LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

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-BF101116.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	5.137	243	245	255	rBV	216874	365804	5.93%	0.727%
2	5.560	280	282	304	rBV	1148057	2492831	40.40%	4.957%
3	6.589	369	372	381	rBV	887876	1672742	27.11%	3.326%
4	6.715	381	383	397	rVV	2901317	4485406	72.69%	8.919%
5	6.943	401	403	414	rVB	755691	1209755	19.60%	2.406%
6	7.103	414	417	430	rBV	3867011	4044980	65.55%	8.043%
7	7.515	450	453	455	rBV	2651123	3161956	51.24%	6.287%
8	7.629	462	463	468	rVB4	26873	63769	1.03%	0.127%
9	7.880	483	485	490	rVB3	41694	85659	1.39%	0.170%
10	7.972	490	493	497	rBV	90467	176772	2.86%	0.351%
11	8.166	506	510	513	rBV4	127188	181954	2.95%	0.362%
12	8.235	513	516	522	rVV	1638000	1961924	31.79%	3.901%
13	8.475	536	537	540	rBV3	34970	67526	1.09%	0.134%
14	8.703	552	557	560	rBV5	70134	134194	2.17%	0.267%
15	8.795	564	565	569	rVB4	46933	75136	1.22%	0.149%
16	8.966	578	580	585	rVB2	100446	151392	2.45%	0.301%
17	9.058	585	588	589	rBV3	63432	143637	2.33%	0.286%
18	9.080	589	590	593	rVB2	97265	87685	1.42%	0.174%
19	9.172	595	598	600	rVB3	56170	109881	1.78%	0.218%
20	9.218	600	602	604	rBV2	52168	69469	1.13%	0.138%
21	9.309	608	610	613	rVV	5073823	6170723	100.00%	12.270%
22	9.389	615	617	620	rVB4	58974	85455	1.38%	0.170%
23	9.652	638	640	643	rVB4	66432	92974	1.51%	0.185%
24	9.766	648	650	655	rVB5	57803	165517	2.68%	0.329%
25	9.846	655	657	659	rBV2	48134	83002	1.35%	0.165%
26	9.995	667	670	672	rBV	1843668	1885310	30.55%	3.749%
27	10.189	685	687	690	rBV3	50035	75637	1.23%	0.150%
28	10.303	693	697	702	rBV	629721	1098063	17.79%	2.183%
29	10.475	709	712	718	rBV3	318712	774909	12.56%	1.541%
30	10.635	723	726	728	rVB	59929	93782	1.52%	0.186%
31	10.726	732	734	736	rBV	131578	152371	2.47%	0.303%
32	10.783	736	739	742	rBV	3483989	4007338	64.94%	7.968%
33	10.898	747	749	753	rVB2	62336	117106	1.90%	0.233%
34	11.481	798	800	802	rBV	2086171	1879733	30.46%	3.738%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

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-BF101116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.006	844	846	849	rBV2	144319	224065	3.63%	0.446%
36	12.795	913	915	920	rBV	59935	71071	1.15%	0.141%
37	13.069	936	939	941	rBV	6034973	5563697	90.16%	11.063%
38	13.961	1015	1017	1020	rBV	98845	111071	1.80%	0.221%
39	14.121	1029	1031	1034	rBV	1615285	1448992	23.48%	2.881%
40	14.601	1071	1073	1078	rVB	49510	84485	1.37%	0.168%
41	15.001	1105	1108	1113	rVB	116108	184956	3.00%	0.368%
42	15.435	1143	1146	1149	rBV	256434	381856	6.19%	0.759%
43	15.595	1157	1160	1163	rBV	811971	1099633	17.82%	2.187%
44	15.938	1186	1190	1196	rVB	359141	655531	10.62%	1.303%
45	16.544	1238	1243	1253	rVB	378823	948994	15.38%	1.887%
46	17.264	1301	1306	1315	rVB	325487	891835	14.45%	1.773%
47	18.156	1378	1384	1394	rVB	213730	724455	11.74%	1.441%
48	19.253	1473	1480	1489	rBV	111670	475906	7.71%	0.946%

