LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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	3.530	167	170	177	rBV	16253	36227	1.70%	0.196%
2	3.747	187	189	193	rBV	39187	71203	3.34%	0.385%
3	4.090	216	219	222	rVB	242004	353653	16.57%	1.910%
4	4.410	243	247	255	rBV	819984	1592172	74.59%	8.599%
5	4.913	288	291	293	rBV	1444124	1848367	86.59%	9.982%
6	6.033	386	389	391	rBV	1609325	2075376	97.22%	11.208%
7	6.125	395	397	399	rBV	1929565	1755906	82.26%	9.483%
8	6.353	415	417	420	rVB	396595	351202	16.45%	1.897%
9	6.513	429	431	433	rBV	1632314	1430268	67.00%	7.724%
10	6.936	465	468	470	rBV	1238760	1207149	56.55%	6.519%
11	7.645	528	530	532	rBV	545422	451075	21.13%	2.436%
12	8.730	622	625	627	rBV	2301370	2134629	100.00%	11.528%
13	9.131	658	660	663	rBV	485886	429098	20.10%	2.317%
14	9.382	680	682	685	rVB	486632	445662	20.88%	2.407%
15	9.828	718	721	725	rVB2	21970	38838	1.82%	0.210%
16	10.171	748	751	753	rBV	1206713	1195228	55.99%	6.455%
17	10.319	762	764	768	rVB	30554	32951	1.54%	0.178%
18	10.845	808	810	813	rBV	470384	446782	20.93%	2.413%
19	11.428	859	861	866	rBV	90410	105206	4.93%	0.568%
20	12.297	934	937	939	rBV	67556	82703	3.87%	0.447%
21	12.434	946	949	952	rBV	1541055	1681909	78.79%	9.083%
22	12.994	996	998	1000	rBV	57733	56276	2.64%	0.304%
23	13.360	1028	1030	1036	rBV	56896	130008	6.09%	0.702%
24	13.451	1036	1038	1041	rVB	335518	325152	15.23%	1.756%
25	14.765	1150	1153	1155	rBV	192788	239082	11.20%	1.291%

Sum of corrected areas: 18516122

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
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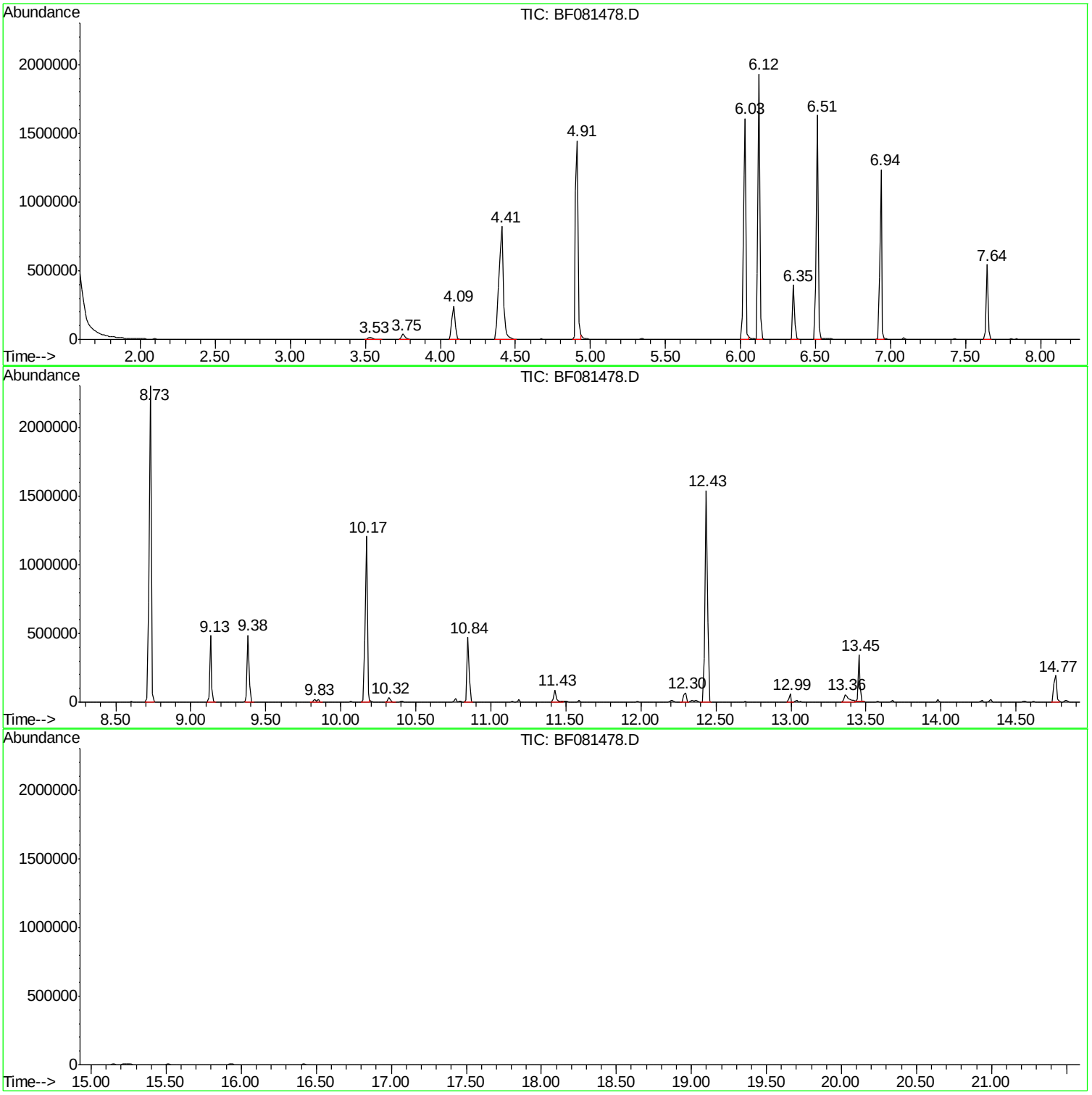
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
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Instrument : BNA_F
ClientSampleId : SB-3

