Supporting Information

Potent Anticancer Activity with High Selectivity of a chiral Palladium N-heterocyclic Carbene Complex

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MKG: Department of Chemistry, IIT Kanpur, Kanpur, 208016, India.

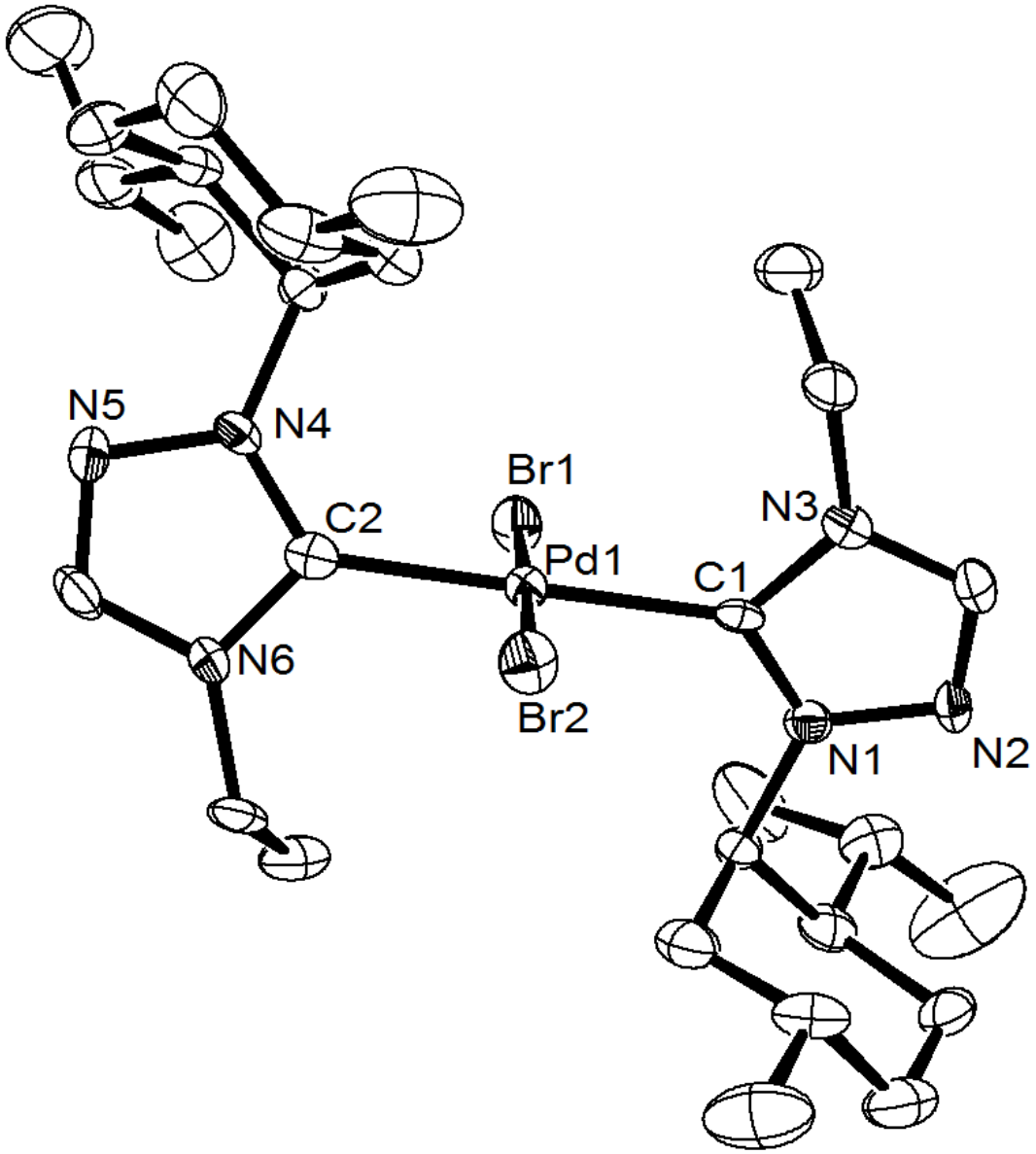


Figure S1. ORTEP of *1R,2R,5S*-**1b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd(1)−C(1) 2.025(3), Pd(1)−C(2) 2.020(3), Pd(1)−Br(1) 2.4352(7), Pd(1)−Br(2) 2.4551(7), C(1)−Pd(1)−C(2) 179.41(15), Br(1)−Pd(1)−Br(2) 177.984(17), C(1)−Pd(1)−Br(2) 91.57(10), C(1)−Pd(1)−Br(1) 90.02(10).

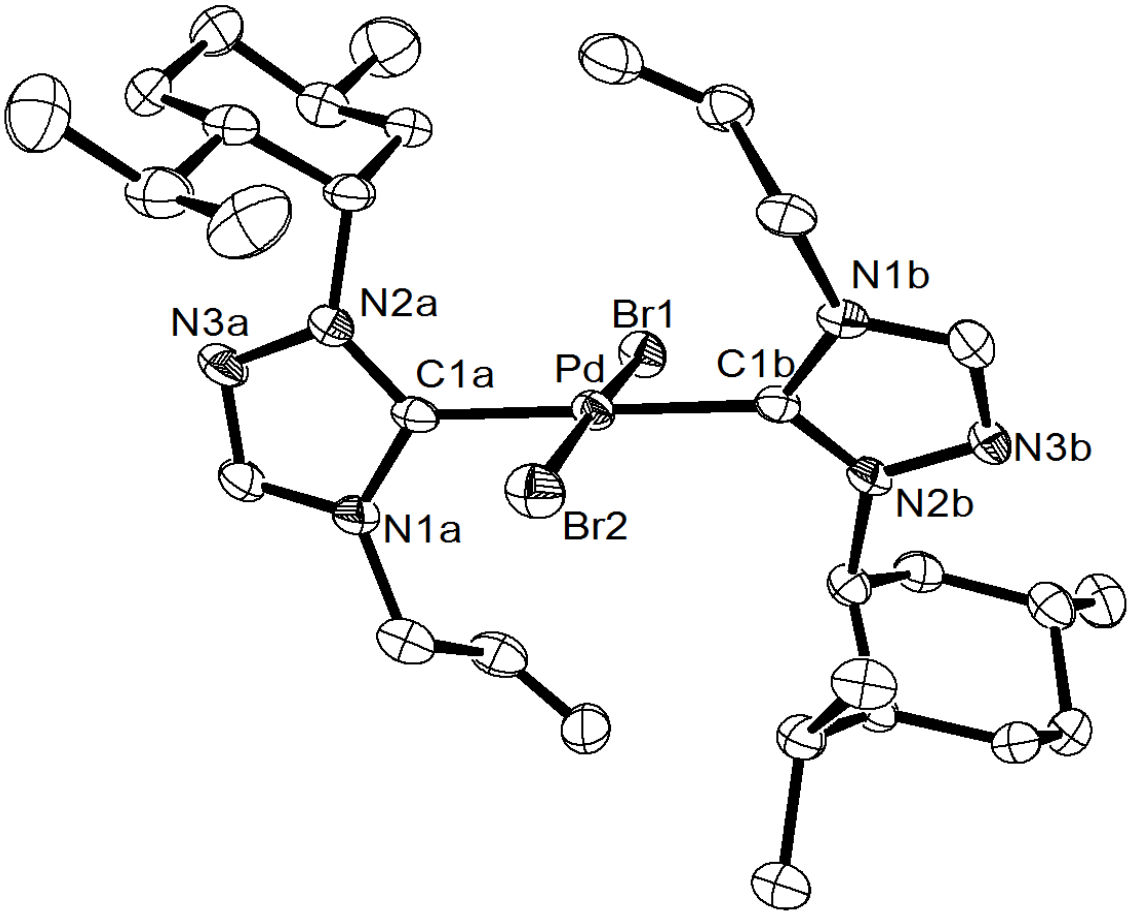


Figure S2. ORTEP of *1S,2S,5R*-**2b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd−C(1a) 2.008(6), Pd−C(1b) 2.028(5), Pd−Br(1) 2.4479(9), Pd−Br(2) 2.4319(10), C(1a)−Pd−C(1b) 179.2(2), Br(1)−Pd−Br(2) 175.32(5), C(1a)−Pd−Br(2) 89.72(15), C(1b)−Pd−Br(1) 90.24(15).

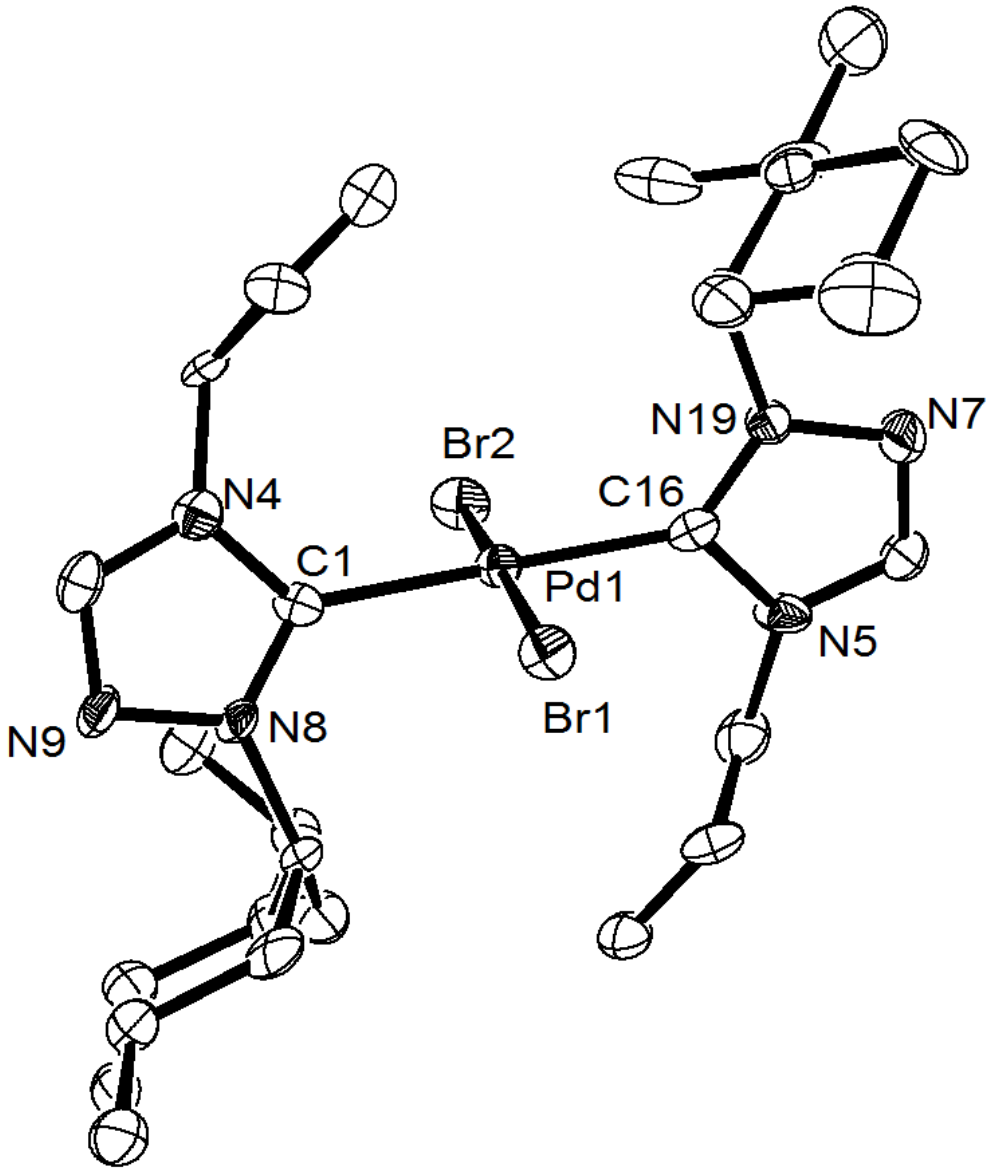


Figure S3. ORTEP of *1R,2R,5S*-**2b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd(1)−C(1) 2.049(11), Pd(1)−C(16) 2.012(12), Pd(1)−Br(1) 2.4369(15), Pd(1)−Br(2) 2.4446(15), C(1)−Pd(1)−C(16) 178.8(5), Br(1)−Pd(1)−Br(2) 175.39(7), C(1)−Pd(1)−Br(2) 90.9(3), C(1)−Pd(1)−Br(1) 90.1(3).

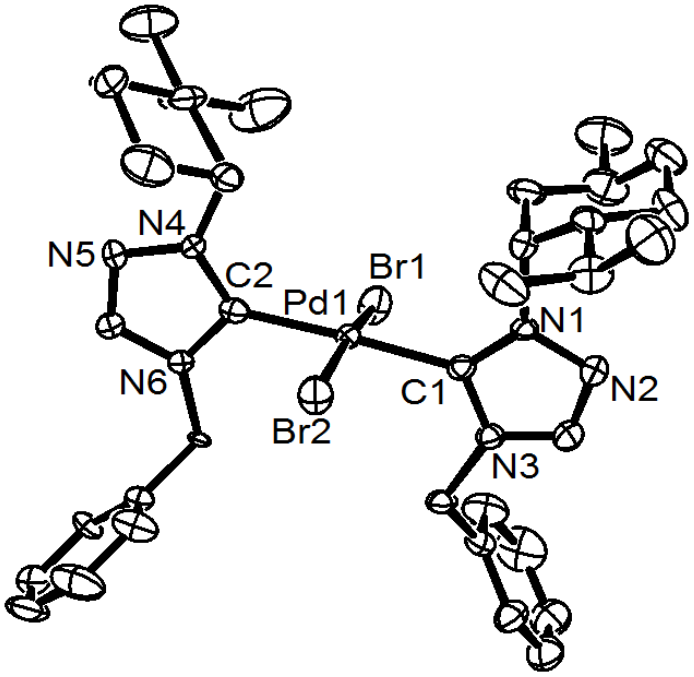


Figure S4. ORTEP of *1R,2R,5S*-**3b** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd(1)−C(1) 2.018(9), Pd(1)−C(2) 2.022(9), Pd(1)−Br(1) 2.4354(12), Pd(1)−Br(2) 2.4370(12), C(1)−Pd(1)−C(2) 177.5(5), Br(1)−Pd(1)−Br(2) 169.51(5), C(1)−Pd(1)−Br(2) 91.3(3), C(1)−Pd(1)−Br(1) 87.8(3).

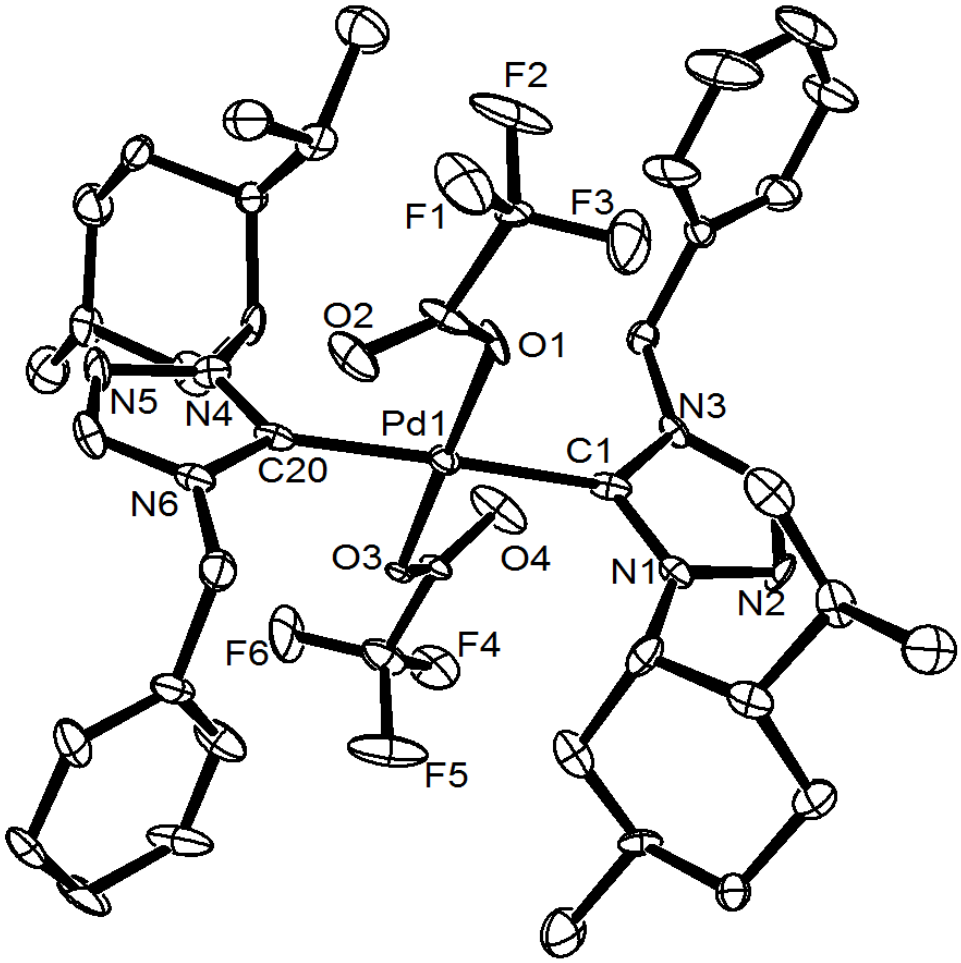


Figure S5. ORTEP of *1S,2S,5R*-**3c** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd(1)−C(1) 2.022(10), Pd(1)−C(20) 2.028(10), Pd(1)−O(1) 2.006(6), Pd(1)−O(3) 2.017(6), C(1)−Pd(1)−C(20) 176.8(5), O(1)−Pd(1)−O(3) 179.1(4), C(1)−Pd(1)−O(1) 87.0(4), C(20)−Pd(1)−O(3) 85.0(3).

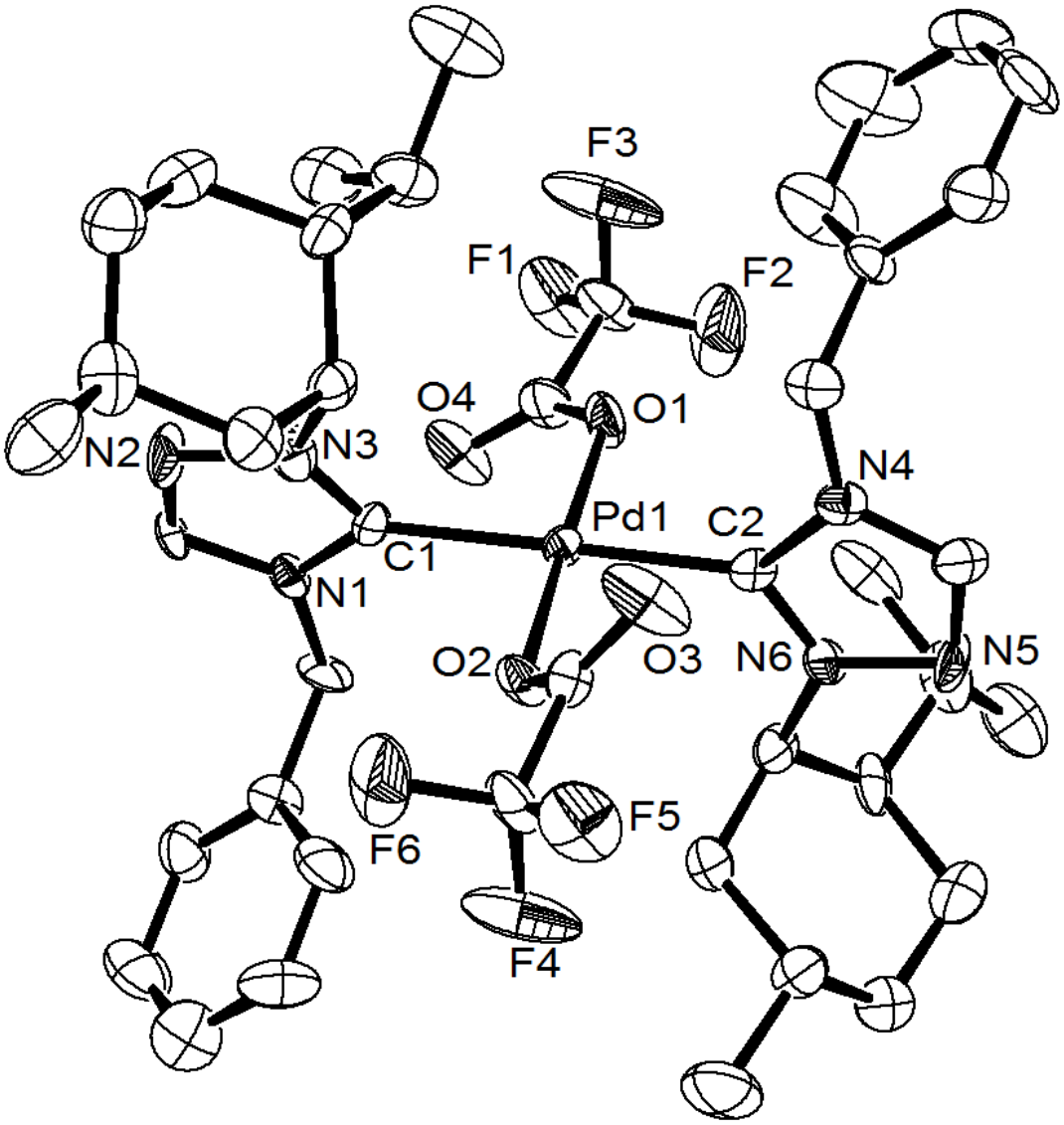


Figure S6. ORTEP of *1R,2R,5S*-**3c** with thermal ellipsoids are shown at the 50 % probability level. Selected bond lengths (Å) and angles (°): Pd(1)−C(1) 2.033(8), Pd(1)−C(2) 2.020(8), Pd(1)−O(1) 2.022(5), Pd(1)−O(2) 2.021(5), C(1)−Pd(1)−C(2) 176.7(3), O(1)−Pd(1)−O(2) 178.7(3), C(1)−Pd(1)−O(1) 95.3(3), C(2)−Pd(1)−O(2) 91.3(3).

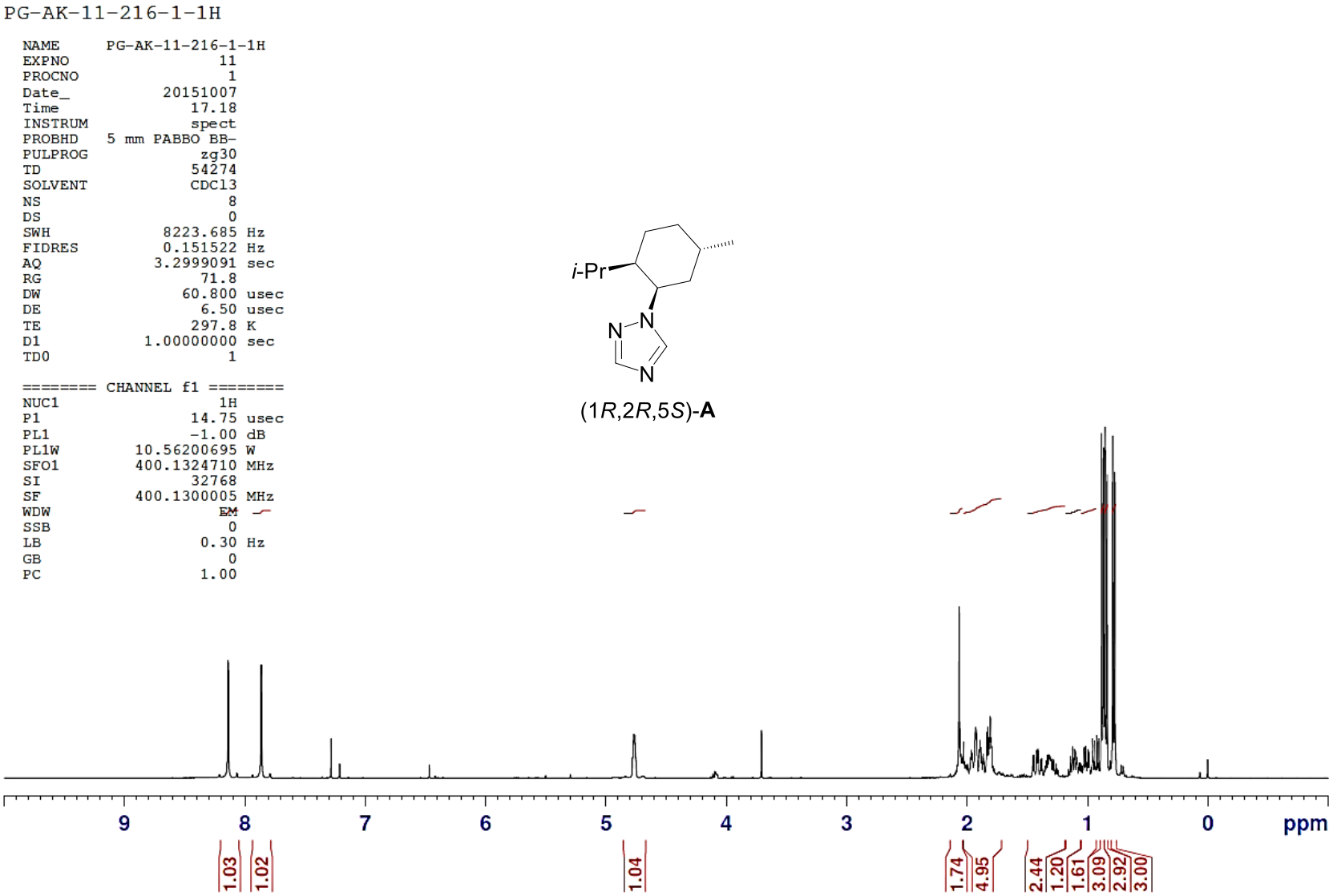


Figure S7. ^{1}H NMR spectrum of 1*R*,2*R*,5*S*-**A** in $CDCl_3$.

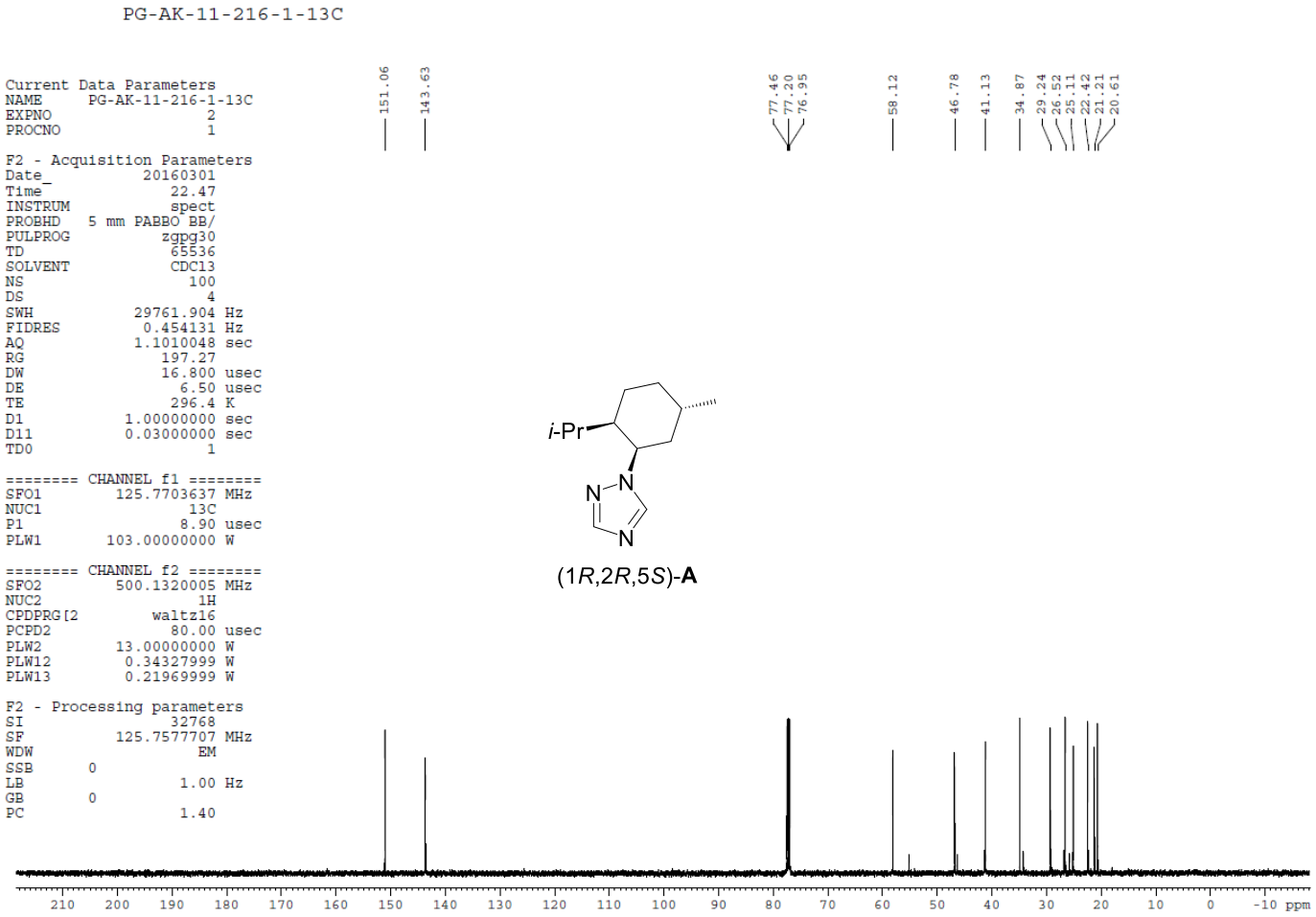


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of 1*R*,2*R*,5*S*-**A** in $CDCl_3$.

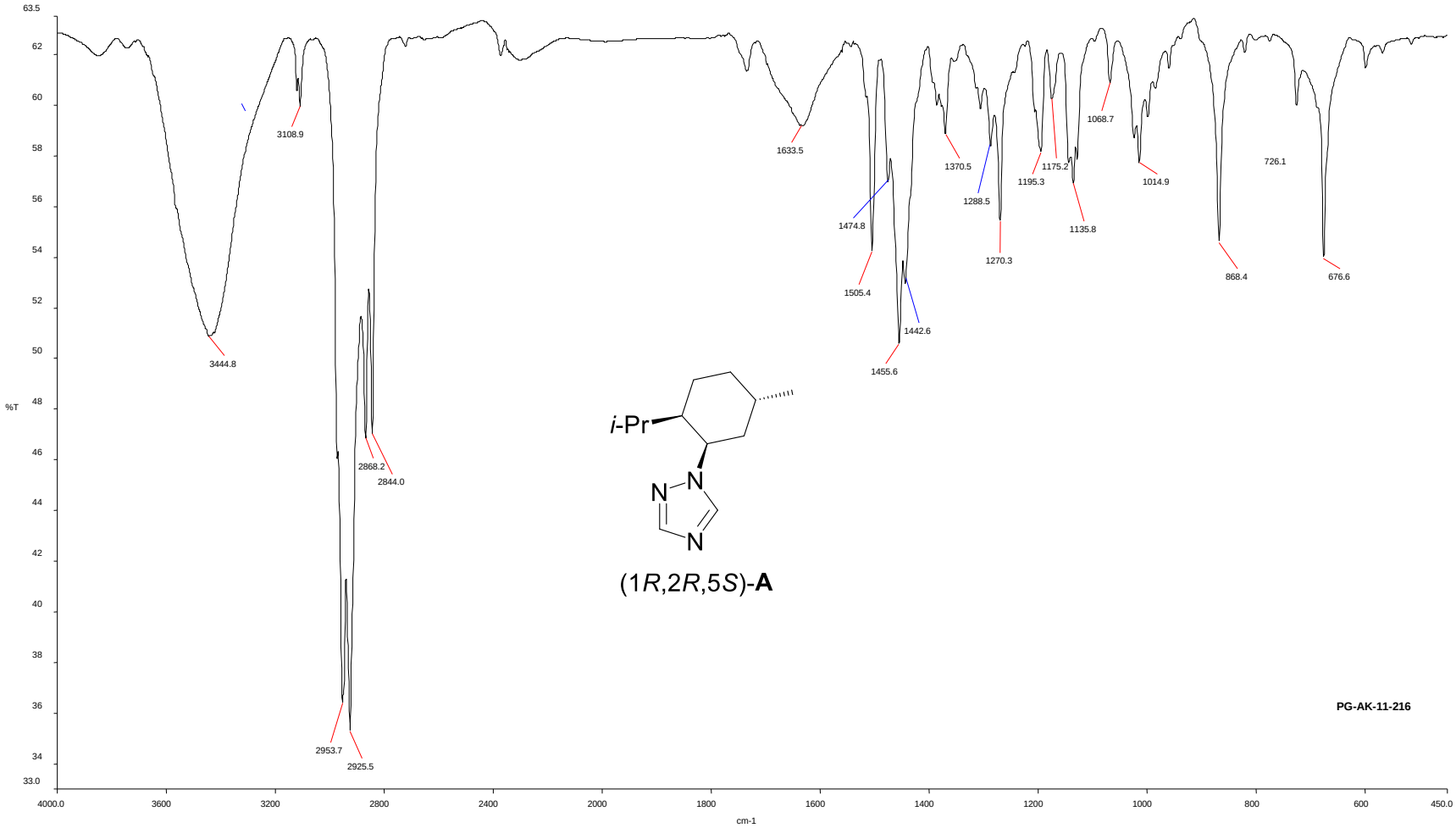


Figure S9. Infrared spectrum of 1*R*,2*R*,5*S*-**A** in KBr.

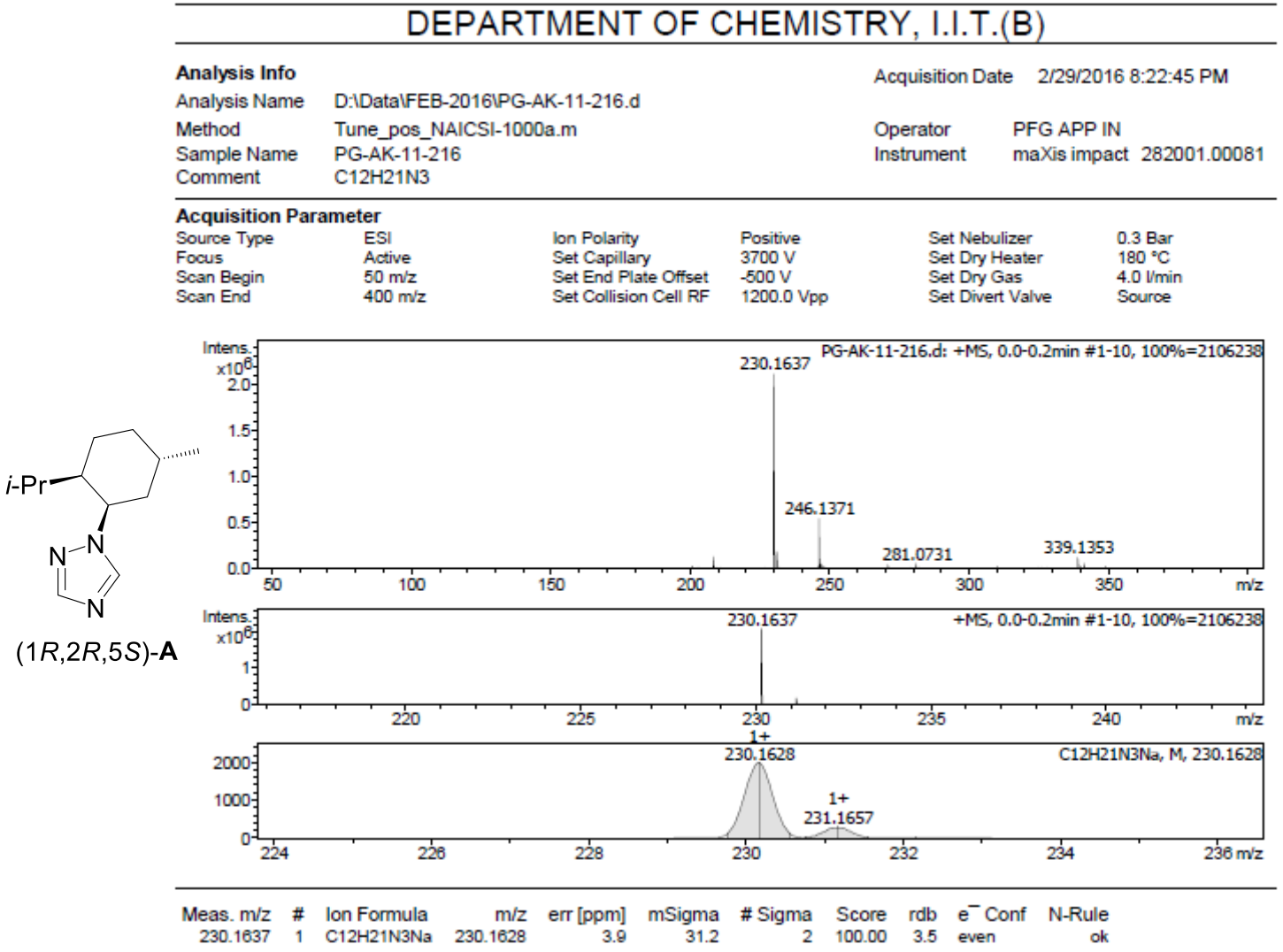
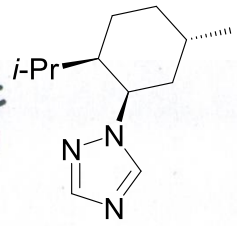


Figure S10. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**A**.