Sum of corrected areas: 50290939

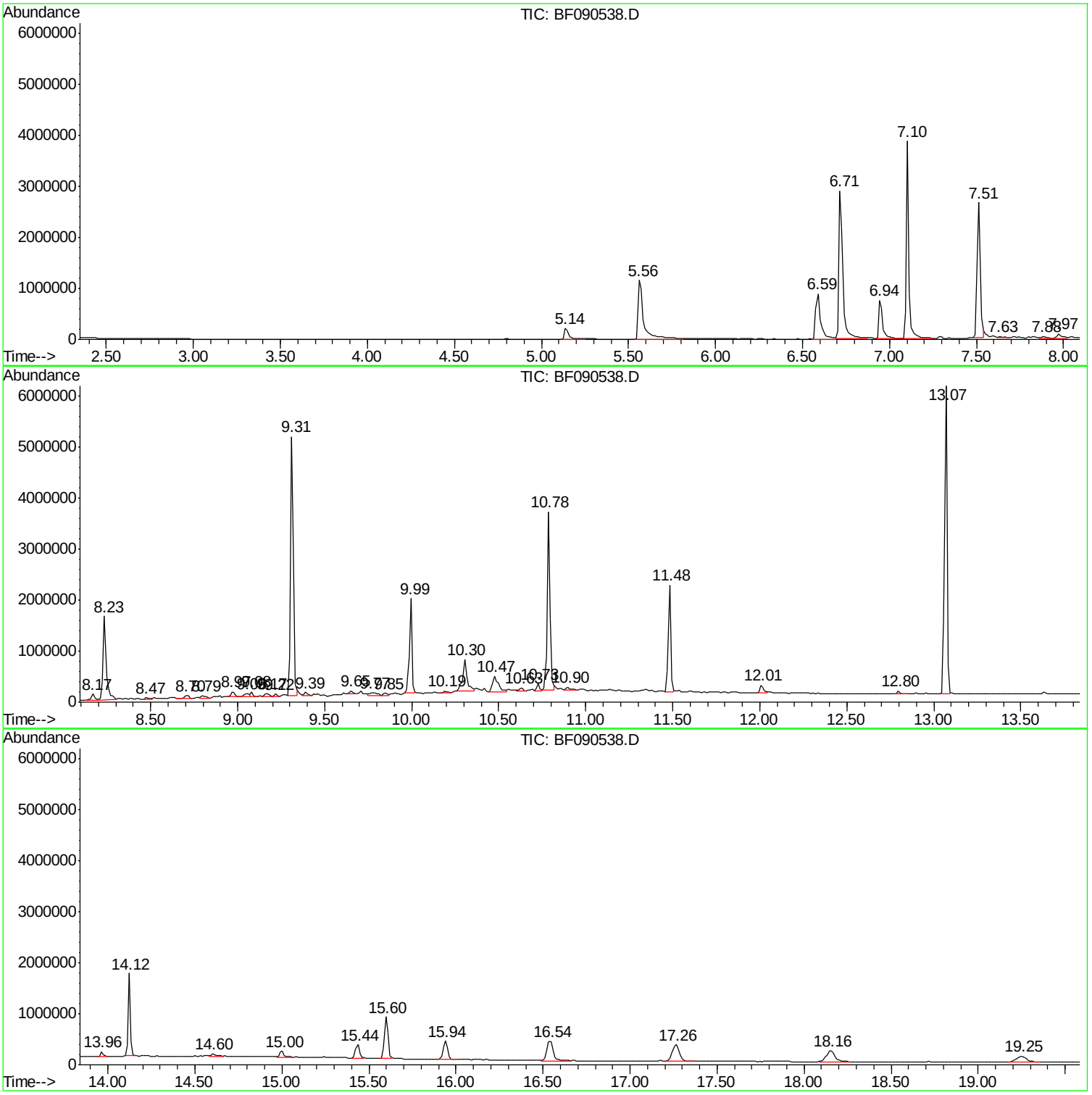
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