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

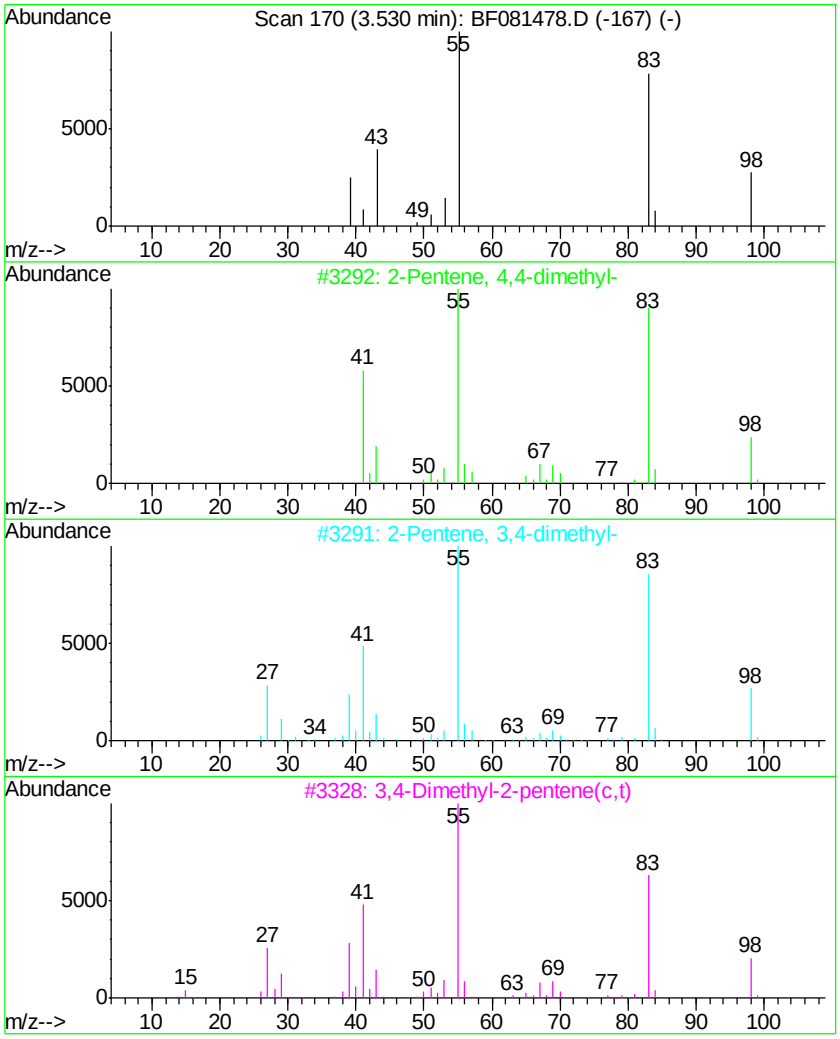
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

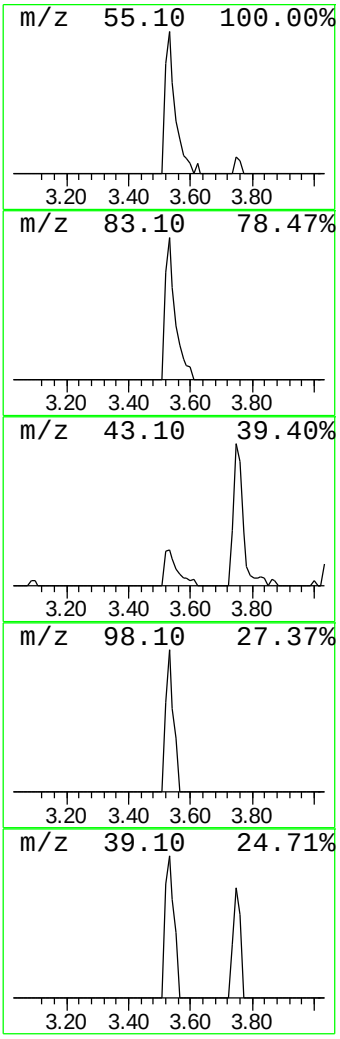
****

Peak Number 1 2-Pentene, 4,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	2.06 ng	36227	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	83
2	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	83
3	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	83
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	83
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83





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Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

