Supporting Information

Cinchonidine Thiourea Catalyzed Asymmetric Addition of Phenols to Oxindole Derivatives

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1) General Methods and Materials.

(A) General Methods:

All reactions were performed in oven-dried glassware. All solvents and commercially available chemical were used without further purification. The molecular sieves were activated at 200 ˚C for 2 hours in an oven. The column chromatography was carried out on a column packed with silica gel 60-120 using mixtures of hexane and ethyl acetate as an eluents. ^{1}H NMR spectra were recorded in $CDCl_3$ on a BRUKER AVANCE III (500 MHz), JNM-ECS400 (400 MHz), BRUKER AVANCE II (400 MHz) and JEOL (300 MHz) spectrometer. ^{13}C NMR spectra were recorded in $CDCl_3$ on BRUKER AVANCE III (125 MHz), JNM-ECS400 (100 MHz), BRUKER AVANCE II (100 MHz) and JEOL (75 MHz). Chemical shifts (δ) are expressed in ppm downfield from internal TMS. MS were recorded on micrOTOF-Q II 10356 Mass Spectrometer. Optical rotation was determined with AUTOPOL IV polarimeter at 25 ˚C using sodium D light. Enantiomeric excess was determined by using Shimadzu LC-20AD using Daicel Chiralpak IA, IB and IC column.

(B) Material:

Catalysts **1a**, **1b, 2a and 2b** were purchased from Sigma Aldrich. The catalysts **1c**, **1d**, **2c, 2d, 3a, 3b, 4a, 4b, 6a and 6b** were synthesized by the procedures reported in literature.[1] The catalyst **5** was synthesized by the reported procedure by S. Mukherjee and et al.[2] The catalyst **7** and **8** was prepared according to our previously reported method.[3] Isatins were commercially available from Spectrochem, India. The *N*-methyl, *N*-allyl or *N*-benzyl protected isatins were prepared according to the literature method.[4]

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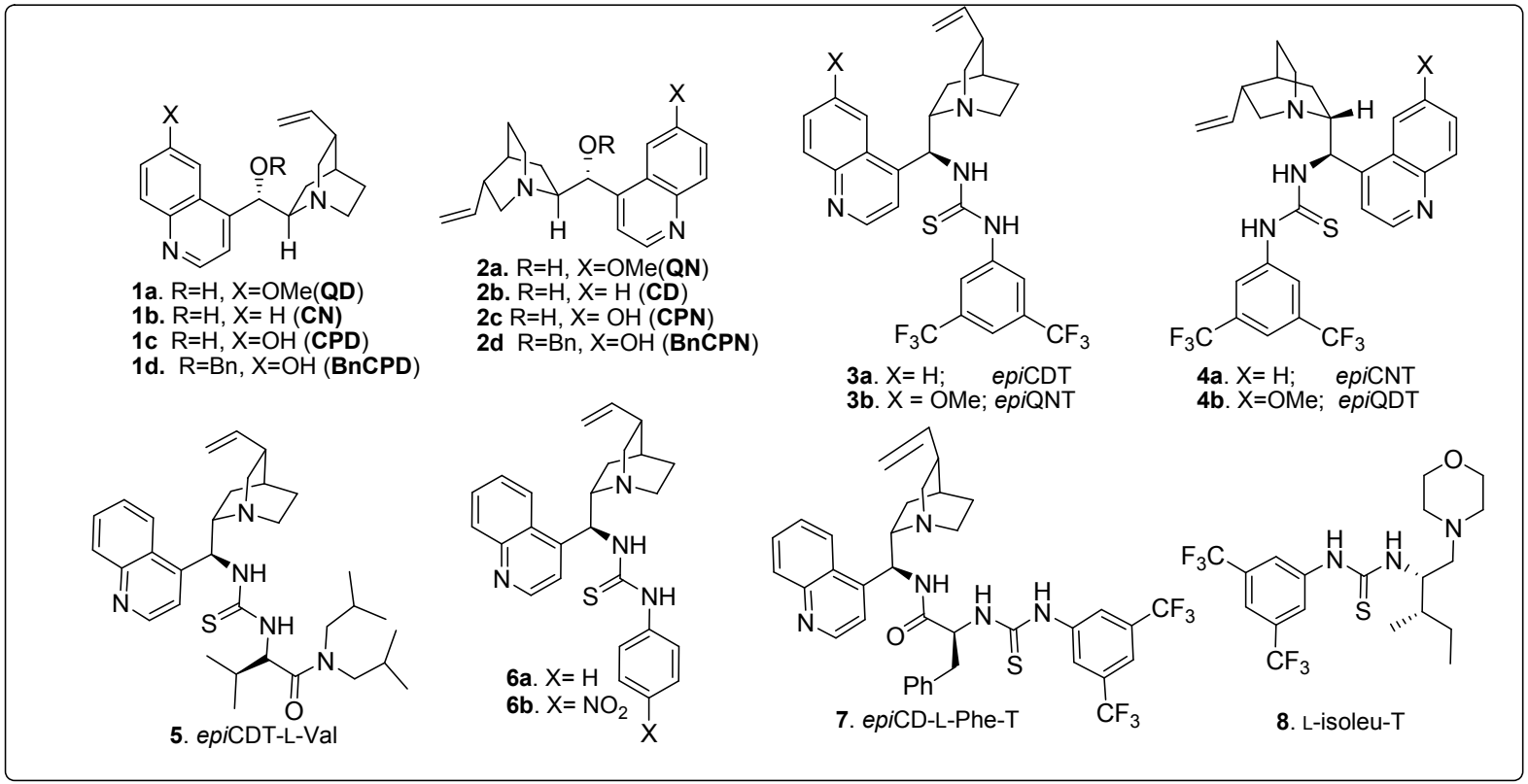
[1] (a) Li, H.; Wang, Y.; Tang, L.; Deng, L. *J. Am. Chem. Soc.* **2004**, *126*, 9906. (b) Li, H.; Wang, B.; Deng, L. *J. Am. Chem. Soc.* **2006**, *128*, 732. (c) Wang, Y.; Liu, X.; Deng, L. *J. Am. Chem. Soc.* **2006**, *128*, 3928. (d) Iwabuchi, Y.; Nakatani, M.; Yokoyama, N.; Hatakeyama S. *J. Am. Chem. Soc.* **1998**, *121*, 10219. (e).Vakulya, V; Varga, S.; Csámpai, A.; Soos, T. *Org. Lett.* **2005**, *7*, 1967.

[2] Manna, M.S.; Kumar, V.; Mukherjee, S. *Chem. Commun*., **2012**,*48*, 5193.

[3] (a) Kumar, A.; Singh, S.; Kumar, V.; Chimni, S. S. *Org. Biomol. Chem*. **2011**, *9*, 2731. (b) Kaur, J.; Kumar, A.; Chimni, S.S. *Tetrahedron Lett*. **2014**, *55*, 2138.

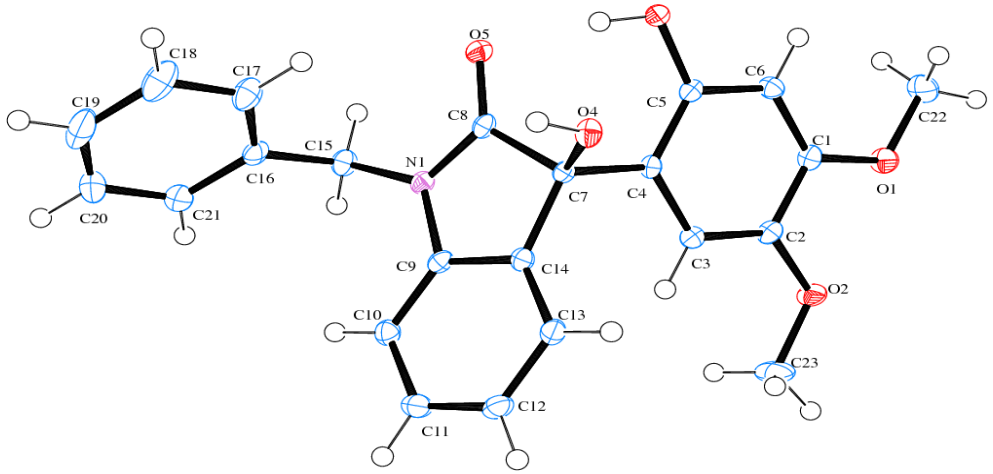
2) Experimental details and characterization data.