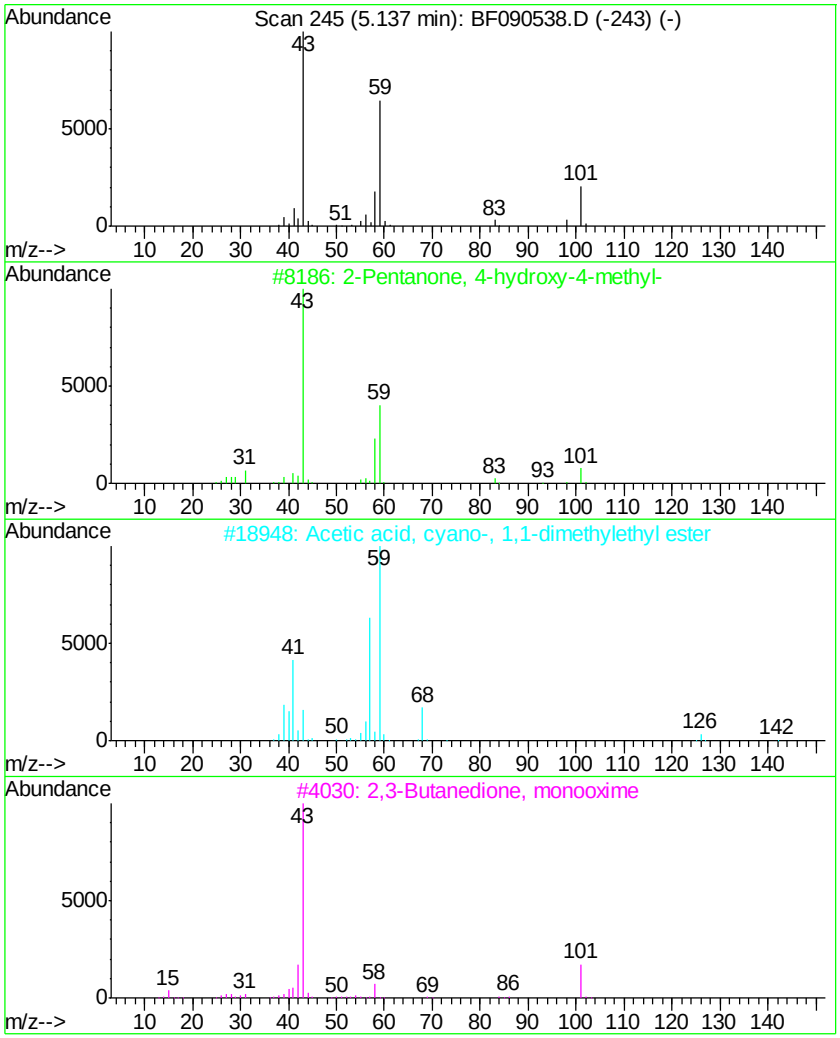
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

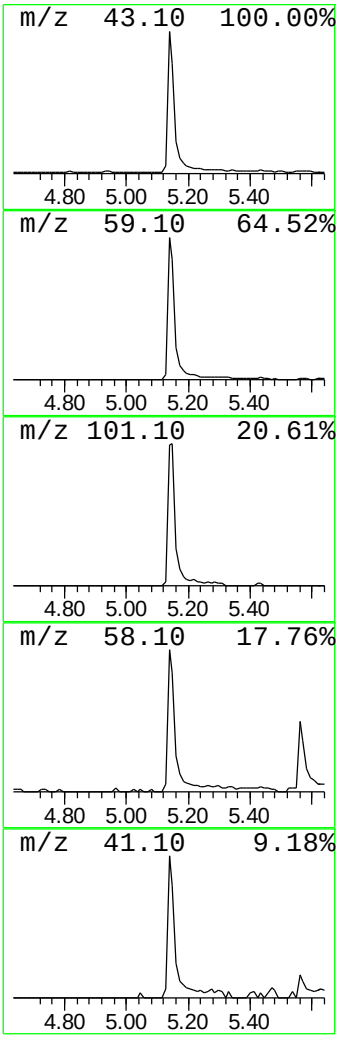
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.05 ng	365804	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