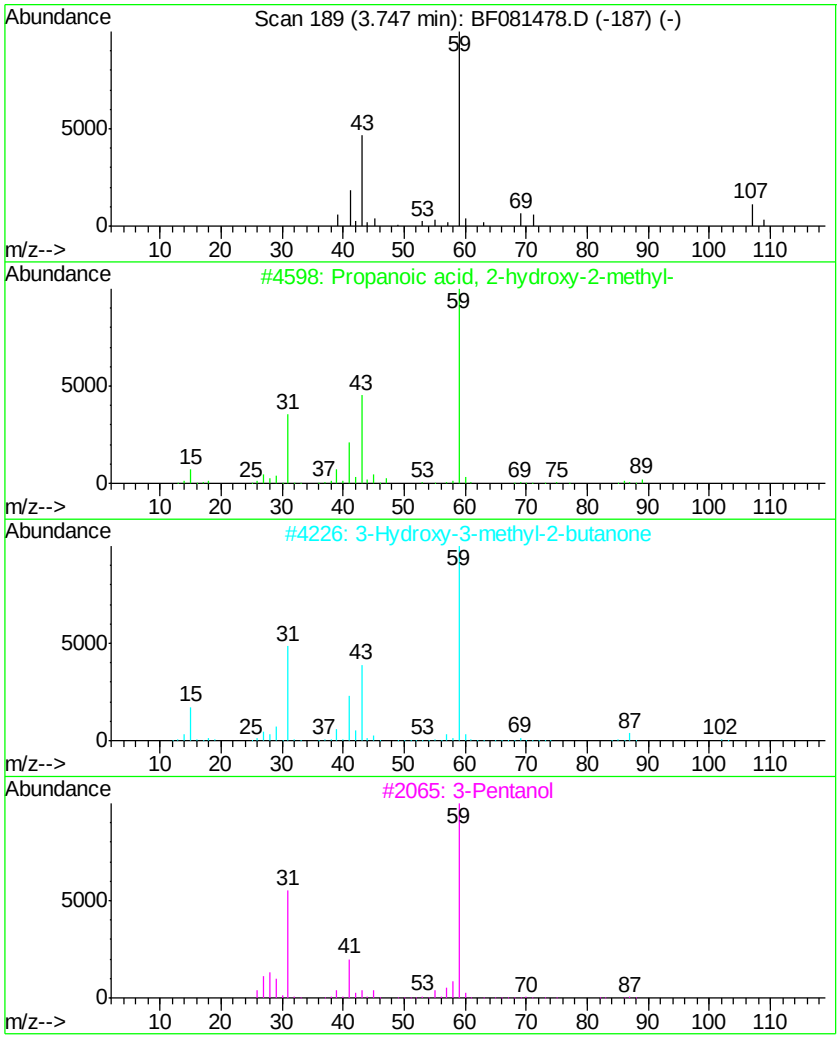
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

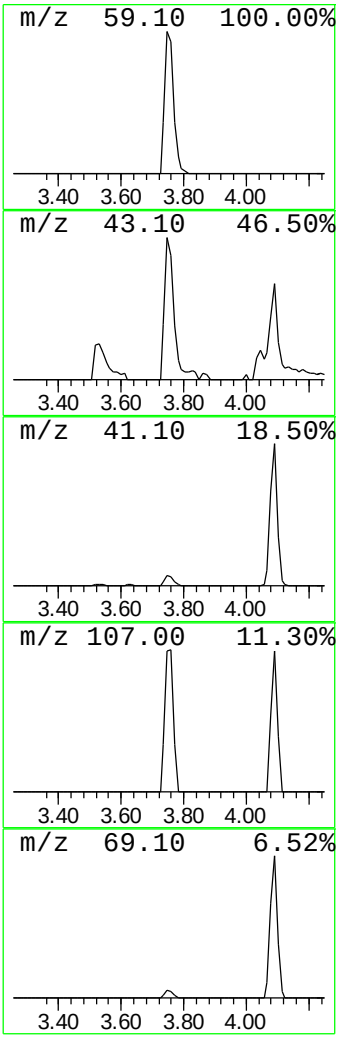
****

Peak Number 2 unknown3.75 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.75	4.05 ng	71203	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	45
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
3	3-Pentanol	88	C5H12O	000584-02-1	36
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	9
5	1,1-Dimethyl-3-chloropropanol	122	C5H11ClO	001985-88-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

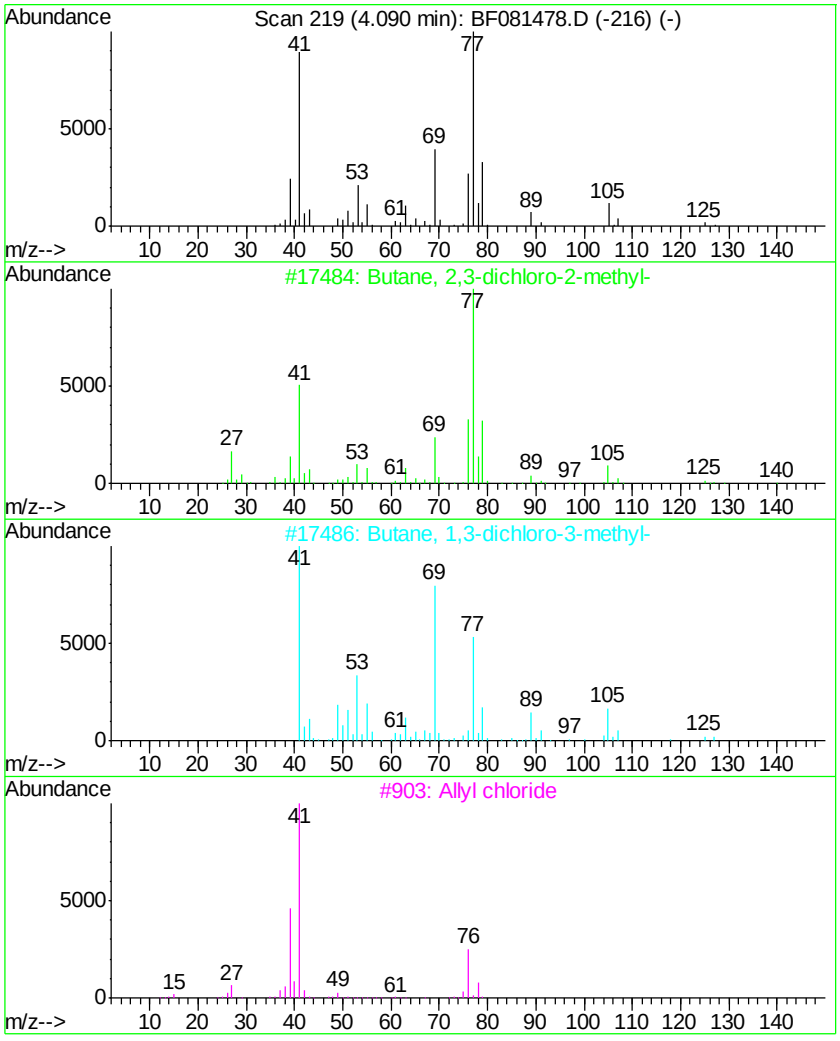
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

