LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

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-BF122415.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	3.698	139	141	146	rBB	10367	18330	1.14%	0.185%
2	4.967	250	252	260	rBB	49689	61992	3.87%	0.627%
3	5.413	288	291	301	rBB	387826	422647	26.39%	4.276%
4	6.442	380	381	390	rBB	181490	275622	17.21%	2.789%
5	6.567	390	392	395	rBV	1036412	905159	56.52%	9.158%
6	6.796	410	412	415	rBV	345213	287207	17.93%	2.906%
7	6.956	424	426	428	rBV	901418	937612	58.55%	9.486%
8	7.367	459	462	464	rBV	659398	761466	47.55%	7.704%
9	7.699	489	491	495	rBV	9256	16772	1.05%	0.170%
10	7.825	500	502	504	rBV	82994	69936	4.37%	0.708%
11	8.087	522	525	527	rBV	272314	373122	23.30%	3.775%
12	9.162	616	619	621	rBV	1638673	1601384	100.00%	16.202%
13	9.425	639	642	644	rBV2	7922	16210	1.01%	0.164%
14	9.505	647	649	652	rVV3	7986	17131	1.07%	0.173%
15	9.550	652	653	655	rVB	71146	75146	4.69%	0.760%
16	9.836	675	678	680	rBV	461744	440018	27.48%	4.452%
17	10.271	712	716	718	rBV	22652	28050	1.75%	0.284%
18	10.625	744	747	749	rBV	968602	925488	57.79%	9.364%
19	10.751	756	758	762	rVB3	21507	39531	2.47%	0.400%
20	10.922	770	773	776	rBV4	8454	17759	1.11%	0.180%
21	11.185	795	796	802	rVB4	14284	32099	2.00%	0.325%
22	11.322	806	808	810	rBV	338315	403032	25.17%	4.078%
23	11.551	826	828	830	rBV	13245	18663	1.17%	0.189%
24	11.859	853	855	859	rBV2	84079	96231	6.01%	0.974%
25	12.636	921	923	928	rBV3	29131	51448	3.21%	0.521%
26	12.785	935	936	940	rVB3	26766	36788	2.30%	0.372%
27	12.899	943	946	948	rBV	1385607	1280366	79.95%	12.954%
28	13.802	1023	1025	1030	rVB3	55399	80569	5.03%	0.815%
29	13.951	1036	1038	1041	rBV2	238245	305884	19.10%	3.095%
30	14.122	1051	1053	1059	rVB6	8908	17522	1.09%	0.177%
31	14.785	1109	1111	1116	rVB	16987	20574	1.28%	0.208%
32	15.380	1161	1163	1168	rVB	202438	249965	15.61%	2.529%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

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-BF122415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