(1*R*,2*R*,5*S*)-**A**

Eager 300 Report

Page: 1 Sample: PG-AK-11-216-1 (PG-AK-11-216-1)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-216-1
Operator ID : CHANDNI
Analysed : 10/13/2015 15:28
Sample ID : PG-AK-11-216-1 (# 22)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/13/2015 18:36
Instrument N. : Instrument #1
Sample weight : .881

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	19.3771	40	184872	FU	8.597494	.108295E+07
Carbon	69.0840	63	1589435	FU	1.000000	.260680E+07
Hydrogen	9.9775	178	599593	RS	2.650857	.665180E+07
Totals	98.4386		2373900			

Figure S11. Elemental analysis data of (1*R*,2*R*,5*S*)-**A**.

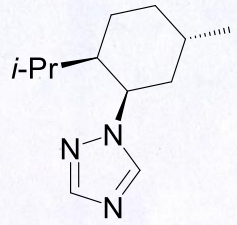
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Monday, 30-NOV-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**A**

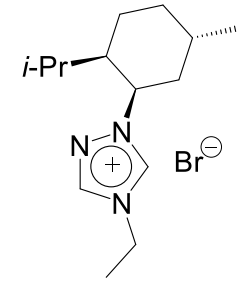
n	Average	Std.Dev.	Maximum	Minimum
5	-40.941	0.0822	-40.851	-41.001

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-216-a2	16:53:19	-41.001	SR	-0.205	589	50	1	24.8
2	pg-ak-11-216-a2	16:53:26	-41.001	SR	-0.205	589	50	1	24.8
3	pg-ak-11-216-a2	16:53:33	-41.001	SR	-0.205	589	50	1	24.8
4	pg-ak-11-216-a2	16:53:42	-40.851	SR	-0.204	589	50	1	24.8
5	pg-ak-11-216-a2	16:53:49	-40.851	SR	-0.204	589	50	1	24.9

Figure S12. Specific rotation of (1*R*,2*R*,5*S*)-**A** in $CHCl_3$.

PG-AK-11-219-1-1H

NAME	PG-AK-11-219-1-1H
EXPNO	1
PROCNO	1
Date_	20151008
Time	22.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	54274
SOLVENT	CDCl3
NS	9
DS	0
SWH	8223.685 Hz
FIDRES	0.151522 Hz
AQ	3.2999091 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	297.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	-1.00 dB
PL1W	10.56200695 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



(1*R*,2*R*,5*S*)-**1a**

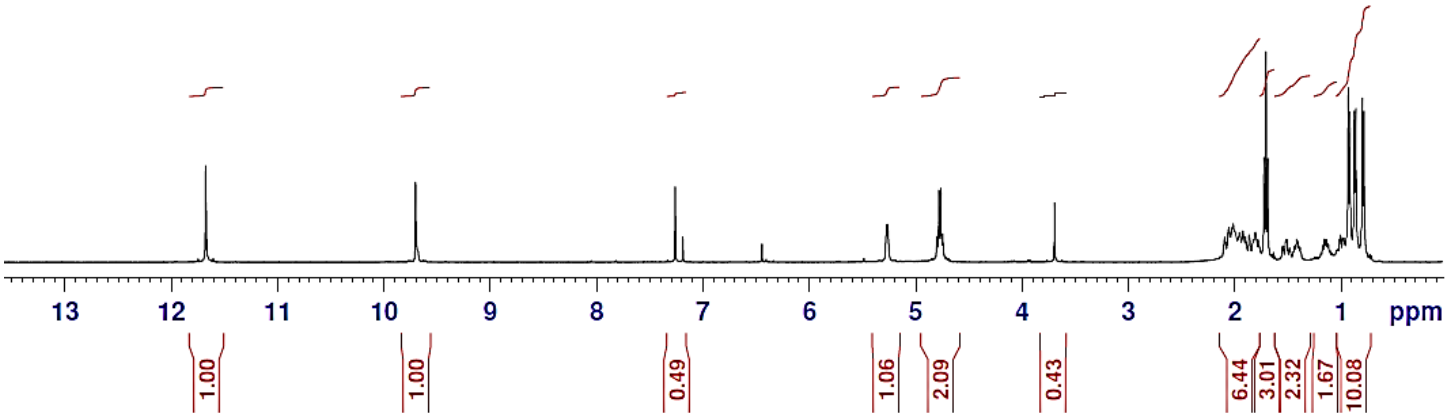


Figure S13. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**1a** in $CDCl_3$.

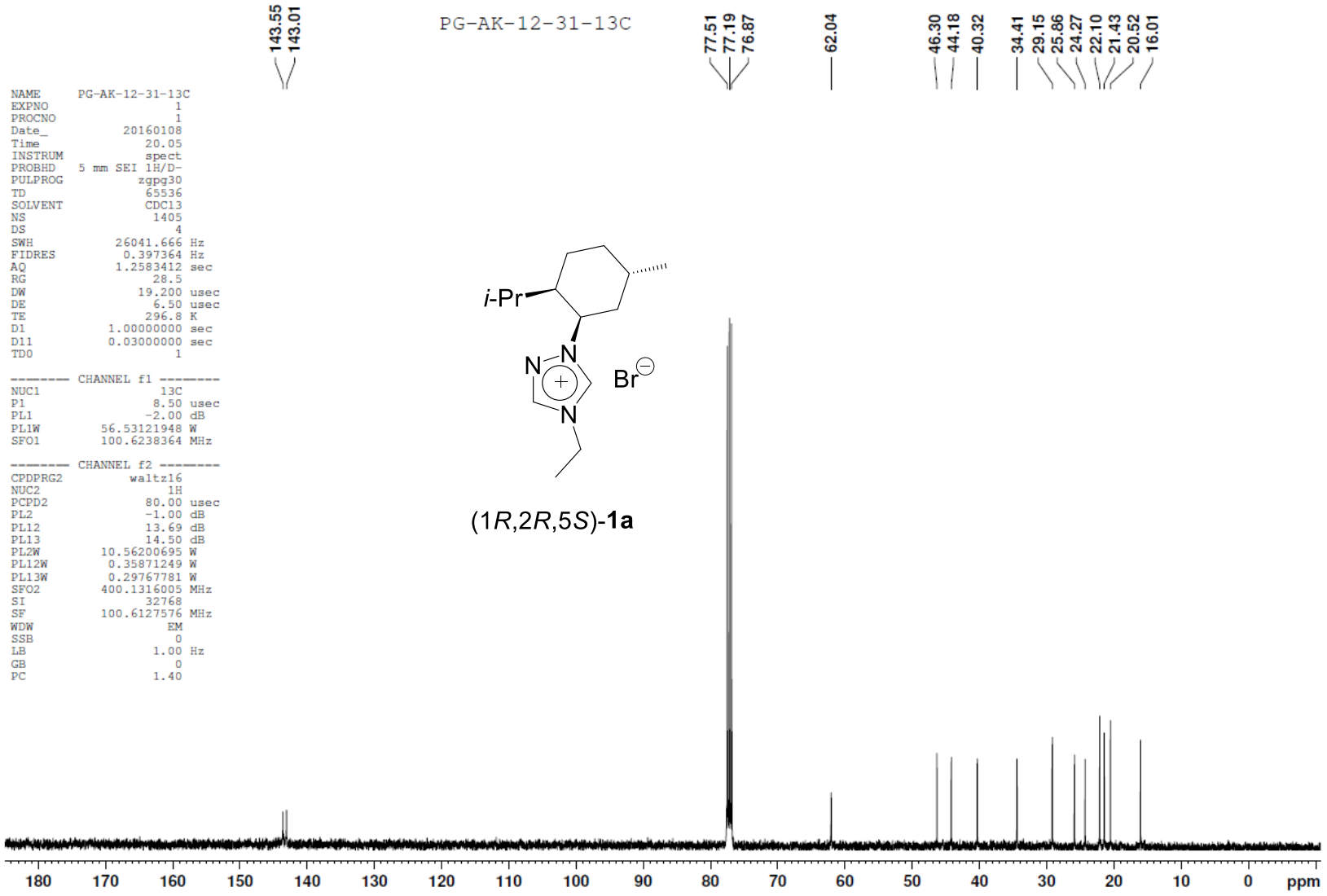


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of 1*R*,2*R*,5*S*-**1a** in $CDCl_3$.

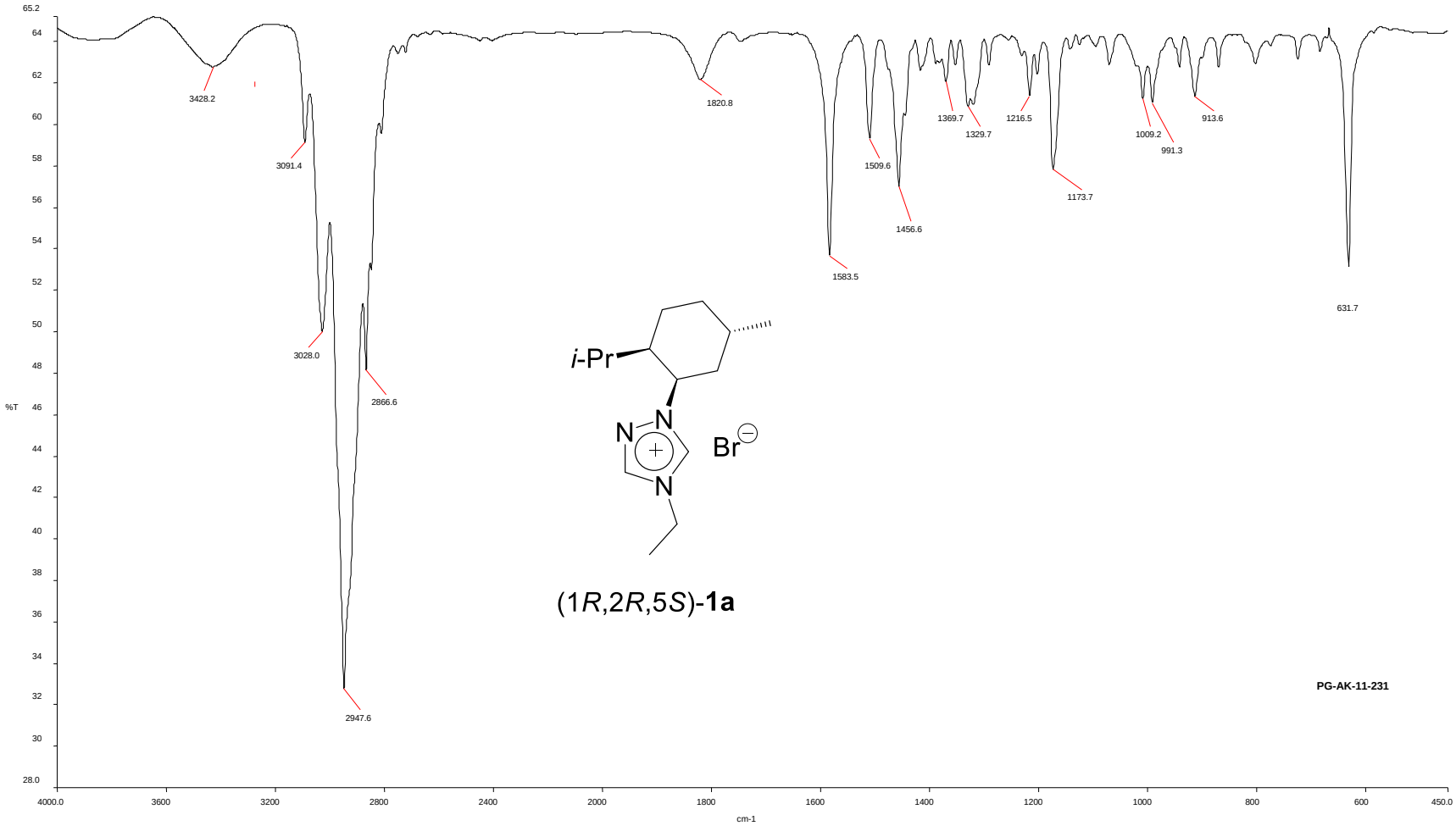


Figure S15. Infrared spectrum of 1*R*,2*R*,5*S*-**1a** in KBr.

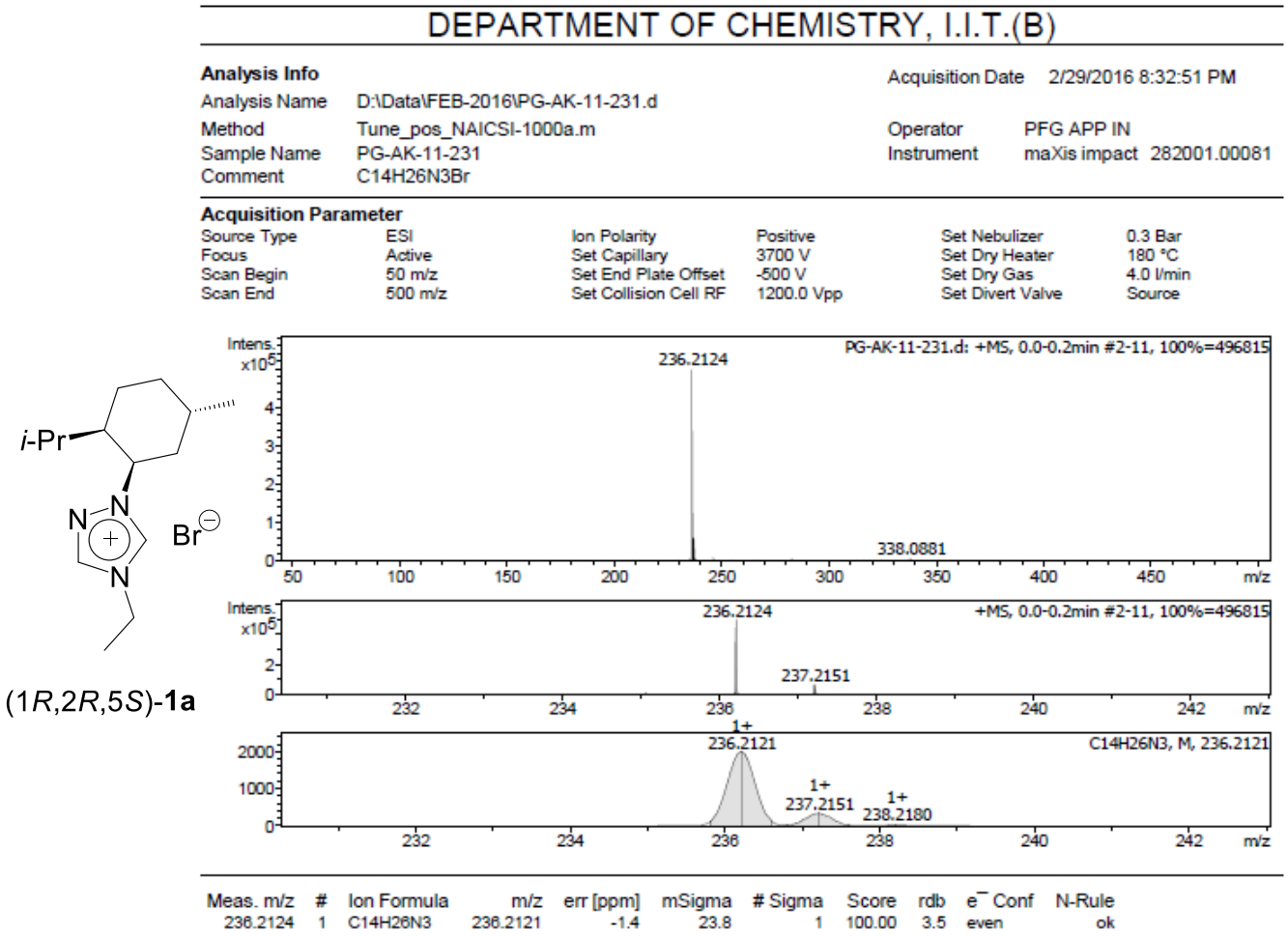
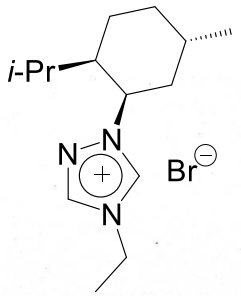


Figure S16. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**1a**.



(1*R*,2*R*,5*S*)-**1a**

Eager 300 Report

Page: 1 Sample: PG-AK-11-231-2 (PG-AK-11-231-2)

Method Name : PGCP26102015
Method File : D:\CHNS-2015\PGCP26102015.mth
Chromatogram : PG-AK-11-231-2
Operator ID : CHANDNI
Analysed : 10/26/2015 12:13
Sample ID : PG-AK-11-231-2 (# 7)
Analysis Type : UnkNown (Area)

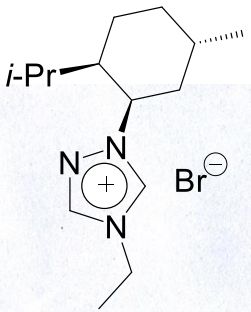
Company Name : C.E. Instruments
Printed : 10/30/2015 09:57
Instrument N. : Instrument #1
Sample weight : .788

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	13.2688	41	121875	RS	9.069481	.116562E+07
Carbon	53.9449	65	1105343	RS	1.000000	.260028E+07
Hydrogen	8.3895	178	446363	RS	2.476332	.655078E+07
Totals	75.6032		1673581			

Figure S17. Elemental analysis data of (1*R*,2*R*,5*S*)-**1a**.



(1*R*,2*R*,5*S*)-**1a**

CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Tuesday, 27-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF

n	Average	Std.Dev.	Maximum	Minimum
5	-21.972	0.1866	-21.820	-22.277

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-231-1	17:28:17	-21.972	SR	-0.110	589	50.00	1.000	24.9
2	pg-ak-11-231-1	17:28:24	-21.820	SR	-0.109	589	50.00	1.000	24.9
3	pg-ak-11-231-1	17:28:31	-21.820	SR	-0.109	589	50.00	1.000	24.9
4	pg-ak-11-231-1	17:28:37	-21.972	SR	-0.110	589	50.00	1.000	24.9
5	pg-ak-11-231-1	17:28:44	-22.277	SR	-0.111	589	50.00	1.000	24.9

Figure S18. Specific rotation of (1*R*,2*R*,5*S*)-**1a** in $CHCl_3$.

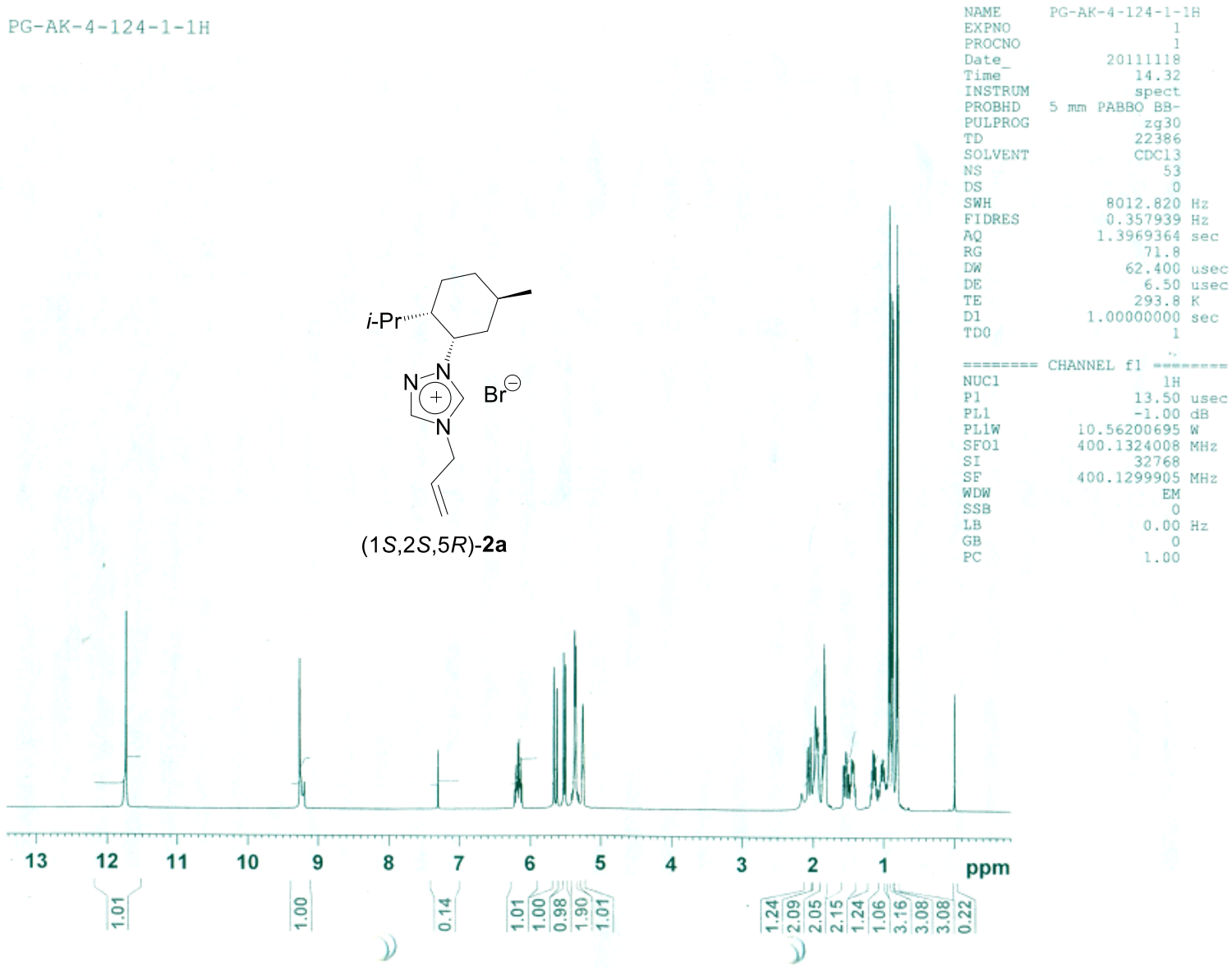


Figure S19. ^{1}H NMR spectrum of 1*S*,2*S*,5*R*-**2a** in $CDCl_3$.

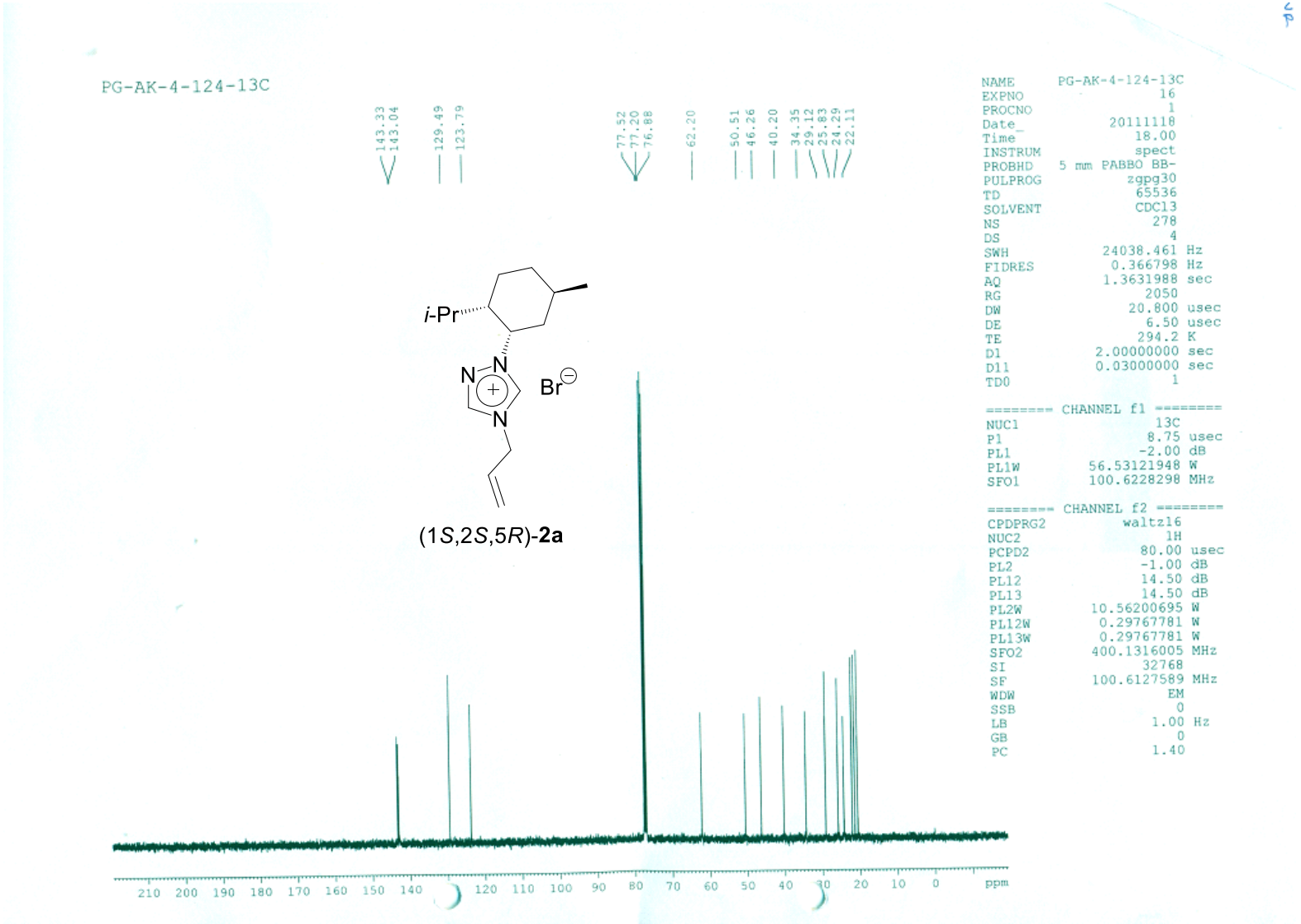


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**2a** in $CDCl_3$.

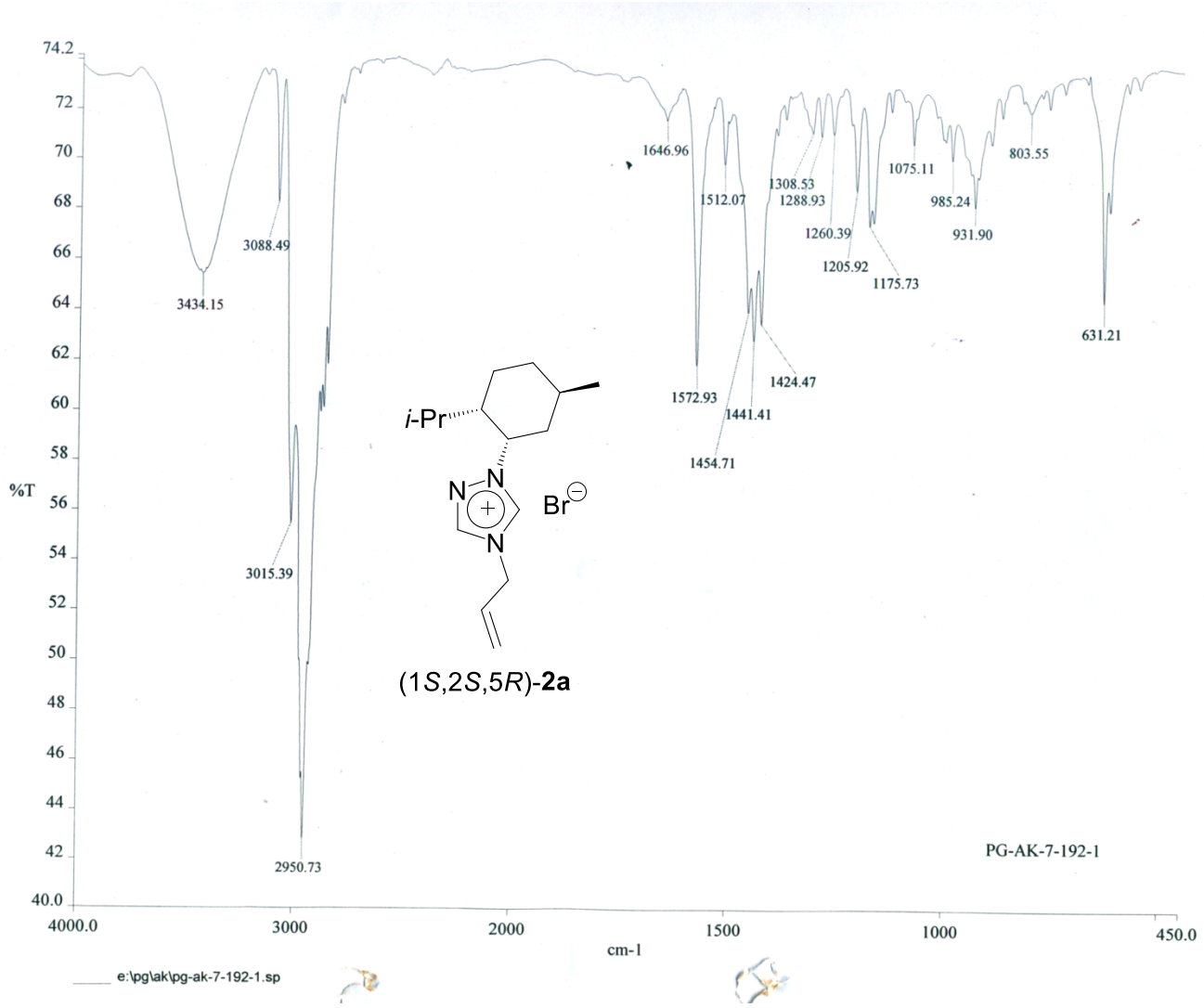


Figure S21. Infrared spectrum of 1*S*,2*S*,5*R*-**2a** in KBr.

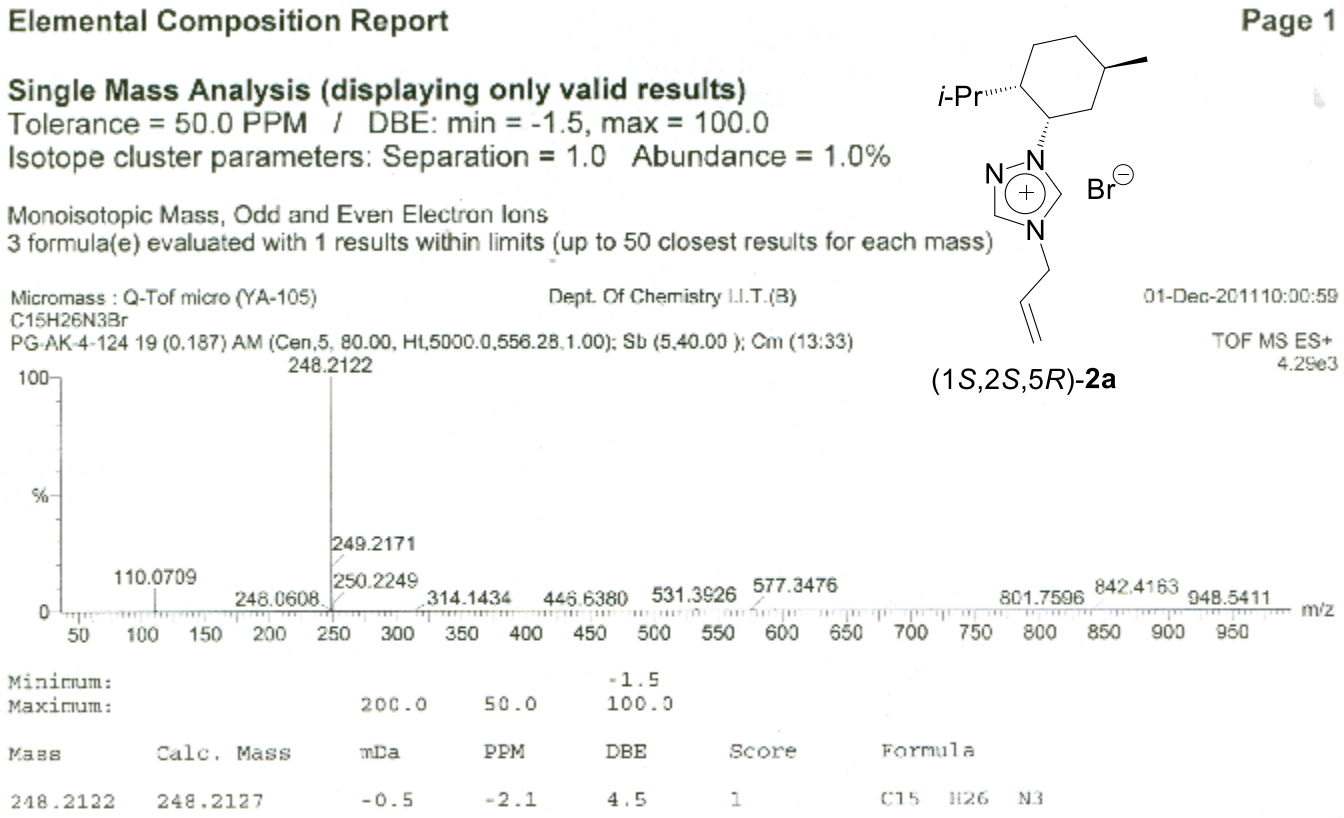
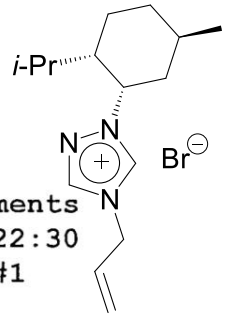


Figure S22. High Resolution Mass Spectrometry (HRMS) data of 1*S*,2*S*,5*R*-**2a**.

Eager 300 Report

Page: 1 Sample: PG-AK-7-192 (PG-AK-7-192)



(1*S*,2*S*,5*R*)-**2a**

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Method File	: D:\CHNS2012-13\SP-190813.mth		
Chromatogram	: PG-AK-7-192		
Operator ID	: MNRAO	Company Name	: C.E. Instruments
Analysed	: 08/19/2013 14:14	Printed	: 8/19/2013 22:30
Sample ID	: PG-AK-7-192 (# 18)	Instrument N.	: Instrument #1
Analysis Type	: UnkNown (Area)	Sample weight	: .671

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
1	0.0000	18	3652	RS		0.0000
Nitrogen	12.6831	43	112844	FU	8.757821	.132596E+07
Carbon	54.9056	66	988271	FU	1.000000	.267626E+07
Hydrogen	7.3224	178	306922	RS	3.219941	.604146E+07
Totals	74.9112		1411689			

Figure S23. Elemental analysis data of 1*S*,2*S*,5*R*-**2a**.

PG-AK-7-192.p1d

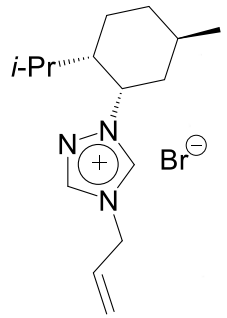
[Comment]
Sample name
Comment
User
Division
Company IITB

[Data Information]
Creation Date 8/1/2013 1 08 PM

[Measurement Information]
Instrument Name JASCO POLARIMETER
Model Name P-2000
Serial No A043361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-203
Accessory S/N A017861234
Path Length 100 mm

Light Source Na
Monitor wavelength 589 nm
D I T 5 sec
No of cycle 5
Cycle interval 5 sec
Temp Monitor Cell
Temp Corr Factor None
Aperture(S) 3 0mm
Aperture(L) Auto
Mode Specific O R
Path Length 100 mm
Concentration 1 w/v
Factor 1



(1*S*,2*S*,5*R*)-**2a**

No	Sample Name	Measurement Date	Temperature[C]	Optical Rotation Monitor	Specific O R	S D	C V	Comment
1	PG-AK-7-192			0 22	21 7280	0 0901	0 4147	CHCl3
2	PG-AK-7-192-1	8/1/2013 1 07 PM	25 00	0 22	21 6800			
3	PG-AK-7-192-2	8/1/2013 1 07 PM	25 00	0 22	21 8400			
4	PG-AK-7-192-3	8/1/2013 1 07 PM	25 00	0 22	21 7000			
5	PG-AK-7-192-4	8/1/2013 1 07 PM	25 00	0 22	21 8000			
6	PG-AK-7-192-5	8/1/2013 1 08 PM	24 99	0 22	21 6200			

Figure S24. Specific rotation of 1*S*,2*S*,5*R*-**2a** in $CHCl_3$.

