

**A Novel Series of Enoyl Reductase Inhibitors Targeting the ESKAPE
Pathogens, *Staphylococcus aureus* and *Acinetobacter baumannii***

Jieun Kwon,^a Tina Mistry,^a + Jinhong Ren,^b Michael E. Johnson,^{a,b,*} and Shahila Mehboob^{a,*}

Supplementary Data

Table S1: Calculated K_i values for N-carboxy pyrrolidine analogs

Compound	SaFabI		AbFabI		Compound	SaFabI		AbFabI	
	IC ₅₀ (μ M)	K _i (μ M)	IC ₅₀ (μ M)	K _i (μ M)		IC ₅₀ (μ M)	K _i (μ M)	IC ₅₀ (μ M)	K _i (μ M)
1	10.7	4.0	3.1	1.6	16	1.8	0.7	>200	>100
2	5.0	1.9	3.9	2.0	17	>100	>37.1	>100	>50
3	4.6	1.7	2.1	1.1	18	>100	>37.1	>100	>50
4	7.3	2.7	9.3	4.7	19	>100	>37.1	>100	>50
5	3.0	1.1	7.4	3.7	20	>100	>37.1	>100	>50
6	1.9	0.7	6.9	3.5	21	>100	>37.1	>100	>50
7	5.7	2.1	3.0	1.5	22	>100	>37.1	>100	>50
8	0.5	0.2	3.6	1.8	23	1.2	0.4	0.5	0.2
9	12.5	4.6	>200	>100	24	3.5	1.3	0.4	0.2
10	18.4	6.8	30.7	15.4	25	3.6	1.3	>200	>100
11	6.0	2.2	14.0	7.0	26	1.1	0.4	8.5	4.3
12	2.5	0.9	7.8	3.9	27	4.5	1.7	20.0	10.0
13	2.7	1.0	32.0	16.0	28	28.4	10.5	7.1	3.6
14	2.3	0.9	54.0	27.0	29	>100	>37.1	>100	>50
15	5.5	2.0	13.7	6.9					

K_i values were calculated by the Cheng-Prusoff equation for competitive inhibition. We assume the mechanism of inhibition to be competitive as we see that in the crystal structure compound **1** occupies the same region in the active site as known FabI inhibitors that are competitive with the substrate (Mehboob *et al*, *J Med Chem.* **2012**, 55: 5933-41). However, this remains to be confirmed experimentally.

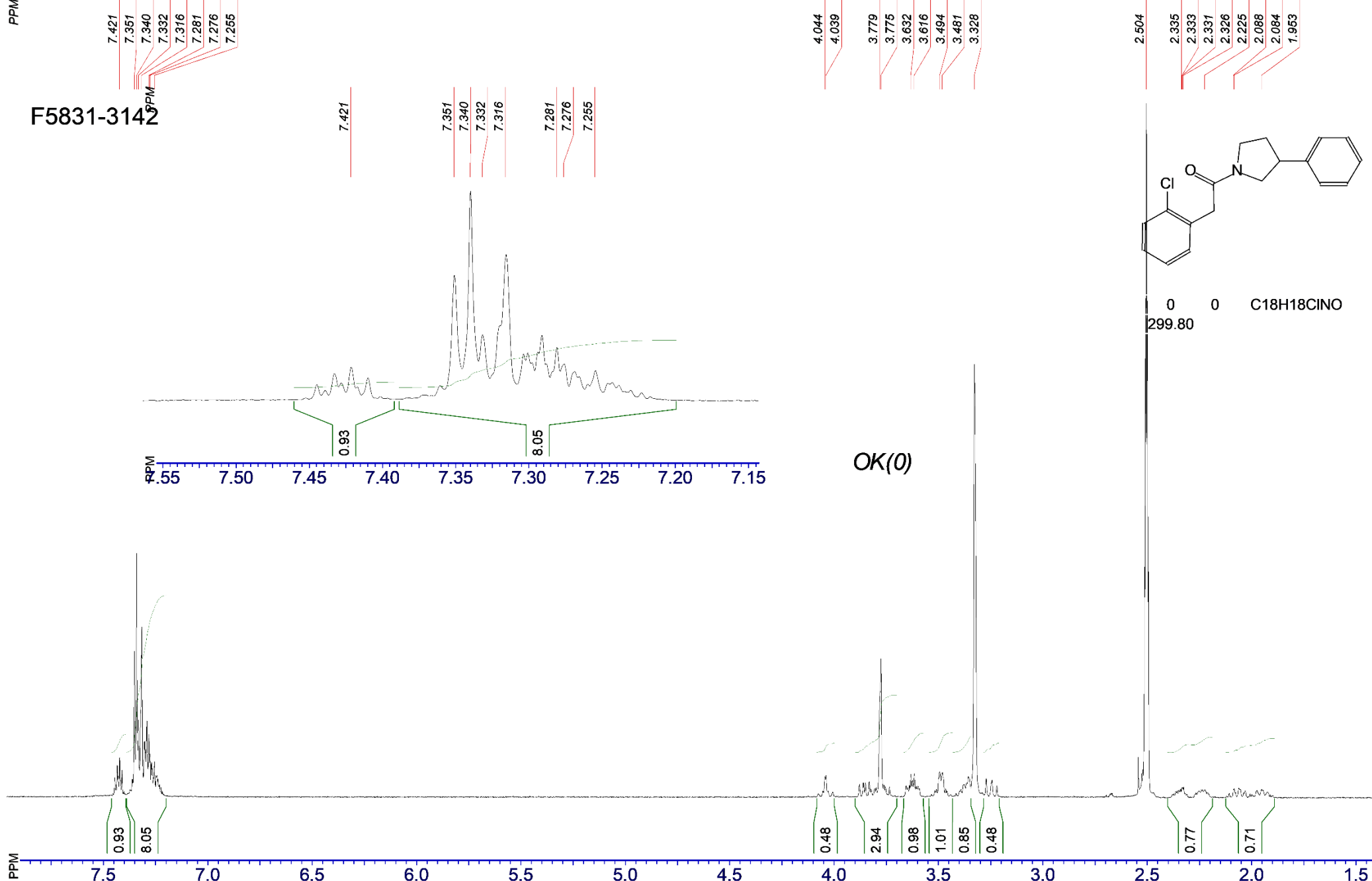
Cheng-Prusoff equation:

$$K_i = IC_{50}/(1 + ([S]/K_m))$$

where [S] (substrate concentration used in the assay) is 400 μ M for SaFabI and 300 μ M for AbFabI and substrate K_m values are 236 μ M for SaFabI and 300 μ M for AbFabI.

NMR Spectra and Mass Spectra for each compound discussed in this article are provided herein. This information provides conclusive evidence confirming identity and purity of the compounds. The compounds were rationally designed and then custom synthesized by Life Chemicals. The compound names provided by Life Chemicals appears on each data sheet. Below is the table correlating the compound numbers appearing in the manuscript with the numbers provided by Life Chemicals.

Compound #	Compound name	% purity as observed by mass spec	identity confirmed by ¹ H- NMR	Spectra displayed on page
1	F5831-3142	>95 %	Yes	4, 5
2	F0687-0495	>95 %	Yes	6, 7
3	F0687-0499	>95 %	Yes	8, 9
4	F0687-0497	>95 %	Yes	10, 11
5	F0687-0501	>95 %	Yes	12, 13
6	F0687-0496	>95 %	Yes	14, 15
7	F0687-0500	>95 %	Yes	16, 17
8	F0687-0473	>95 %	Yes	18, 19
9	F5831-2782	>95 %	Yes	20, 21
10	F6395-0086	>95 %	Yes	22, 23
11	F0687-0483	>95 %	Yes	24, 25
12	F6518-4222	>95 %	Yes	26, 27
13	F0687-0502	>95 %	Yes	28, 29
14	F0687-0503	>95 %	Yes	30, 31
15	F0687-0504	>95 %	Yes	32, 33
16	F6518-4339	>95 %	Yes	34, 35
17	F0687-0489	>95 %	Yes	36,37
18	F0687-0490	>95 %	Yes	38, 39
19	F0687-0491	>95 %	Yes	40, 41
20	F0687-0492	>95 %	Yes	42, 43
21	F0687-0494	>95 %	Yes	44, 45
22	F6518-4320	>95 %	Yes	46, 47
23	F0687-0468	>95 %	Yes	48, 49
24	F0687-0471	>95 %	Yes	50, 51
25	F0687-0493	>95 %	Yes	52, 53
26	F0687-0478	>95 %	Yes	54, 55
27	F0687-0481	>95 %	Yes	56, 57
28	F0687-0475	>95 %	Yes	58, 59
29	F0687-0498	>95 %	Yes	60, 61

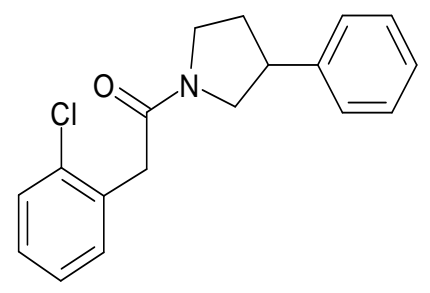


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Date: 10_sep_2015	Solvent: DMSO 0810		TE: 293 K	block: S16696

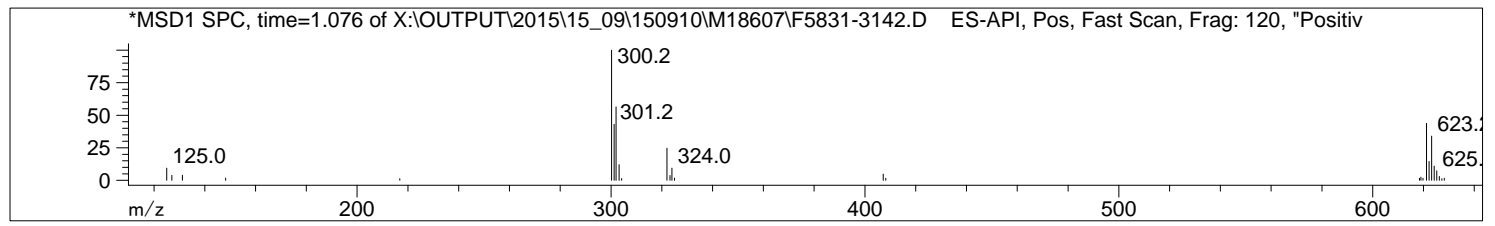
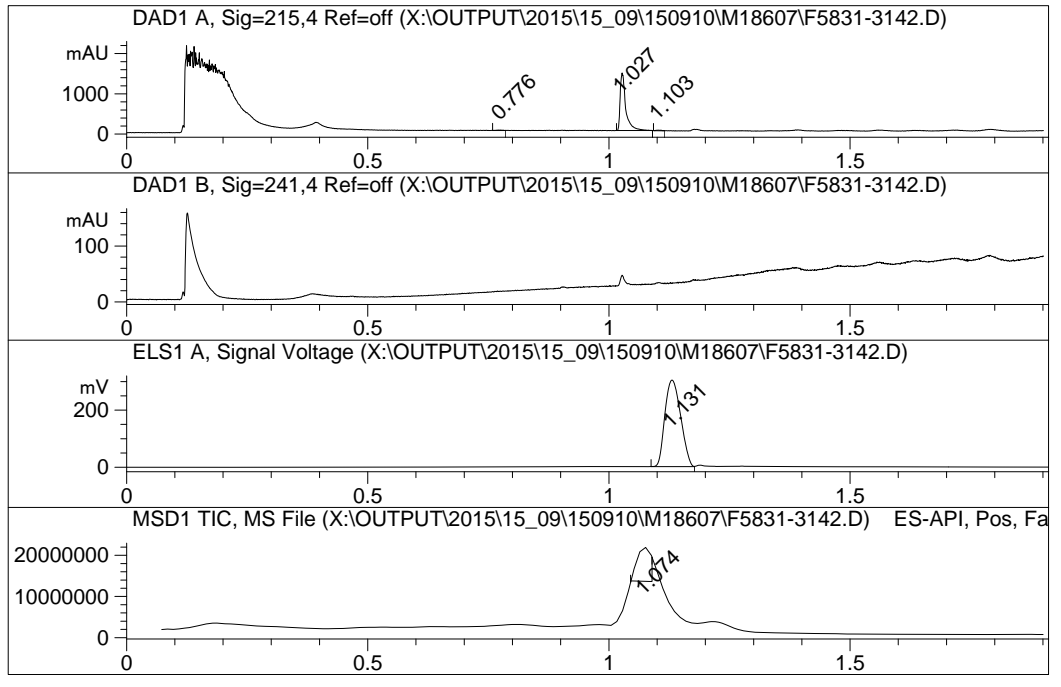
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 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation column: **98 %**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 299.8
 Salt:



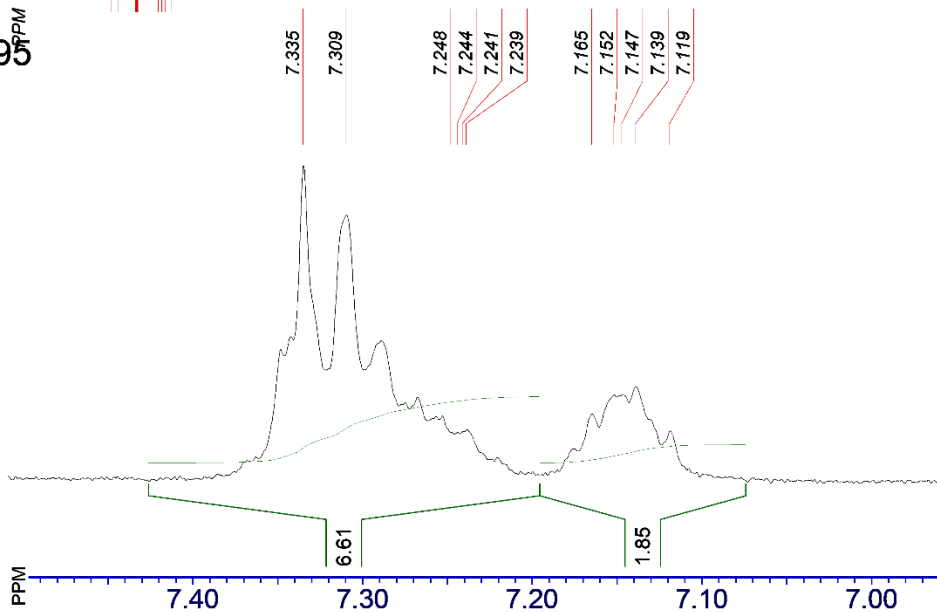
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#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.074	100.000

PPM

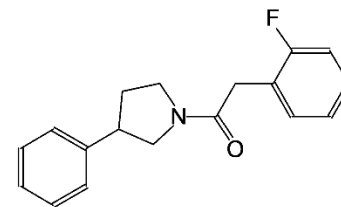
F0687-0495



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3.619
3.479
3.469
3.306
3.288

2.504

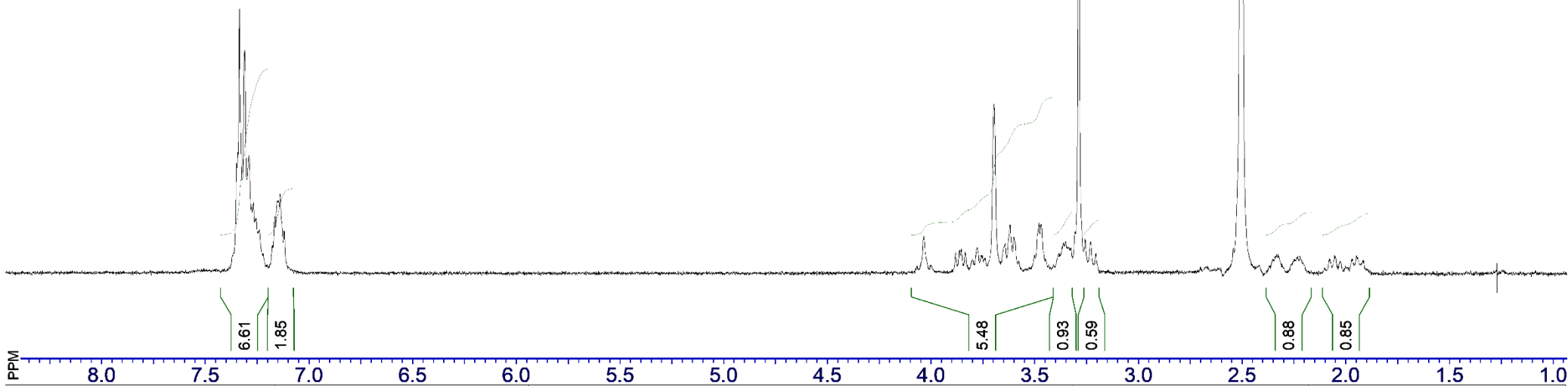
2.220
2.031
1.946



C18H18FNO

283.35

OK(0)



File name: F0687-0495

Expert: M.Pyanova

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NS: ; pw: 9,65 usec

SI: 65536, TD: 24000

Date: 21_Mar_2016

Solvent: DMSO 0315

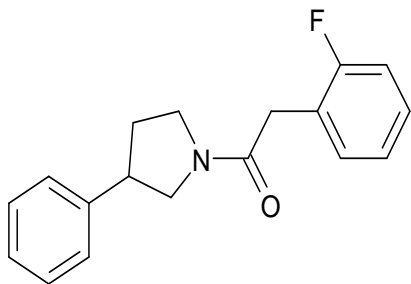
TE: 293 K

block: S18648

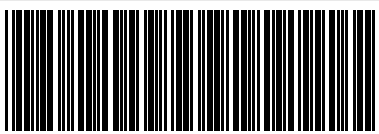
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

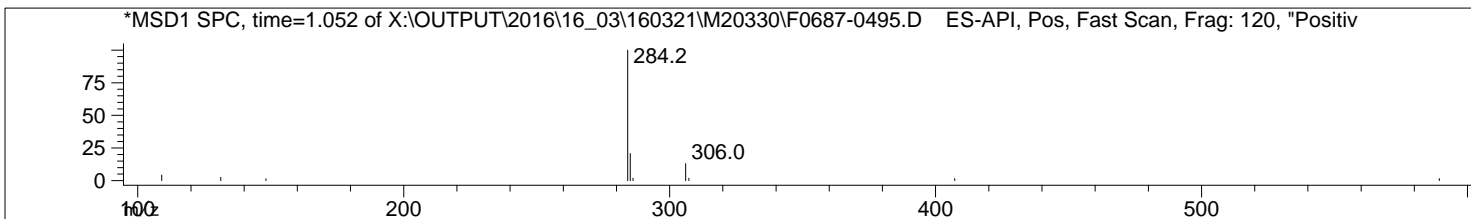
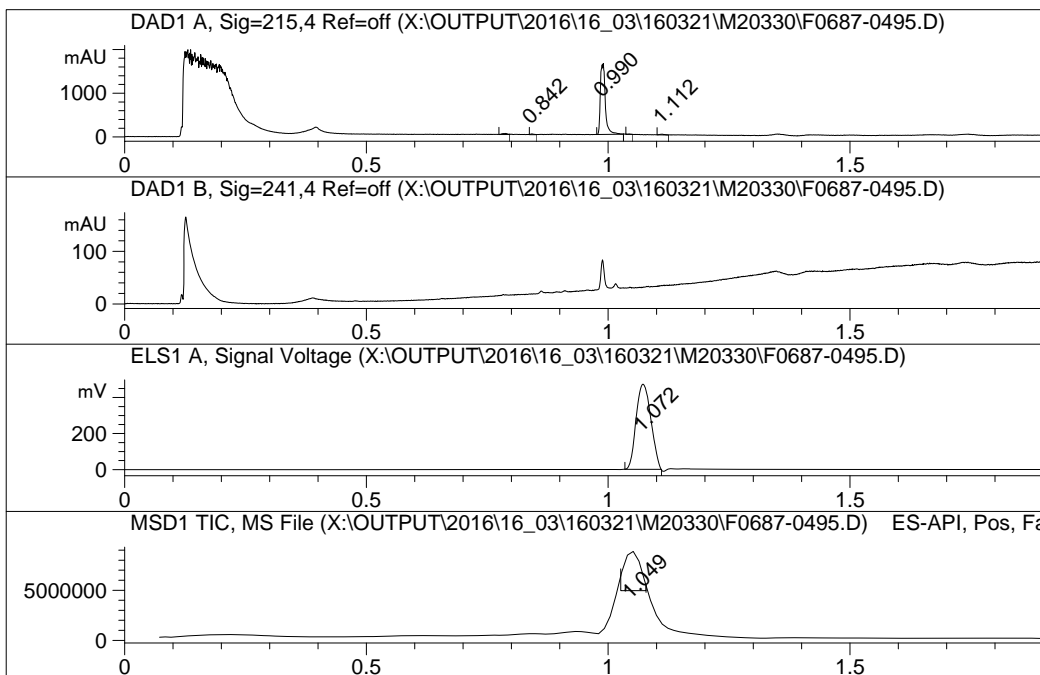
Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation column **96 %**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 283.34
 Salt:



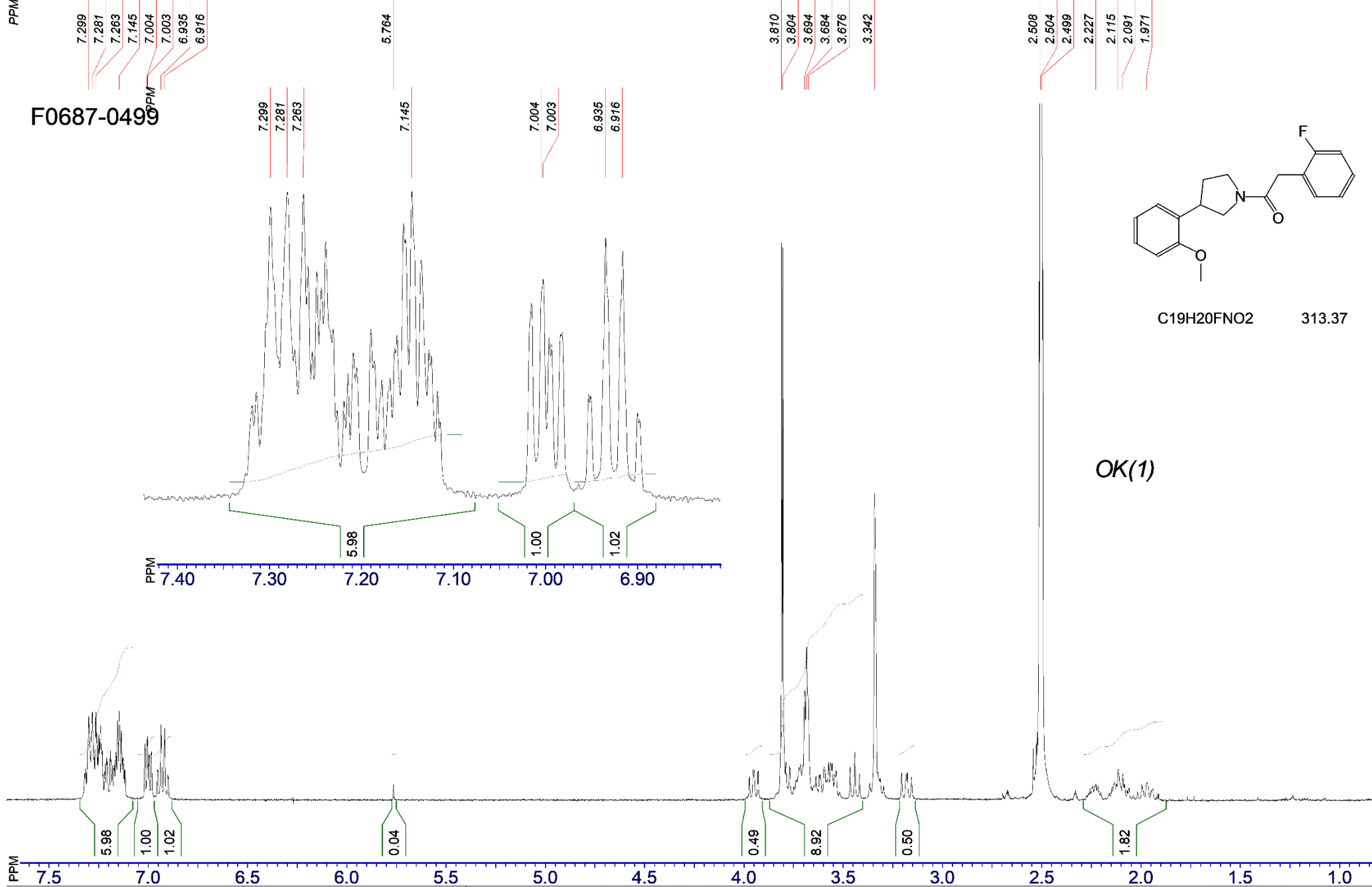
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2		0.842	0.720
3		0.990	96.407
4		1.043	0.265
5		1.112	0.997

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.072	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.049	100.000

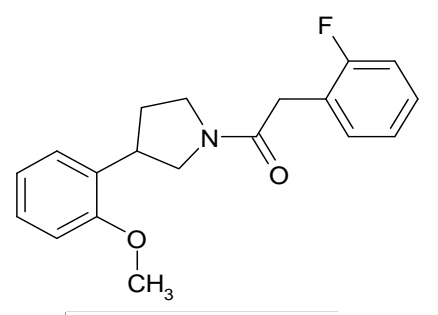


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Date: 28_Mar_2016	Solvent: DMSO 0321		TE: 293 K	block: S18745

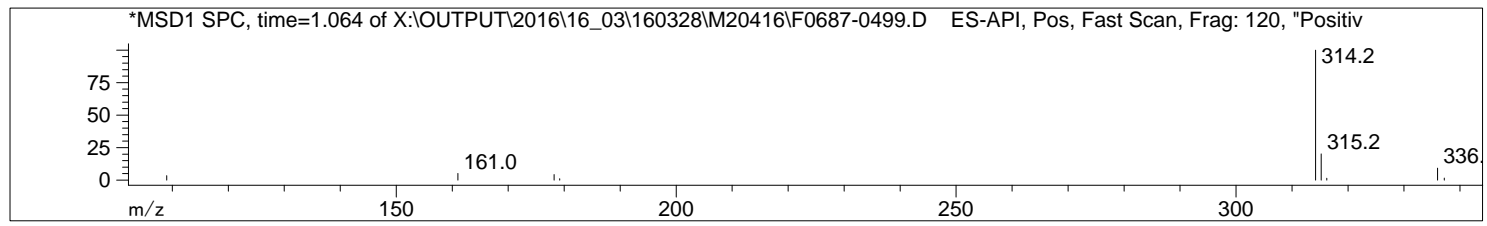
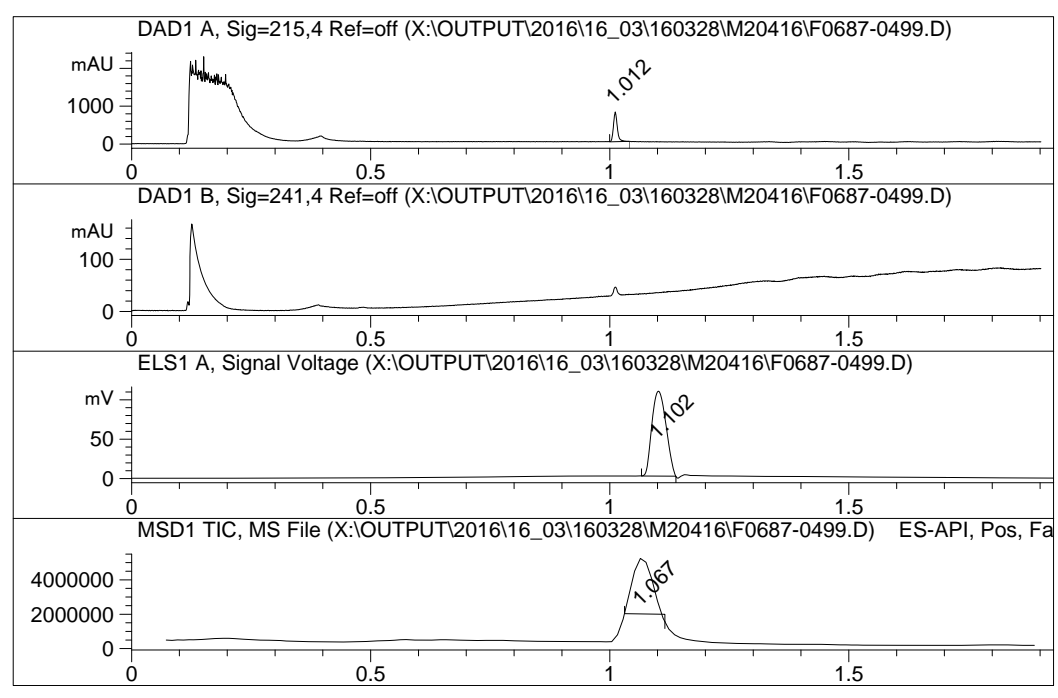
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Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