Structure of organocatalysts used

(3) Crystal data for enantiopure product (11a)

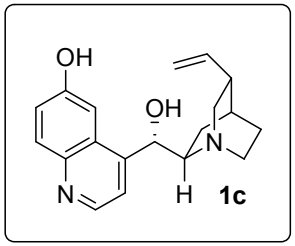
[4] Overman L. E. , Peterson E. A., *Tetrahedron*, **2003**, *59*, 6905.



Chemical formula	$C_{23}H_{21}NO_5$
Formula Mass	391.41
Crystal system	Monoclinic
Colour	Colourless
a/Å	8.4183(14)
b/Å	12.2957(19)
c/Å	9.3671(16)

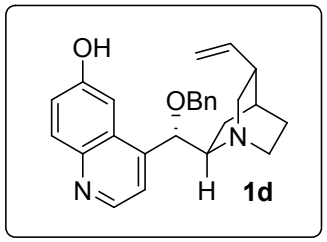
α/°	90.00
β/°	97.016(6)
γ/°	90.00
Unit cell volume/Å^3	962.3(3)
Temperature/K	100(2)
Space group	P 21
No. of formula units per unit cell, Z	2
No. of reflections measured	6247
Final R_1 values (all data)	0.0379
Final $wR(F^2)$ values (all data)	0.0965
Goodness of fit on F^2	1.020
Flack parameter	0.4(7)
CCDC number	1022904

Cupreidine (CPD) (1c)



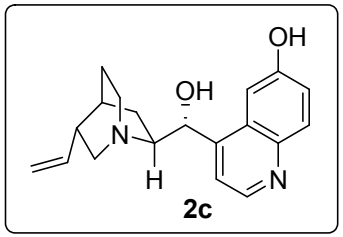
White Solid, mp: 130-140℃ , 90% yield, $[\alpha]_D^{25}$ = +240.0 (c 1.0 EtOH); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (d, J= 5.0 Hz, 1H), 7.94-8.02 (m, 1H), 7.60 (d, J= 5.0 Hz, 1H), 7.28-7.42 (m, 2H), 6.07 (d, J= 5.0 Hz, 2H), 5.02-5.08 (m, 2H), 3.83-3.87 (m, 1H), 2.64-3.05 (m, 2H), 2.17-2.35 (m, 3H), 1.72 (s, 1H), 0.27-1.40 (m, 2H), 0.82-0.91 (m, 1H); ^{13}C (125 MHz, $CDCl_3$) δ 18.38, 25.44, 27.97, 36.51, 39.40, 49.21, 59.29, 70.34, 103.8, 155.4, 117.6, 123.3, 126.5, 131.6, 139.6, 143.0, 146.4, 146.7, 157.8.

9-*O*-Benzylcupreidine (BnCPD) (1d)



White Solid, mp: 125-127℃ , 85% yield, $[\alpha]_D^{25}$ = +154.3.0 (c 1.0 $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (d, J= 5.0 Hz, 1H), 8.03 (d, J= 10.0 Hz, 1H), 7.28-7.46 (m, 8H), 6.83 (s, 1H), 5.77-5.83 (m, 1H), 5.01-5.09 (m, 2H), 4.76 (d, J= 10.0 Hz, 1H), 4.57 (d, J= 10.0 Hz, 1H), 4.15-4.18 (m, 1H), 3.26-3.75 (m, 5H), 2.42-2.62 (m, 2H), 1.81-2.03 (m, 3H), 1.26 (d, J= 15.0 Hz, 2H) ; ^{13}C (125 MHz, $CDCl_3$) δ 18.47, 23.22, 27.42, 36.98, 48.43, 49.40, 59.70, 72.06, 75.27, 103.6, 117.5, 117.8, 122.9, 126.6, 128.1, 128.3, 128.4, 128.6, 132.1, 135.8, 136.8, 139.6, 144.0, 146.6, 156.7; m/z (ESI): 401.2201 $(M+1)^+$.

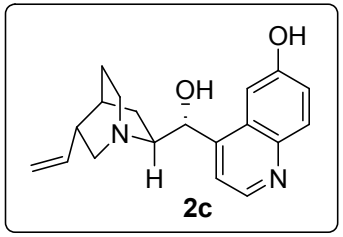
Cupreine (CPN) (2c)



2c

Light Brown Solid, mp: 168-170℃, 90% yield, $[\alpha]_D^{25}$ = -163.0 (c 1.0 EtOH); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (d, J= 4.0 Hz, 1H), 7.93 (d, J= 9.0 Hz, 1H), 7.56 (d, J= 5.0 Hz, 1H), 7.31-7.33 (m, 1H), 7.10 (d, J= 2.0 Hz, 1H), 5.78 (s, 1H), 5.53-5.57 (m, 2H), 4.84-4.88 (m, 2H), 3.90-3.97 (m, 5H), 2.90-3.01 (m, 3H), 2.72 (s, 1H), 2.56 (s, 1H), 2.32 (s, 1H), 1.82-1.92 (m, 3H), 1.55 (d, J= 3.0 Hz, 1H), 1.24 (d, J= 3.0 Hz, 1H); ^{13}C (125 MHz, $CDCl_3$) δ 14.69, 21.54, 24.22, 27.42, 38.71, 40.05, 44.22, 53.44, 53.87, 57.61, 67.39, 74.73, 89.01, 99.98, 111.1, 115.6, 118.5, 123.5, 127.3, 132.3, 141.9, 142.9, 156.9, 161.6; m/z (ESI): 311.1731 $(M+1)^+$.

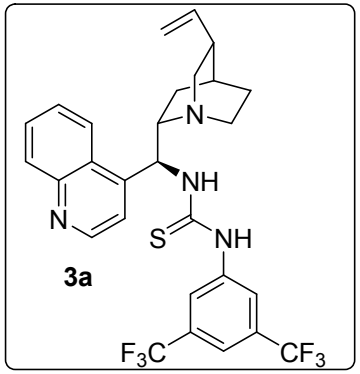
9-*O*-Benzylcupreine (BnCPN) (2d)



2c

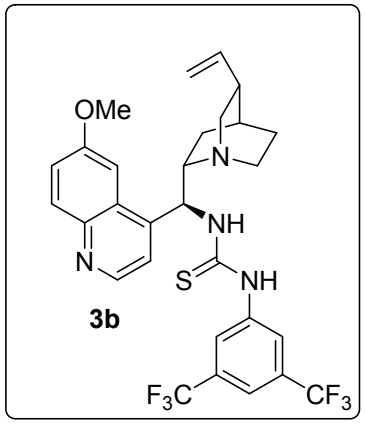
White Solid, mp: 208-210℃, 85% yield, $[\alpha]_D^{25}$ = -79.0 (c 1.0 EtOH); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, J=5.0 Hz, 1H), 8.05 (d, J= 10.0 Hz, 1H), 7.82 (d, J= 5.0 Hz, 1H), 7.49 (s, 1H), 7.28-7.41 (m, 7H), 5.99 (s, 1H), 5.61-5.65 (m, 1H), 5.02-5.07 (m, 2H), 4.50-4.60 (m, 2H), 3.35-3.43 (m, 2H), 3.05 (d, J= 10.0 Hz, 2H), 2.59 (s, 1H), 1.51-2.18 (m, 5H); ^{13}C (75 MHz, $CDCl_3$) δ 23.09, 27.30, 32.70, 46.33, 50.35, 53.92, 56.31, 72.42, 105.4, 118.9, 122.3, 126.9, 131.3, 141.6, 143.1, 146.7, 156.7; m/z (ESI): 401.2204 $(M+1)^+$.