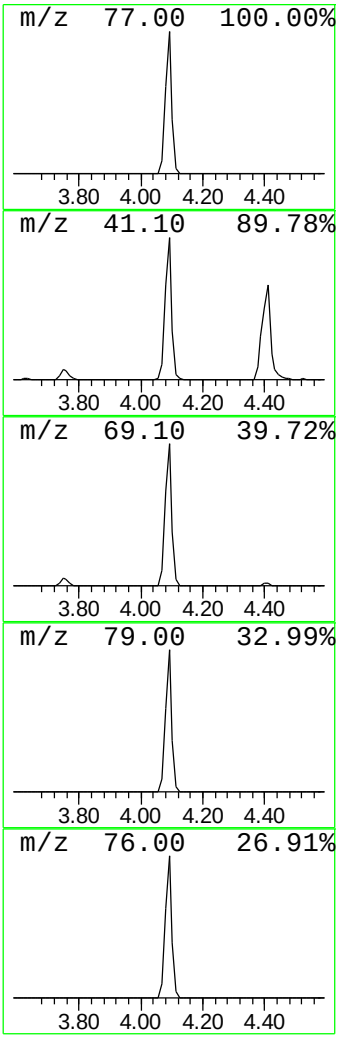
****

Peak Number 3 Butane, 2,3-dichloro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	20.14 ng	353653	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dichloro-2-methyl-	140	C5H10Cl2	000507-45-9	78
2	Butane, 1,3-dichloro-3-methyl-	140	C5H10Cl2	000624-96-4	12
3	Allyl chloride	76	C3H5Cl	000107-05-1	11
4	Propane, 1-chloro-2-nitro-	123	C3H6ClNO2	002425-66-3	9
5	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
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Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

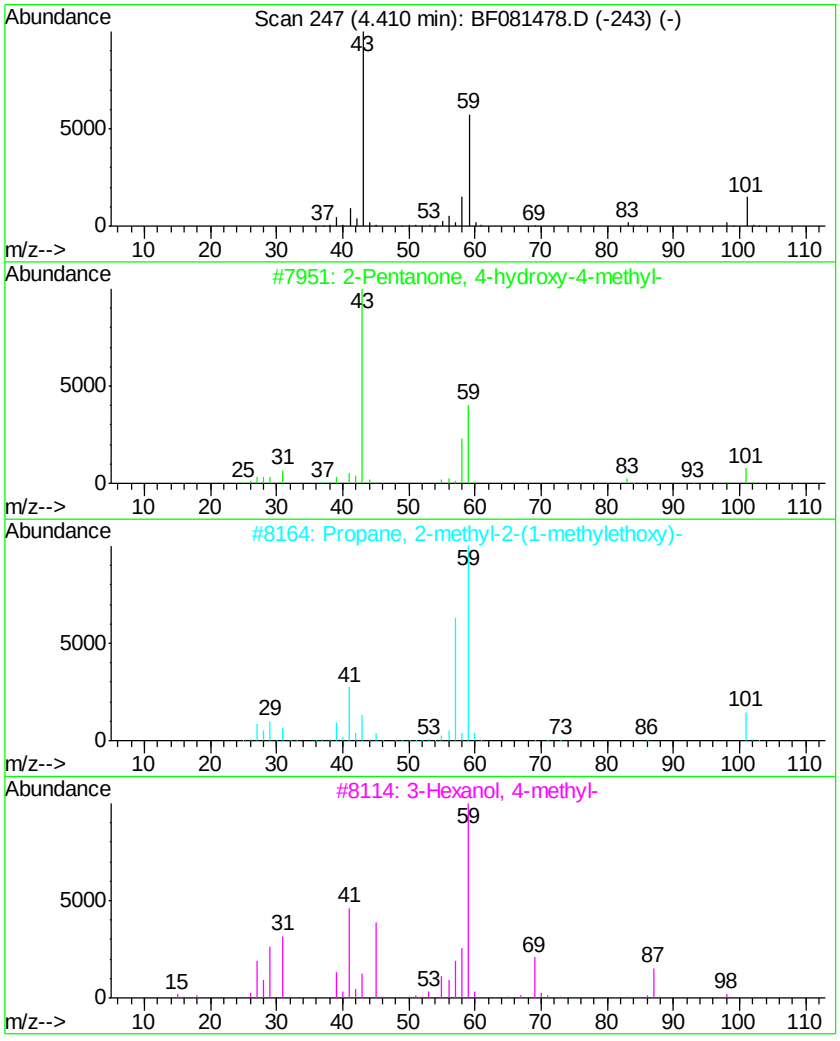
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