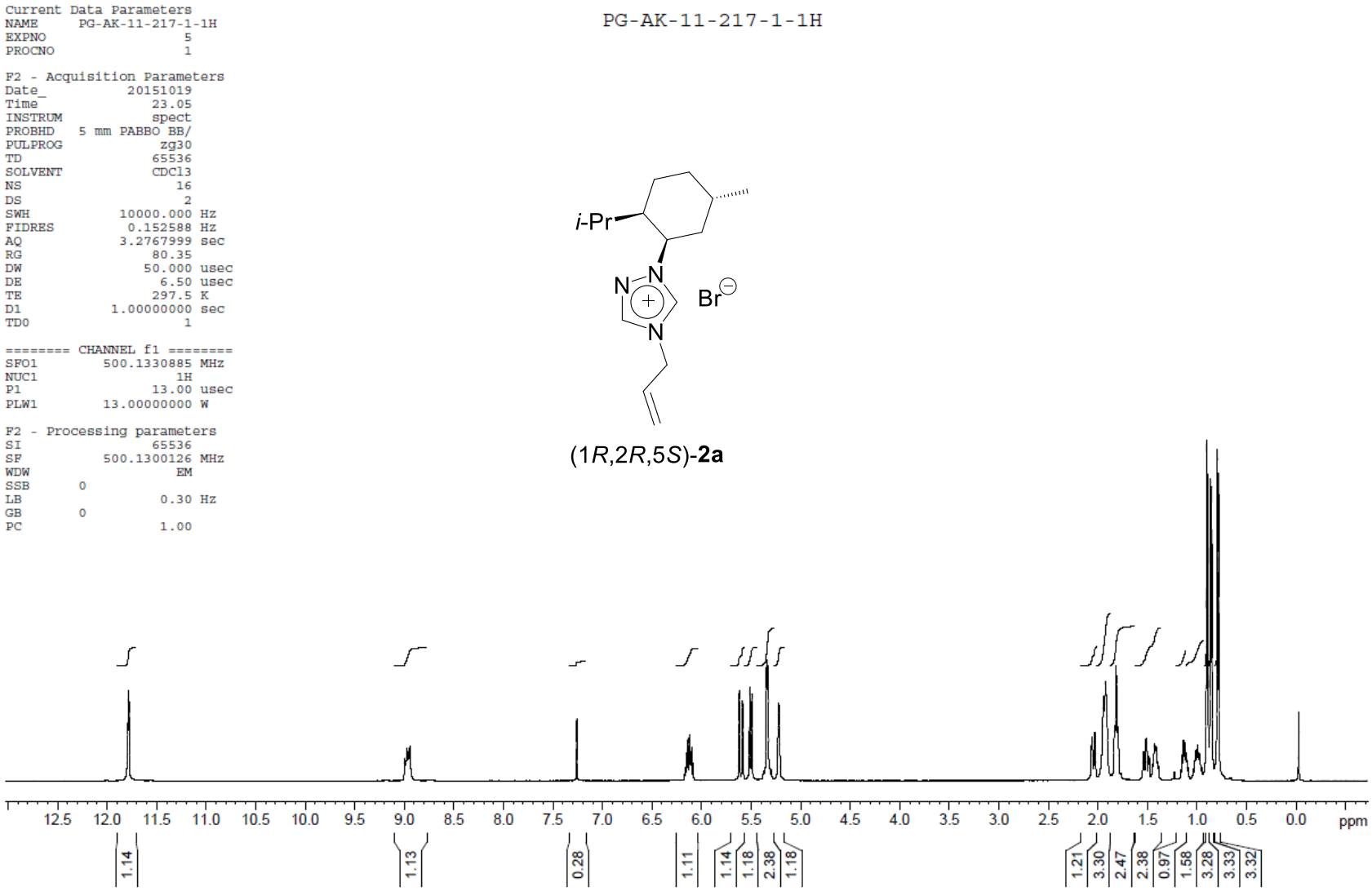


Figure S25. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**2a** in $CDCl_3$.

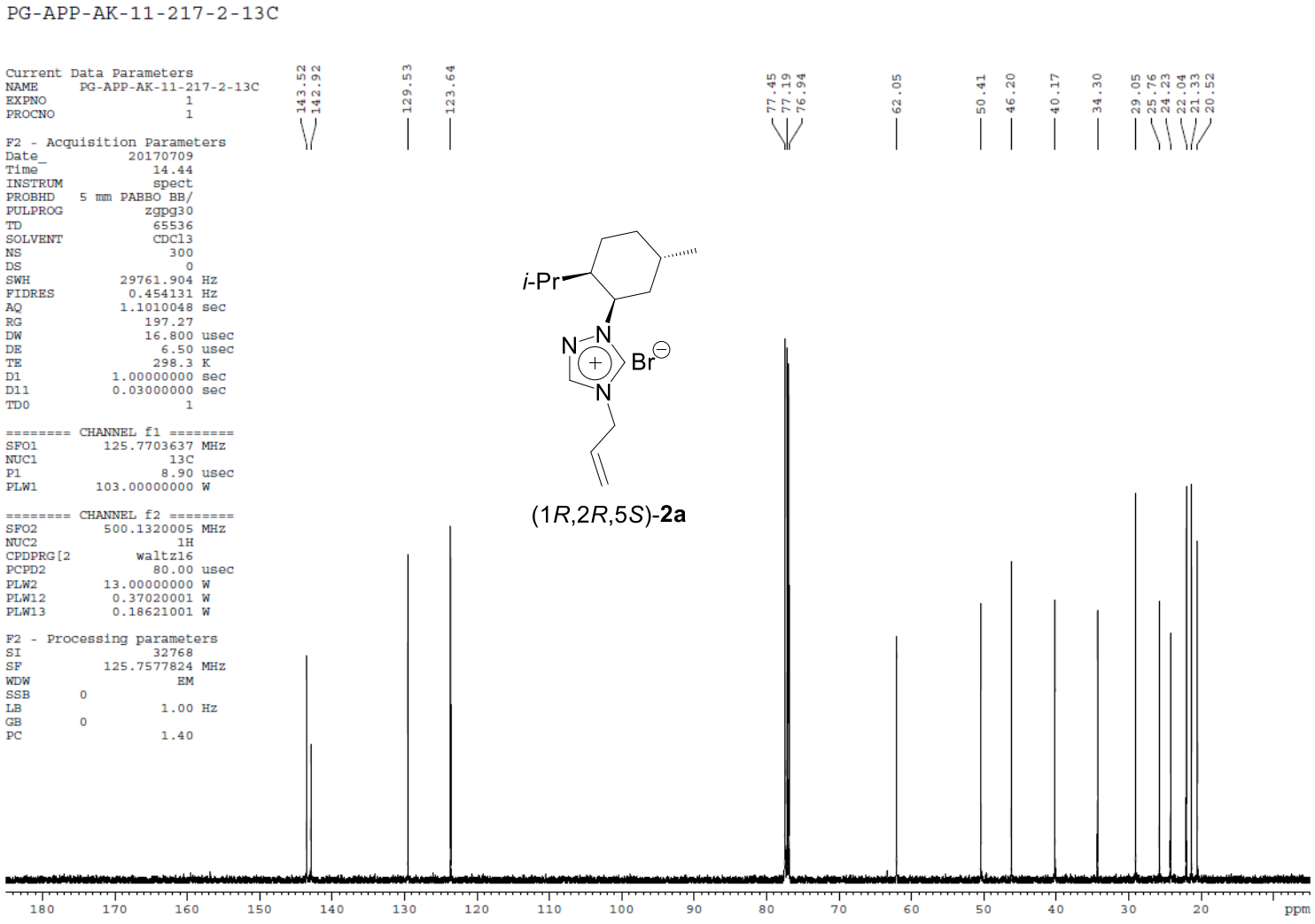


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of 1*R*,2*R*,5*S*-**2a** in $CDCl_3$.

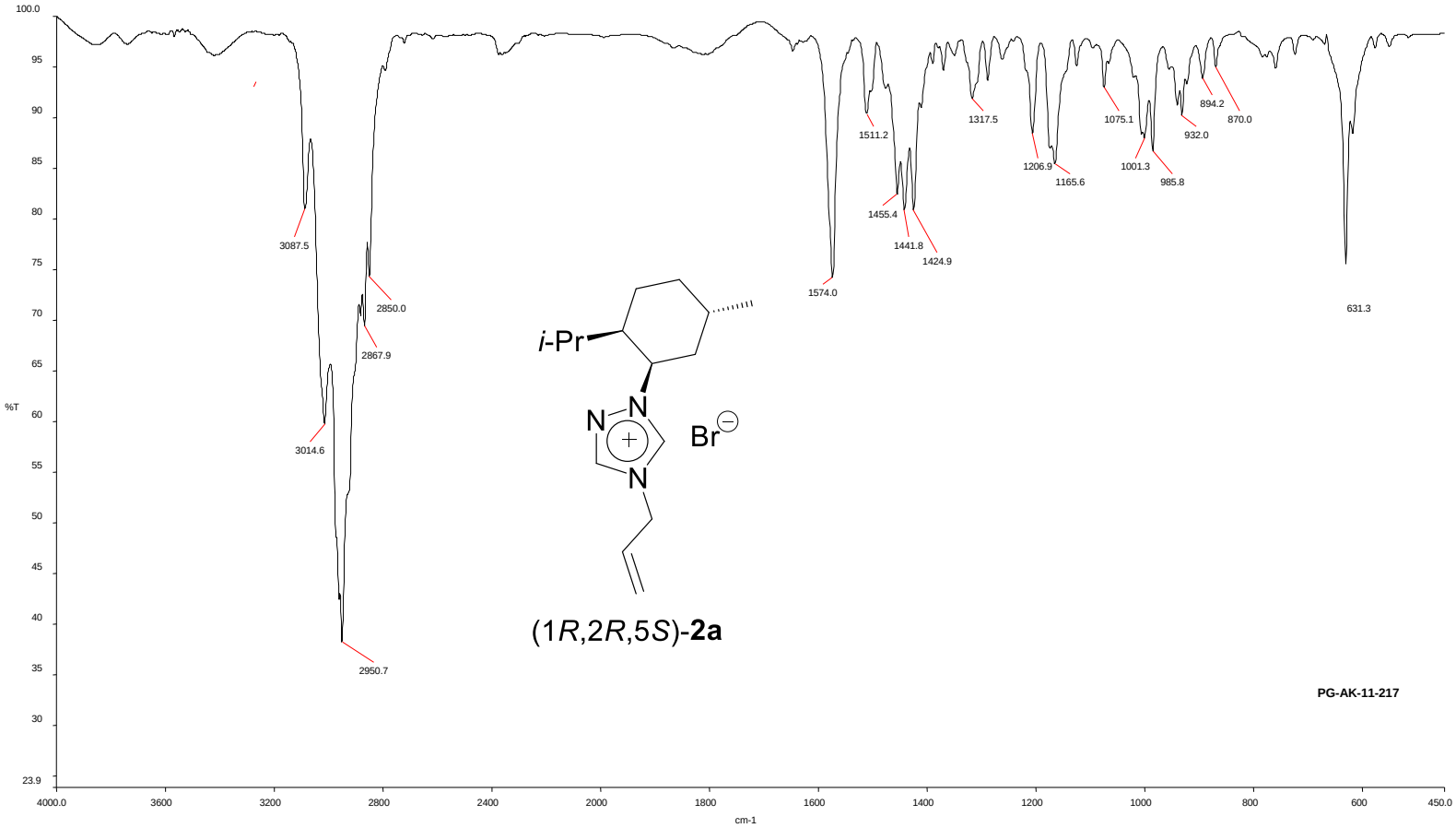


Figure S27. Infrared spectrum of 1*R*,2*R*,5*S*-**2a** in KBr.

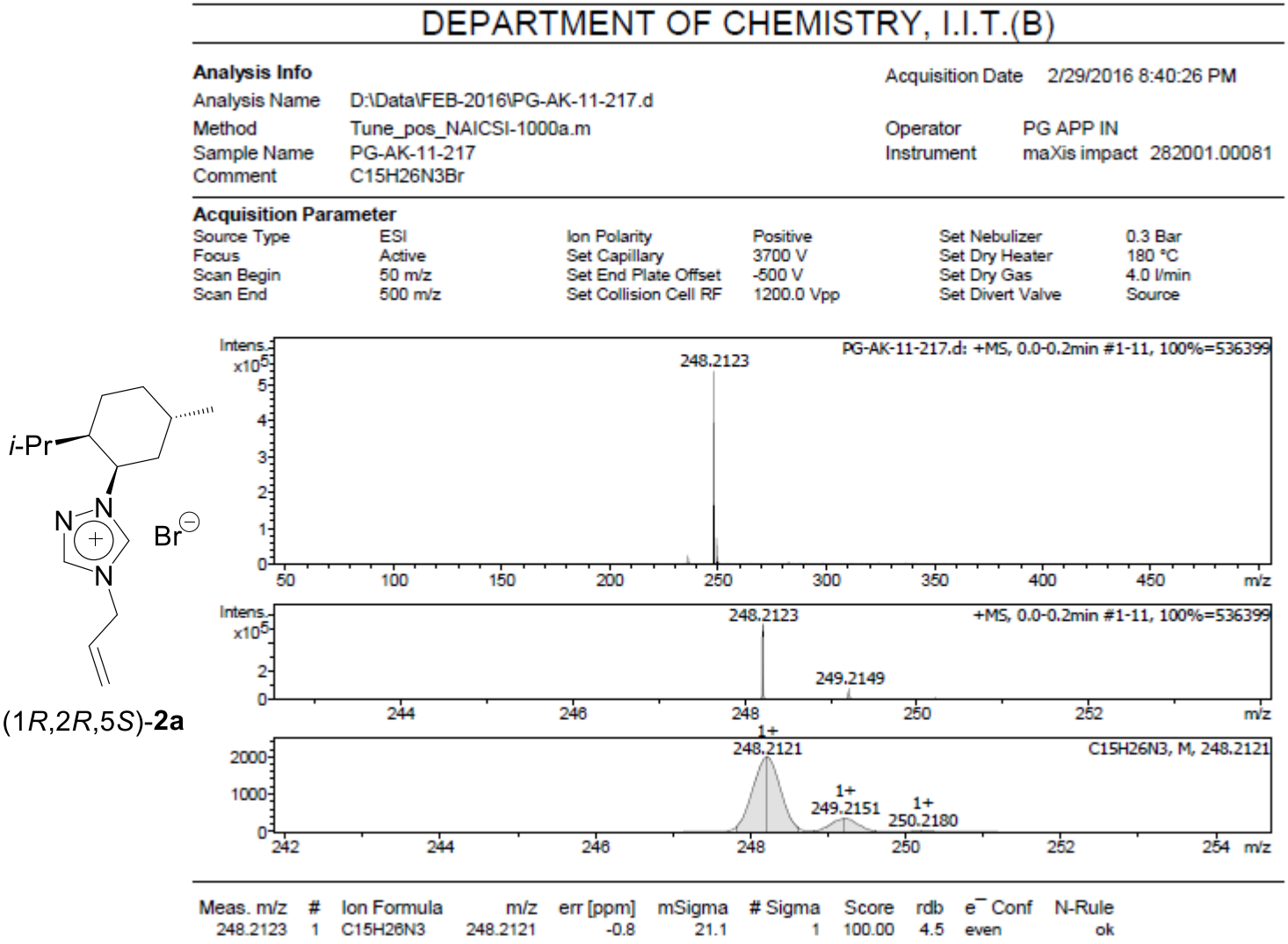
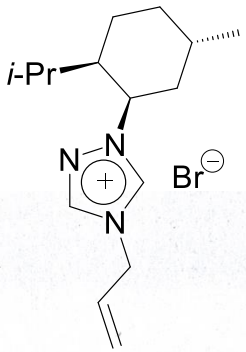


Figure S28. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**2a**.



(1*R*,2*R*,5*S*)-**2a**

Eager 300 Report

Page: 1 Sample: PG-AK-11-217-1 (PG-AK-11-217-1)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-217-1
Operator ID : CHANDNI
Analysed : 10/13/2015 14:19
Sample ID : PG-AK-11-217-1 (# 19)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/13/2015 18:36
Instrument N. : Instrument #1
Sample weight : .566

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	13.0268	41	79848	RS	10.189700	.108295E+07
Carbon	54.9502	64	813622	RS	1.000000	.260680E+07
Hydrogen	7.3945	175	293284	RS	2.774178	.665180E+07
Totals	75.3715		1186754			

Figure S29. Elemental analysis data of (1*R*,2*R*,5*S*)-**2a**.

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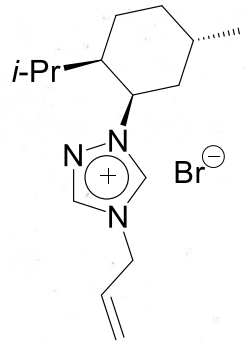
Monday, 12-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**2a**

n	Average	Std.Dev.	Maximum	Minimum
5	-21.599	0.0000	-21.599	-21.599

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-217-1	12:51:46	-21.599	SR	-0.108	589	50	1	24.9
2	pg-ak-11-217-1	12:51:53	-21.599	SR	-0.108	589	50	1	24.9
3	pg-ak-11-217-1	12:52:00	-21.599	SR	-0.108	589	50	1	24.9
4	pg-ak-11-217-1	12:52:07	-21.599	SR	-0.108	589	50	1	24.9
5	pg-ak-11-217-1	12:52:13	-21.599	SR	-0.108	589	50	1	24.9

Figure S30. Specific rotation of (1*R*,2*R*,5*S*)-**2a** in $CHCl_3$.

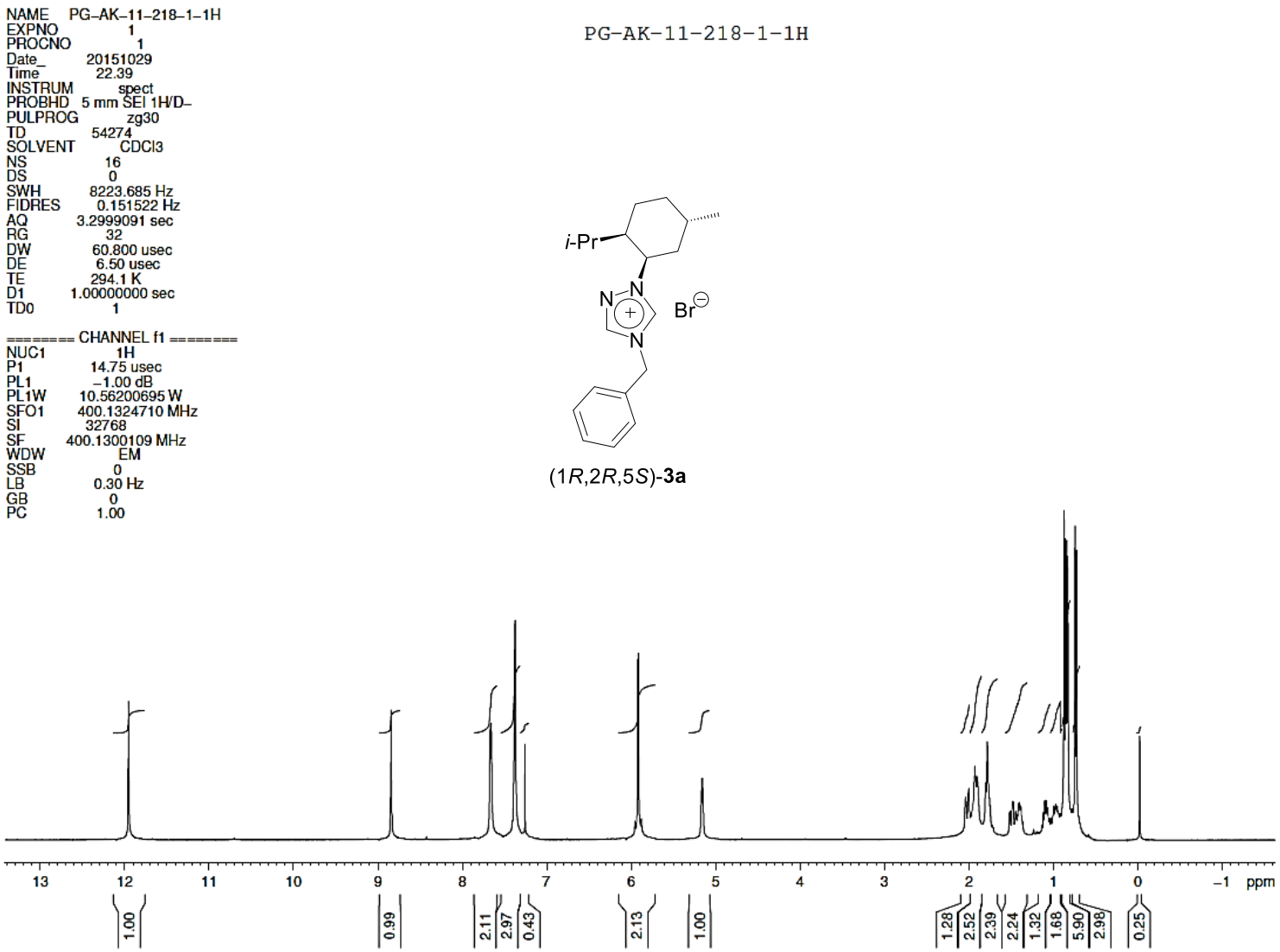


Figure S31. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**3a** in $CDCl_3$.

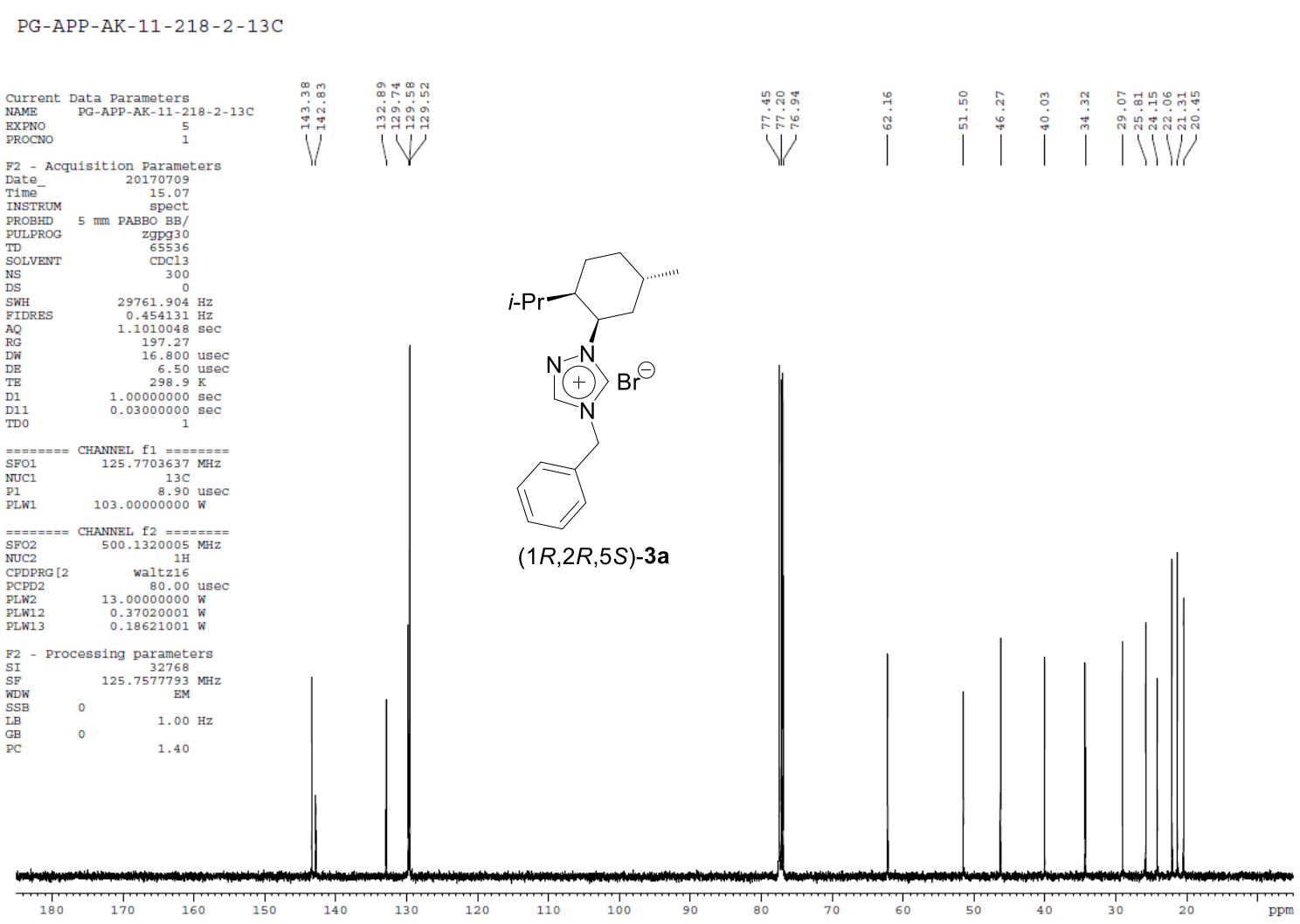


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**3a** in $CDCl_3$.

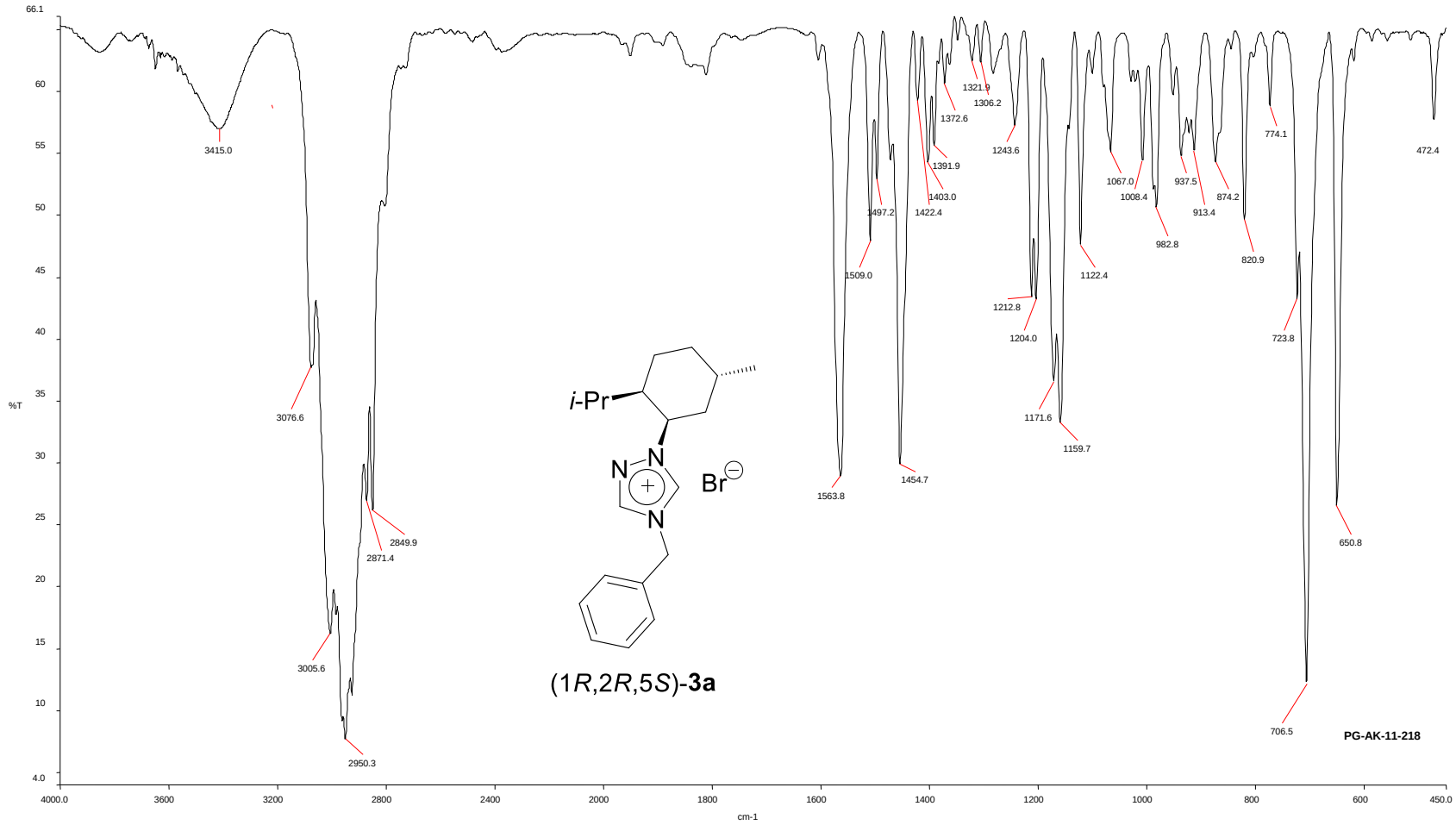


Figure S33. Infrared spectrum of 1*R*,2*R*,5*S*-**3a** in KBr.

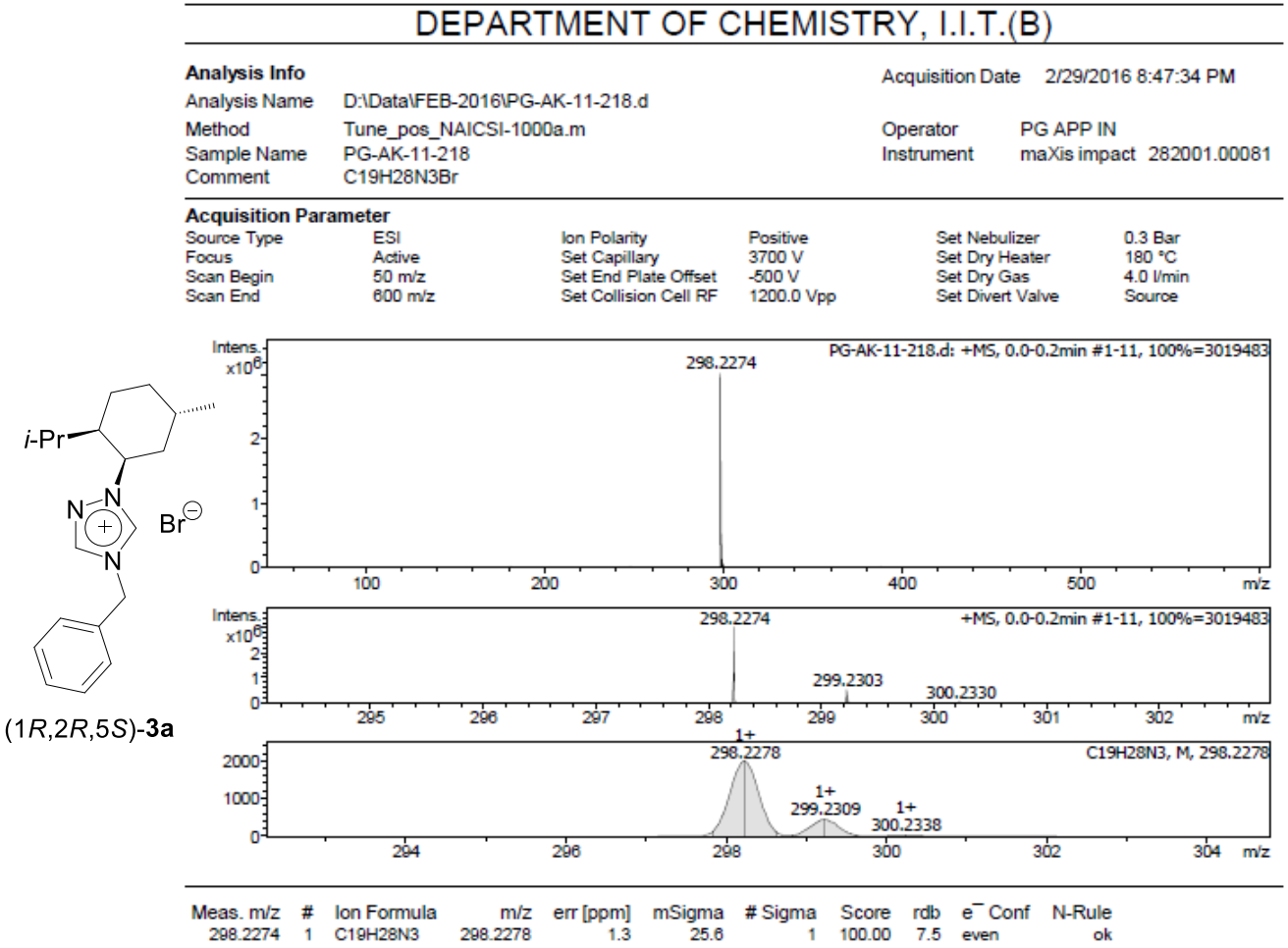
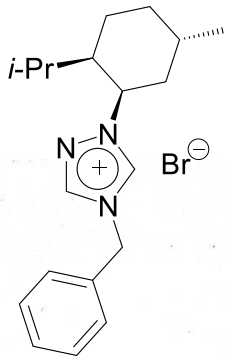


Figure S34. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**3a**.



(1*R*,2*R*,5*S*)-**3a**

Eager 300 Report

Page: 1 Sample: PG-AK-11-218-1 (PG-AK-11-218-1)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-218-1
Operator ID : CHANDNI
Analysed : 10/13/2015 15:18
Sample ID : PG-AK-11-218-1 (# 21)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 10/13/2015 18:36
Instrument N. : Instrument #1
Sample weight : .815

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.2482	41	99276	FU	12.849350	.108295E+07
Carbon	59.9083	64	1275636	FU	1.000000	.260680E+07
Hydrogen	6.6576	178	375811	RS	3.394355	.665180E+07
Totals	77.8141		1750723			

Figure S35. Elemental analysis data of (1*R*,2*R*,5*S*)-**3a**.

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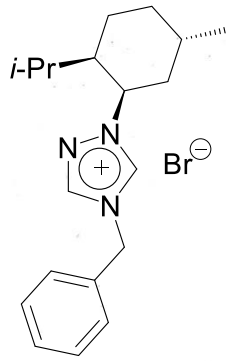
Monday, 12-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**3a**

n	Average	Std.Dev.	Maximum	Minimum
5	-16.174	0.0827	-16.083	-16.234

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-218-1	12:57:21	-16.083	SR	-0.080	589	50	1	24.8
2	pg-ak-11-218-1	12:57:28	-16.083	SR	-0.080	589	50	1	24.8
3	pg-ak-11-218-1	12:57:35	-16.234	SR	-0.081	589	50	1	24.8
4	pg-ak-11-218-1	12:57:41	-16.234	SR	-0.081	589	50	1	24.8
5	pg-ak-11-218-1	12:57:48	-16.234	SR	-0.081	589	50	1	24.9

Figure S36. Specific rotation of (1*R*,2*R*,5*S*)-**3a** in $CHCl_3$.

