LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

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-BF090115.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	1.247	11	14	17	rBV	823166	1037730	76.13%	6.877%
2	1.327	19	21	25	rVB	18074	23469	1.72%	0.156%
3	1.441	30	31	37	rBV	66600	170231	12.49%	1.128%
4	1.533	37	39	72	rVB	373407	1363119	100.00%	9.033%
5	4.459	291	295	315	rBV	247959	686634	50.37%	4.550%
6	5.327	368	371	395	rBB	608308	1178087	86.43%	7.807%
7	7.590	566	569	574	rBV	636322	1219535	89.47%	8.082%
8	7.682	574	577	586	rVB	654426	1261850	92.57%	8.362%
9	8.173	617	620	627	rVB	187559	306793	22.51%	2.033%
10	8.493	644	648	656	rBB	504001	869547	63.79%	5.763%
11	9.465	729	733	743	rBV	400180	793421	58.21%	5.258%
12	11.065	870	873	882	rBV	216429	388997	28.54%	2.578%
13	13.717	1100	1105	1108	rBV	665976	1308268	95.98%	8.670%
14	14.768	1194	1197	1205	rBB	121917	199507	14.64%	1.322%
15	15.191	1230	1234	1240	rBB2	227526	422231	30.98%	2.798%
16	16.597	1354	1357	1360	rBV	8811	14760	1.08%	0.098%
17	17.100	1397	1401	1410	rVB	467705	821731	60.28%	5.446%
18	17.740	1453	1457	1465	rBB	15172	33648	2.47%	0.223%
19	18.700	1537	1541	1544	rBV	266967	443802	32.56%	2.941%
20	18.826	1549	1552	1555	rBV	12954	23228	1.70%	0.154%
21	19.854	1638	1642	1645	rVB	9162	14266	1.05%	0.095%
