LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

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-BF111214.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	1.624	44	47	50	rBV	5711702	6745345	100.00%	27.146%
2	1.761	56	59	63	rBV	145884	271477	4.02%	1.093%
3	1.956	74	76	83	rBV2	230784	376116	5.58%	1.514%
4	5.339	370	372	375	rBV	701954	864600	12.82%	3.480%
5	5.842	413	416	418	rBV	1563186	1690281	25.06%	6.802%
6	7.088	523	525	528	rBV	1306420	1611356	23.89%	6.485%
7	7.259	537	540	542	rBV	1810604	1703571	25.26%	6.856%
8	7.545	563	565	568	rVB	275832	309363	4.59%	1.245%
9	7.739	579	582	584	rBV	1327852	1237761	18.35%	4.981%
10	8.242	623	626	628	rVB	1013701	1016227	15.07%	4.090%
11	9.133	701	704	705	rBV	352637	431032	6.39%	1.735%
12	10.471	819	821	824	rBV	1549580	1660502	24.62%	6.683%
13	10.974	863	865	868	rBV	481240	418659	6.21%	1.685%
14	11.305	892	894	897	rVB	446517	467363	6.93%	1.881%
15	12.288	977	980	983	rBV	1163192	1135889	16.84%	4.571%
16	13.157	1053	1056	1059	rBV	512885	474852	7.04%	1.911%
17	13.854	1115	1117	1120	rBV	127395	150046	2.22%	0.604%
18	14.551	1175	1178	1179	rBV	133862	153877	2.28%	0.619%
19	14.574	1179	1180	1185	rVB	145060	141464	2.10%	0.569%
20	15.157	1228	1231	1233	rBV	1466961	1785131	26.46%	7.184%
21	15.774	1282	1285	1292	rBV	45228	117274	1.74%	0.472%
22	16.048	1306	1309	1312	rBV	74705	73665	1.09%	0.296%
23	16.346	1331	1335	1342	rBV4	90249	348352	5.16%	1.402%
24	16.448	1342	1344	1347	rVV	544400	549432	8.15%	2.211%
25	16.871	1379	1381	1384	rVB	68705	78099	1.16%	0.314%
26	18.197	1494	1497	1500	rBV	378688	550983	8.17%	2.217%
27	18.906	1555	1559	1567	rBV4	32526	99991	1.48%	0.402%
28	20.483	1691	1697	1703	rBV4	71103	202067	3.00%	0.813%
29	20.803	1720	1725	1734	rBV7	42537	183581	2.72%	0.739%

Sum of corrected areas: 24848356

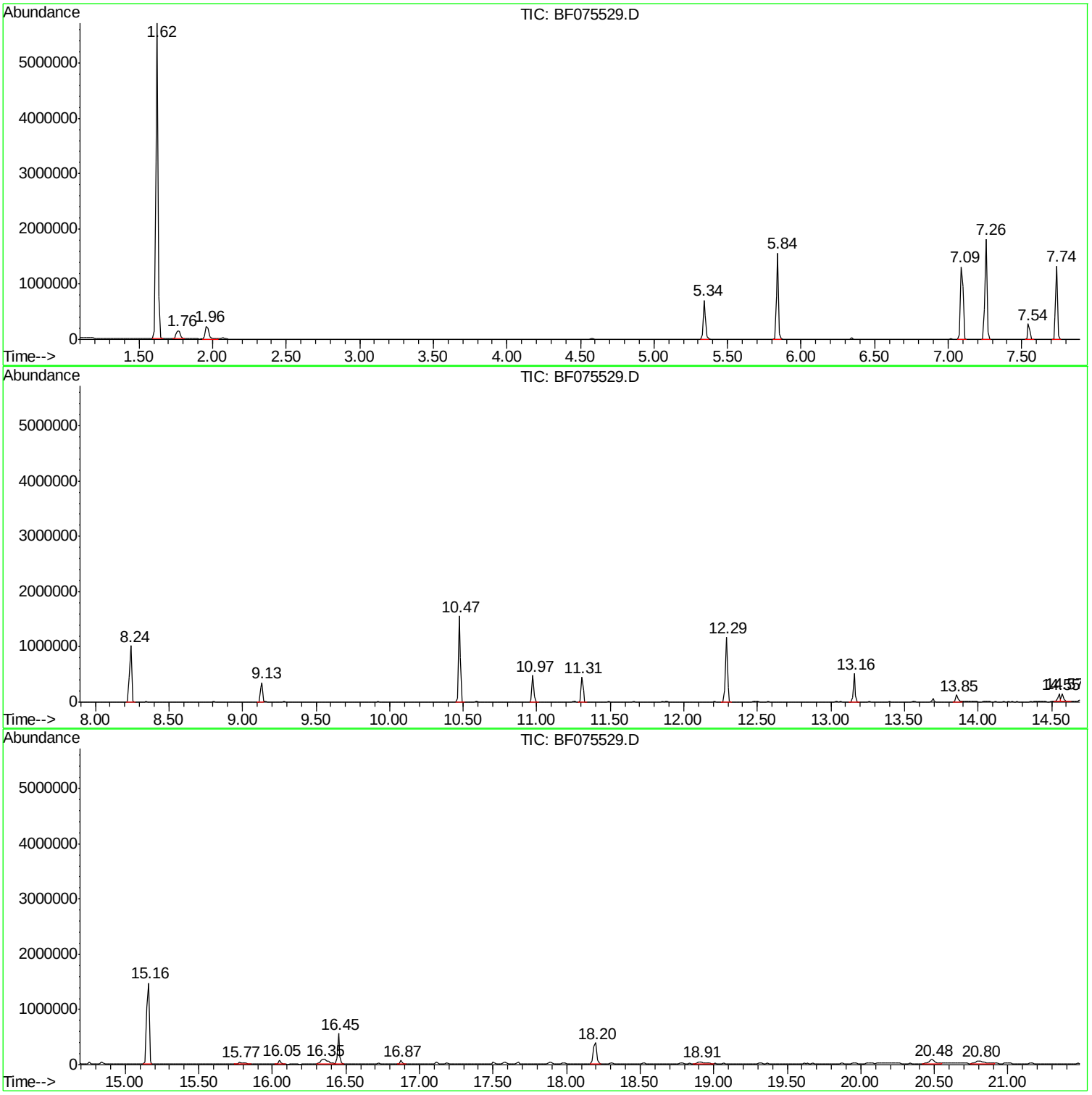
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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

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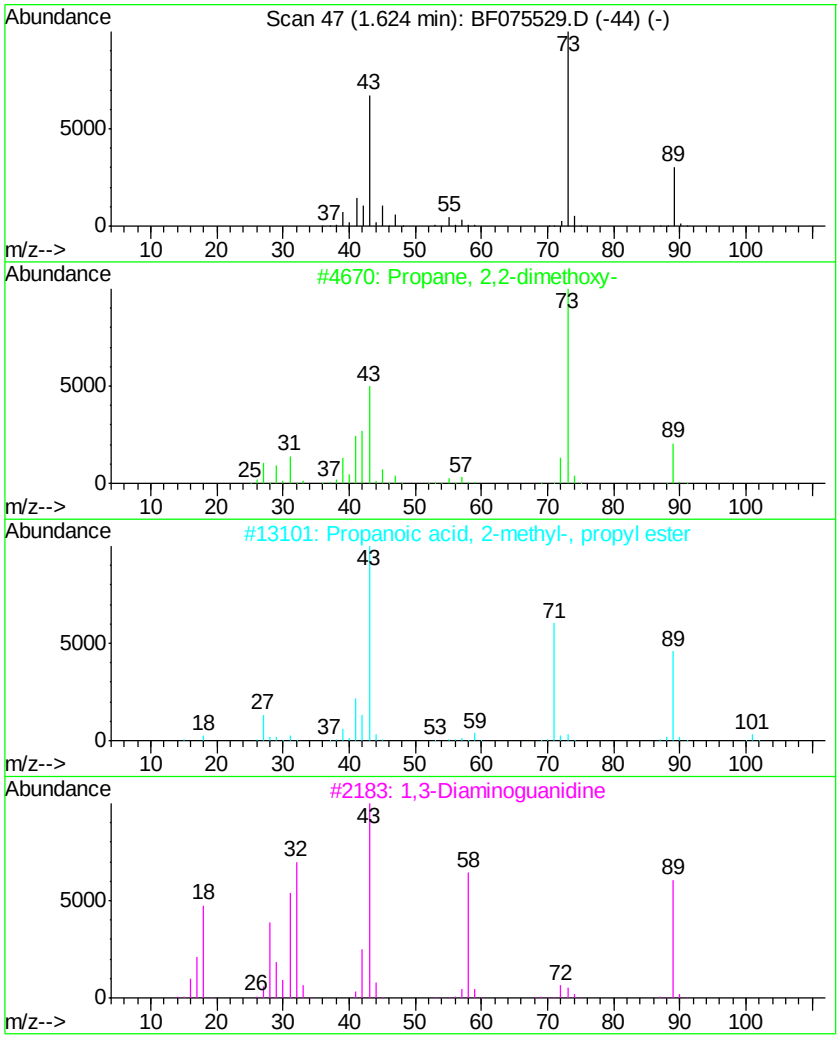
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

