LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(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-BF110715.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	5.024	254	257	260	rBV	1970117	3237491	49.99%	4.945%
2	5.447	291	294	297	rBV	4403985	6053583	93.48%	9.246%
3	6.476	381	384	387	rBV	4532271	6475887	100.00%	9.891%
4	6.613	393	396	399	rBV	5557853	5688036	87.83%	8.688%
5	6.842	414	416	419	rBV	1231998	1576241	24.34%	2.408%
6	7.002	428	430	433	rVB	3855231	4030428	62.24%	6.156%
7	7.413	462	466	468	rBV	3699882	4500639	69.50%	6.874%
8	7.516	472	475	480	rBV	37237	71519	1.10%	0.109%
9	8.133	526	529	531	rBV	2407041	2150445	33.21%	3.285%
10	9.093	611	613	620	rBV3	32417	69669	1.08%	0.106%
11	9.207	620	623	626	rBV	4768753	6370846	98.38%	9.731%
12	9.608	655	658	660	rBV	1908033	1821667	28.13%	2.782%
13	9.882	680	682	685	rBV	1977475	2413423	37.27%	3.686%
14	10.305	717	719	720	rBV	283901	240389	3.71%	0.367%
15	10.328	720	721	723	rVB	113271	107651	1.66%	0.164%
16	10.556	737	741	743	rBV2	50366	83498	1.29%	0.128%
17	10.671	748	751	754	rBV	4105657	4242291	65.51%	6.480%
18	10.808	761	763	767	rVB	139900	226039	3.49%	0.345%
19	11.253	799	802	803	rBV2	215214	189767	2.93%	0.290%
20	11.288	803	805	807	rVB	49761	65752	1.02%	0.100%
21	11.368	809	812	814	rVV	2967366	2587645	39.96%	3.952%
22	11.436	815	818	820	rVB2	54750	80088	1.24%	0.122%
23	11.676	837	839	842	rBV	157820	147109	2.27%	0.225%
24	11.916	857	860	864	rBV2	340381	564928	8.72%	0.863%
25	12.088	871	875	877	rBV	58953	86205	1.33%	0.132%
26	12.694	926	928	934	rBV	62582	80657	1.25%	0.123%
27	12.956	948	951	953	rBV	6398256	6065288	93.66%	9.264%
28	13.894	1029	1033	1040	rBV	371775	1328959	20.52%	2.030%
29	13.997	1040	1042	1045	rVB2	2087798	2414169	37.28%	3.687%
30	14.579	1088	1093	1094	rBV4	24492	71499	1.10%	0.109%
31	14.865	1115	1118	1120	rBV	330824	314330	4.85%	0.480%
32	15.425	1164	1167	1170	rBV	1634726	2009098	31.02%	3.069%
33	16.020	1213	1219	1220	rBV4	48594	105522	1.63%	0.161%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