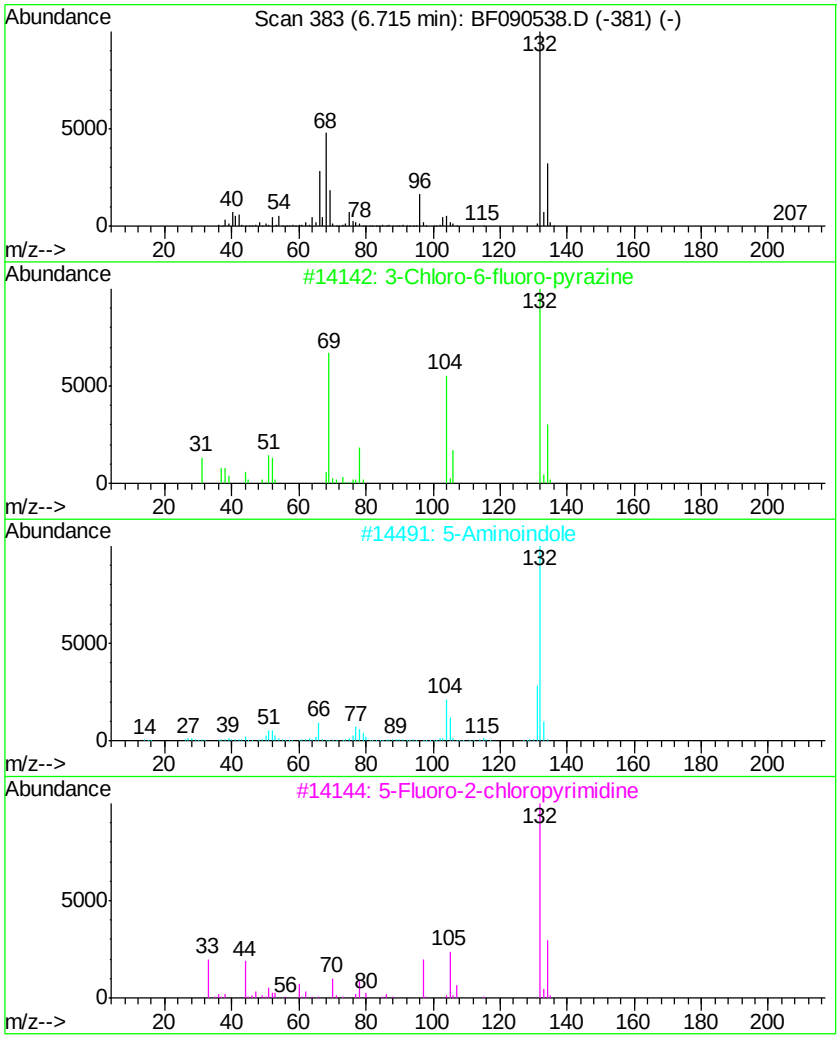
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

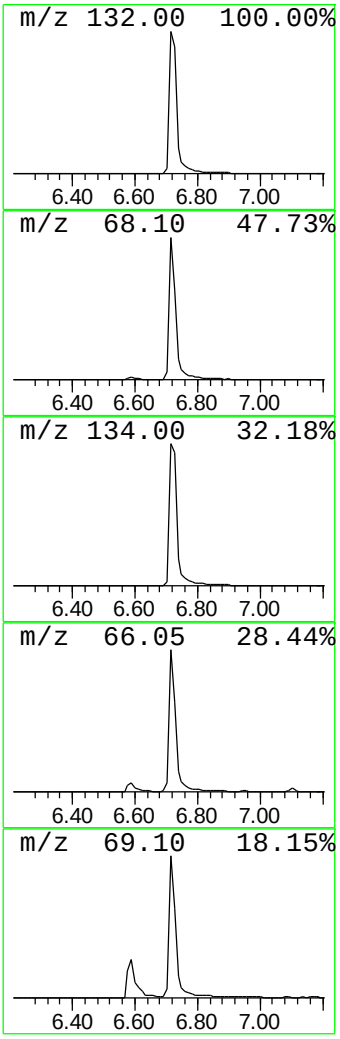
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	74.15 ng	4485410	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