1-(3,5-Bis(trifluoromethyl)phenyl)-3-(*S*)-(quinolin-4-yl)(8-vinylquinuclidin-2-yl)methyl thiourea (CDT) (3a)



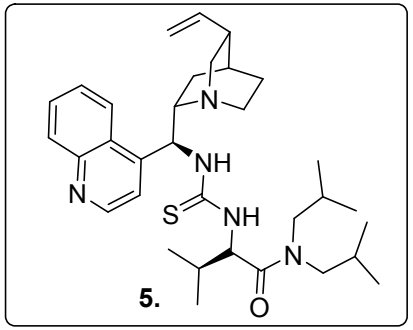
Yellow Solid, mp: 122-123 ℃, 92% yield, $[\alpha]_D^{25}$ = -53.7 (c 0.37 $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.91 (d, J= 5.0 Hz, 1H), 8.50 (s, 1H), 8.18 (d, J= 10.0 Hz, 1H), 8.01 (s, 1H), 7.05-7.81 (m, 5H), 5.65 (d, J= 10.0 Hz, 1H), 5.05-5.08 (m, 2H), 3.00-3.72 (m, 5H), 2.54 (s, 1H), 2.33 (s, 1H), 1.89-1.97 (m, 2H), 1.52 (d, J= 15.0 Hz, 1H), 1.27 (s, 1H), 1.15 (br, s, 1H); ^{13}C (125 MHz, $CDCl_3$) δ 24.78, 26.18, 26.98, 26.69, 38.13, 41.64, 54.63, 57.05, 116.0, 123.9, 124.4, 125.3, 126.1, 127.0, 129.2, 129.4, 130.4, 148.6, 150.3, 180.9; m/z (ESI): 565.1 $(M+1)^+$.

1-(3,5-bis(trifluoromethyl)phenyl)-3-((*S*)-(6-methoxyquinolin-4-yl)(8-vinylquinuclidin-2-yl)methyl)thiourea (QNT) (3b)



Yellow Solid, mp: 120-121 ℃, 93% yield, $[\alpha]_D^{25}$ = -127.0 (c 0.5 $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.05-8.17 (m, 3H), 7.41-7.58 (m, 3H), 6.81 (s, 1H), 5.64-5.71 (m, 1H), 5.15-5.21 (m, 2H), 4.06 (s, 3H), 3.21-3.72 (m, 5H), 2.74 (s, 1H), 2.06-2.16 (s, 1H), 1.78 (d, J= 15.0 Hz, 1H), 0.86-1.22 (m, 3H); ^{13}C (125 MHz, $CDCl_3$) δ 24.40, 26.67, 29.68, 36.94, 41.84, 54.13, 57.95, 64.90, 102.7, 115.2, 122.9, 127.6, 128.6, 128.7, 129.8, 131.5, 131.9, 132.1, 156.2, 179.3; HRMS calcd. for $[C_{29}H_{28}F_6N_4OS]^+$: 594.1882; found: 594.1876.

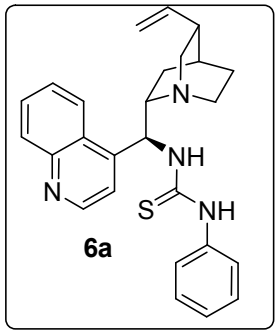
1-((*S*)-1-(diisobutylcarbamoyl)-2-methylpropyl)-3-((*S*)-(quinolin-4-yl)(8-vinylquinuclidin-2-yl)methyl)thiourea (5)



5.

White Solid, mp: 109-110 ℃, 84% yield, ^1H NMR (500 MHz, $CDCl_3$) δ 8.88 (d, J= 5.0 Hz, 1H), 8.50 (d, J= 10.0 Hz, 1H), 8.13 (d, J= 10.0 Hz, 1H), 7.25-7.73 (m, 3H), 7.28 (s, 1H), 6.69 (s, 1H), 5.59-5.66 (m, 2H), 5.38 (s, 1H), 4.90-4.97 (m, 2H), 3.59 (s, 1H), 2.78-3.28 (m, 10H), 2.33 (s, 1H), 1.03-1.98 (m, 8H), 0.76-0.92 (m, 21H); ^{13}C (125 MHz, $CDCl_3$) δ 16.23, 19.41, 19.49, 19.68, 19.75, 19.99, 20.22, 20.30, 25.23, 25.60, 26.23, 27.34, 28.02, 29.66, 31.86, 39.15, 40.76, 53.35, 55.45, 59.29, 76.82, 115.0, 123.4, 127.3, 129.5, 130.5, 140.6, 148.7, 150.2, 172.1, 181.6.

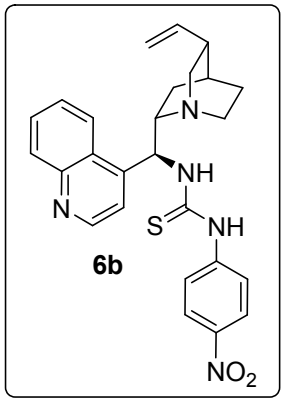
1-phenyl-3-((*S*)-(quinolin-4-yl)(8-vinylquinuclidin-2-yl)methyl)thiourea (6a)



6a

Brown Solid, mp: 125-127℃, 90% yield, ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.54 (s, 1H), 8.15 (d, J= 10.0 Hz, 1H), 7.22-7.76 (m, 8H), 6.29 (s, 1H), 5.54-5.65 (m, 1H), 5.01-5.03 (m, 2H), 2.93-3.58 (m, 4H), 2.44 (s, 1H), 1.78-1.91 (m, 2H), 1.13-1.47 (m, 4H); ^{13}C (125 MHz, $CDCl_3$) δ 24.78, 26.17, 26.98, 27.52, 29.70, 38.11, 41.62, 54.62, 116.1, 123.8, 124.4, 125.3, 126.1, 127.1, 129.2, 129.4, 129.6, 130.4, 148.6, 150.3, 150.7, 180.9.

1-(4-nitrophenyl)-3-((*S*)-(quinolin-4-yl)(8-vinylquinuclidin-2-yl)methyl)thiourea (6b)



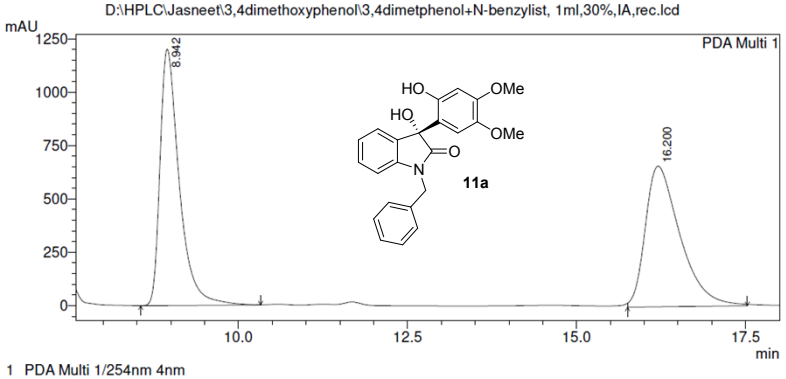
6b

White Solid, mp: 110-112℃, 92% yield, ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.93 (d, J=5.0 Hz, 1H), 8.50 (s, 1H), 8.12-8.17 (m, 2H), 7.28-7.79 (m, 5H), 6.63 (d, J= 10.0 Hz, 1H), 5.61-5.68 (m, 1H), 5.04-5.08 (m, 2H), 3.37-3.74 (m, 3H), 3.01-3.03 (m, 2H), 2.51 (s, 1H),

1.87-2.06 (m, 3H), 1.12-1.54 (m, 3H); ^{13}C (125 MHz, $CDCl_3$) δ 24.62, 25.87, 26.80, 37.84, 41.88, 54.53, 61.13, 113.3, 116.4, 121.6, 123.7, 124.5, 126.5, 127.5, 129.7, 130.4, 143.5, 145.0, 148.5, 156.2, 180.5.