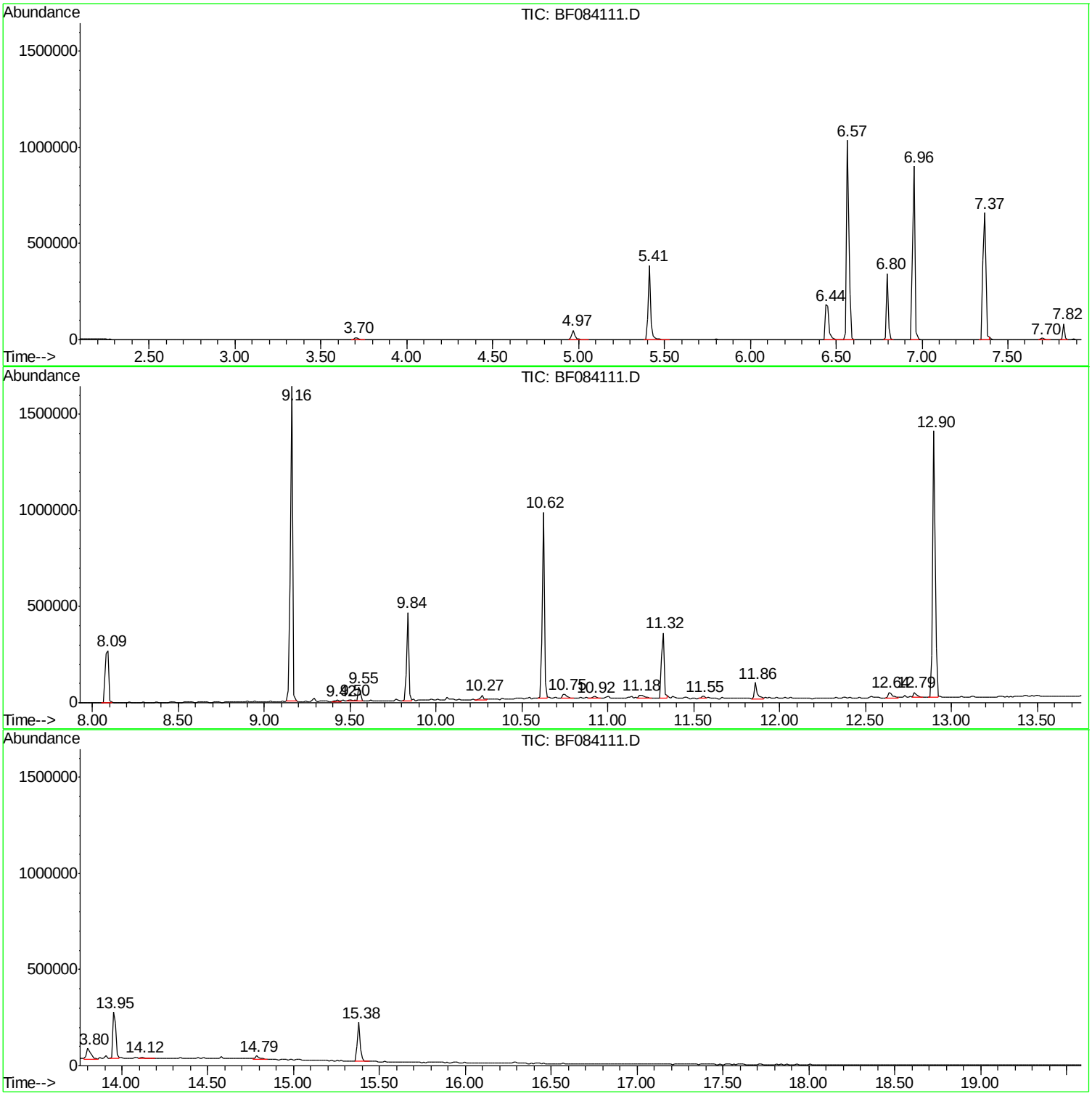
Sum of corrected areas: 9883723

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

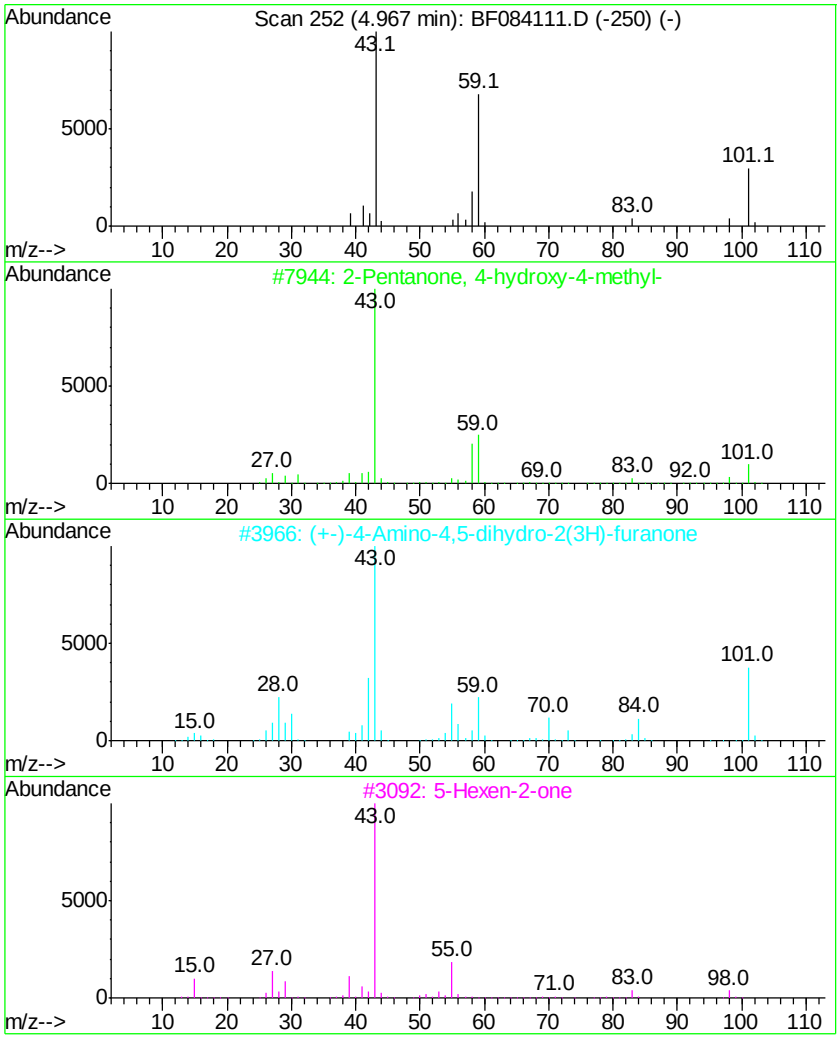
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