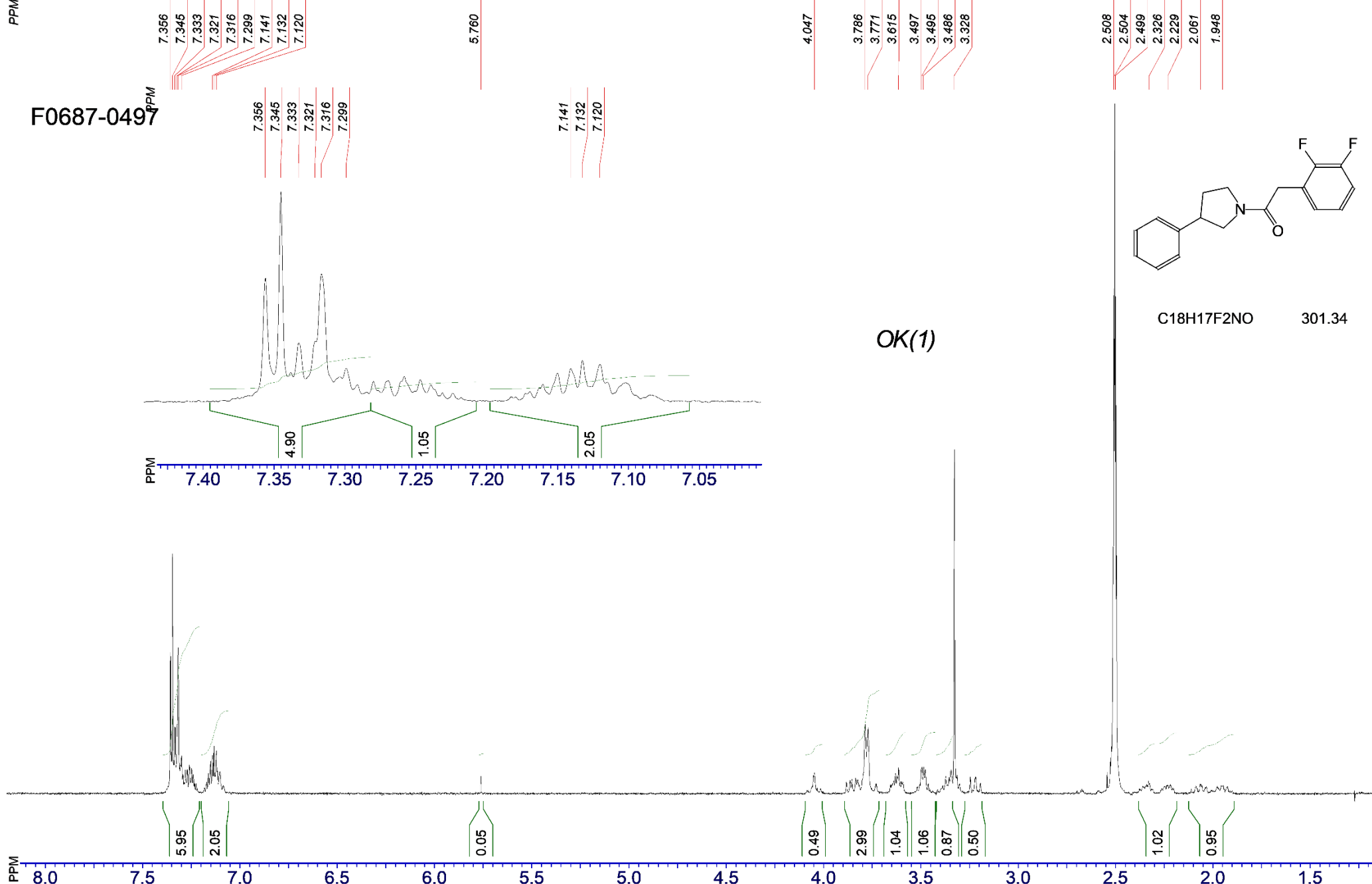
Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
Separation colu **100 %**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 313.37
Salt:



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.012	100.000
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.102	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.067	100.000

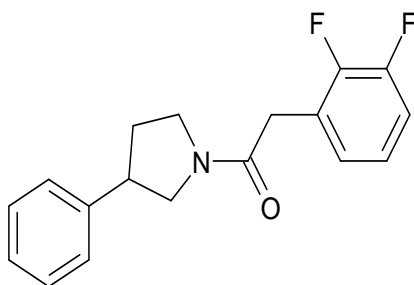


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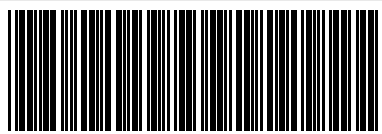
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Agilent 1200 LC/MSD
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 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

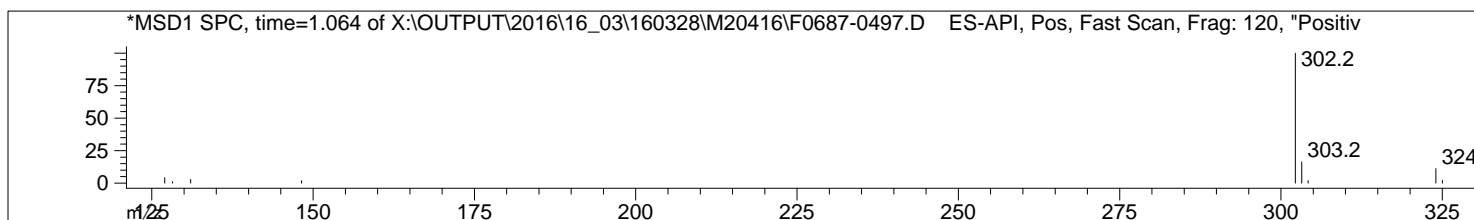
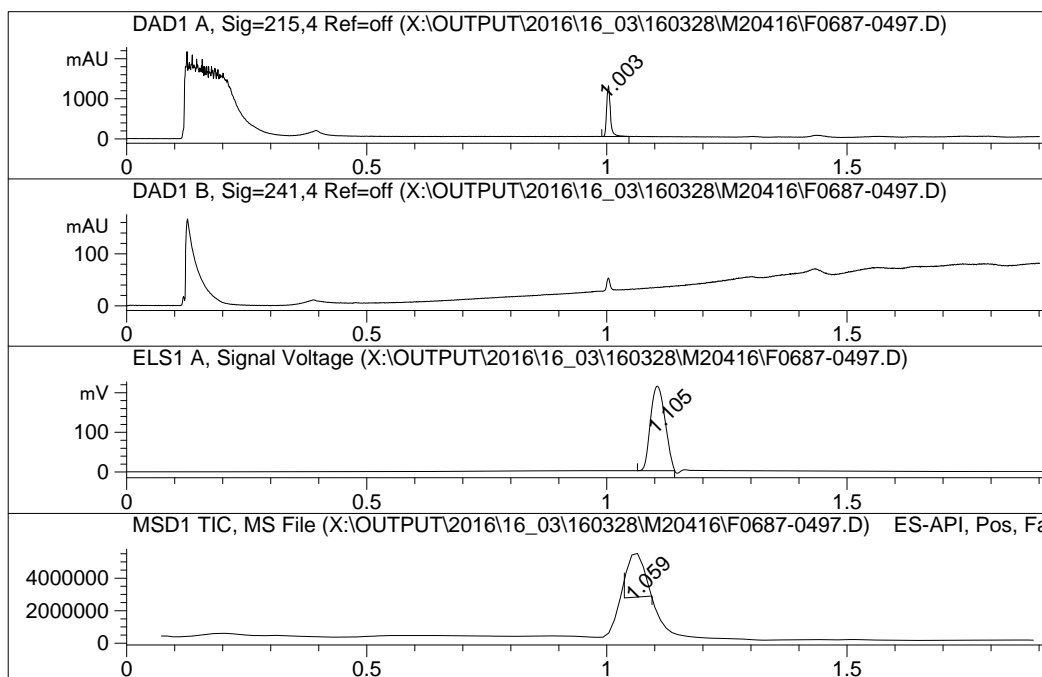
Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation colour **100 %**
 Rapid Resolution HPLC Cartidge 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



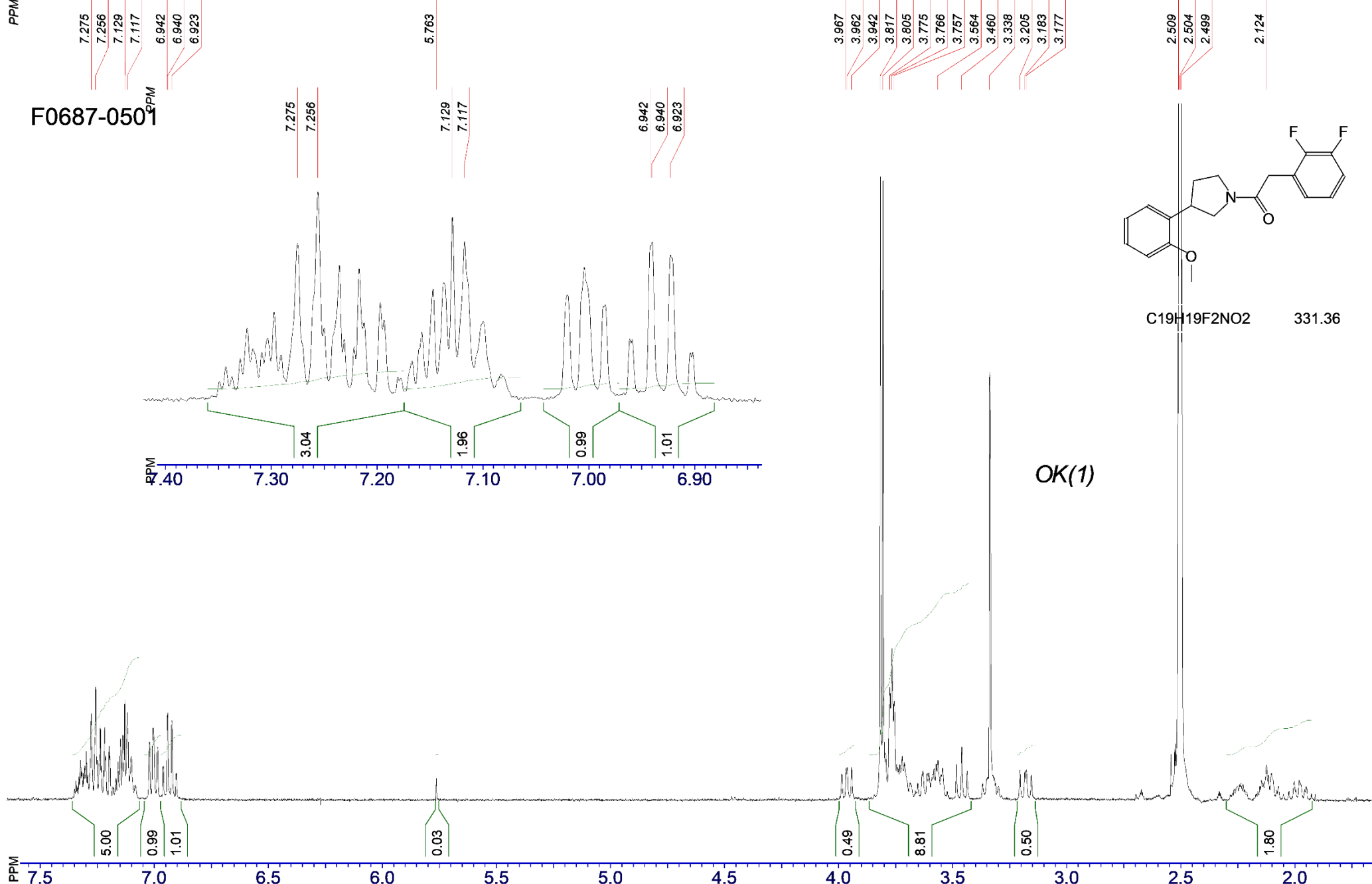
Mol.Weight: 301.33
 Salt:



F0687-0497



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.003	100.000
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.105	100.000
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1	MSD1 TIC, MS File	1.059	100.000

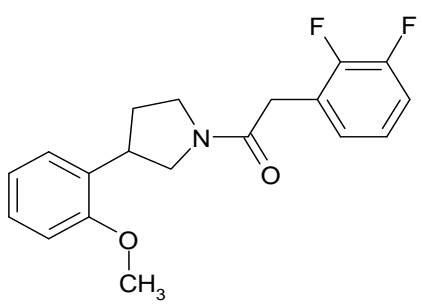


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Date: 28_Mar_2016	Solvent: DMSO 0321		TE: 293 K	block: S18745

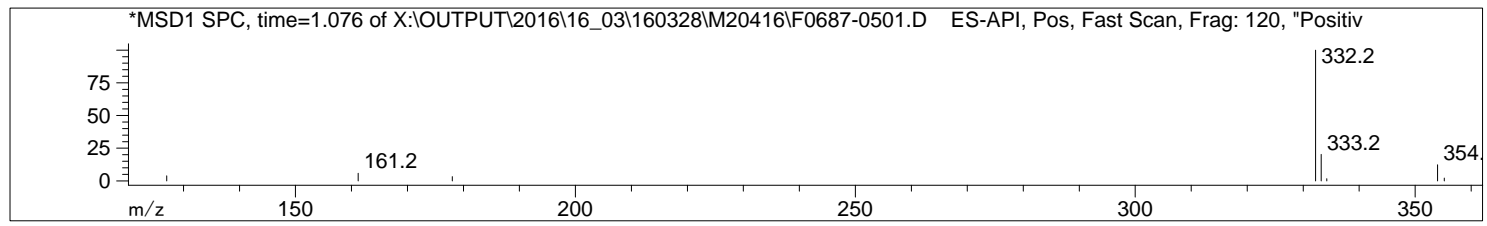
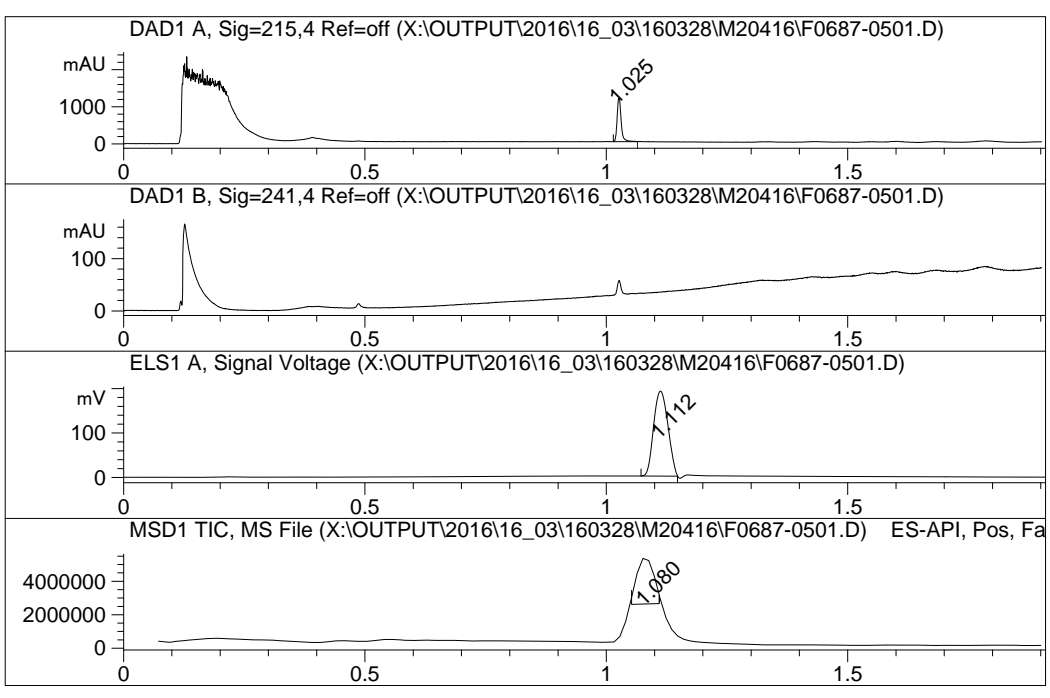
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

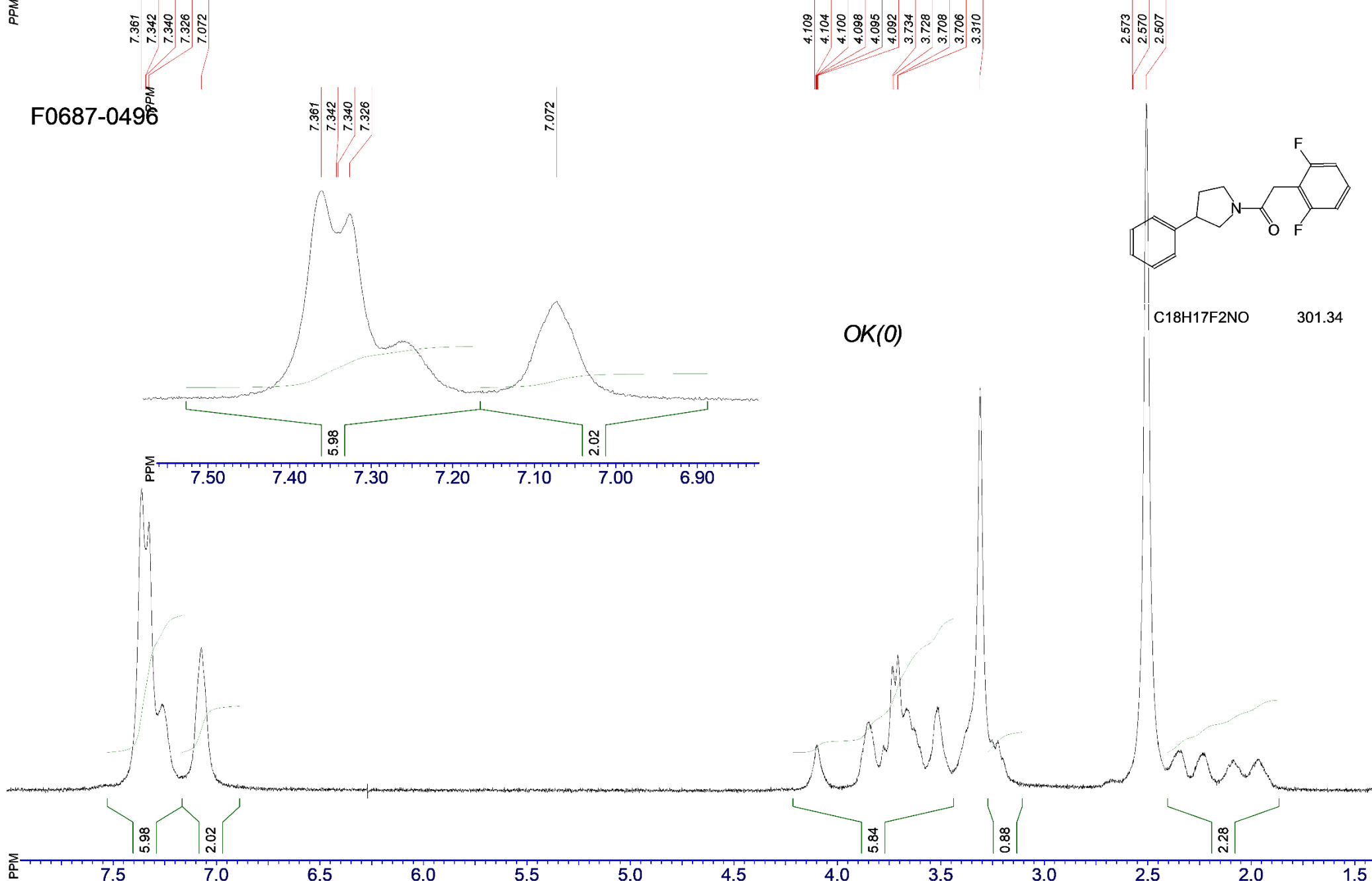
Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation colu **100%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 331.36
 Salt:



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.025	100.000
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.112	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.080	100.000

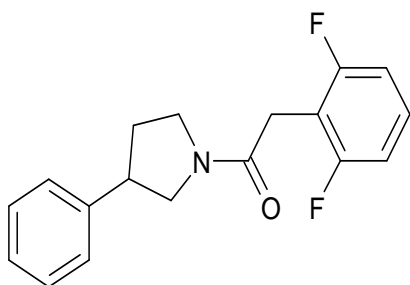


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Date: 21_Mar_2016	Solvent: DMSO 0315		TE: 293 K	block: S18648

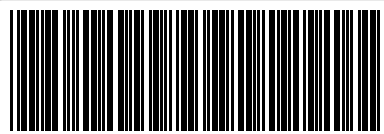
-.o.-Syntez Purity Report -.o.-

Agilent 1200 LC/MSD
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 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

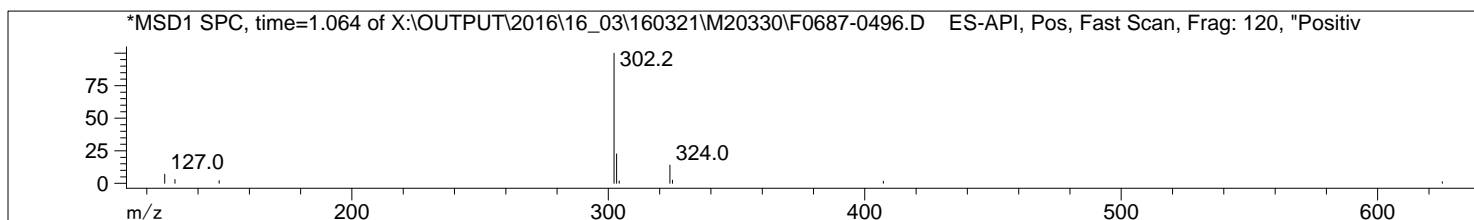
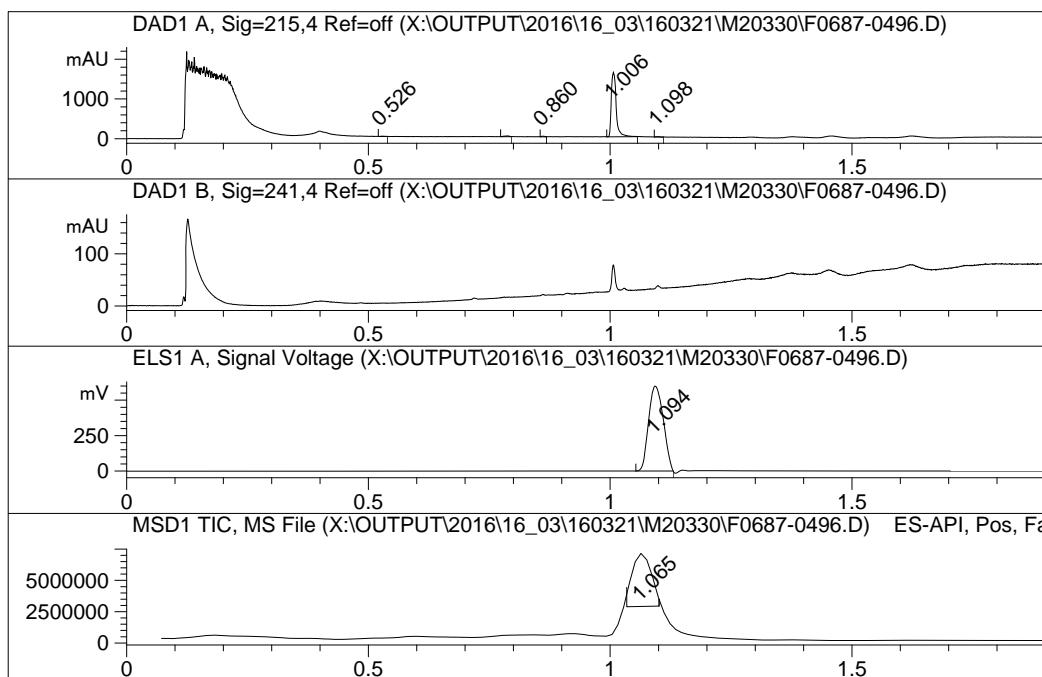
Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation colun **97%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 301.33
 Salt:



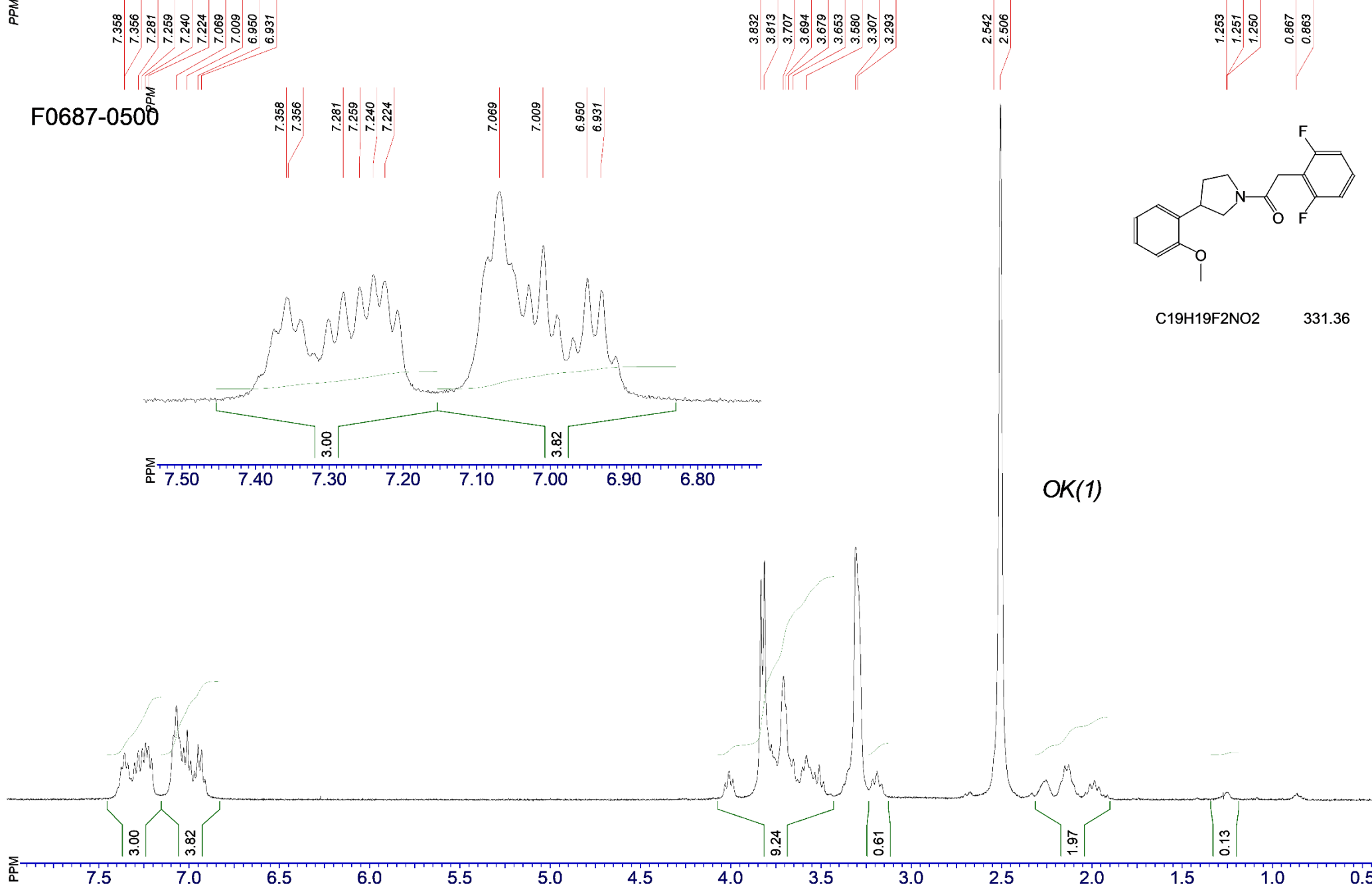
F0687-0496



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1	DAD1 A, Sig=215,4 Ref=off	0.526	0.534
2		0.787	1.249
3		0.860	0.632
4		1.006	97.073
5		1.098	0.512

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.094	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.065	100.000

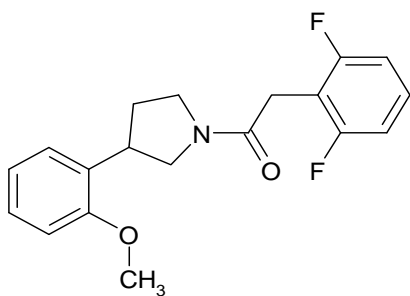


File name: F0687-0500	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 22_Mar_2016	Solvent: DMSO 0315		TE: 293 K	block: S18666

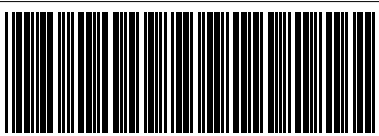
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
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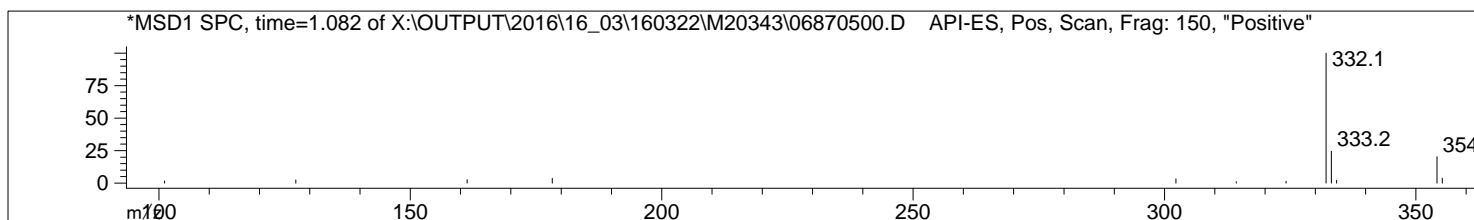
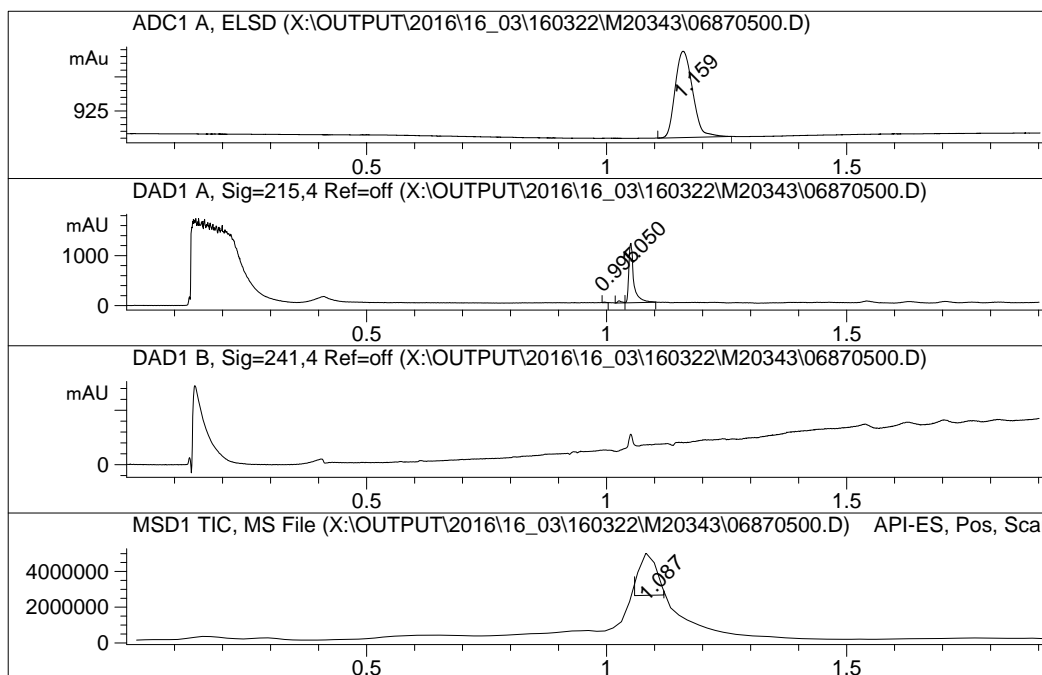
Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column: **96 %**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