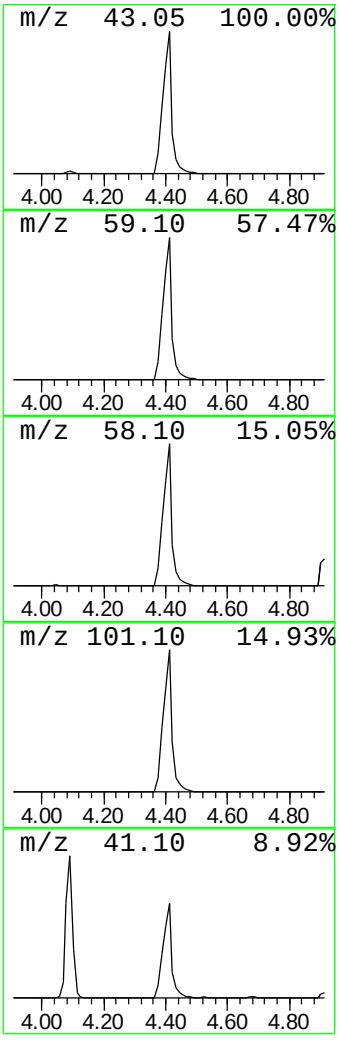
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	90.67 ng	1592170	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	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	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
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Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

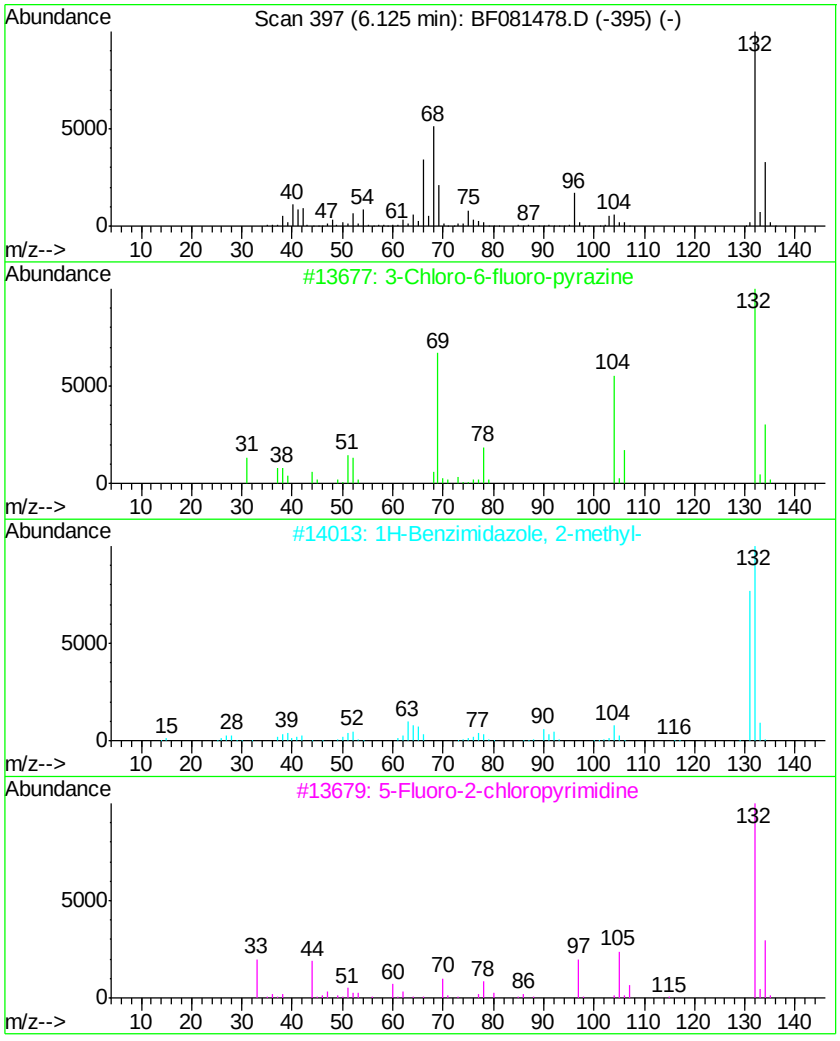
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

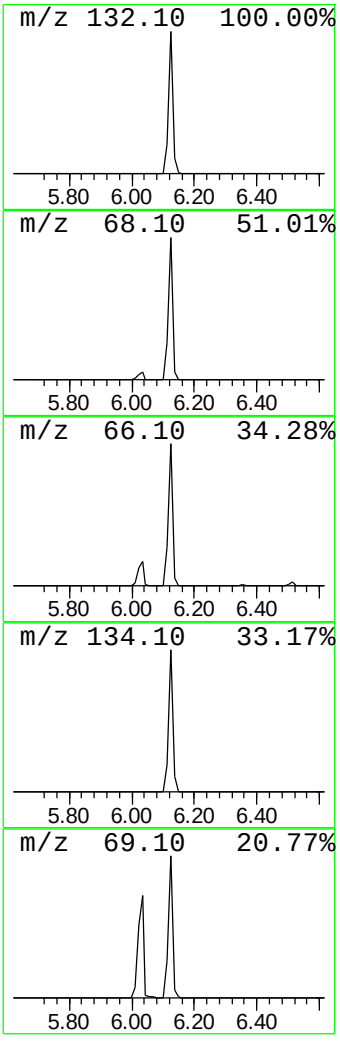
****

Peak Number 5 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	99.99 ng	1755910	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

