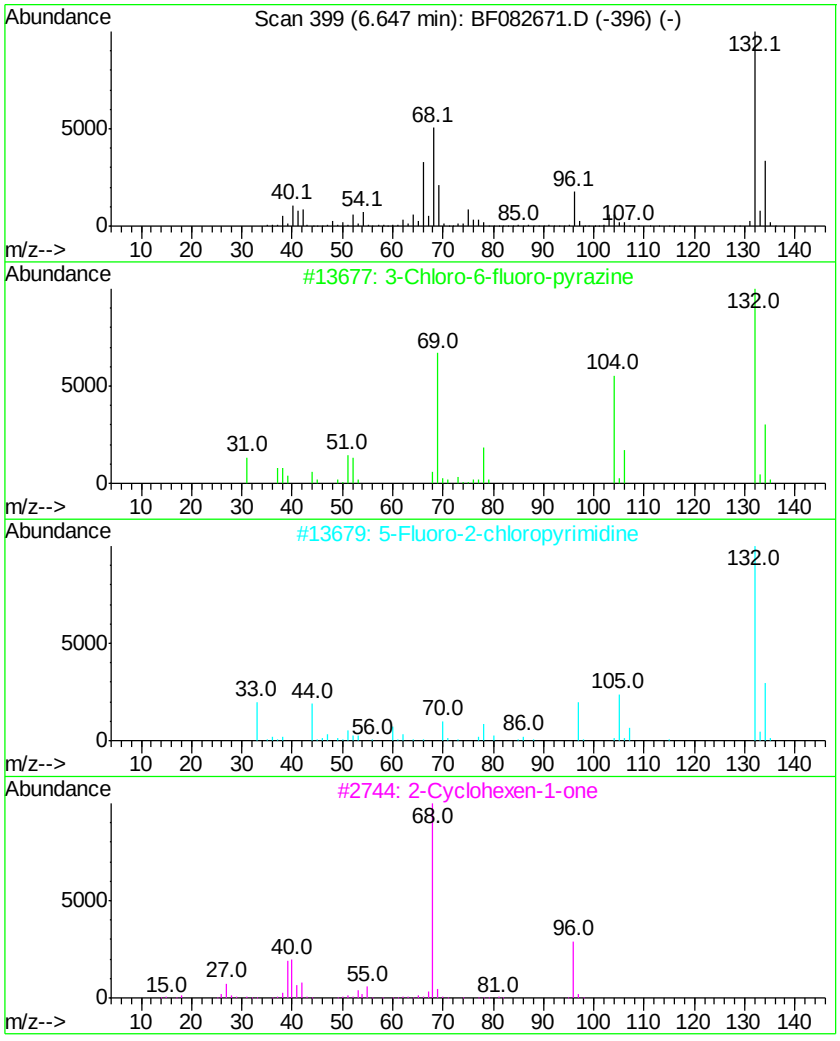
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

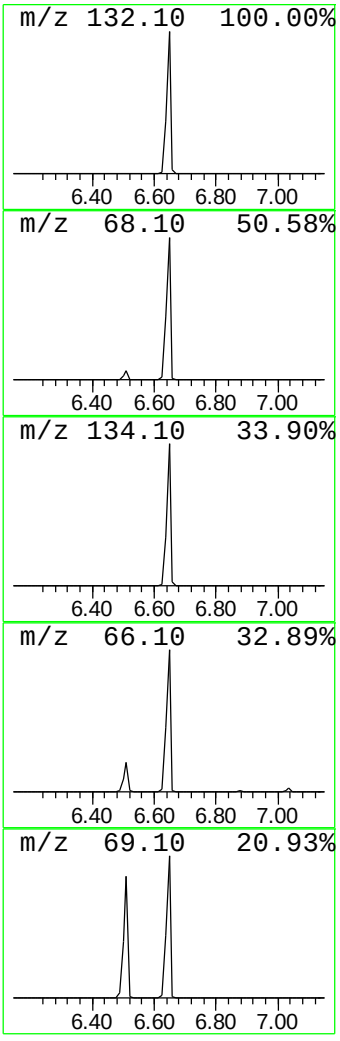
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	100.31 ng	6017640	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	16
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