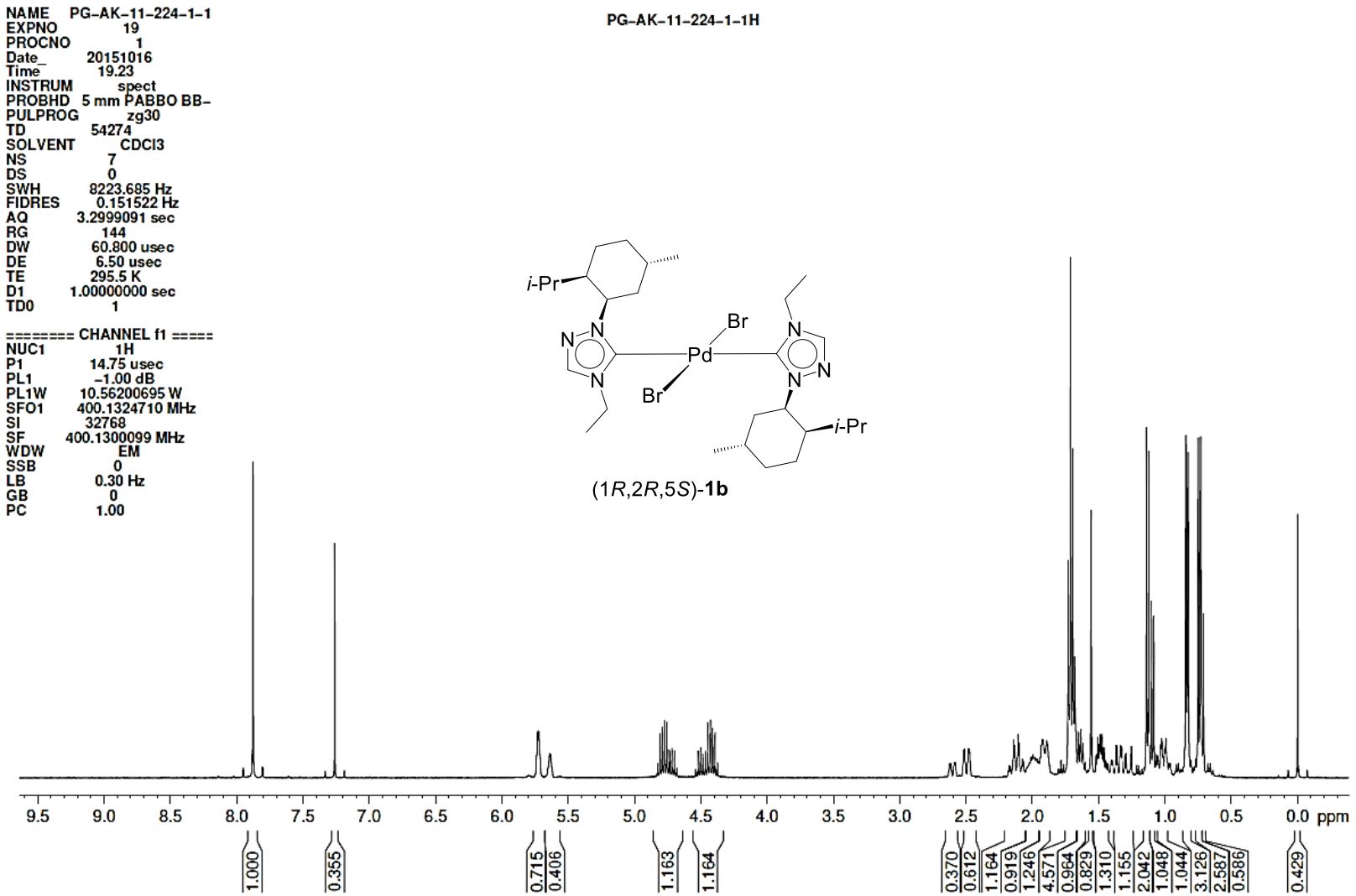


Figure S37. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**1b** in $CDCl_3$.

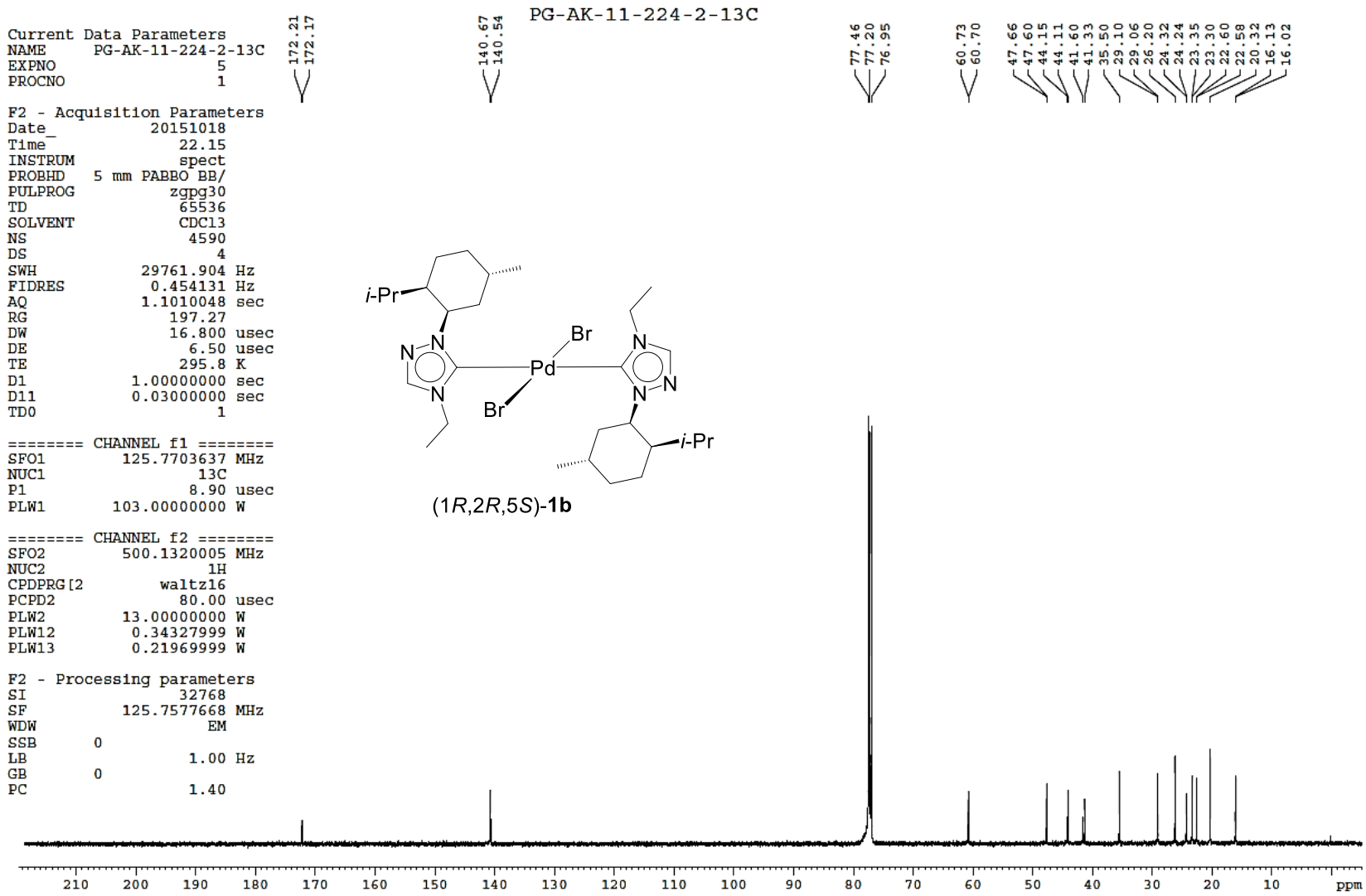


Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**1b** in $CDCl_3$.

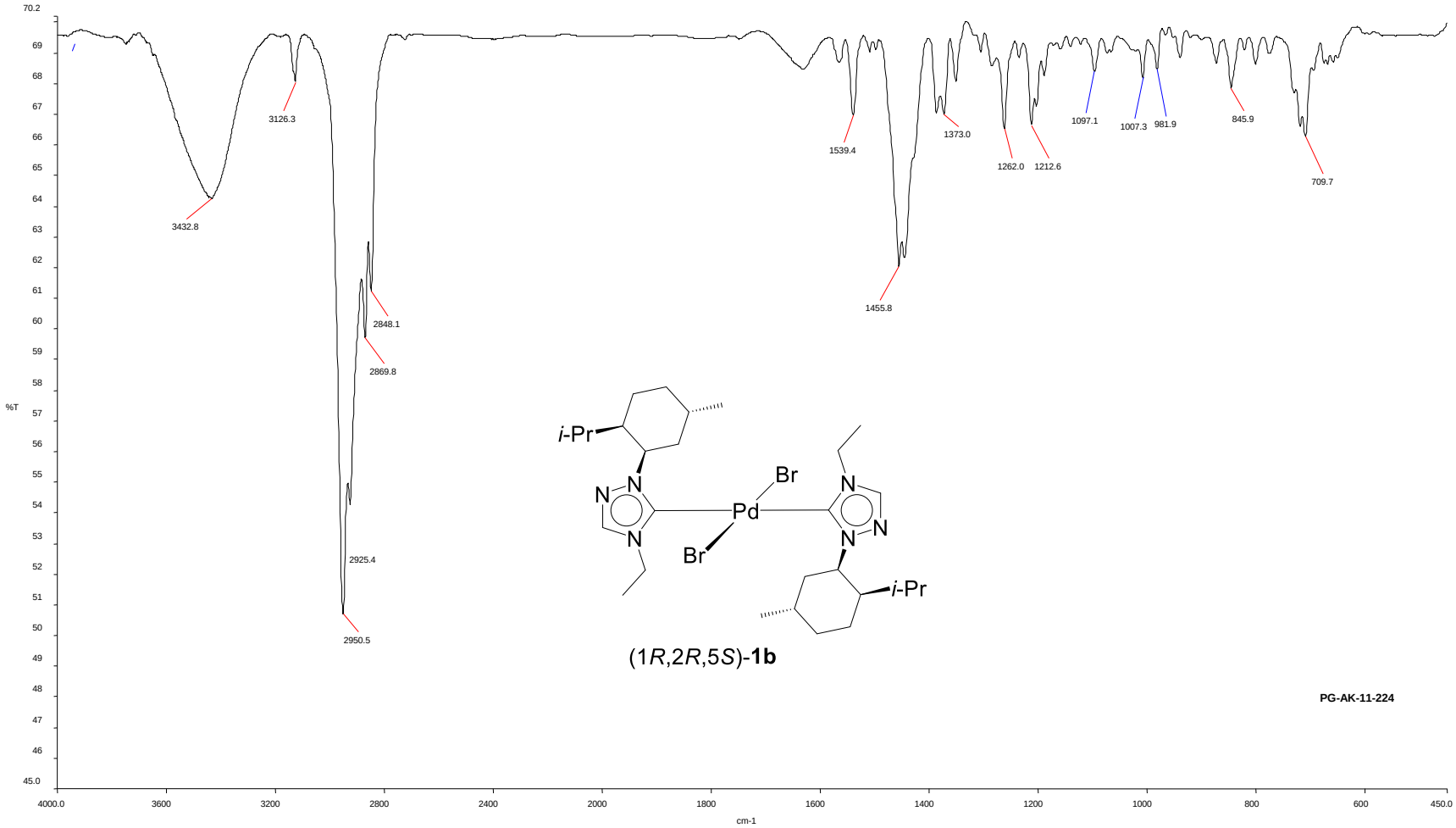


Figure S39. Infrared spectrum of 1*R*,2*R*,5*S*-**1b** in KBr.

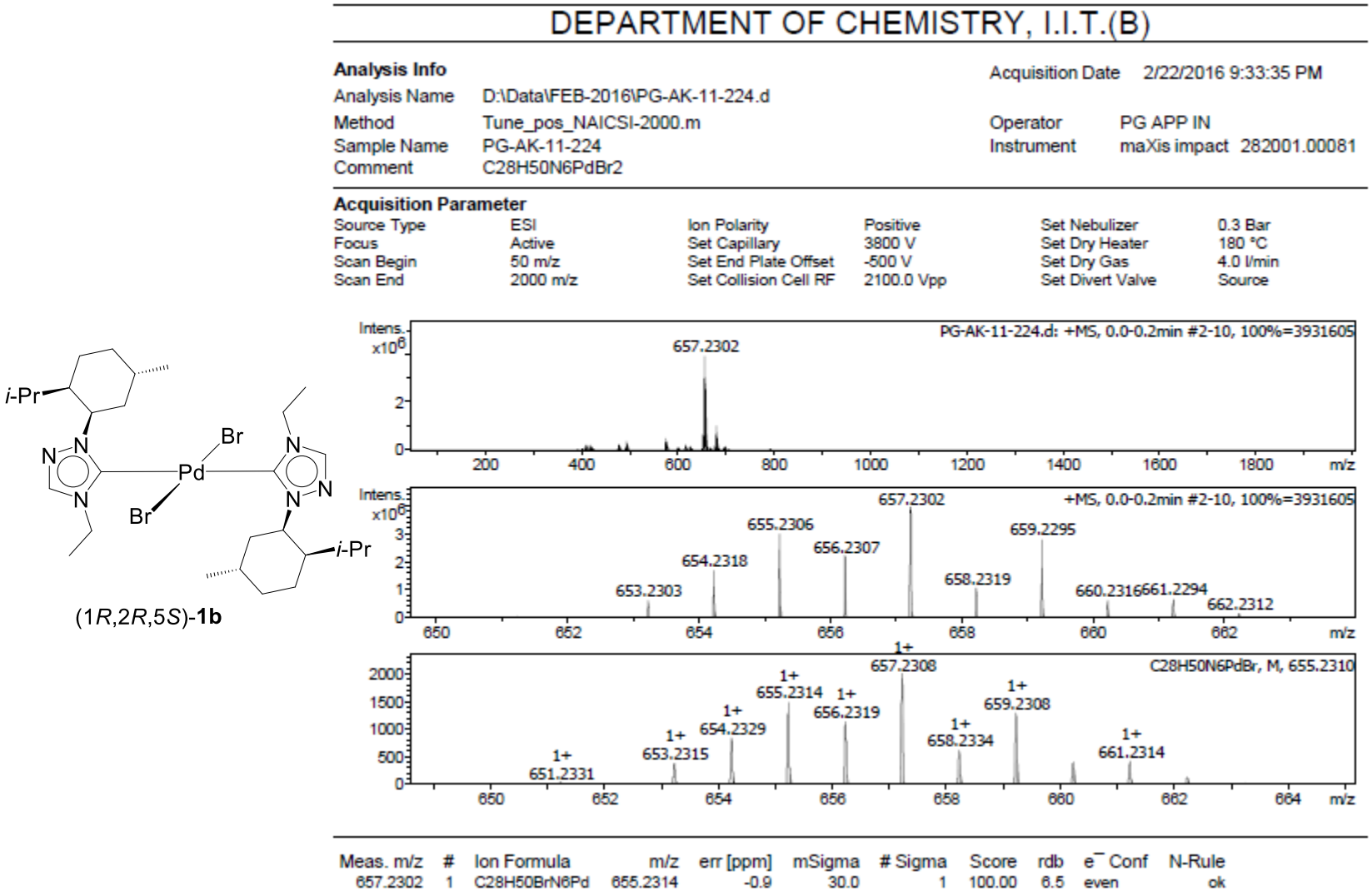
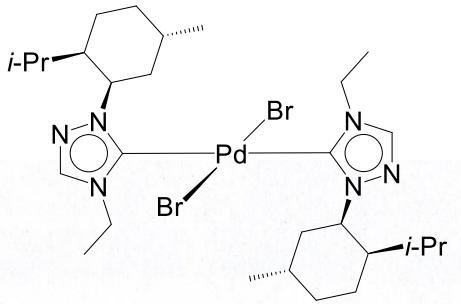


Figure S40. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**1b**.



(1*R*,2*R*,5*S*)-**1b**

Eager 300 Report

Page: 1 Sample: PG-AK-11-224-1 (PG-AK-11-224-1)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-224-1
Operator ID : CHANDNI Company Name : C.E. Instruments
Analysed : 10/13/2015 12:46 Printed : 10/13/2015 18:36
Sample ID : PG-AK-11-224-1 (# 10) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .677

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.6158	41	85162	RS	9.577969	.108295E+07
Carbon	46.0572	65	815679	RS	1.000000	.260680E+07
Hydrogen	6.4525	175	305461	RS	2.670321	.665180E+07
Totals	64.1256		1206302			

Figure S41. Elemental analysis data of (1*R*,2*R*,5*S*)-**1b**.

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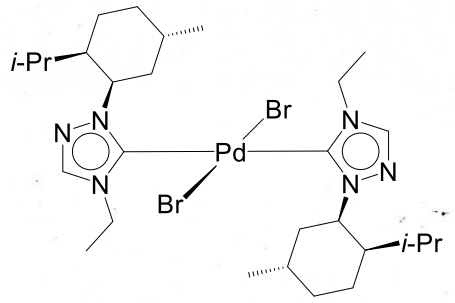
Monday, 12-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**1b**

n	Average	Std.Dev.	Maximum	Minimum
5	29.857	0.0680	29.887	29.735

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-224-2	12:03:38	29.735	SR	0.149	589	50	1	24.9
2	pg-ak-11-224-2	12:03:44	29.887	SR	0.149	589	50	1	24.9
3	pg-ak-11-224-2	12:03:51	29.887	SR	0.149	589	50	1	25.0
4	pg-ak-11-224-2	12:03:58	29.887	SR	0.149	589	50	1	25.0
5	pg-ak-11-224-2	12:04:05	29.887	SR	0.149	589	50	1	25.0

Figure S42. Specific rotation of (1*R*,2*R*,5*S*)-**1b** in $CHCl_3$.

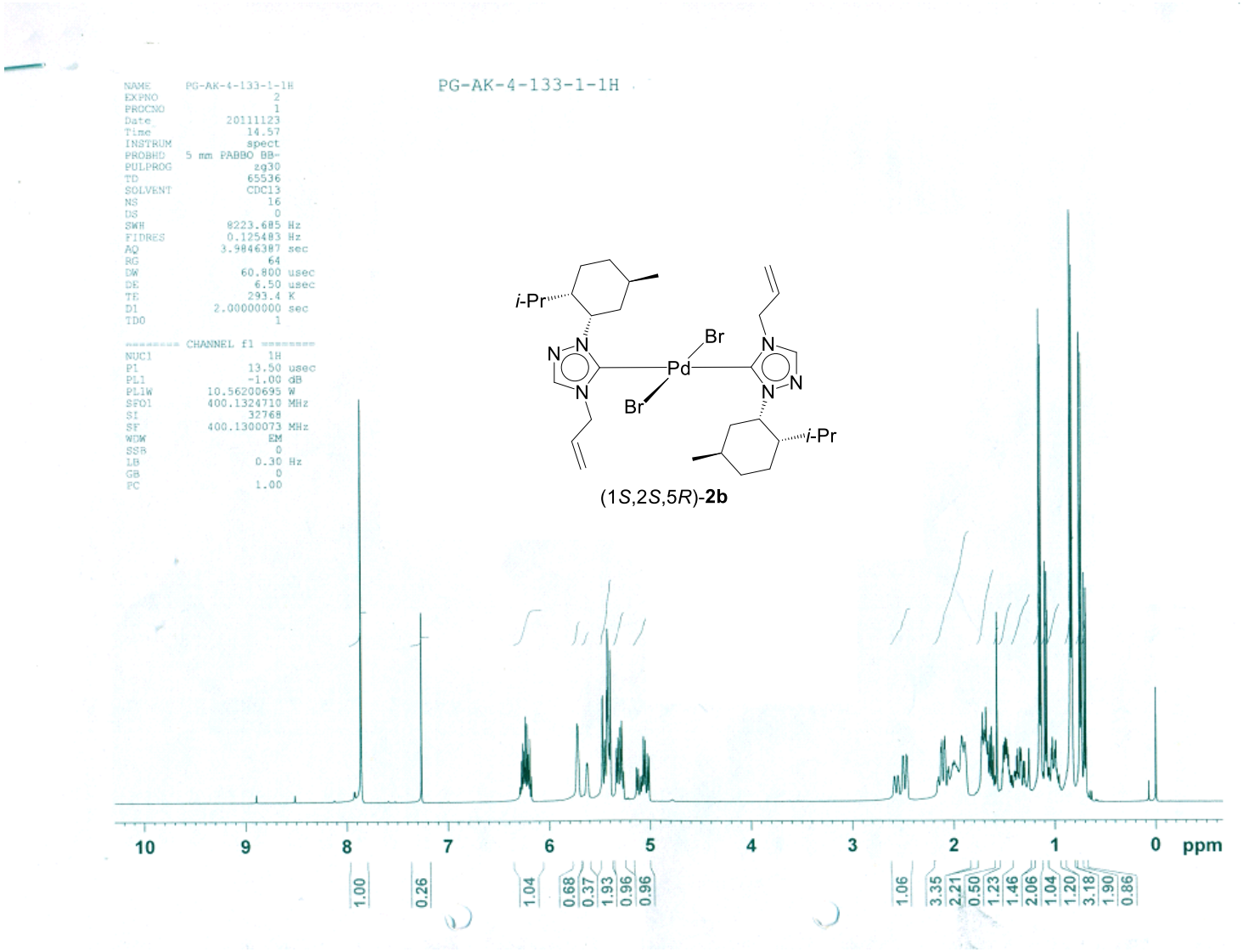


Figure S43. ^{1}H NMR spectrum of 1*S*,2*S*,5*R*-**2b** in $CDCl_3$.

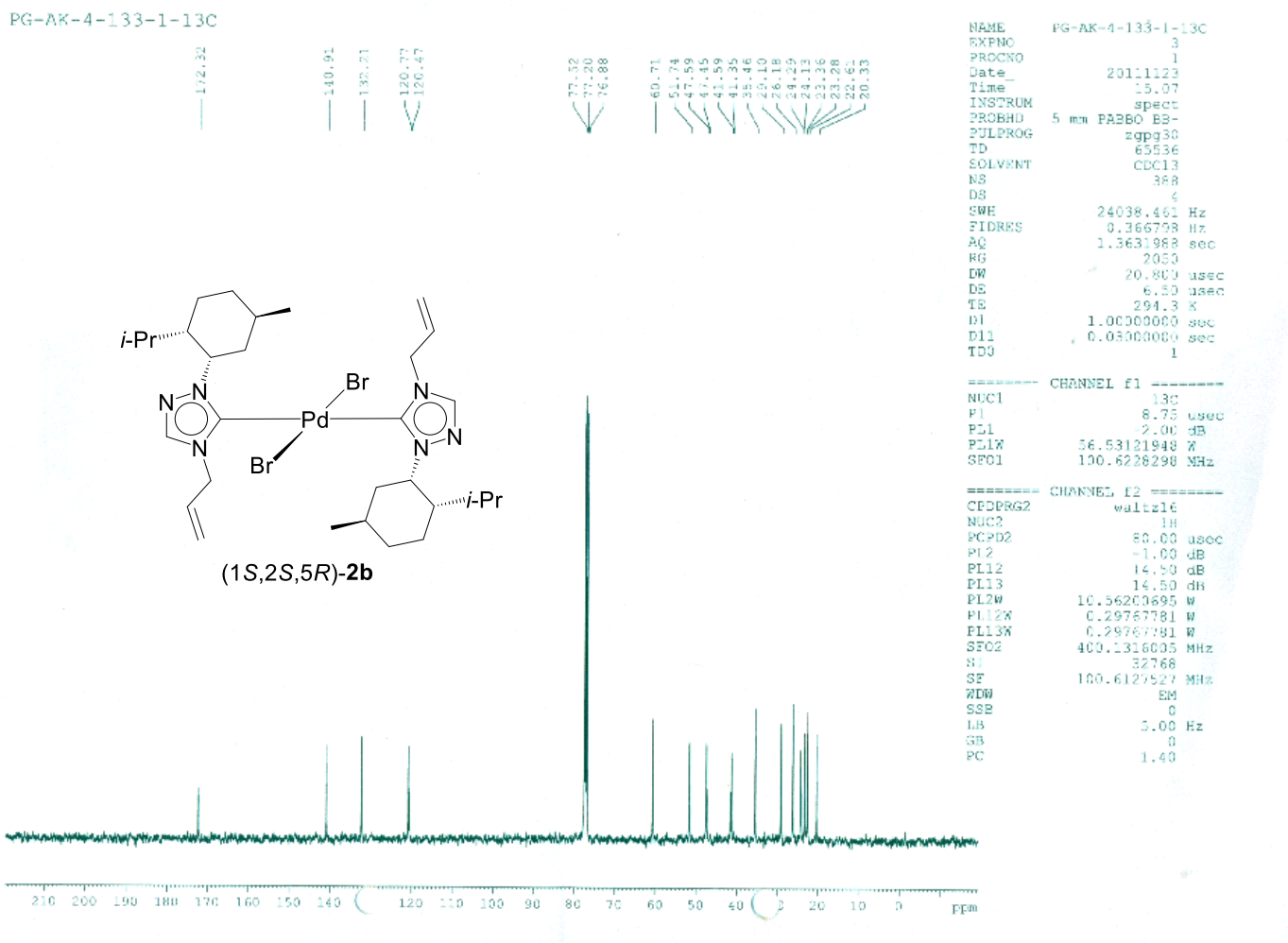


Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**2b** in $CDCl_3$.

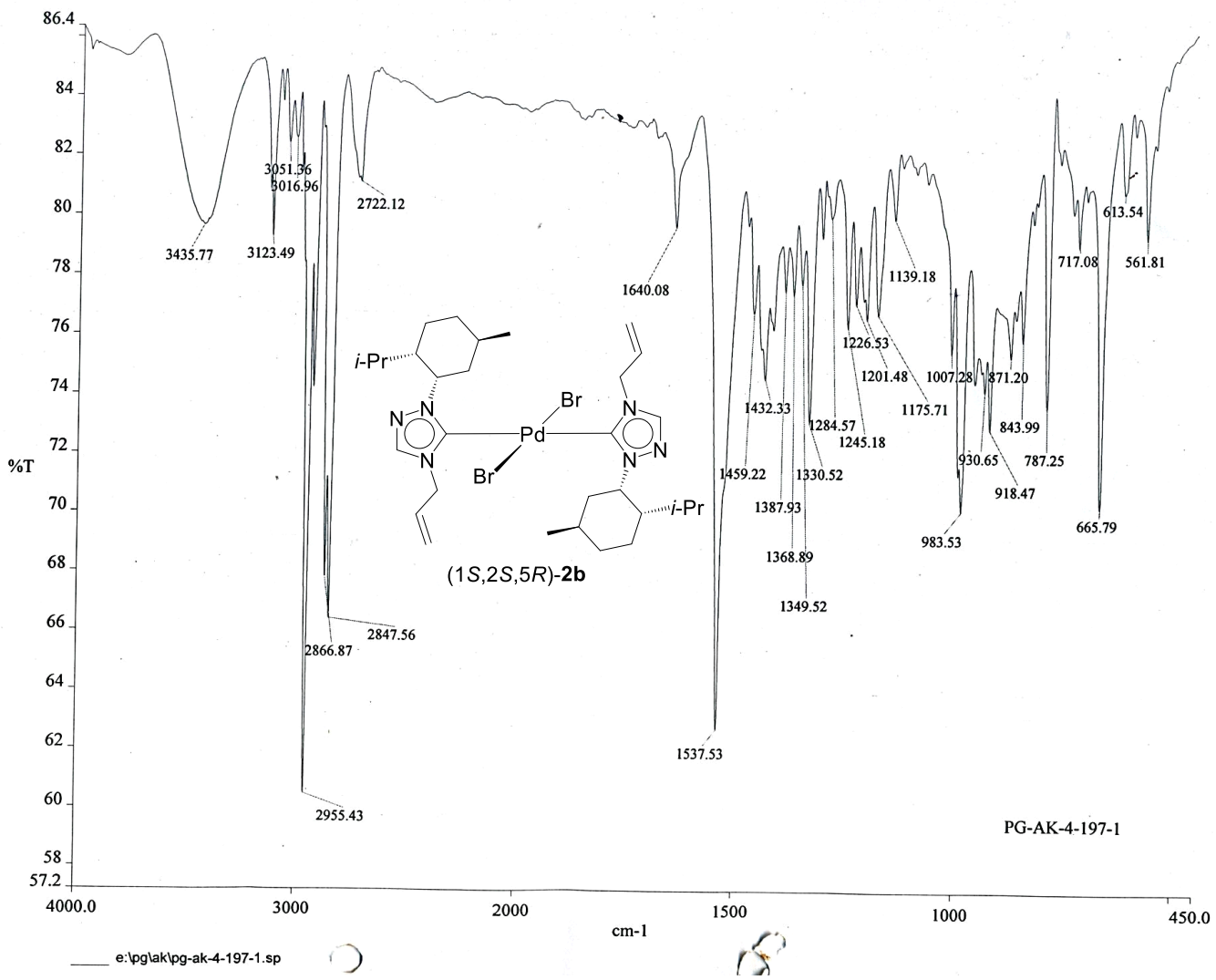


Figure S45. Infrared spectrum of 1*S*,2*S*,5*R*-**2b** in KBr.

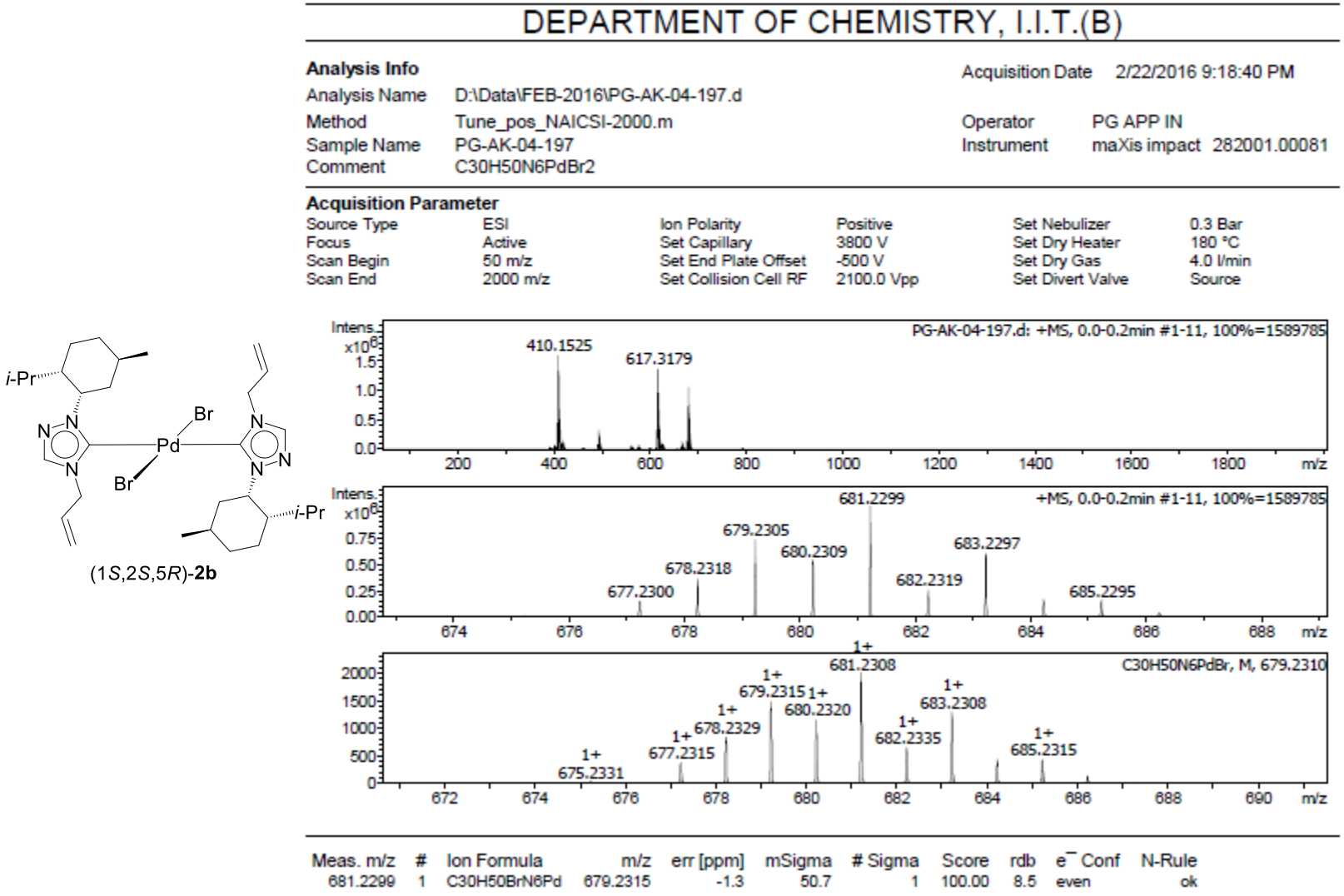
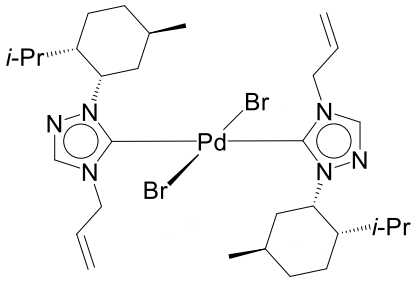


Figure S46. High Resolution Mass Spectrometry (HRMS) data of 1*S*,2*S*,5*R*-**2b**.



(1*S*,2*S*,5*R*)-**2b**

Eager 300 Report

Page: 1 Sample: PG-AK-4-197-2 (PG-AK-4-197-2)

Method Name	: SP-050312		
Method File	: D:\CHNS2012\SP-050312.mth		
Chromatogram	: PG-AK-4-197-2		
Operator ID	: MNRAO	Company Name	: C.E. Instruments
Analysed	: 03/05/2012 18:24	Printed	: 3/5/2012 19:58
Sample ID	: PG-AK-4-197-2 (# 23)	Instrument N.	: Instrument #1
Analysis Type	: UnkNown (Area)	Sample weight	: .755

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.1258	44	113335	FU	8.001876	.134923E+07
Carbon	47.7199	68	906896	FU	1.000000	.251716E+07
Hydrogen	6.5555	178	283533	RS	3.198556	.572859E+07
Totals	65.4013		1303765			

Figure S47. Elemental analysis data of 1*S*,2*S*,5*R*-**2b**.

pg-ak-6-150-2 p1d

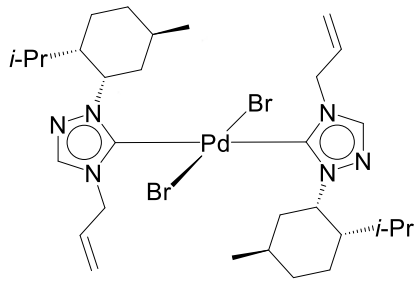
[Comment]
Sample name
Comment
User
Division
Company IITB

[Data Information]
Creation Date 6/10/2013 3 53 PM

[Measurement Information]
Instrument Name JASCO POLARIMETER
Model Name P-2000
Serial No A043361232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-203
Accessory S/N A017861234
Path Length 100 mm

Light Source Na
Monitor wavelength 589 nm
D I T 5 sec
No of cycle 5
Cycle interval 5 sec
Temp Monitor Cell
Temp Corr Factor None
Aperture(S) 3 0mm
Aperture(L) Auto
Mode Specific O R
Path Length 100 mm
Concentration 1 w/v
Factor 1



(1*S*,2*S*,5*R*)-**2b**

[Comment]
Sample name
Comment
User
Division
Company IITB

		No	Sample No	Mode	Calc Data	Meas Data	Temperature(C)	Comment
1	*	1	PG-AK-6-150-1	Specific O R	-41 6360	-0 4164	24 99	CHCl3
2	*	2	PG-AK-6-150-2	Specific O R	-41 7160	-0 4172	24 99	CHCl3
3	*	3	PG-AK-6-150-3	Specific O R	-41 7260	-0 4173	24 99	CHCl3
4	*	4	PG-AK-6-150-4	Specific O R	-41 4760	-0 4148	24 99	CHCl3
5	*	5	PG-AK-6-150-5	Specific O R	-41 8560	-0 4186	24 99	CHCl3
6	*	6	Avg		-41 6820			
7		7	S D		0 1396			
8		8	C V		0 3348			

Figure S48. Specific rotation of 1*S*,2*S*,5*R*-**2b** in $CHCl_3$.

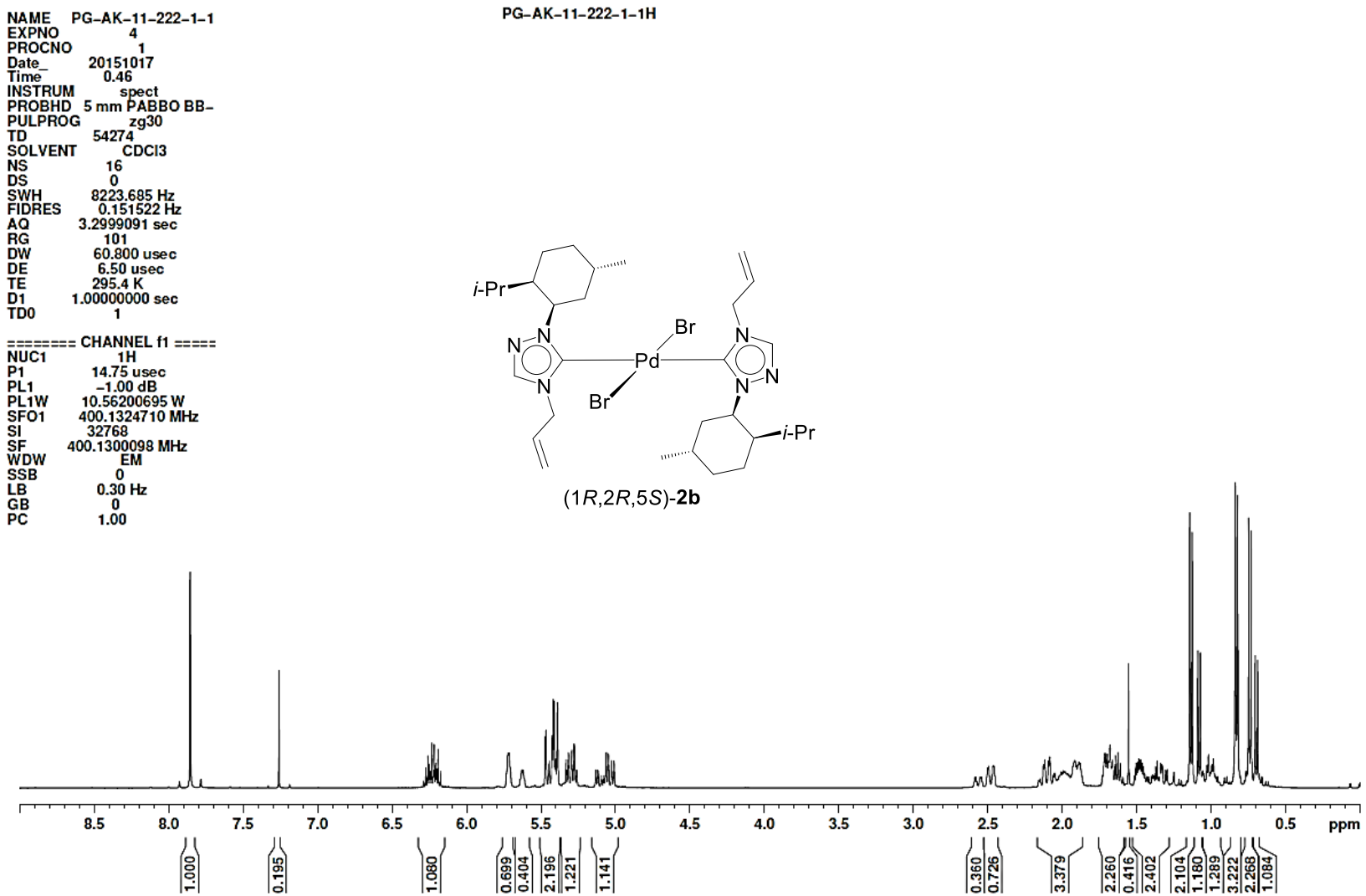


Figure S49. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**2b** in $CDCl_3$.