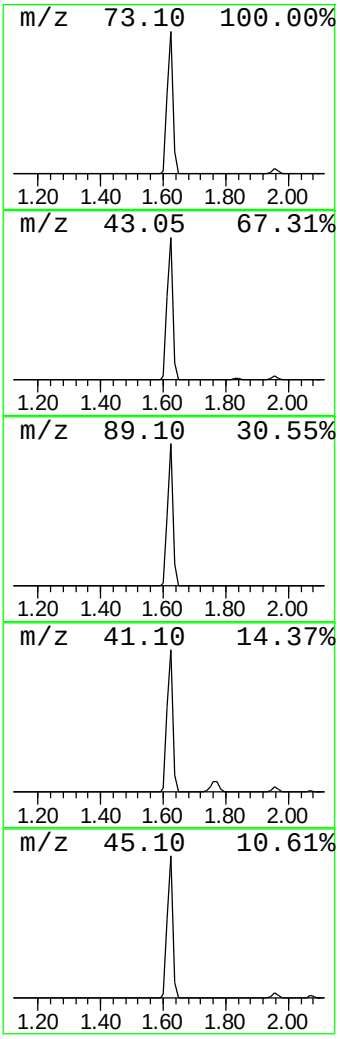
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	436.08 ng	6745350	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	23
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF075529.D
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Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

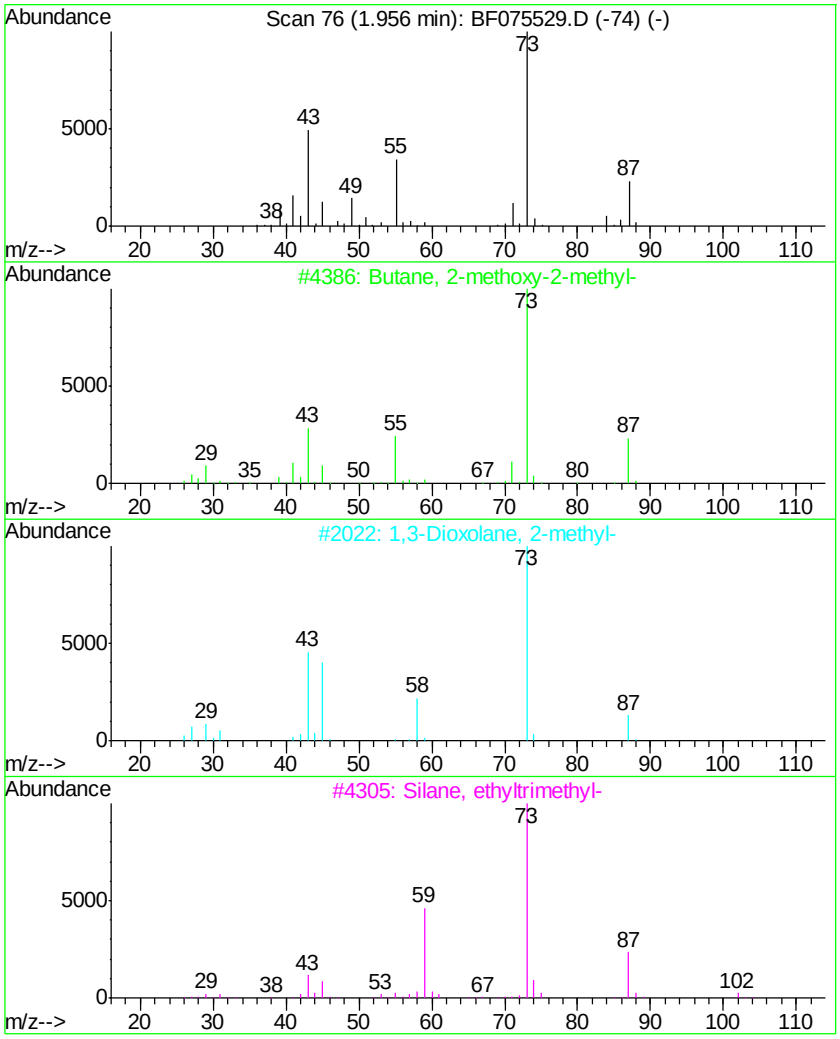
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

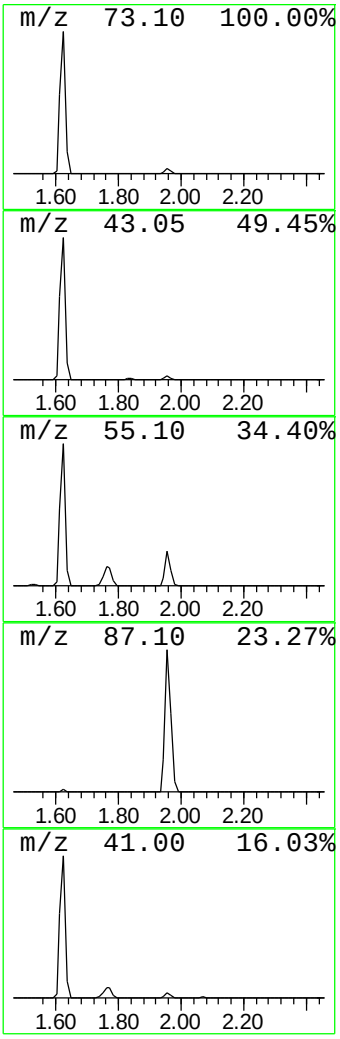
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	24.32 ng	376116	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	22
5	1-Pentanamine	87	C5H13N	000110-58-7	9





Library Search Compound Report

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Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

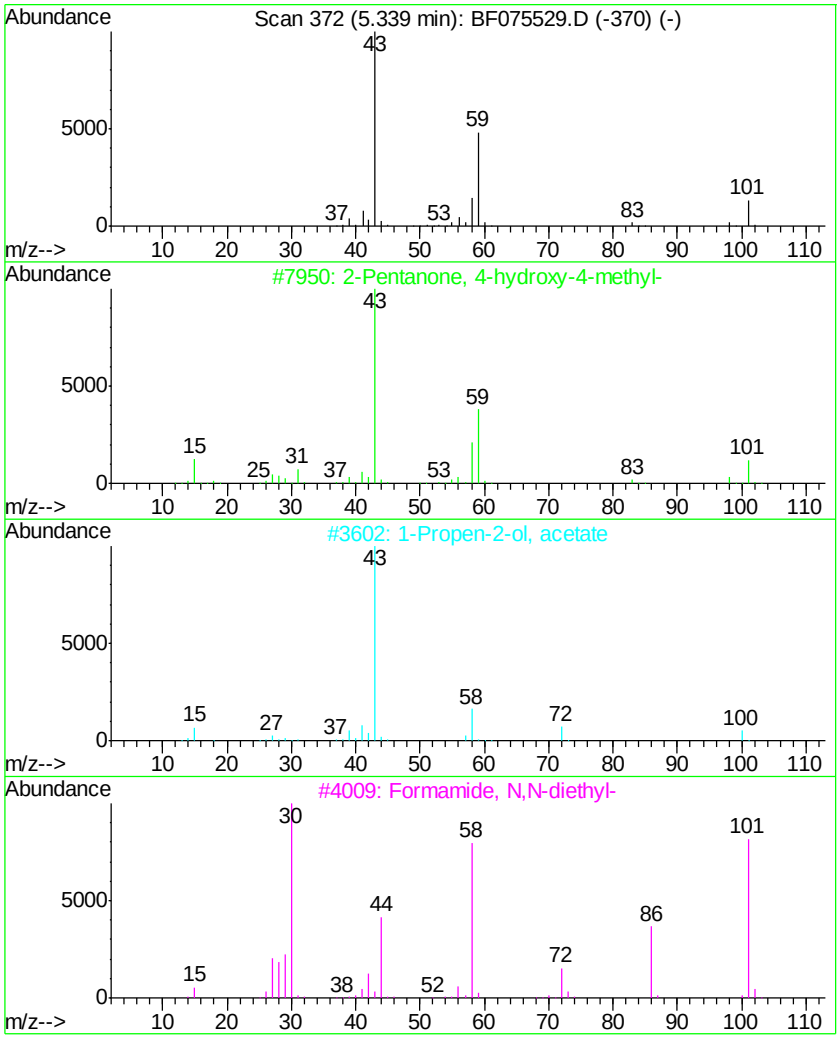
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

