LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081480.D
Acq On : 5 Sep 2015 23:31
Operator : UM/IZ
Sample : G3555-05
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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	3.518	167	169	180	rBV	44264	99917	5.73%	0.604%
2	4.410	243	247	260	rVB	788237	1474450	84.57%	8.917%
3	4.913	288	291	293	rBV	1412714	1734649	99.49%	10.490%
4	6.022	386	388	391	rBV	1219545	1686993	96.76%	10.202%
5	6.124	395	397	399	rBV	1853685	1653805	94.86%	10.001%
6	6.353	415	417	420	rVB	399698	357095	20.48%	2.160%
7	6.513	429	431	433	rBV	1434020	1273336	73.03%	7.700%
8	6.936	465	468	470	rBV	1143061	1166250	66.89%	7.053%
9	7.645	528	530	532	rBV	536302	453694	26.02%	2.744%
10	8.730	622	625	627	rBV	1868163	1743494	100.00%	10.544%
11	9.130	658	660	663	rBV	367777	322471	18.50%	1.950%
12	9.382	680	682	685	rVB	480131	450807	25.86%	2.726%
13	10.171	748	751	753	rBV	1069549	1067053	61.20%	6.453%
14	10.319	762	764	768	rBV	23242	25278	1.45%	0.153%
15	10.765	801	803	804	rBV	24095	21236	1.22%	0.128%
16	10.845	808	810	813	rBV	419187	445551	25.56%	2.694%
17	11.428	859	861	866	rBV	59467	69655	4.00%	0.421%
18	12.296	934	937	939	rBV	97514	124508	7.14%	0.753%
19	12.342	939	941	942	rBV	17749	20617	1.18%	0.125%
20	12.365	942	943	946	rVB	27904	25046	1.44%	0.151%
21	12.434	946	949	951	rBV	1539086	1373648	78.79%	8.307%
22	12.994	995	998	1000	rBV	91388	92567	5.31%	0.560%
23	13.039	1000	1002	1003	rBV	19929	19347	1.11%	0.117%
24	13.359	1027	1030	1036	rBV	79534	156344	8.97%	0.945%
