LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082378.D
Acq On : 20 Oct 2015 3:07
Operator : UM/IZ
Sample : G4040-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

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-BF101015.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	4.971	244	248	256	rBV	899171	1343724	52.88%	5.987%
2	5.406	283	286	288	rBV	1511506	1989771	78.30%	8.865%
3	5.794	318	320	323	rVB	32618	33773	1.33%	0.150%
4	6.446	374	377	385	rBV	1849335	1941330	76.39%	8.649%
5	6.572	385	388	390	rBV	2376778	2154355	84.78%	9.599%
6	6.800	406	408	411	rBV	605549	519557	20.45%	2.315%
7	6.960	419	422	424	rBV	1787637	1774761	69.84%	7.907%
8	7.372	455	458	461	rBV	1139690	1167228	45.93%	5.200%
9	8.092	519	521	523	rBV	793602	673753	26.51%	3.002%
10	9.178	613	616	618	rBV	2290468	2541195	100.00%	11.322%
11	9.566	648	650	653	rBV	368397	403935	15.90%	1.800%
12	9.852	673	675	677	rBV	933838	805759	31.71%	3.590%
13	10.275	711	712	714	rVB	47275	45661	1.80%	0.203%
14	10.492	729	731	734	rBV	17424	28904	1.14%	0.129%
15	10.641	742	744	747	rBV	1246549	1351234	53.17%	6.020%
16	10.755	751	754	758	rVB	75716	101192	3.98%	0.451%
17	11.201	791	793	794	rVV	90341	80043	3.15%	0.357%
18	11.235	794	796	798	rVB	25929	37328	1.47%	0.166%
19	11.338	803	805	809	rBV2	826492	882042	34.71%	3.930%
20	11.418	809	812	813	rVB2	19725	34703	1.37%	0.155%
21	11.578	824	826	829	rBV4	20576	38689	1.52%	0.172%
22	11.623	829	830	832	rVB	26362	34773	1.37%	0.155%