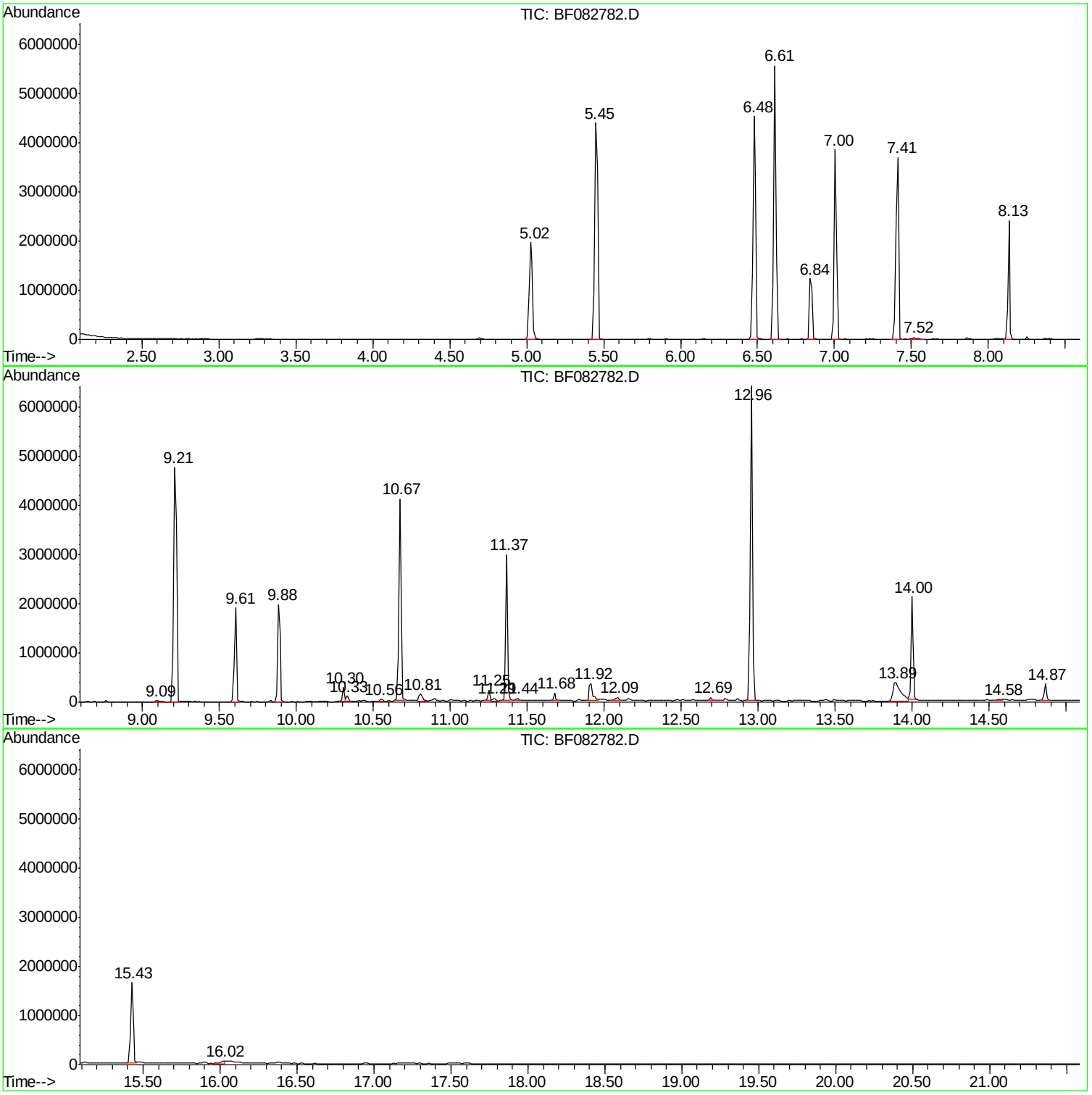
Sum of corrected areas: 65470758

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

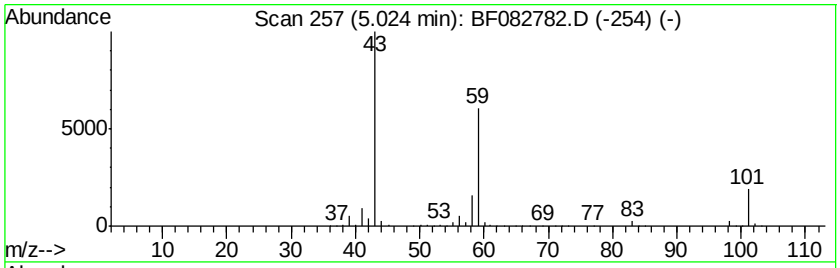
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