HPLC chromatograms

==== Shimadzu LCsolution Analysis Report ====



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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1	8.942	23807734	1201821	50.202	64.580
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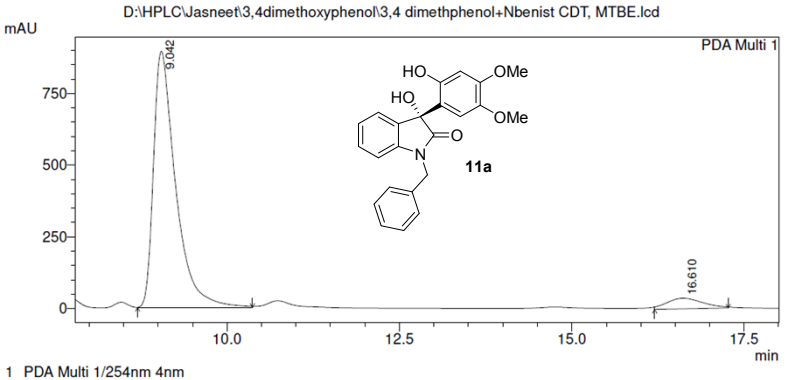
Total		47423847	1860984	100.000	100.000



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PeakTable

PDA Ch1 254nm 4nm

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1	9.042	19949335	894002	93.736	96.028
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Total		21282440	930985	100.000	100.000

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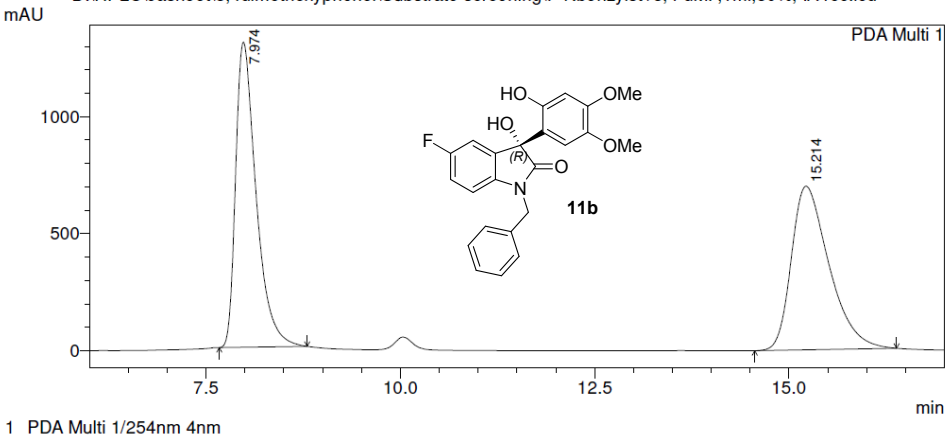

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PeakTable

PDA Ch1 254nm 4nm

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1	7.974	23876611	1303855	50.340	65.094
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Total		47431094	2003048	100.000	100.000

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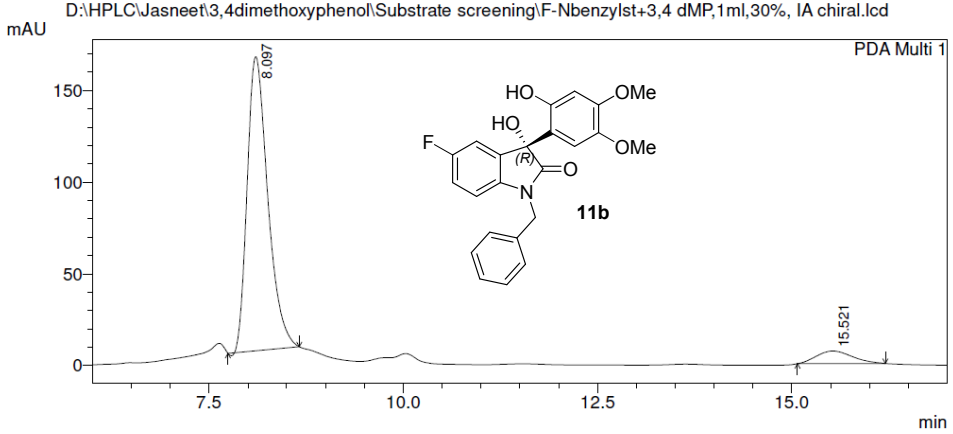

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PeakTable

PDA Ch1 254nm 4nm

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1	8.097	2957524	160303	93.068	95.900
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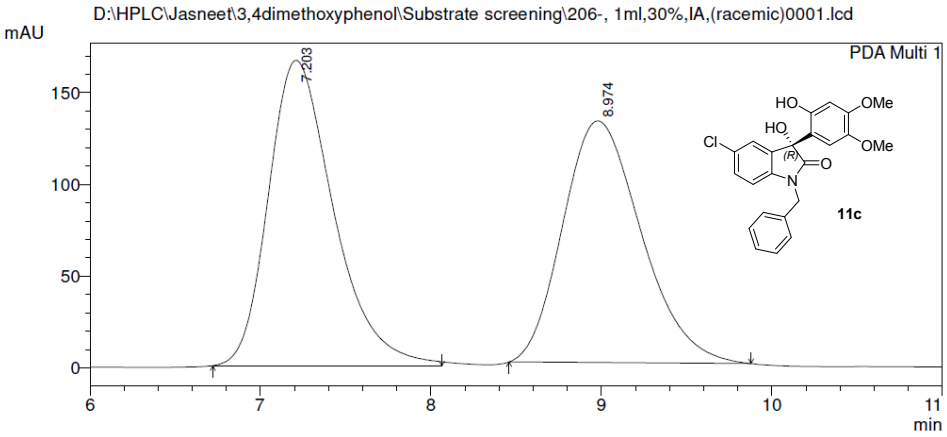
Total		3177799	167157	100.000	100.000



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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1	7.203	4437178	166637	51.278	55.848
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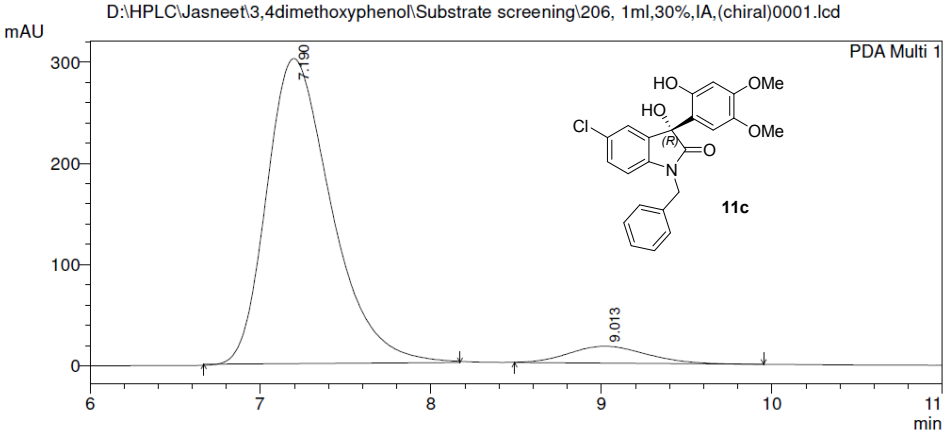
Total		8653210	298376	100.000	100.000