25	13.451	1036	1038	1041	rVB	351110	333142	19.11%	2.015%
26	13.679	1055	1058	1060	rBV	29159	31602	1.81%	0.191%
27	13.977	1082	1084	1087	rBV	30551	29745	1.71%	0.180%
28	14.274	1108	1110	1112	rBV	21623	23156	1.33%	0.140%
29	14.548	1132	1134	1137	rBV	17898	19619	1.13%	0.119%
30	14.765	1150	1153	1155	rBV	183014	240753	13.81%	1.456%

Sum of corrected areas: 16535828

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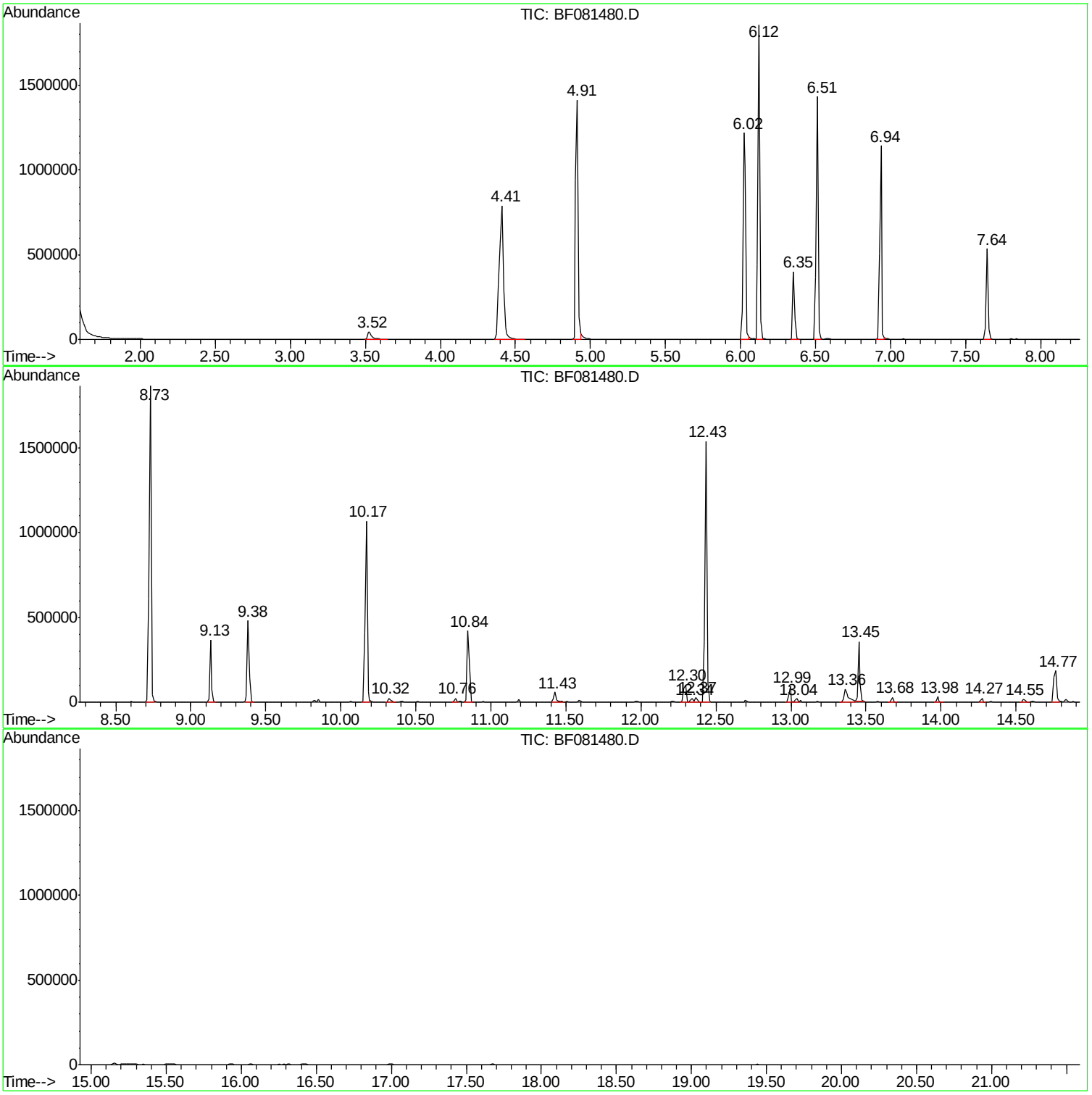
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-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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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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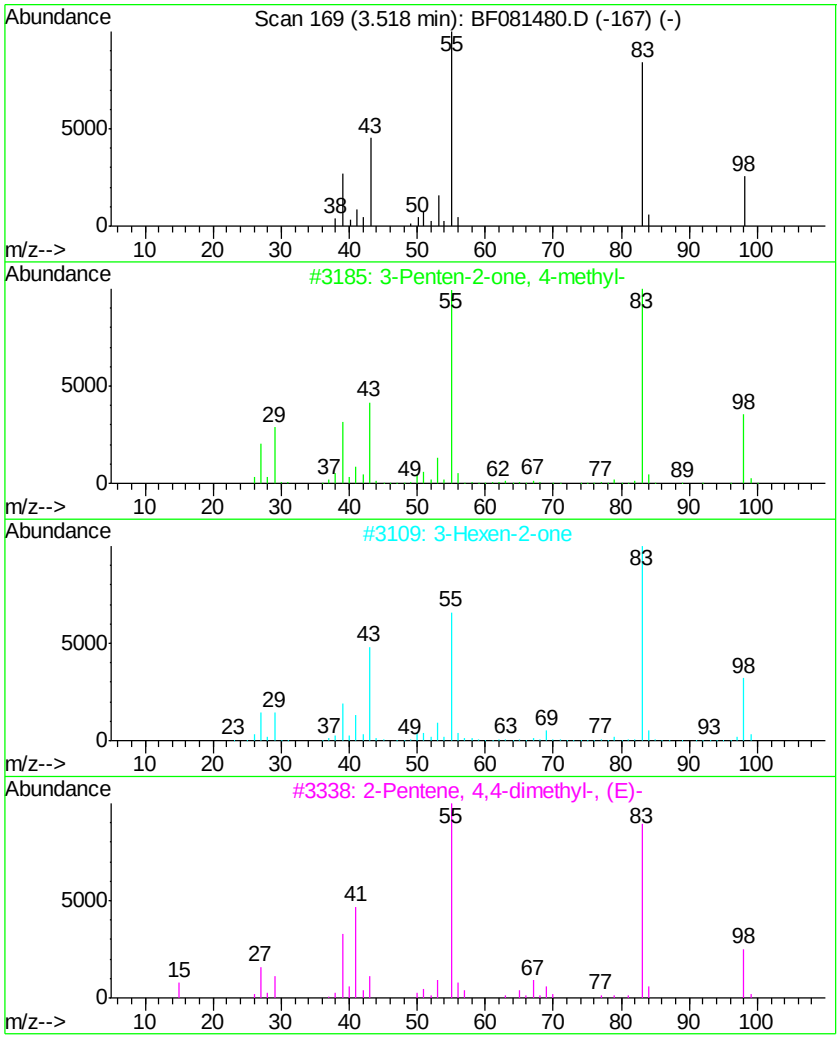