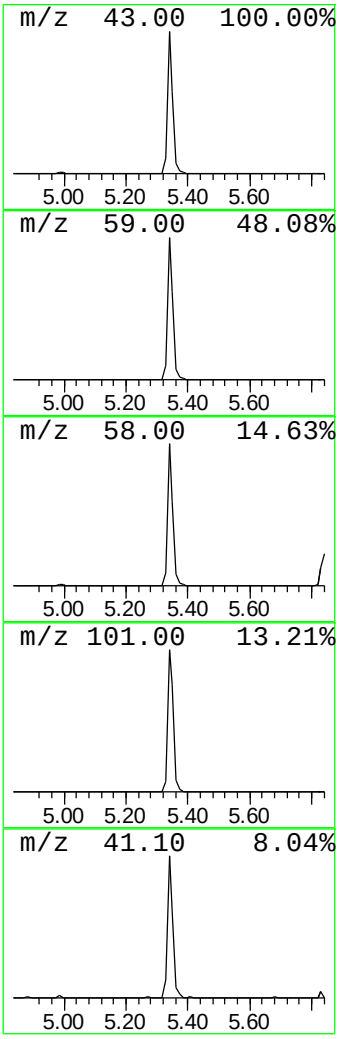
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	55.90 ng	864600	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7
5	Butane	58	C4H10	000106-97-8	5





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
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Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

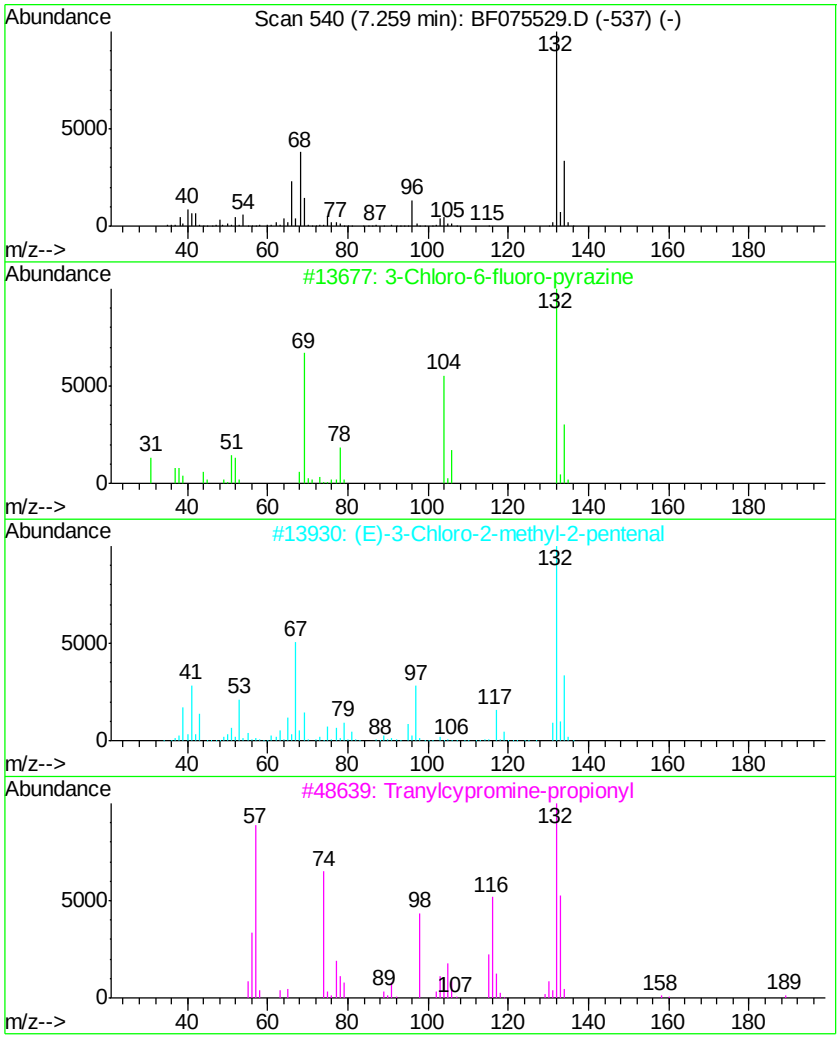
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

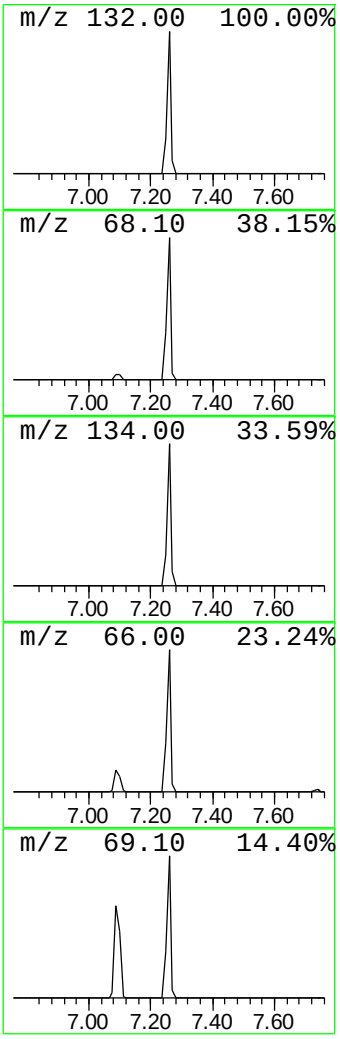
****

Peak Number 5 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	110.13 ng	1703570	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





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Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

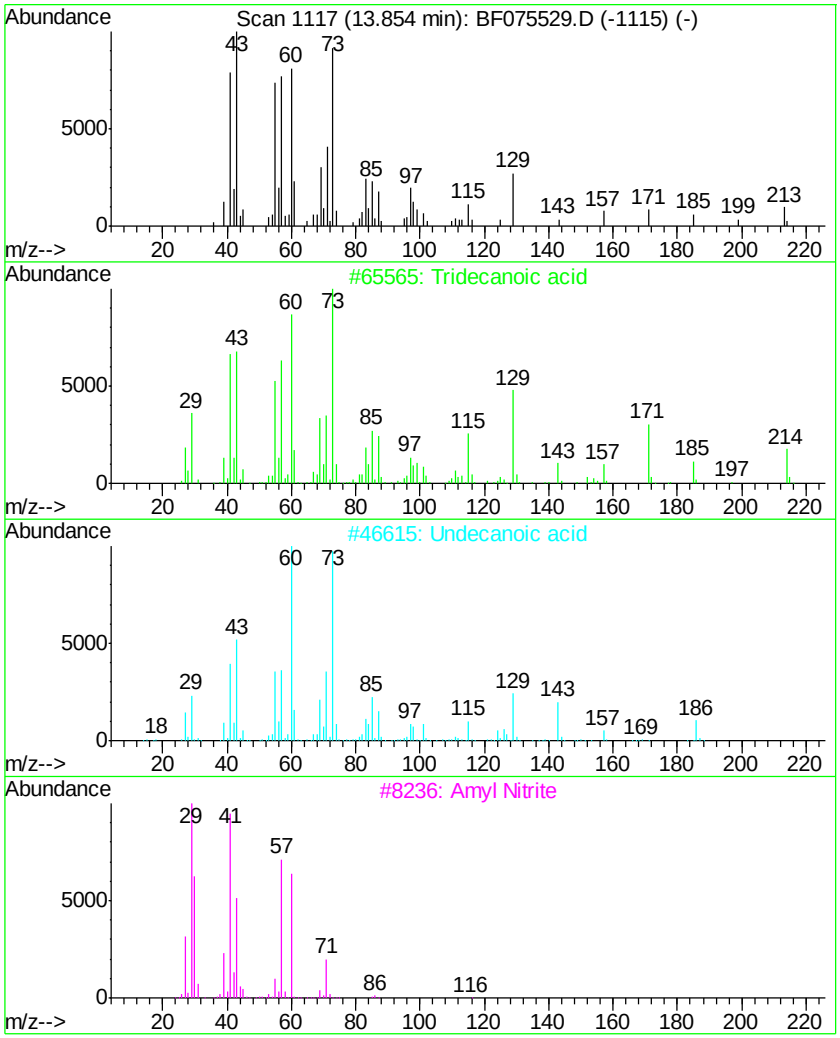
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