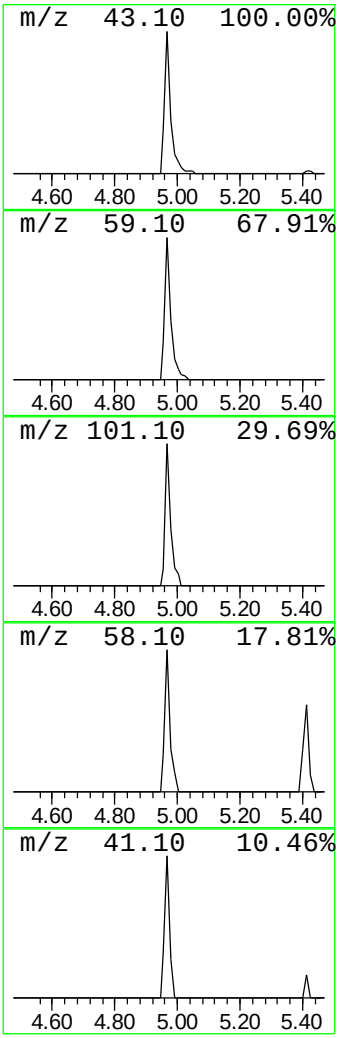
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	4.32 ng	61992	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

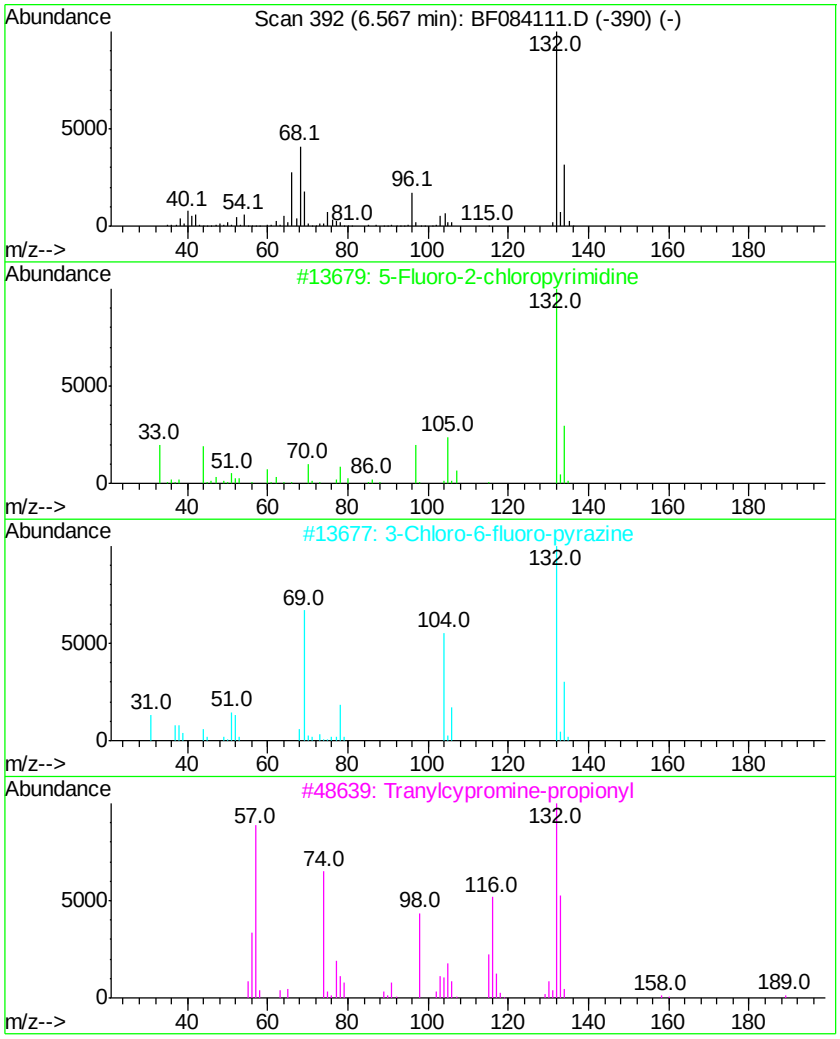
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