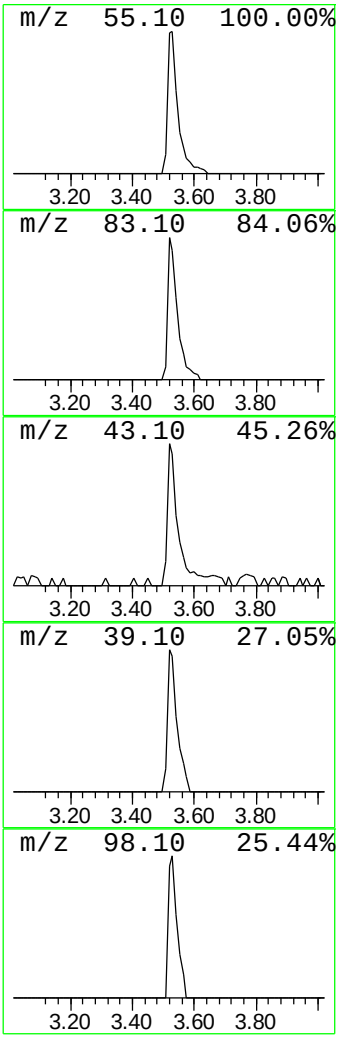
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.52	5.60 ng	99917	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





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Acq On : 5 Sep 2015 23:31
Operator : UM/IZ
Sample : G3555-05
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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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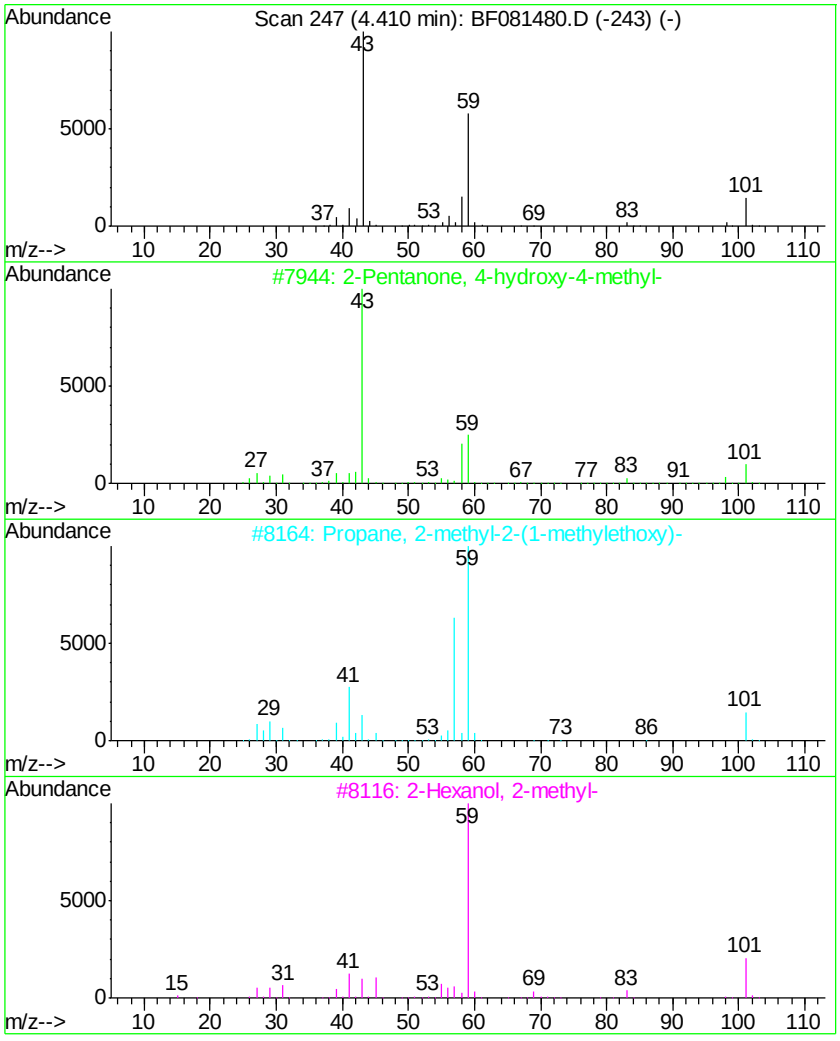
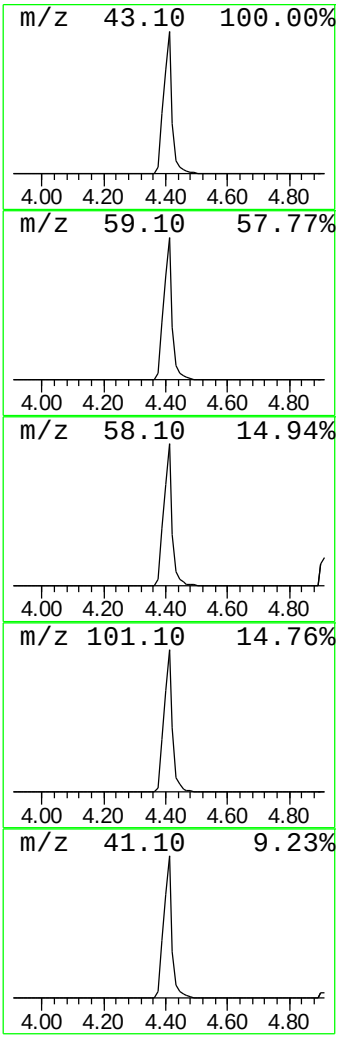
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	82.58 ng	1474450	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	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\BF090515\
Data File : BF081480.D
Acq On : 5 Sep 2015 23:31