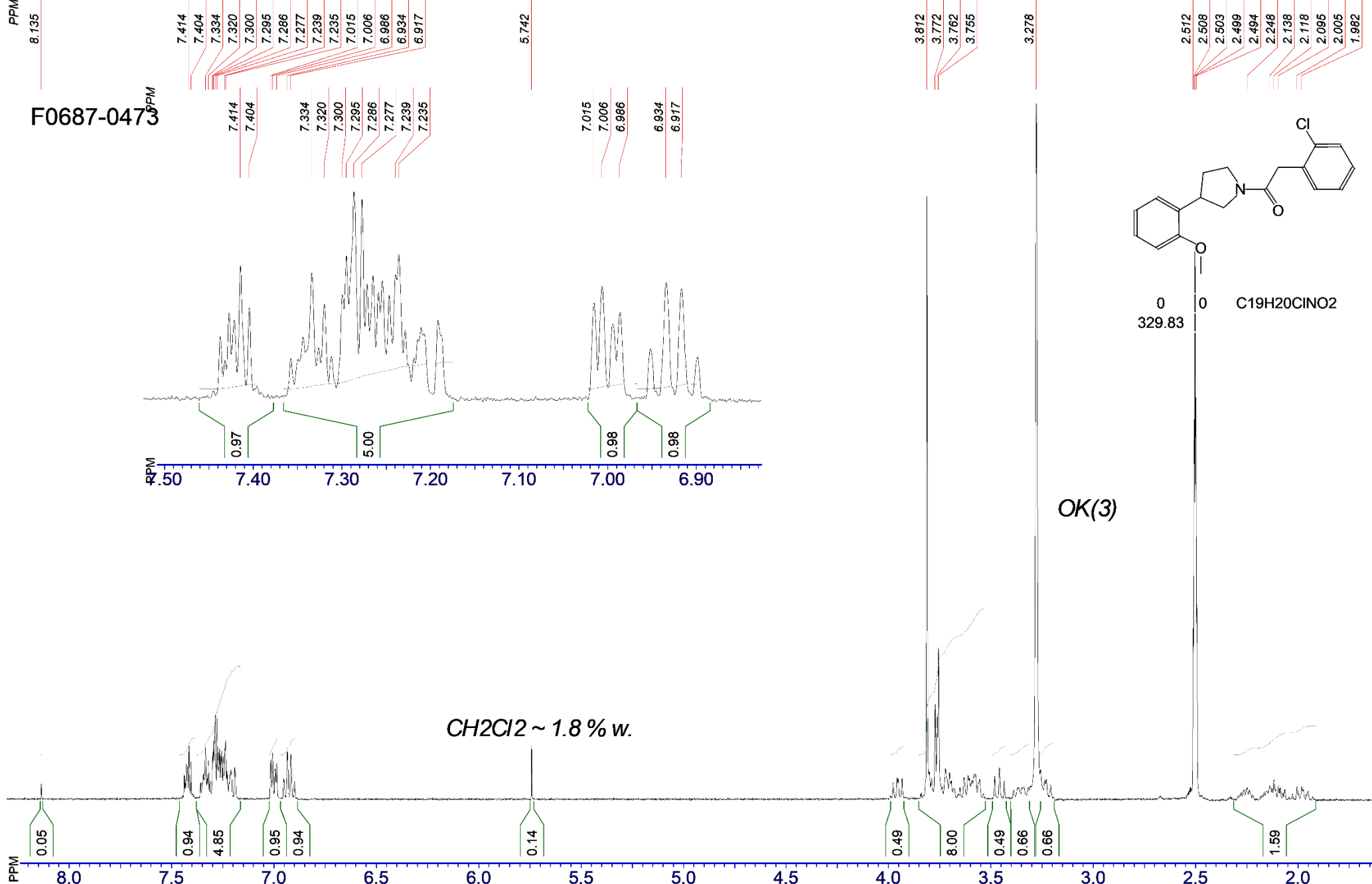
Mol.Weight: 331.36
 Salt:



F0687-0500



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1	DAD1 A, Sig=215,4 Ref=off	0.995	0.528
2		1.025	2.825
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#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.087	100.000

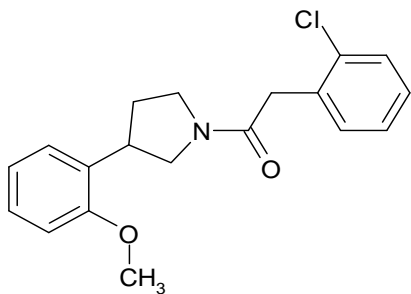


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Date: 26_Oct_2015	Solvent: DMSO new		TE: 293 K	block: S17133

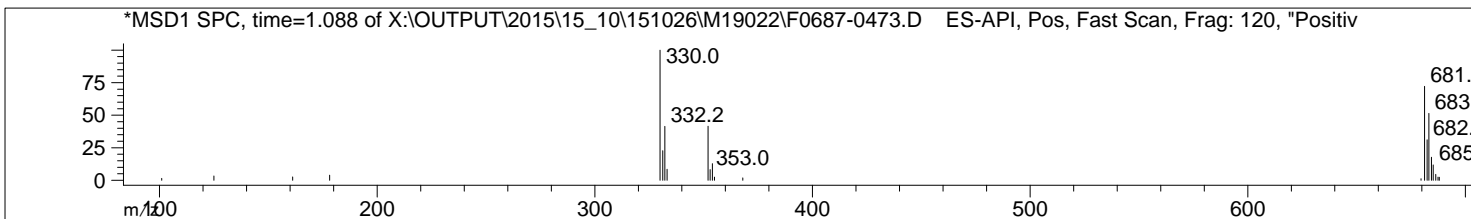
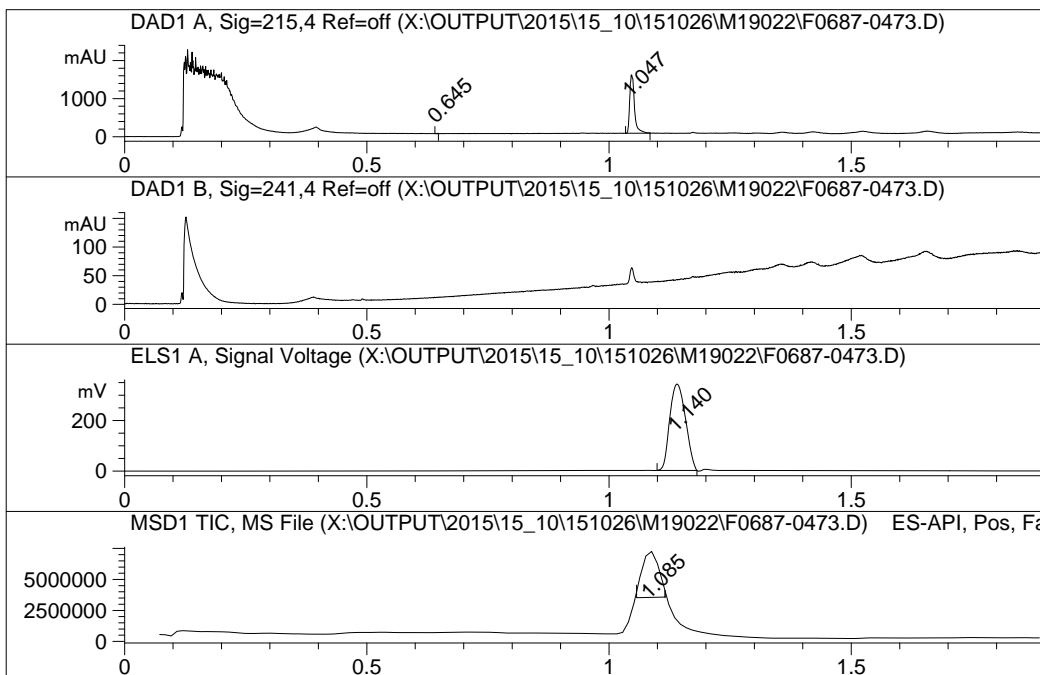
- .o. - Syntez Purity Report - .o. -

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation colu **99%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



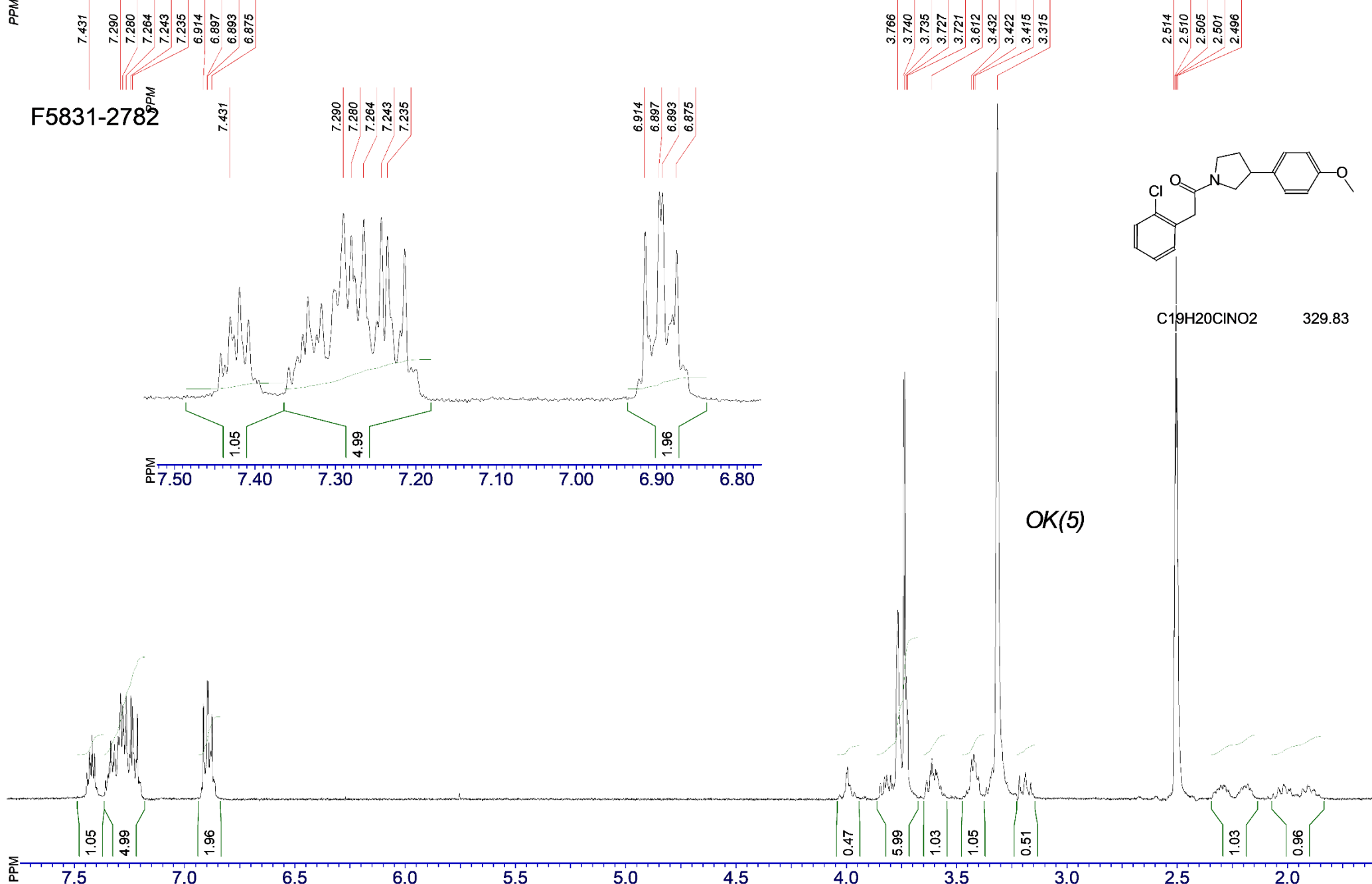
Mol.Weight: 329.83
 Salt:



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.645	0.306
2		1.047	99.694

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.140	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.085	100.000



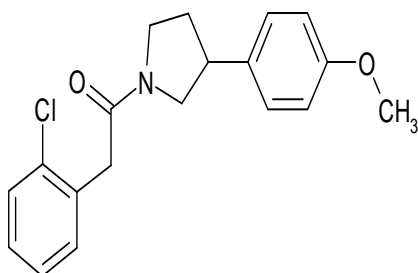
File name: F5831-2782	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO new		TE: 293 K	block: S17623

-.o.-Syntez Purity Report -.o.-

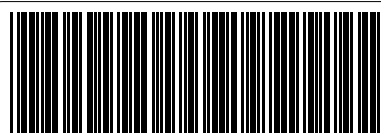
Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column
 Rapid Resolutionn HPLC Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18

99%



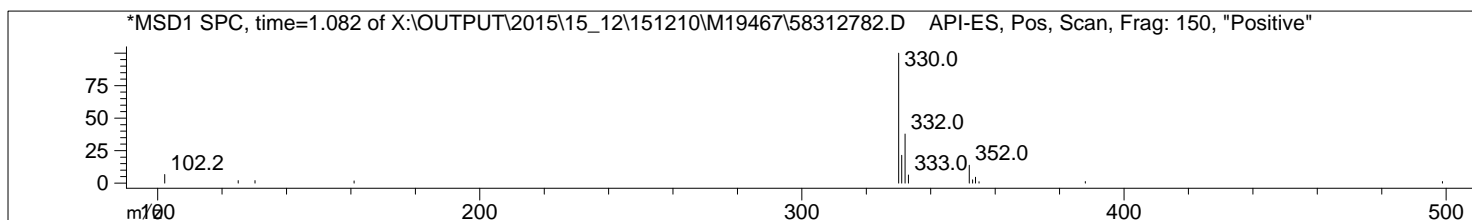
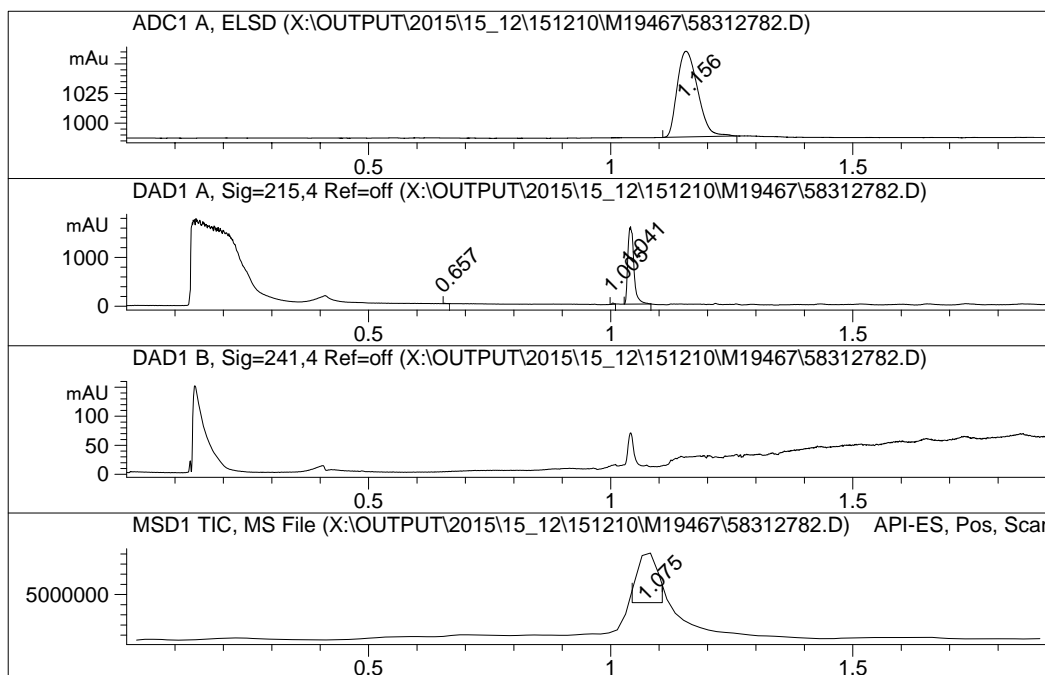
Mol.Weight: 329.83
 Salt:



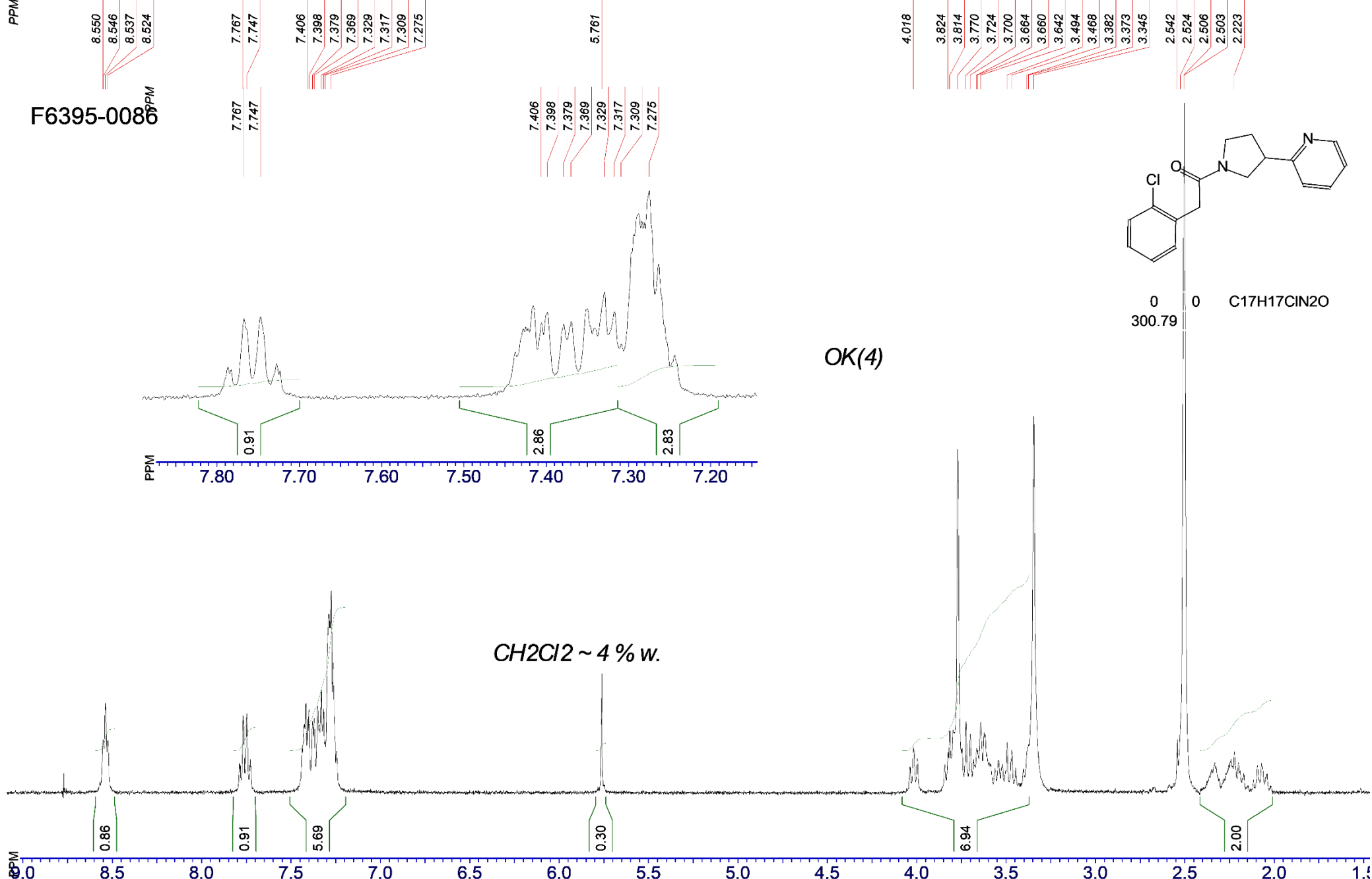
F5831-2782

M19467

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.156	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.657	0.234
2		1.005	0.598
3		1.041	99.168
#	Signal	R.Time	Area %
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.075	100.000

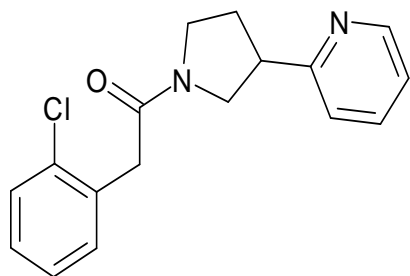


File name: F6395-0086	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 06_Nov_2015	Solvent: DMSO 1027		TE: 293 K	block: S17287

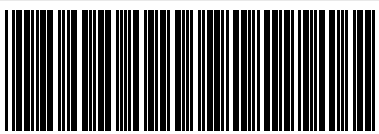
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

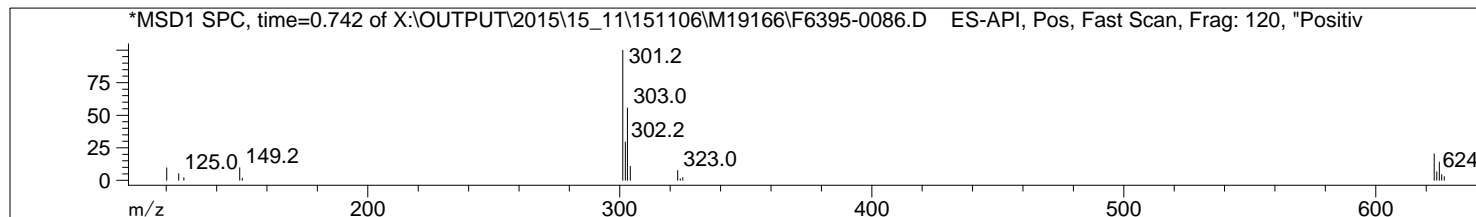
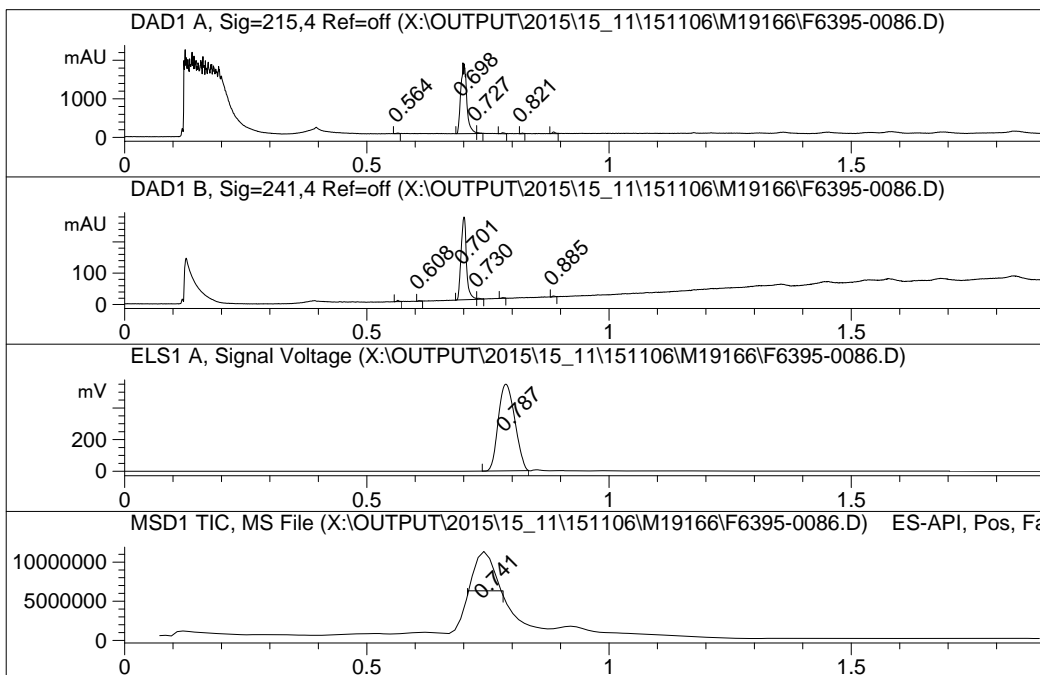
Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation colu **96%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 300.79
 Salt:



F6395-0086

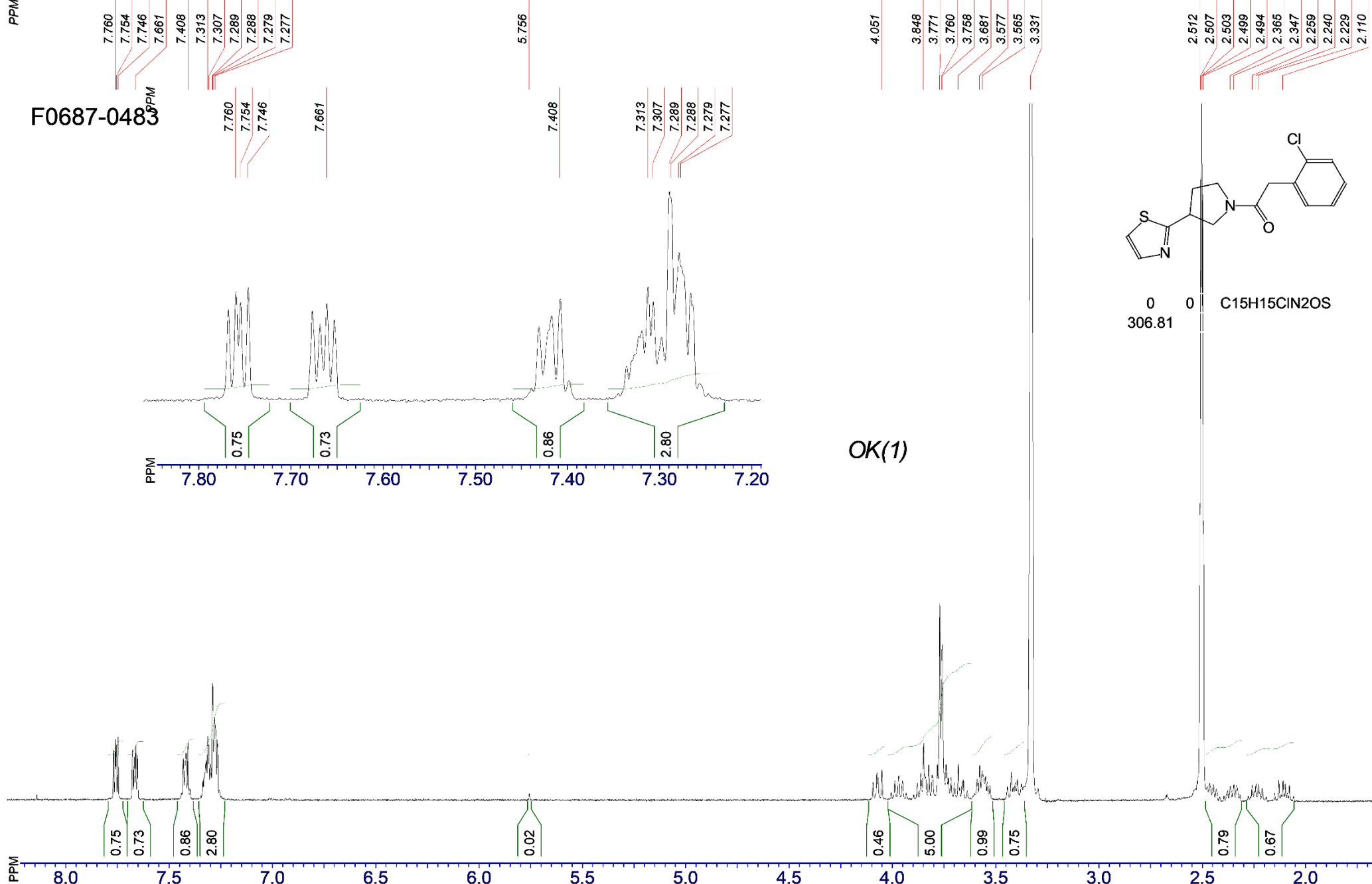


#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.564	0.435
2		0.698	96.784
3		0.727	0.516
4		0.780	0.670
5		0.821	0.399
6		0.885	1.196

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.564	0.622
2		0.608	0.372
3		0.701	97.190
4		0.730	0.742
5		0.781	0.435
6		0.885	0.639

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.787	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.741	100.000

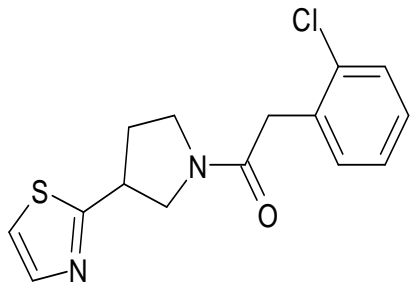


File name: F0687-0483	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 26_Oct_2015	Solvent: DMSO new		TE: 293 K	block: S17133