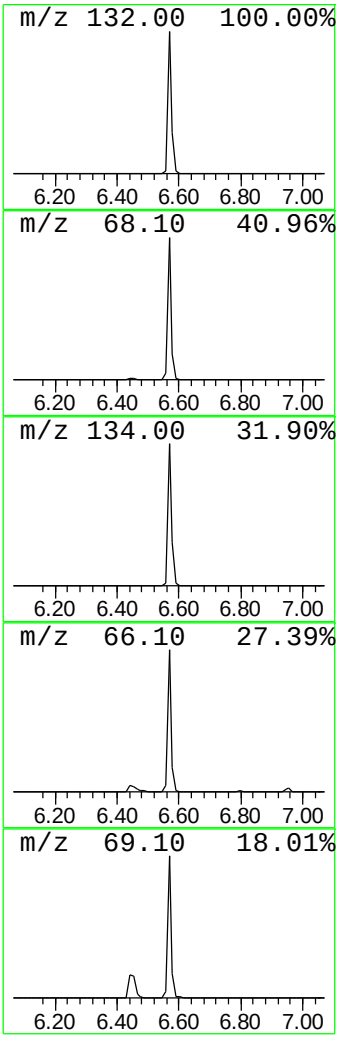
****

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.03 ng	905159	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

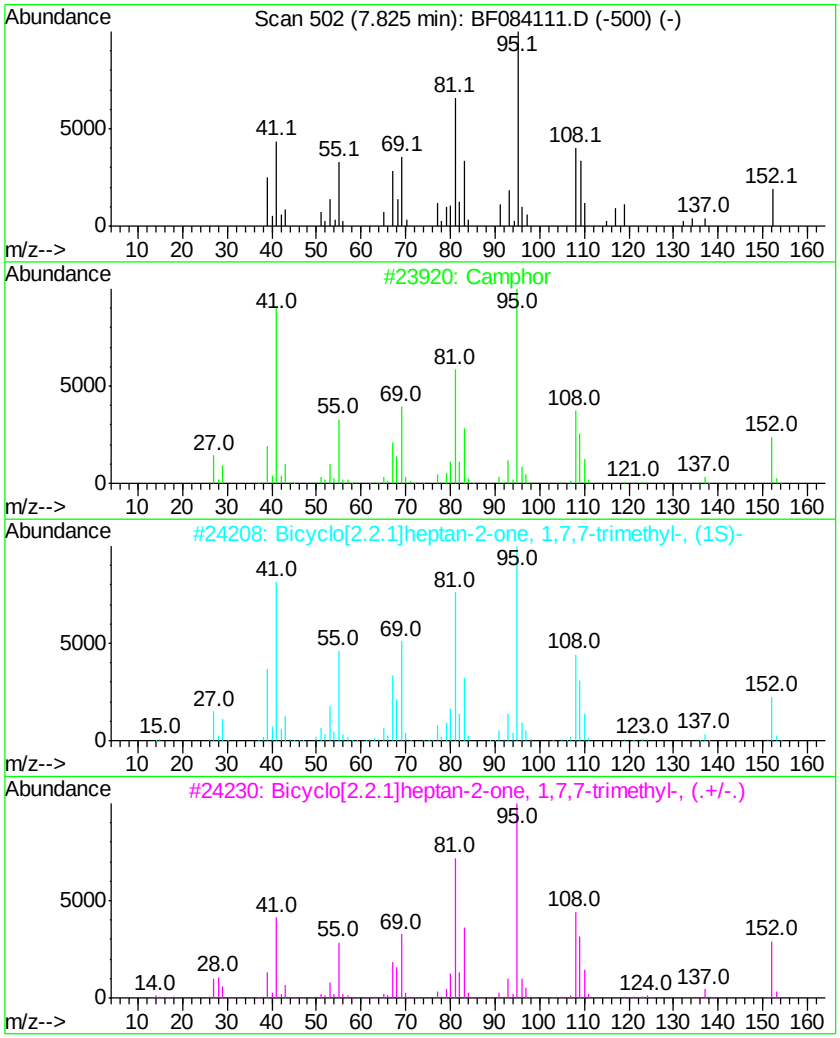
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

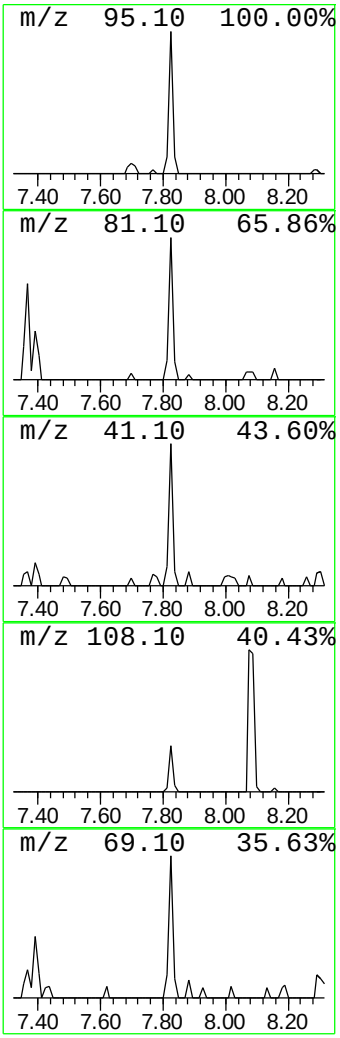
****

Peak Number 4 Camphor Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	3.75 ng	69936	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphor	152	C10H16O	000076-22-2	95
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	94
4	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	94
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