Operator : UM/IZ
Sample : G3555-05
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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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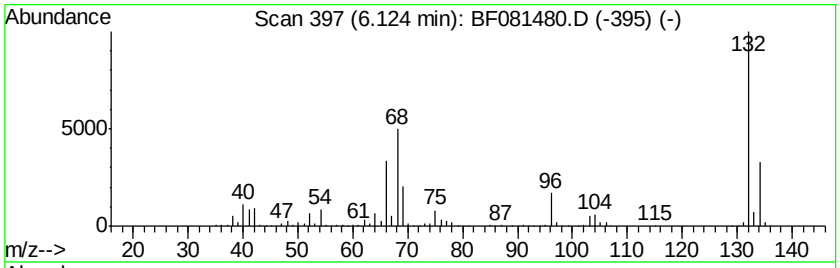
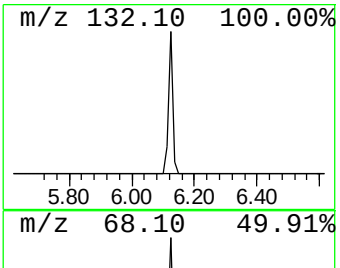
Peak Number 3 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	92.63 ng	1653810	1,4-Dichlorobenzene-d4	6.35

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	16
3	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Xenon	132	Xe	007440-63-3	9





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Operator : UM/IZ
Sample : G3555-05
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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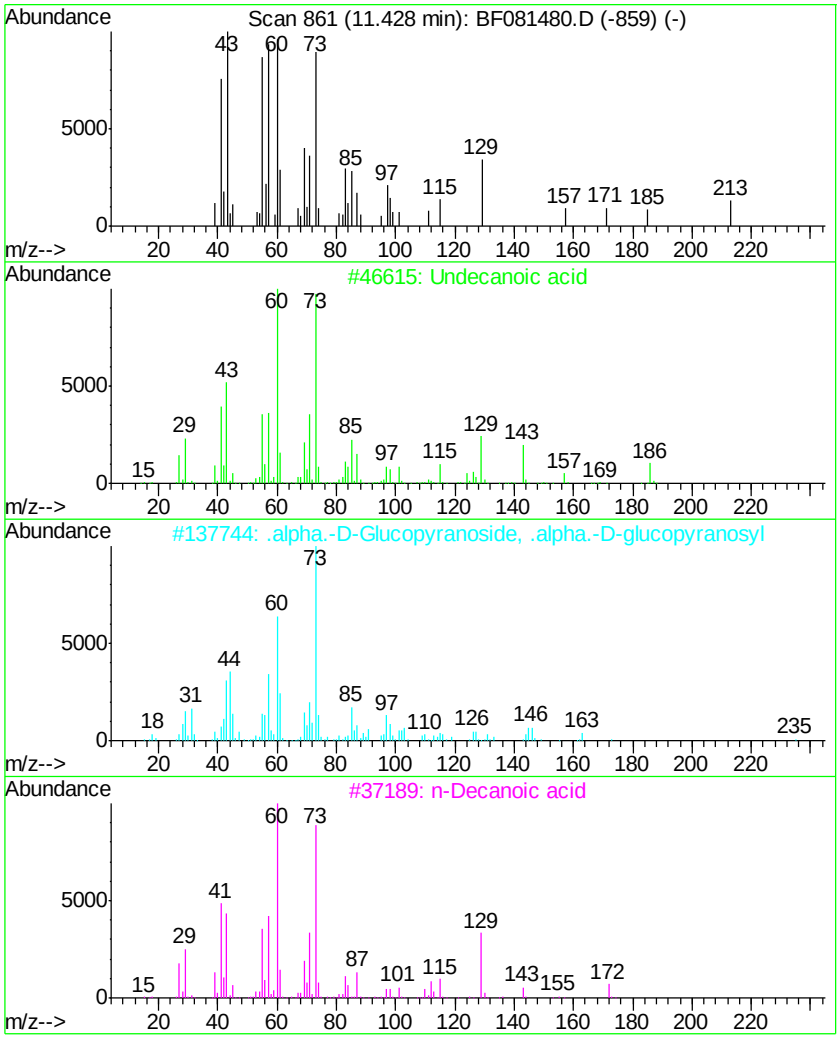