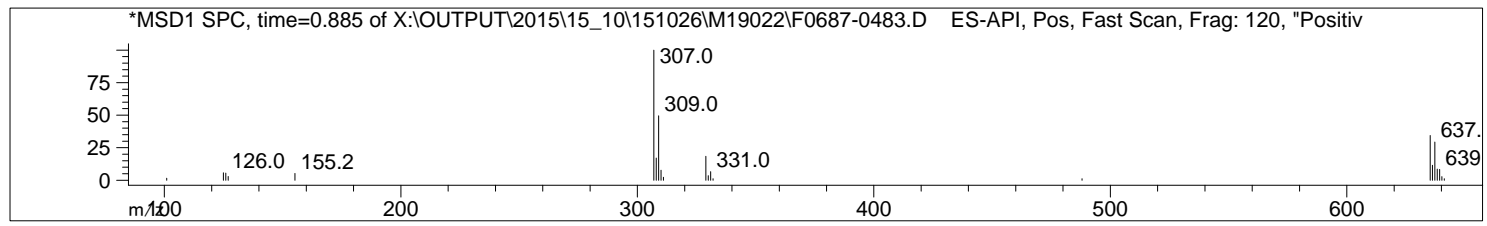
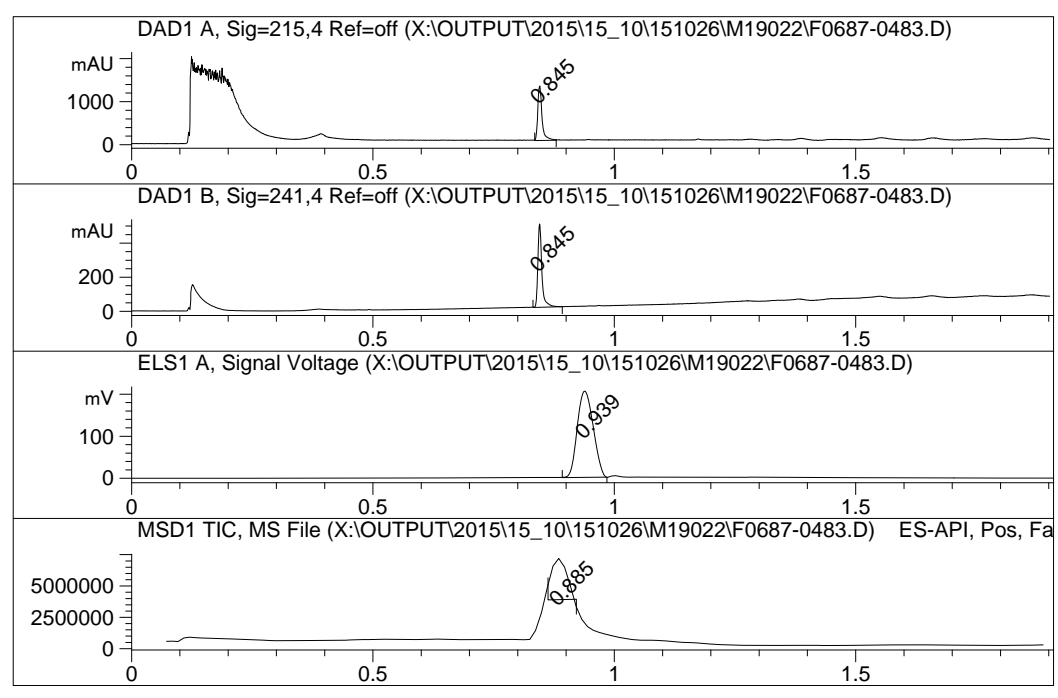
- .o.-Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

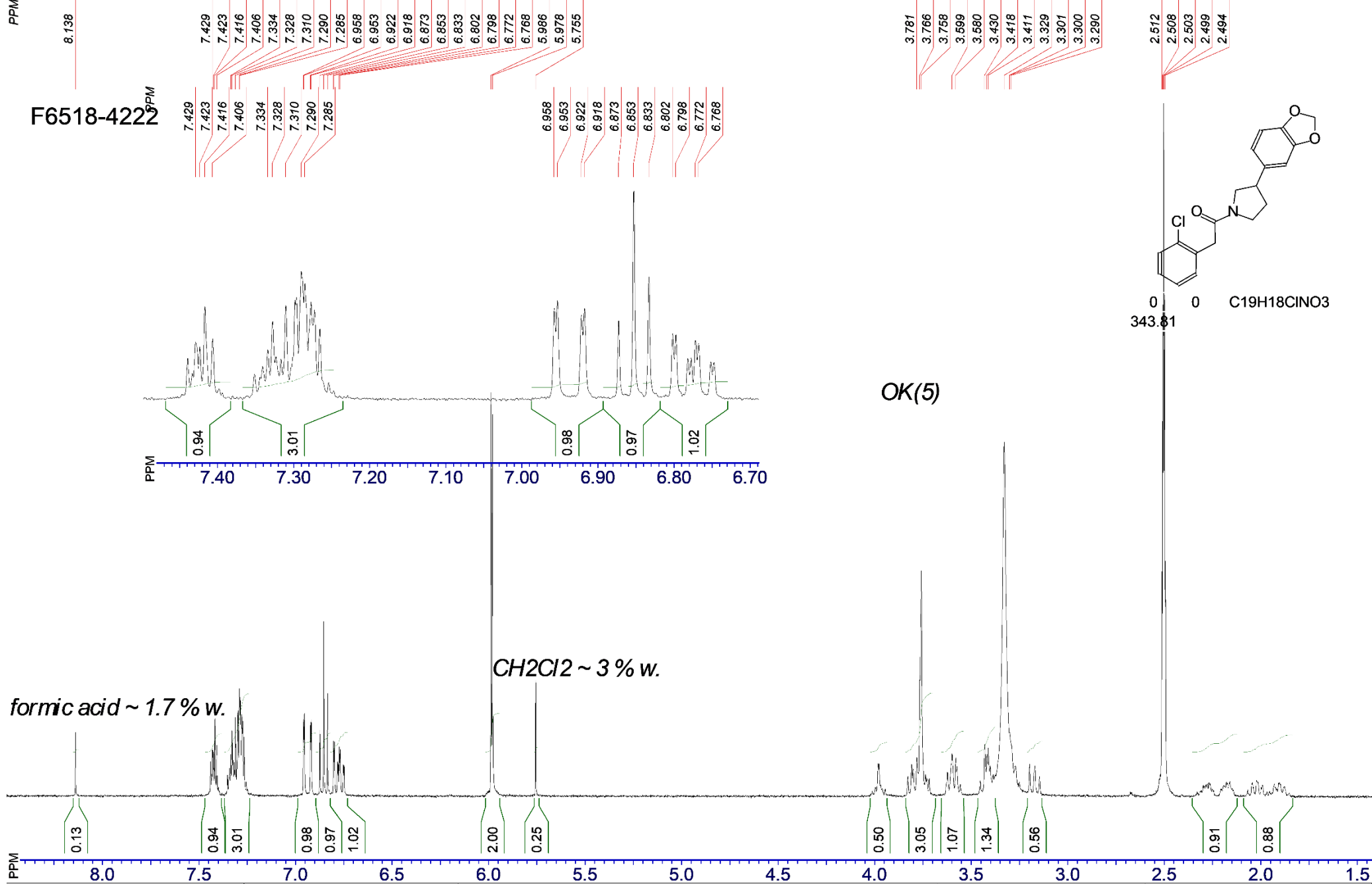
Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
Separation col: **100 %**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 306.82
Salt:



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.845	100.000
1	DAD1 B, Sig=241,4 Ref=off	0.845	100.000
1	ELS1 A, Signal Voltage	0.939	100.000
1	MSD1 TIC, MS File	0.885	100.000

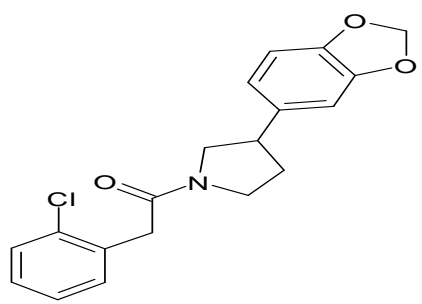


File name: F6518-4222	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 26_Oct_2015	Solvent: DMSO new		TE: 293 K	block: S17133

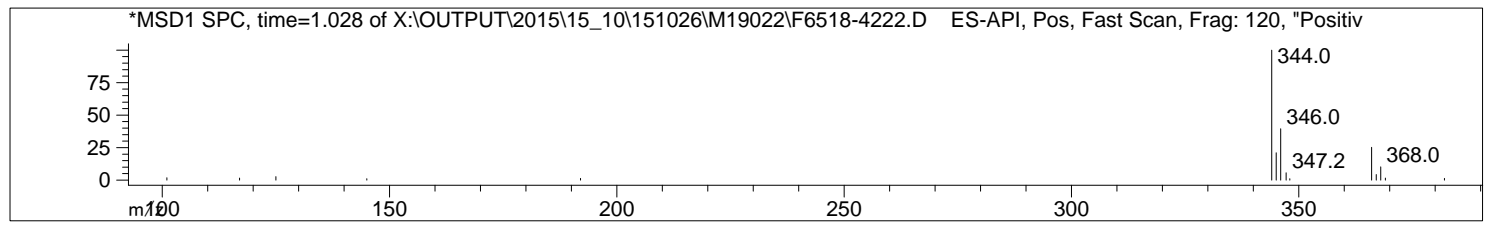
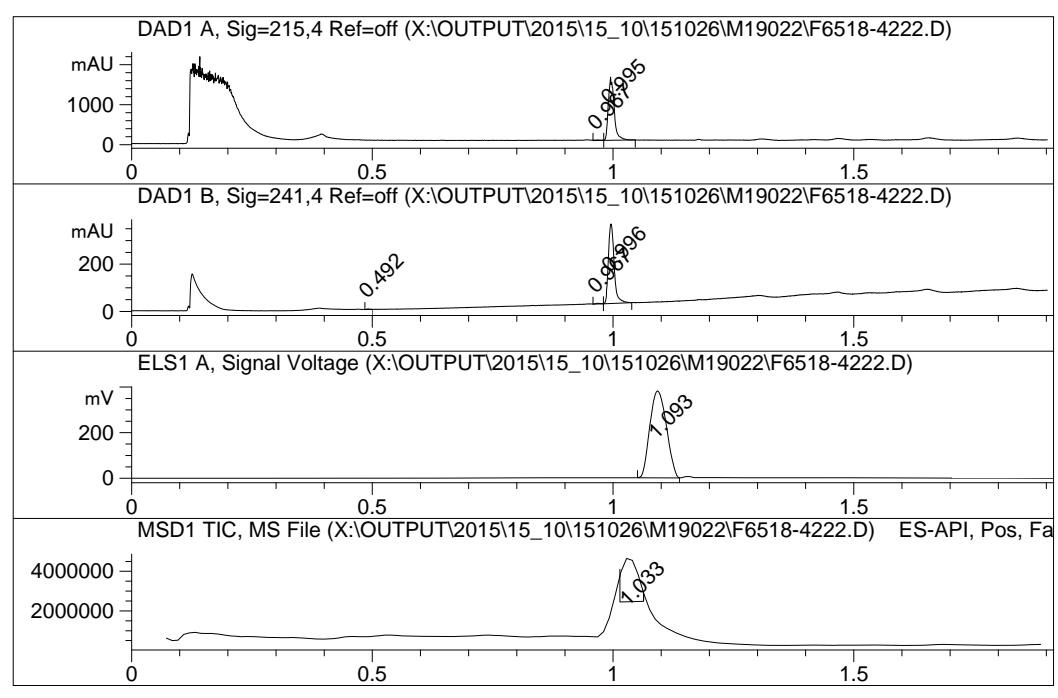
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

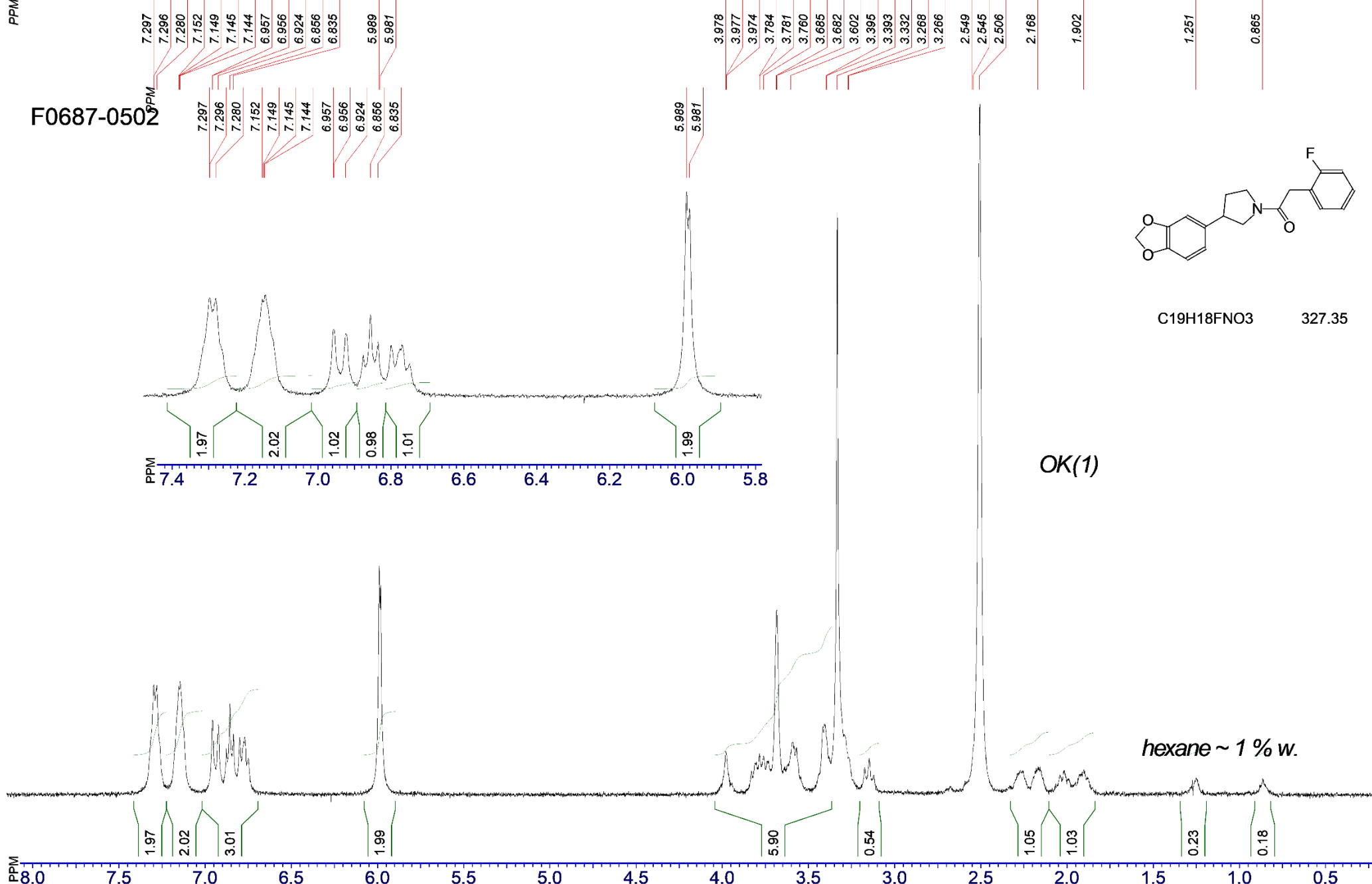
Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
Separation col: **99%**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 343.81
Salt:



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.967	0.953
2		0.995	99.047
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.492	0.489
2		0.967	0.699
3		0.996	98.812
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.093	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.033	100.000

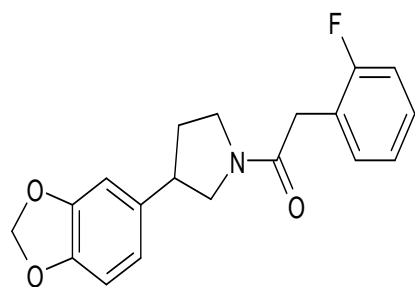


File name: F0687-0502	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 22_Mar_2016	Solvent: DMSO 0315		TE: 293 K	block: S18666

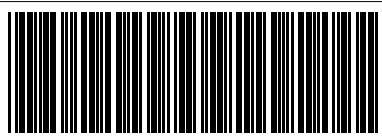
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

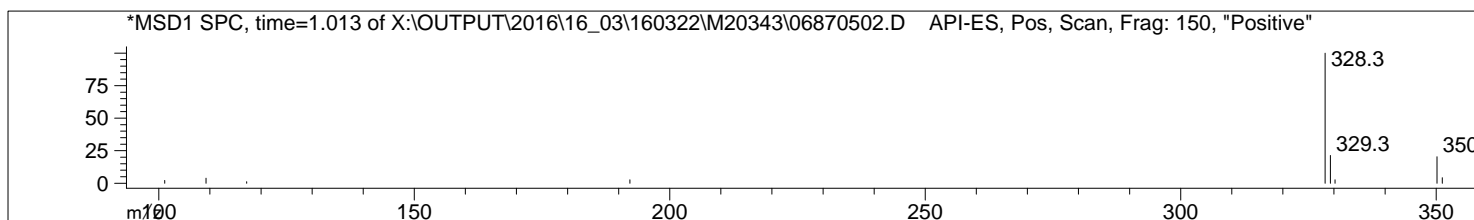
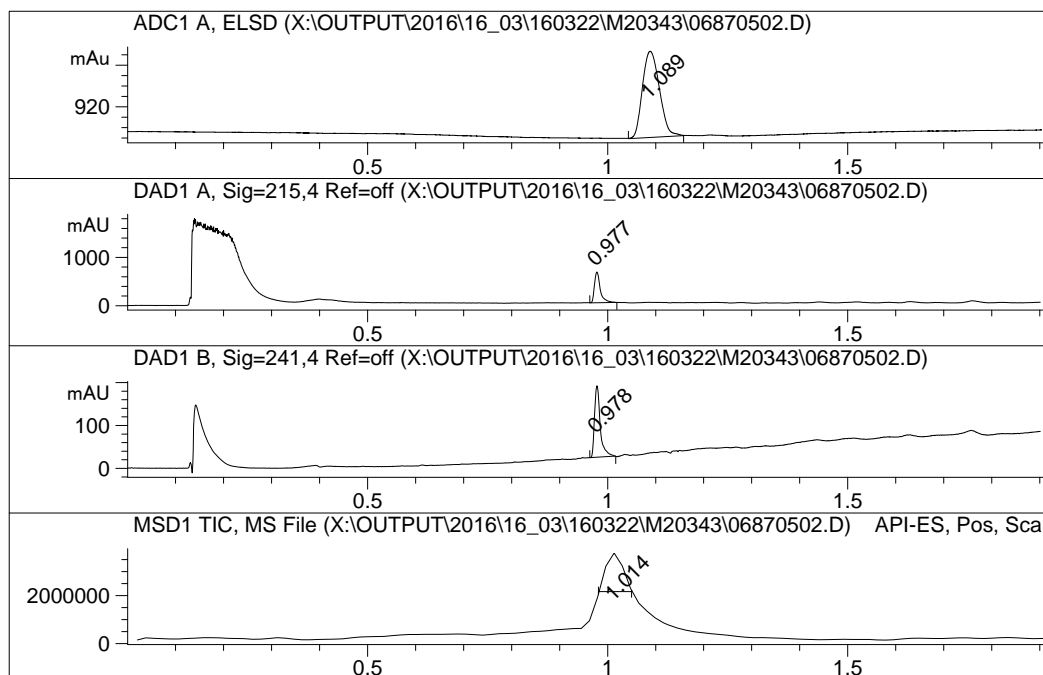
Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column
 Rapid Resolutionn HPL Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18

100 %

Mol.Weight: 327.35
 Salt:



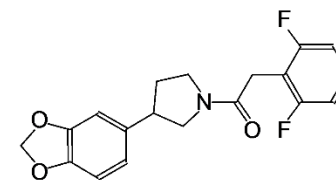
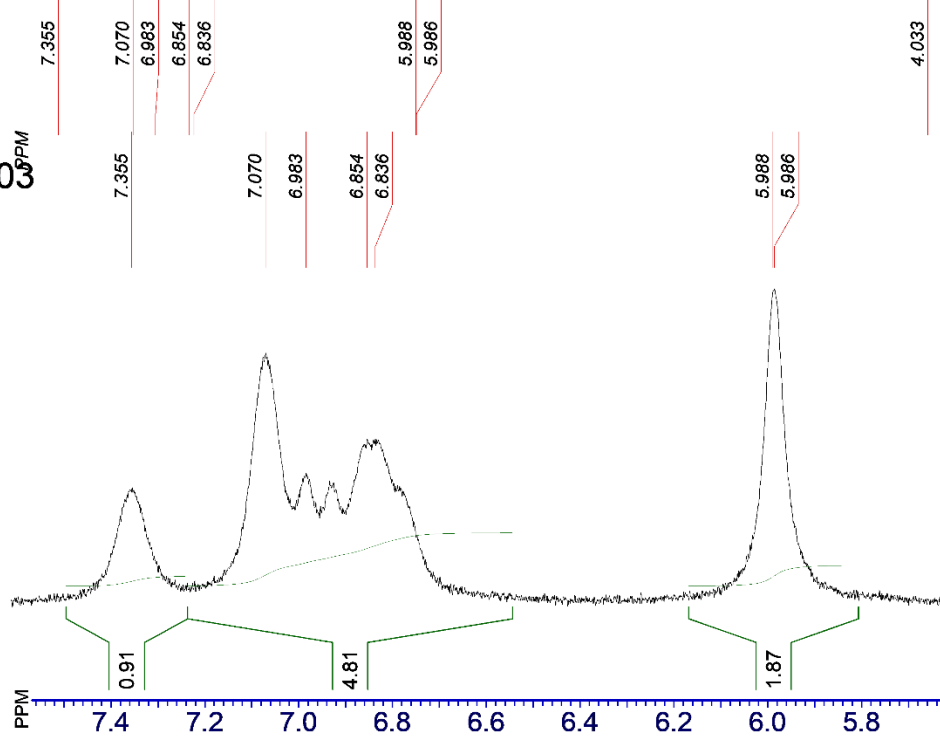
F0687-0502



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.089	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.977	100.000
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.978	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.014	100.000

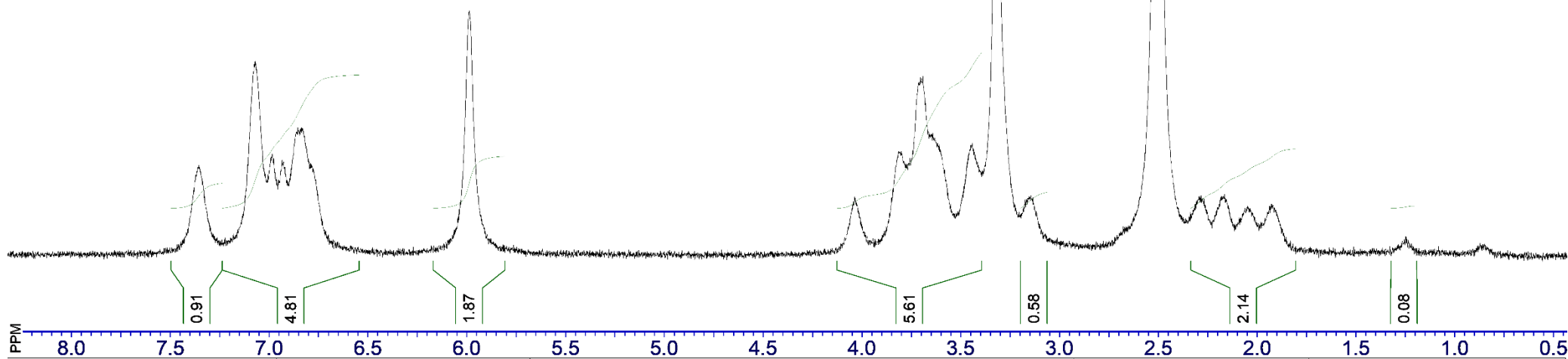
PPM

F0687-0503

C₁₉H₁₇F₂NO₃

345.34

OK(1)



File name: F0687-0503

Expert: M.Pyanova

SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec

NS: ; pw: 9,65 usec

SI: 65536, TD: 24000

Date: 21_Mar_2016

Solvent: DMSO 0315

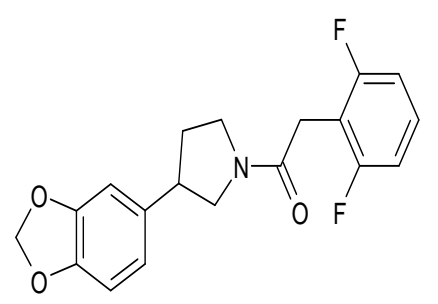
TE: 293 K

block: S18648

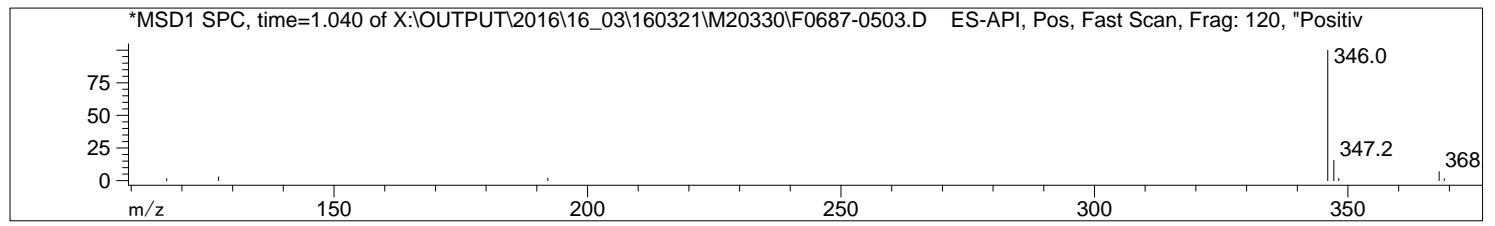
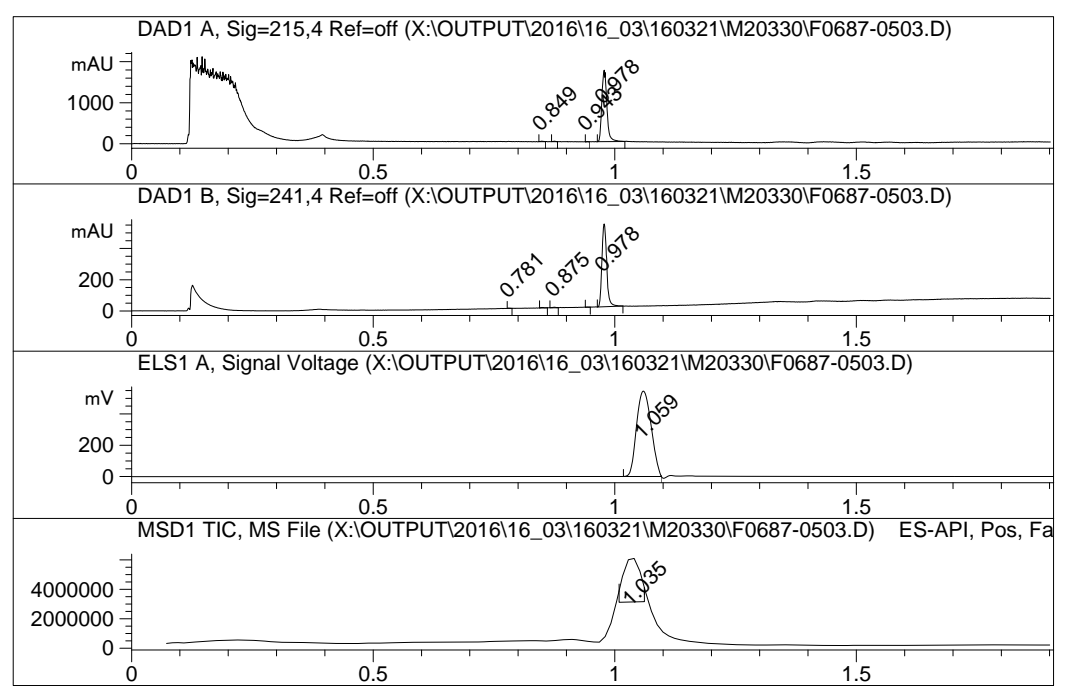
-.o.-Syntez Purity Report -.o.-

Agilent 1200 LC/MSD
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1HCOOH;B-MeCN+0.1HCOOH
Separation column **99 %**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 345.34
Salt:

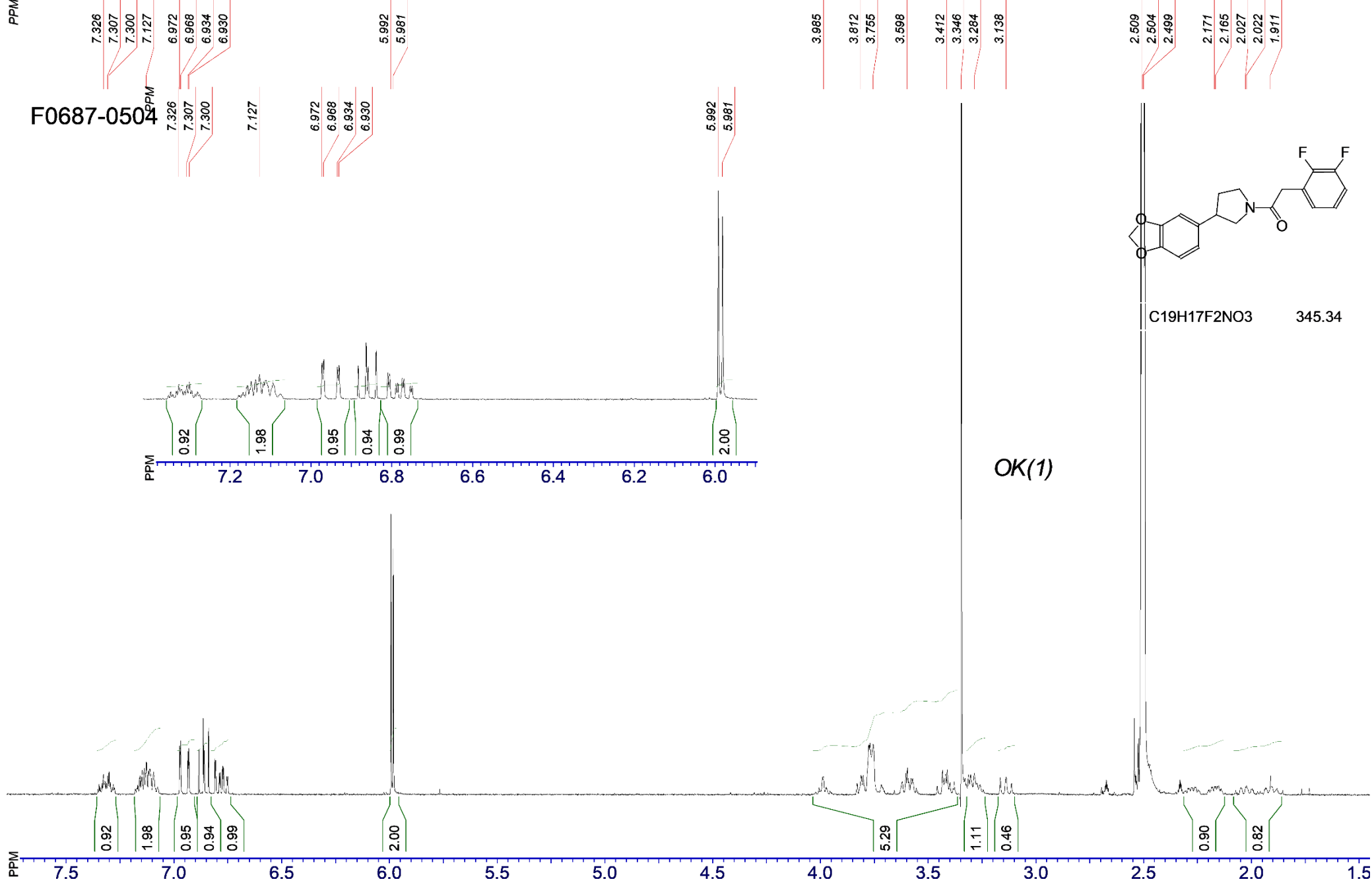


#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.849	0.442
2		0.876	0.399
3		0.943	0.152
4		0.978	99.007

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.781	0.249
2		0.849	0.528
3		0.875	0.495
4		0.941	0.171
5		0.978	98.556

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.059	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.035	100.000

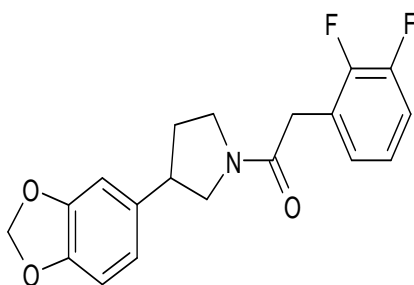


File name: F0687-0504	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 28_Mar_2016	Solvent: DMSO 0321		TE: 293 K	block: S18745

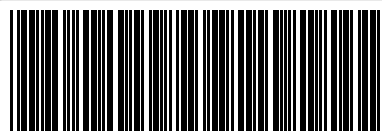
-.o.-Syntez Purity Report -.o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

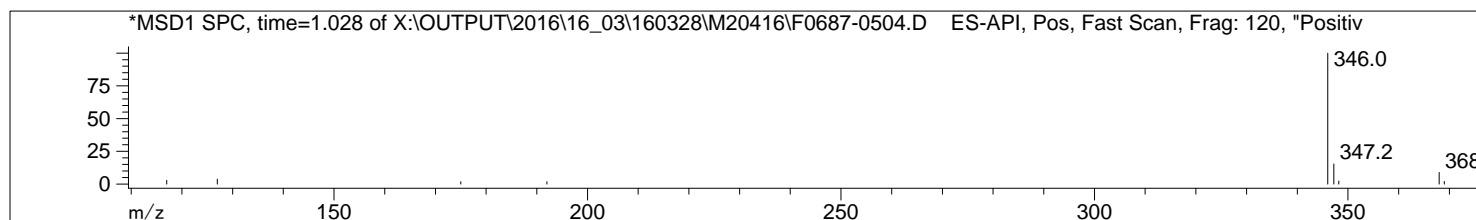
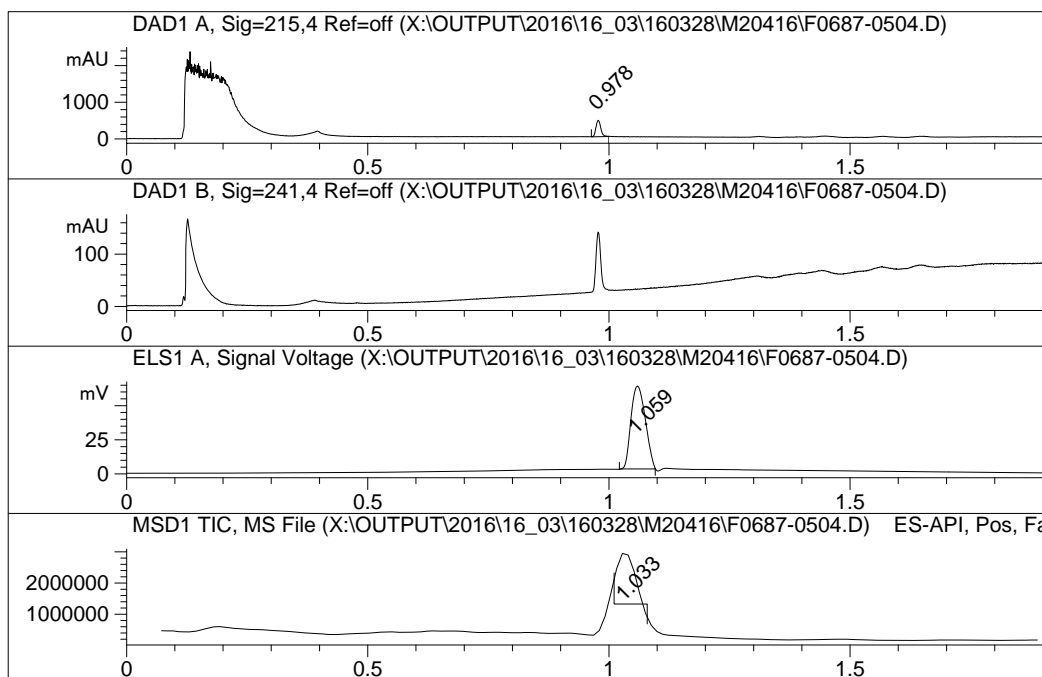
Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation colour **Non-informative**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



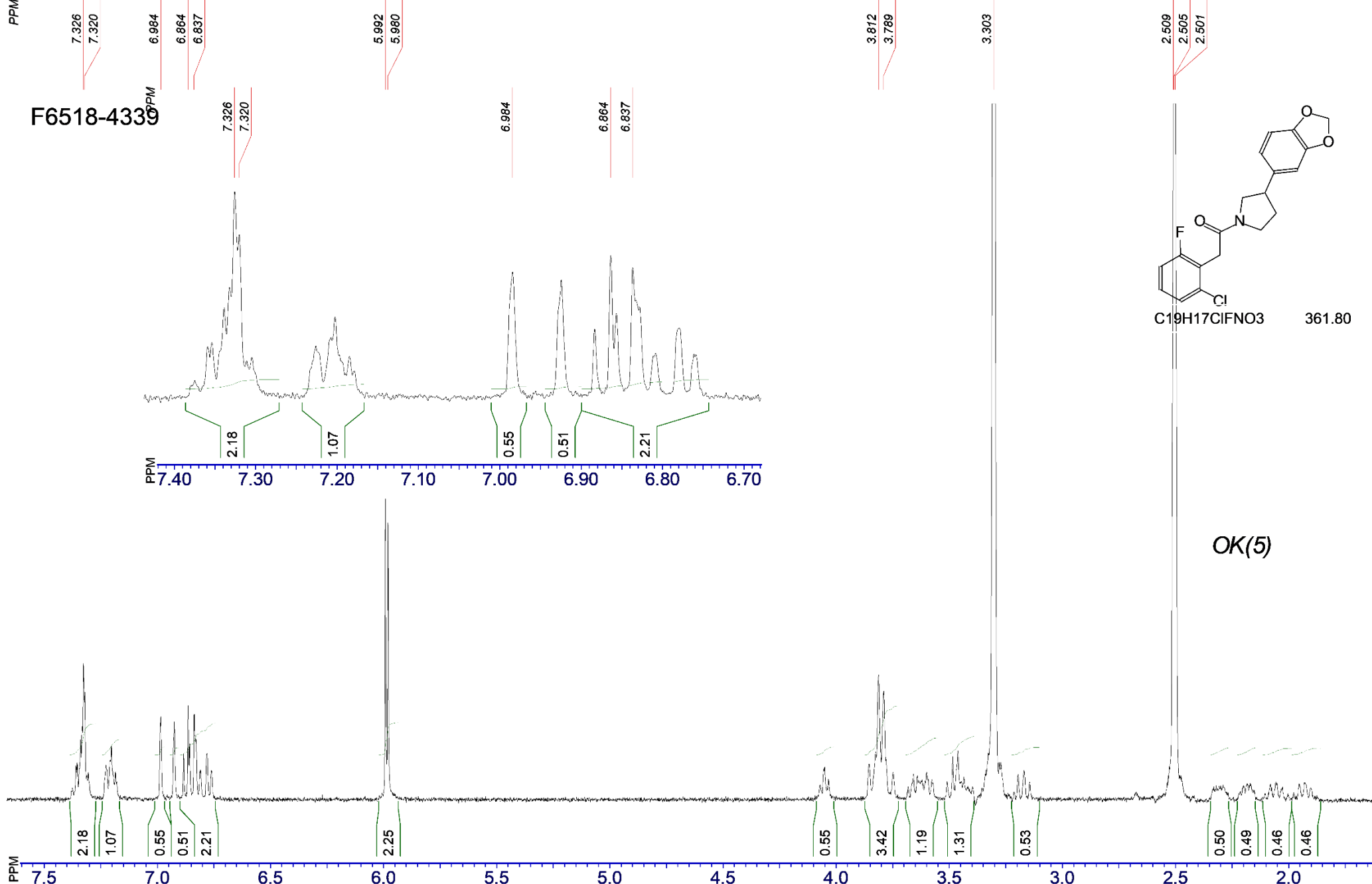
Mol.Weight: 345.34
 Salt:



F0687-0504



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.978	100.000
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	1.059	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.033	100.000

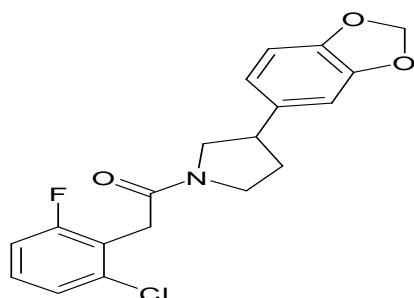


File name: F6518-4339	Expert: A.Ryabitsky	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 09_dec_2015	Solvent: DMSO new		TE: 293 K	block: S17623

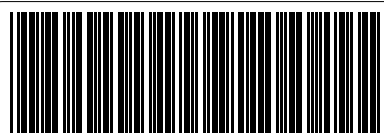
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolution HPLC Cartridge 4.6x300mm,
 1.8-Micron, Zorbax SB C-18

100 %

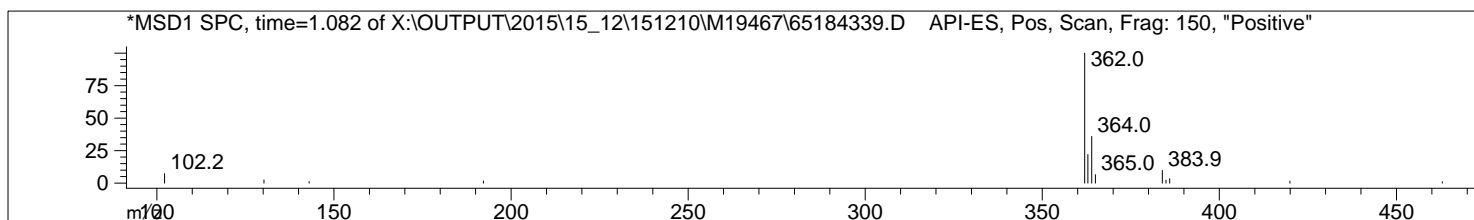
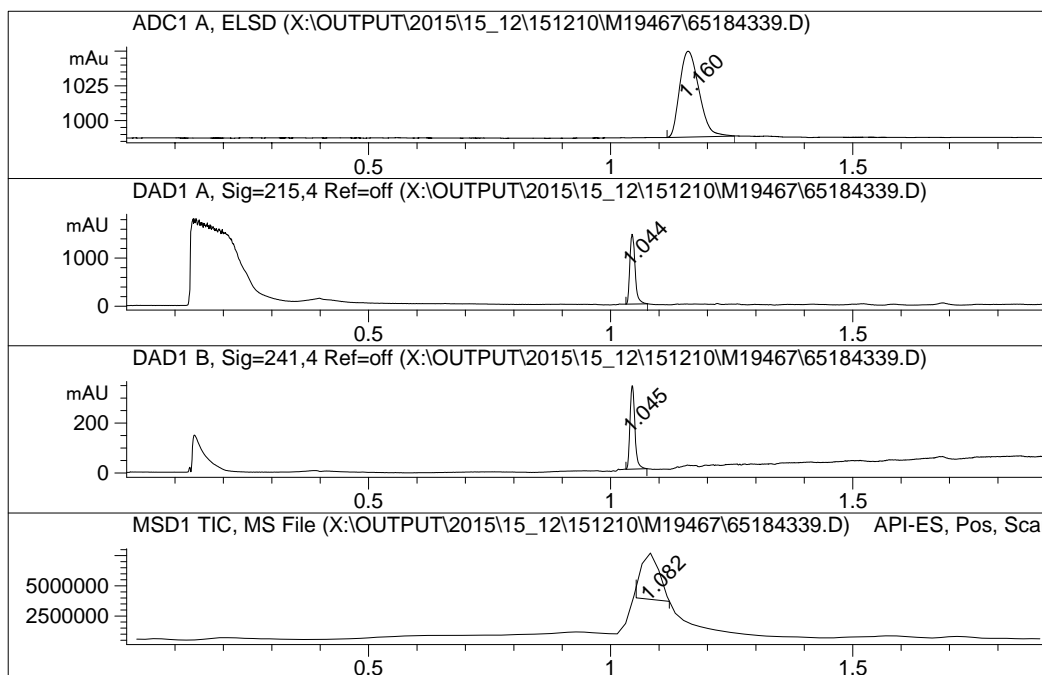
Mol.Weight: 361.8
 Salt:



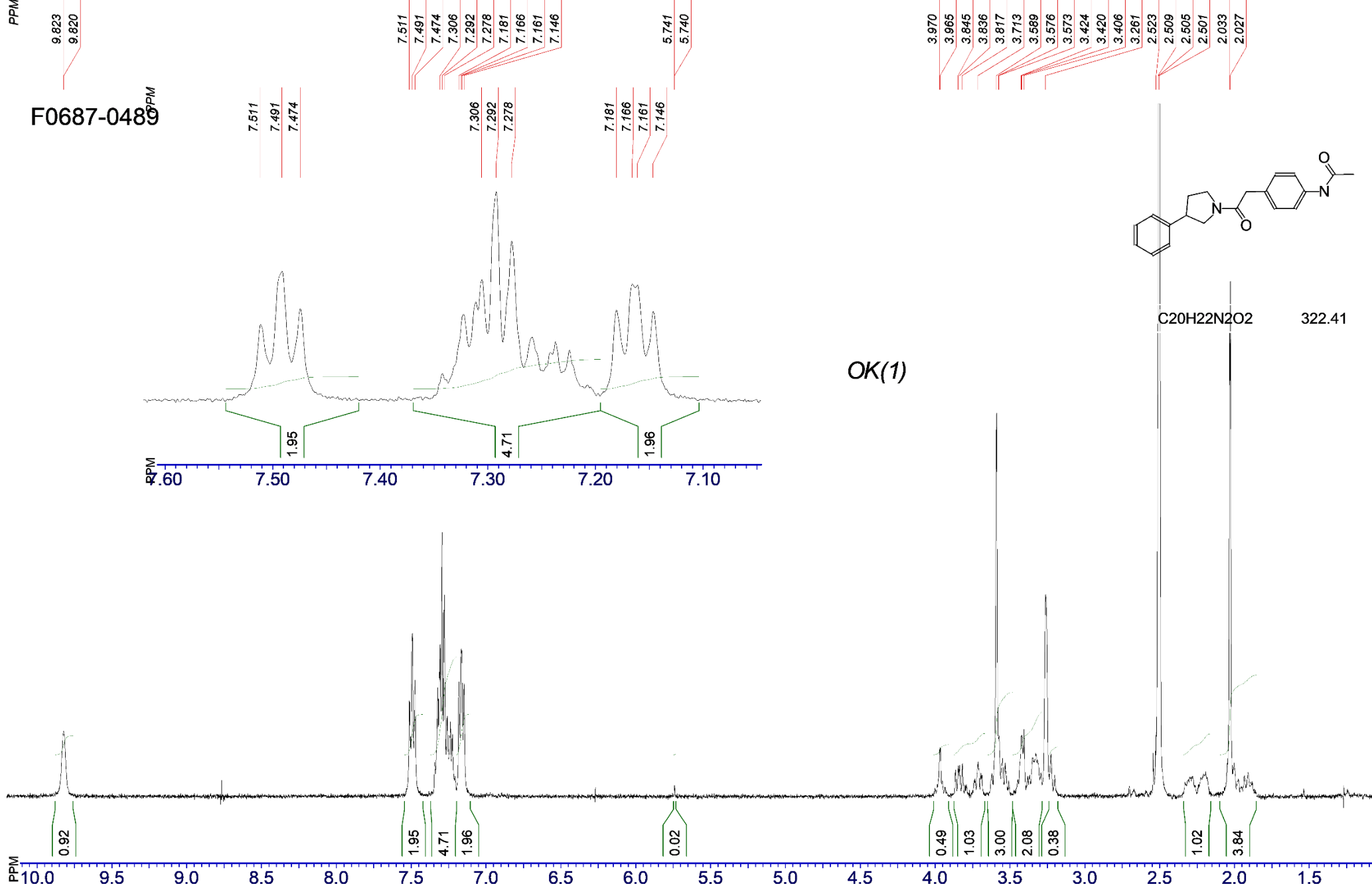
F6518-4339

M19467

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.160	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	1.044	100.000
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	1.045	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	1.082	100.000

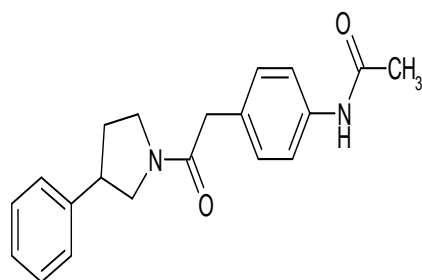


File name: F0687-0489	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

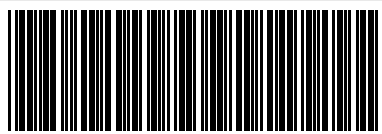
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation colun **Non-informative**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



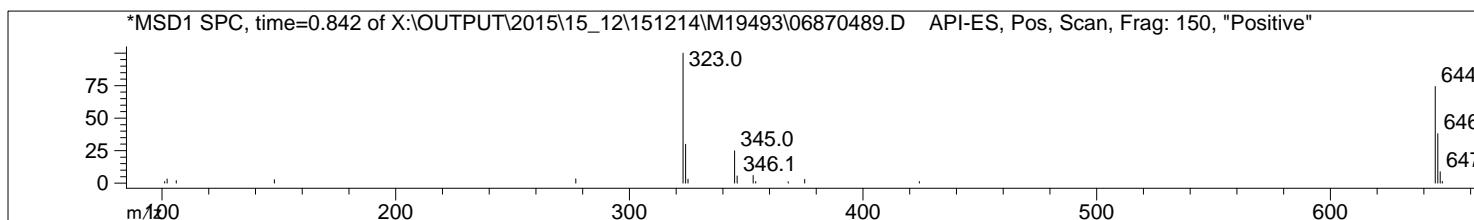
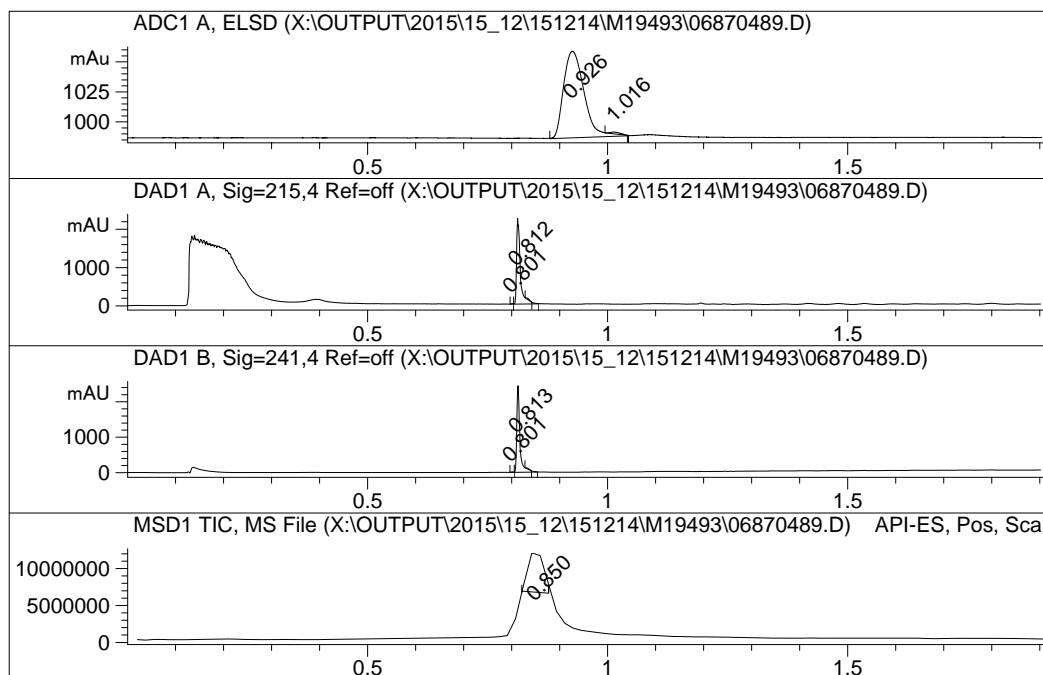
Mol.Weight: 322.41
 Salt:



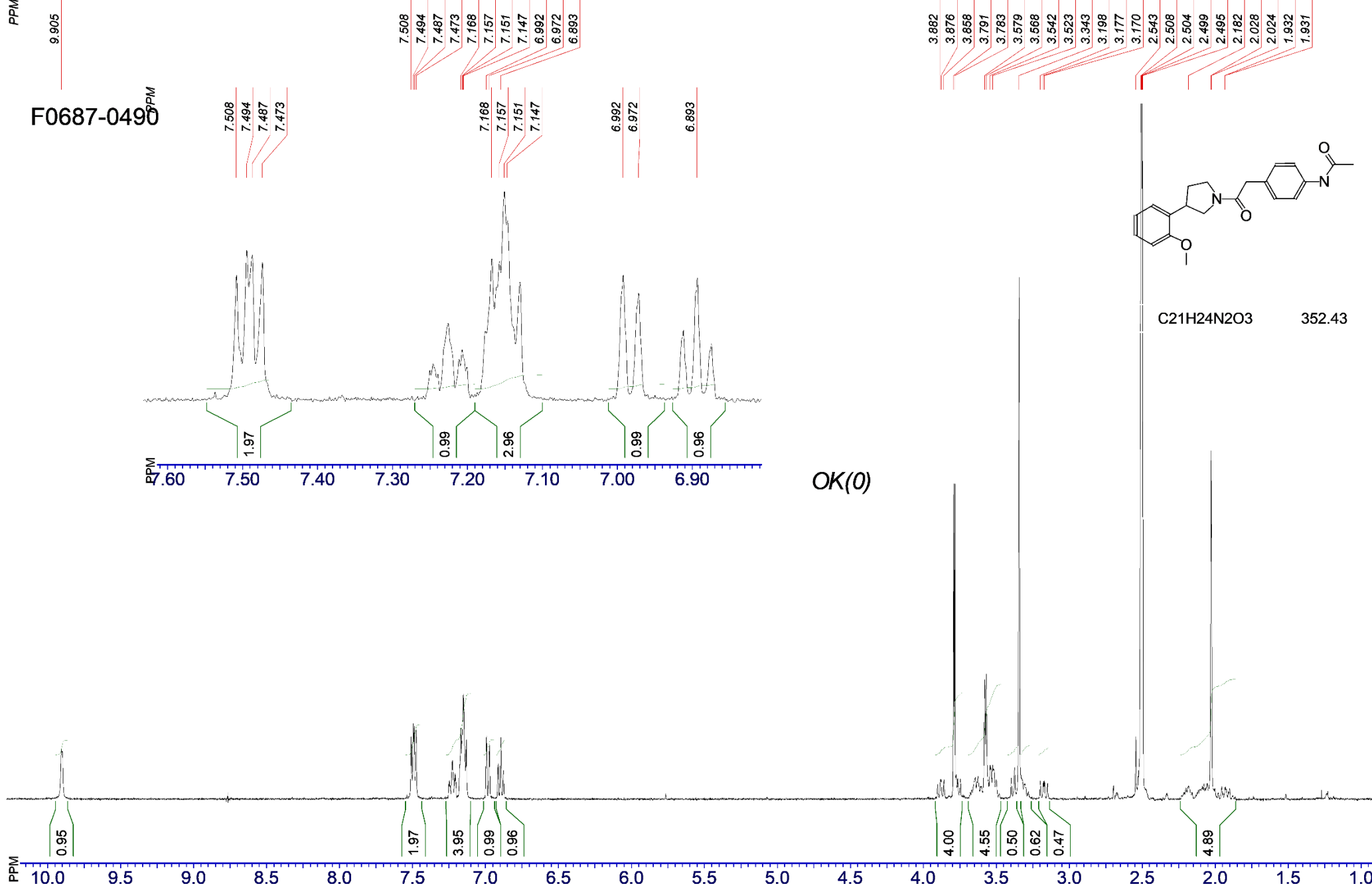
F0687-0489

M19493

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.926	98.943
2		1.016	1.057
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.801	0.306
2		0.812	98.455
3		0.834	1.239
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.801	0.437
2		0.813	98.722
3		0.834	0.841
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.850	100.000

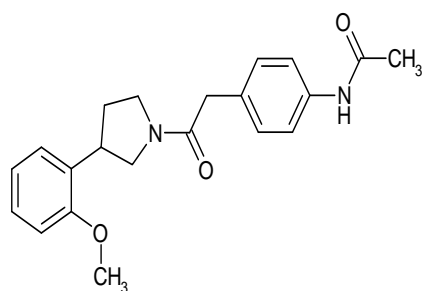


File name: F0687-0490	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

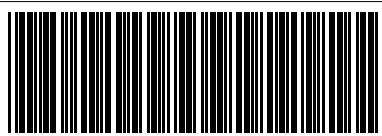
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column **99%**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



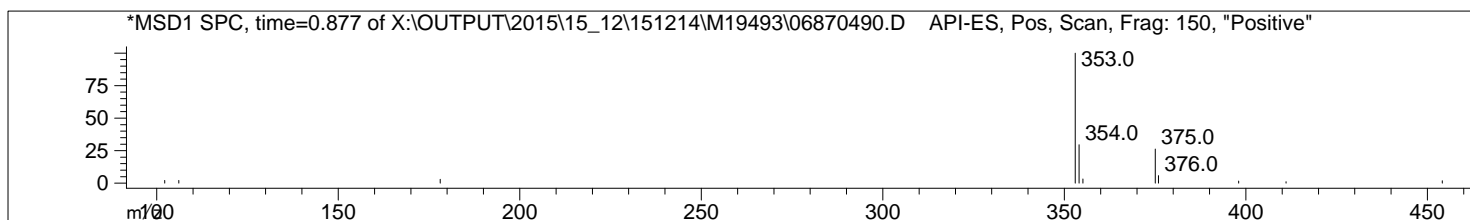
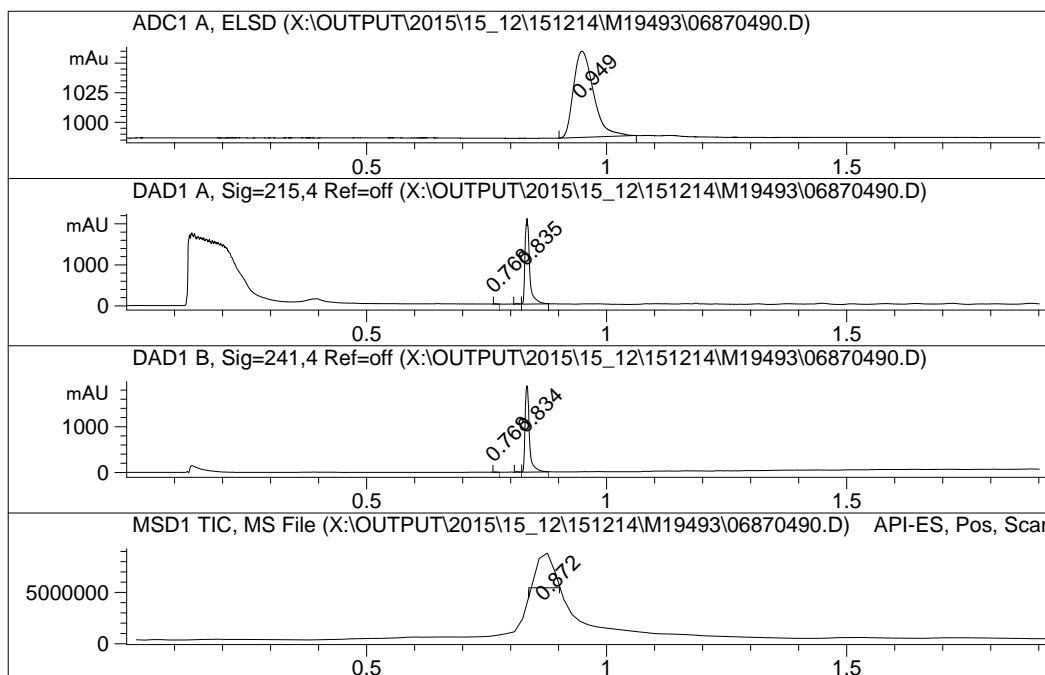
Mol.Weight: 352.43
 Salt:



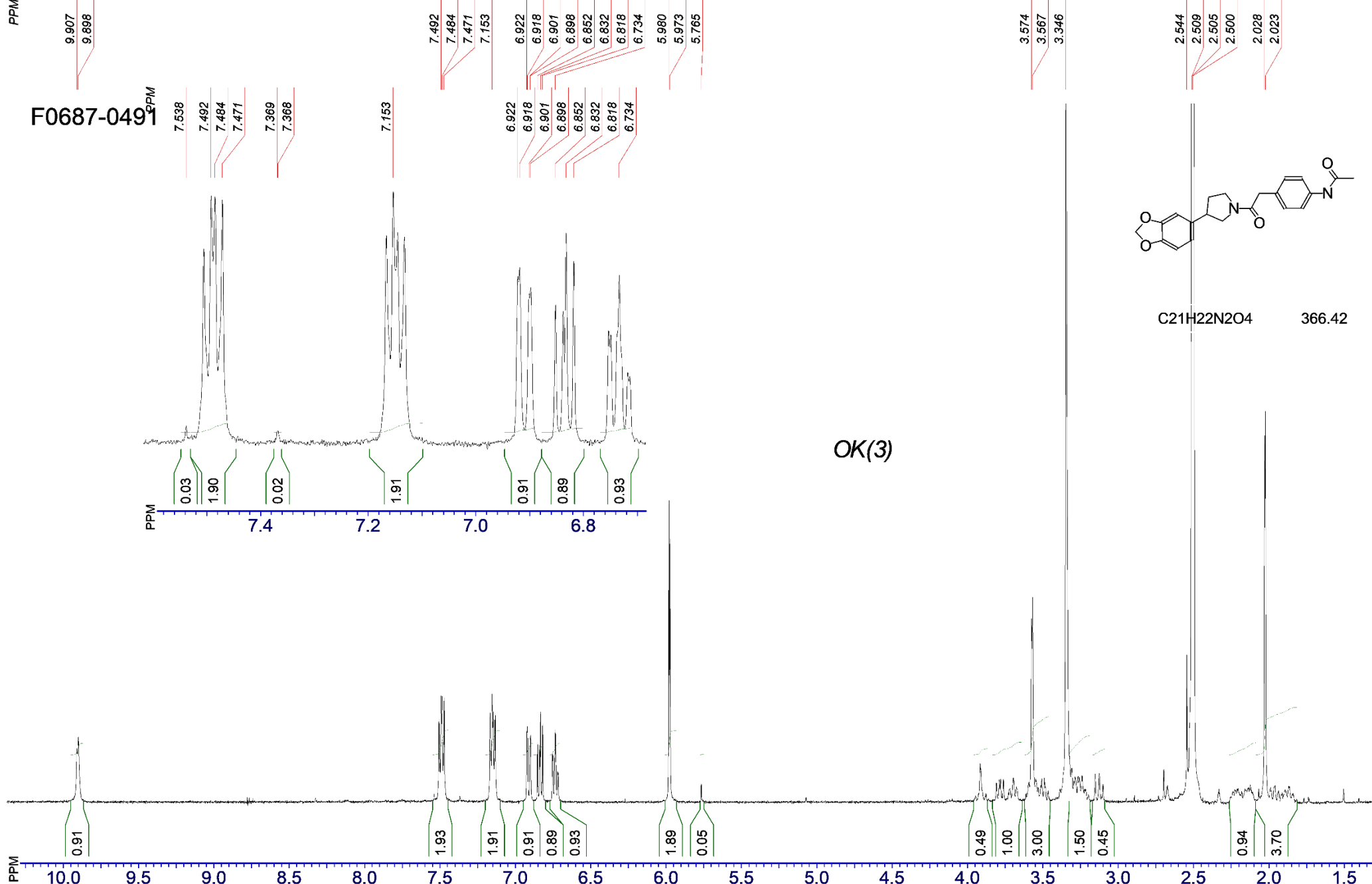
F0687-0490

M19493

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.949	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.768	0.323
2		0.813	0.625
3		0.835	99.052
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.768	0.285
2		0.813	0.521
3		0.834	99.194
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.872	100.000

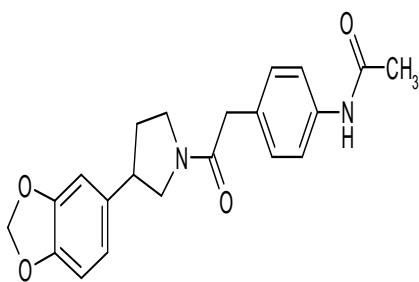


File name: F0687-0491	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

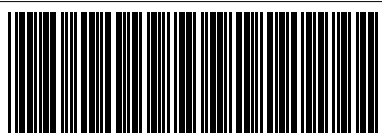
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation colu **100 %**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



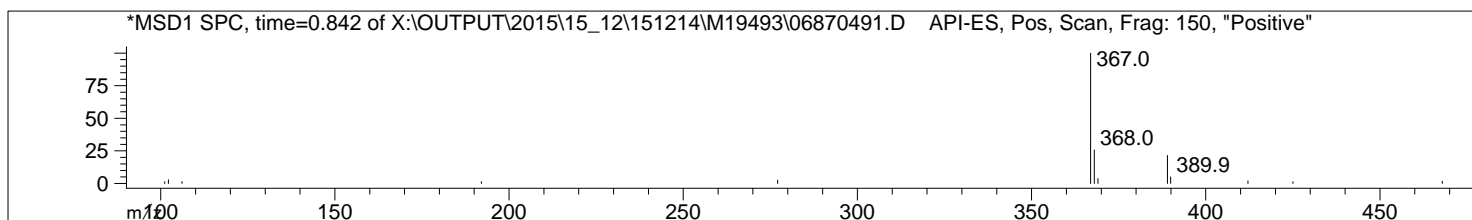
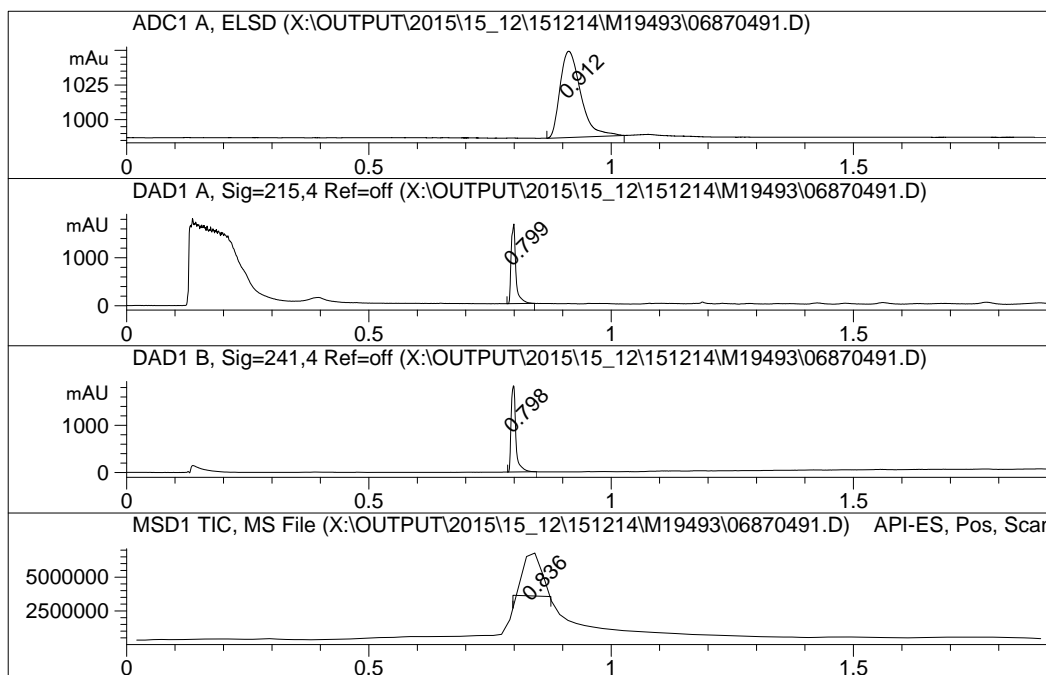
Mol.Weight: 366.41
 Salt:



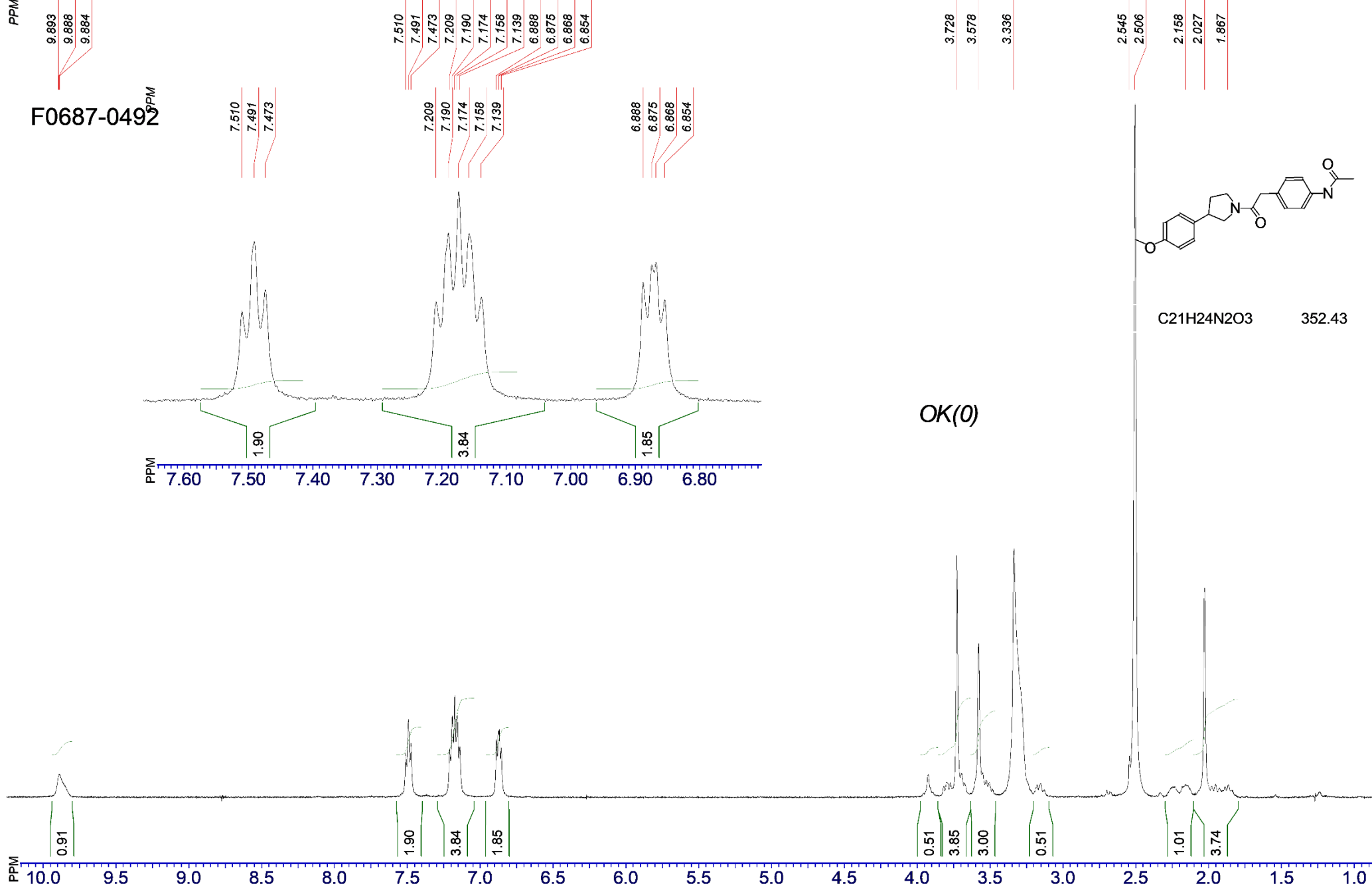
F0687-0491

M19493

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.912	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.799	100.000
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.798	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.836	100.000

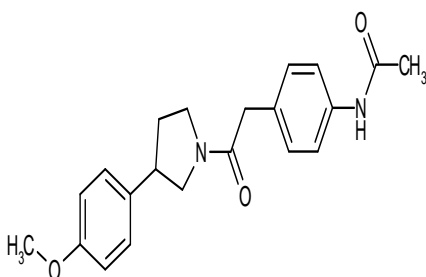


File name: F0687-0492	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

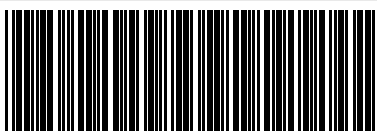
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation col **Non-informative**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



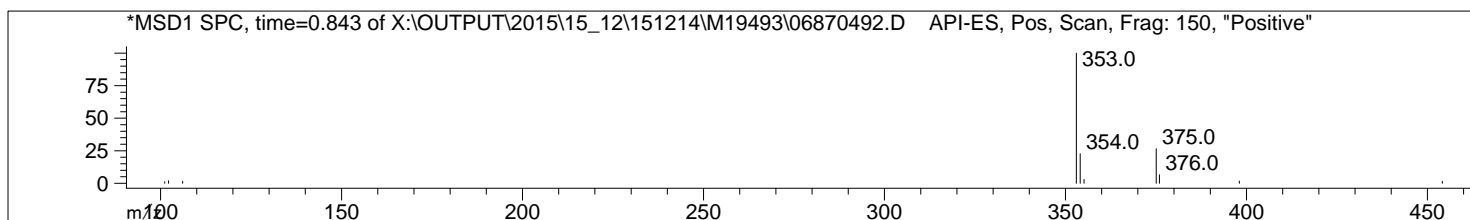
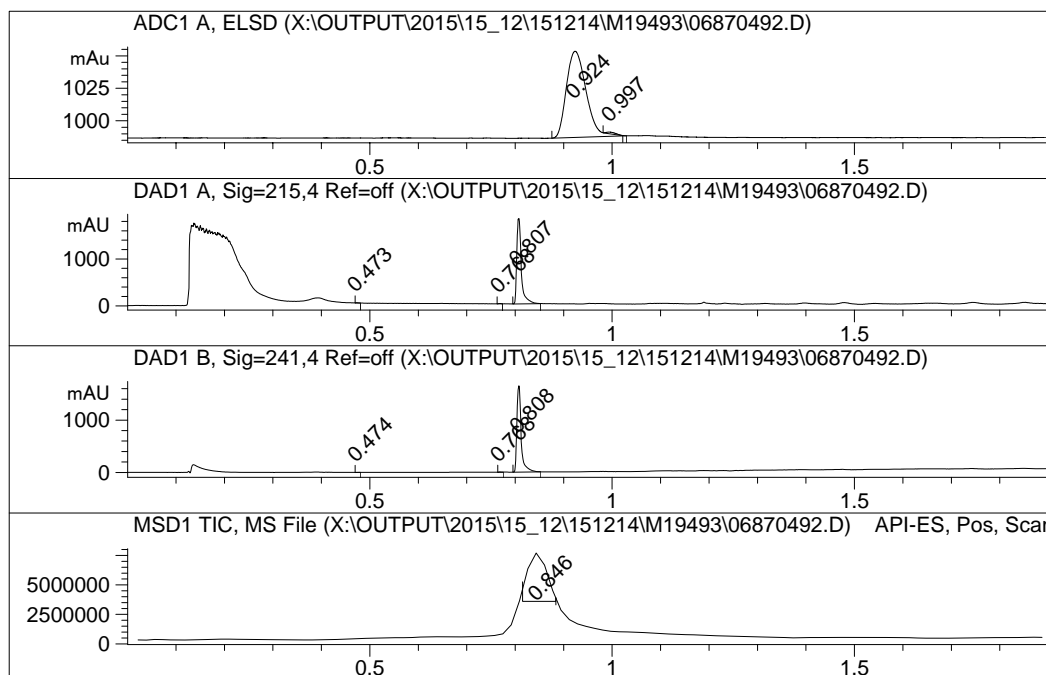
Mol.Weight: 352.43
 Salt:



F0687-0492

M19493

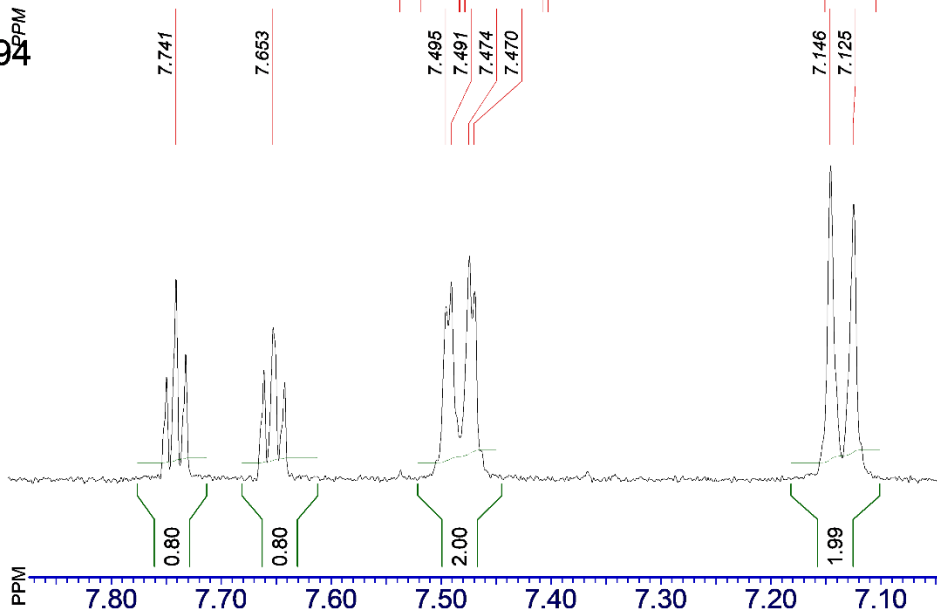
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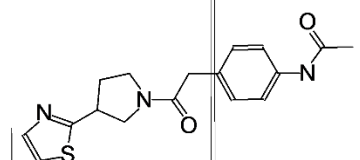
#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.924	99.038
2		0.997	0.962
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.473	0.275
2		0.768	0.172
3		0.807	99.554
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.474	0.107
2		0.768	0.250
3		0.808	99.643
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.846	100.000

PPM

F0687-0494

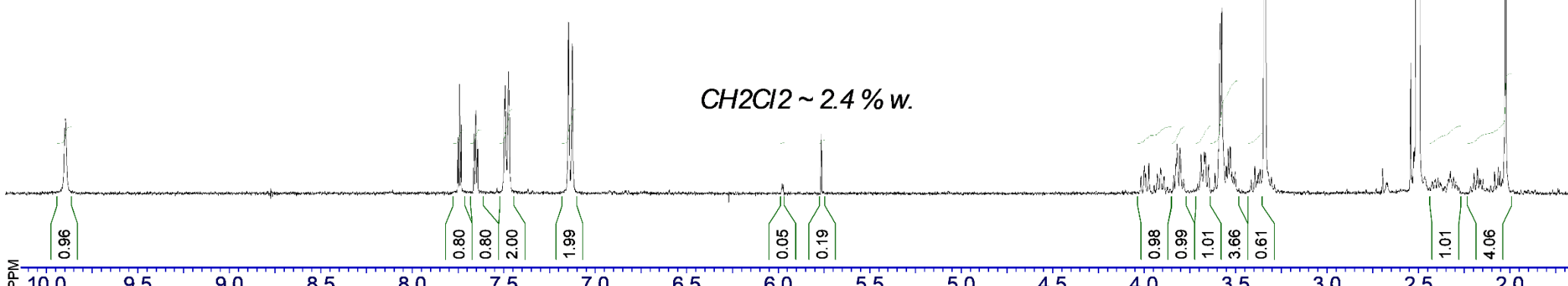


3.999
3.974
3.970
3.908
3.826
3.820
3.804
3.689
3.671
3.664
3.585
3.576
3.529
3.341
2.543
2.508
2.504
2.499
2.326
2.179
2.025



C₁₇H₁₉N₃O₂S 329.42

OK(5)

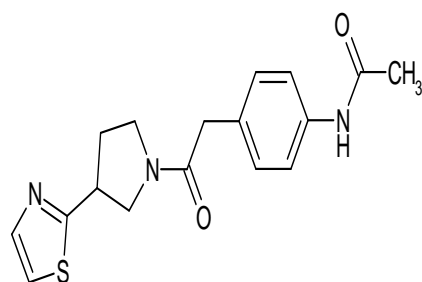


File name: F0687-0494	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

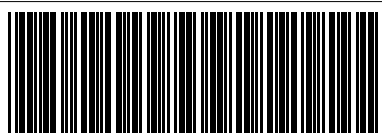
-.o.-Syntez Purity Report -.o.-

Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column **96 %**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



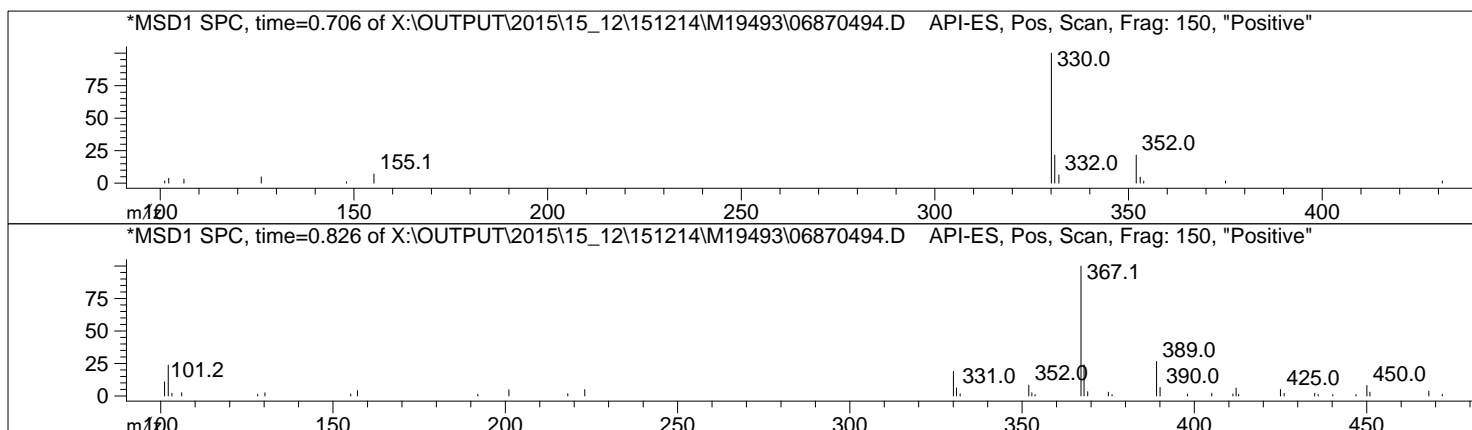
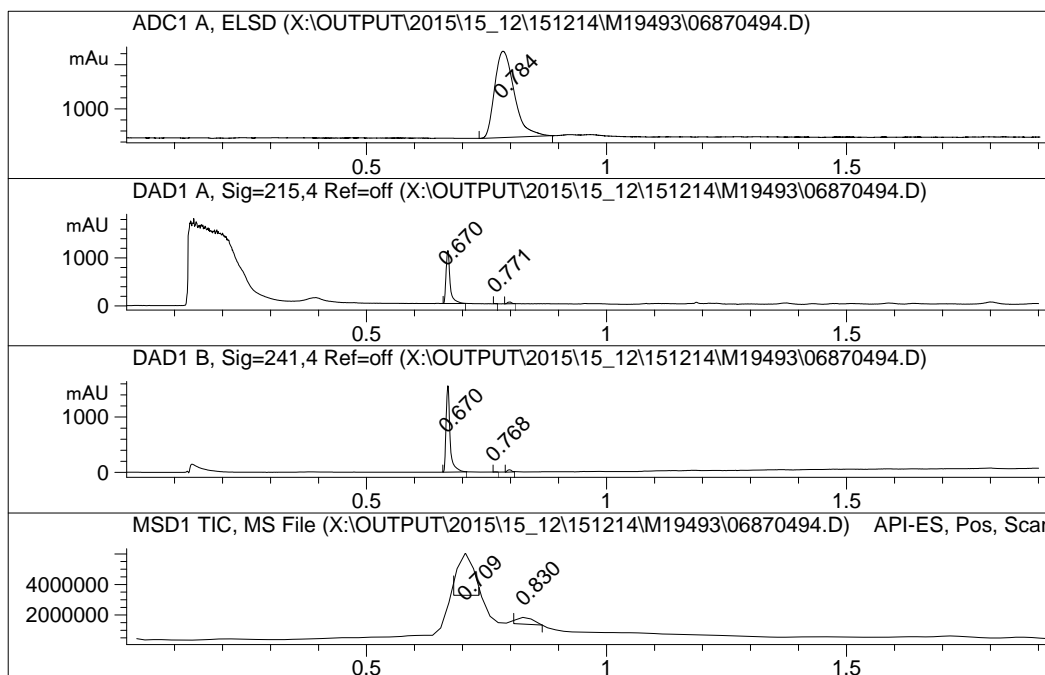
Mol.Weight: 329.42
 Salt:



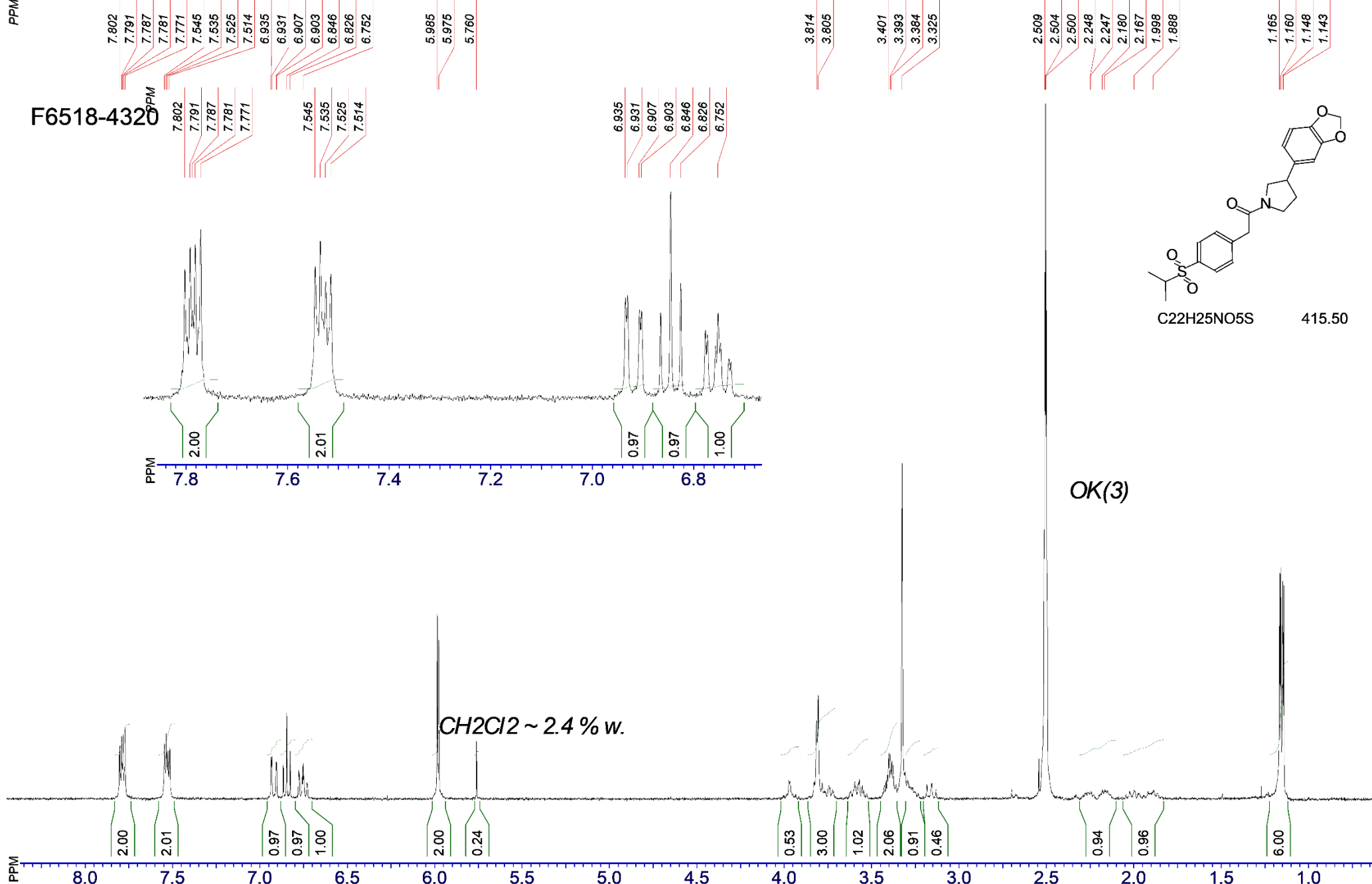
F0687-0494

M19493

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#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.784	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.670	96.275
2		0.771	0.298
3		0.798	3.427
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.670	97.226
2		0.768	0.129
3		0.799	2.645
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.709	88.151
2		0.830	11.849