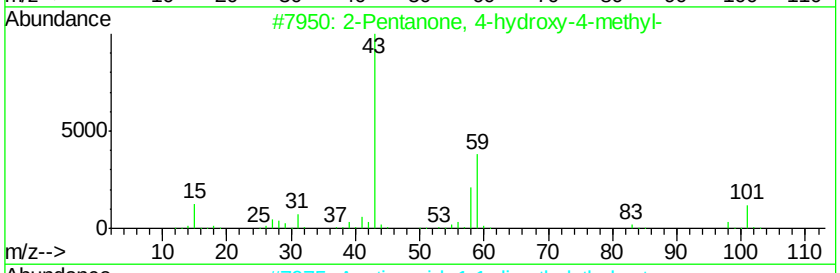
****

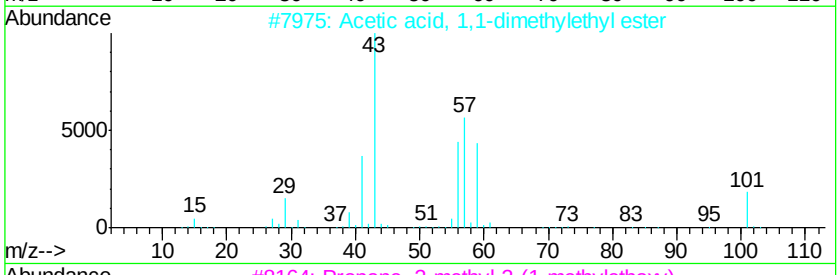
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

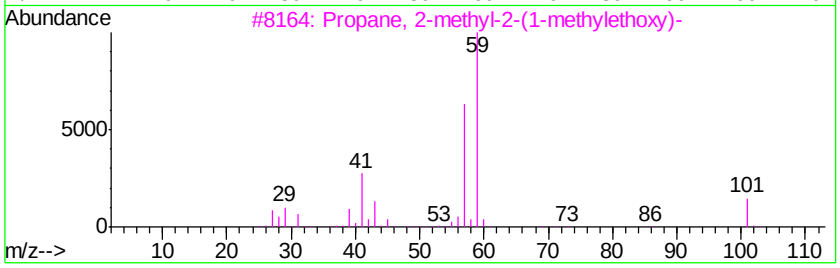
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	41.08 ng	3237490	1,4-Dichlorobenzene-d4	6.85

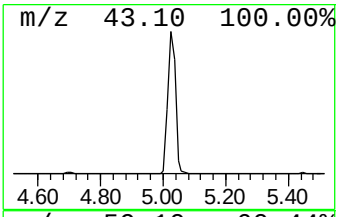
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32