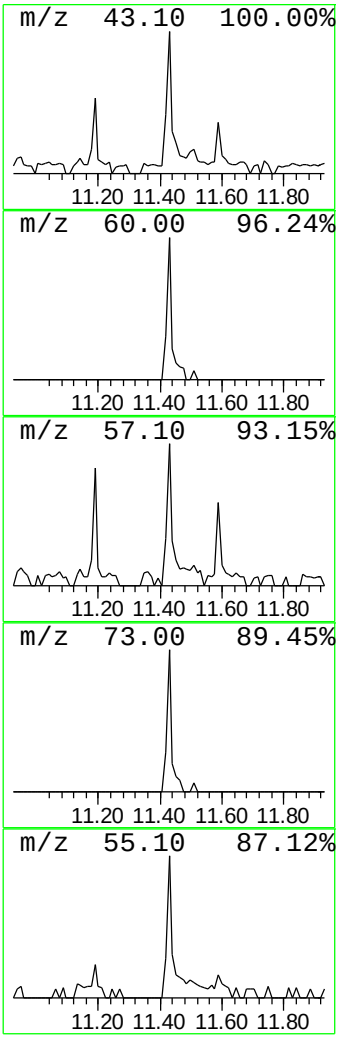
Peak Number 5 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	3.13 ng	69655	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





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Data File : BF081480.D
Acq On : 5 Sep 2015 23:31
Operator : UM/IZ
Sample : G3555-05
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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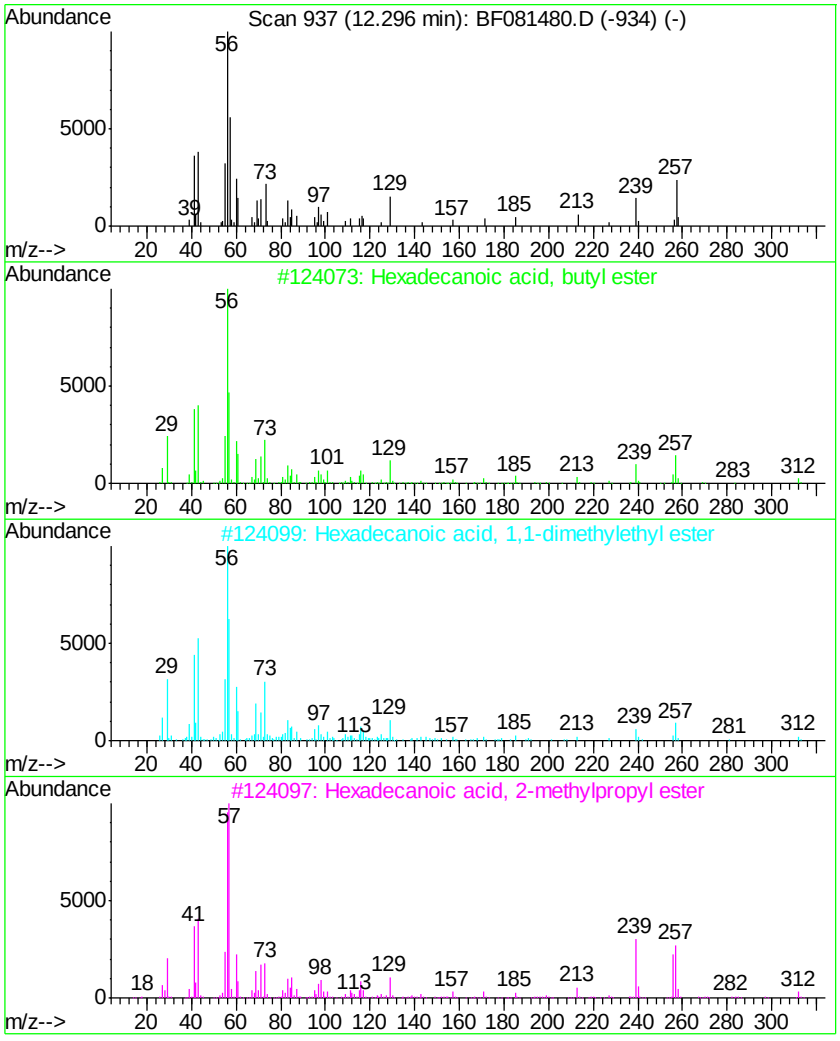
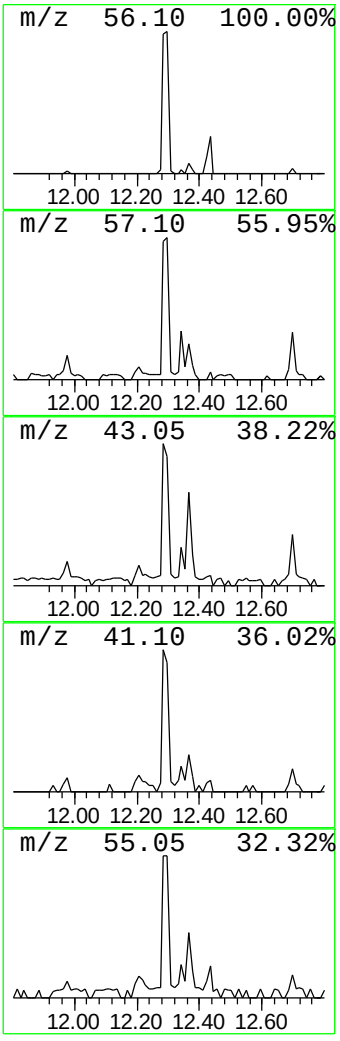
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	7.47 ng	124508	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	56
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	35