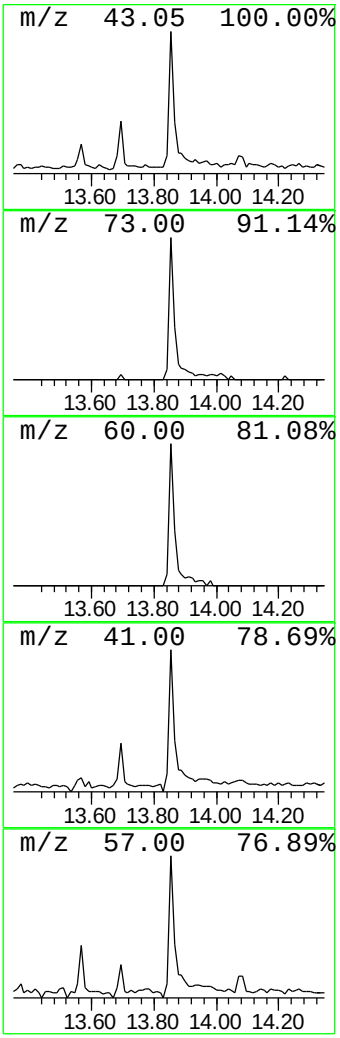
****

Peak Number 7 Tridecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	6.32 ng	150046	Phenanthrene-d10	13.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	70
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Amyl Nitrite	117	C5H11NO2	000110-46-3	35
4	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	14
5	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	10





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Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

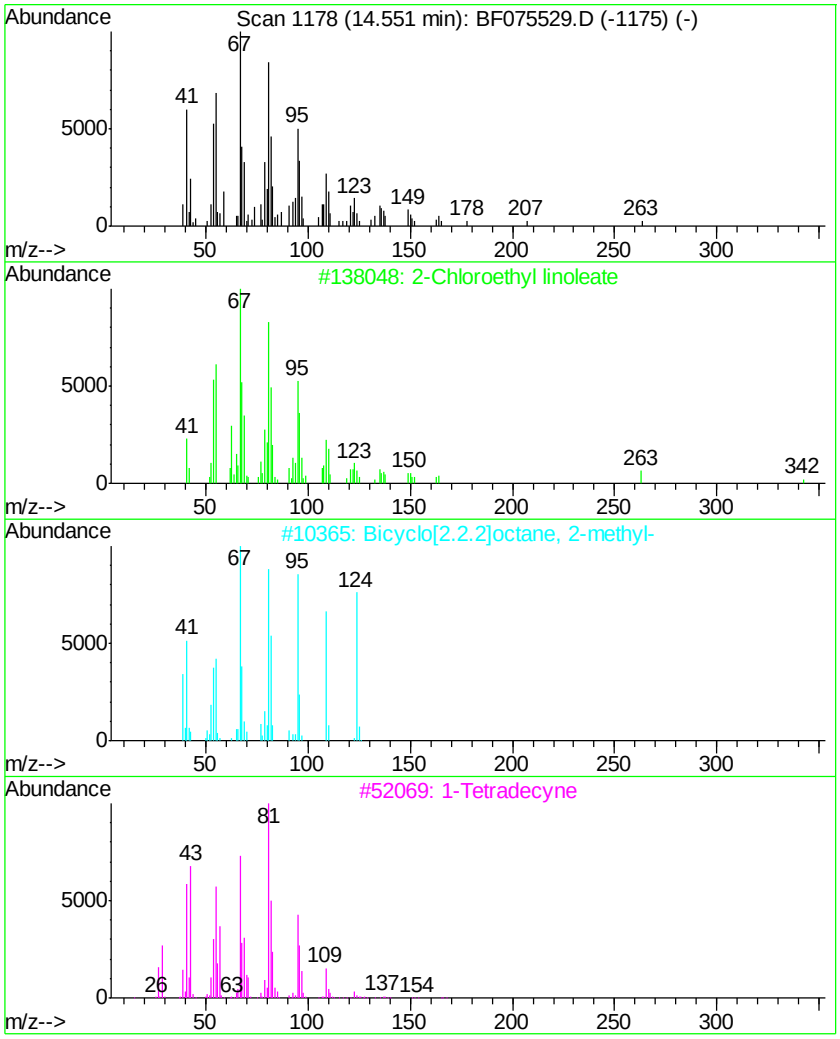
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

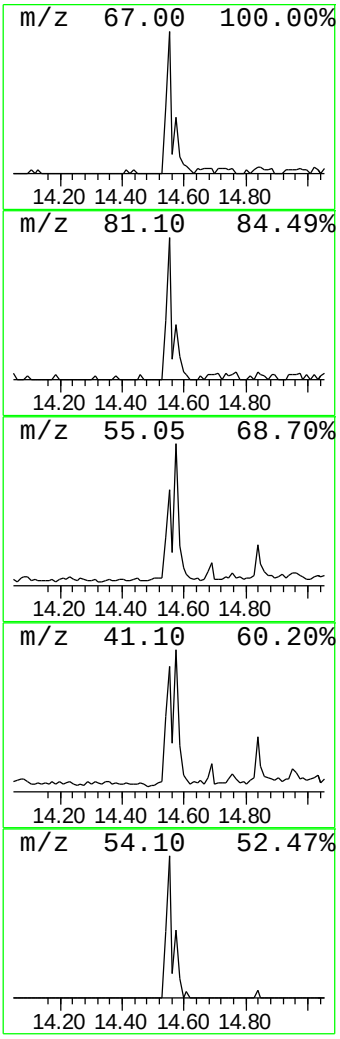
****

Peak Number 8 2-Chloroethyl linoleate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	6.48 ng	153877	Phenanthrene-d10	13.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
2	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	90
3	1-Tetradecyne	194	C14H26	000765-10-6	87
4	1,9-Cyclohexadecadiene	220	C16H28	004277-06-9	87
5	1-Hexadecyne	222	C16H30	000629-74-3	87





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

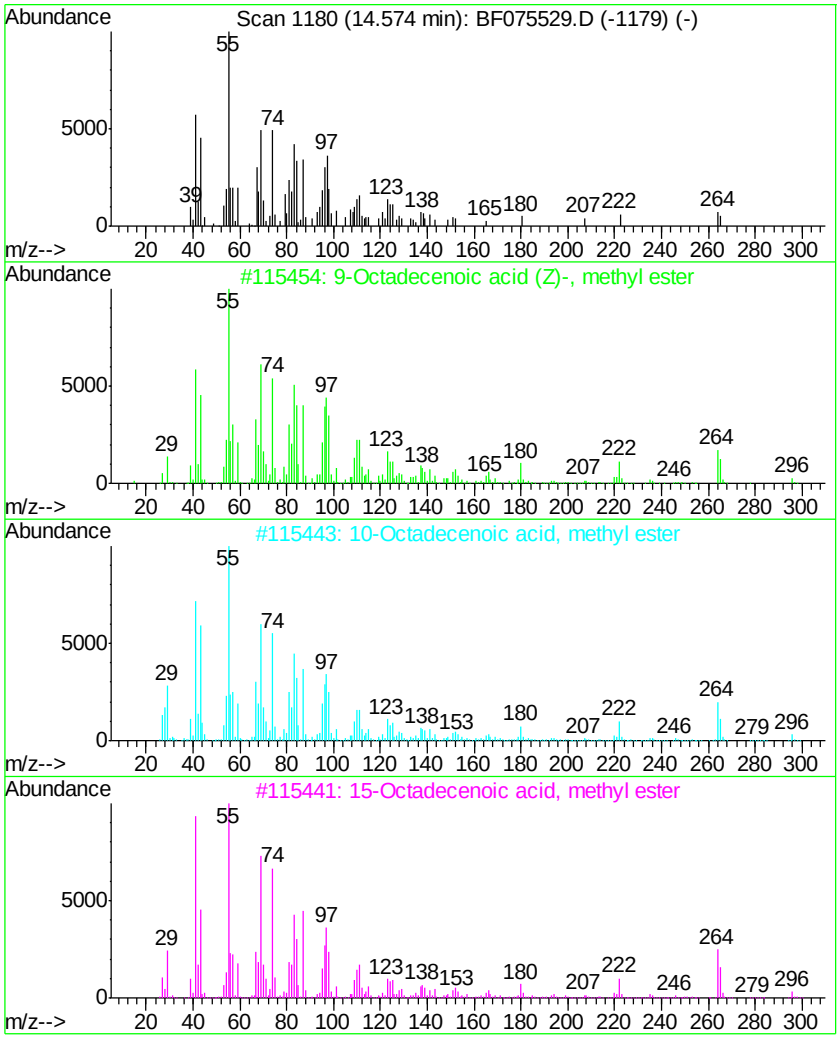
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