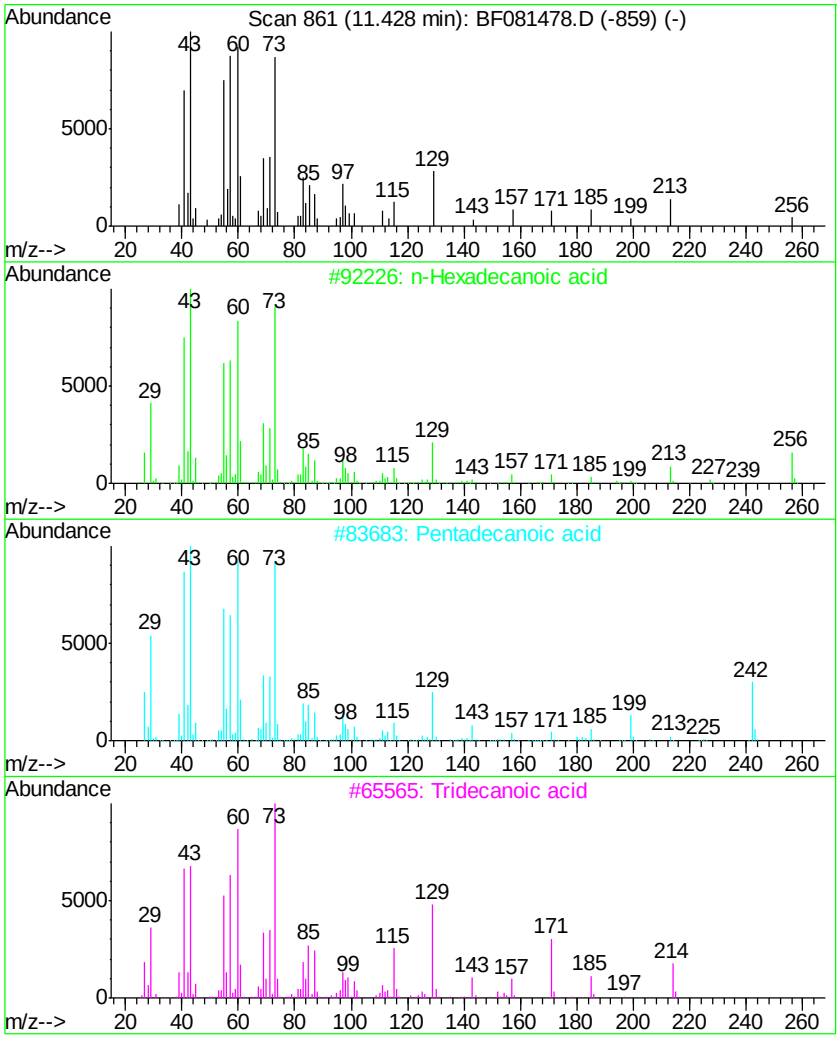
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

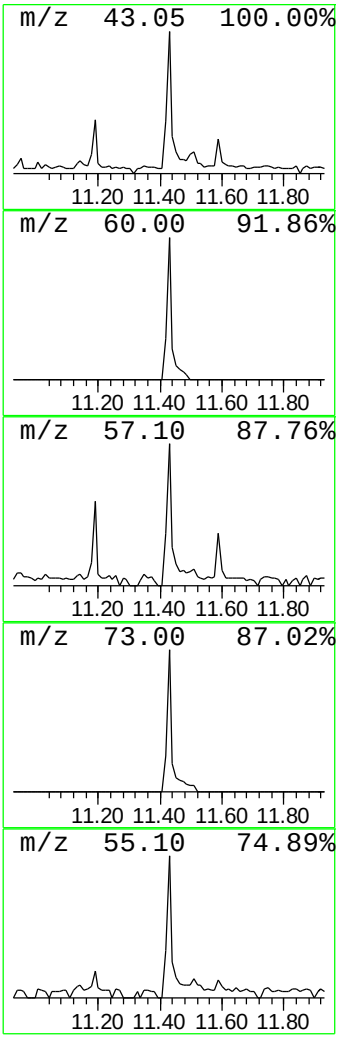
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	4.71 ng	105206	Phenanthrene-d10	10.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Sample : G3555-03
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Instrument : BNA_F
ClientSampleId : SB-3

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

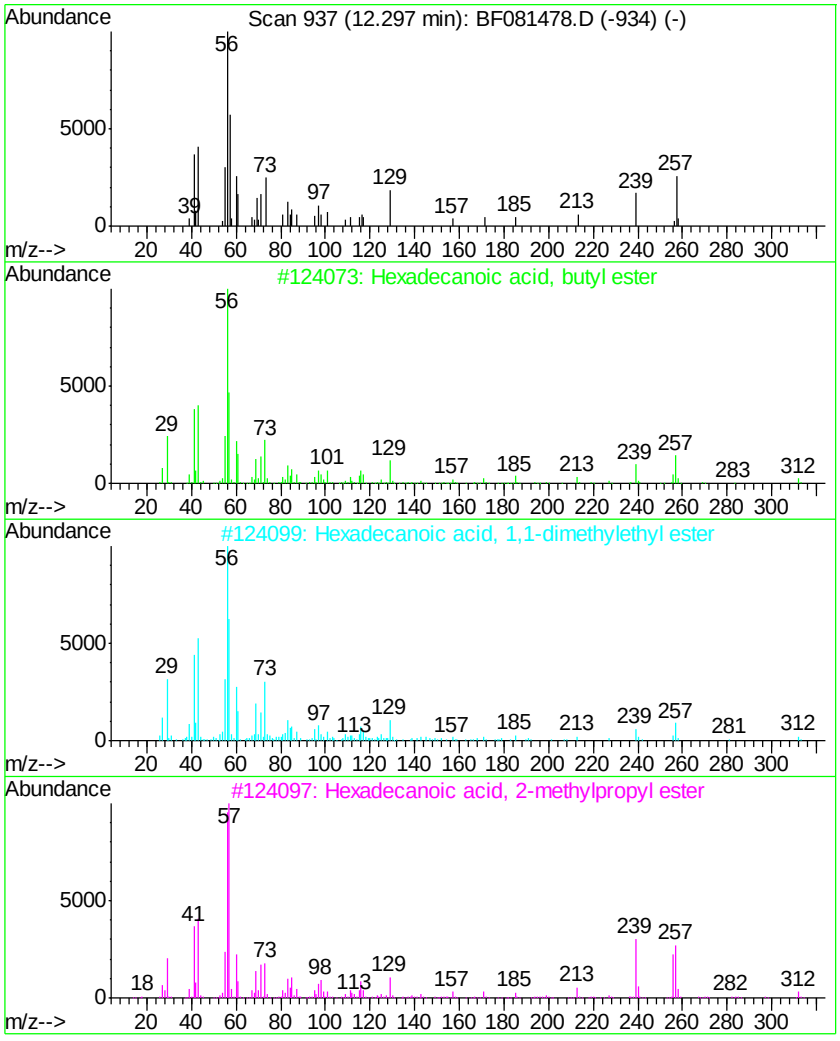
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