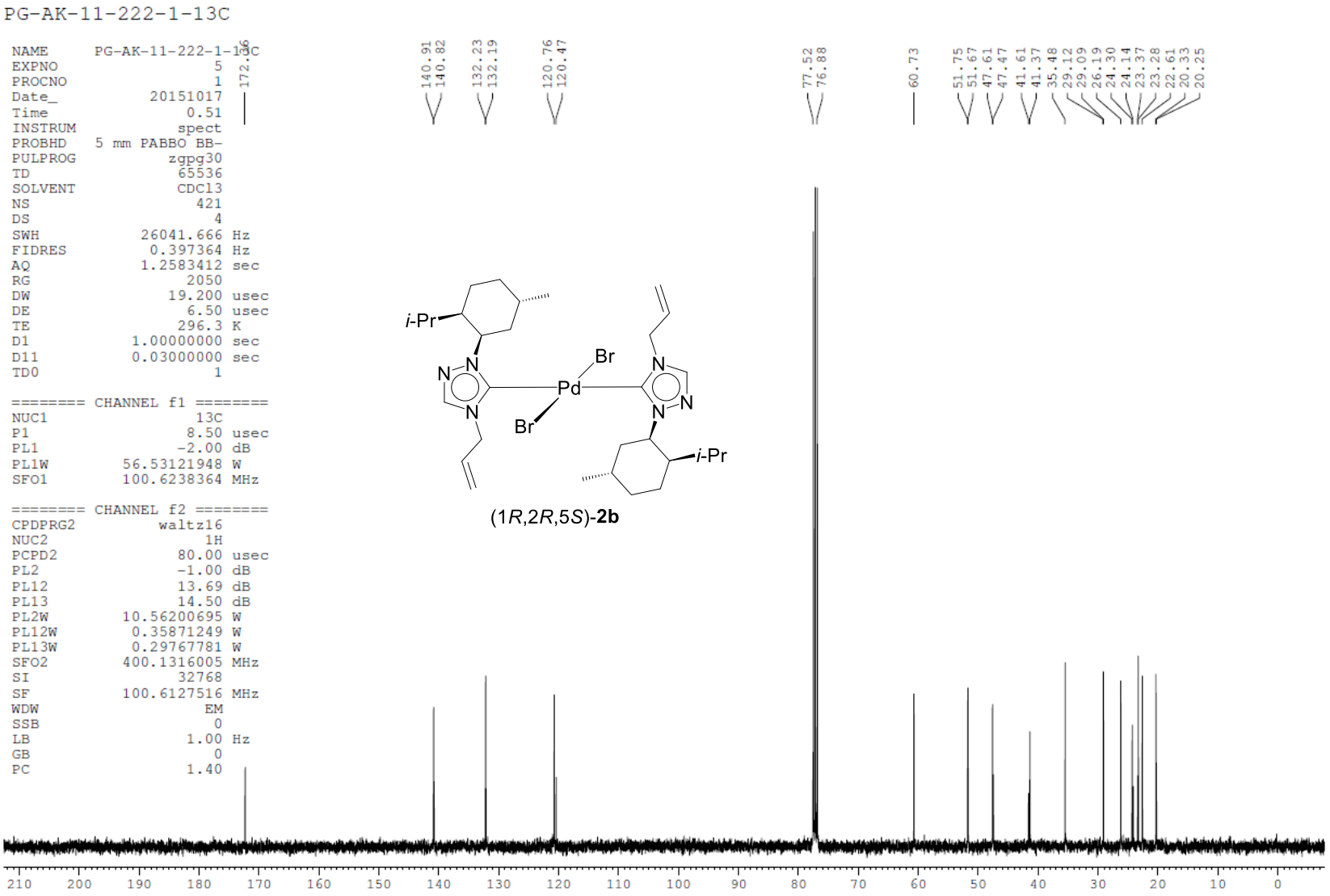


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**2b** in $CDCl_3$.

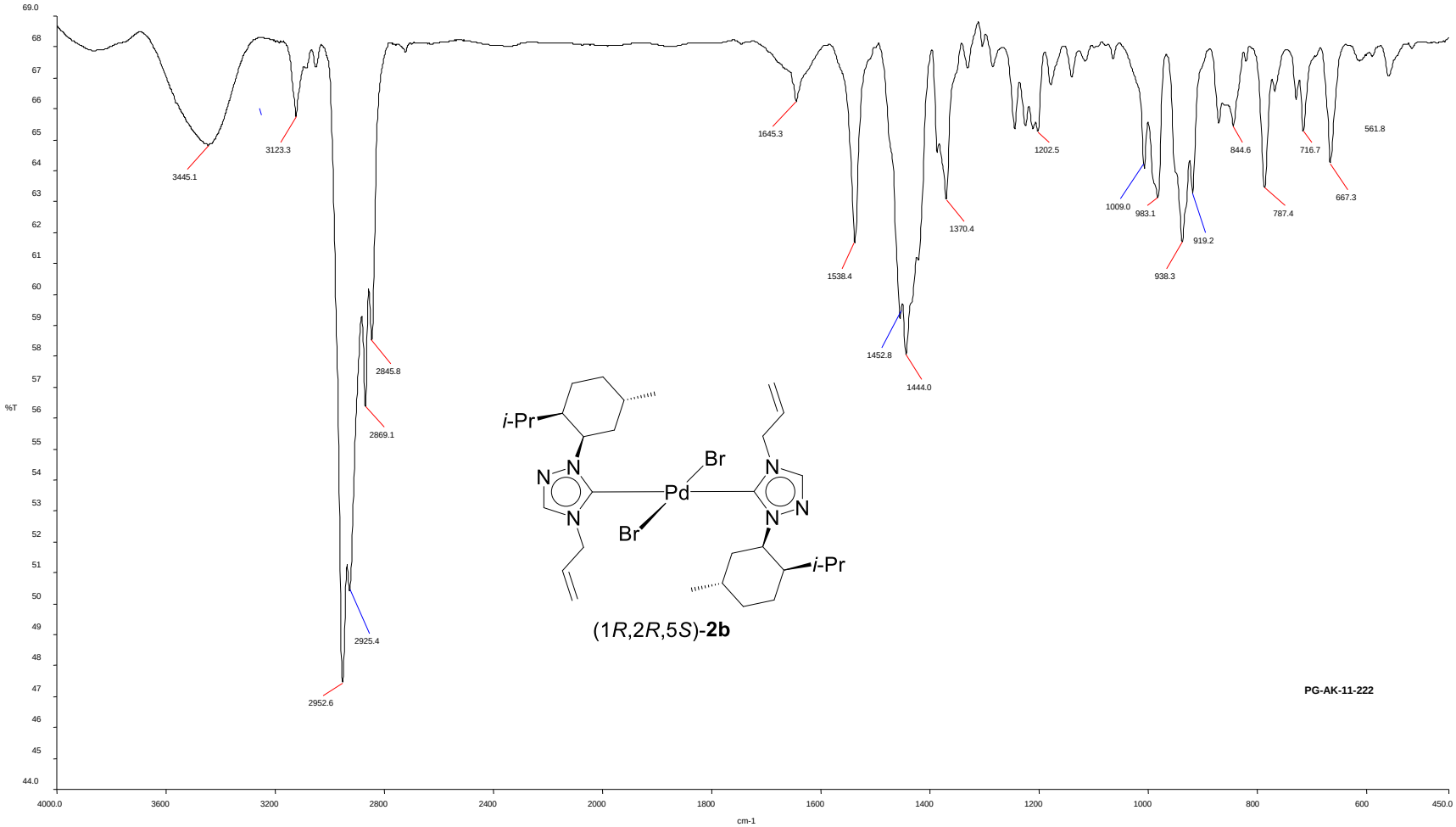


Figure S51. Infrared spectrum of 1*R*,2*R*,5*S*-**2b** in KBr.

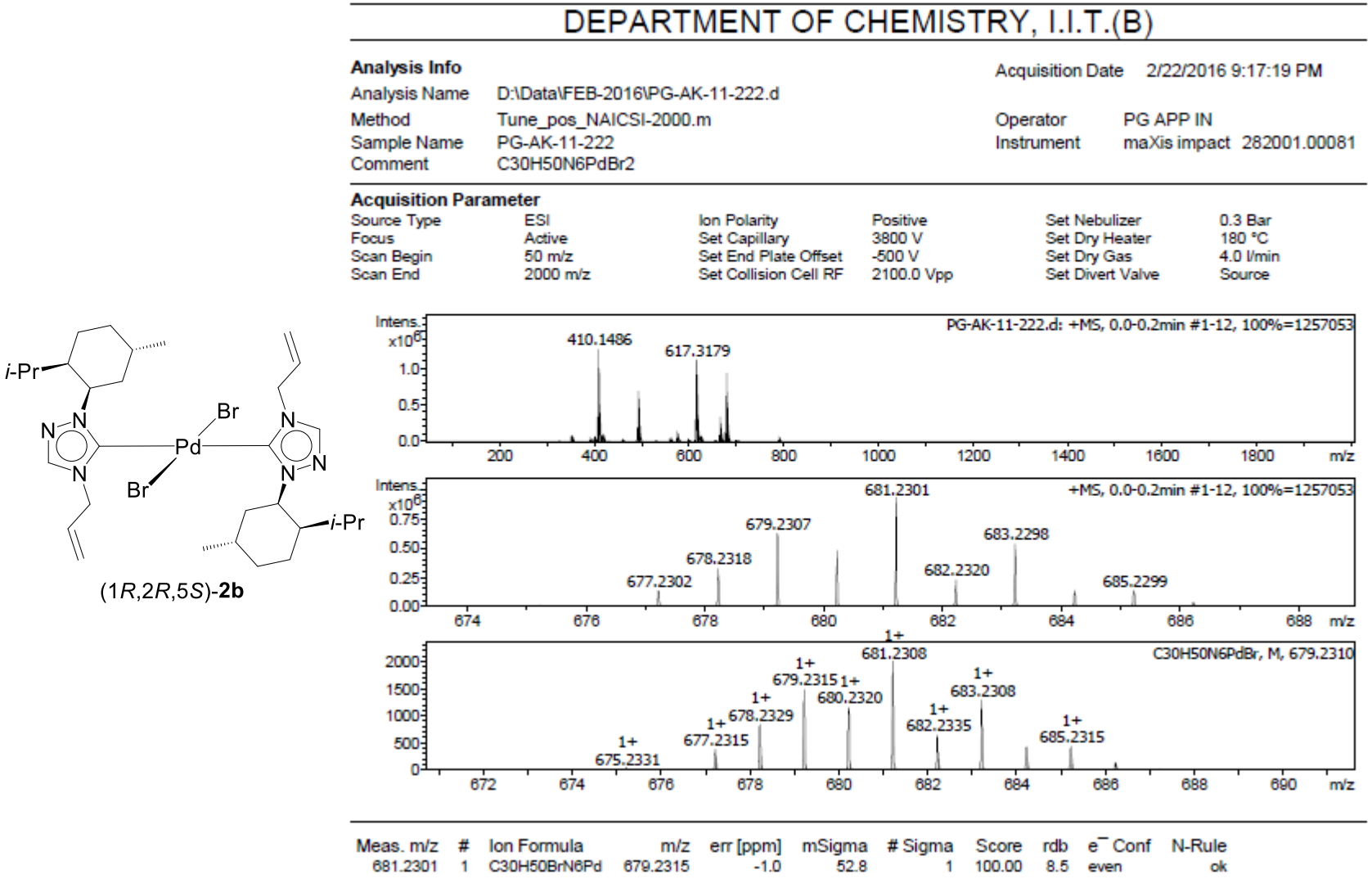
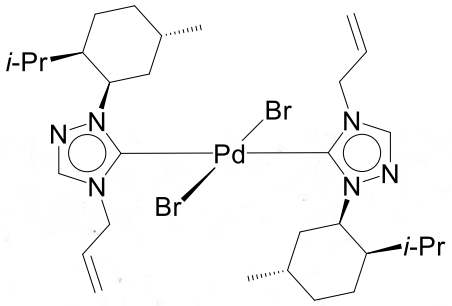


Figure S52. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**2b**.



(1*R*,2*R*,5*S*)-**2b**

Eager 300 Report

Page: 1 Sample: PG-AK-11-222-2 (PG-AK-11-222-2)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-222-2
Operator ID : CHANDNI Company Name : C.E. Instruments
Analysed : 10/13/2015 13:17 Printed : 10/13/2015 18:36
Sample ID : PG-AK-11-222-2 (# 13) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .784

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	11.1318	41	94512	RS	10.356680	.108295E+07
Carbon	47.7544	64	978831	RS	1.000000	.260680E+07
Hydrogen	6.3743	175	347305	RS	2.818360	.665180E+07
Totals	65.2604		1420648			

Figure S53. Elemental analysis data of (1*R*,2*R*,5*S*)-**2b**.

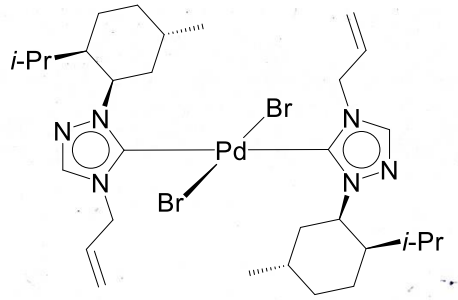
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Monday, 12-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**2b**

n	Average	Std.Dev.	Maximum	Minimum
5	39.430	0.1341	39.639	39.340

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-222-1	12:20:47	39.340	SR	0.197	589	50	1	25.1
2	pg-ak-11-222-1	12:20:54	39.340	SR	0.197	589	50	1	25.1
3	pg-ak-11-222-1	12:21:00	39.340	SR	0.197	589	50	1	25.1
4	pg-ak-11-222-1	12:21:07	39.493	SR	0.197	589	50	1	25.1
5	pg-ak-11-222-1	12:21:19	39.639	SR	0.198	589	50	1	25.1

Figure S54. Specific rotation of (1*R*,2*R*,5*S*)-**2b** in $CHCl_3$.

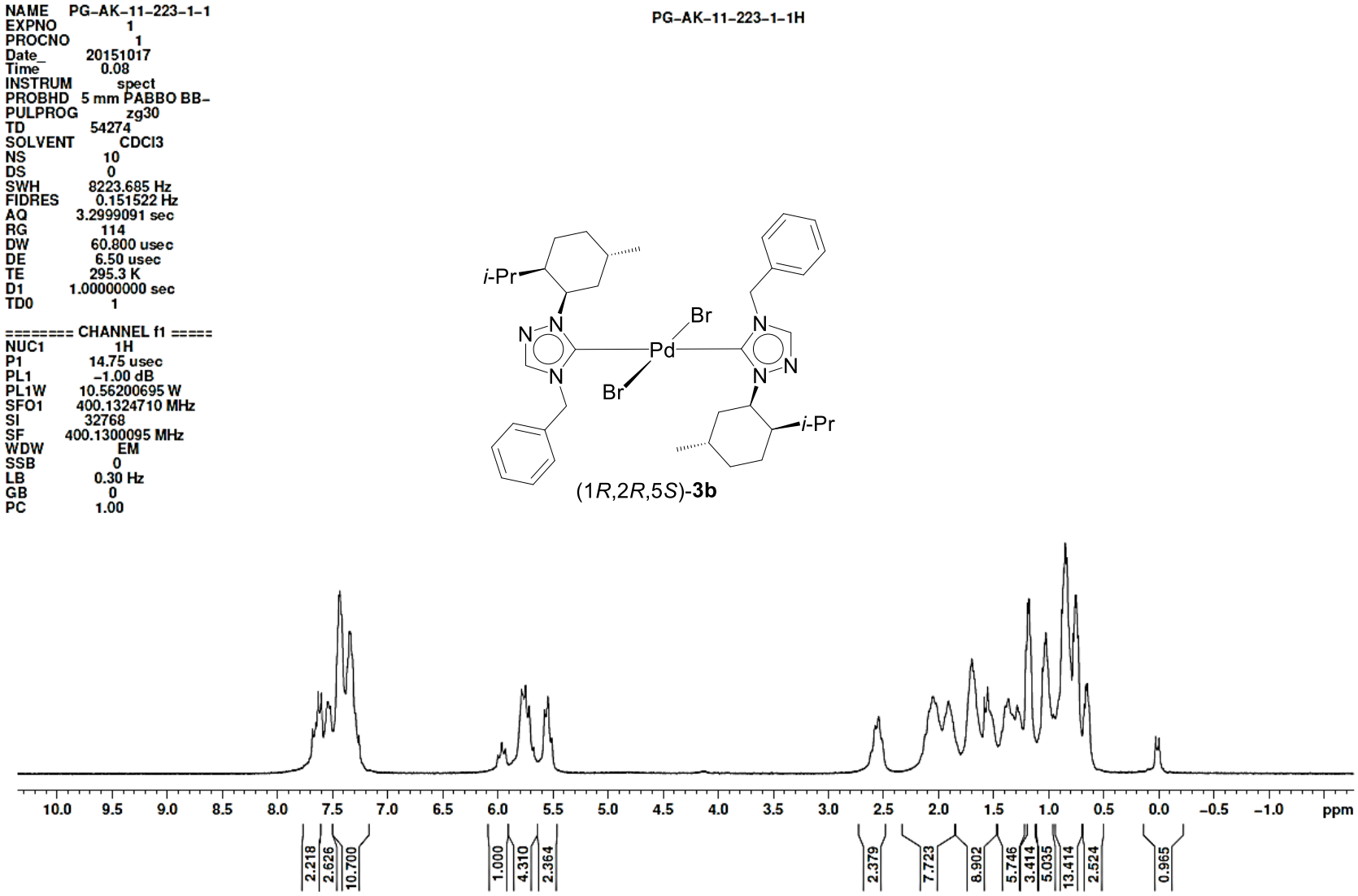


Figure S55. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**3b** in $CDCl_3$.

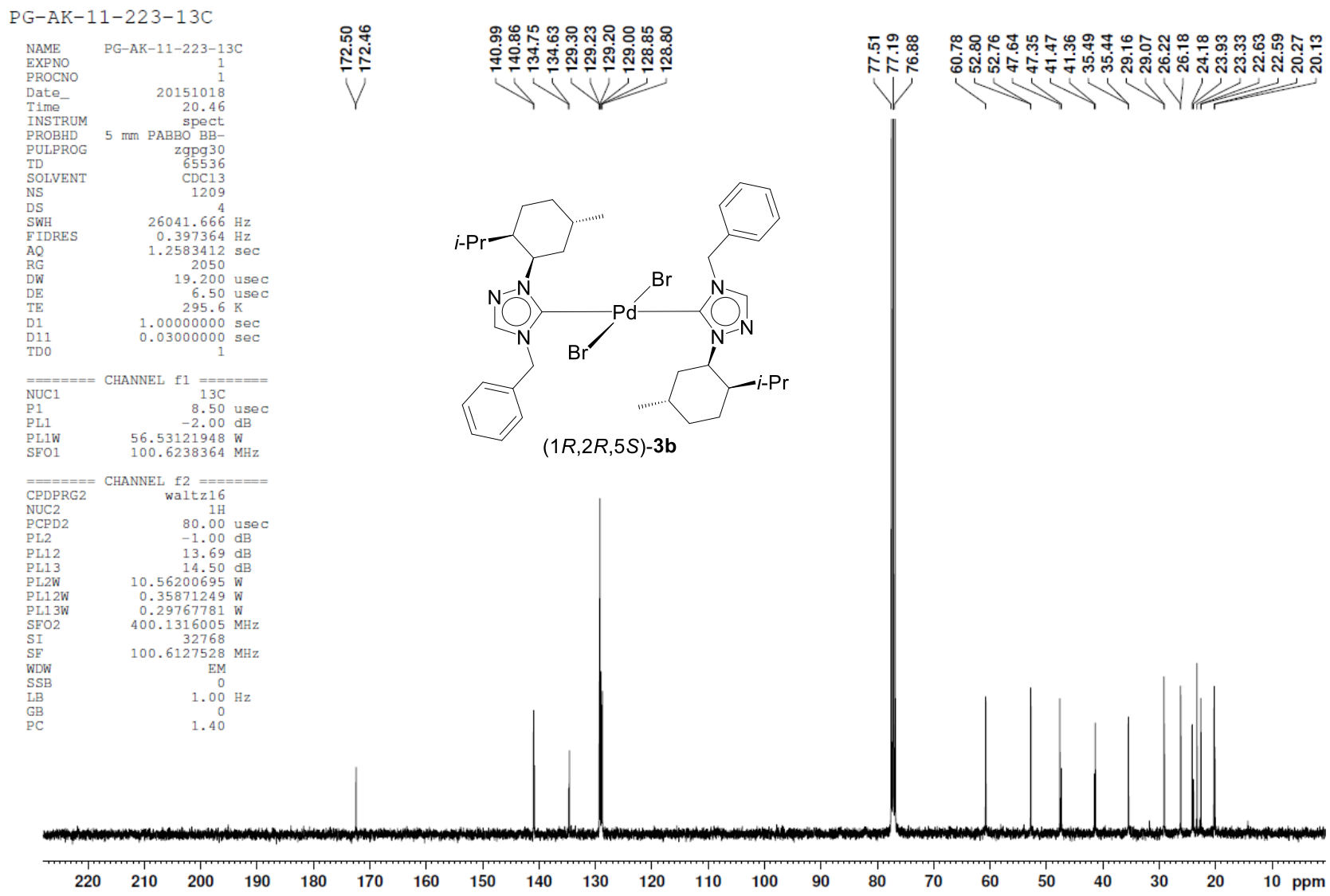


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**3b** in $CDCl_3$.

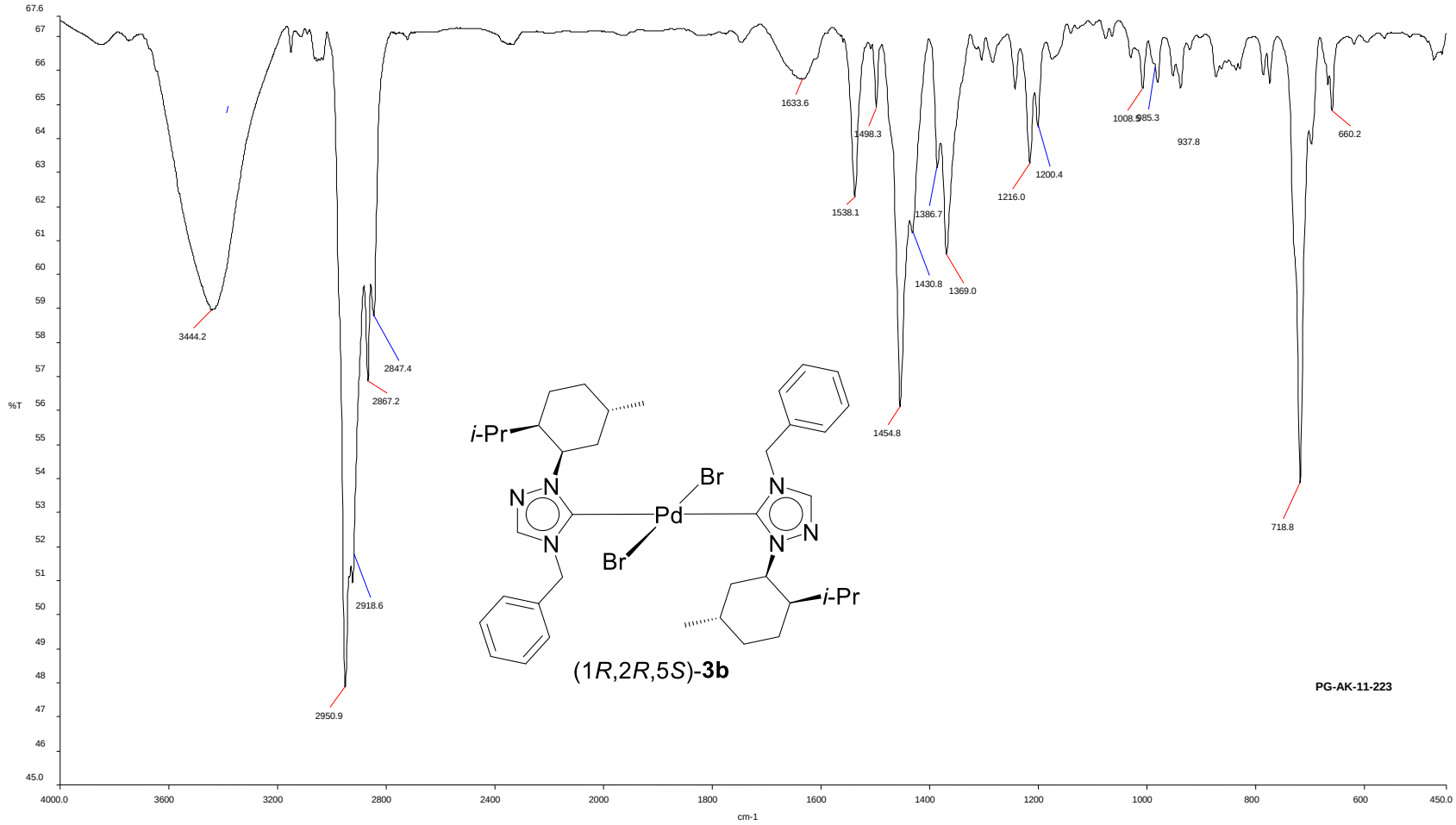


Figure S57. Infrared spectrum of 1*R*,2*R*,5*S*-**3b** in KBr.

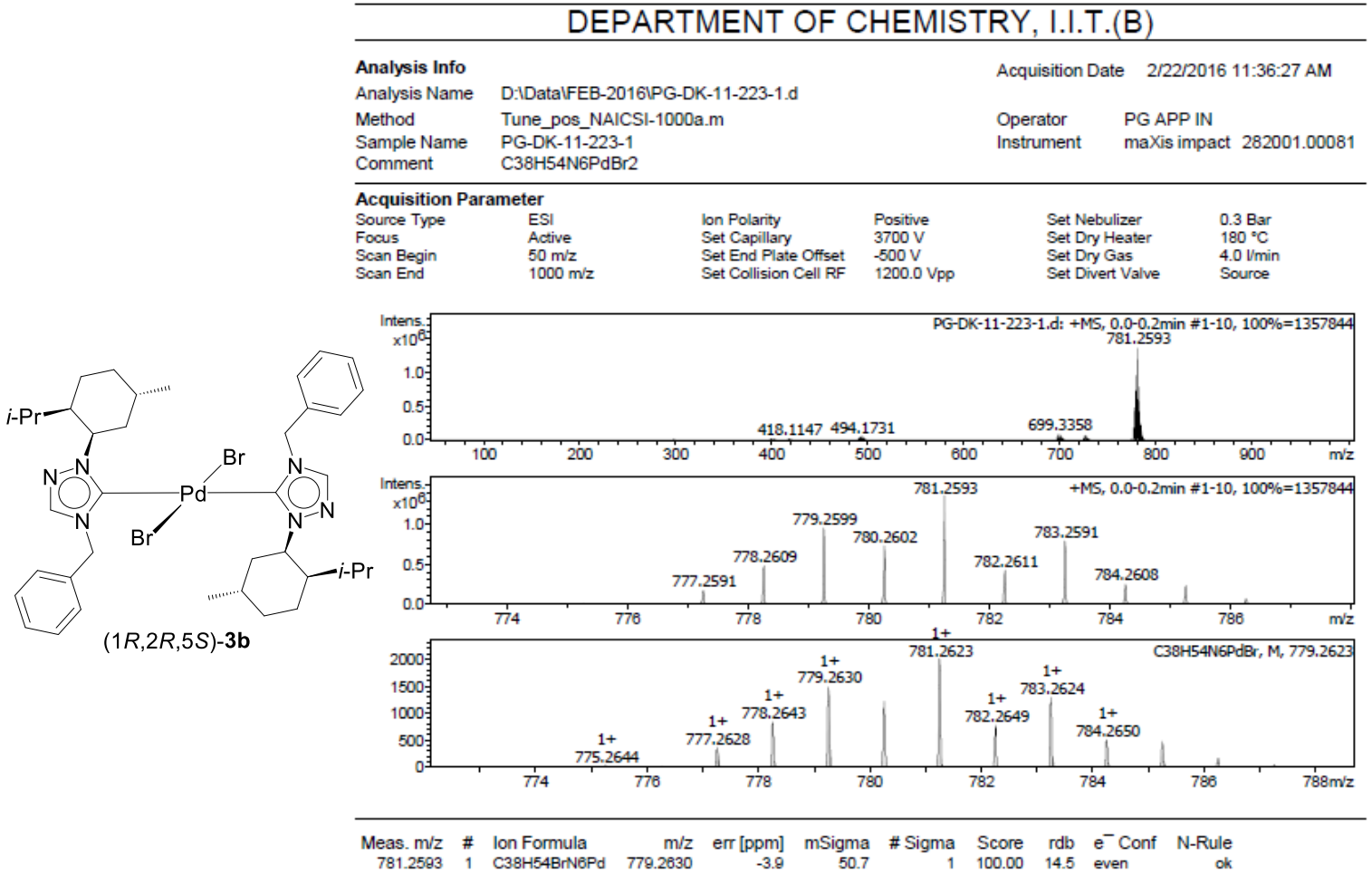
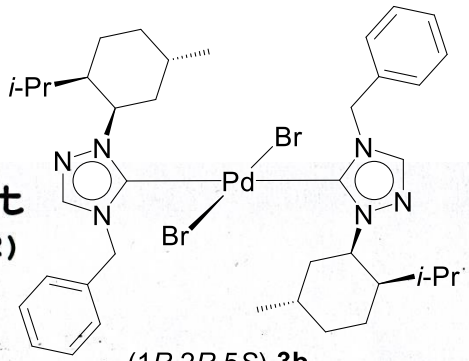


Figure S58. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**3b**.



(1*R*,2*R*,5*S*)-**3b**

Eager 300 Report

Page: 1 Sample: PG-AK-11-223-2 (PG-AK-11-223-2)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-223-2
Operator ID : CHANDNI
Company Name : C.E. Instruments
Analysed : 10/13/2015 13:37
Printed : 10/13/2015 18:36
Sample ID : PG-AK-11-223-2 (# 15)
Instrument N. : Instrument #1
Analysis Type : UnkNown (Area)
Sample weight : 1.004

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	9.5675	41	104025	RS	13.525010	.108295E+07
Carbon	53.6476	63	1406939	RS	1.000000	.260680E+07
Hydrogen	6.2084	178	429505	RS	3.275722	.665180E+07
Totals	69.4235		1940469			

Figure S59. Elemental analysis data of (1*R*,2*R*,5*S*)-**3b**.

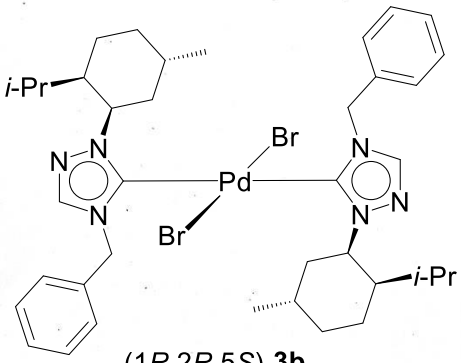
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Monday, 12-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**3b**

n	Average	Std.Dev.	Maximum	Minimum
5	44.991	0.0000	44.991	44.991

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-223-1	12:13:09	44.991	SR	0.225	589	50	1	24.9
2	pg-ak-11-223-1	12:13:16	44.991	SR	0.225	589	50	1	24.9
3	pg-ak-11-223-1	12:13:23	44.991	SR	0.225	589	50	1	24.9
4	pg-ak-11-223-1	12:13:29	44.991	SR	0.225	589	50	1	24.9
5	pg-ak-11-223-1	12:13:36	44.991	SR	0.225	589	50	1	24.9

Figure S60. Specific rotation of (1*R*,2*R*,5*S*)-**3b** in $CHCl_3$.

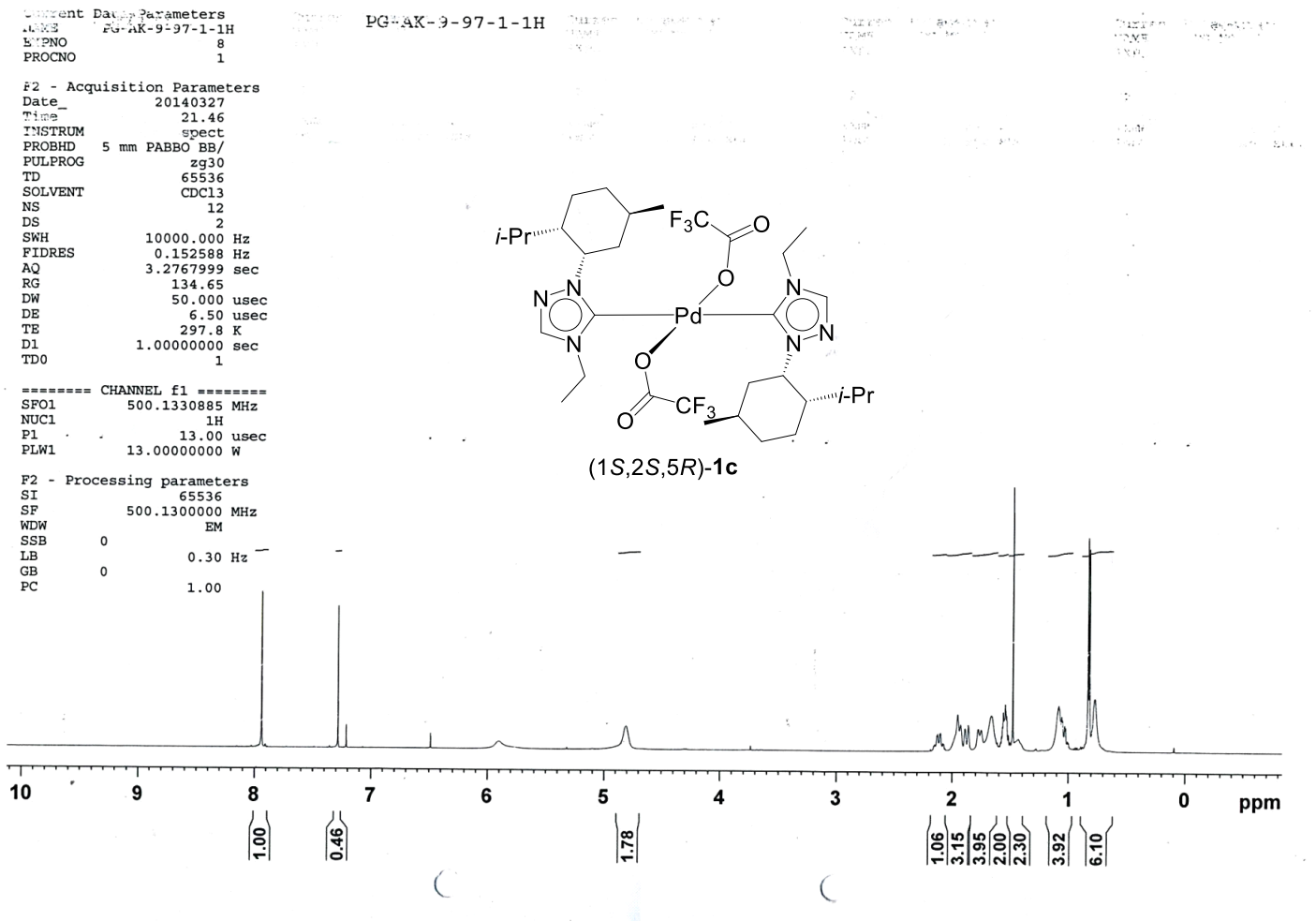


Figure S61. ^{1}H NMR spectrum of 1*S*,2*S*,5*R*-**1c** in $CDCl_3$.