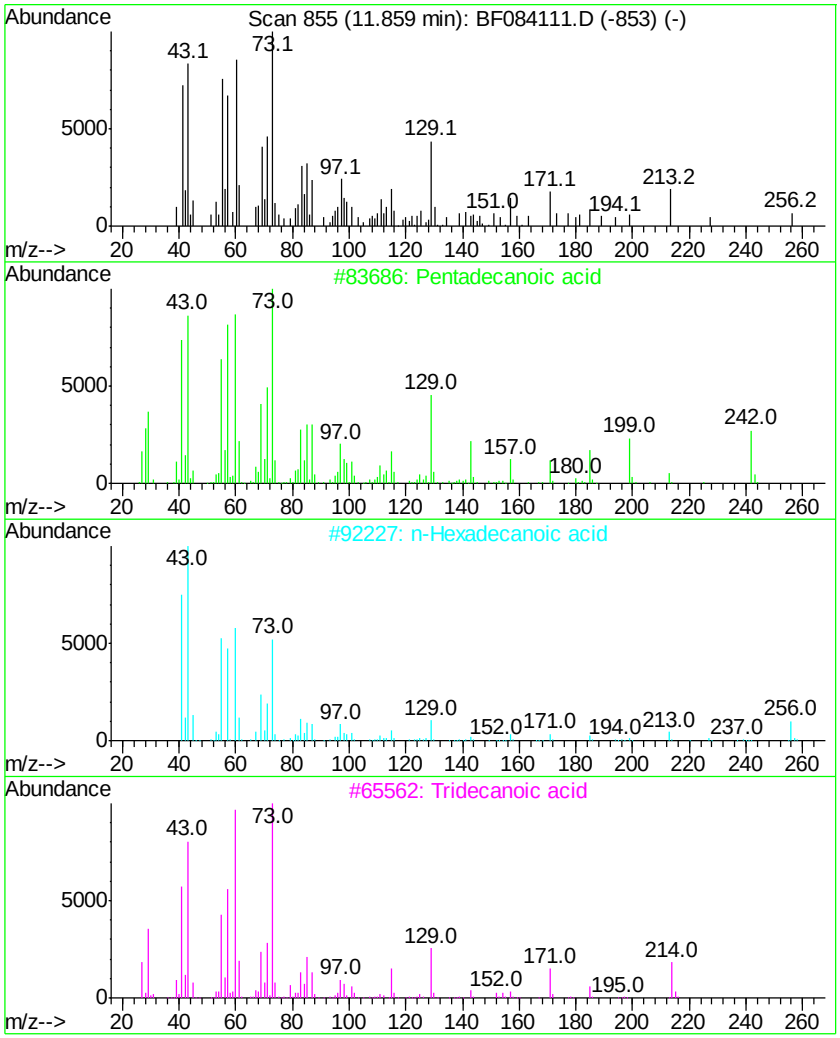
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

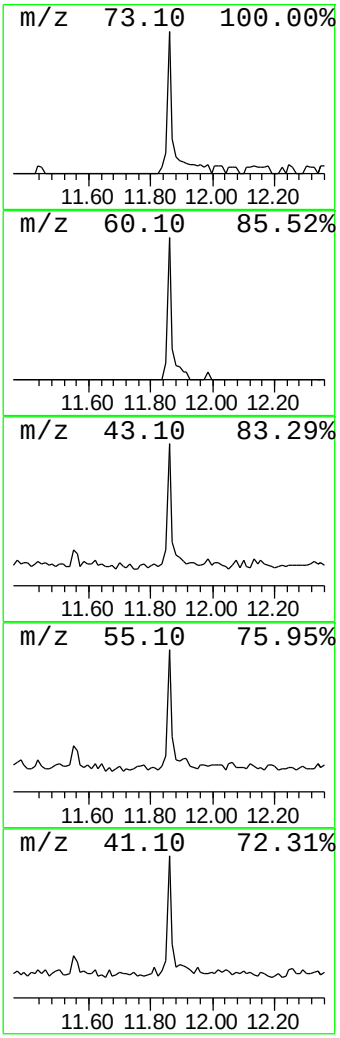
****

Peak Number 5 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.78 ng	96231	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
5	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