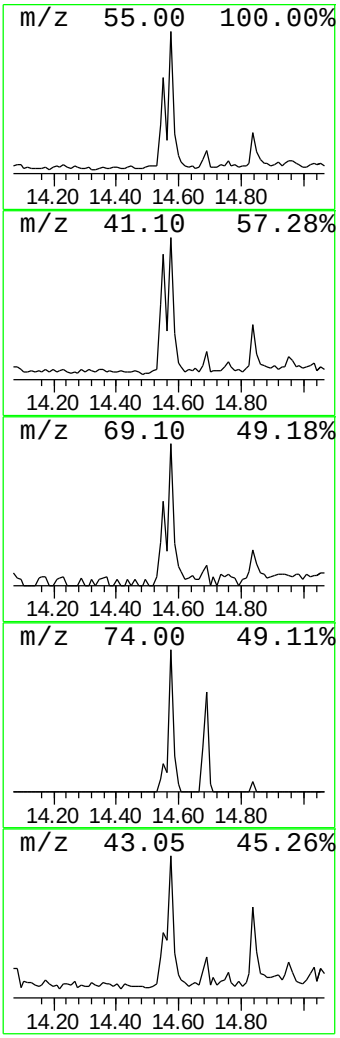
****

Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	5.96 ng	141464	Phenanthrene-d10	13.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	90
5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	83





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TIC Library : C:\DATABASE\NIST02.L
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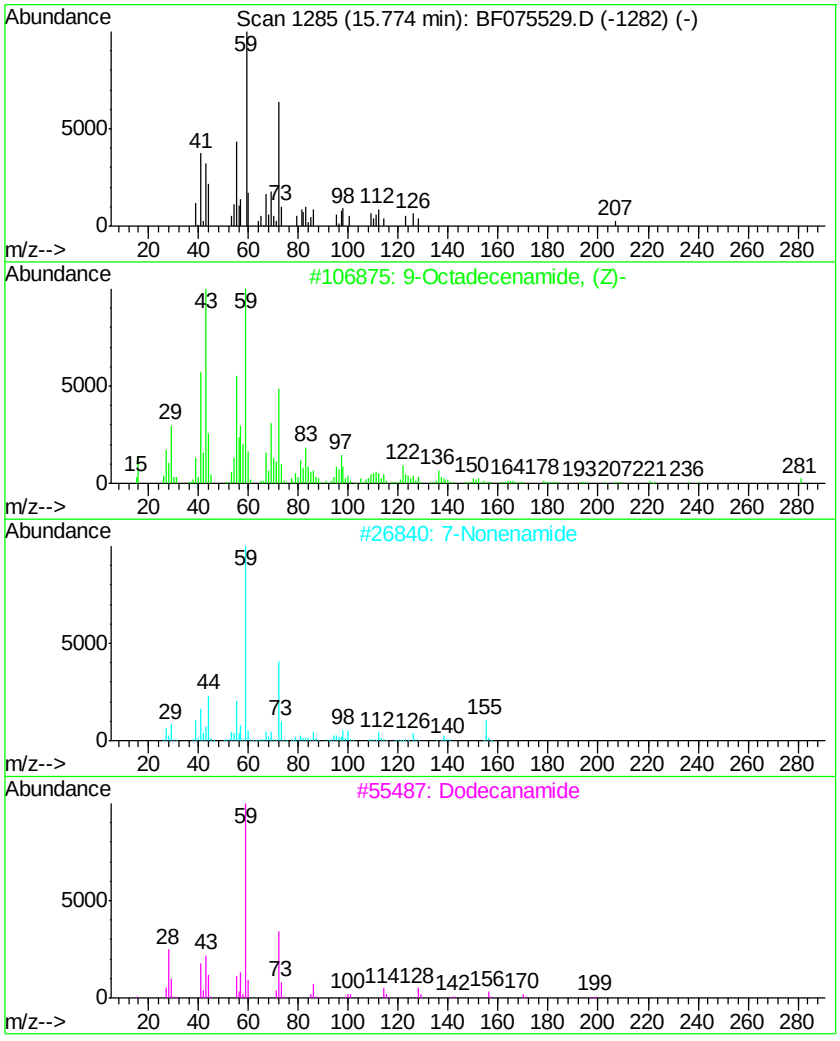
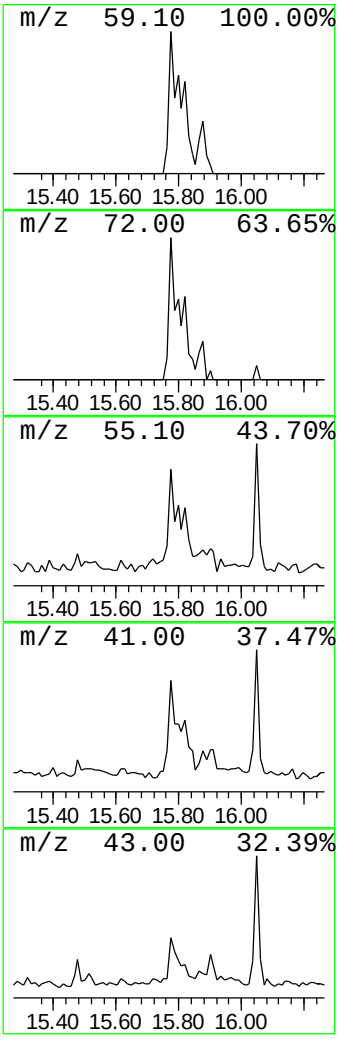
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	4.27 ng	117274	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	7-Nonenamide	155	C9H17NO	090949-53-4	53
3	Dodecanamide	199	C12H25NO	001120-16-7	42
4	Nonanamide	157	C9H19NO	001120-07-6	42
5	Mannosamine hydrochloride	179	C6H13NO5	1000127-68-8	40





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Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

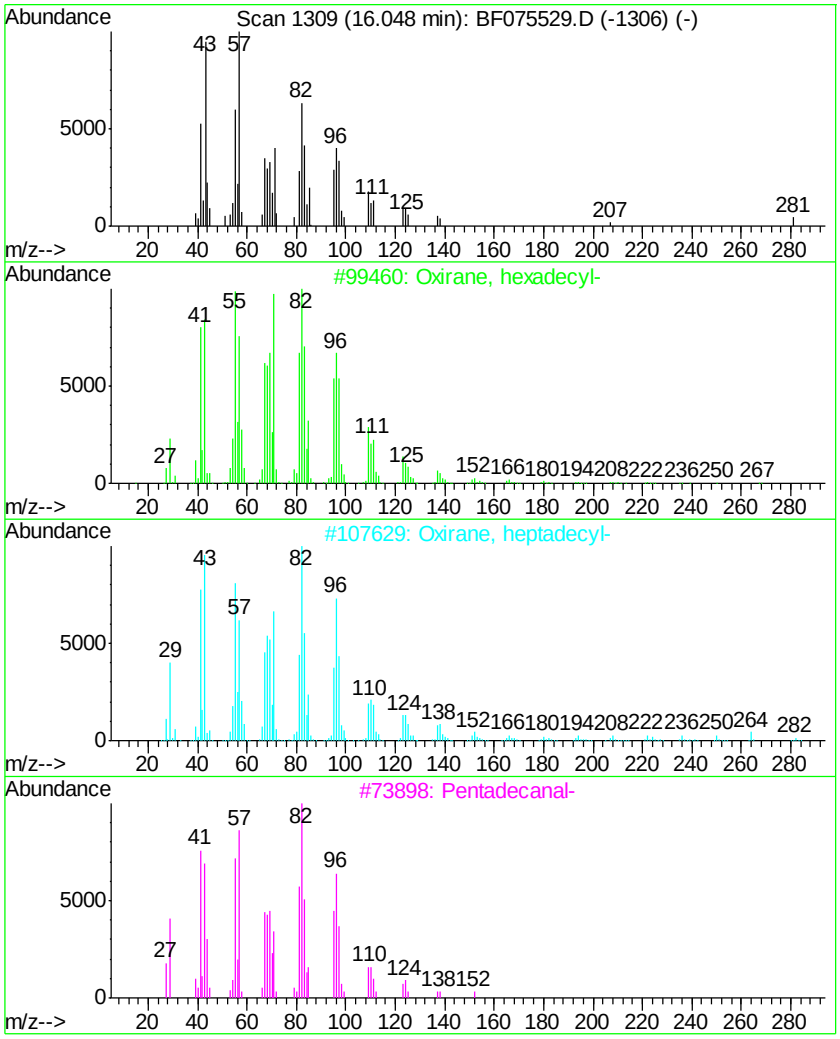
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