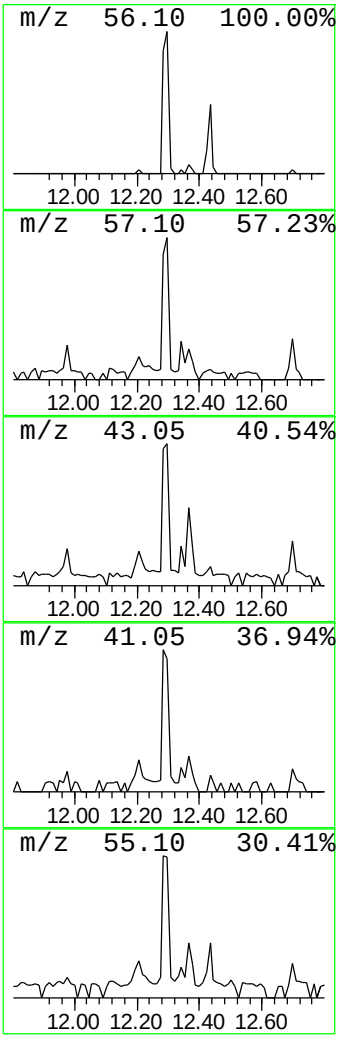
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	5.09 ng	82703	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	32
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





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Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

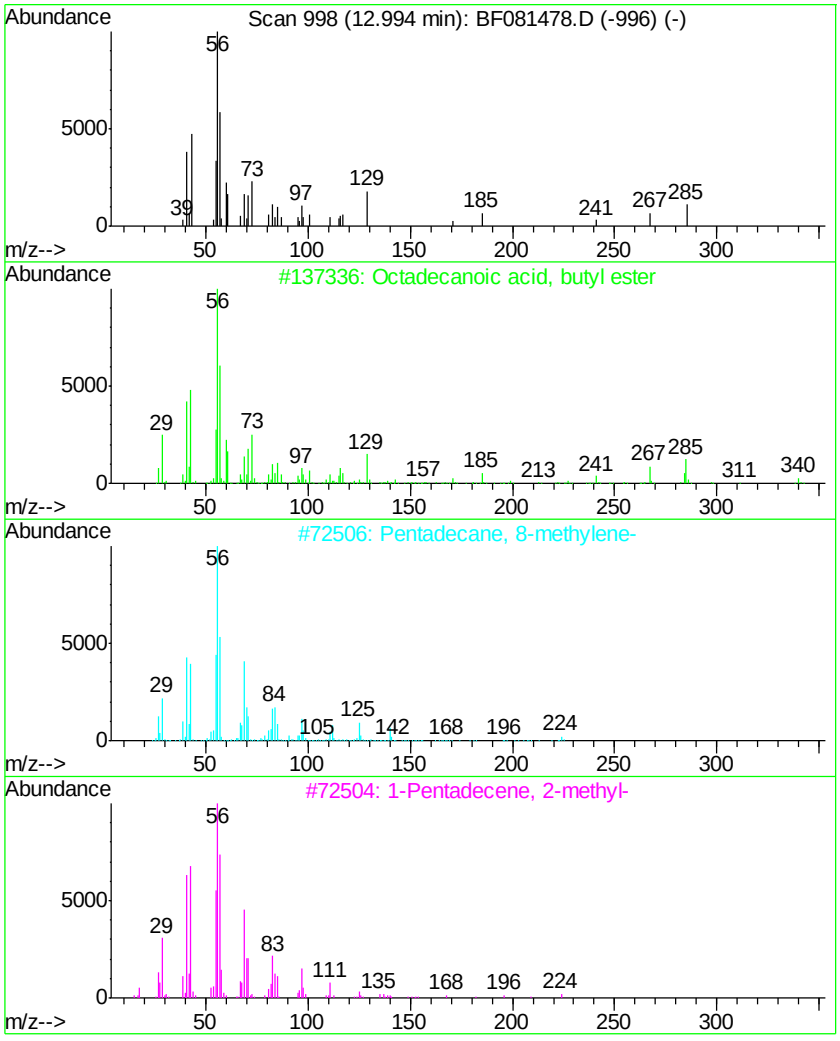
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

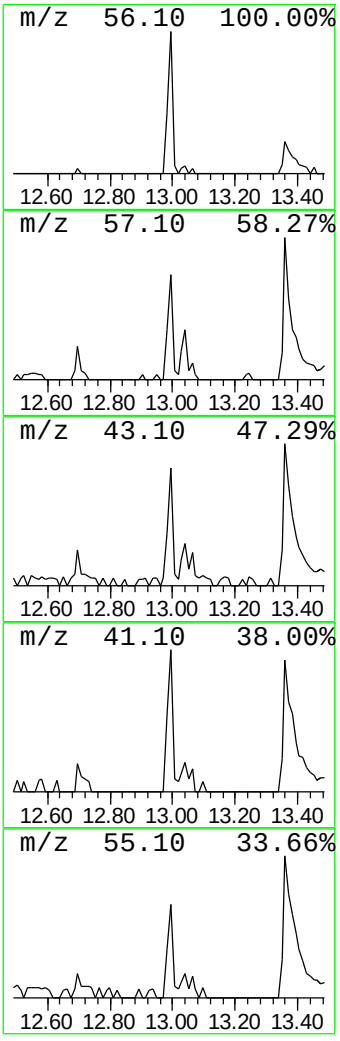
****

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	3.46 ng	56276	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
3	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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