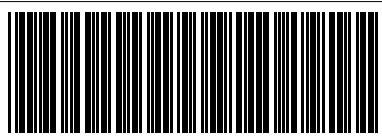
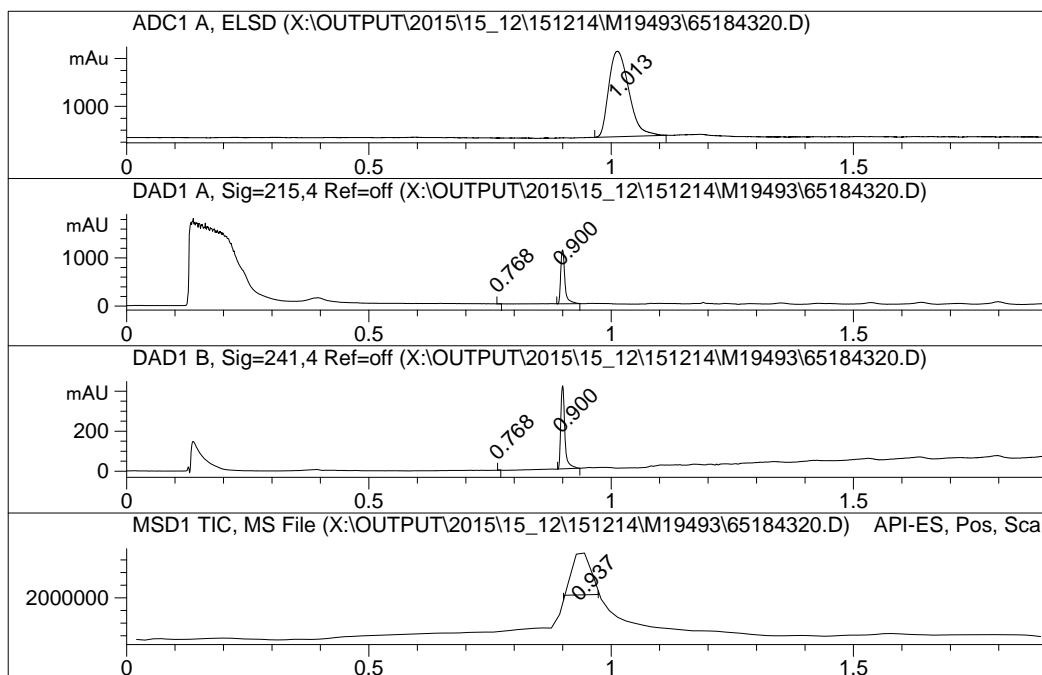
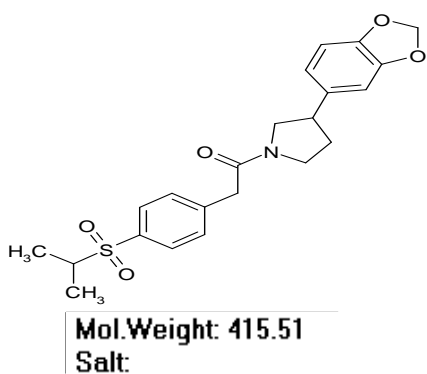


File name: F6518-4320	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 11_Dec_2015	Solvent: DMSO 1207		TE: 293 K	block: S17655

-.o.-Syntez Purity Report -.o.-

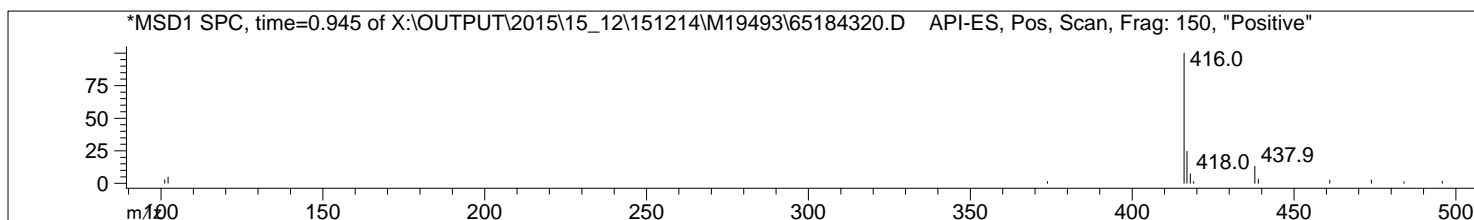
Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolutionn HPLC Cartridge 4.6x300mm,
 1.8-Micron, Zorbax SB C-18

99 %**F6518-4320**

M19493

->



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.013	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.768	0.334
2		0.900	99.666
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.768	0.252
2		0.900	99.748
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.937	100.000

PPM

F0687-0468

10.642

PPM

8.599
8.594

8.154
8.116
8.084

8.154
8.116
8.084

7.452
7.361
7.355
7.347

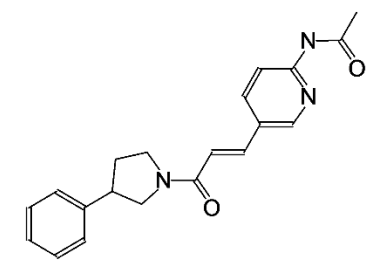
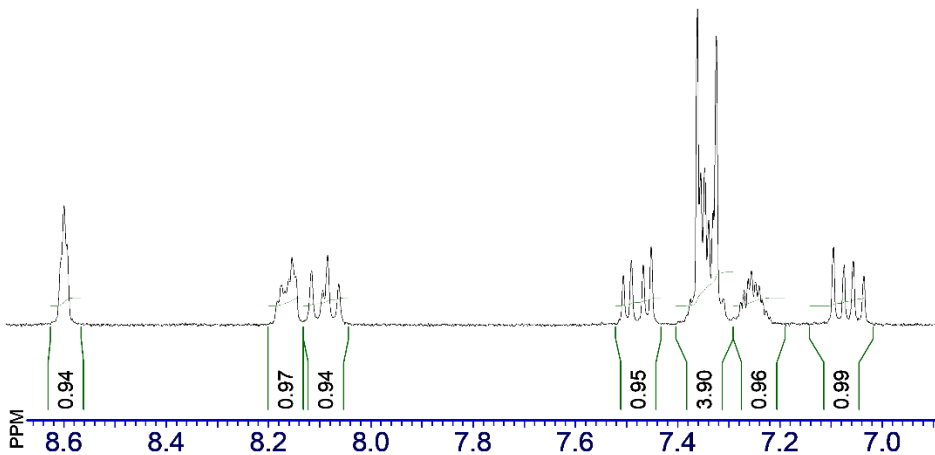
7.339
7.330
7.324
7.095

7.452
7.361
7.355
7.347
7.339
7.330
7.324
7.095

4.226
4.207
4.203
4.201
4.182
3.955
3.931
3.723
3.717
3.699
3.566
3.326

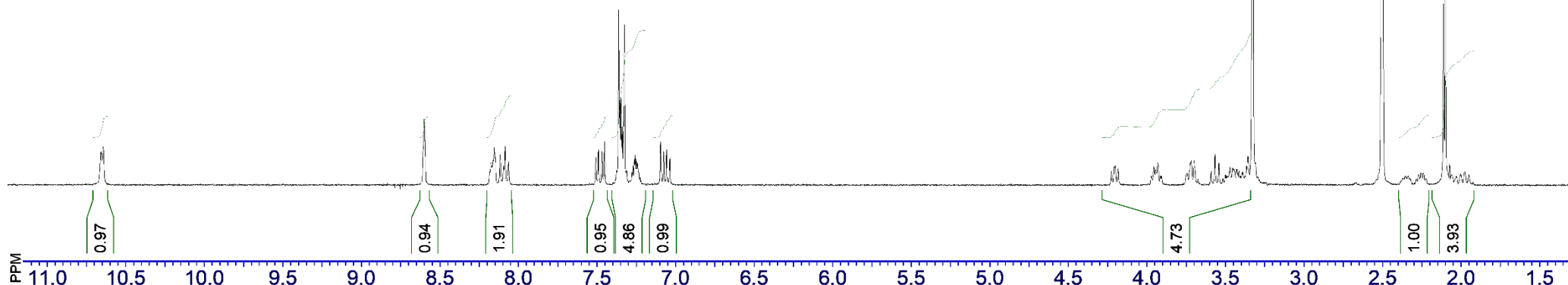
2.502

2.112
2.099



0 0 C20H21N3O2
335.40

OK(0)

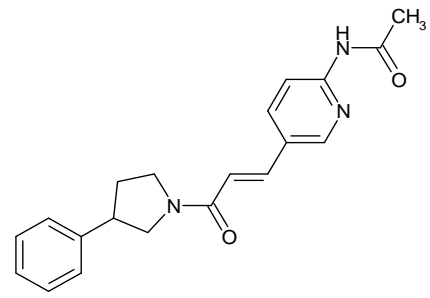


File name: F0687-0468	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 29_Oct_2015	Solvent: DMSO new		TE: 293 K	block: S17188

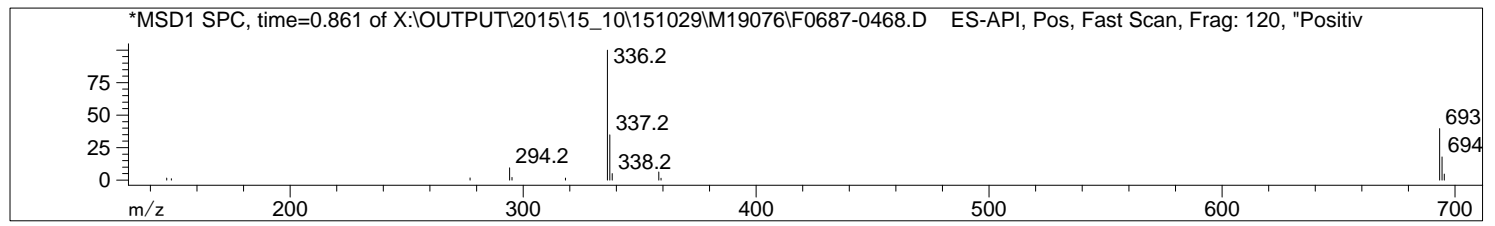
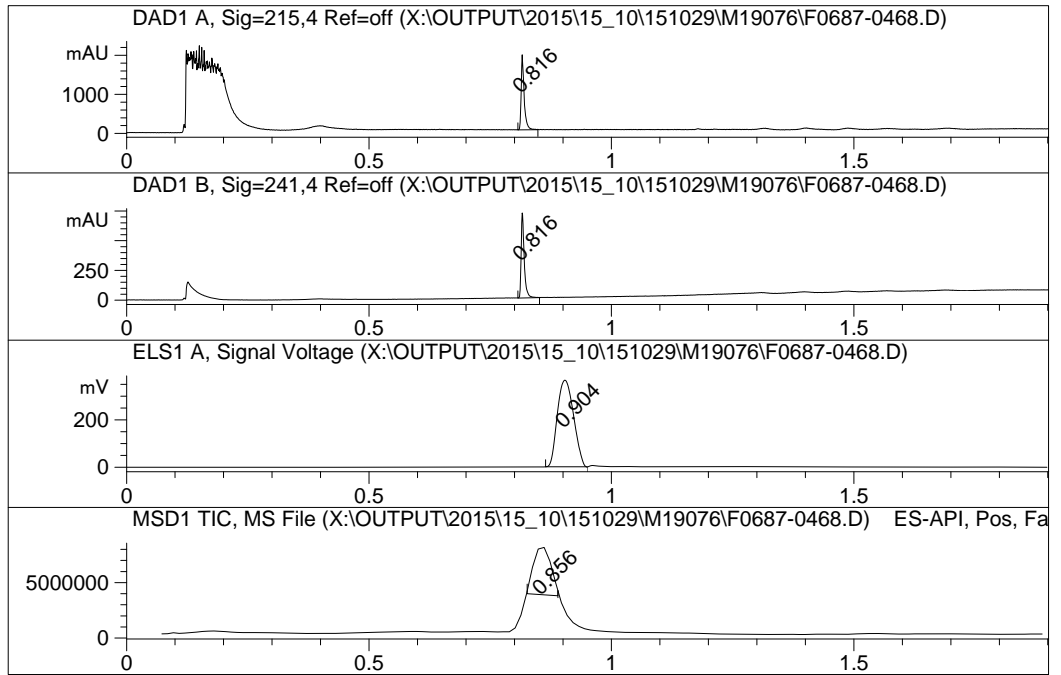
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation column **100 %**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



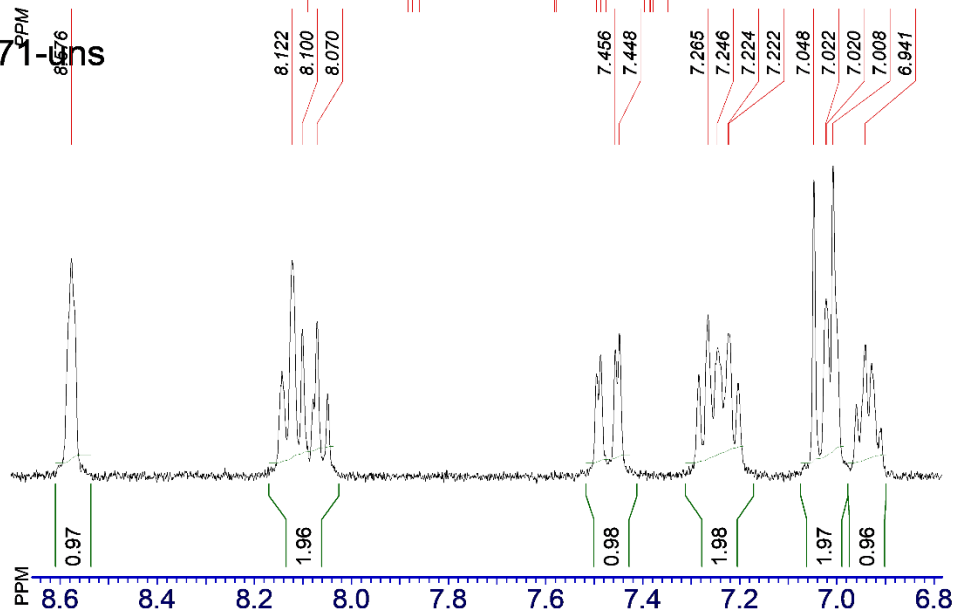
Mol.Weight: 335.4
 Salt:



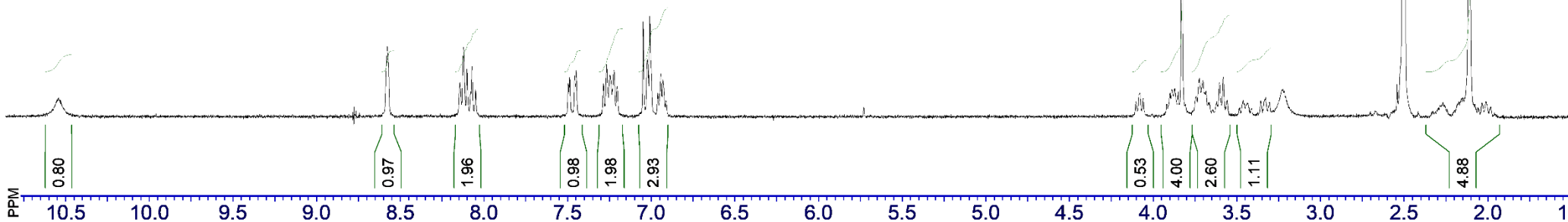
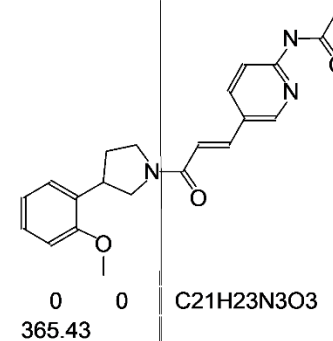
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.816	100.000
1	DAD1 B, Sig=241,4 Ref=off	0.816	100.000
1	ELS1 A, Signal Voltage	0.904	100.000
1	MSD1 TIC, MS File	0.856	100.000

PPM

F0687-0471-uns



UNS



File name: F0687-0471-uns

Expert: M.Pyanova

SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec

NS: ; pw: 9,65 usec

SI: 65536, TD: 24000

Date: 02_Nov_2015

Solvent: DMSO 1028

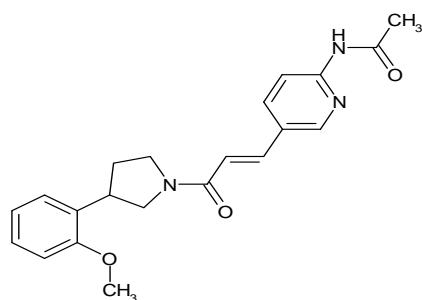
TE: 293 K

block: S17224

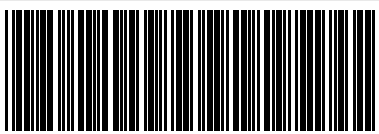
-.o.-Syntez Purity Report -.o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

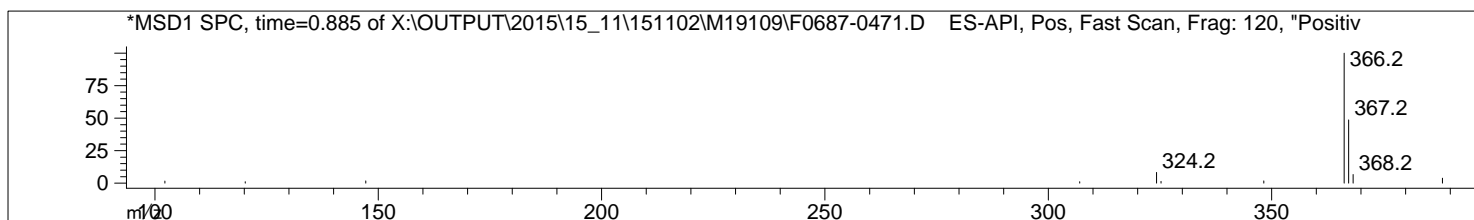
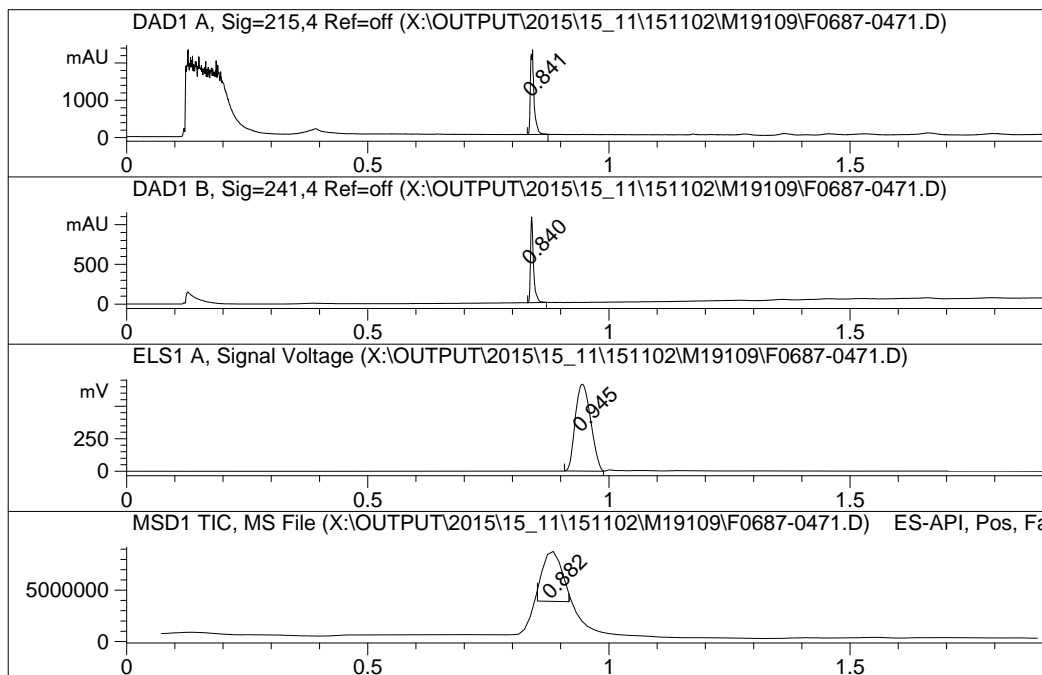
Mobile Phase:A-H₂O+0.1HCOOH;B-MeCN+0.1HCOOH
 Separation col **100 %**
 Rapid Resolutionn HPLC Cartidge 4.6x50mm,
 1.8-Micron, Zorbax SB-C18



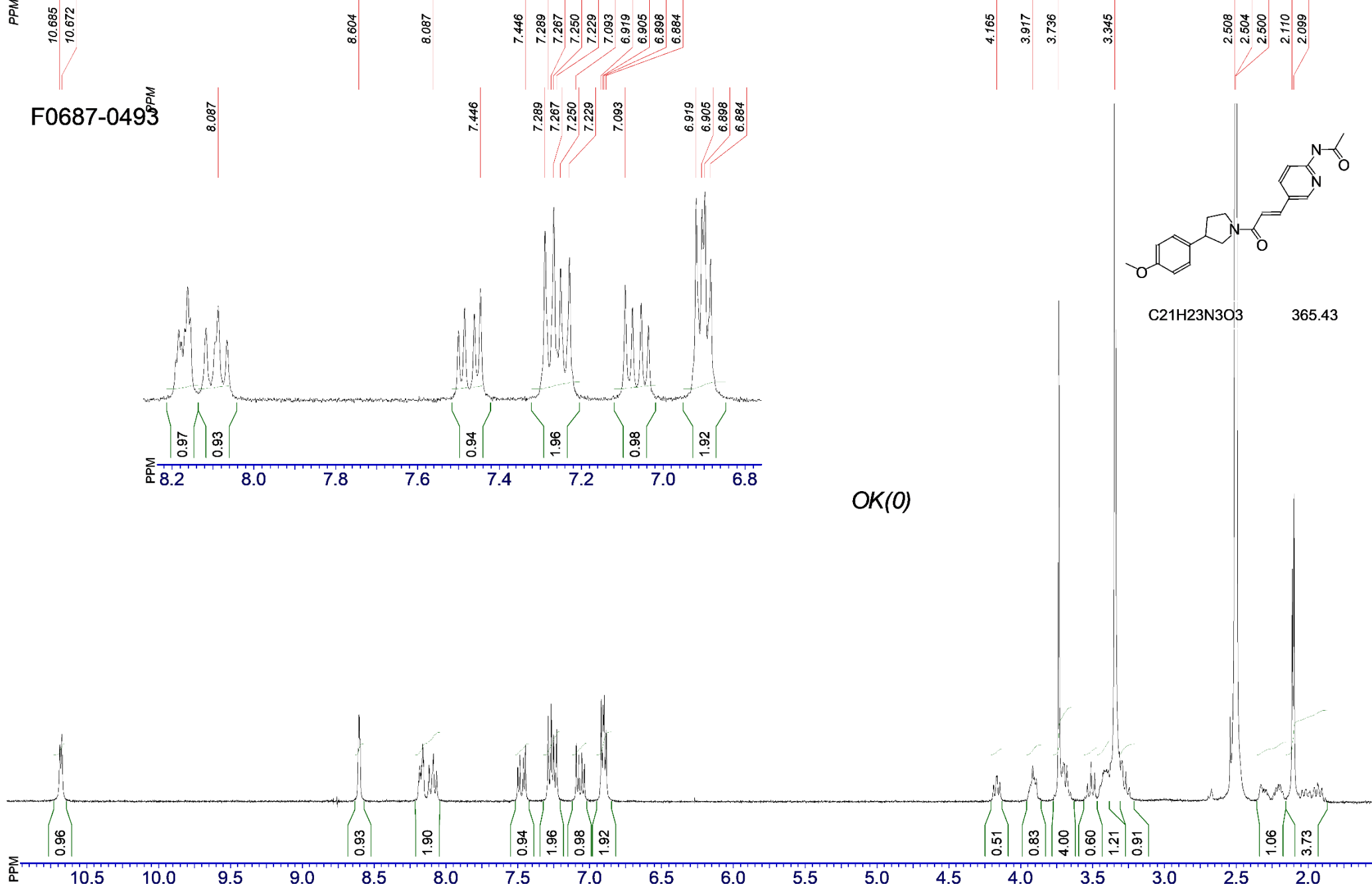
Mol.Weight: 365.43
 Salt:



F0687-0471



#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.841	100.000
1	DAD1 B, Sig=241,4 Ref=off	0.840	100.000
1	ELS1 A, Signal Voltage	0.945	100.000
1	MSD1 TIC, MS File	0.882	100.000



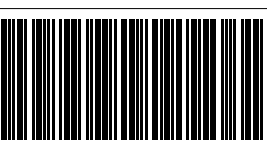
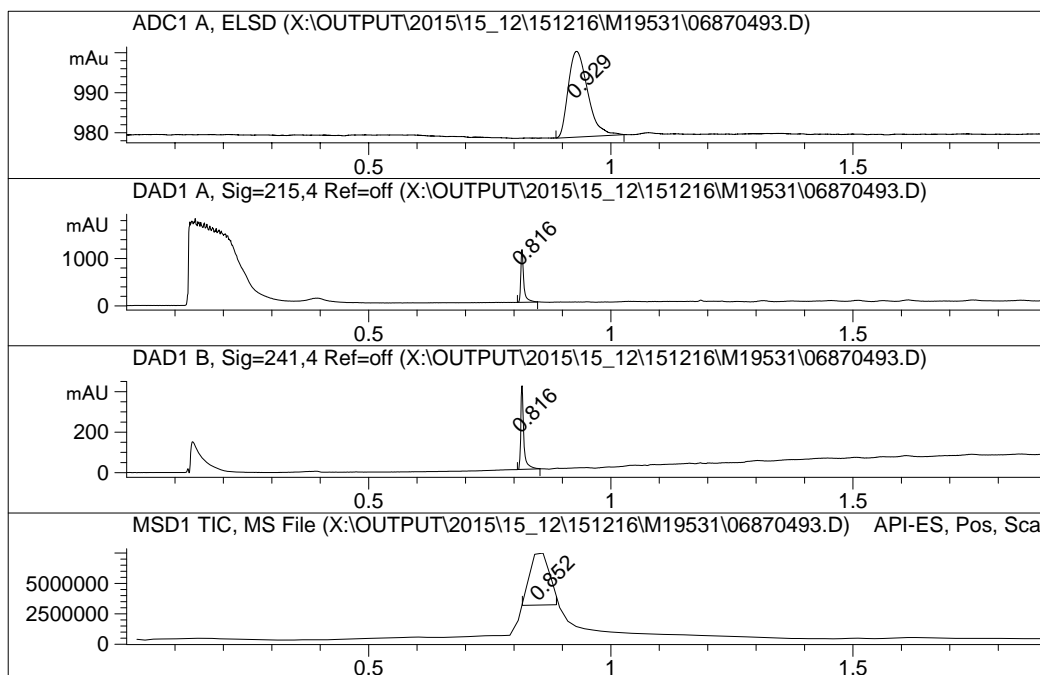
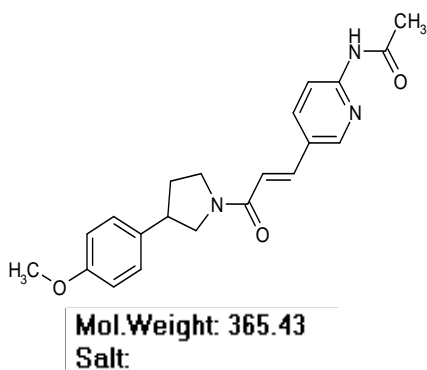
OK(0)

File name: F0687-0493	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 16_Dec_2015	Solvent: DMSO 1211		TE: 293 K	block: S17697

-.o.-Syntez Purity Report -.o.-

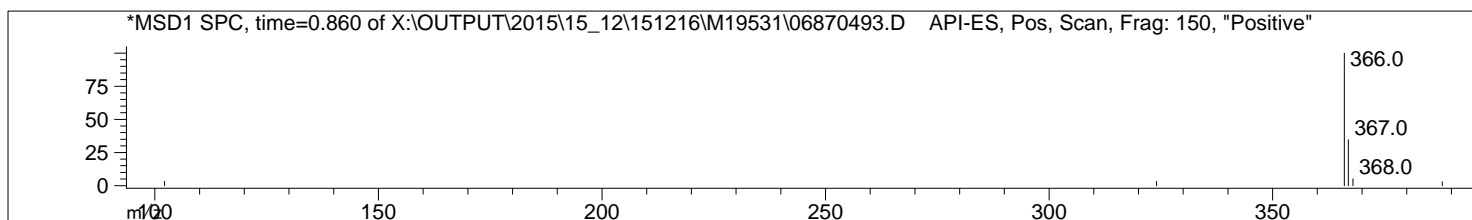
Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H₂O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation colun **100 %**
 Rapid Resolutionn HT Cartridge 4.6x30mm,
 1.8-Micron, Zorbax SB C-18