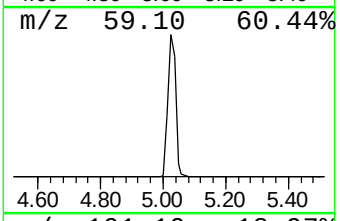


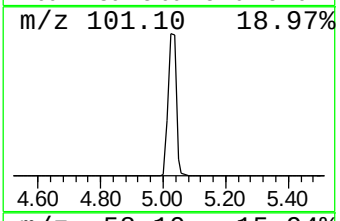


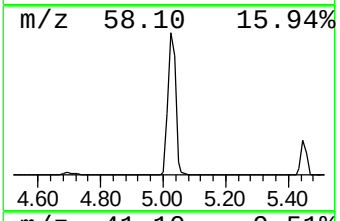


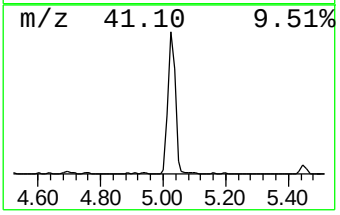












Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

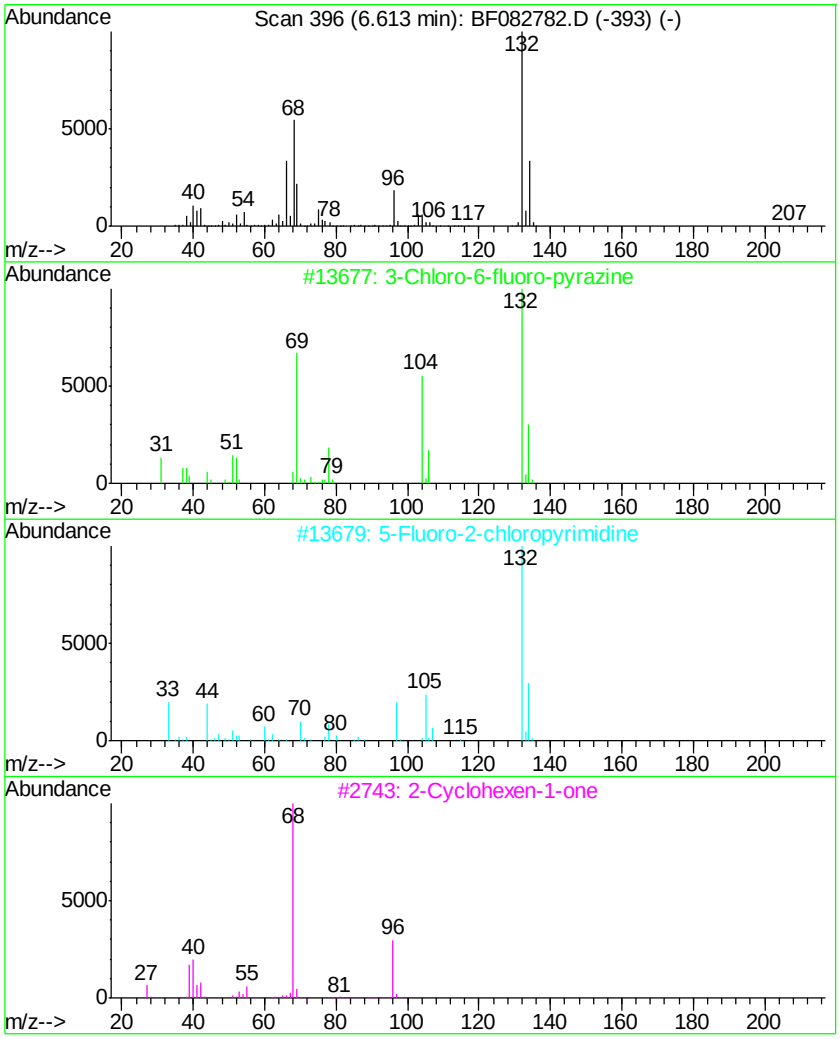
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

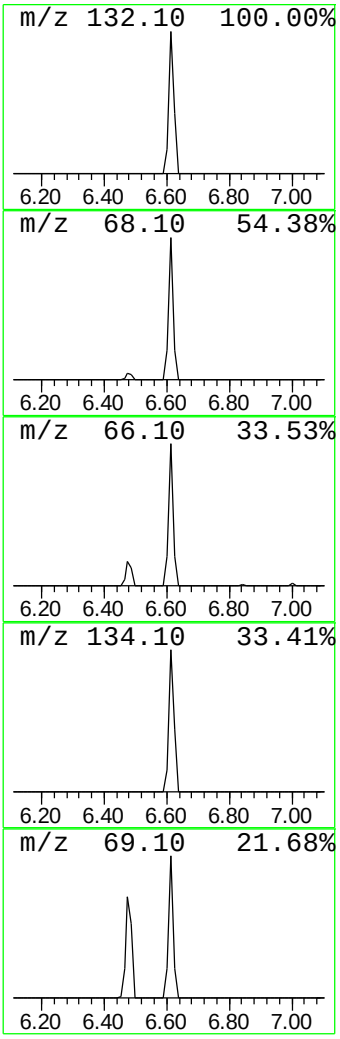
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.17 ng	5688040	1,4-Dichlorobenzene-d4	6.85

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	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