23	11.875	850	852	854	rVV	122166	146222	5.75%	0.651%
24	11.955	857	859	864	rVB2	31693	56720	2.23%	0.253%
25	12.115	871	873	876	rBV	32733	48472	1.91%	0.216%
26	12.549	909	911	914	rBV	102153	117760	4.63%	0.525%
27	12.652	918	920	924	rBV4	16153	32653	1.28%	0.145%
28	12.778	929	931	934	rBV	101672	154680	6.09%	0.689%
29	12.938	942	945	947	rBV	1733703	2214011	87.12%	9.864%
30	13.864	1023	1026	1030	rBV	87421	177336	6.98%	0.790%
31	14.012	1036	1039	1046	rBV	620455	794900	31.28%	3.542%
32	15.464	1164	1166	1169	rVV	40876	59219	2.33%	0.264%
33	15.521	1169	1171	1178	rVB	407044	601623	23.67%	2.680%
34	16.184	1227	1229	1232	rVB	39493	57231	2.25%	0.255%

LSC Area Percent Report

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Operator : UM/IZ
Sample : G4040-03
Misc :
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Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

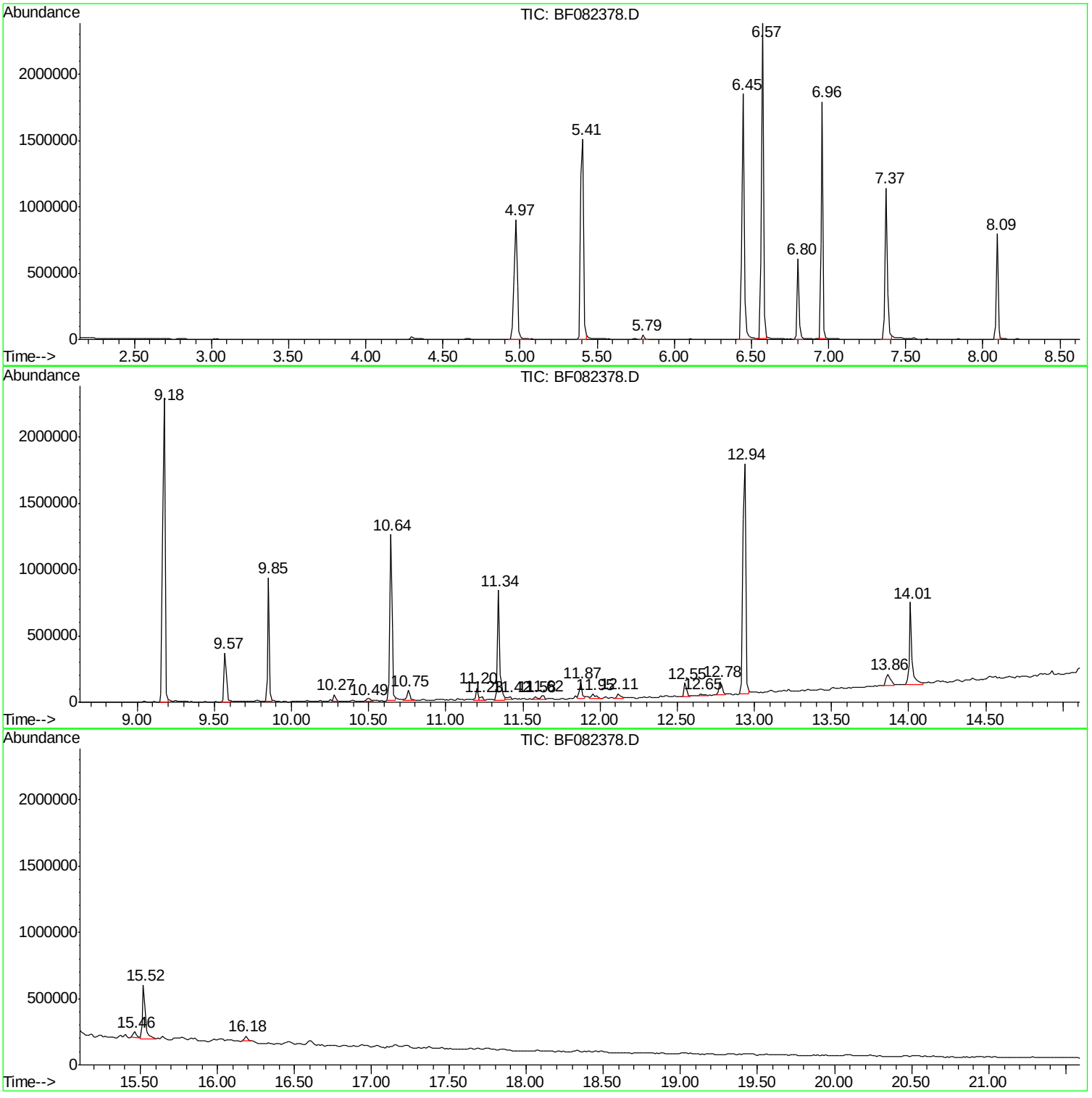
Sum of corrected areas: 22444537

Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
Data File : BF082378.D
Acq On : 20 Oct 2015 3:07
Operator : UM/IZ
Sample : G4040-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-MLA-2.5-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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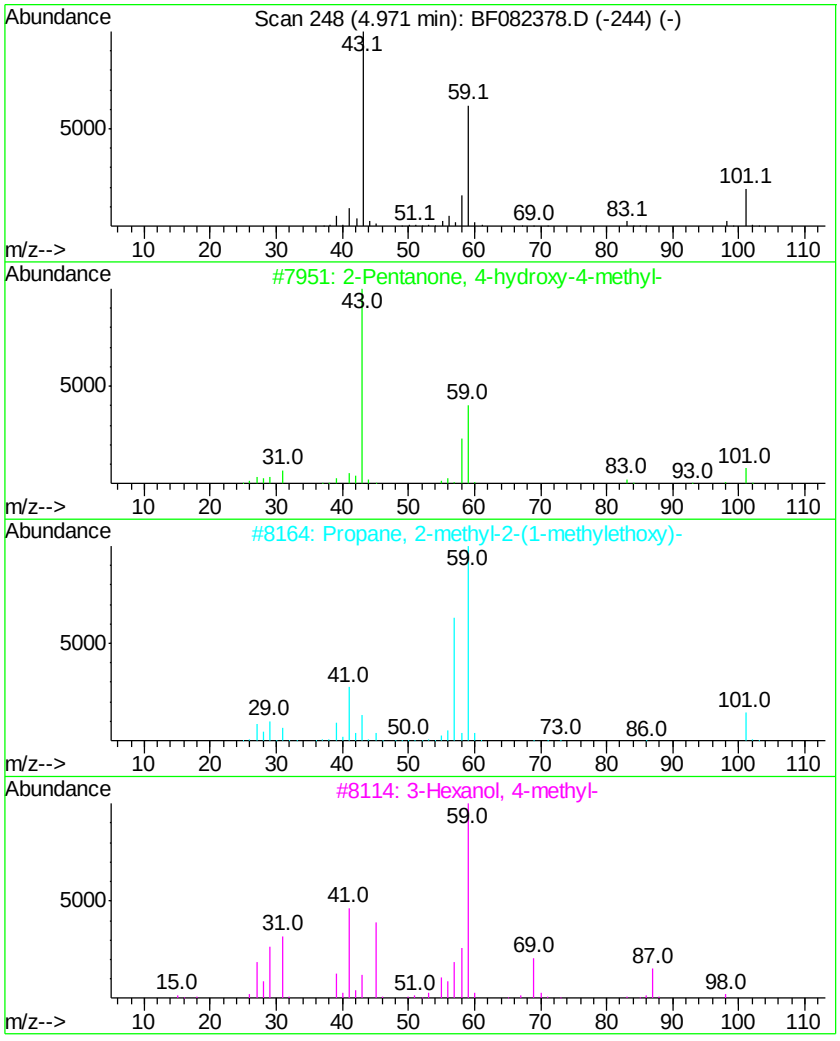
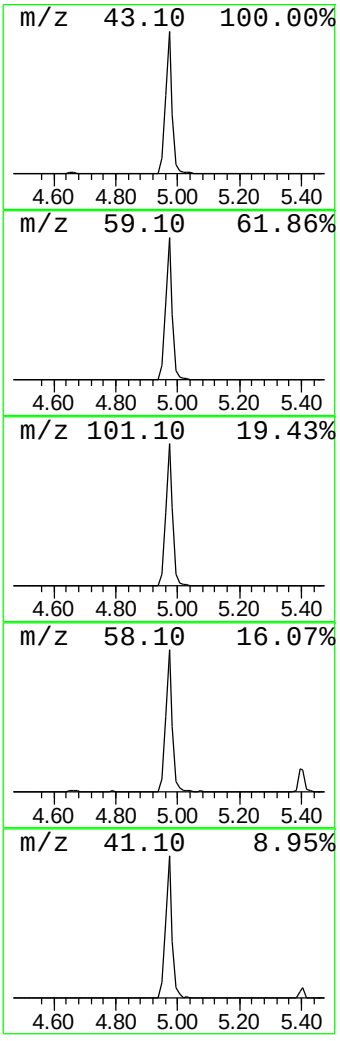
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	51.73 ng	1343720	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	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