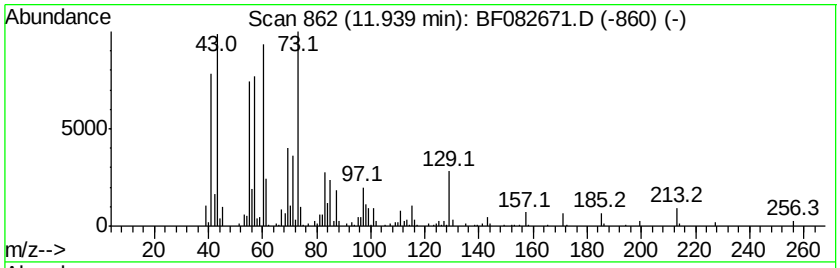
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

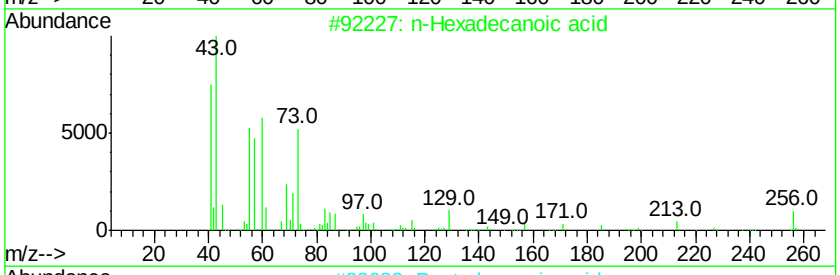
****

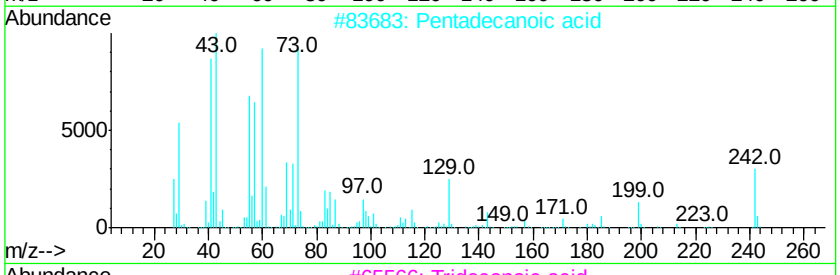
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

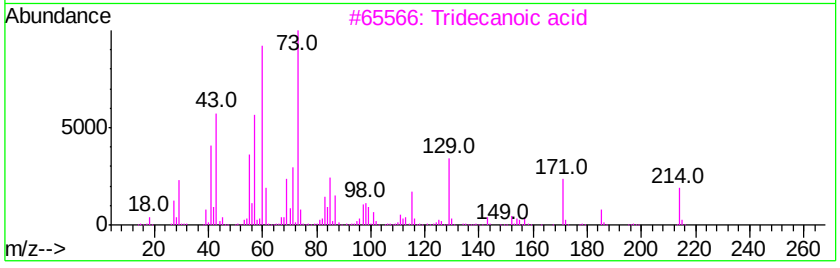
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	8.29 ng	762095	Phenanthrene-d10	11.40

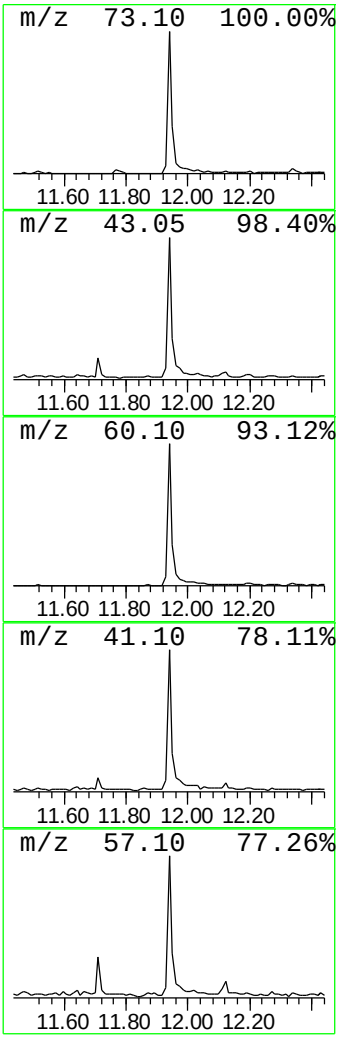
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64











Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

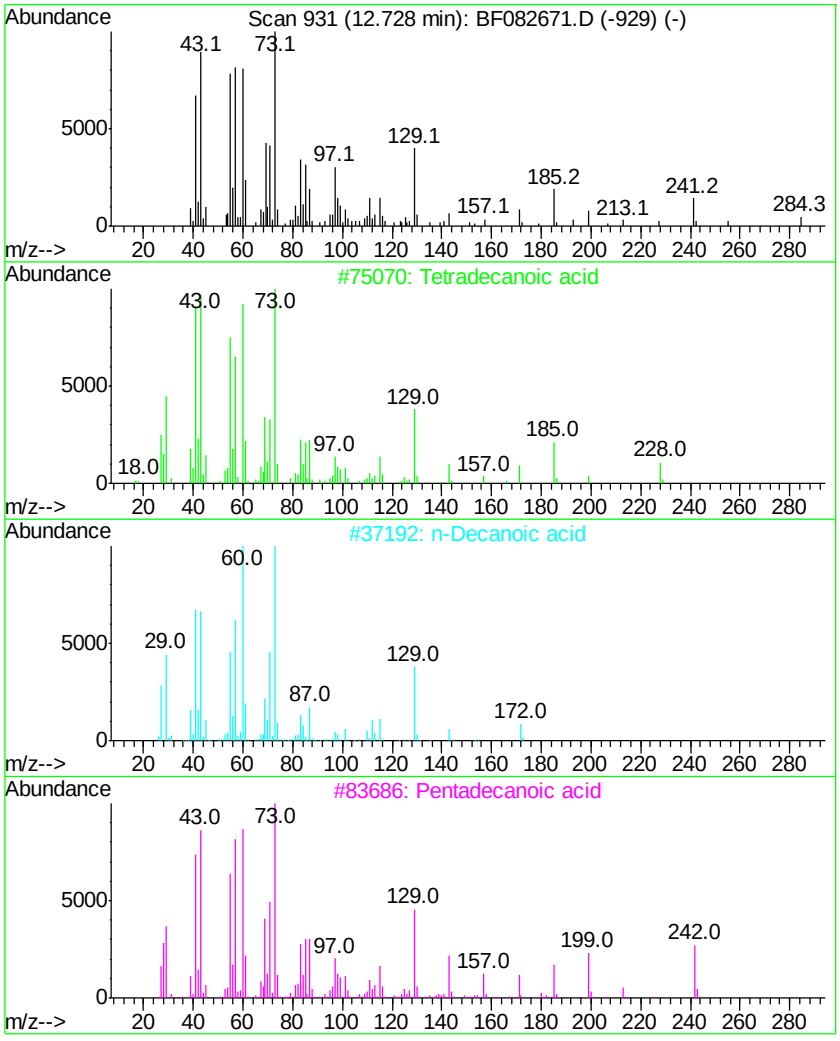
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

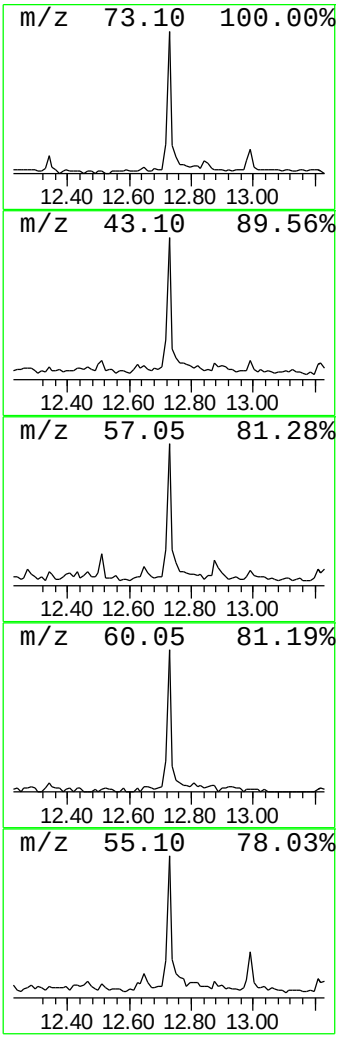
****

Peak Number 6 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.73 ng	235158	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
2	n-Decanoic acid	172	C10H20O2	000334-48-5	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tridecane	184	C13H28	000629-50-5	11
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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