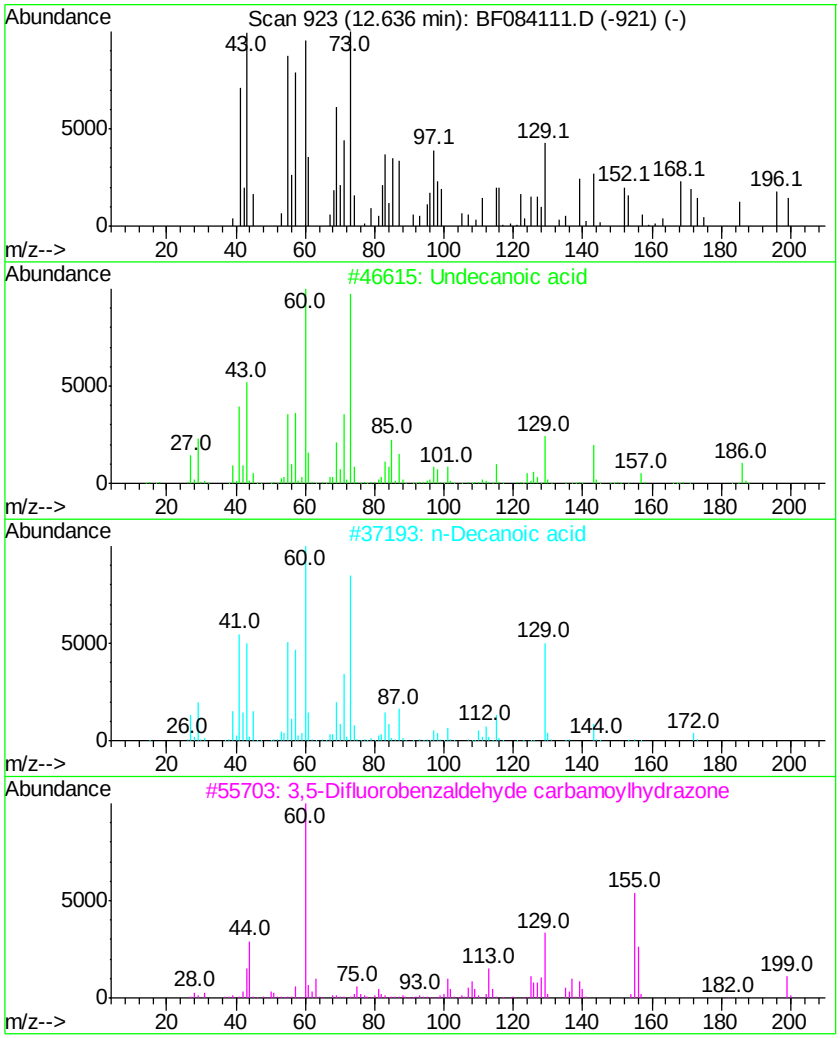
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

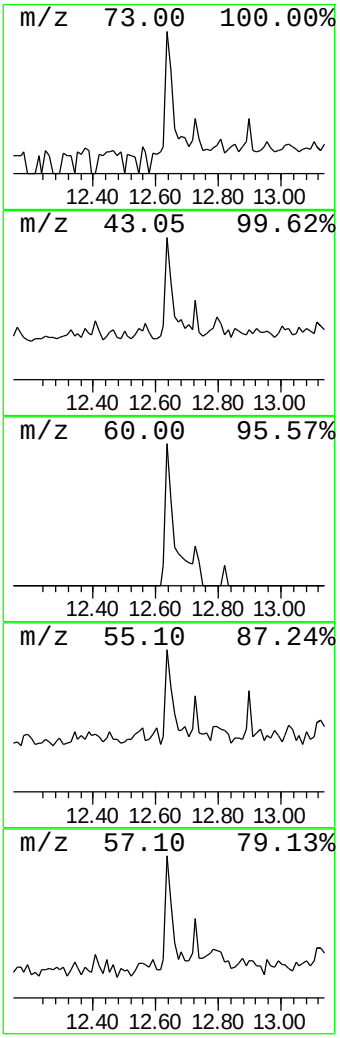
****

Peak Number 6 unknown12.64 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.55 ng	51448	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	38
2	n-Decanoic acid	172	C10H20O2	000334-48-5	35
3	3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	30
4	Acetamide, N-(4-hydroxycyclohexy...	157	C8H15NO2	027489-60-7	27
5	Lactose	342	C12H22O11	000063-42-3	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