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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1	7.190	7950834	301712	93.827	94.770
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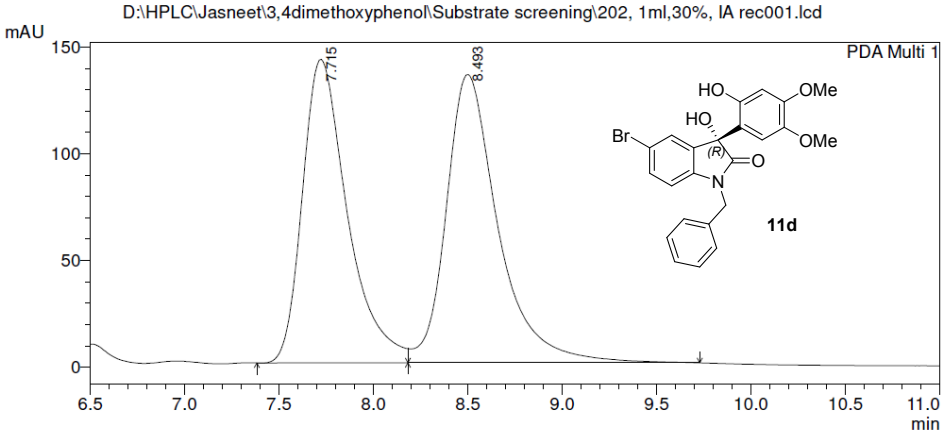
Total		8473895	318363	100.000	100.000



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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1	7.715	2354799	142219	47.651	51.284
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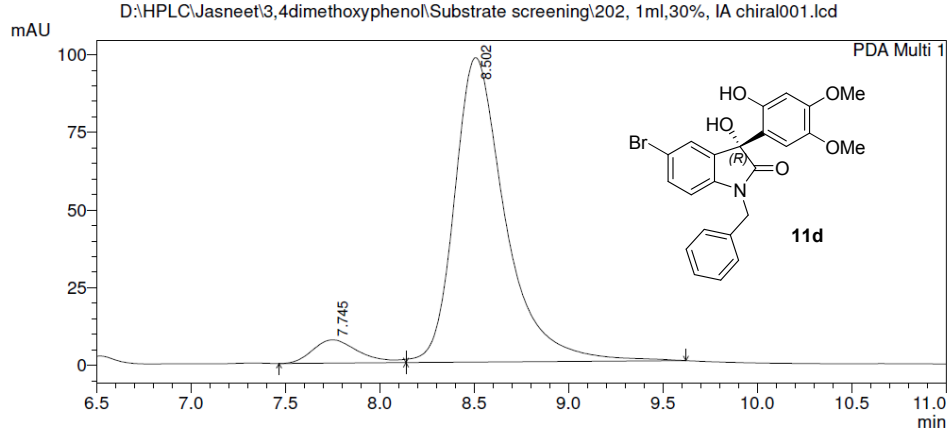

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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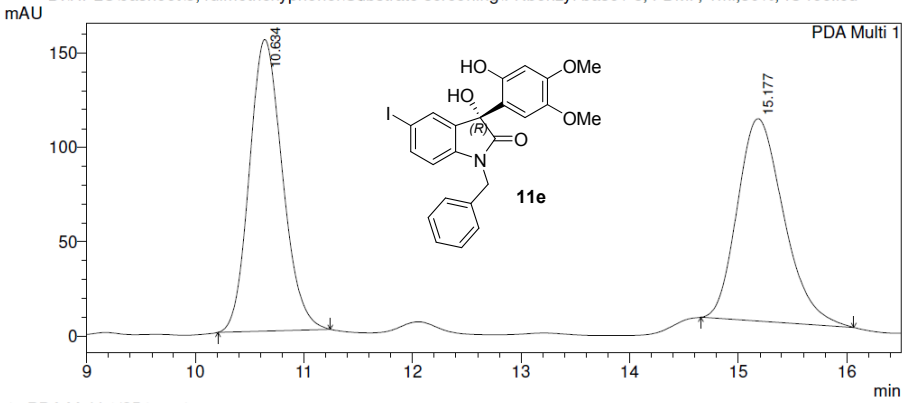
1	7.745	128400	7530	6.525	7.137
2	8.502	1839299	97974	93.475	92.863
Total		1967699	105504	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\I-Nbenzyl base+ 3,4 DMP, 1ml,30%, IC rec.lcd



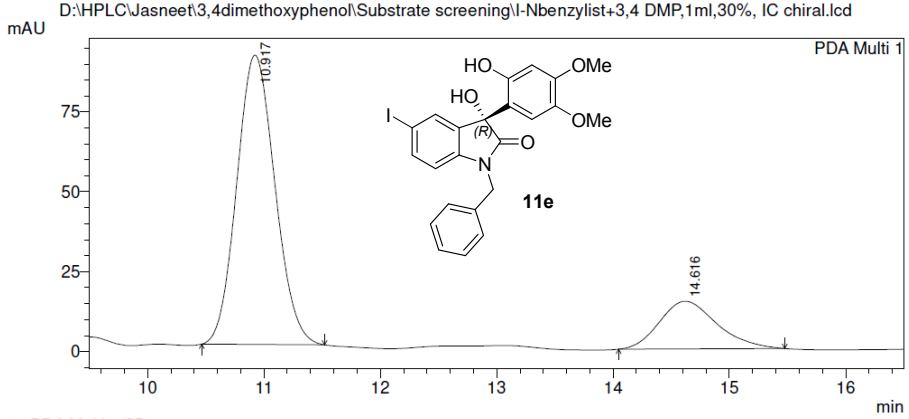
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.634	3277769	154570	50.711	59.032
2	15.177	3185879	107272	49.289	40.968
Total		6463648	261842	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\I-Nbenzylist+3,4 DMP,1ml,30%, IC chiral.lcd

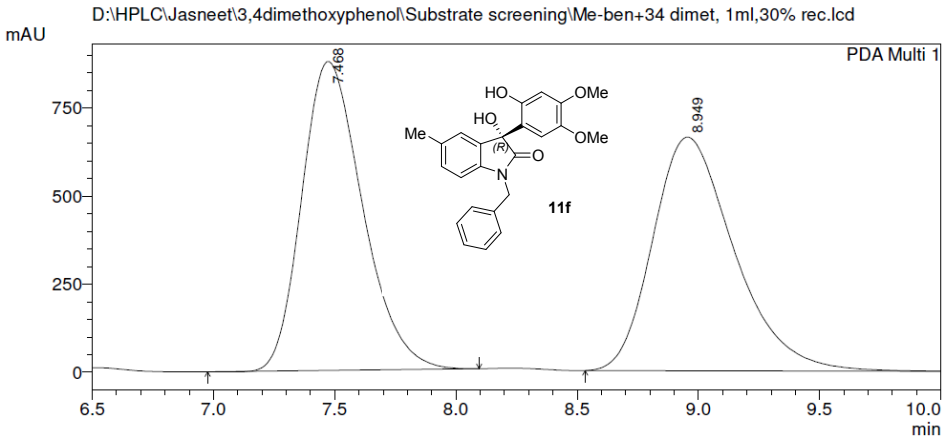


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.917	2067832	90585	80.101	85.869
2	14.616	513688	14908	19.899	14.131
Total		2581521	105493	100.000	100.000