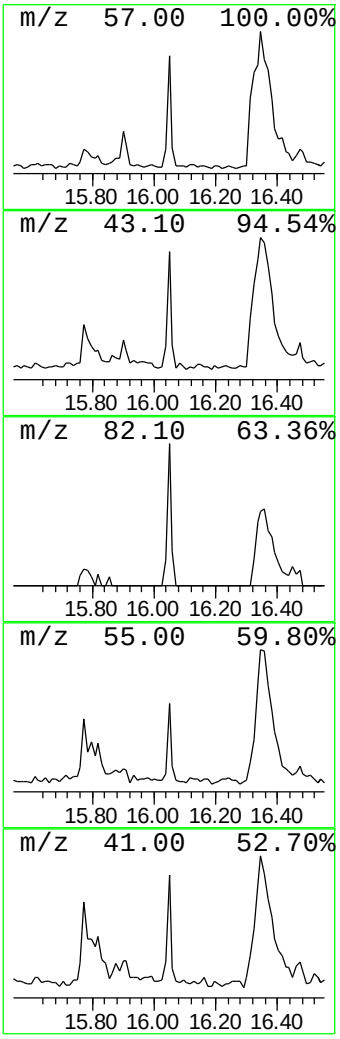
****

Peak Number 11 Oxirane, hexadecyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.68 ng	73665	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3	Pentadecanal-	226	C15H30O	002765-11-9	87
4	Octadecanal	268	C18H36O	000638-66-4	86
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
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Sample : F4695-07
Misc :
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Instrument : BNA_F
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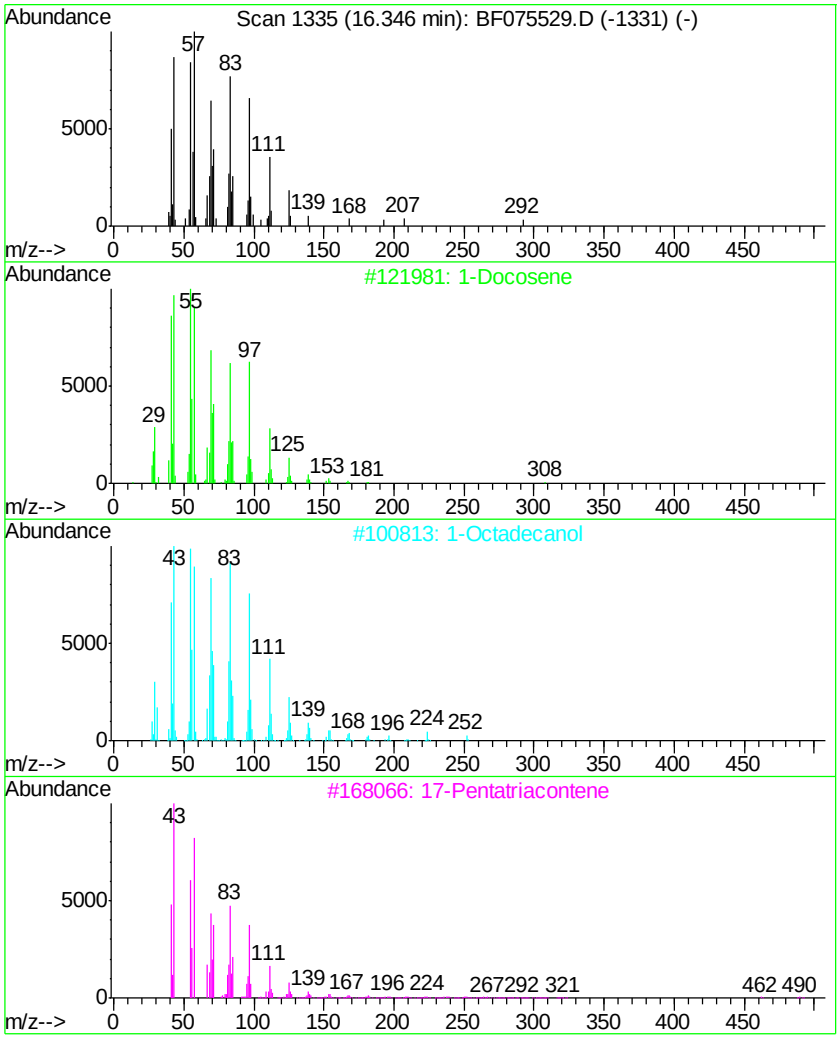
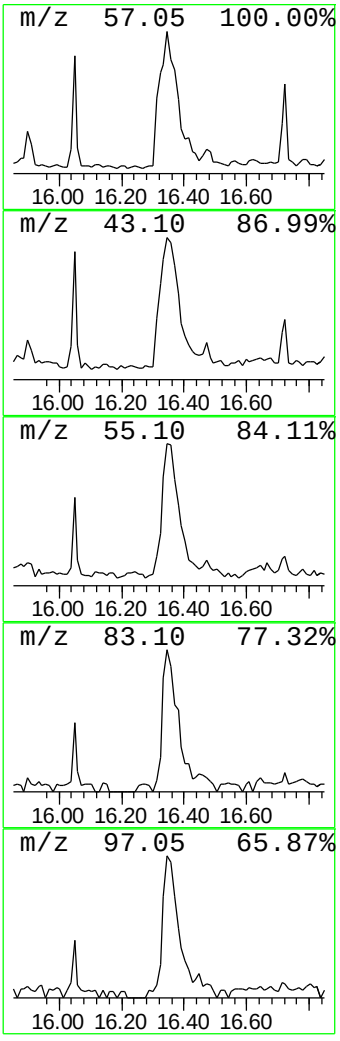
****