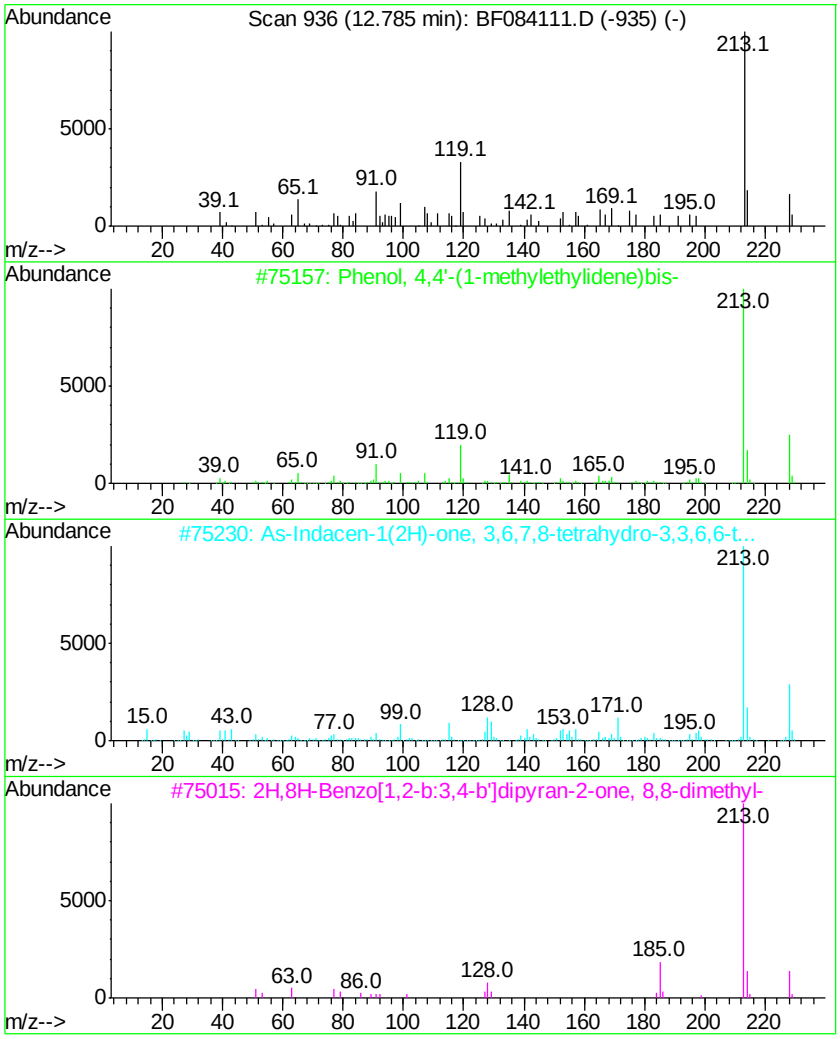
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

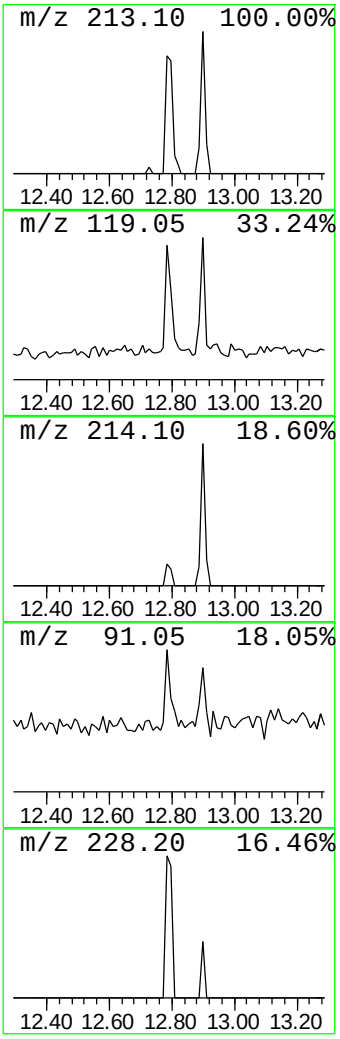
****

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.41 ng	36788	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	As-Indacen-1(2H)-one, 3,6,7,8-te...	228	C16H20O	055591-18-9	50
3	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	49
4	Benzene, 1-nitro-3-(phenylmethyl)-	213	C13H11NO2	005840-41-5	49
5	1-(7-Methyl-6H-imidazo[1,2-a]pyr...	213	C12H11N3O	1000147-75-1	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