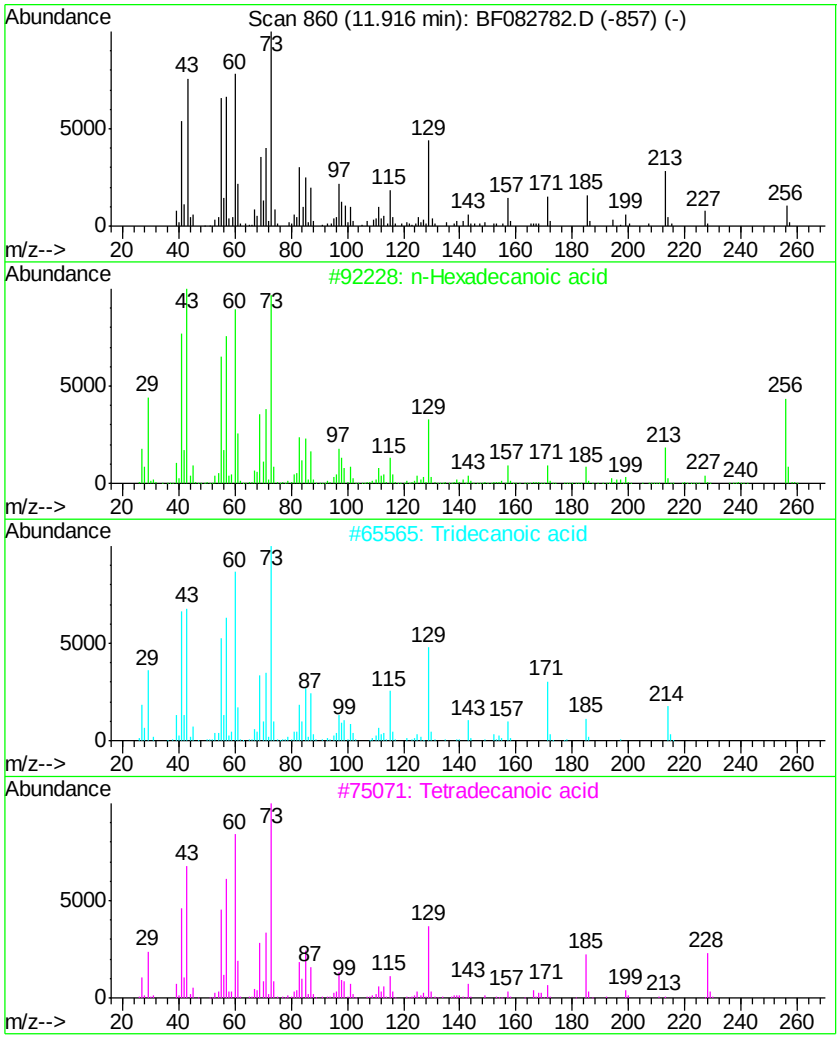
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

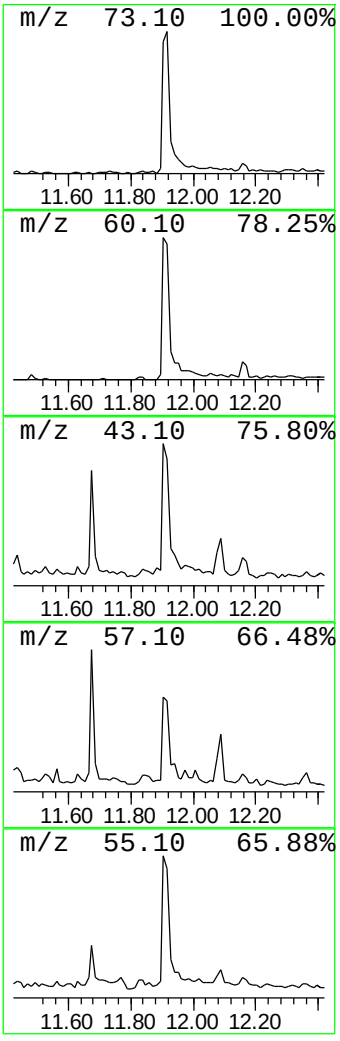
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.37 ng	564928	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