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Operator : UM/IZ
Sample : G4040-03
Misc :
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Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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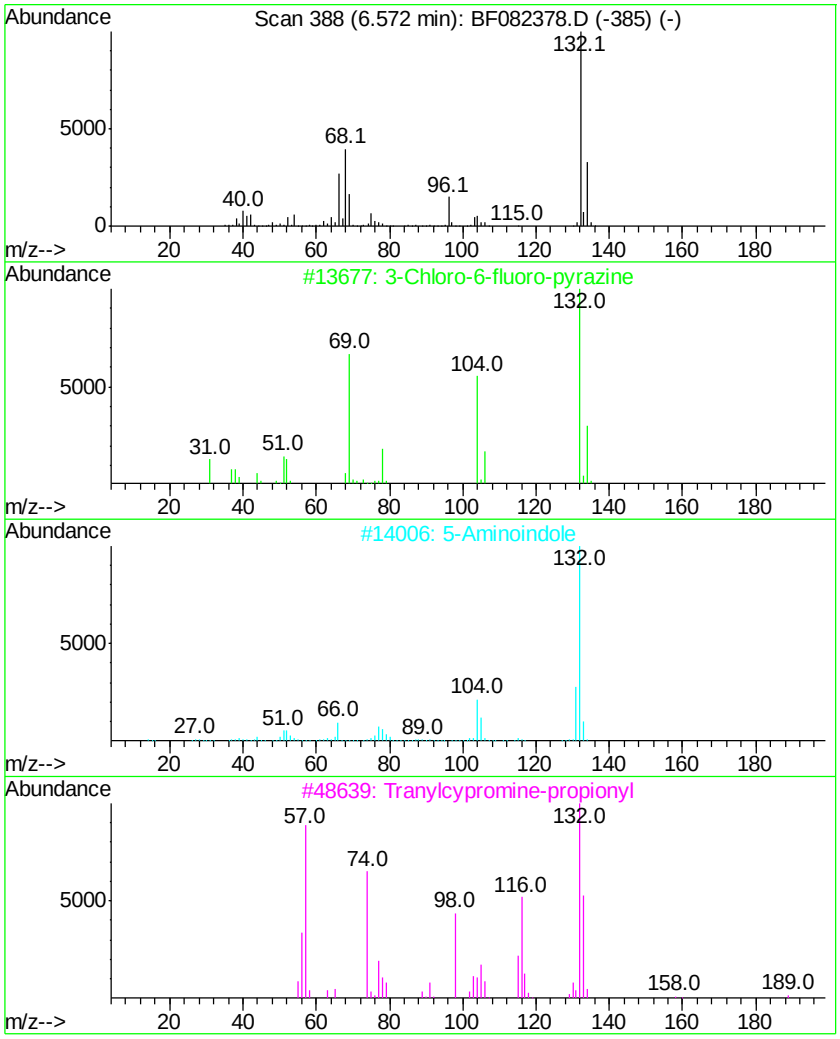
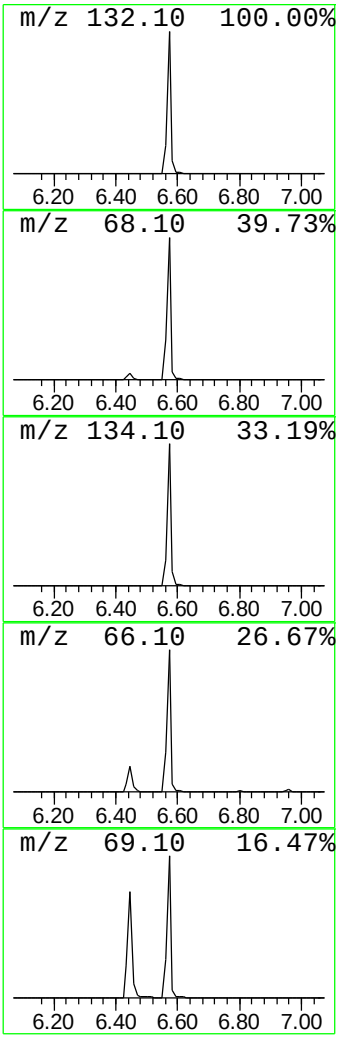
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	82.93 ng	2154360	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : G4040-03
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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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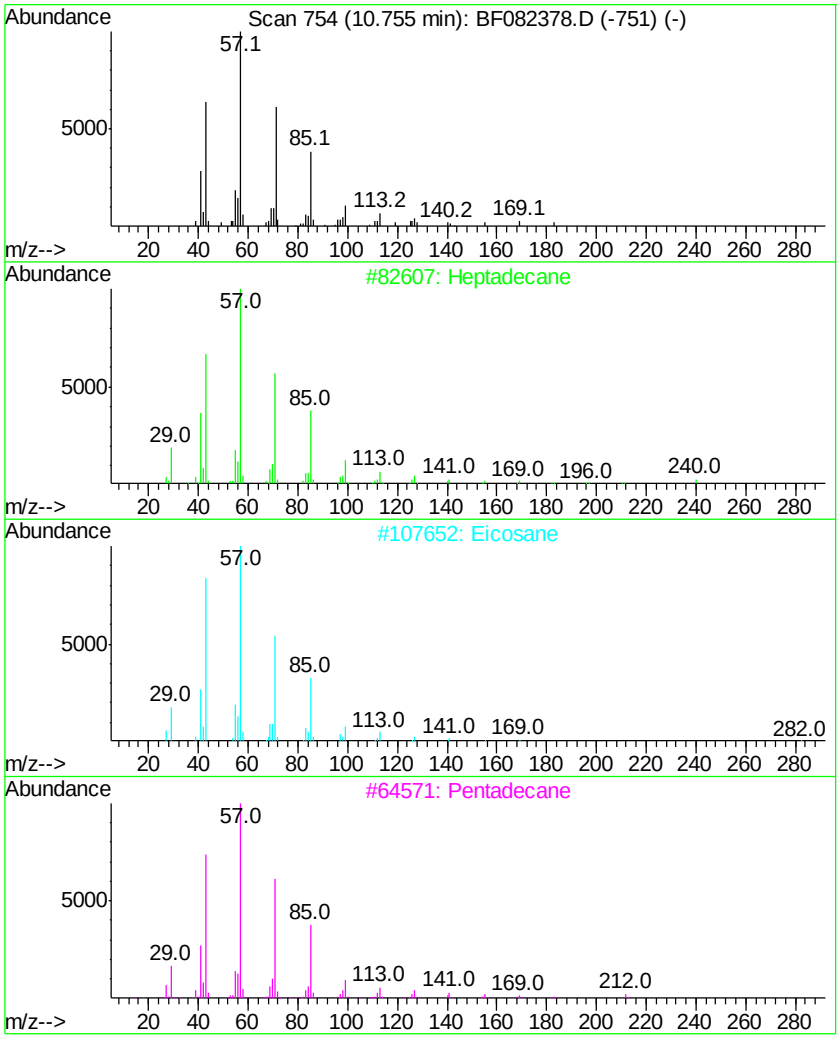