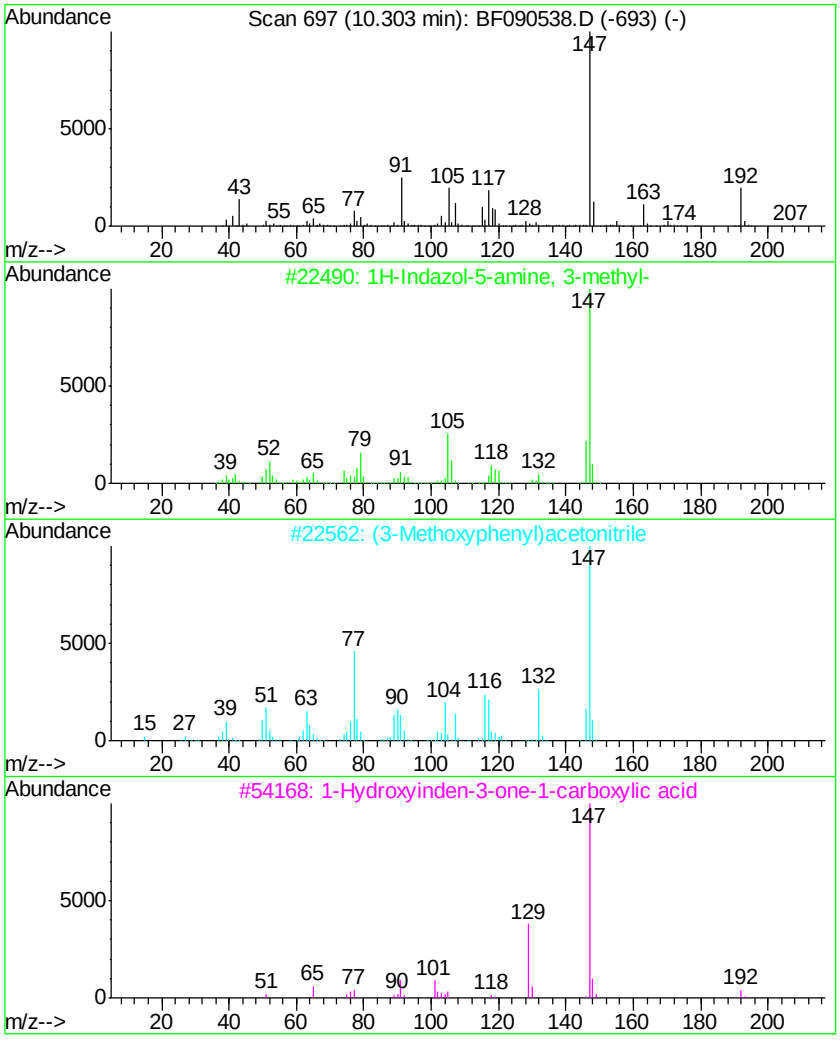
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