22	20.460	1692	1695	1709	rBV	73651	147800	10.84%	0.979%
23	21.352	1764	1773	1775	rBV	20750	40655	2.98%	0.269%
24	21.866	1816	1818	1826	rBV	19336	33084	2.43%	0.219%
25	21.992	1826	1829	1833	rVB	11103	13771	1.01%	0.091%
26	22.072	1833	1836	1839	rBV	1095100	1289447	94.60%	8.545%
27	23.352	1942	1948	1950	rBV2	306457	603714	44.29%	4.001%
28	23.455	1955	1957	1960	rBV	15638	21324	1.56%	0.141%
29	24.015	2003	2006	2008	rBV	12381	19802	1.45%	0.131%
30	24.609	2055	2058	2062	rBV4	5965	14737	1.08%	0.098%
31	24.781	2071	2073	2076	rBV	250205	281114	20.62%	1.863%
32	25.215	2109	2111	2118	rVB2	22854	43422	3.19%	0.288%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-3(0-5)

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

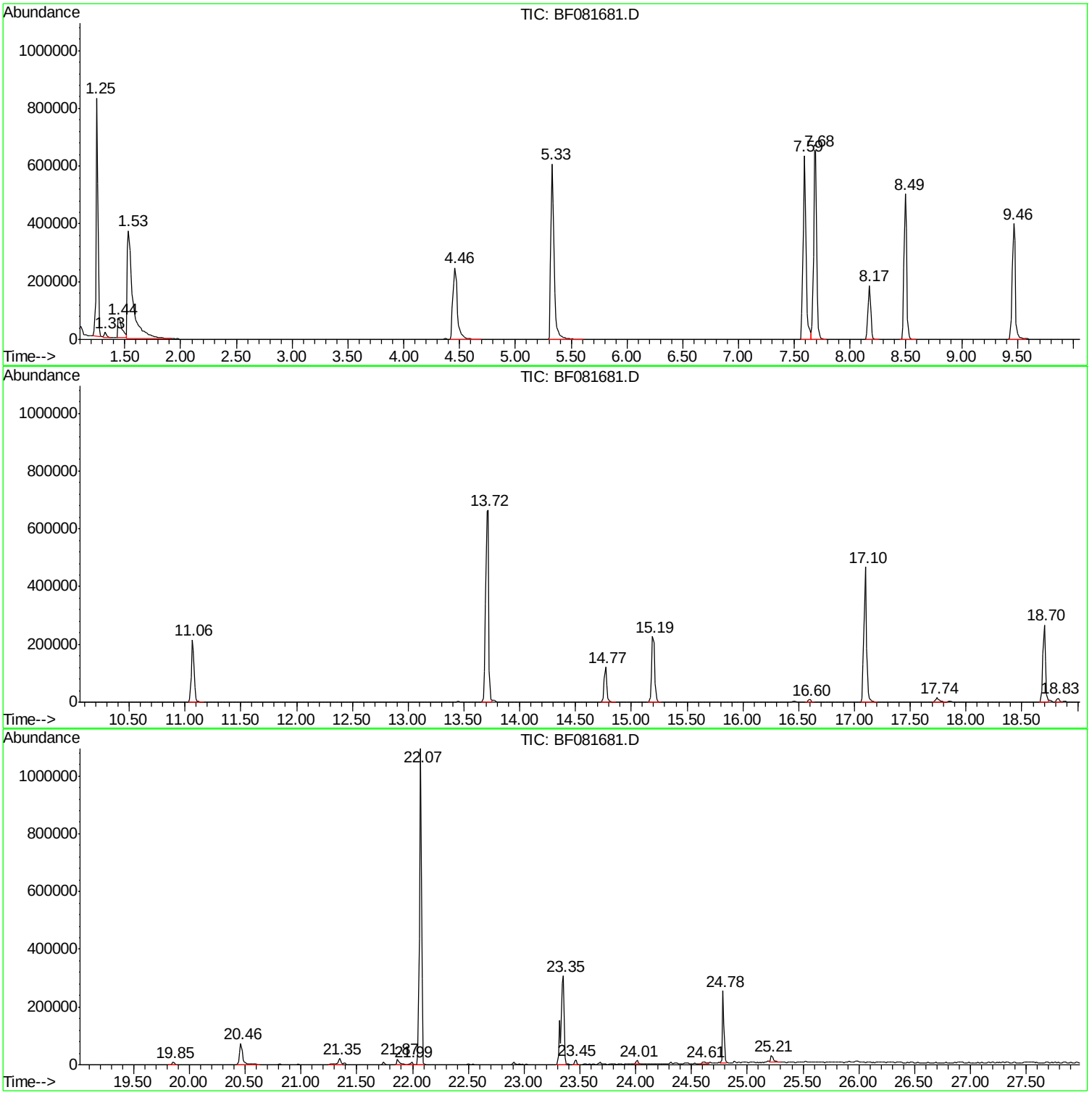
Sum of corrected areas: 15089724

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF091715\
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ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

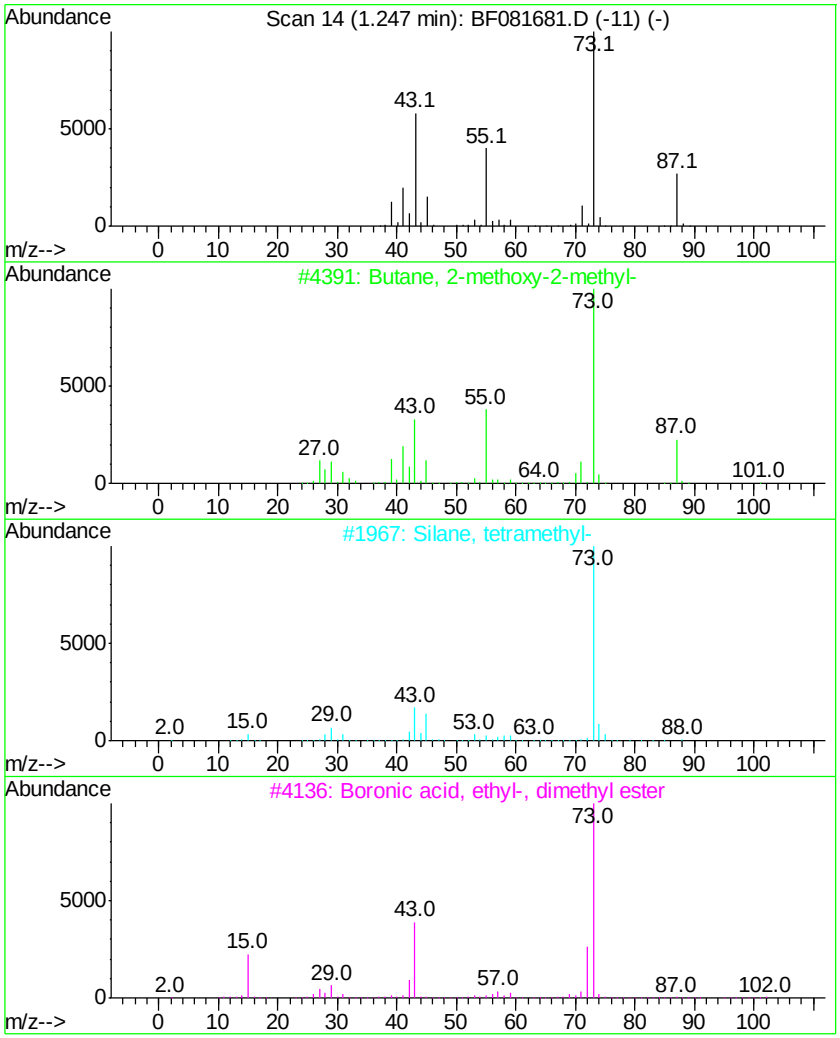
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

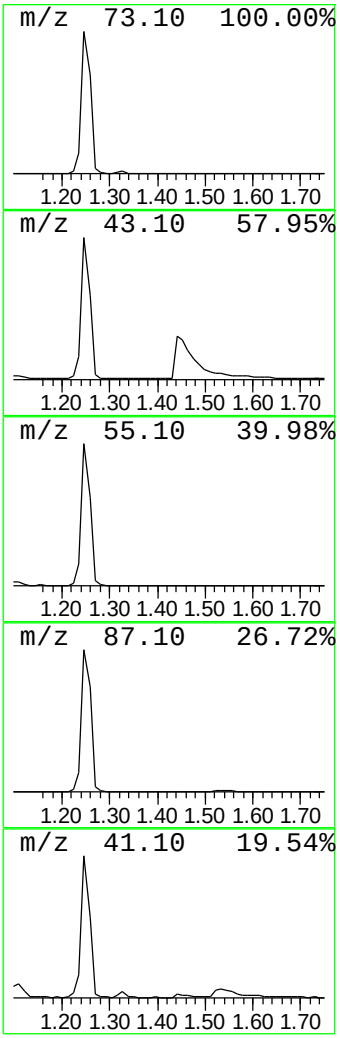
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.25	67.65 ng	1037730	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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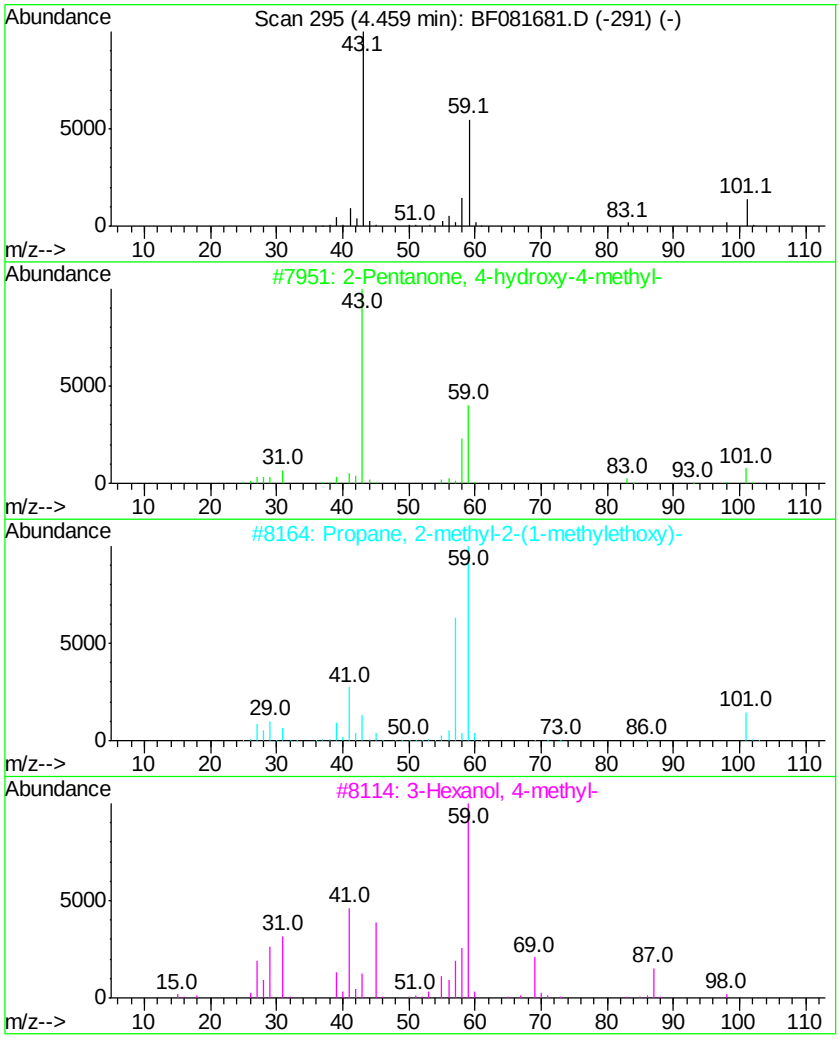