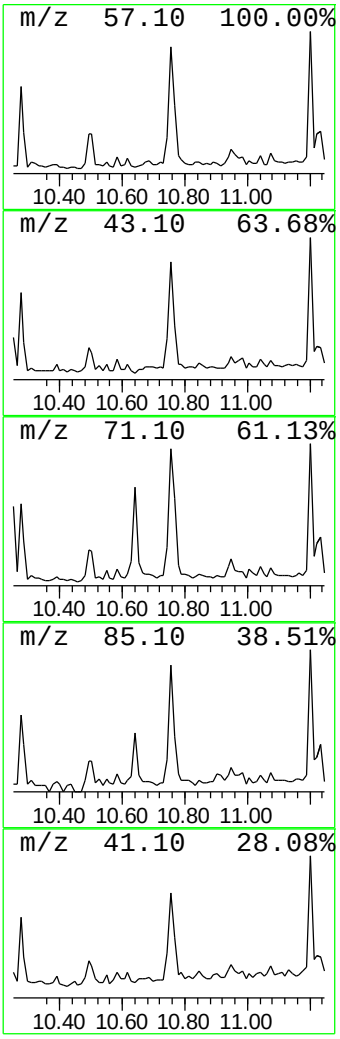
Peak Number 4 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.29 ng	101192	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Hexadecane	226	C16H34	000544-76-3	90





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF101915\
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Sample : G4040-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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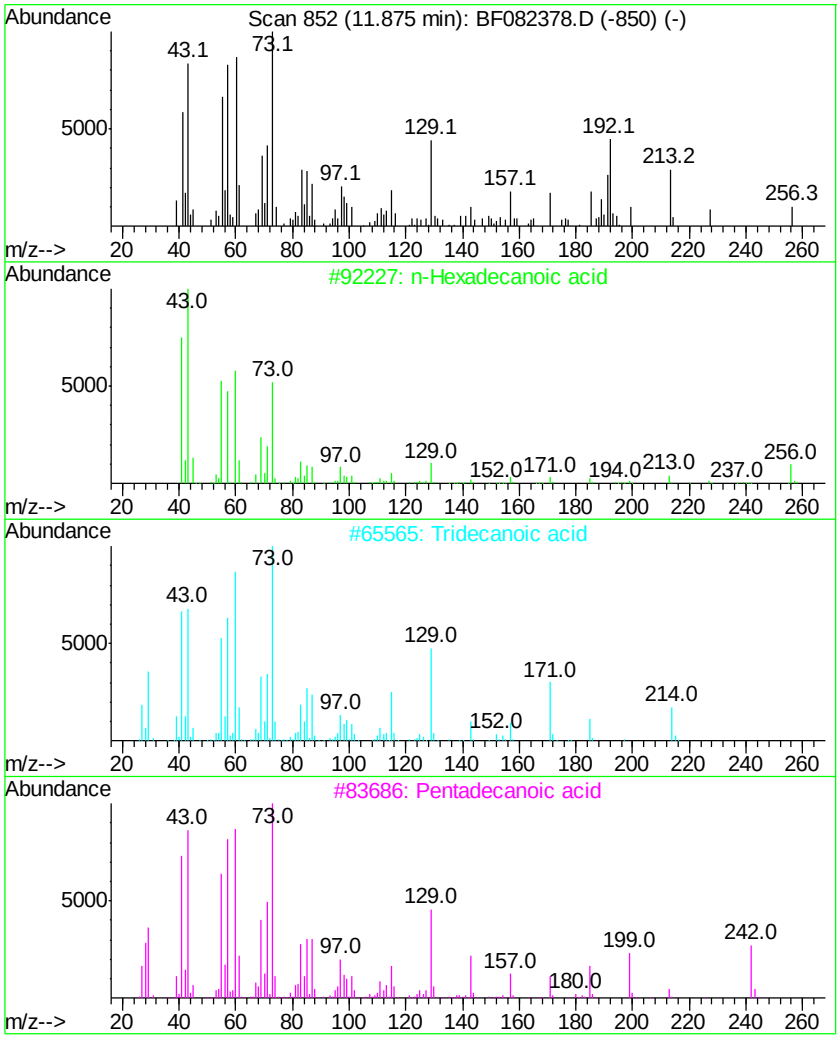
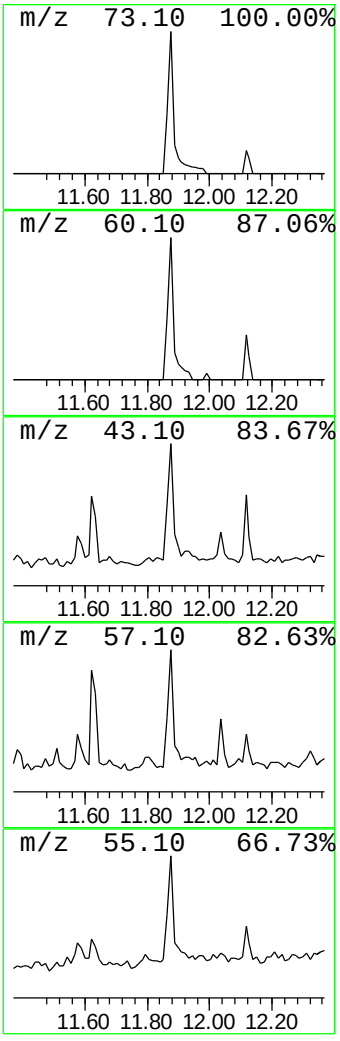
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.32 ng	146222	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Sample : G4040-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MLA-2.5-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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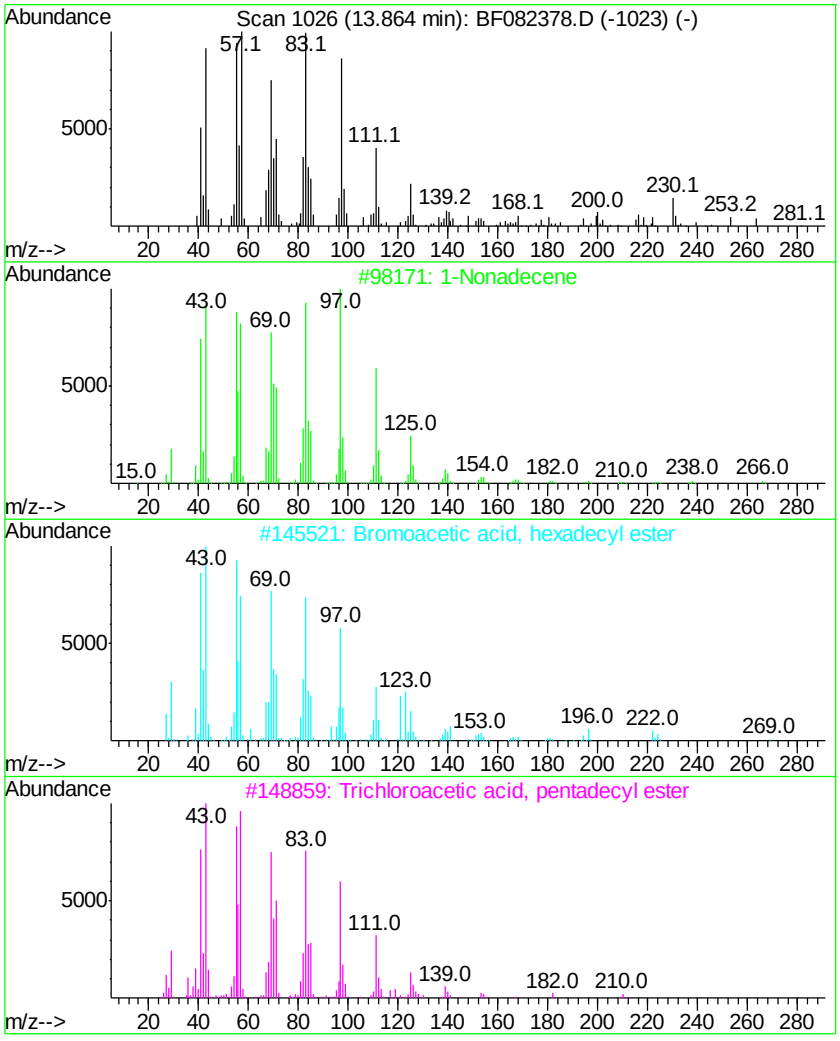
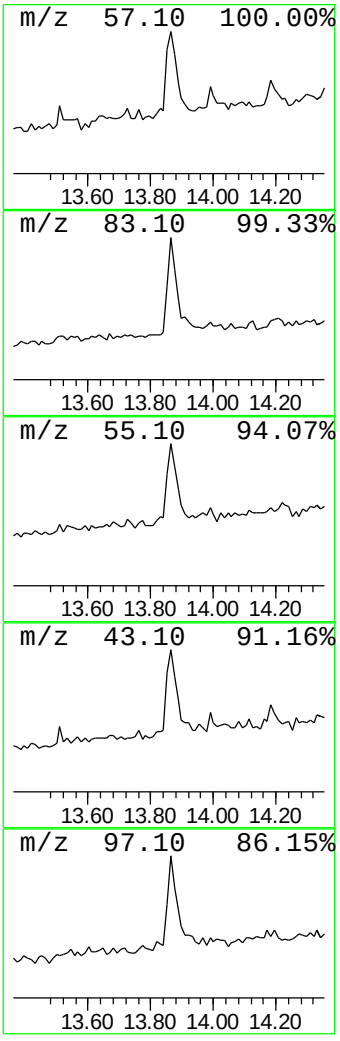
Peak Number 6 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.46 ng	177336	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	87
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	76
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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...	4.97	51.7	ng	1343720	1	6.80	519557	20.0
unknown6.57	6.57	82.9	ng	2154360	1	6.80	519557	20.0
Heptadecane	10.75	2.3	ng	101192	4	11.34	882042	20.0
n-Hexadecanoic acid	11.87	3.3	ng	146222	4	11.34	882042	20.0
1-Nonadecene	13.86	4.5	ng	177336	5	14.01	794900	20.0