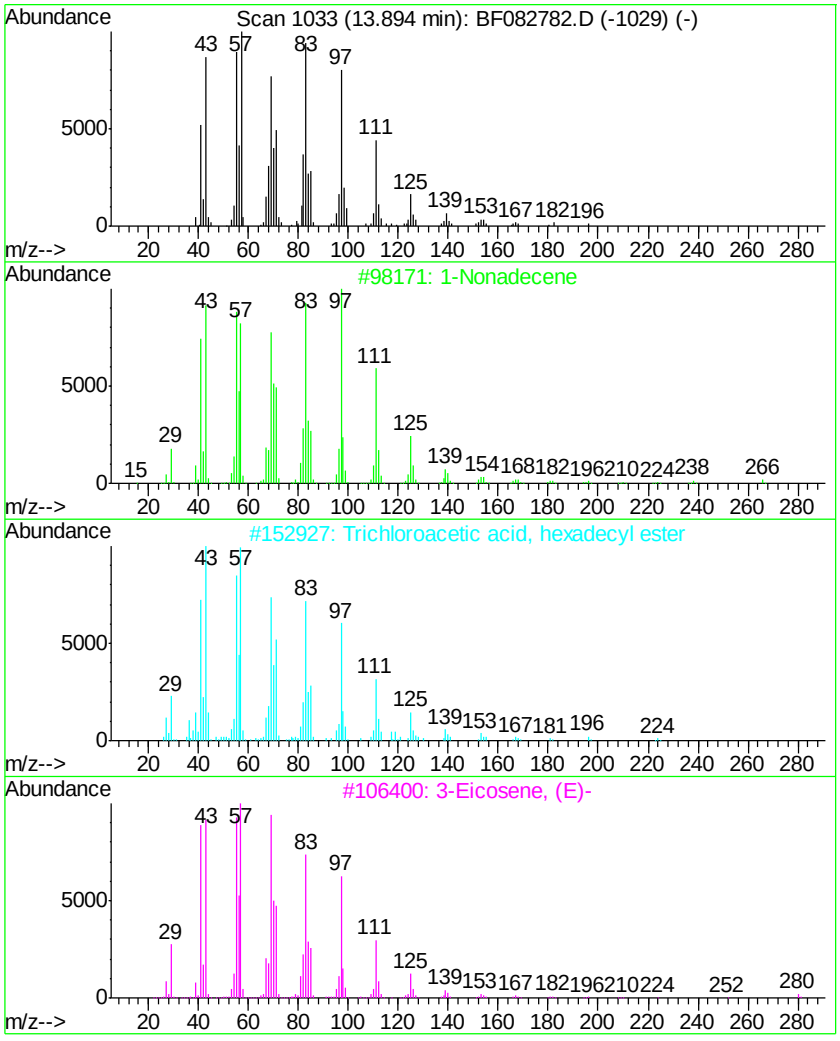
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

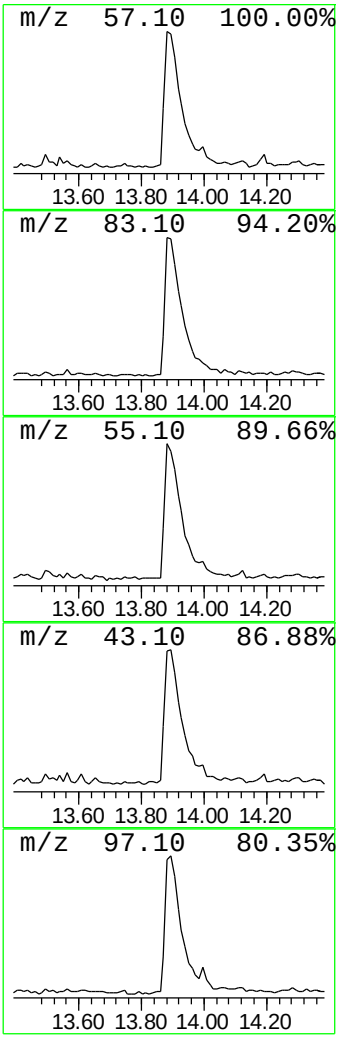
****

Peak Number 5 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	11.01 ng	1328960	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4	1-Hexadecanol	242	C16H34O	036653-82-4	83
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