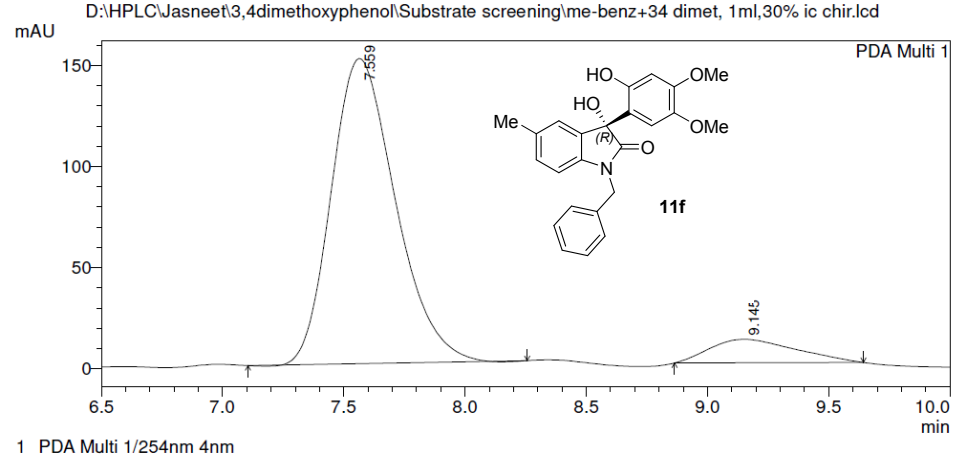


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.468	15304461	877518	49.694	56.950
2	8.949	15492955	663332	50.306	43.050
Total		30797417	1540850	100.000	100.000



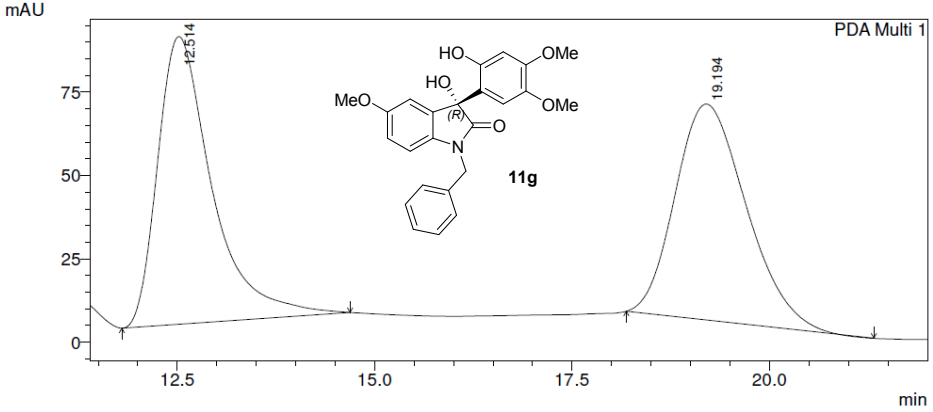
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.559	2767603	150820	90.631	92.858
2	9.145	286100	11600	9.369	7.142
Total		3053703	162420	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\OMebenzlyist+3,4 DMP,1ml,30%, IA rec.lcd



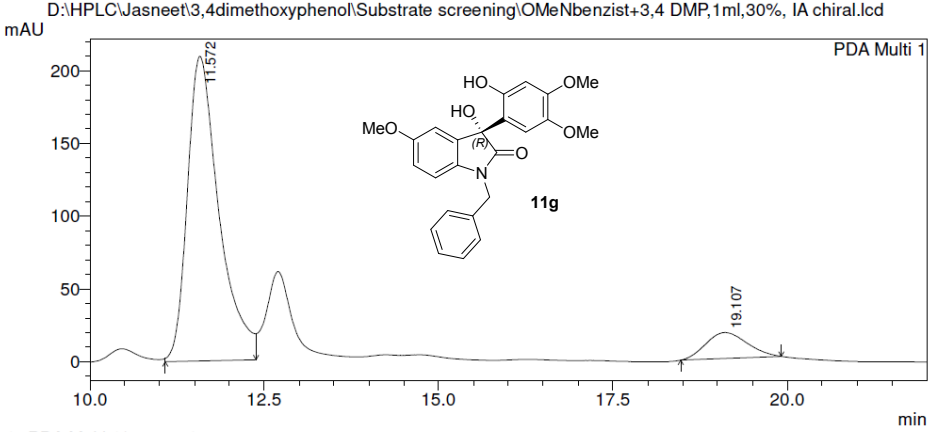
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.514	4137048	86274	50.482	57.139
2	19.194	4058060	64715	49.518	42.861
Total		8195109	150989	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\OMeNbenzist+3,4 DMP,1ml,30%, IA chiral.lcd



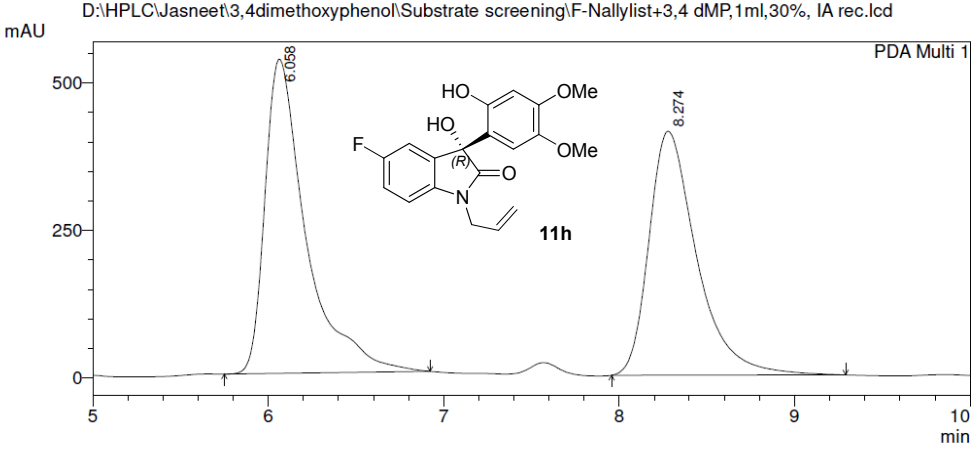
1 PDA Multi 1/209nm 4nm

PeakTable

PDA Ch1 209nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.572	6604725	209326	89.949	92.145
2	19.107	738006	17844	10.051	7.855
Total		7342731	227170	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\F-Nallylist+3,4 dMP,1ml,30%, IA rec.lcd



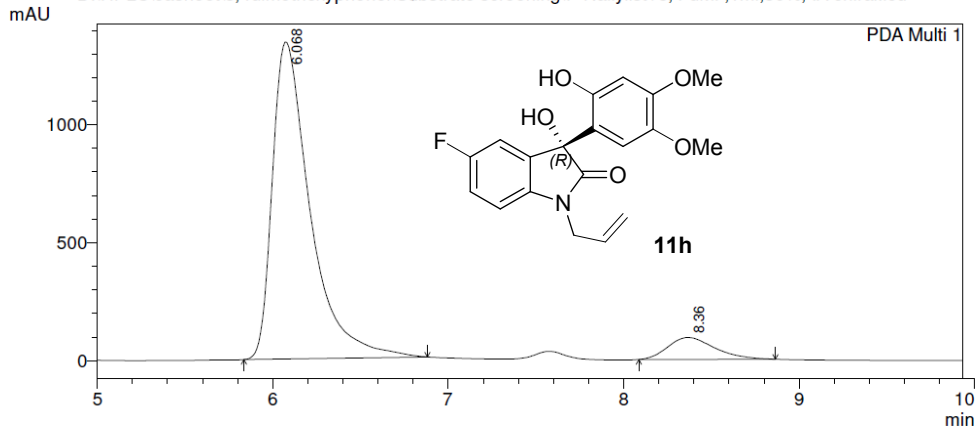
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.058	8657208	531650	52.581	56.276
2	8.274	7807402	413068	47.419	43.724
Total		16464610	944718	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\F-Nallylist+3,4 dMP,1ml,30%, IA chiral.lcd