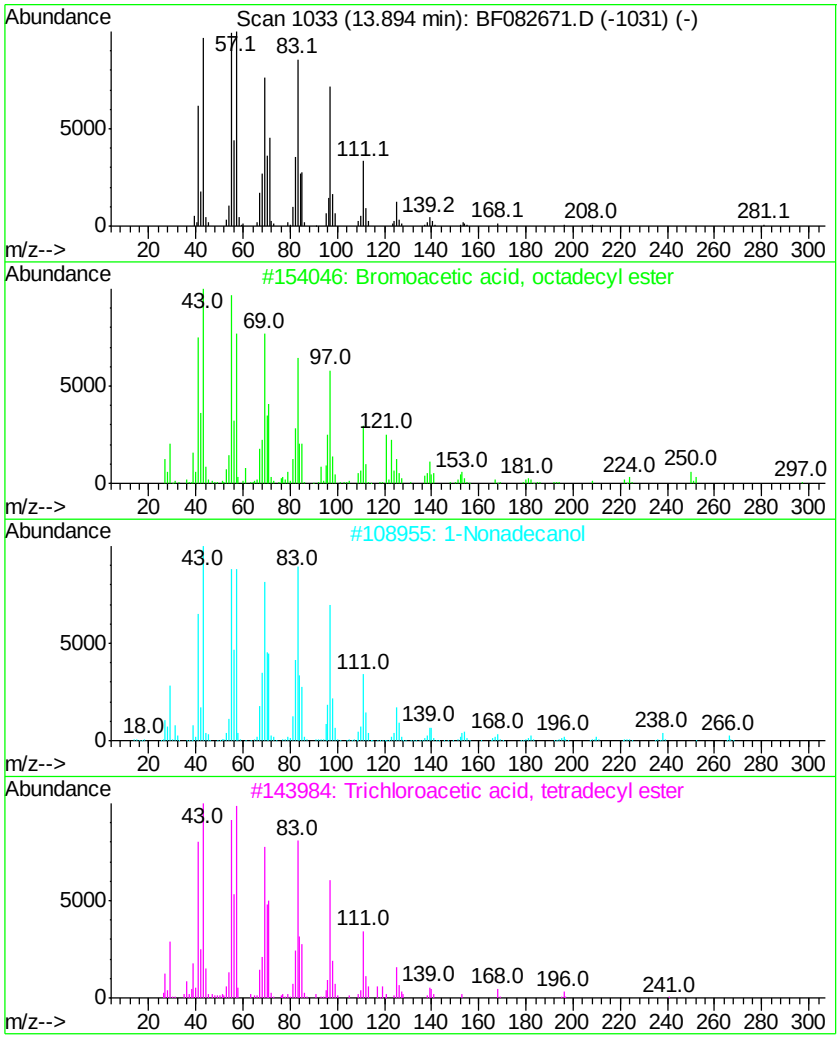
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

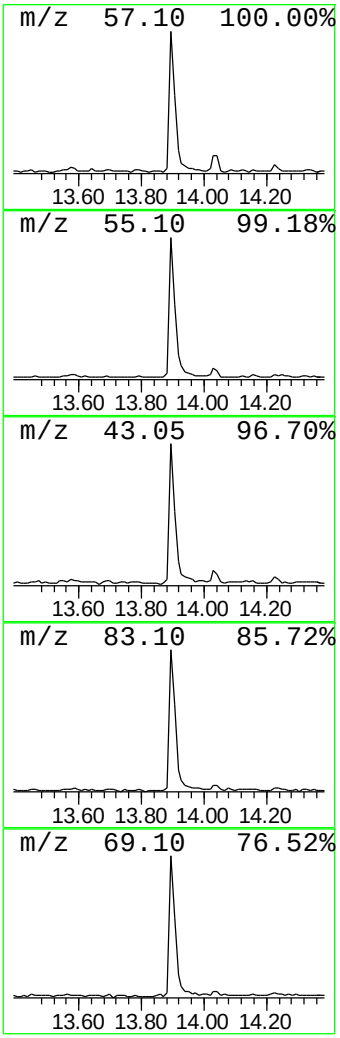
****

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.75 ng	669043	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2	1-Nonadecanol	284	C19H40O	001454-84-8	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5	1-Tetracosanol	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110315\
Data File : BF082671.D
Acq On : 3 Nov 2015 20:17
Operator : UM/IZ
Sample : G4240-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-05(16-18)

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
Hexane	2.21	10.9	ng	651224	1	6.88	1199840	20.0
2-Pentanone, 4-hy...	5.07	48.5	ng	2909320	1	6.88	1199840	20.0
unknown6.65	6.65	100.3	ng	6017640	1	6.88	1199840	20.0
n-Hexadecanoic acid	11.94	8.3	ng	762095	4	11.40	1838290	20.0
Tetradecanoic acid	12.73	2.7	ng	235158	5	14.04	1725480	20.0
Bromoacetic acid,...	13.89	7.8	ng	669043	5	14.04	1725480	20.0