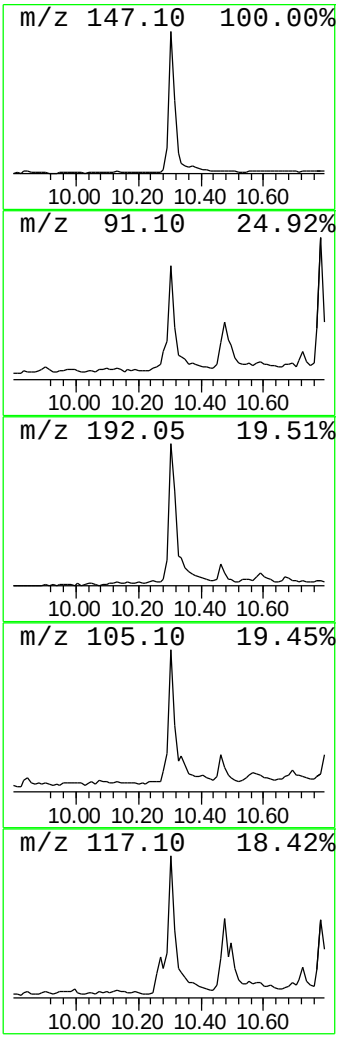
****

Peak Number 4 1H-Indazol-5-amine, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	11.65 ng	1098060	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indazol-5-amine, 3-methyl-	147	C8H9N3	1000338-20-2	53
2	(3-Methoxyphenyl)acetonitrile	147	C9H9NO	019924-43-7	53
3	1-Hydroxyinden-3-one-1-carboxyli...	192	C10H8O4	1000215-33-8	49
4	Benzoic acid, 4-propyl-, 4-cyano...	265	C17H15NO2	056131-49-8	47
5	2,6-Dimethylphenyl isocyanate	147	C9H9NO	028556-81-2	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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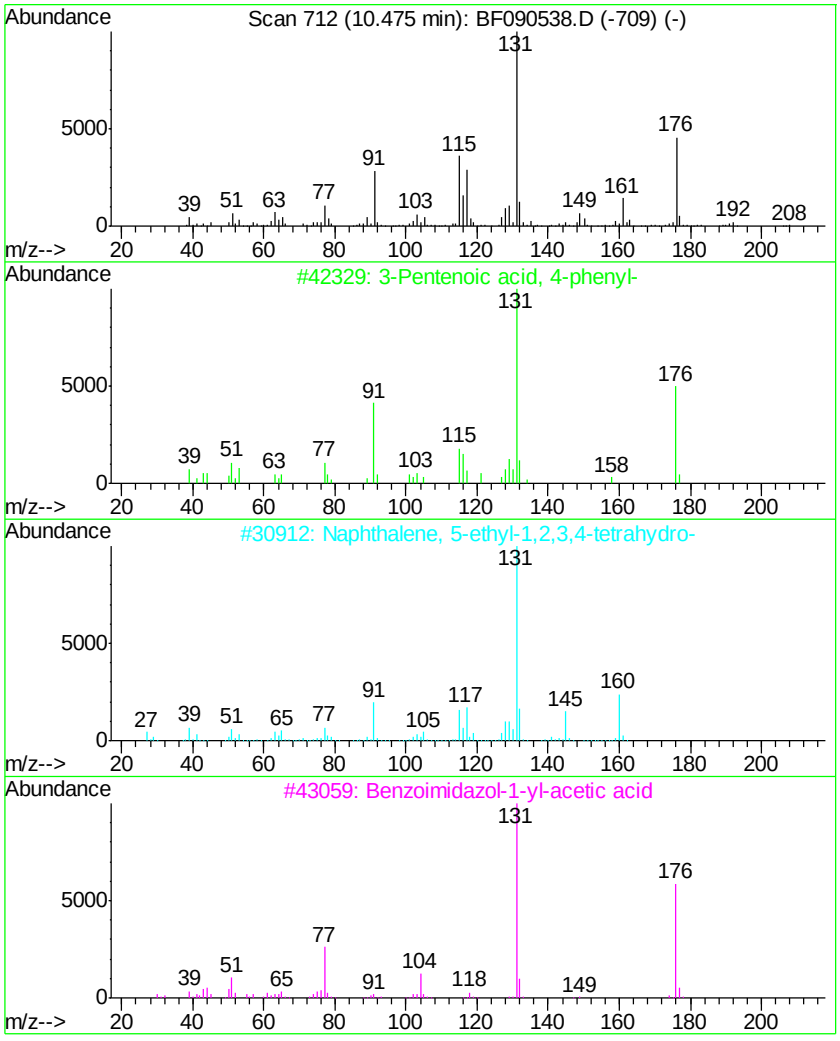
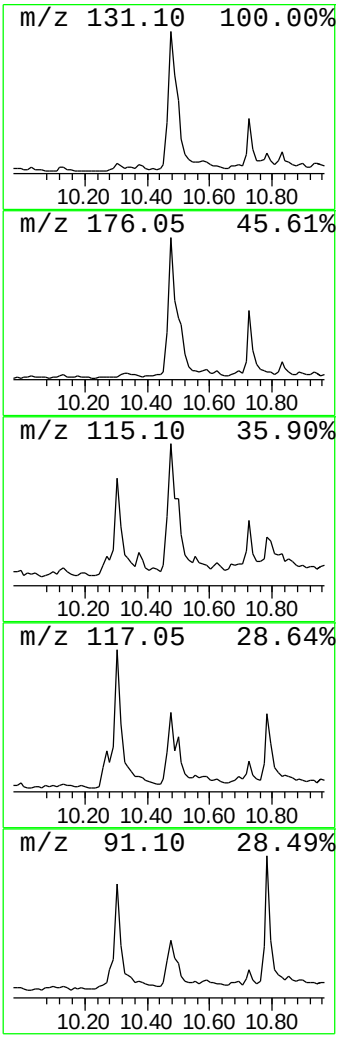
Peak Number 5 3-Pentenoic acid, 4-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	8.22 ng	774909	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	74
2	Naphthalene, 5-ethyl-1,2,3,4-tet...	160	C12H16	042775-75-7	58
3	Benzoimidazol-1-yl-acetic acid	176	C9H8N2O2	1000317-79-2	50
4	2-Propenoic acid, 3-phenyl-, eth...	176	C11H12O2	000103-36-6	50
5	3-Phenyl-4,5-dimethyl-2,1-oxabor...	202	C13H19BO	1000062-26-1	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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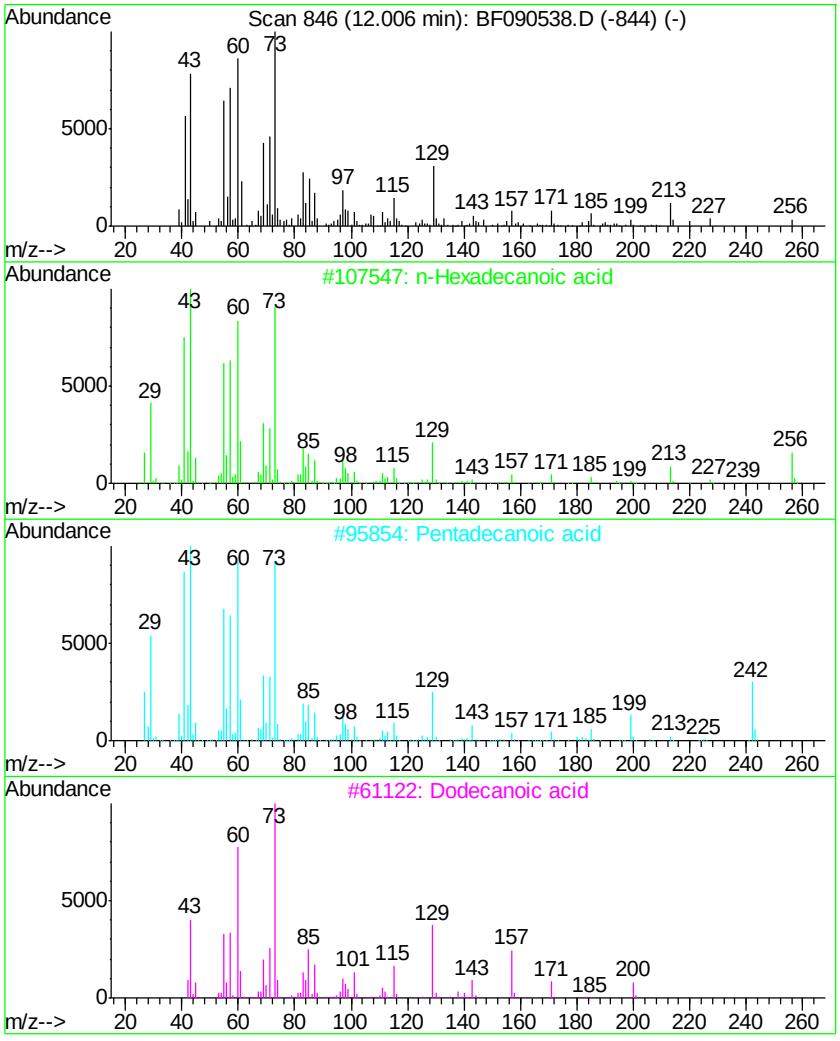
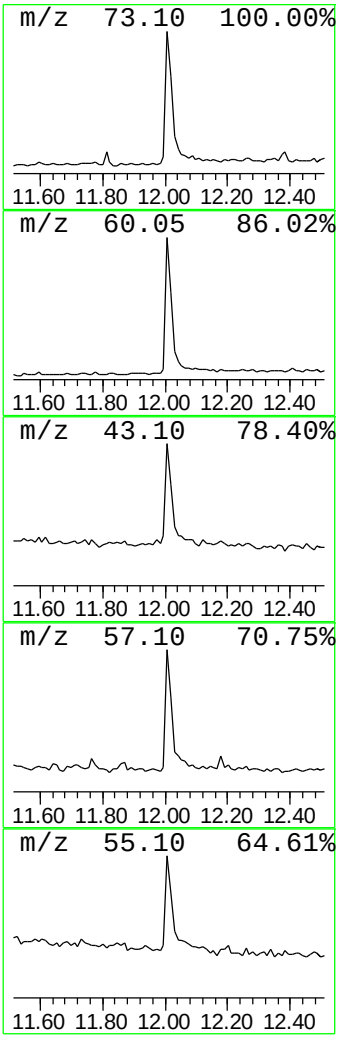
Peak Number 6 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.38 ng	224065	Phenanthrene-d10	11.48