Peak Number 12 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	12.68 ng	348352	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Octadecanol	270	C18H38O	000112-92-5	87
3	17-Pentatriacontene	491	C35H70	006971-40-0	74
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	72
5	1-Nonadecene	266	C19H38	018435-45-5	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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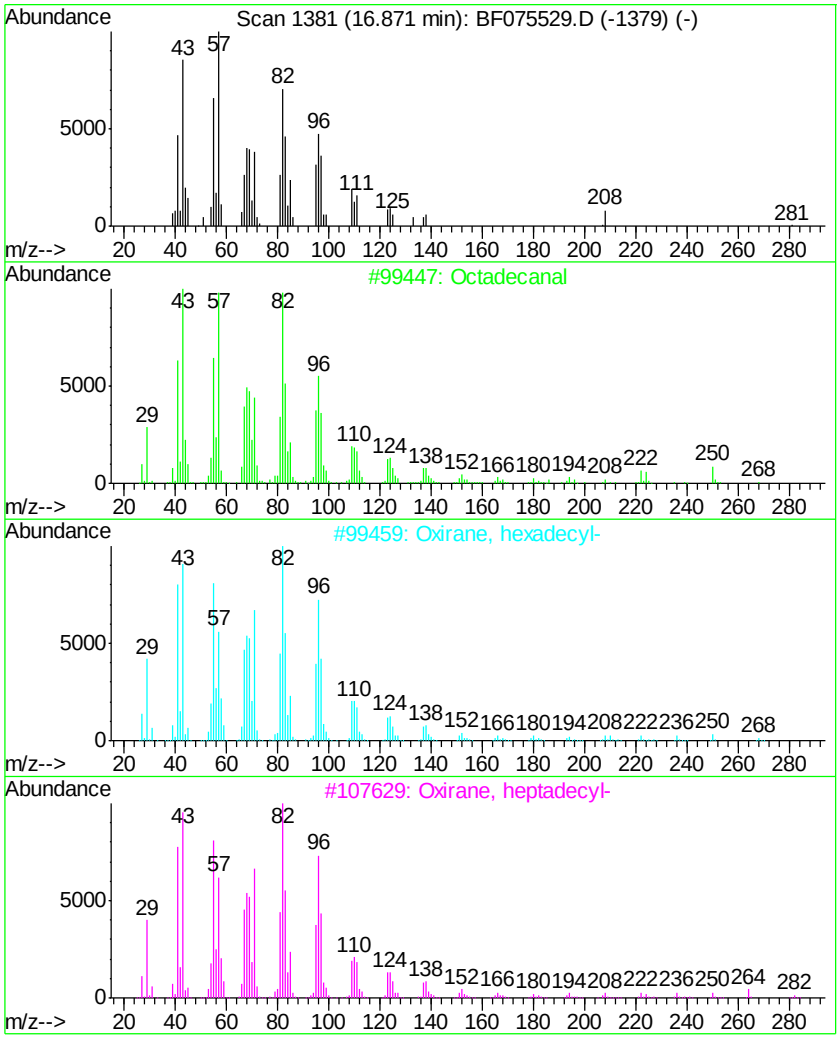
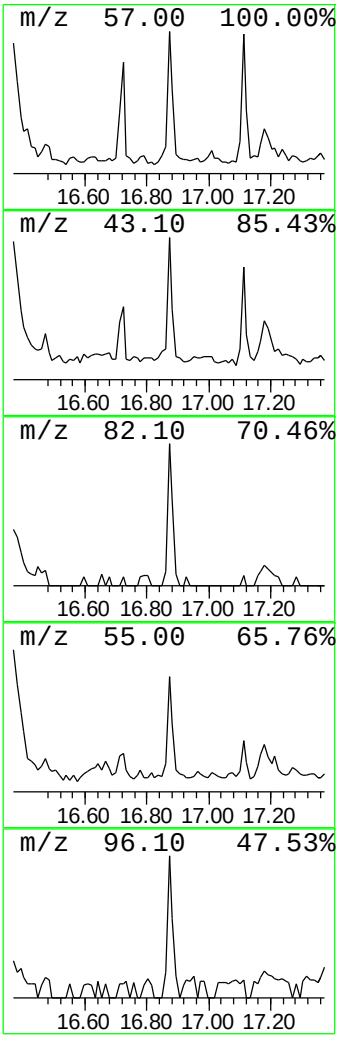
Peak Number 13 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	2.84 ng	78099	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4	1,19-Eicosadiene	278	C20H38	014811-95-1	87
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	86