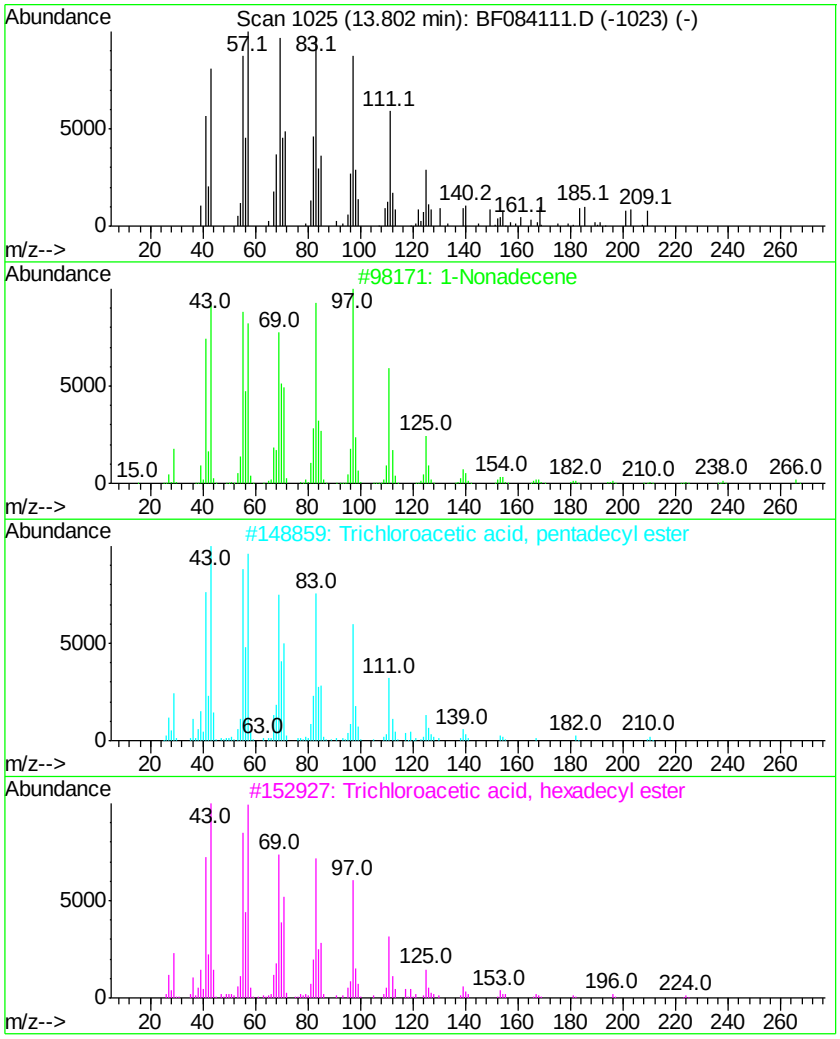
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

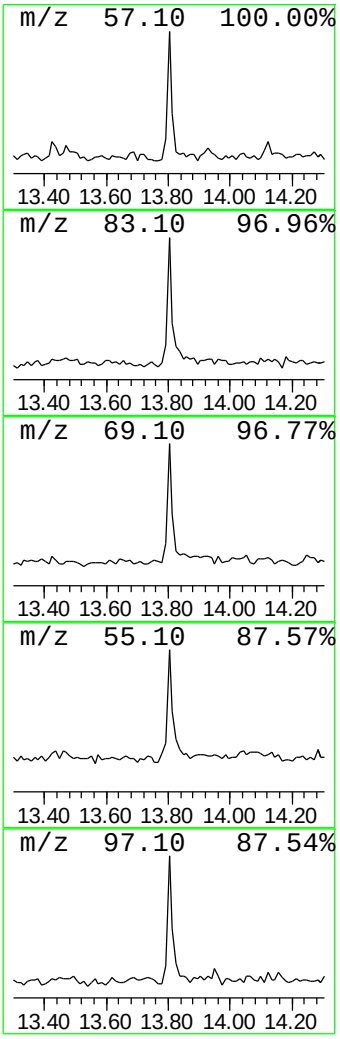
****

Peak Number 8 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.27 ng	80569	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
4	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	80
5	1-Docosene	308	C22H44	001599-67-3	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084111.D
Acq On : 25 Dec 2015 6:27
Operator : UM/SJ
Sample : G4951-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5-122215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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...	4.97	4.3	ng	61992	1	6.80	287207	20.0
unknown6.57	6.57	63.0	ng	905159	1	6.80	287207	20.0
Camphor	7.82	3.8	ng	69936	2	8.09	373122	20.0
Pentadecanoic acid	11.86	4.8	ng	96231	4	11.32	403032	20.0
unknown12.64	12.64	2.5	ng	51448	4	11.32	403032	20.0
Phenol, 4,4'-(1-m...	12.79	2.4	ng	36788	5	13.95	305884	20.0
1-Nonadecene	13.80	5.3	ng	80569	5	13.95	305884	20.0