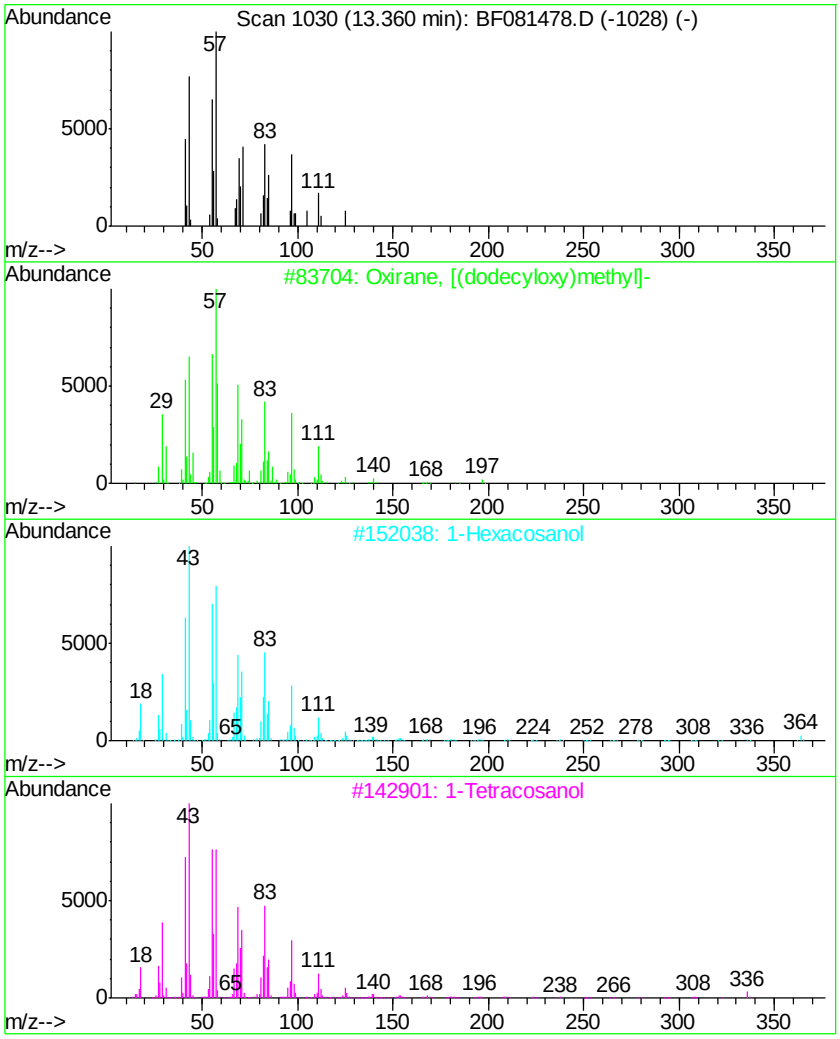
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

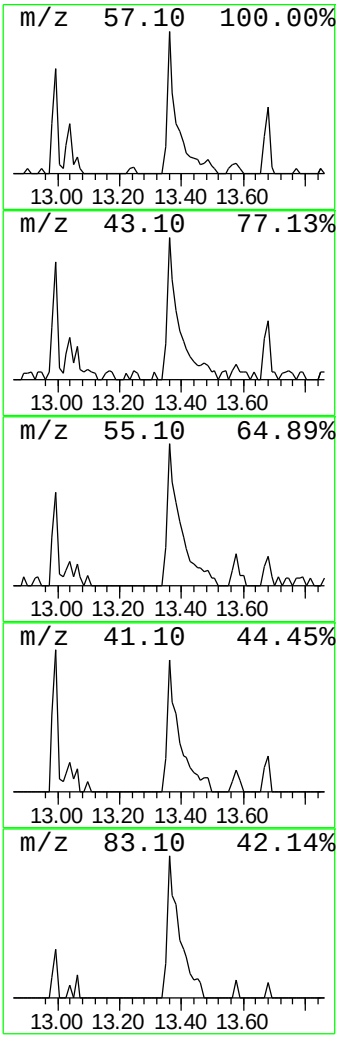
****

Peak Number 10 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	8.00 ng	130008	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	80
2	1-Hexacosanol	382	C26H54O	000506-52-5	68
3	1-Tetracosanol	354	C24H50O	000506-51-4	68
4	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	58
5	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081478.D
Acq On : 5 Sep 2015 22:30
Operator : UM/IZ
Sample : G3555-03
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3

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
2-Pentene, 4,4-di...	3.53	2.1	ng	36227	1	6.35	351202	20.0
unknown3.75	3.75	4.0	ng	71203	1	6.35	351202	20.0
Butane, 2,3-dichl...	4.09	20.1	ng	353653	1	6.35	351202	20.0
2-Pentanone, 4-hy...	4.41	90.7	ng	1592170	1	6.35	351202	20.0
unknown6.12	6.12	100.0	ng	1755910	1	6.35	351202	20.0
n-Hexadecanoic acid	11.43	4.7	ng	105206	4	10.85	446782	20.0
Hexadecanoic acid...	12.30	5.1	ng	82703	5	13.45	325152	20.0
Octadecanoic acid...	12.99	3.5	ng	56276	5	13.45	325152	20.0
Oxirane, [(dodecy...	13.36	8.0	ng	130008	5	13.45	325152	20.0