F0687-0493

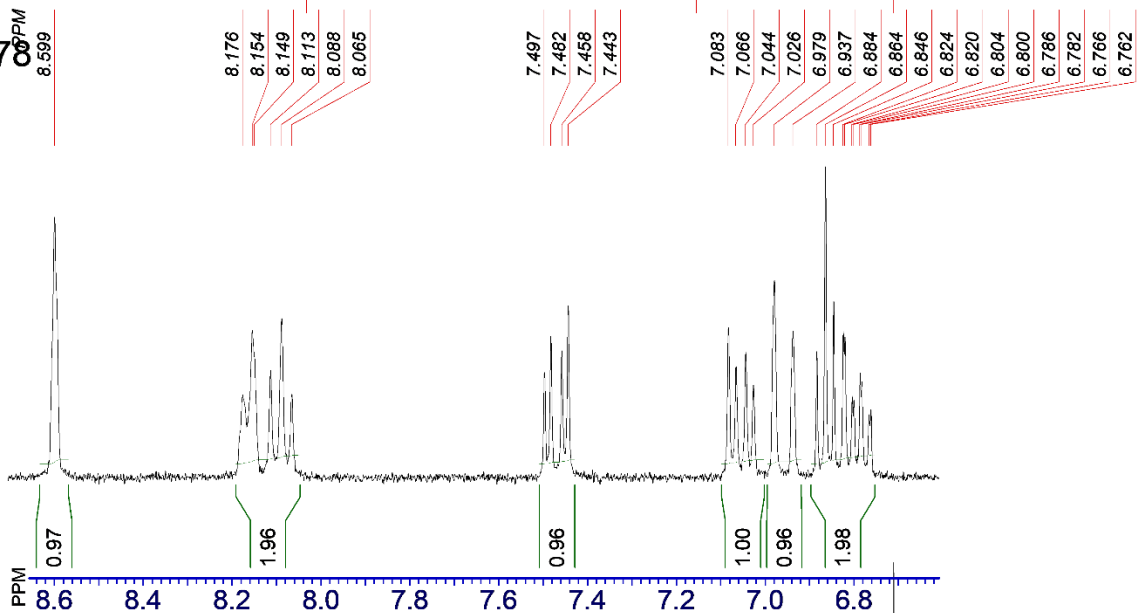
151216-1 ->



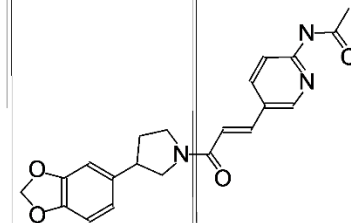
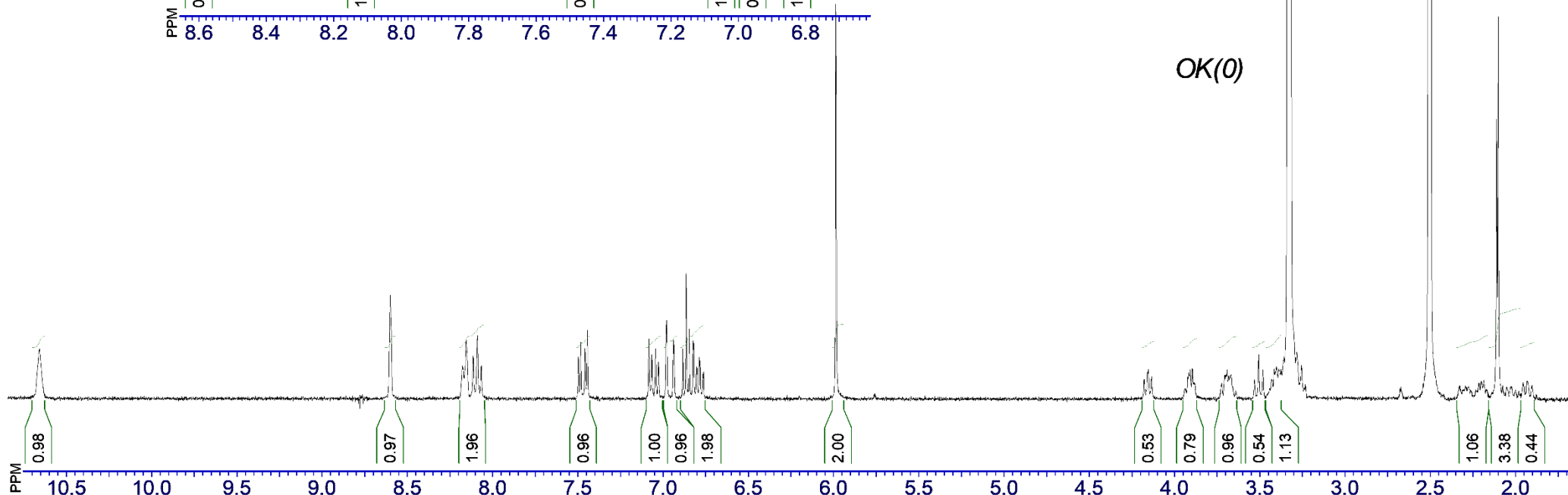
#	Signal	R.Time	Area %
1	ADC1 A, ELSD	0.929	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.816	100.000
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.816	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.852	100.000

PPM

F0687-0478



OK(0)



0 0 C₂₁H₂₁N₃O₄
379.41

File name: F0687-0478

Expert: A.Ryabitsky

SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec

NS: ; pw: 9,65 usec

SI: 65536, TD: 24000

Date: 03_nov_2015

Solvent: DMSO new

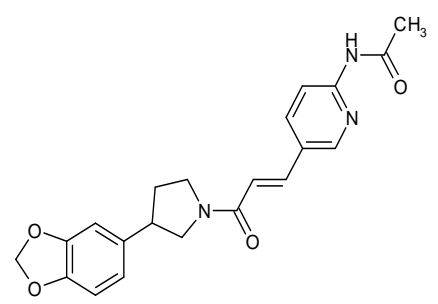
TE: 293 K

block: S17233

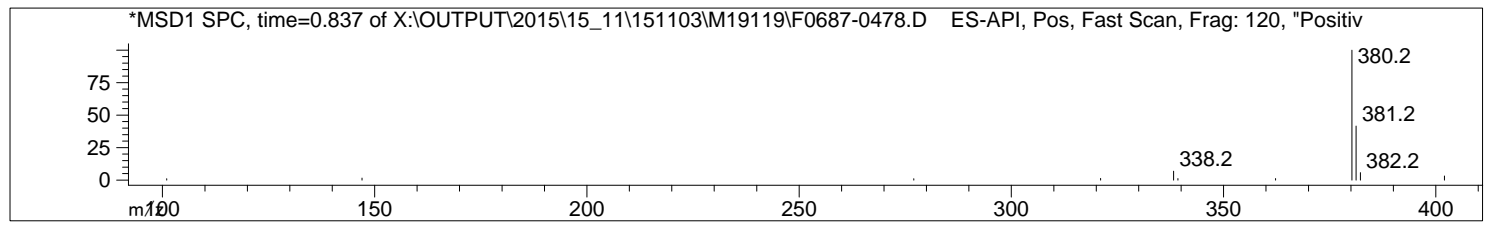
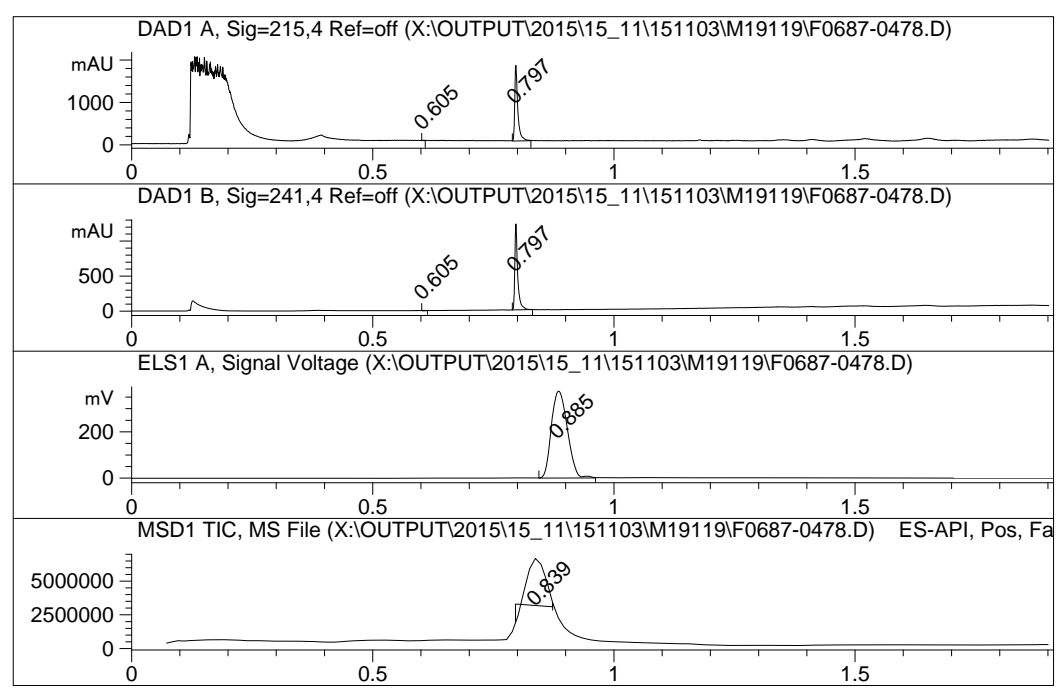
- .o. - Syntez Purity Report - .o. -

Agilent 1200 LC/MSD
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
Separation colun **99 %**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 379.41
Salt:

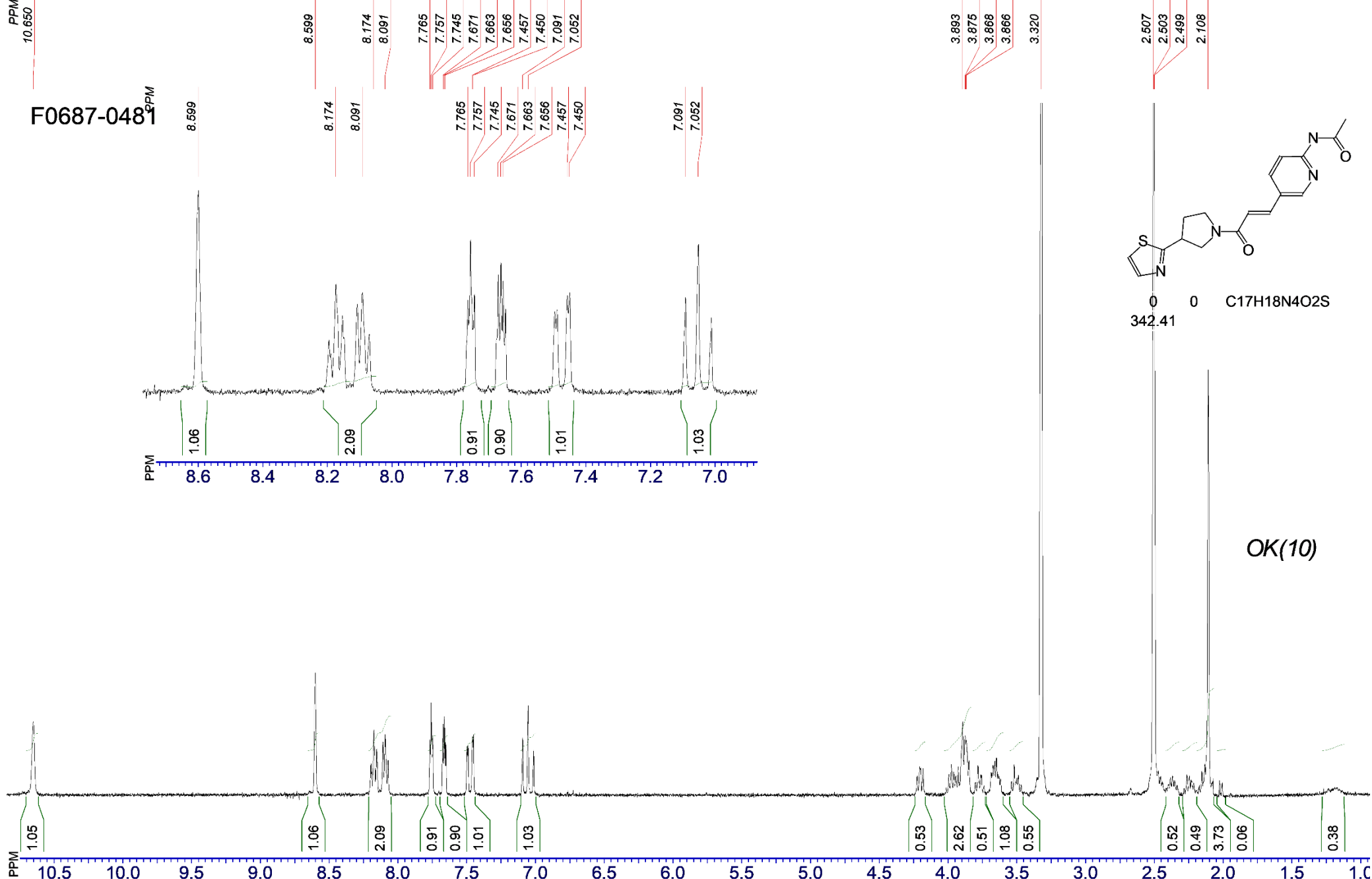


#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.605	0.240
2		0.797	99.760

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.605	0.516
2		0.797	99.484

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.885	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.839	100.000

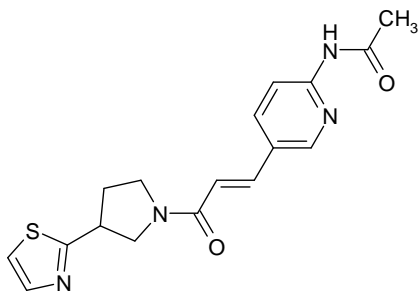


File name: F0687-0481	Expert: A.Ryabitsky	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 03_nov_2015	Solvent: DMSO new		TE: 293 K	block: S17233

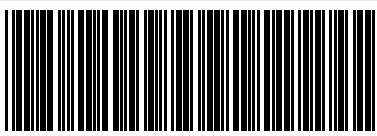
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
ELSD Altech 3300 (ADC1 A, ELSD)

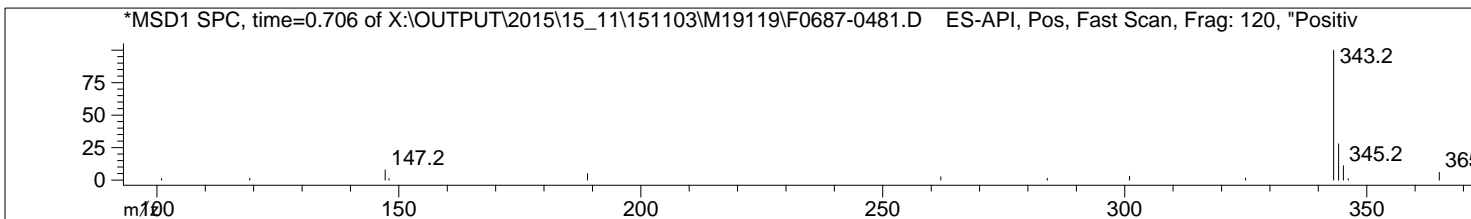
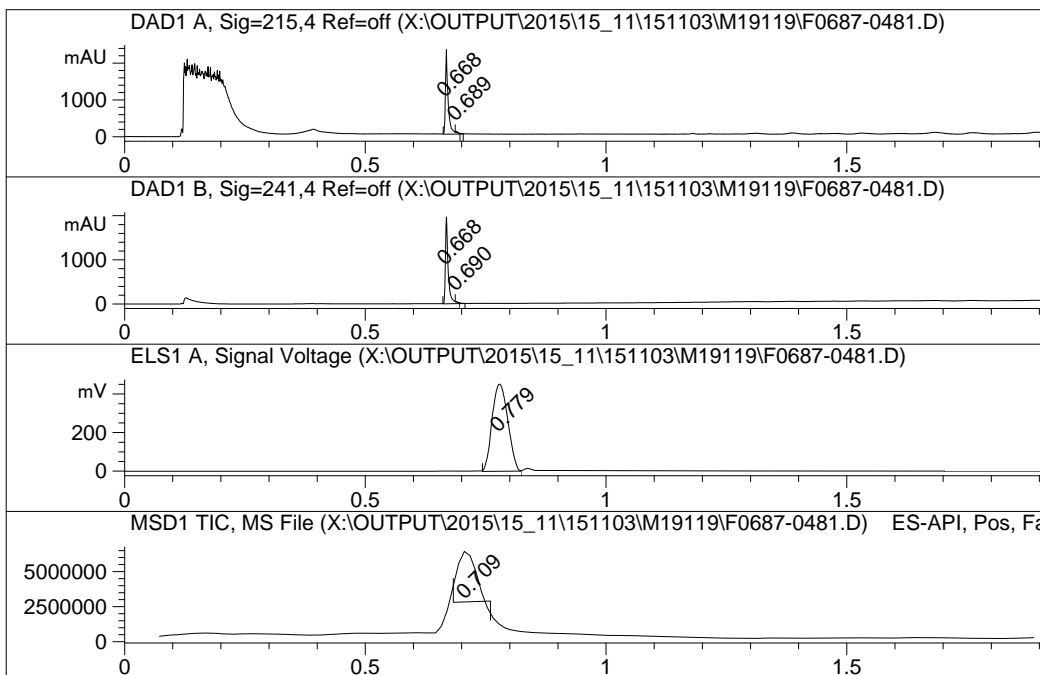
Mobile Phase: A-H2O+0.1HCOOH; B-MeCN+0.1HCOOH
Separation colu **Non-informative**
Rapid Resolutionn HT Cartige 4.6x30mm,
1.8-Micron, Zorbax SB-C18



Mol.Weight: 342.42
Salt:



F0687-0481

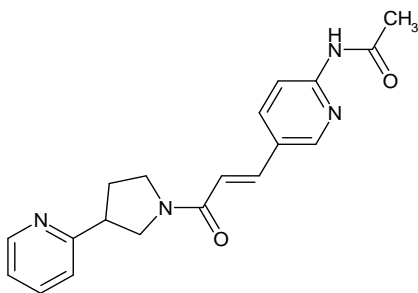


#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.668	98.872
2		0.689	1.128
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.668	99.639
2		0.690	0.361
#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.779	100.000
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.709	100.000

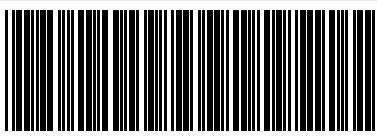
- .o.- Syntez Purity Report - .o.-

Agilent 1200 LC/MSD
 Diodearray G1315B (DAD1A-215nm; DAD1B-240nm)
 Mass Quad G6140A (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

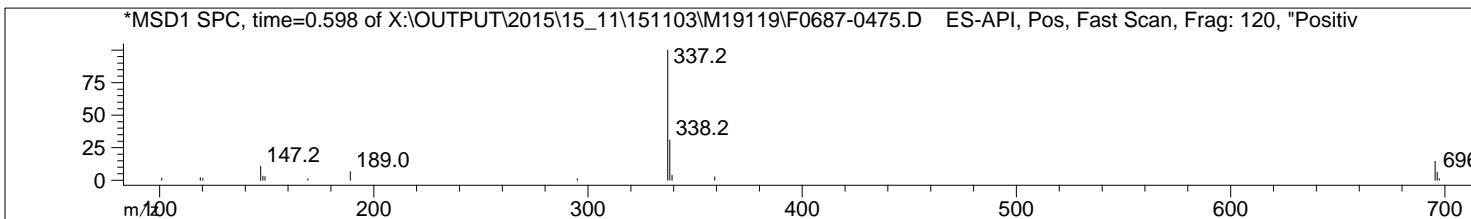
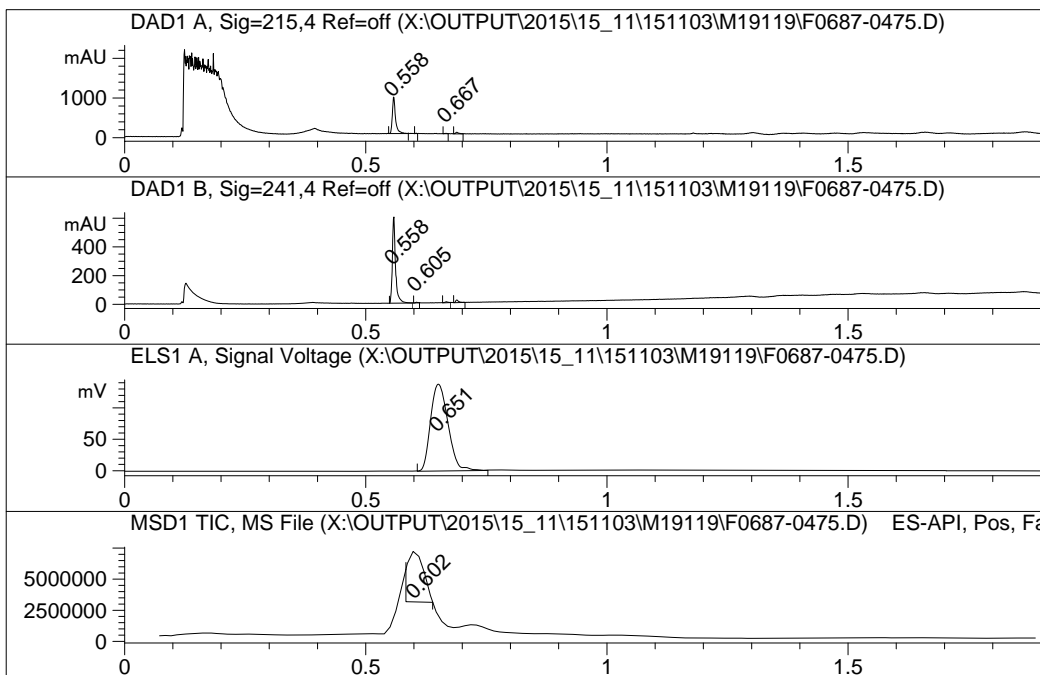
Mobile Phase: A-H₂O+0.1HCOOH; B-MeCN+0.1HCOOH
 Separation column: **95%**
 Rapid Resolutionn HT Cartige 4.6x30mm,
 1.8-Micron, Zorbax SB-C18



Mol.Weight: 336.39
 Salt:



F0687-0475

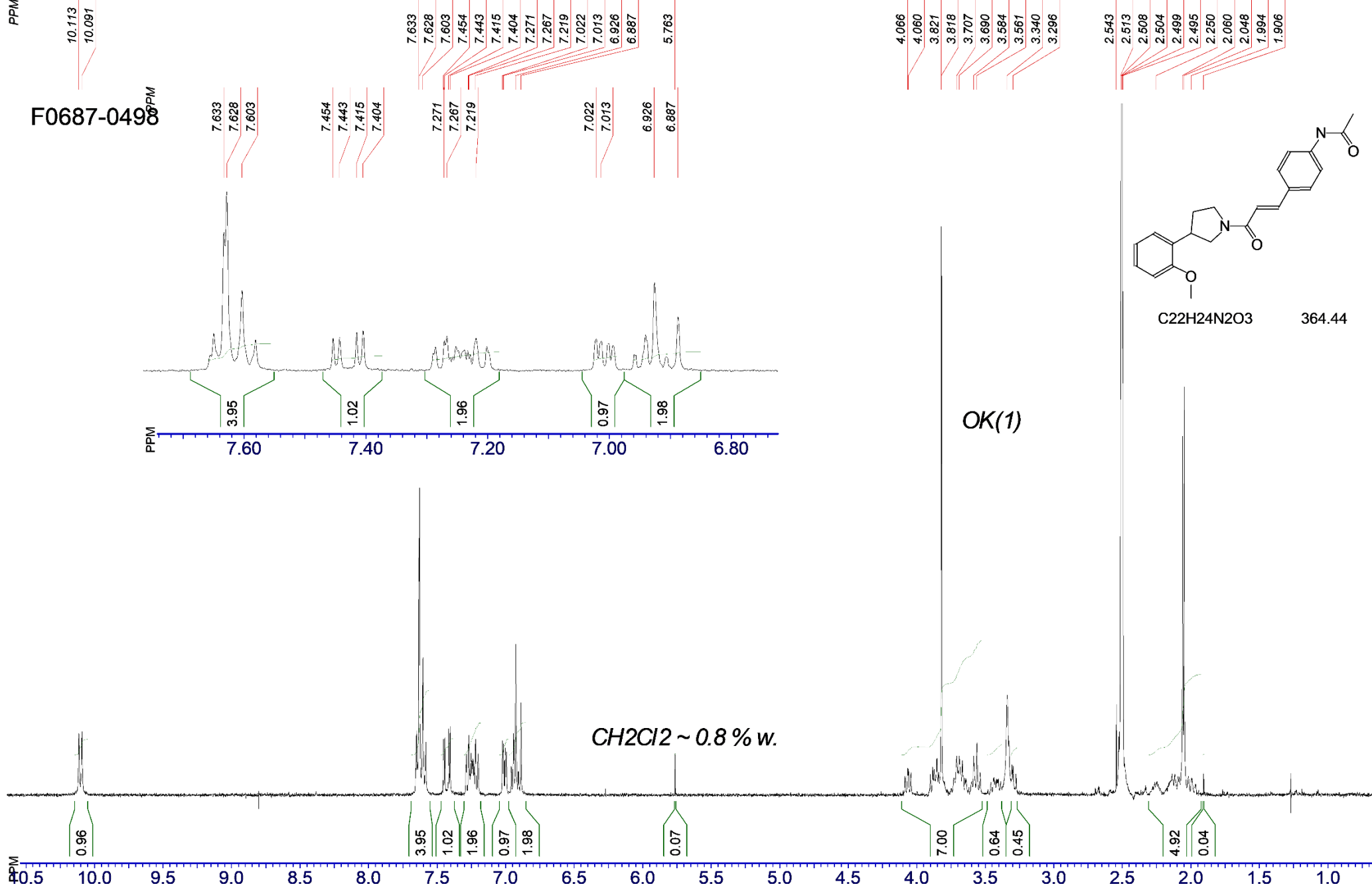


#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.558	95.055
2		0.605	0.412
3		0.667	0.902
4		0.688	3.631

#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.558	95.697
2		0.605	0.427
3		0.667	1.169
4		0.688	2.707

#	Signal	R.Time	Area %
1	ELS1 A, Signal Voltage	0.651	100.000

#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.602	100.000



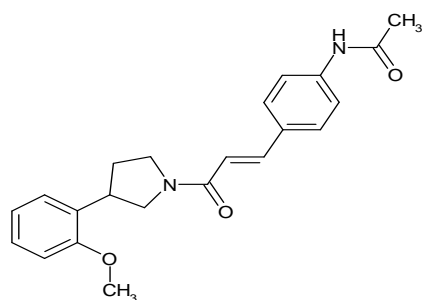
File name: F0687-0498	Expert: M.Pyanova	SF: 400.0778 MHz; sw: 8000 Hz; at: 1.50 sec	NS: ; pw: 9,65 usec	SI: 65536, TD: 24000
Date: 06_Apr_2016	Solvent: DMSO 0325		TE: 293 K	block: S18865

-.o.-Syntez Purity Report -.o.-

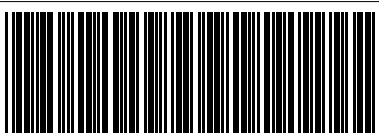
Agilent 1100 LC/MSD SL
 Diodearray G1315B (DAD1A-215nm; DAD1B-254nm)
 Mass Quad G1956B (MSD1-Pos, MSD2-Neg)
 ELSD Altech 3300 (ADC1 A, ELSD)

Mobile Phase:A-H2O+0.1%HCOOH;B-MeCN+0.1HCOOH
 Separation column:
 Rapid Resolution II cartridge 1.0x250mm,
 1.8-Micron, Zorbax SB C-18

99 %

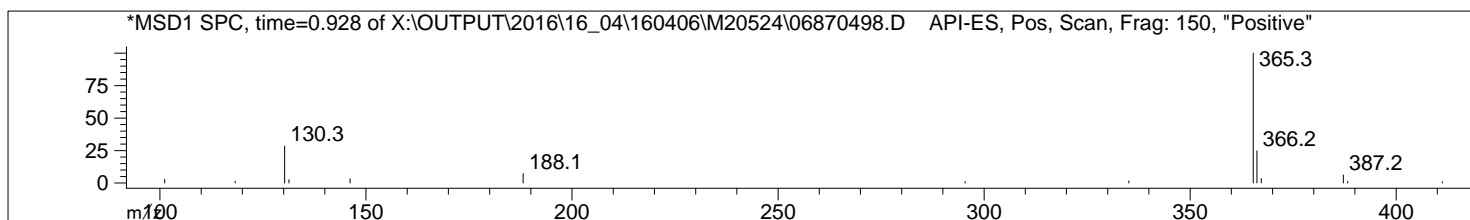
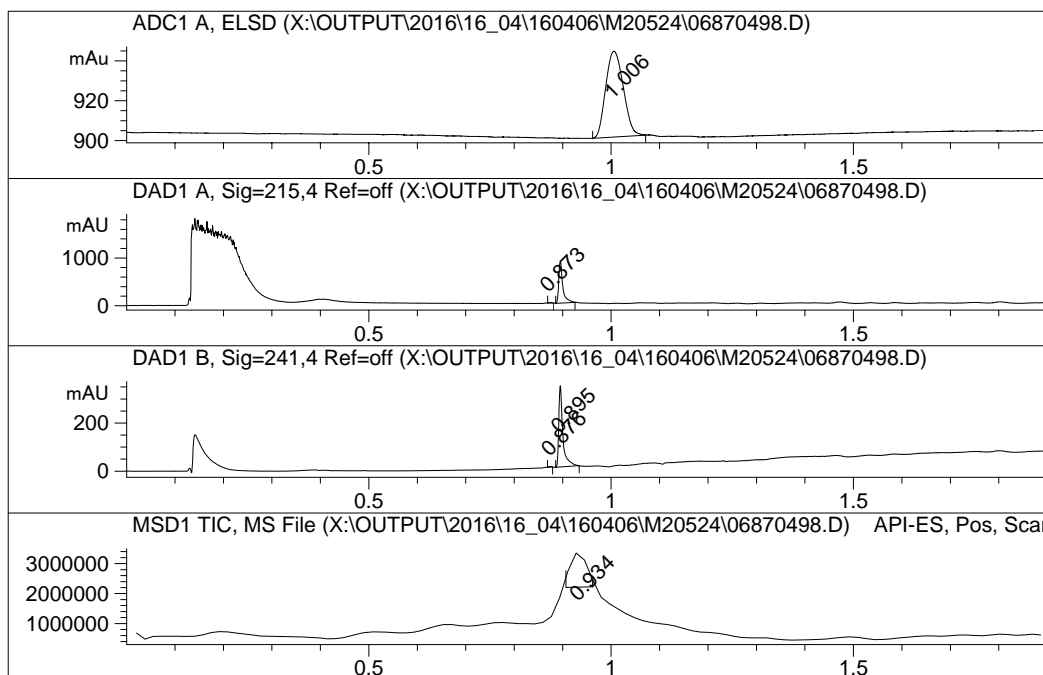


Mol.Weight: 364.44
 Salt:



F0687-0498

160406 ->



#	Signal	R.Time	Area %
1	ADC1 A, ELSD	1.006	100.000
#	Signal	R.Time	Area %
1	DAD1 A, Sig=215,4 Ref=off	0.873	0.975
2		0.895	99.025
#	Signal	R.Time	Area %
1	DAD1 B, Sig=241,4 Ref=off	0.876	0.772
2		0.895	99.228
#	Signal	R.Time	Area %
1	MSD1 TIC, MS File	0.934	100.000