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Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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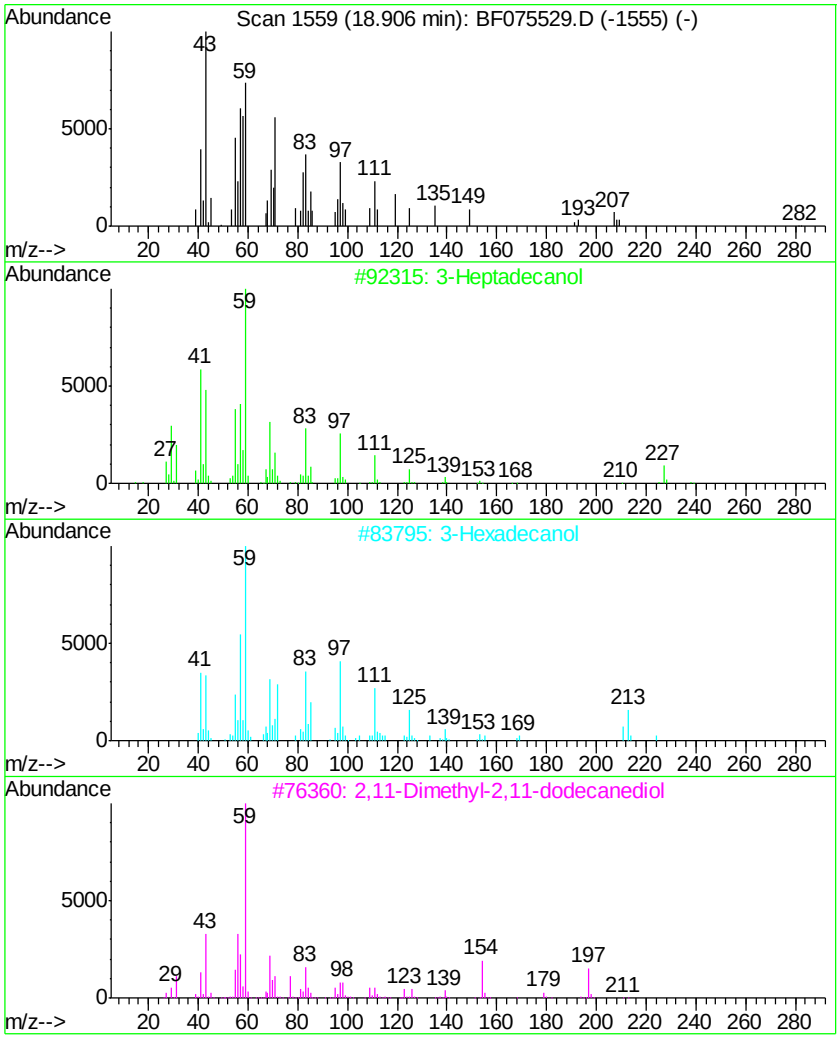
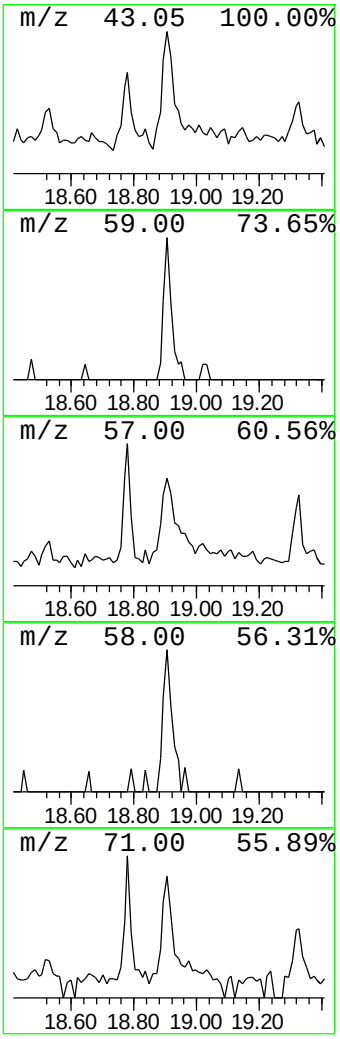
Peak Number 14 unknown18.91 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.91	3.63 ng	99991	Perylene-d12	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptadecanol	256	C17H36O	084534-30-5	47
2	3-Hexadecanol	242	C16H34O	000593-03-3	43
3	2,11-Dimethyl-2,11-dodecanediol	230	C14H30O2	022092-59-7	38
4	2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	35
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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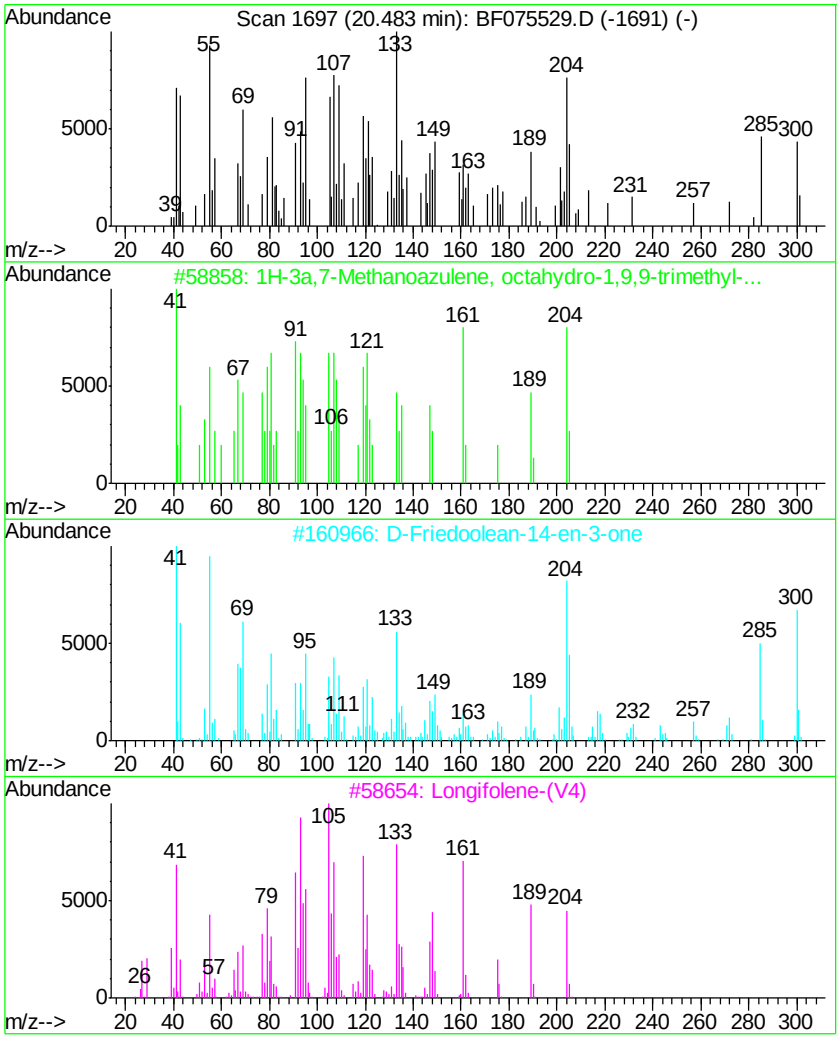
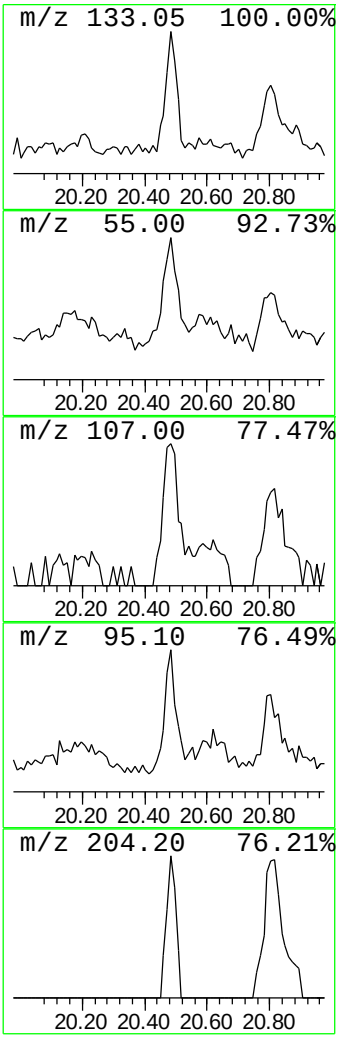
Peak Number 15 1H-3a,7-Methanoazulene, oct... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.48	7.33 ng	202067	Perylene-d12	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	64
2	D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	62
3	Longifolene-(V4)	204	C15H24	061262-67-7	58
4	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	50
5	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	000489-39-4	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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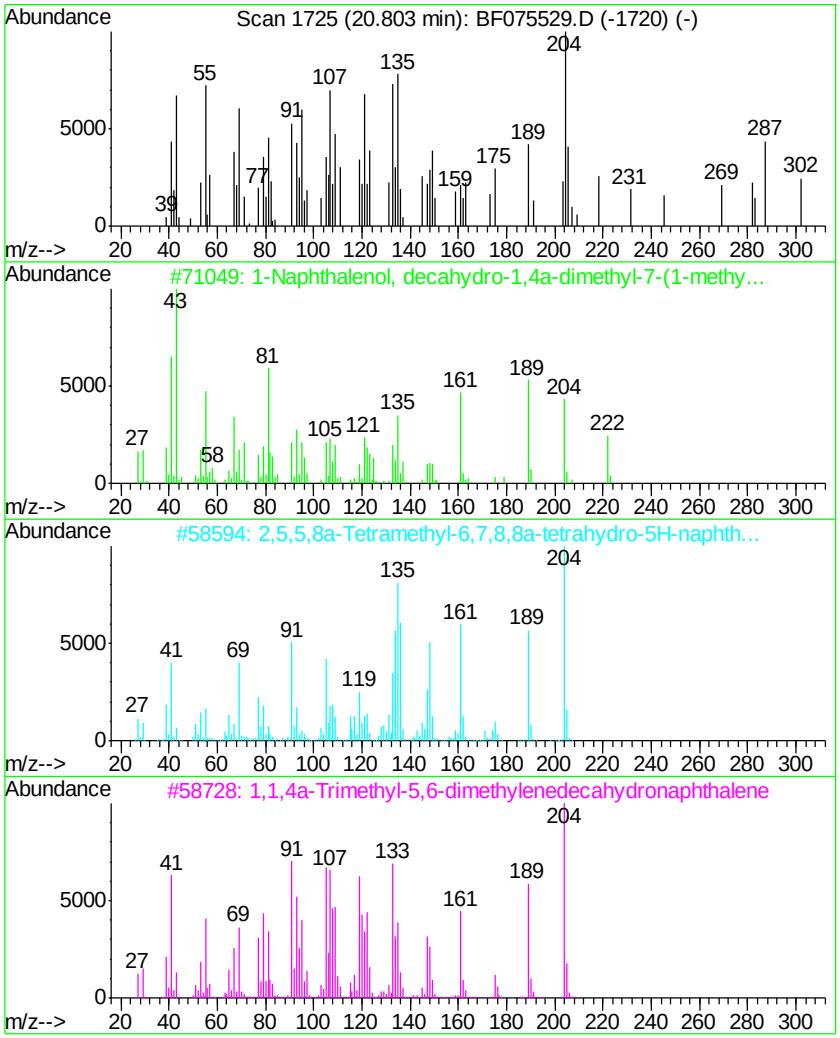
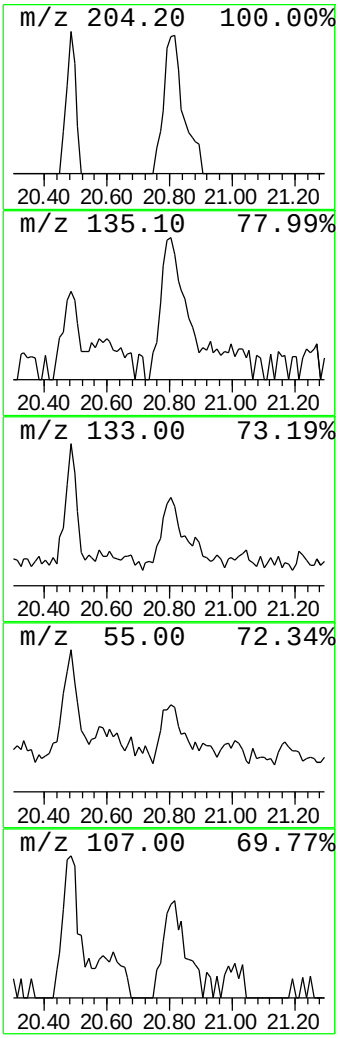
Peak Number 16 unknown20.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.80	6.66 ng	183581	Perylene-d12	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenol, decahydro-1,4a-d...	222	C15H26O	000473-04-1	43
2	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	38
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	30
4	Benzene-1,2-dicarboxylic acid, m...	283	C16H13NO4	194784-73-1	25
5	Aciphyllene	204	C15H24	087745-31-1	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
Data File : BF075529.D
Acq On : 15 Nov 2014 9:15
Operator : TP / JJ
Sample : F4695-07
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-74(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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
Propane, 2,2-dime...	1.62	436.1	ng	6745350	1	7.54	309363	20.0
Butane, 2-methoxy...	1.96	24.3	ng	376116	1	7.54	309363	20.0
2-Pentanone, 4-hy...	5.34	55.9	ng	864600	1	7.54	309363	20.0
unknown7.26	7.26	110.1	ng	1703570	1	7.54	309363	20.0
Tridecanoic acid	13.85	6.3	ng	150046	4	13.16	474852	20.0
2-Chloroethyl lin...	14.55	6.5	ng	153877	4	13.16	474852	20.0
9-Octadecenoic ac...	14.57	6.0	ng	141464	4	13.16	474852	20.0
9-Octadecenamide,...	15.77	4.3	ng	117274	5	16.45	549432	20.0
Oxirane, hexadecyl-	16.05	2.7	ng	73665	5	16.45	549432	20.0
1-Docosene	16.35	12.7	ng	348352	5	16.45	549432	20.0
Octadecanal	16.87	2.8	ng	78099	5	16.45	549432	20.0
unknown18.91	18.91	3.6	ng	99991	6	18.20	550983	20.0
1H-3a,7-Methanoaz...	20.48	7.3	ng	202067	6	18.20	550983	20.0
unknown20.80	20.80	6.7	ng	183581	6	18.20	550983	20.0