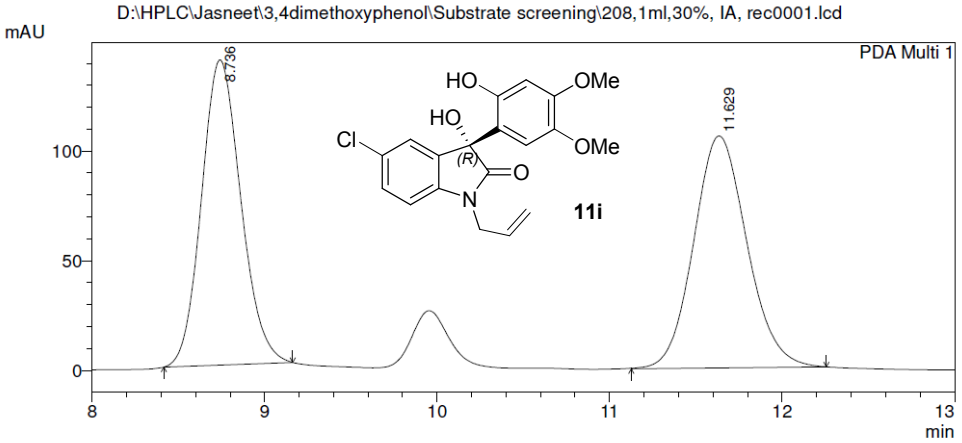


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.068	20086271	1342304	92.115	93.545
2	8.360	1719320	92620	7.885	6.455
Total		21805591	1434924	100.000	100.000

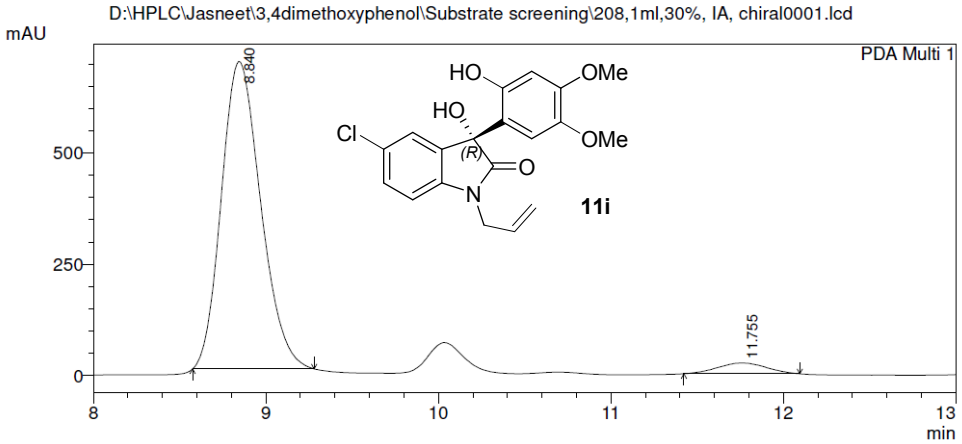


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.736	2206091	139052	49.307	56.792
2	11.629	2268131	105793	50.693	43.208
Total		4474222	244845	100.000	100.000

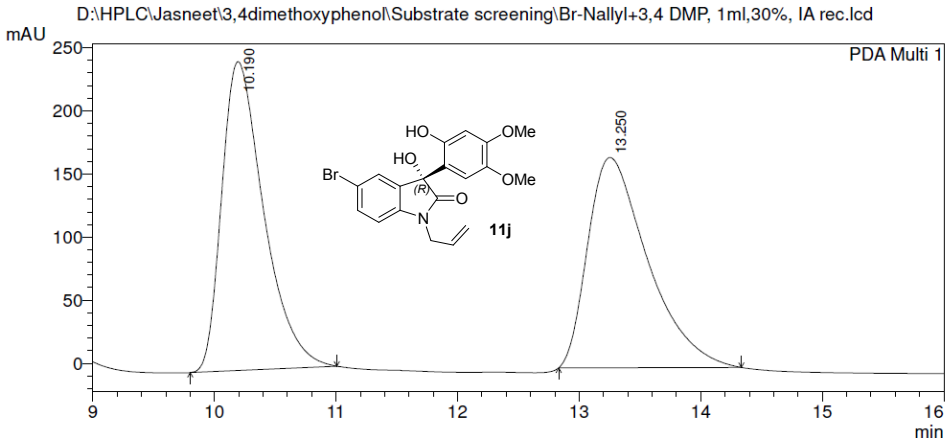


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.840	10949651	690664	95.834	96.616
2	11.755	476038	24187	4.166	3.384
Total		11425688	714851	100.000	100.000

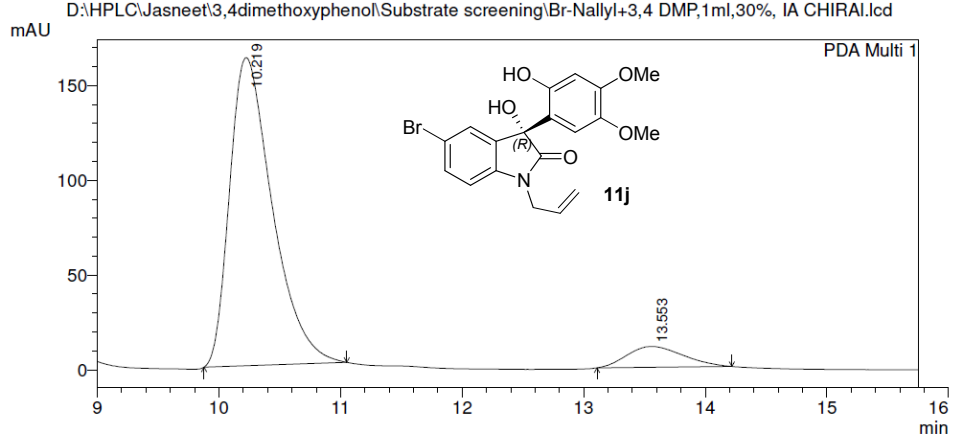


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.190	5882704	244664	50.750	59.490
2	13.250	5708895	166605	49.250	40.510
Total		11591599	411269	100.000	100.000



1 PDA Multi 1/254nm 4nm

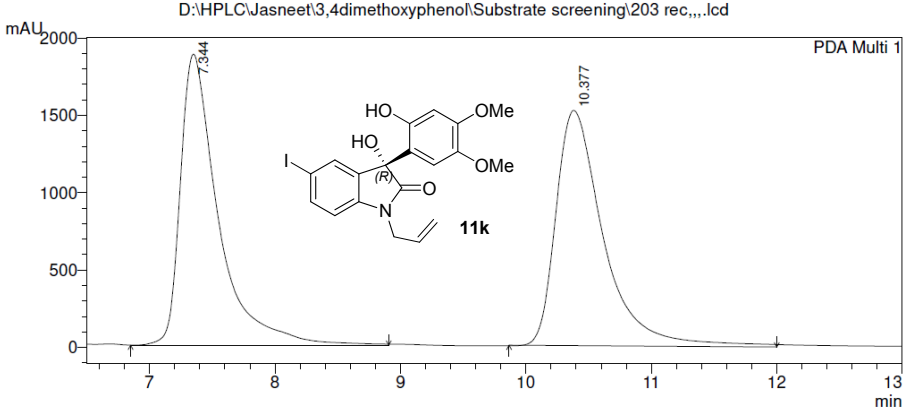
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.219	3976877	162665	91.844	93.653
2	13.553	353146	11025	8.156	6.347
Total		4330022	173689	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\203 rec,,,.lcd