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	90
3	Dodecanoic acid	200	C12H24O2	000143-07-7	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Tridecane	184	C13H28	000629-50-5	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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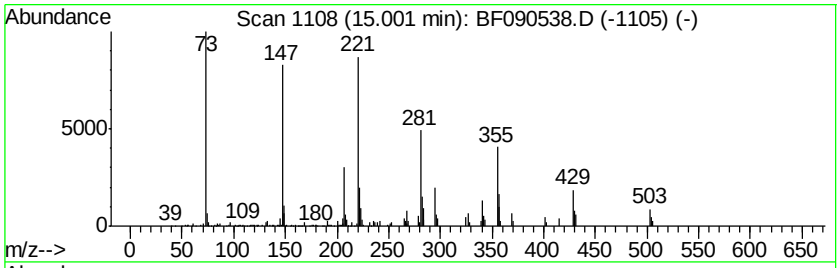
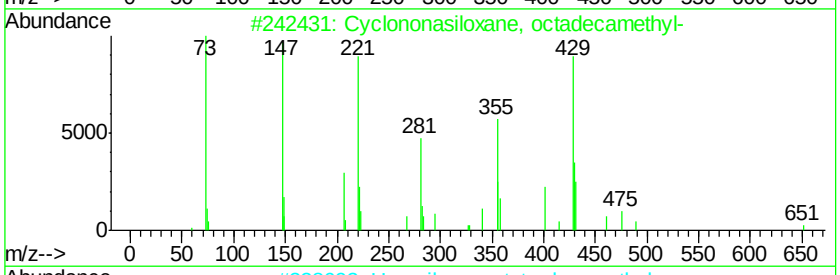
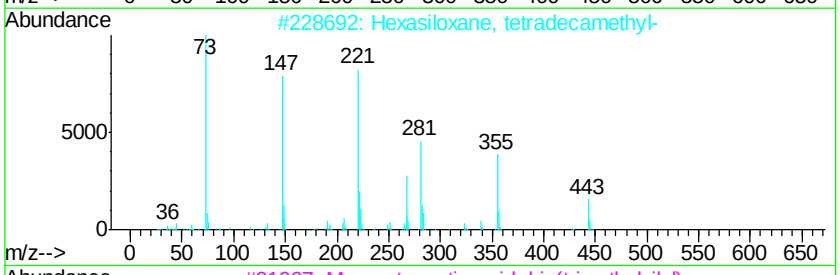
Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 12