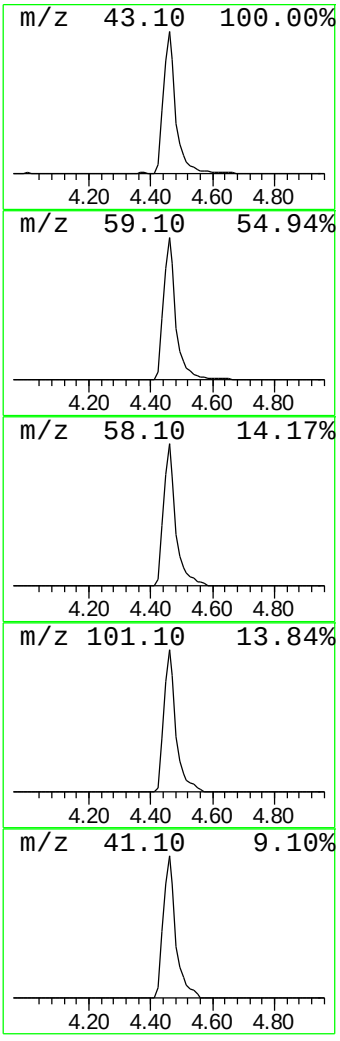
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	44.76 ng	686634	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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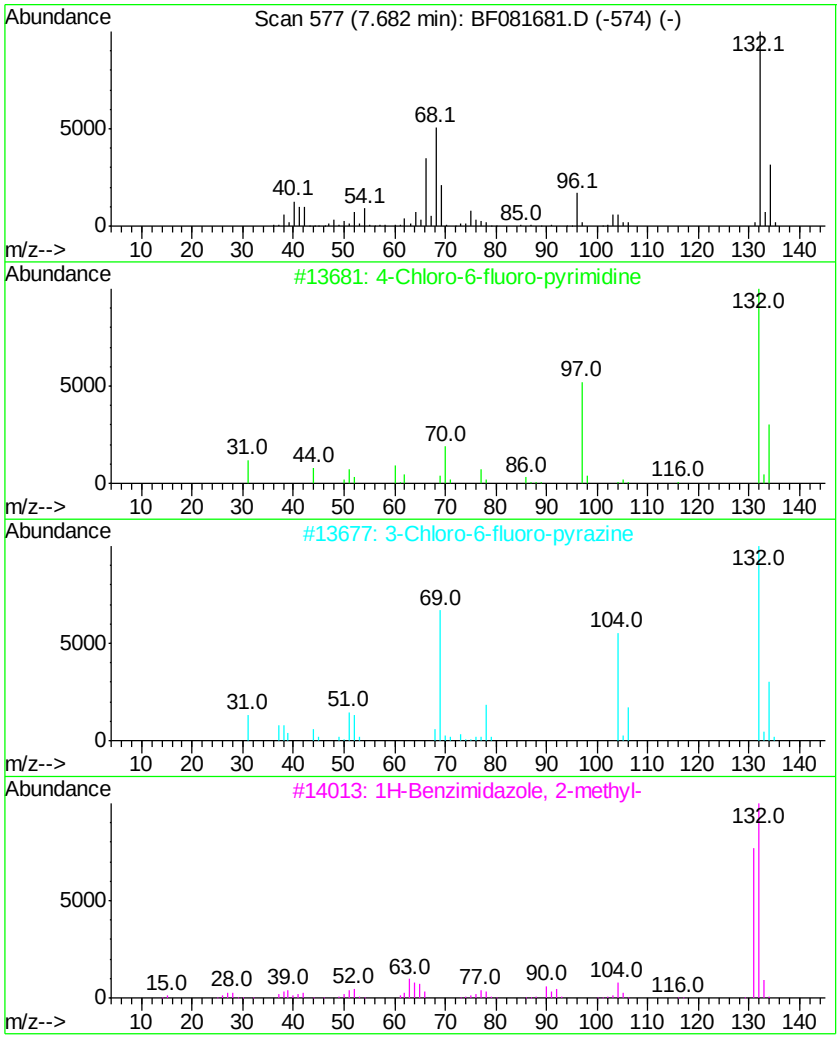
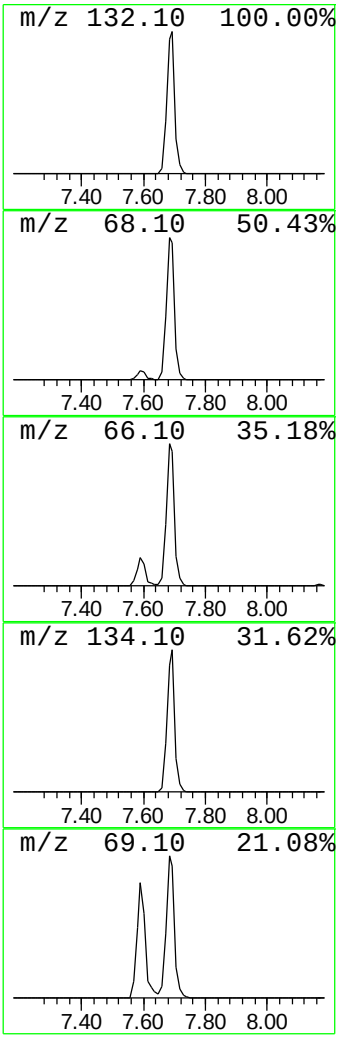
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	82.26 ng	1261850	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





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Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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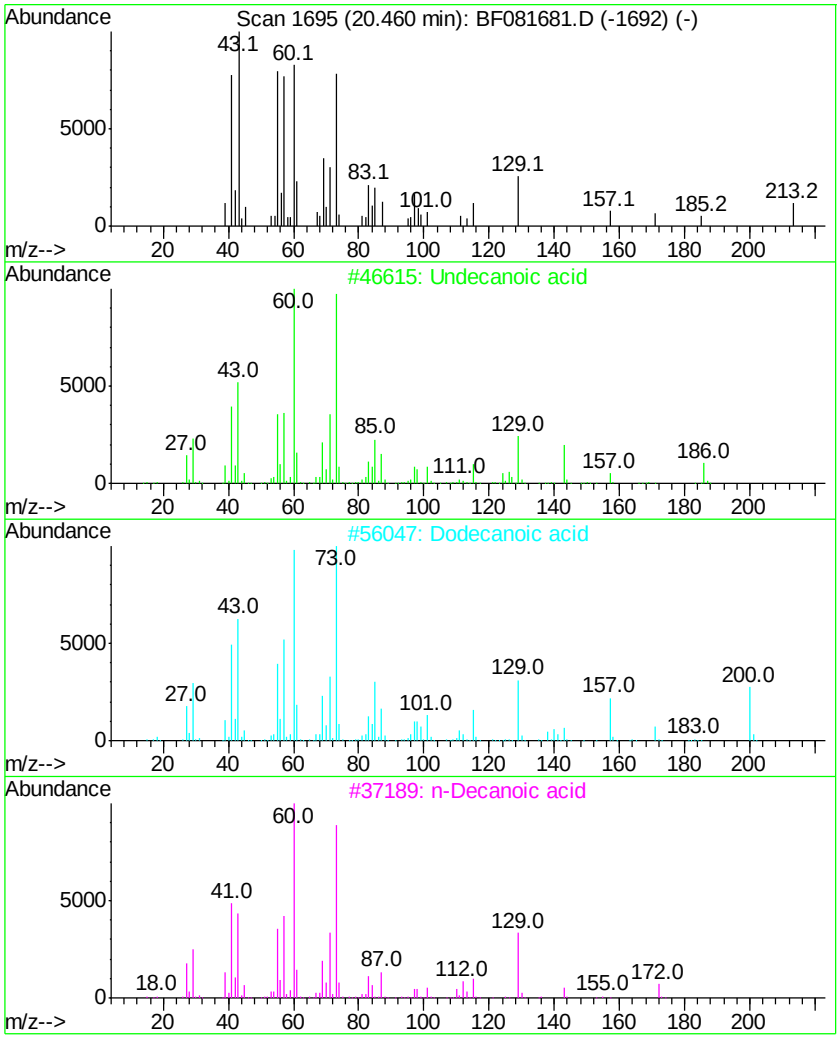