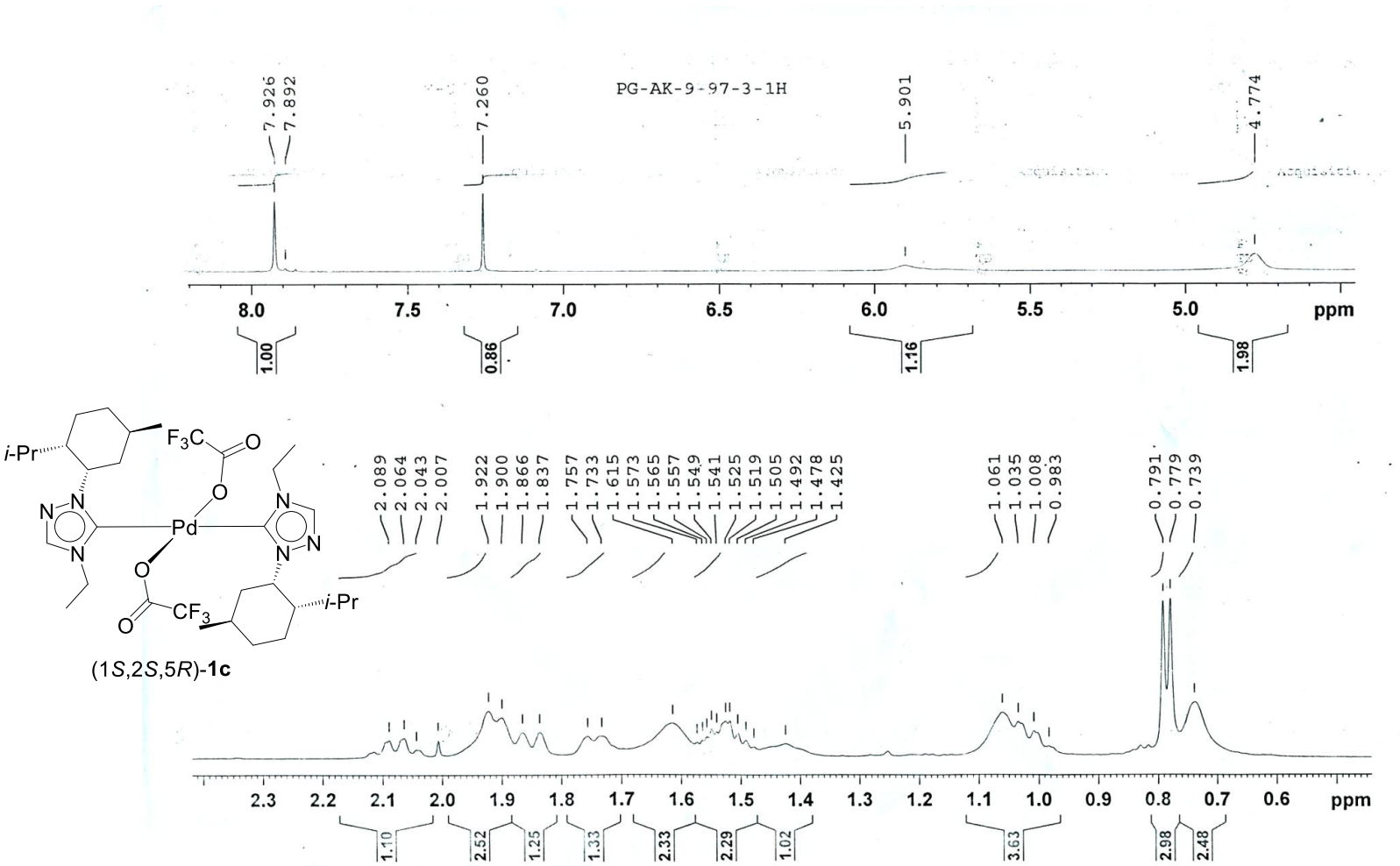


Figure S62. Expanded ^{1}H NMR spectrum of 1*S*,2*S*,5*R*-**1c** in $CDCl_3$.

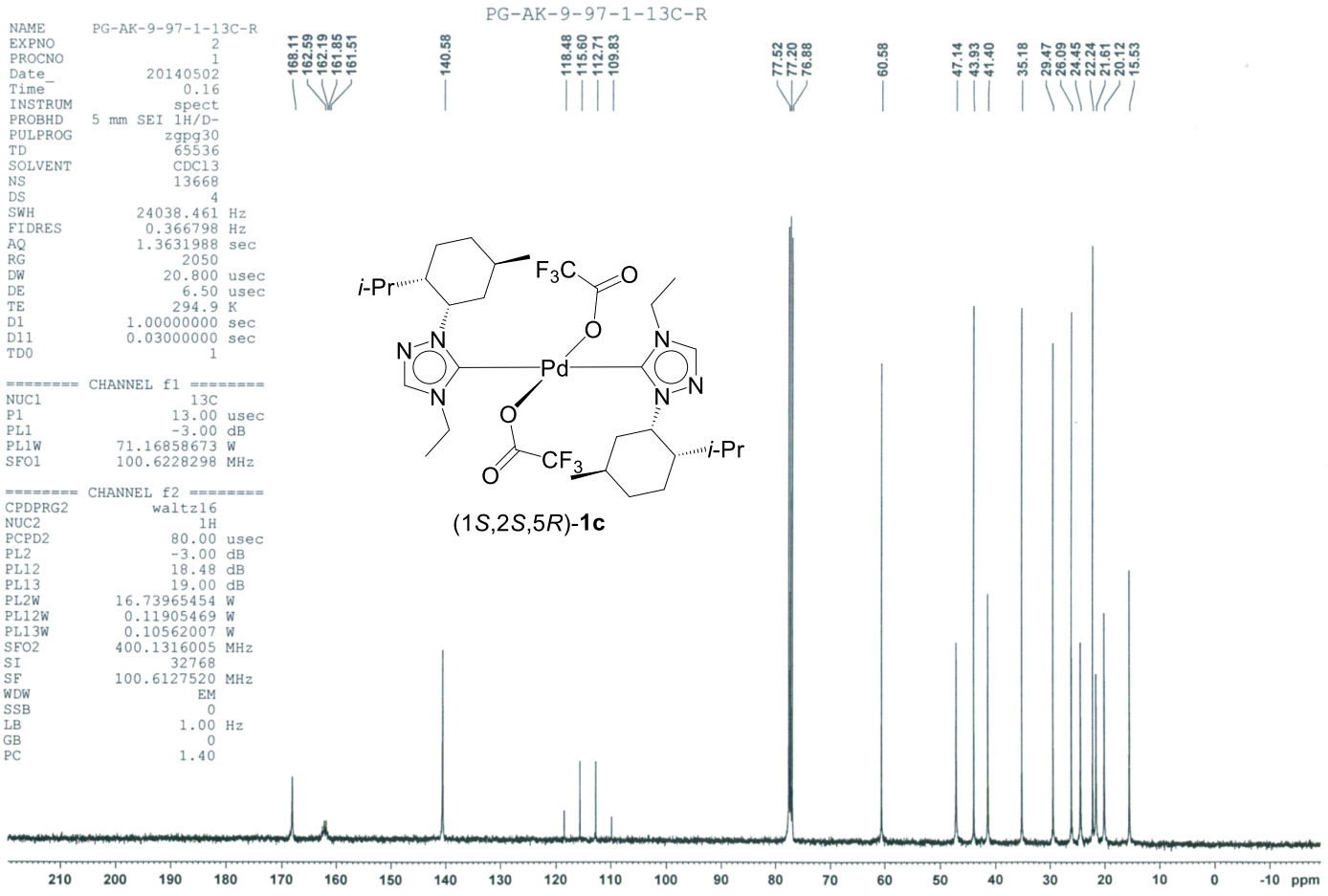


Figure S63. $^{13}C\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**1c** in $CDCl_3$.

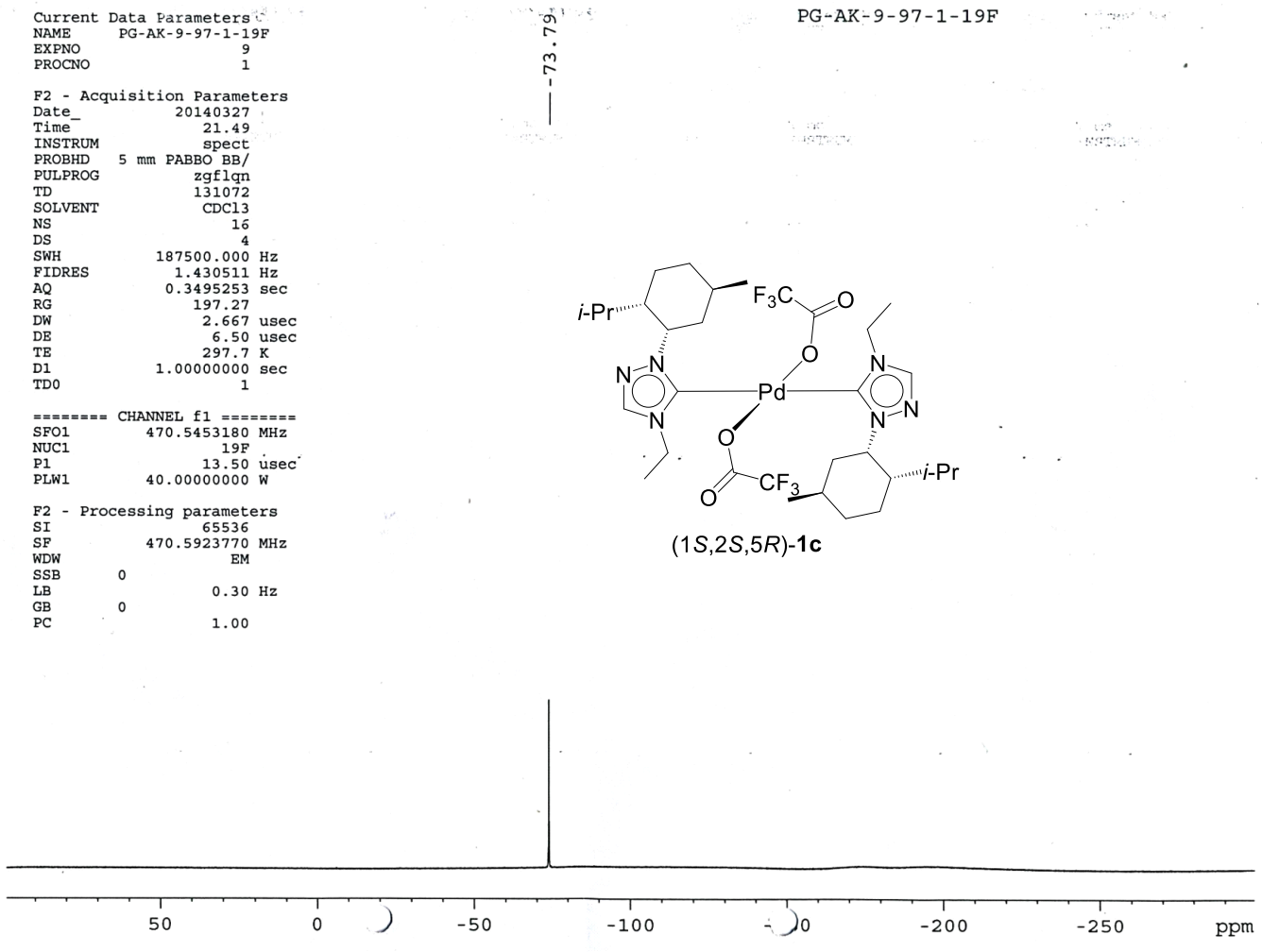


Figure S64. $^{19}F\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**1c** in $CDCl_3$.

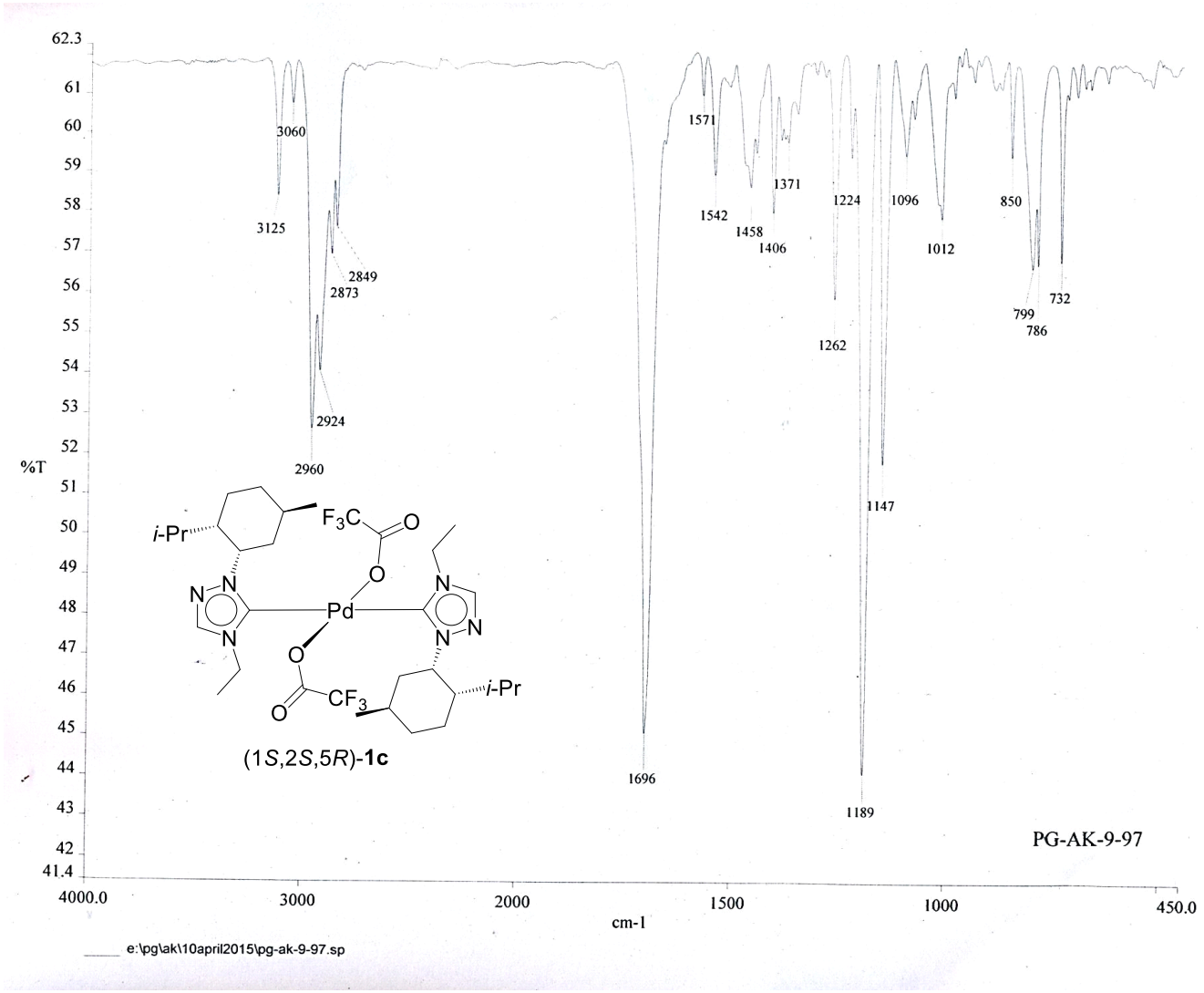


Figure S65. Infrared spectrum of 1*S*,2*S*,5*R*-**1c** in KBr.

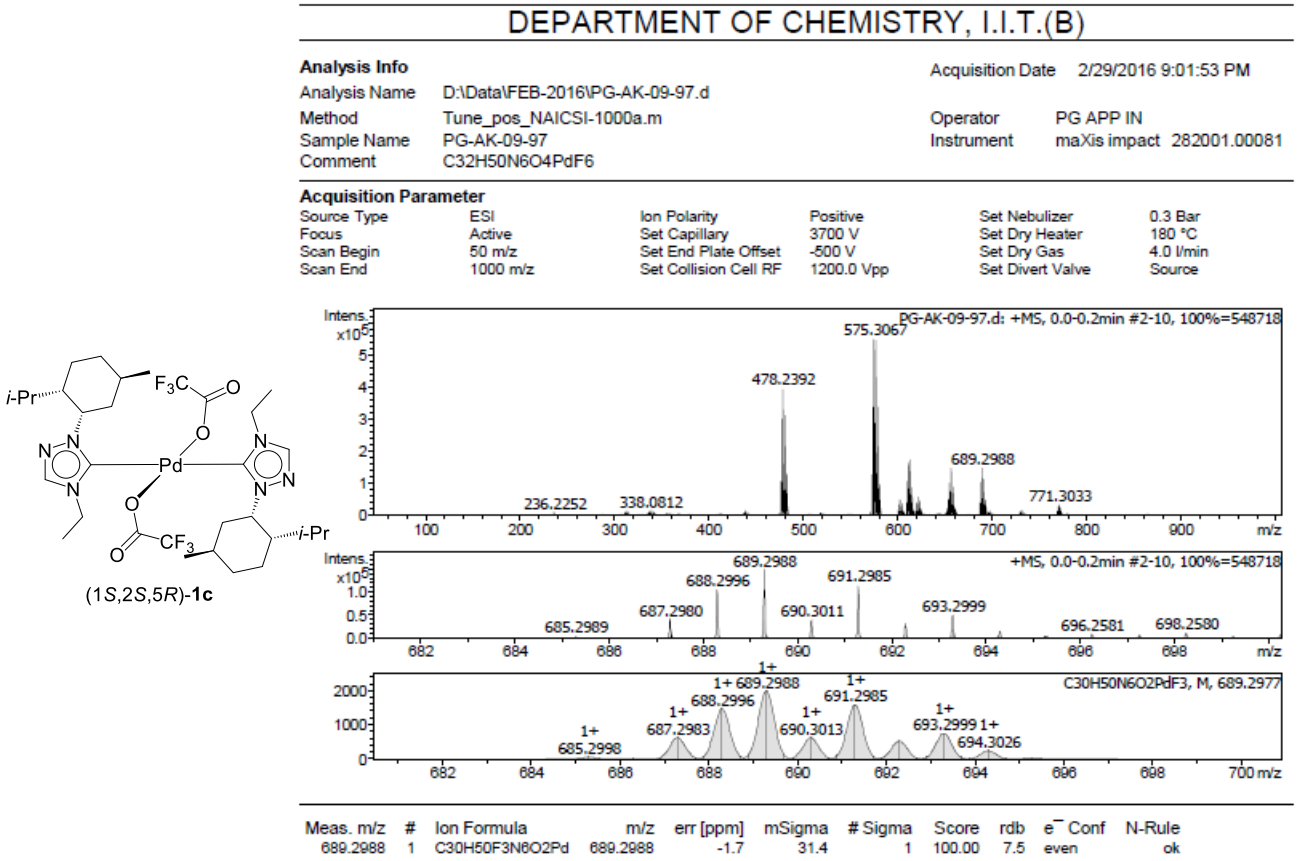
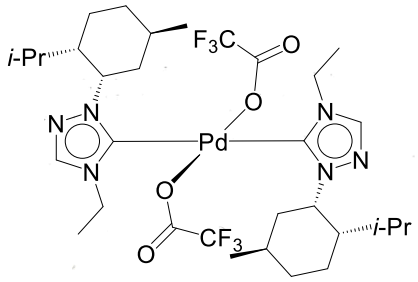


Figure S66. High Resolution Mass Spectrometry (HRMS) data of 1*S*,2*S*,5*R*-**1c**.



(1*S*,2*S*,5*R*)-**1c**

Eager 300 Report

Page: 1 Sample: PG-AK-9-97-1 (PG-AK-9-97-1)

Method Name : PGCP11052015
Method File : D:\CHNS-2015\PGCP11052015.mth
Chromatogram : PG-AK-9-97-1
Operator ID : CHANDNI
Analysed : 05/11/2015 11:48
Sample ID : PG-AK-9-97-1 (# 6)
Analysis Type : UnkNown (Area)

Company Name : C.E. Instruments
Printed : 5/13/2015 19:41
Instrument N. : Instrument #1
Sample weight : .815

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.7128	42	103089	RS	10.013580	.118073E+07
Carbon	48.3356	65	1032285	RS	1.000000	.262045E+07
Hydrogen	5.9624	175	340944	RS	3.027726	.667788E+07
Totals	65.0108		1476318			

Figure S67. Elemental analysis data of 1*S*,2*S*,5*R*-**1c**.

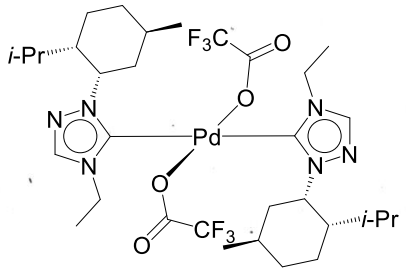
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Monday, 01-DEC-2014

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*S*,2*S*,5*R*)-**1c**

n	Average	Std.Dev.	Maximum	Minimum
5	47.857	0.0671	47.902	47.752

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-9-111	11:54:32	47.752	SR	0.478	589	100	1	25.1
2	pg-ak-9-111	11:54:39	47.827	SR	0.478	589	100	1	25.1
3	pg-ak-9-111	11:54:46	47.902	SR	0.479	589	100	1	25.0
4	pg-ak-9-111	11:54:53	47.902	SR	0.479	589	100	1	25.0
5	pg-ak-9-111	11:54:59	47.902	SR	0.479	589	100	1	25.0

Figure S68. Specific rotation of 1*S*,2*S*,5*R*-**1c** in $CHCl_3$.

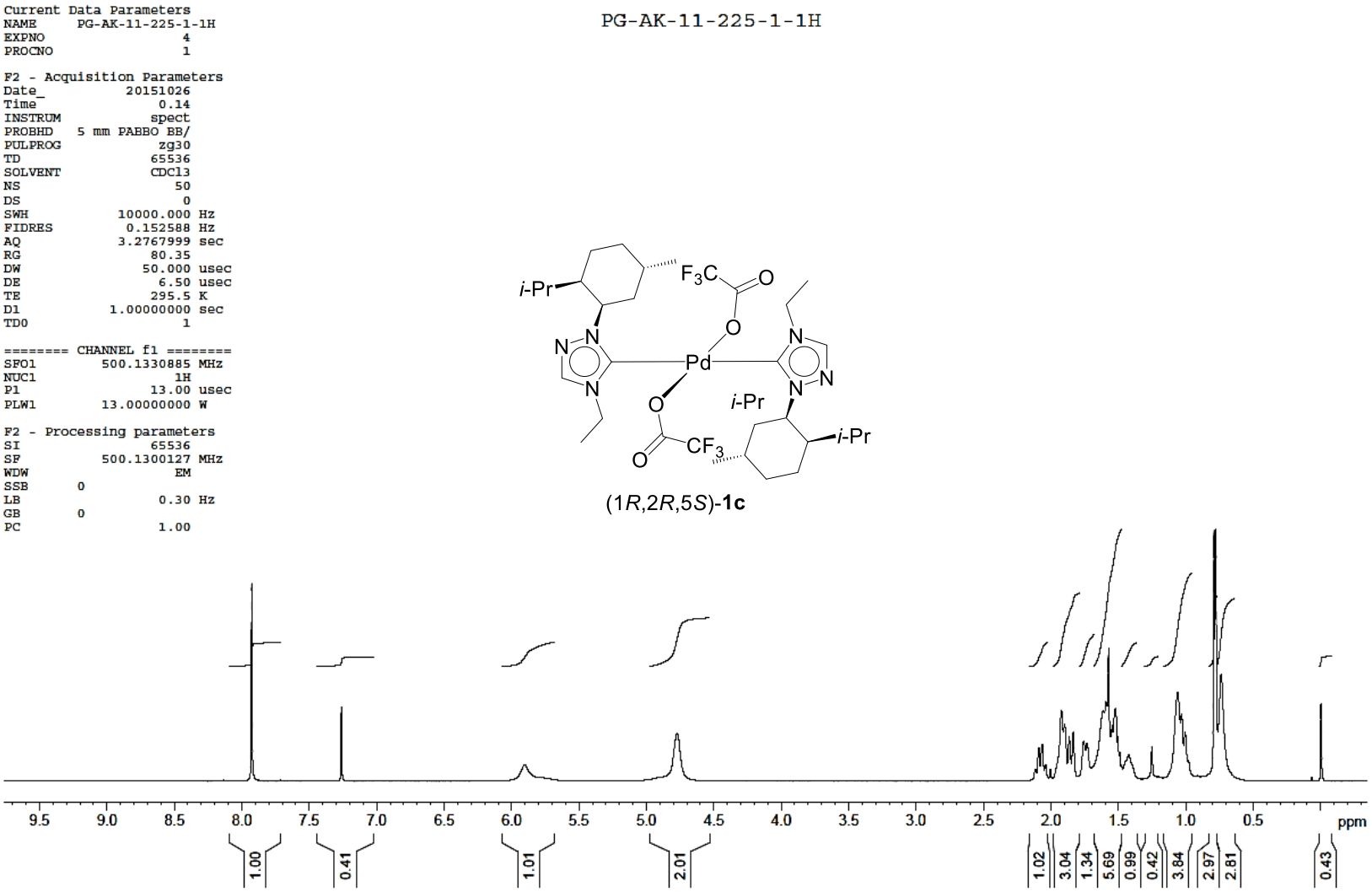


Figure S69. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**1c** in $CDCl_3$.

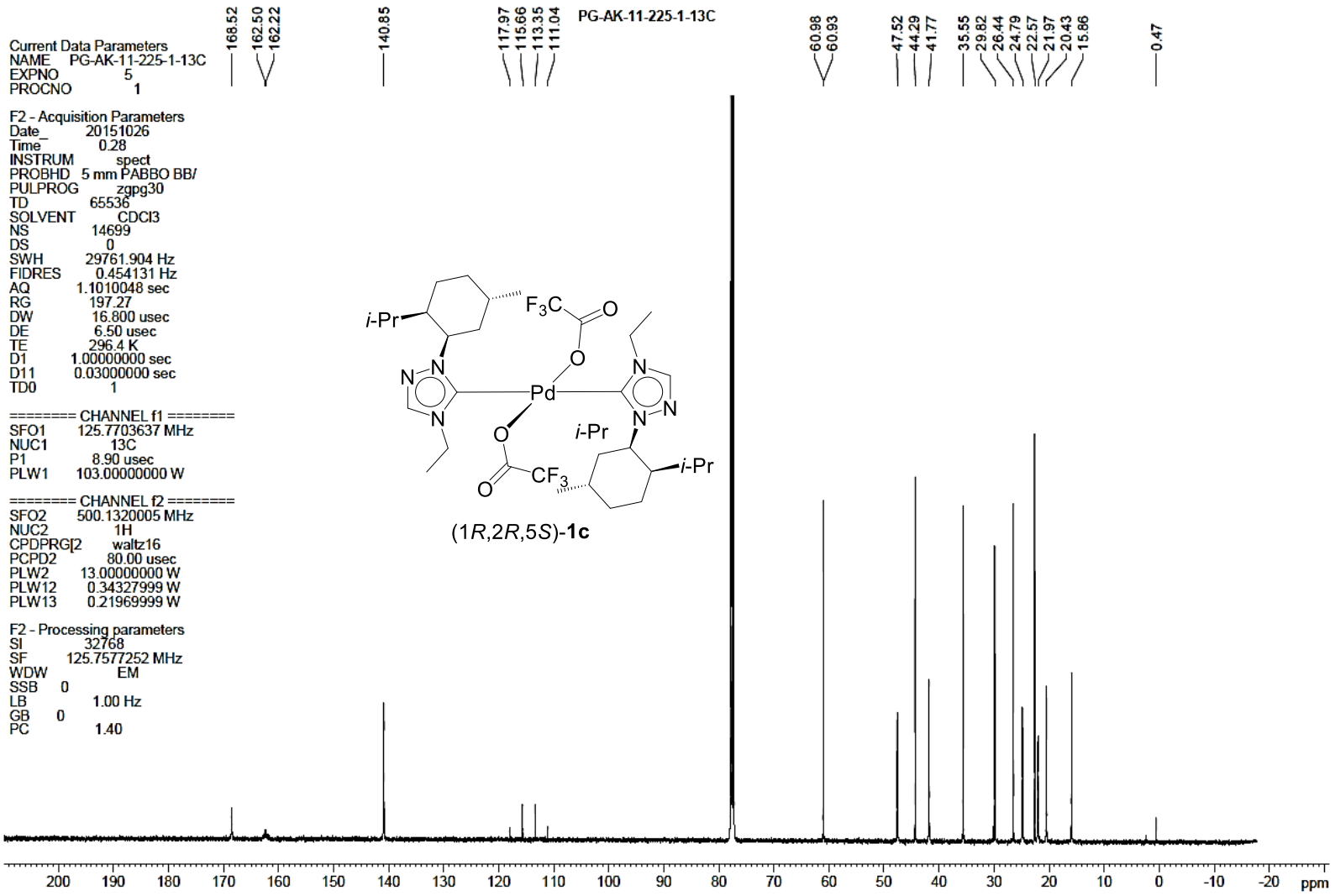


Figure S70. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**1c** in $CDCl_3$.

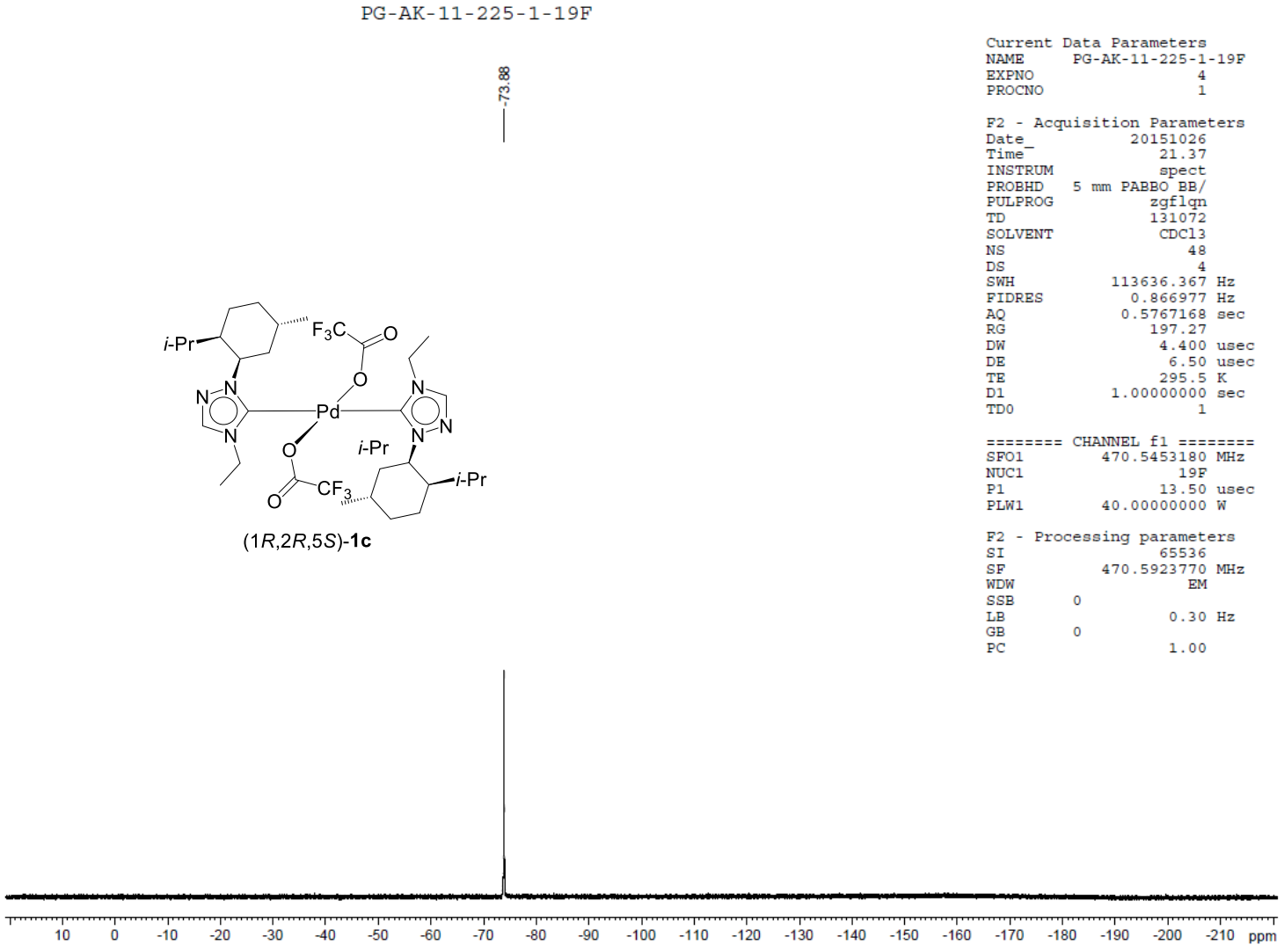


Figure S71. $^{19}F\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**1c** in $CDCl_3$.