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ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-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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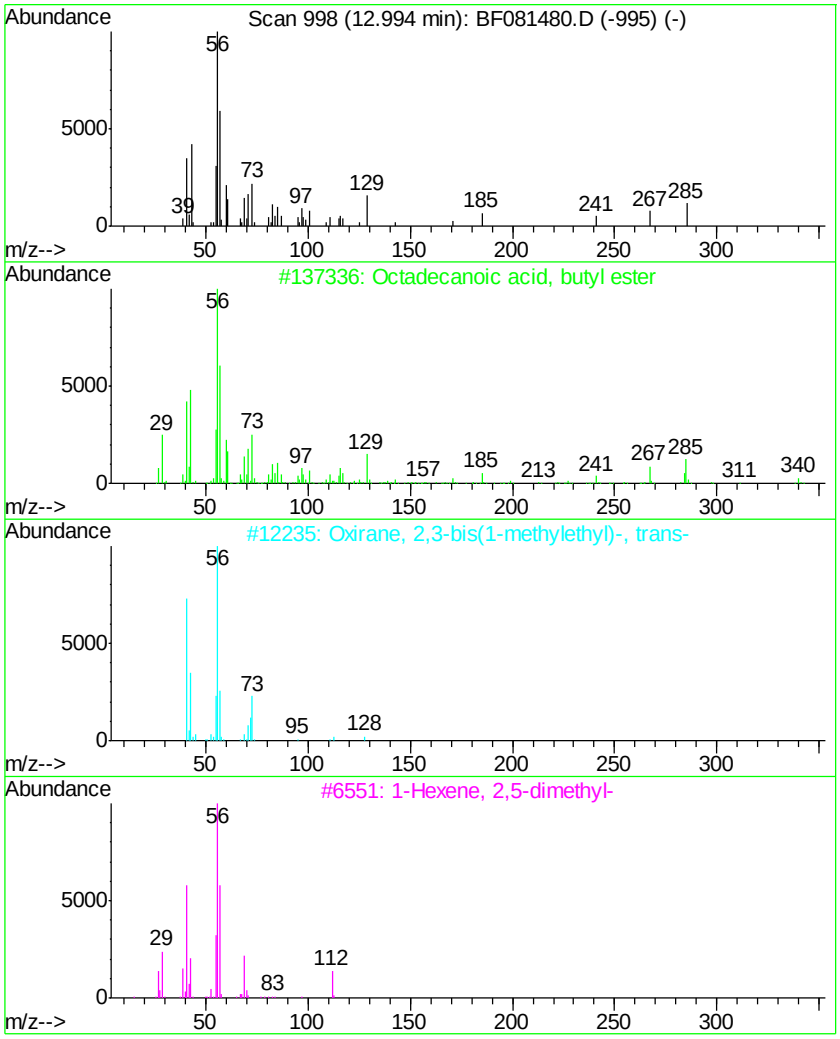
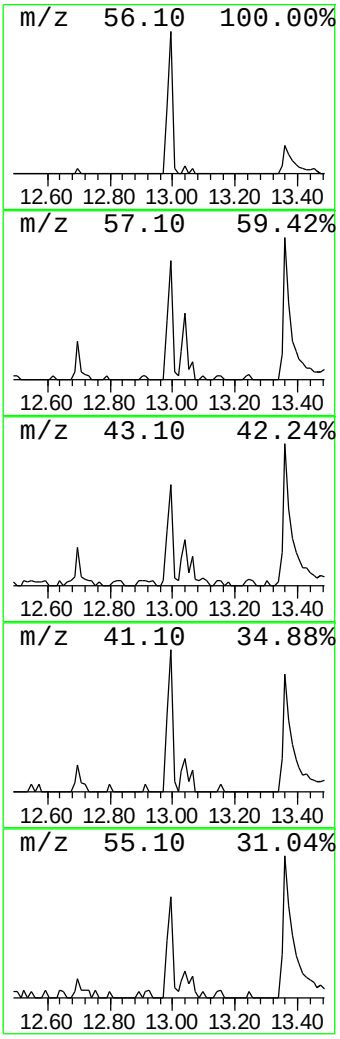
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	5.56 ng	92567	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	68
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35





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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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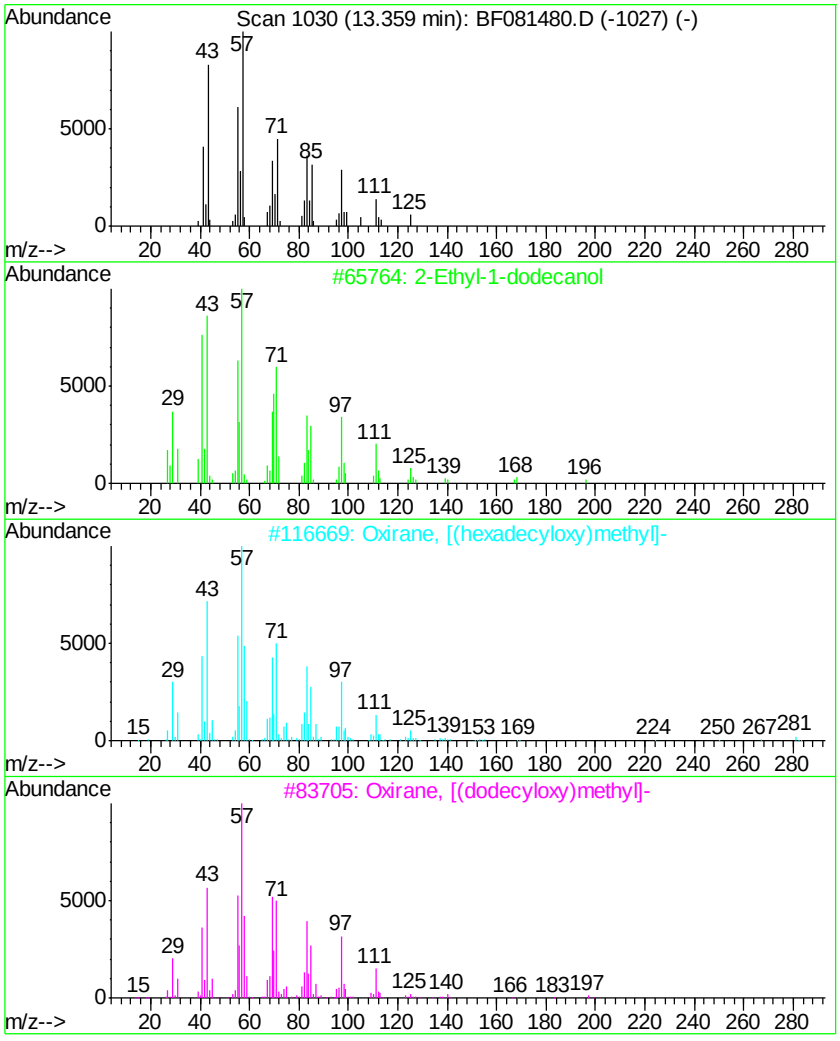
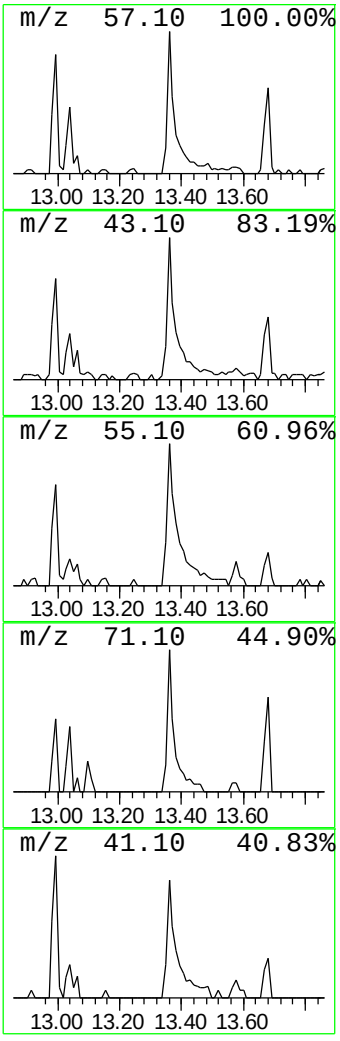
Peak Number 8 2-Ethyl-1-dodecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	9.39 ng	156344	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	90
2	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	83
3	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	64
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	59
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	58





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	3.52	5.6	ng	99917	1	6.35	357095	20.0
2-Pentanone, 4-hy...	4.41	82.6	ng	1474450	1	6.35	357095	20.0
unknown6.12	6.12	92.6	ng	1653810	1	6.35	357095	20.0
Undecanoic acid	11.43	3.1	ng	69655	4	10.84	445551	20.0
Hexadecanoic acid...	12.30	7.5	ng	124508	5	13.45	333142	20.0
Octadecanoic acid...	12.99	5.6	ng	92567	5	13.45	333142	20.0
2-Ethyl-1-dodecanol	13.36	9.4	ng	156344	5	13.45	333142	20.0