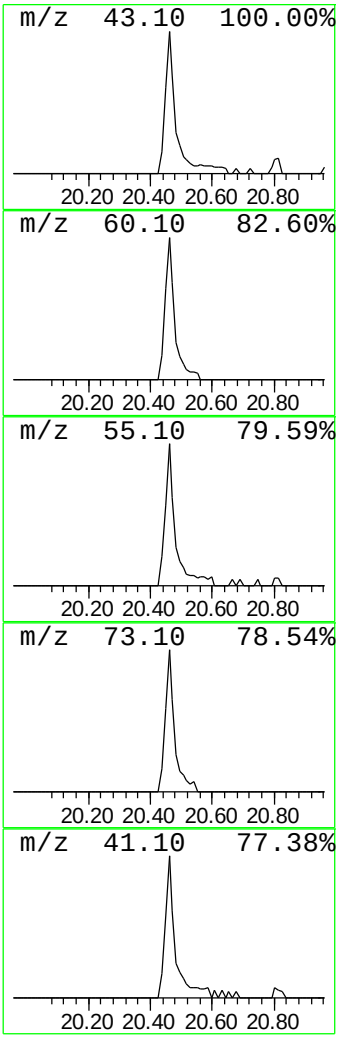
Peak Number 7 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	6.66 ng	147800	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
5	N-(5-Oxo-tetrahydro-furan-2-ylme...	157	C7H11NO3	1000188-71-2	35





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Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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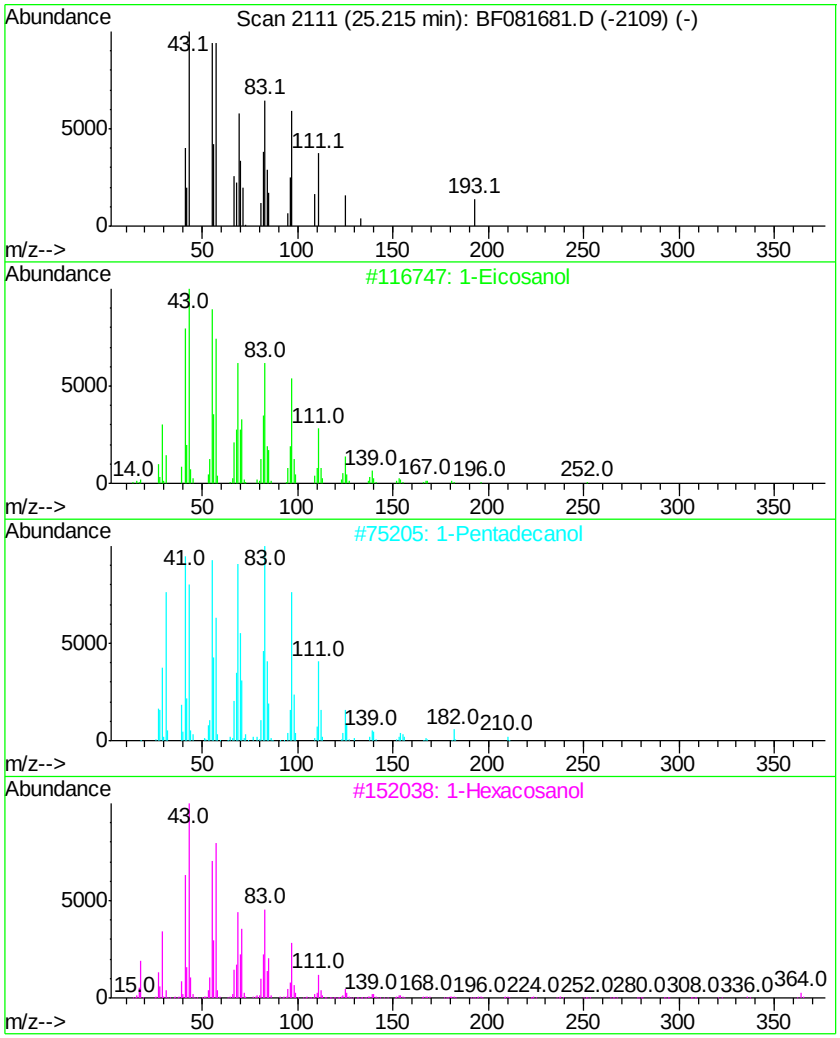
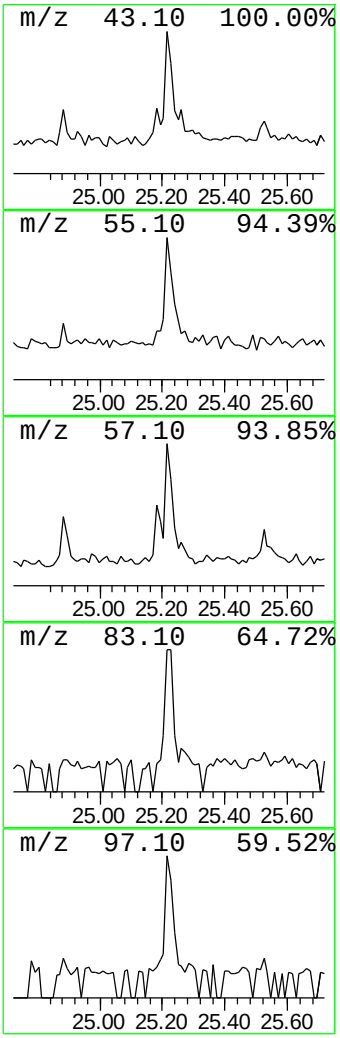
Peak Number 8 1-Eicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.22	3.09 ng	43422	Perylene-d12	24.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	87
2	1-Pentadecanol	228	C15H32O	000629-76-5	72
3	1-Hexacosanol	382	C26H54O	000506-52-5	58
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	53
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091715\
Data File : BF081681.D
Acq On : 17 Sep 2015 16:20
Operator : UM/IZ
Sample : G3664-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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
Butane, 2-methoxy...	1.25	67.7	ng	1037730	1	8.17	306793	20.0
2-Pentanone, 4-hy...	4.46	44.8	ng	686634	1	8.17	306793	20.0
unknown7.68	7.68	82.3	ng	1261850	1	8.17	306793	20.0
Undecanoic acid	20.46	6.7	ng	147800	4	18.70	443802	20.0
1-Eicosanol	25.22	3.1	ng	43422	6	24.78	281114	20.0