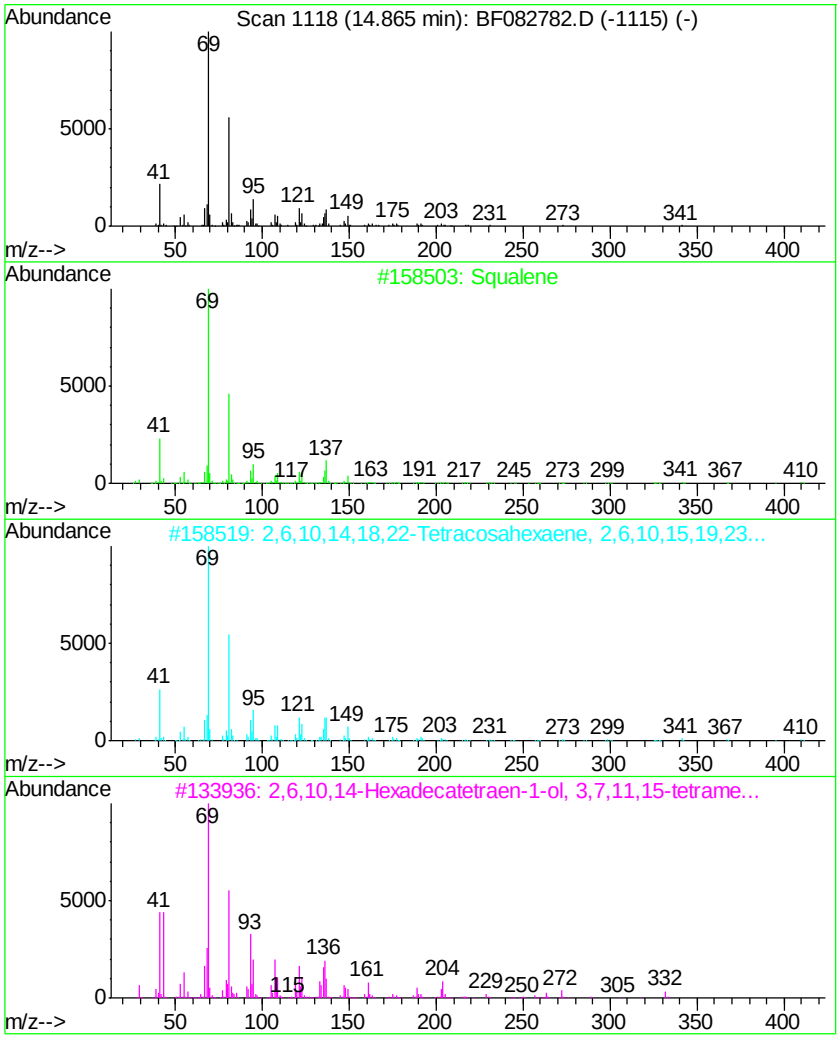
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

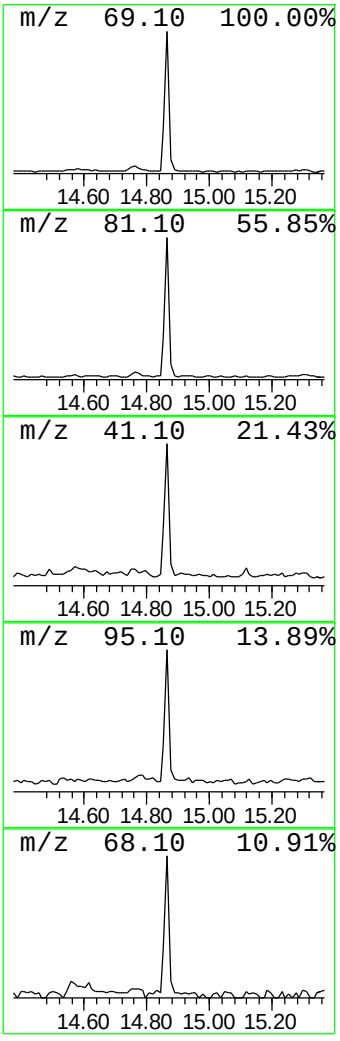
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.13 ng	314330	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110715\
Data File : BF082782.D
Acq On : 7 Nov 2015 1:18
Operator : UM/IZ
Sample : G4258-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-WP11-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	5.02	41.1	ng	3237490	1	6.85	1576240	20.0
unknown6.61	6.61	72.2	ng	5688040	1	6.85	1576240	20.0
n-Hexadecanoic acid	11.92	4.4	ng	564928	4	11.37	2587650	20.0
1-Nonadecene	13.89	11.0	ng	1328960	5	14.00	2414170	20.0
Squalene	14.87	3.1	ng	314330	6	15.43	2009100	20.0