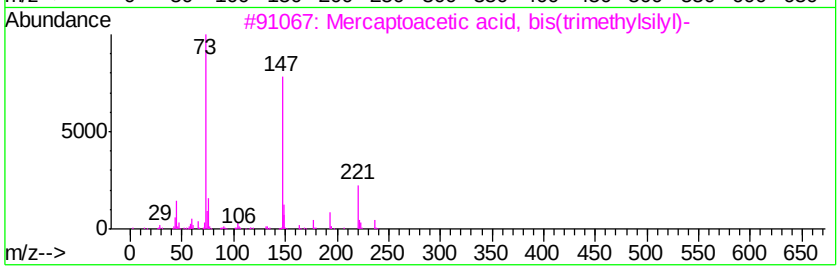
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	3.36 ng	184956	Perylene-d12	15.60

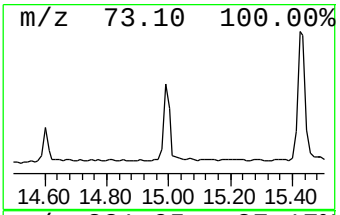
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	83
3	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	28
5	4-Hydroxybenzyl alcohol, bis(ter...	352	C19H36O2Si2	1000364-43-9	17

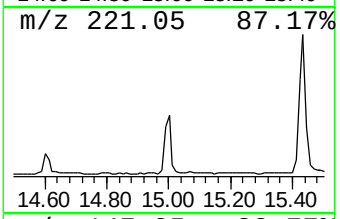


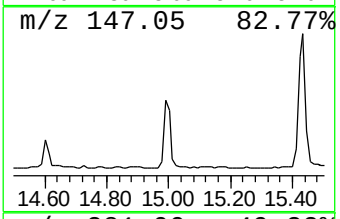


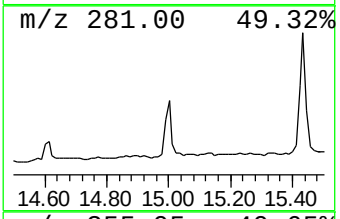


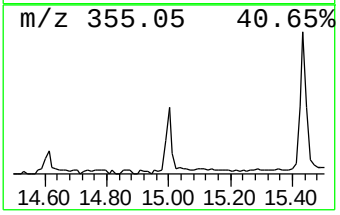












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101216\
Data File : BF090538.D
Acq On : 12 Oct 2016 16:32
Operator : UM/SJ
Sample : H5158-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RAV-GT-113

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	6.0	ng	365804	1	6.94	1209760	20.0
unknown6.71	6.71	74.2	ng	4485410	1	6.94	1209760	20.0
1H-Indazol-5-amin...	10.30	11.7	ng	1098060	3	9.99	1885310	20.0
3-Pentenoic acid,...	10.47	8.2	ng	774909	3	9.99	1885310	20.0
n-Hexadecanoic acid	12.01	2.4	ng	224065	4	11.48	1879730	20.0
Cyclononasiloxane...	15.00	3.4	ng	184956	6	15.60	1099630	20.0