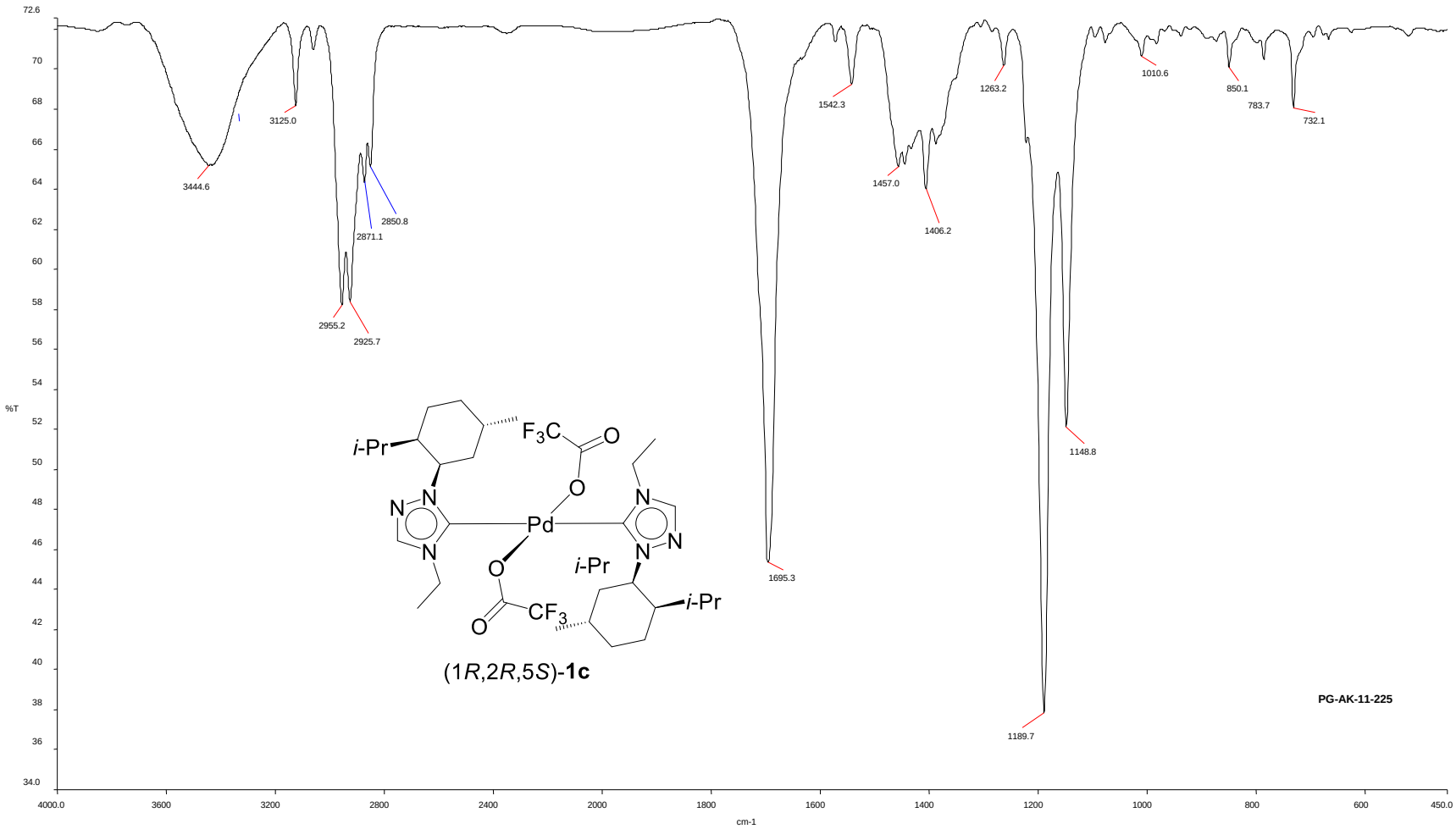
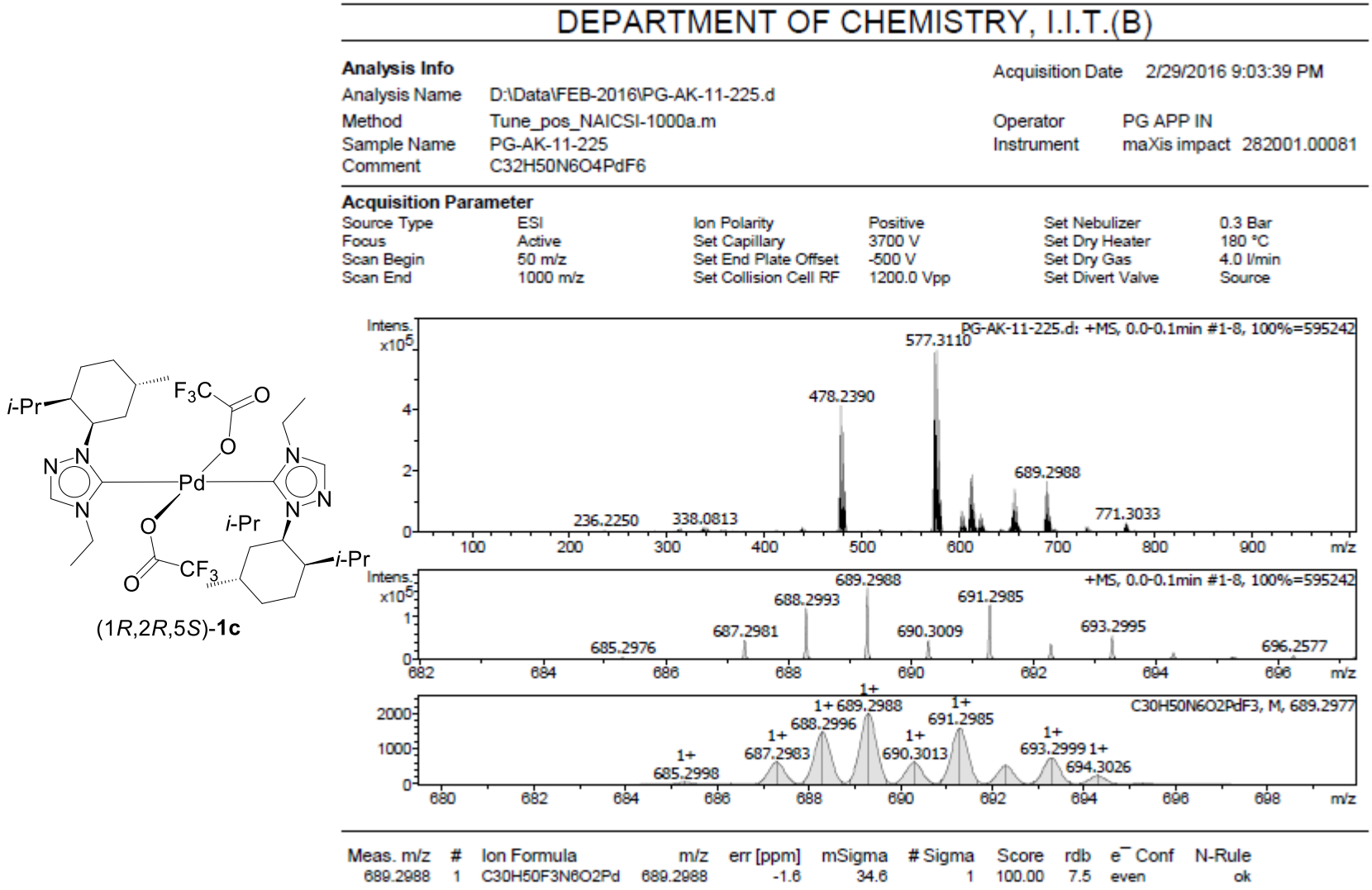
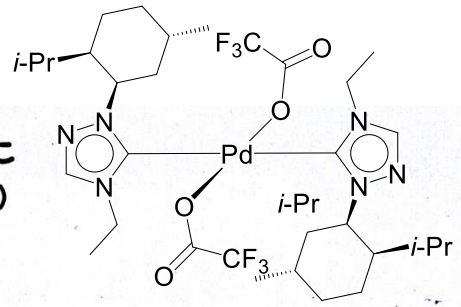


Figure S72. Infrared spectrum of 1*R*,2*R*,5*S*-**1c** in KBr.



(1*R*,2*R*,5*S*)-**1c**

Figure S73. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**1c**.



(1*R*,2*R*,5*S*)-**1c**

Eager 300 Report

Page: 1 Sample: PG-AK-11-225-1 (PG-AK-11-225-1)

Method Name : PGCP13102015
Method File : D:\CHNS-2015\PGCP13102015.mth
Chromatogram : PG-AK-11-225-1
Operator ID : CHANDNI Company Name : C.E. Instruments
Analysed : 10/13/2015 14:08 Printed : 10/13/2015 18:36
Sample ID : PG-AK-11-225-1 (# 18) Instrument N. : Instrument #1
Analysis Type : UnkNown (Area) Sample weight : .644

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	10.6417	41	74217	RS	10.955020	.108295E+07
Carbon	48.2606	64	813049	RS	1.000000	.260680E+07
Hydrogen	5.7098	178	259480	RS	3.133376	.665180E+07
Totals	64.6121		1146746			

Figure S74. Elemental analysis data of (1*R*,2*R*,5*S*)-**1c**.

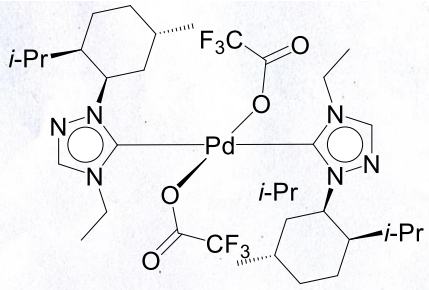
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Tuesday, 27-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**1c**

n	Average	Std.Dev.	Maximum	Minimum
5	-47.974	0.1665	-47.792	-48.096

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-225-1	17:20:17	-47.792	SR	-0.239	589	50.00	1.000	25.1
2	pg-ak-11-225-1	17:20:24	-47.792	SR	-0.239	589	50.00	1.000	25.1
3	pg-ak-11-225-1	17:20:31	-48.096	SR	-0.240	589	50.00	1.000	25.1
4	pg-ak-11-225-1	17:20:38	-48.096	SR	-0.240	589	50.00	1.000	25.1
5	pg-ak-11-225-1	17:20:45	-48.096	SR	-0.240	589	50.00	1.000	25.1

Figure S75. Specific rotation of (1*R*,2*R*,5*S*)-**1c** in $CHCl_3$.

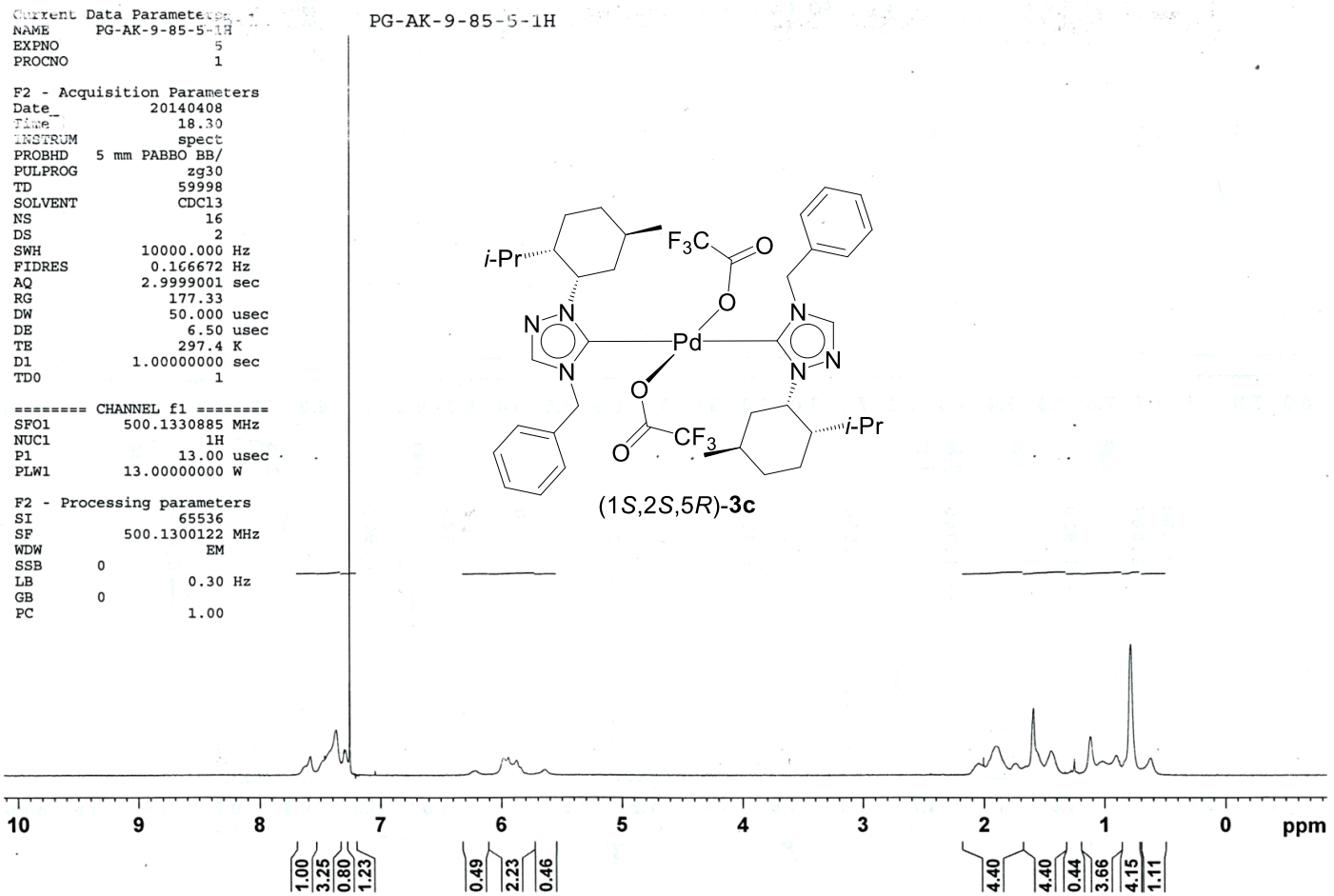


Figure S76. ^{1}H NMR spectrum of 1*S*,2*S*,5*R*-**3c** in $CDCl_3$.

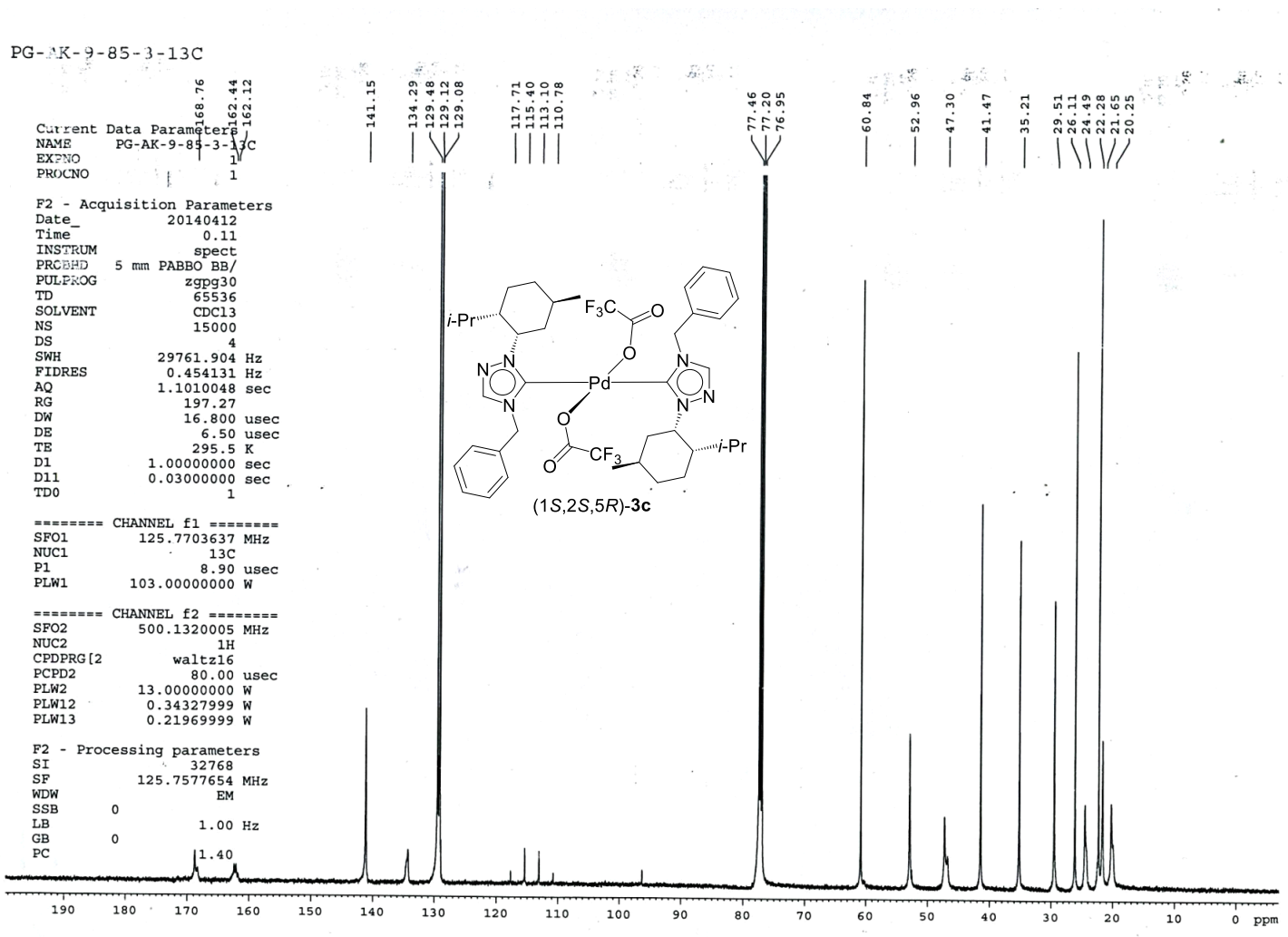


Figure S77. $^{13}C\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**3c** in $CDCl_3$.

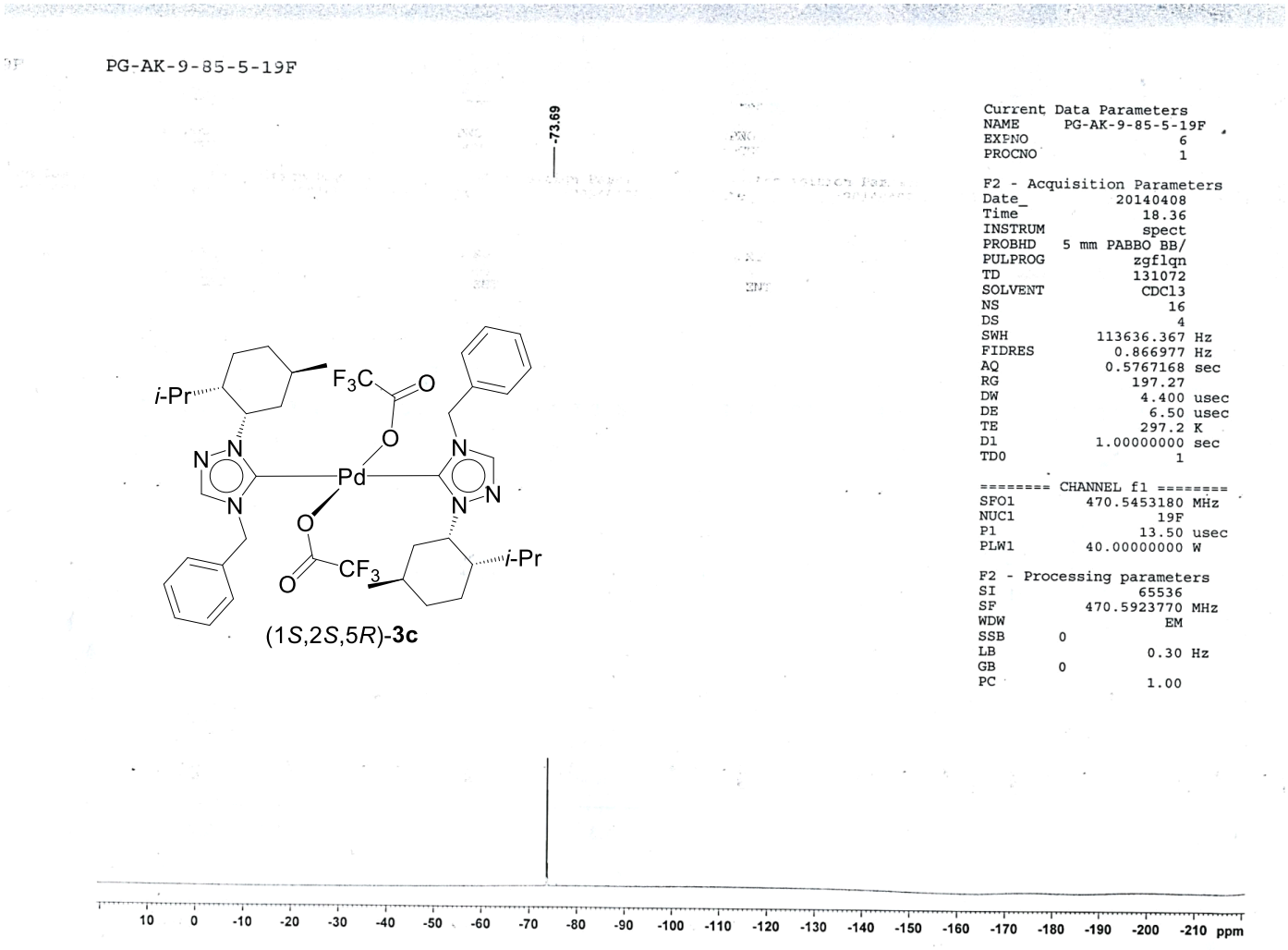


Figure S78. $^{19}F\{^{1}H\}$ NMR spectrum of 1*S*,2*S*,5*R*-**3c** in $CDCl_3$.

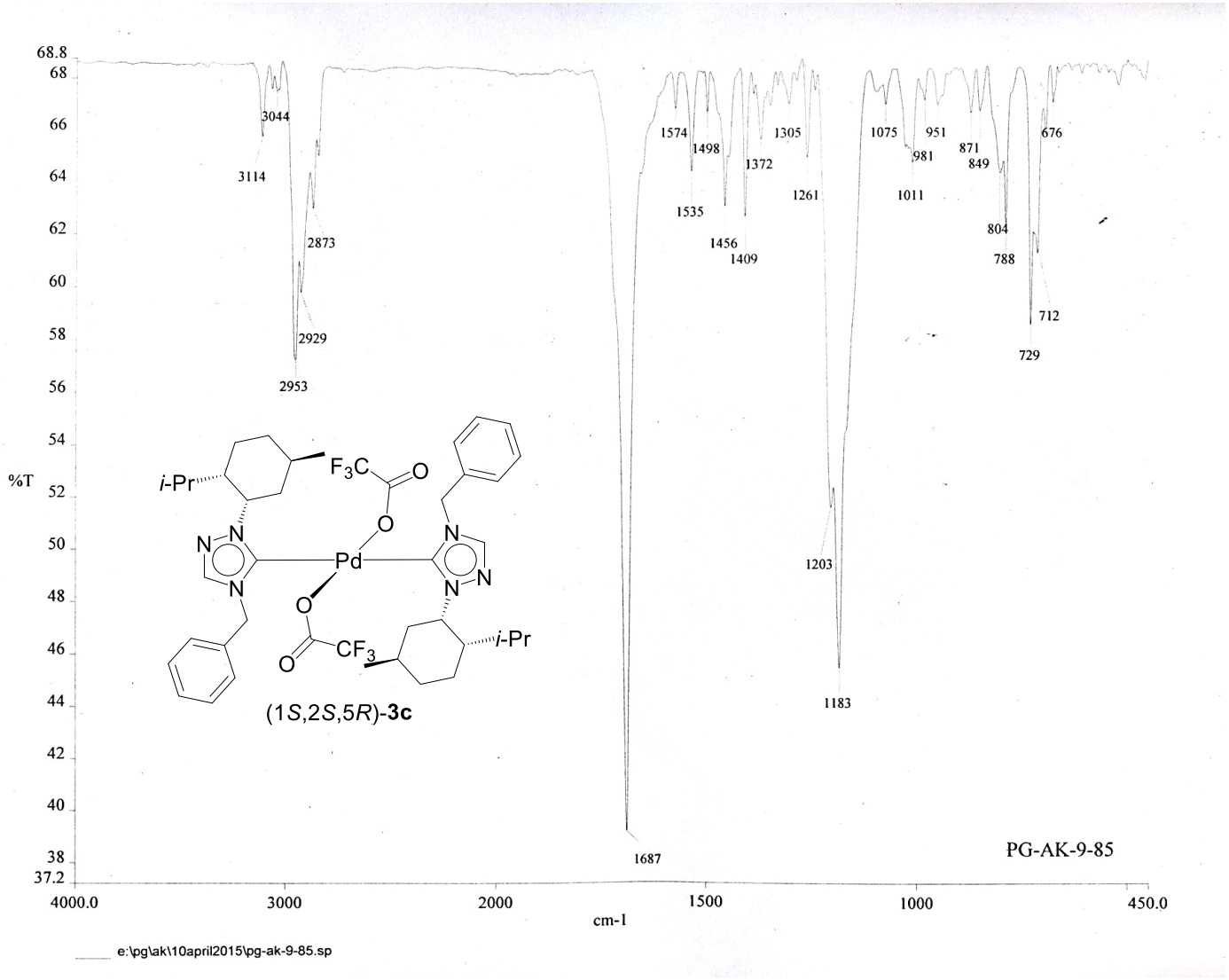


Figure S79. Infrared spectrum of 1*S*,2*S*,5*R*-**3c** in KBr.

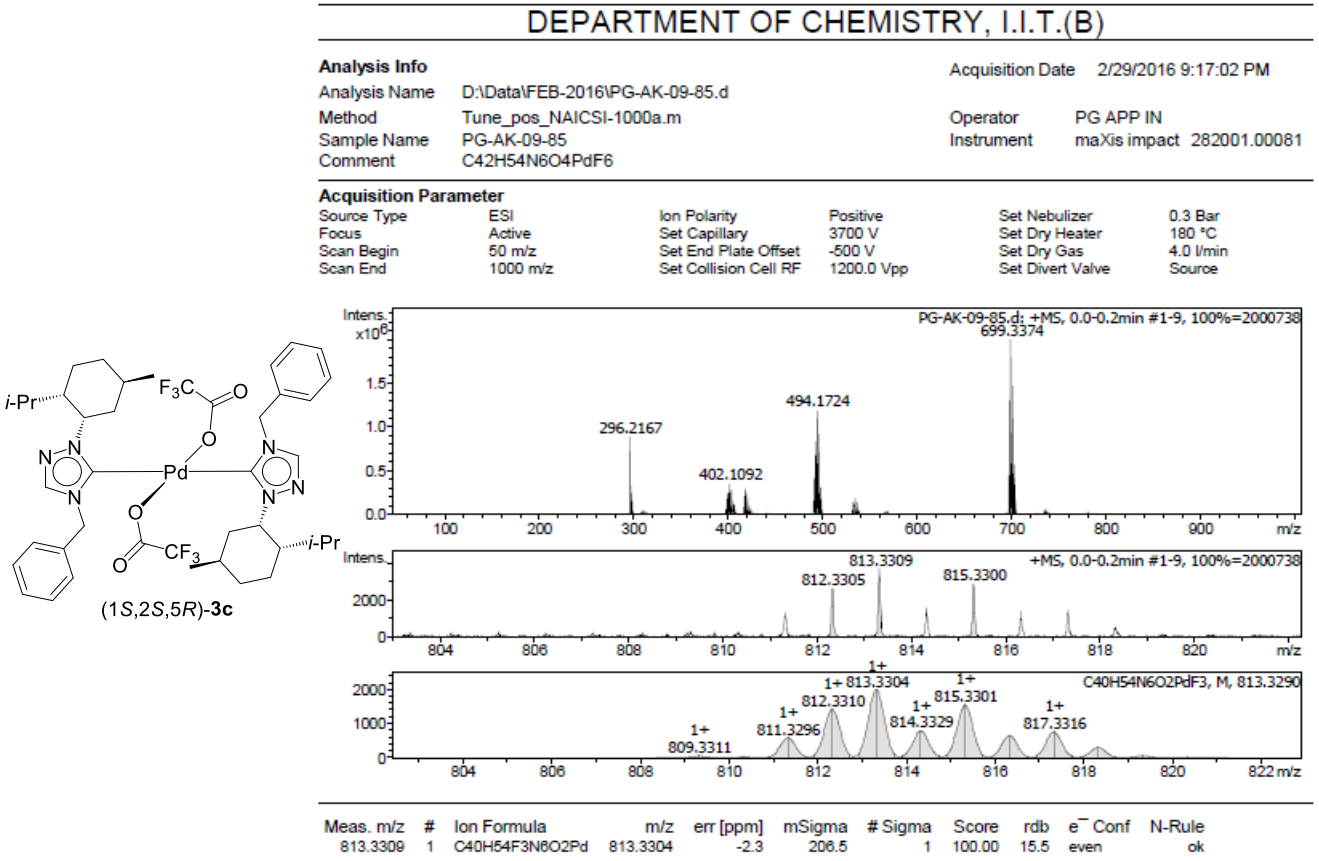
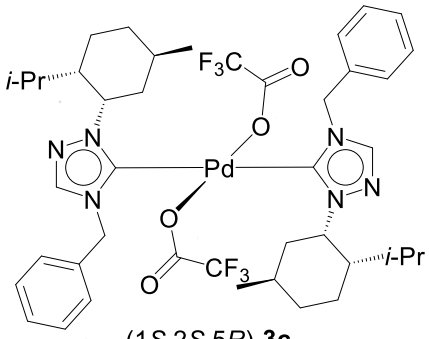


Figure S80. High Resolution Mass Spectrometry (HRMS) data of 1*S*,2*S*,5*R*-**3c**.



(1*S*,2*S*,5*R*)-**3c**

Eager 300 Report

Page: 1 Sample: PG-AK-9-85 (PG-AK-9-85)

Method Name	: SP-070414		
Method File	: D:\CHNS-2014\SP-070414.mth		
Chromatogram	: PG-AK-9-85		
Operator ID	: MNRAO	Company Name	: C.E. Instruments
Analysed	: 04/07/2014 17:54	Printed	: 4/8/2014 01:06
Sample ID	: PG-AK-9-85 (# 10)	Instrument N.	: Instrument #1
Analysis Type	: UnkNown (Area)	Sample weight	: .568

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.6513	40	76436	FU	10.880470	.155549E+07
Carbon	54.3093	64	831657	FU	1.000000	.269601E+07
Hydrogen	5.5081	175	251404	RS	3.308051	.686517E+07
Totals	68.4687		1159497			

Figure S81. Elemental analysis data of 1*S*,2*S*,5*R*-**3c**.

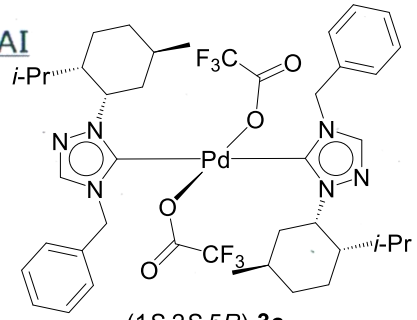
CENTRAL FACILITY LAB CHEMISTRY DEPT. IIT MUMBAI

Monday, 01-DEC-2014

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*S*,2*S*,5*R*)-**3c**

n	Average	Std.Dev.	Maximum	Minimum
5	40.237	1.2469	40.945	38.017

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-9-85	12:04:50	38.017	SR	0.380	589	100.00	1.000	25.1
2	pg-ak-9-85	12:05:08	40.871	SR	0.409	589	100.00	1.000	25.0
3	pg-ak-9-85	12:05:15	40.718	SR	0.407	589	100.00	1.000	25.0
4	pg-ak-9-85	12:05:22	40.945	SR	0.409	589	100.00	1.000	25.0
5	pg-ak-9-85	12:05:29	40.632	SR	0.406	589	100.00	1.000	25.0

Figure S82. Specific rotation of 1*S*,2*S*,5*R*-**3c** in $CHCl_3$.

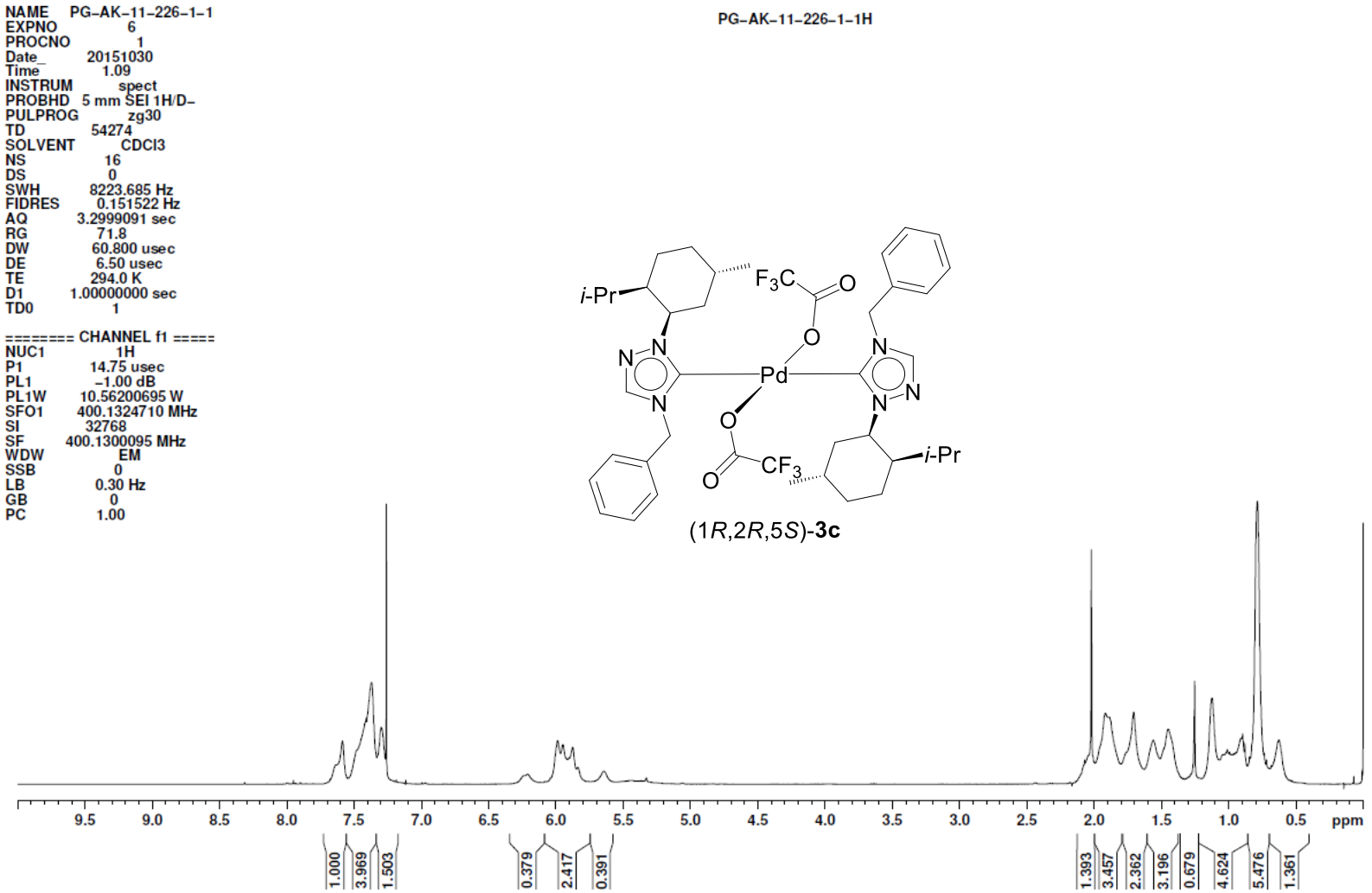


Figure S83. ^{1}H NMR spectrum of (1*R*,2*R*,5*S*)-**3c** in $CDCl_3$.

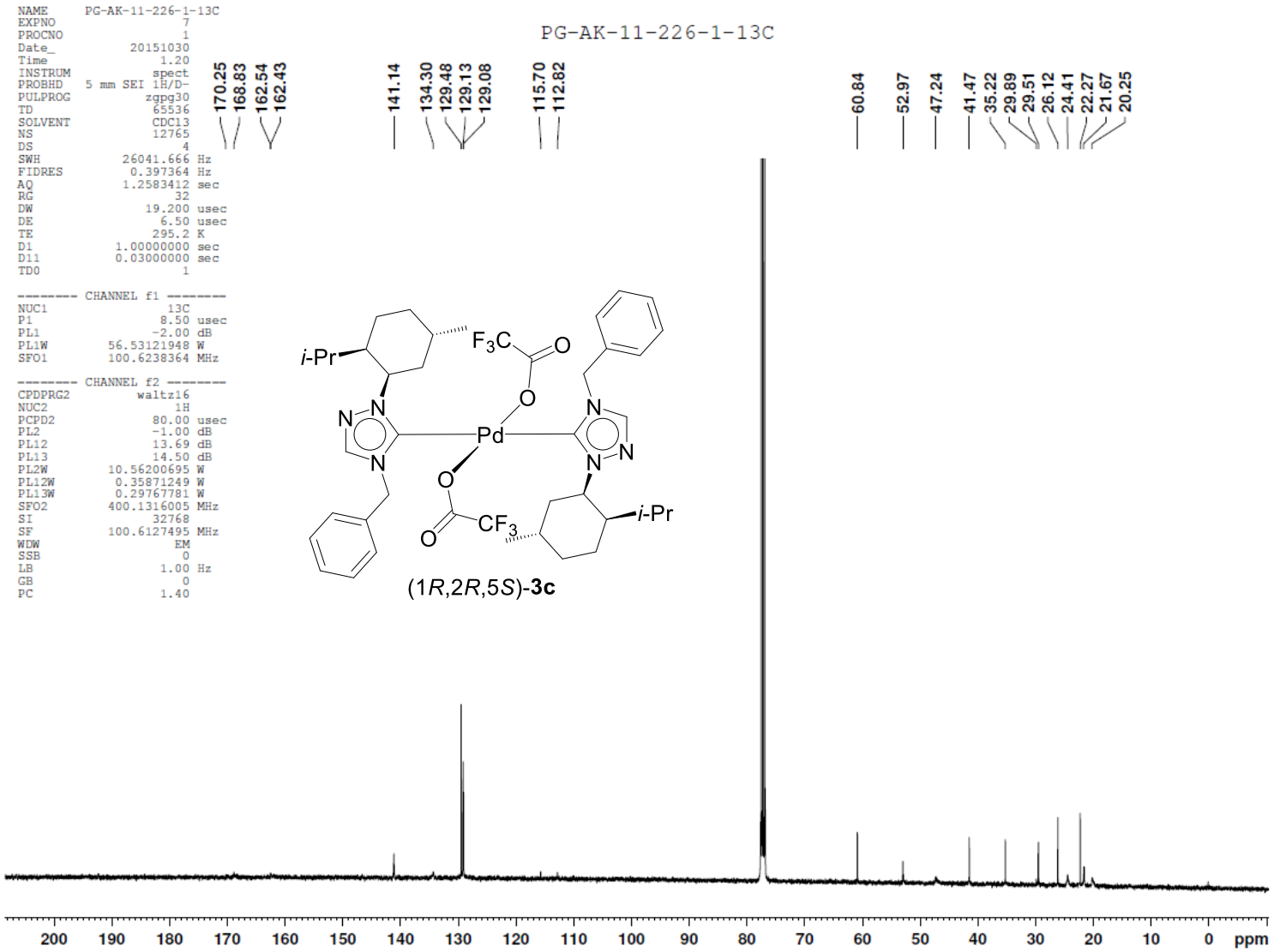


Figure S84. $^{13}C\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**3c** in $CDCl_3$.

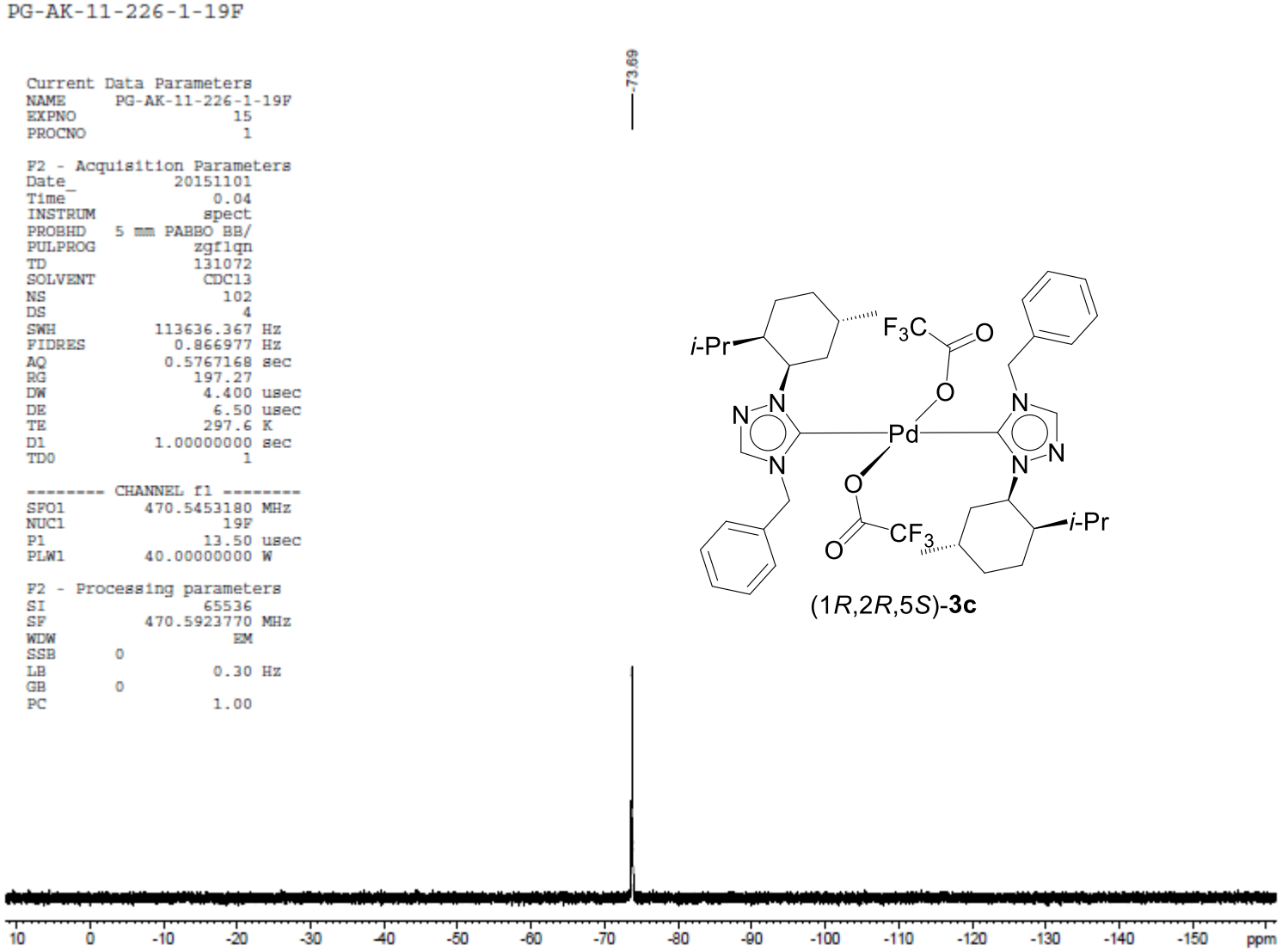


Figure S85. $^{19}F\{^{1}H\}$ NMR spectrum of (1*R*,2*R*,5*S*)-**3c** in $CDCl_3$.

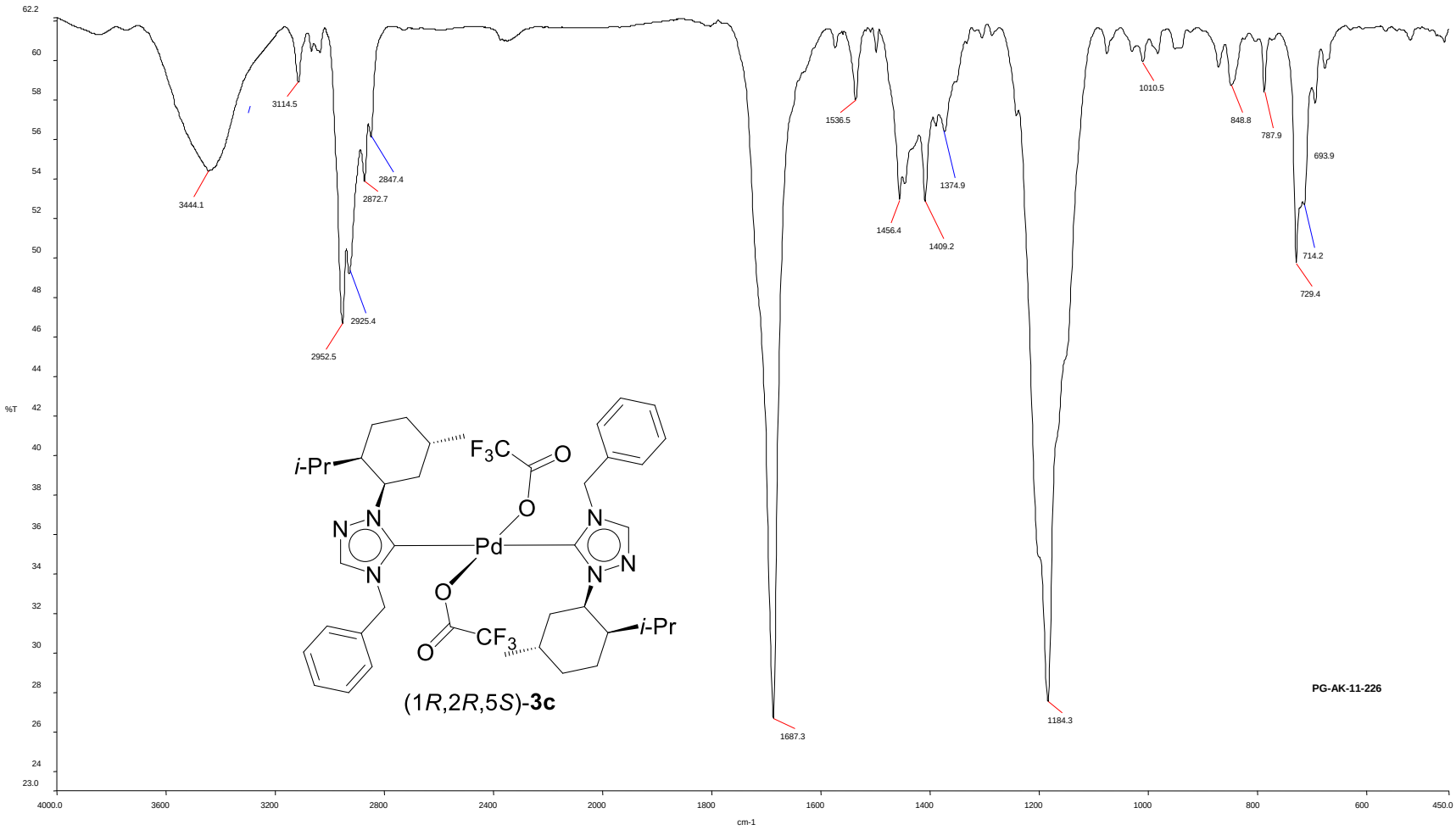


Figure S86. Infrared spectrum of 1*R*,2*R*,5*S*-**3c** in KBr.

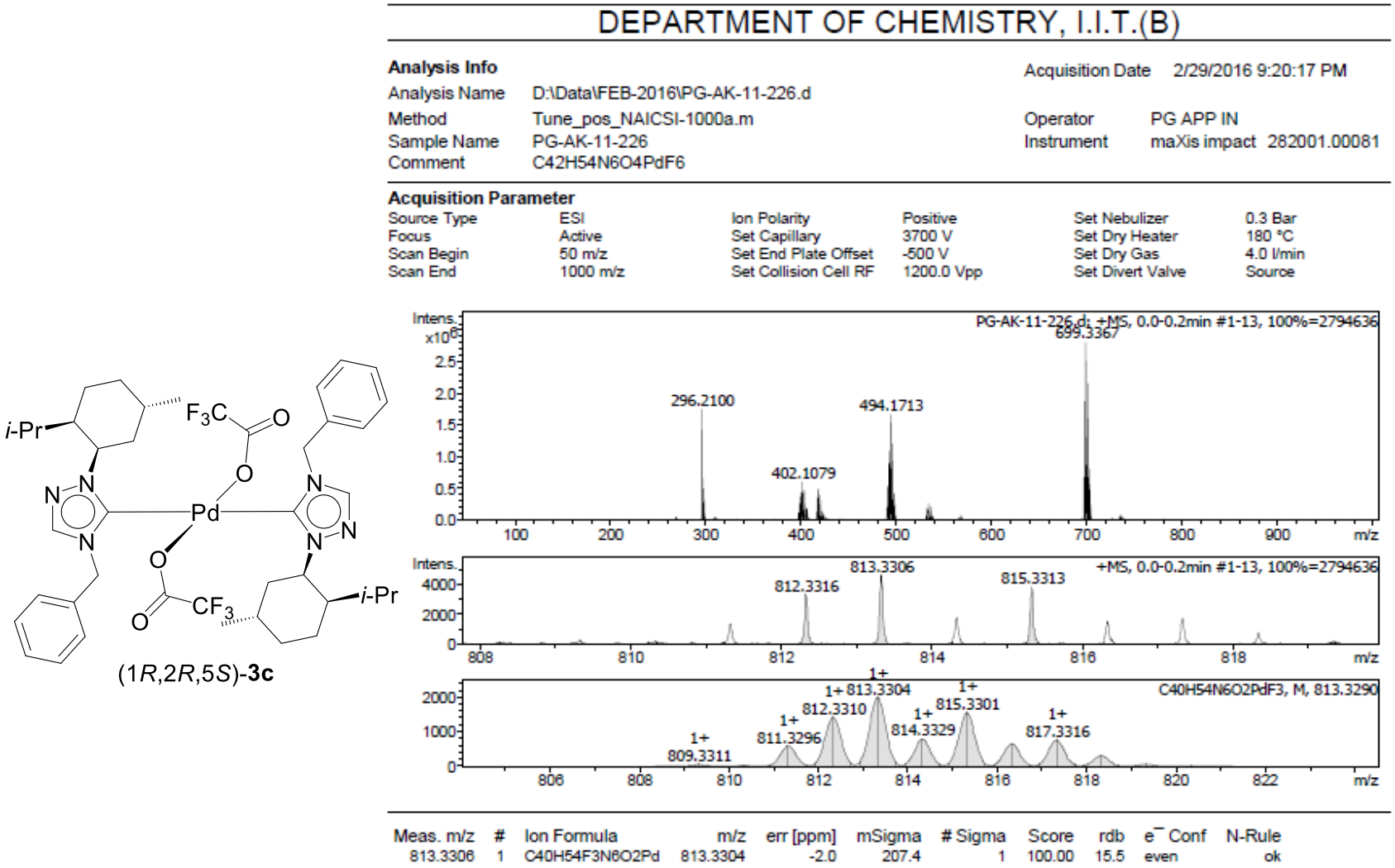
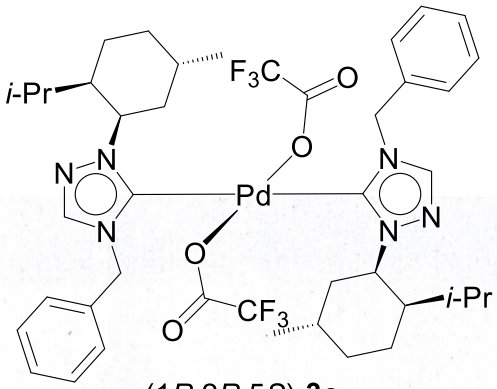


Figure S87. High Resolution Mass Spectrometry (HRMS) data of 1*R*,2*R*,5*S*-**3c**.



(1*R*,2*R*,5*S*)-**3c**

Eager 300 Report

Page: 1 Sample: PG-AK-11-226-1 (PG-AK-11-226-1)

Method Name	: PGCP13102015		
Method File	: D:\CHNS-2015\PGCP13102015.mth		
Chromatogram	: PG-AK-11-226-1		
Operator ID	: CHANDNI	Company Name	: C.E. Instruments
Analysed	: 10/13/2015 14:29	Printed	: 10/13/2015 18:36
Sample ID	: PG-AK-11-226-1 (# 20)	Instrument N.	: Instrument #1
Analysis Type	: UnkNown (Area)	Sample weight	: 1.044

Calib. method : using 'K Factors'

!!! Warning missing one or more peaks.

Element Name	%	Ret.Time	Area	BC	Area ratio	K factor
Nitrogen	8.7208	41	98597	RS	14.867610	.108295E+07
Carbon	53.7587	63	1465902	RS	1.000000	.260680E+07
Hydrogen	5.5882	178	402959	RS	3.637844	.665180E+07
Totals	68.0677		1967458			

Figure S88. Elemental analysis data of (1*R*,2*R*,5*S*)-**3c**.

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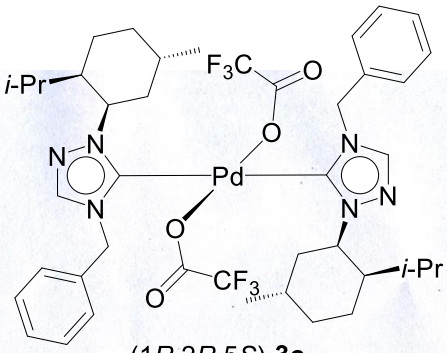
Tuesday, 27-OCT-2015

This sample was measured on an Autopol IV, Serial #82083
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Lot ID : pg

Set Temperature : 25.0
Time Delay : Disabled
Temperature Correction : OFF



(1*R*,2*R*,5*S*)-**3c**

n	Average	Std.Dev.	Maximum	Minimum
5	-44.424	0.0675	-44.303	-44.454

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	pg-ak-11-226-1	17:12:09	-44.454	SR	-0.222	589	50.00	1.000	24.9
2	pg-ak-11-226-1	17:12:16	-44.454	SR	-0.222	589	50.00	1.000	24.9
3	pg-ak-11-226-1	17:12:23	-44.454	SR	-0.222	589	50.00	1.000	24.9
4	pg-ak-11-226-1	17:12:29	-44.454	SR	-0.222	589	50.00	1.000	24.9
5	pg-ak-11-226-1	17:12:36	-44.303	SR	-0.222	589	50.00	1.000	24.9

Figure S89. Specific rotation of (1*R*,2*R*,5*S*)-**3c** in $CHCl_3$.

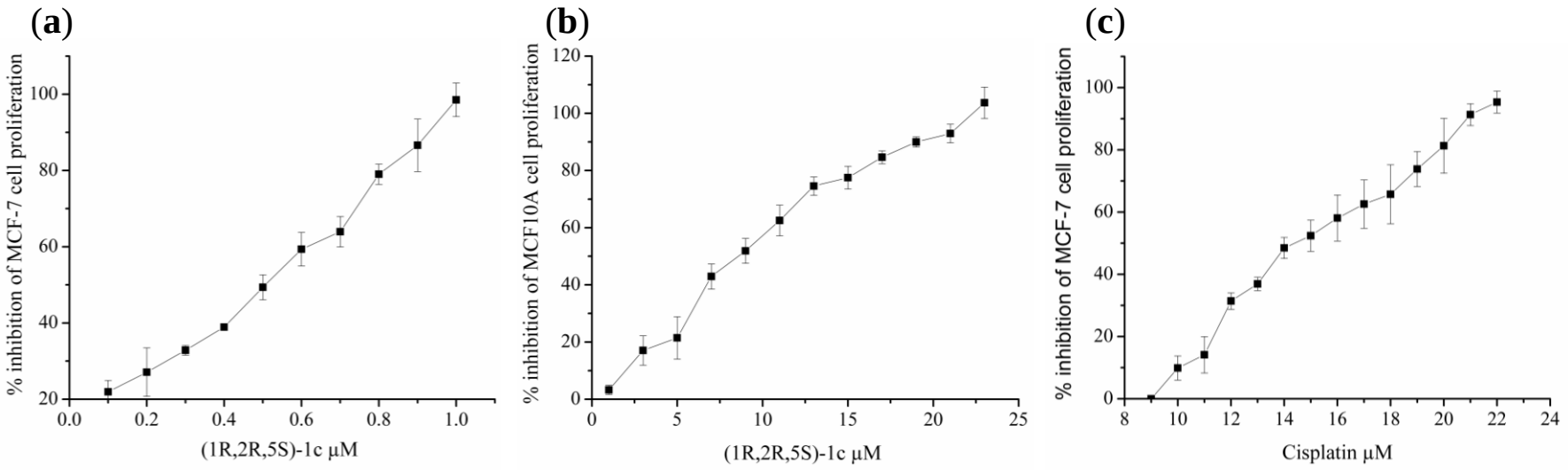


Figure S90. Antiproliferative activity of (*1R,2R,5S*)-**1c** against (**a**) MCF-7 and (**b**) MCF10A. (**c**) Antiproliferative activity of cisplatin against MCF7 measured using sulforhodamine B assay. The experiment was performed three times and average data was plotted. Error bars indicate standard deviation.

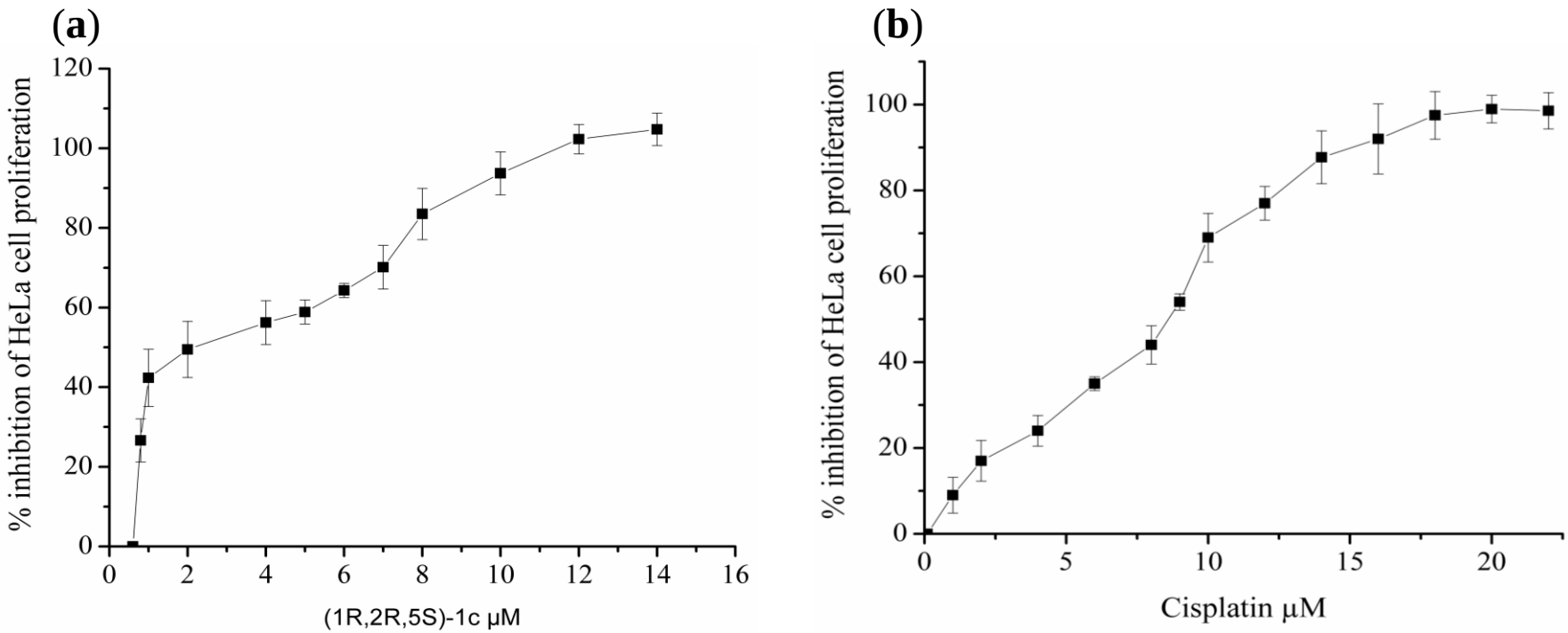


Figure S91. Antiproliferative activity of (**a**) (*1R,2R,5S*)-**1c** and (**b**) cisplatin against HeLa measured using sulforhodamine B assay. The experiment was performed three times and average data was plotted. Error bars indicate standard deviation.

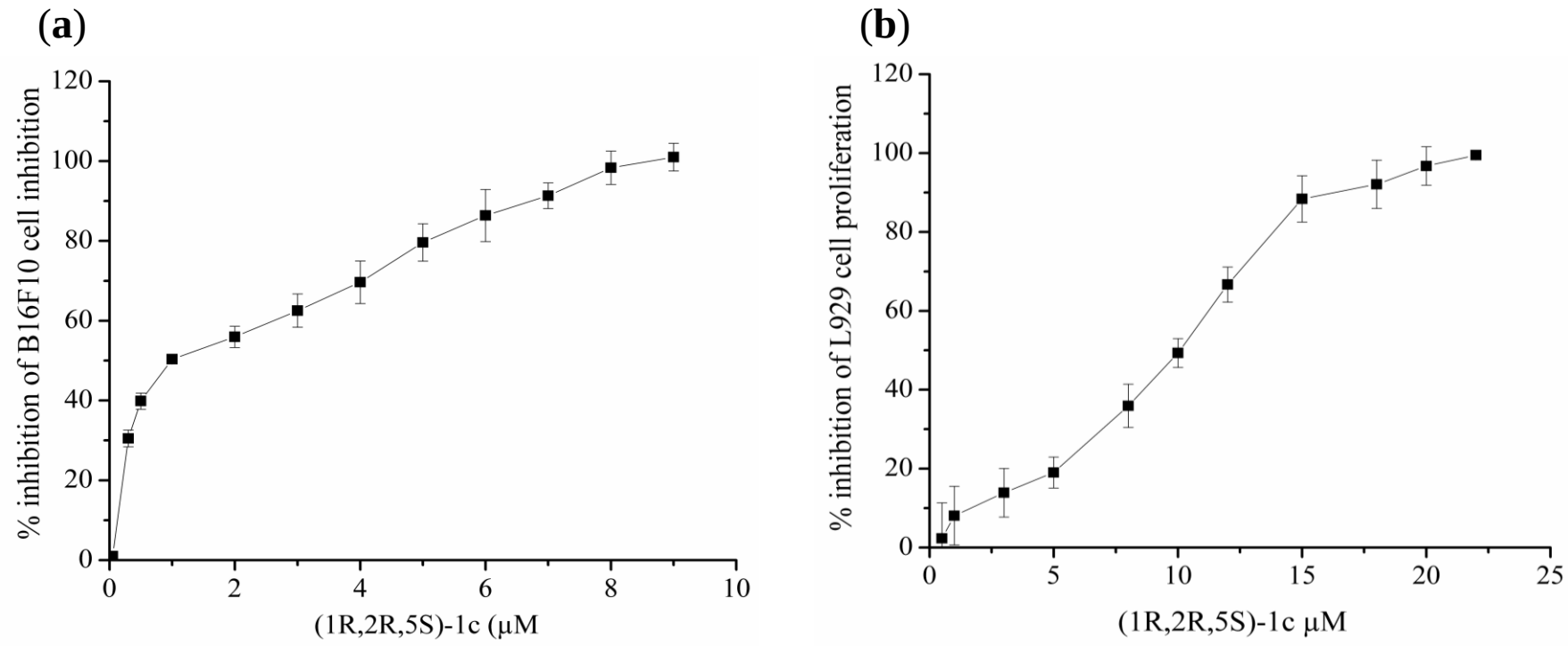


Figure S92. Antiproliferative activity of (*1R,2R,5S*)-**1c** against (**a**) B16F10 and (**b**) L929 measured using sulforhodamine B assay. The experiment was performed three times and average data was plotted. Error bars indicate standard deviation.

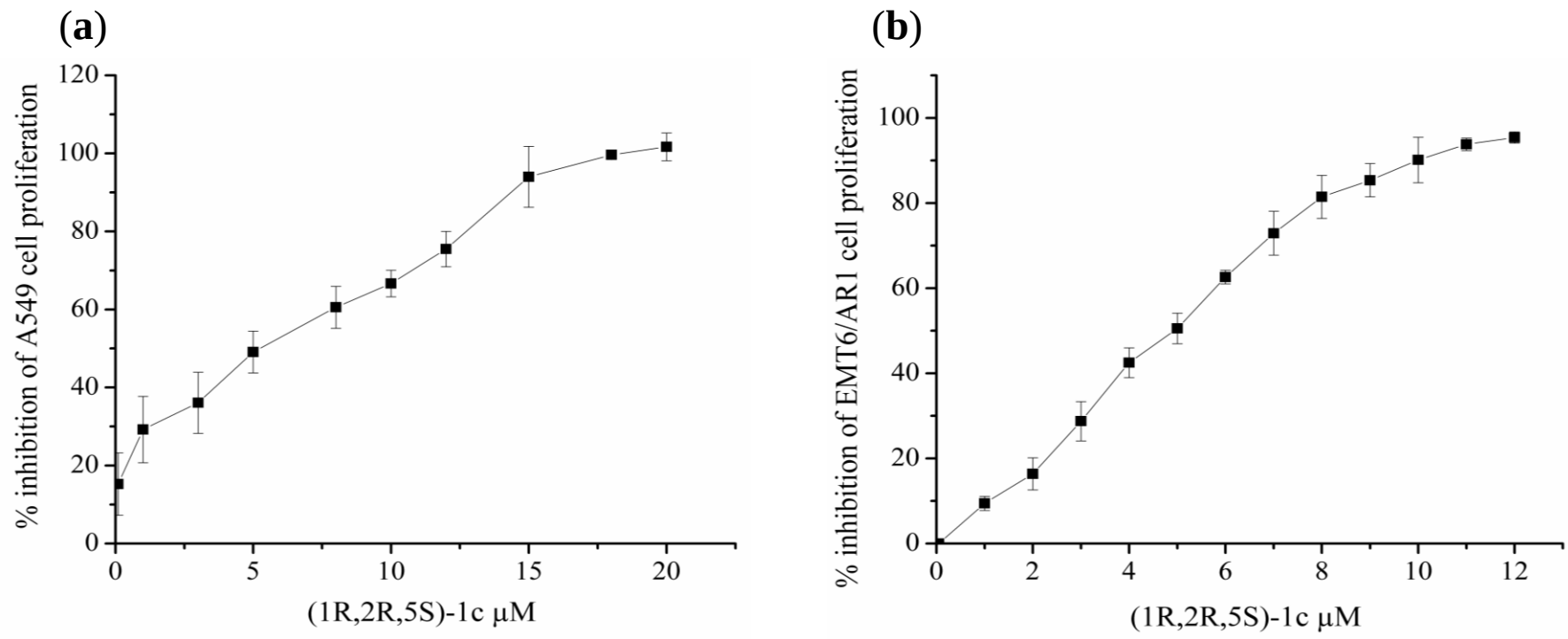
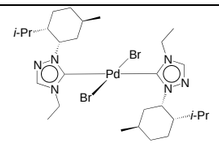
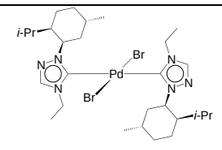
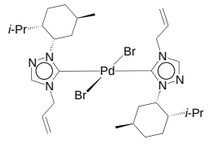
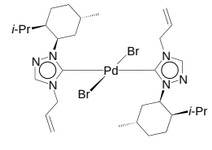
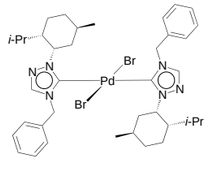
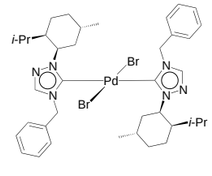
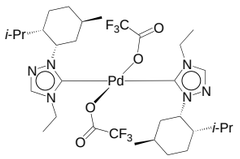
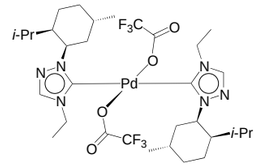
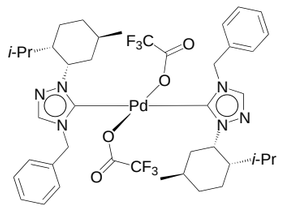
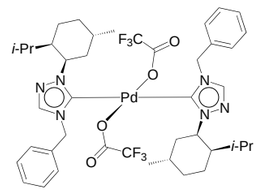


Figure S93. Antiproliferative activity of (*1R,2R,5S*)-**1c** against (**a**) A549 and (**b**) EMT6/AR1 cells measured using sulforhodamine B assay. The experiment was performed three times and average data was plotted. Error bars indicate standard deviation.

Table S1. X-ray crystallographic data for (1*R*,2*R*,5*S*)(**1**−**3**)**b**, (1*S*,2*S*,5*R*)-**2b**, (1*S*,2*S*,5*R*)-**1c**, (1*R*,2*R*,5*S*)-**1c**, (1*S*,2*S*,5*R*)-**3c** and (1*R*,2*R*,5*S*)-**3c**.

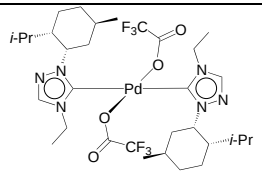
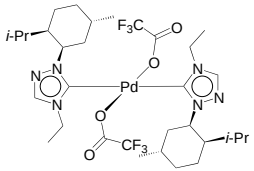
Compound	(1*R*,2*R*,5*S*)-**1b**	(1*S*,2*S*,5*R*)-**2b**	(1*R*,2*R*,5*S*)-**2b**	(1*R*,2*R*,5*S*)-**3b**	(1*S*,2*S*,5*R*)-**1c**	(1*R*,2*R*,5*S*)-**1c**	(1*S*,2*S*,5*R*)-**3c**	(1*R*,2*R*,5*S*)-**3c**
Lattice	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Formula	$C_{28}H_{50}N_6PdBr_2$	$C_{30}H_{50}N_6PdBr_2$	$C_{30}H_{50}N_6PdBr_2$	$C_{76}H_{108}N_{12}Pd_2Br_4$	$C_{32}H_{50}N_6F_6PdO_4$	$C_{96}H_{150}N_{18}F_{18}Pd3O_{12}$	$C_{42}H_{54}N_6F_6PdO_4$	$C_{42}H_{54}N_6F_6PdO_4$
Formula weight	736.96	760.98	760.97	1722.18	803.18	2409.53	927.31	927.31
Space group	*P*1	*P*1	*P*1	*P*1	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a/Å	8.095(2)	7.7060(15)	7.715(4)	11.565(3)	10.561(2)	18.899(5)	9.702(3)	9.734(6)
b/Å	14.812(4)	7.8581(16)	7.865(4)	13.039(3)	11.169(2)	11.212(3)	20.111(6)	20.3275(10)
c/Å	15.641(4)	14.256(3)	14.299(7)	13.719(3)	16.133(3)	27.511(7)	11.874(4)	11.937(7)
α/°	66.874(12)	101.44(3)	101.479(8)	98.396(4)	90.00	90.00	90.00	90.00
β/°	76.588(14)	95.42(3)	95.384(5)	95.925(4)	92.303(3)	95.294(4)	109.578(3)	109.531(8)
γ/°	77.346(14)	90.11(3)	90.079(7)	101.192(3)	90.00	90.00	90.00	90.00
V/Å^3	1660.4(7)	842.1(3)	846.3(7)	1989.1(8)	1901.4(6)	5805(3)	2182.9(12)	2226.0(19)
Z	2	1	1	1	2	2	2	2
Temperature (K)	150(2)	150(2)	273	150(2)	100(2)	150(2)	100(2)	150(2)
Radiation (λ,Å)	0.71075	0.71073	0.71070	0.71075	0.7107	0.71075	0.7107	0.71070
ρ (calcd.), g cm^{-3}	1.474	1.501	1.493	1.438	1.403	1.379	1.411	1.383
θ max, deg.	25.00	32.4597	29.13	25.00	29.20	25.00	29.14	25.00
No. of data	11225	7372	5340	13098	6953	18768	5437	7729
No. of parameters	683	358	352	859	450	1348	538	538
R_1	0.0258	0.0373	0.0553	0.0369	0.0397	0.0719	0.0571	0.0763
wR_2	0.0529	0.0670	0.1204	0.0823	0.0793	0.1488	0.0925	0.1545
GOF	0.892	0.929	1.151	1.086	1.030	1.057	0.857	1.044
Flack	0.007(5)	0.009(6)	0.941(17)	0.015(6)	-0.035(14)	-0.02(2)	-0.03(4)	0.05(4)

Table S2. Anticancer activity of chiral Pd–NHC complexes, (*1S,2S,5R*)-(**1–3)b** and (*1R,2R,5S*)-(**1–3)b,** (*1S,2S,5R*)-(**1**, **3)c** and (*1R,2R,5S*)-(**1,3)c**, against MCF-7 cells.

S. No.	compound	$[\alpha]_D^{25}$	IC_{50} (μM)	compound	$[\alpha]_D^{25}$	IC_{50} (μM)
1	 (*1S,2S,5R*)-**1b**	– 29.4	2.2 ± 0.1	 (*1R,2R,5S*)-**1b**	+ 29.8	2.3 ± 1
2	 (*1S,2S,5R*)-**2b**	– 41.7	≈ 10	 (*1R,2R,5S*)-**2b**	+ 39.4	≈ 10
3	 (*1S,2S,5R*)-**3b**	– 45.2	> 10	 (*1R,2R,5S*)-**3b**	+ 45.0	> 10
4	 (*1S,2S,5R*)-**1c**	+ 47.8	0.7 ± 0.005	 (*1R,2R,5S*)-**1c**	– 48.0	0.55 ± 0.02
5	 (*1S,2S,5R*)-**3c**	+ 40.2	>10	 (*1R,2R,5S*)-**3c**	– 44.4	> 10

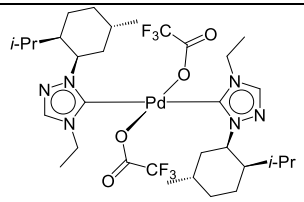
Data are average IC_{50} values from three independent set of experiments and ± indicates S.D.

Table S3. Anticancer activity of chiral Pd–NHC complexes (*1S,2S,5R*)-**1c** and (*1R,2R,5S*)-**1c**, against MCF-7 and HeLa cells in comparison to cisplatin.

S. No.	compound	MCF-7 IC_{50} (μM)	Hela IC_{50} (μM)
1	 (*1S,2S,5R*)-**1c**	0.7 ± 0.005	2.6 ± 1.6
2	 (*1R,2R,5S*)-**1c**	0.55 ± 0.02	2.3 ± 1
3	cisplatin	14.9 ± 0.4	8.5 ± 0.7

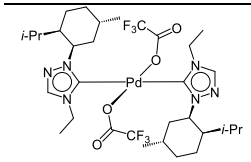
Data are average IC_{50} values from three independent set of experiments and ± indicates S.D.

Table S4. Anticancer activity of the most potent complex (*1R,2R,5S*)-**1c** against various cancer cell lines.

compound	IC_{50} (μM) values				
	MCF-7 (breast cancer)	HeLa (cervical cancer)	A549 (lung cancer)	B16F10 (skin cancer)	EMT6/AR1 (multidrug resistant mammary cancer)
 (1*R*,2*R*,5*S*)-**1c**	0.55 ± 0.02	2.3 ± 1	5.7 ± 1.6	1.3 ± 0.4	4.8 ± 0.3

Data are average IC_{50} values from three independent set of experiments and ± indicates S.D.

Table S5. IC_{50} values of complex (*1R,2R,5S*)-**1c** against MCF-7 and B16F10 in comparison to their respective noncancerous counterparts MCF10A and L929.

compound	MCF-7 IC_{50} (µM)	MCF10A IC_{50} (µM)	B16F10 IC_{50} (µM)	L929 IC_{50} (µM)
 (*1R,2R,5S*)-**1c**	0.55 ± 0.02	8.6 ± 0.9	1.3 ± 0.4	10.5 ± 0.2

Data are average IC_{50} values from three independent set of experiments and ± indicates S.D.