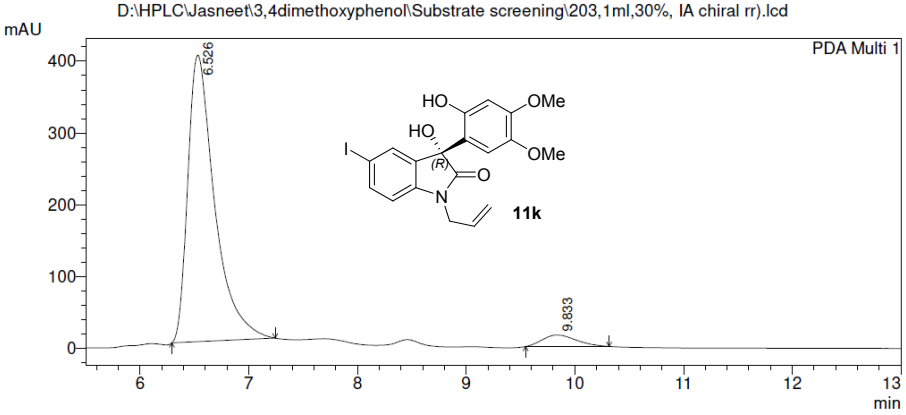
1 PDA Multi 1/209nm 4nm

PeakTable

PDA Ch1 209nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.344	39534485	1881713	49.663	55.327
2	10.377	40070939	1519338	50.337	44.673
Total		79605424	3401051	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\203,1ml,30%, IA chiral rr).lcd



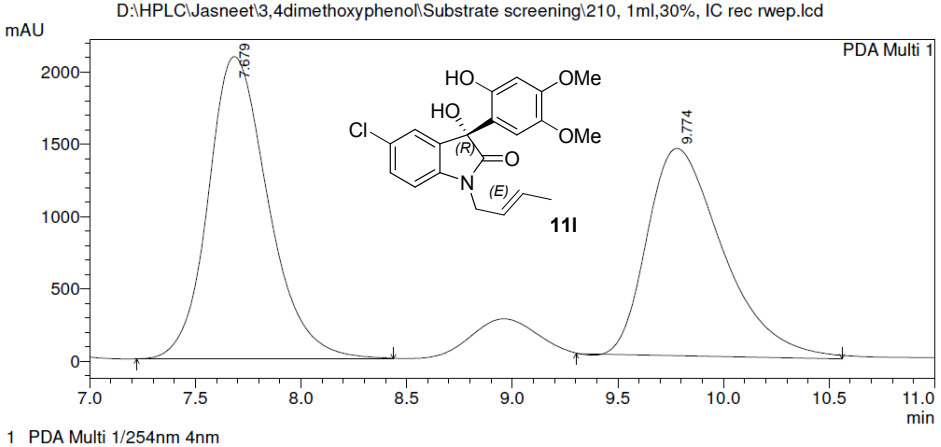
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.526	6858972	399435	95.203	96.163
2	9.833	345590	15938	4.797	3.837
Total		7204562	415373	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\210, 1ml,30%, IC rec rwep.lcd



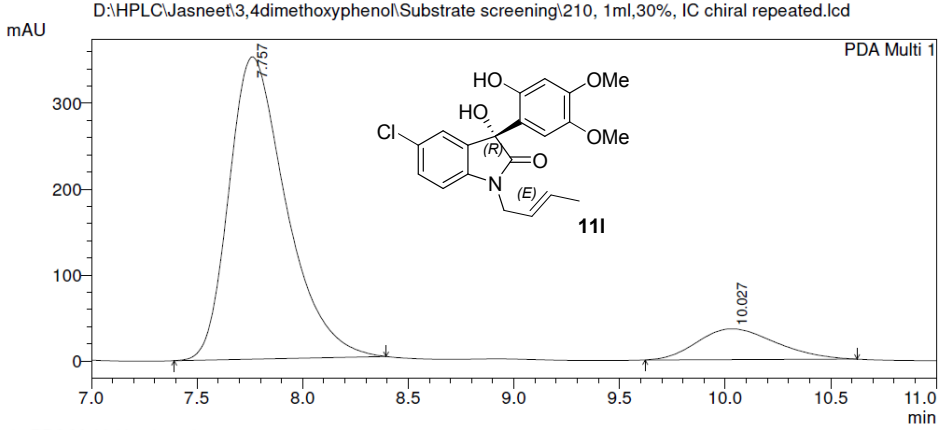
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.679	41414574	2088700	53.713	59.333
2	9.774	35688404	1431618	46.287	40.667
Total		77102978	3520318	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\210, 1ml,30%, IC chiral repeated.lcd



1 PDA Multi 1/254nm 4nm

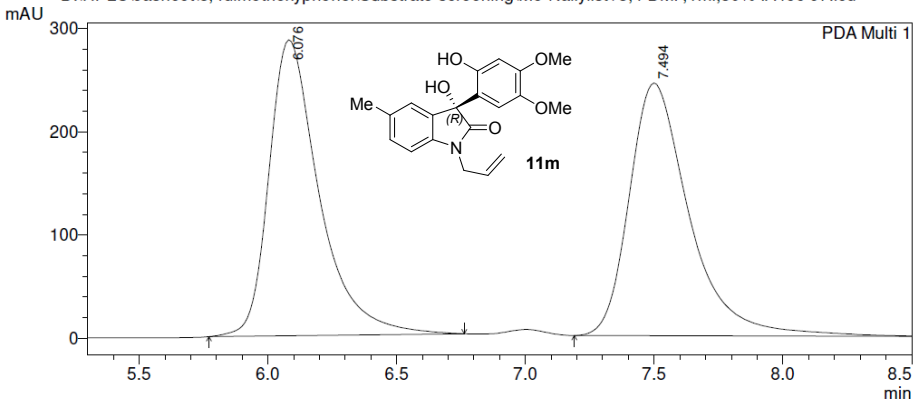
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.757	6621480	351508	87.693	90.765
2	10.027	929303	35763	12.307	9.235
Total		7550783	387272	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\Me-Nallylist+3,4 DMP,1ml,30% IA rec 97.lcd



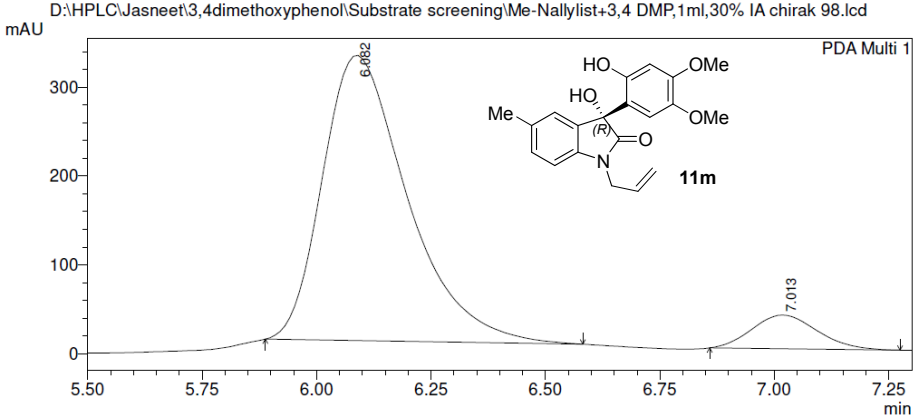
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.076	3901192	286881	49.522	53.950
2	7.494	3976580	244868	50.478	46.050
Total		7877772	531749	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\Me-Nallylist+3,4 DMP,1ml,30% IA chirak 98.lcd

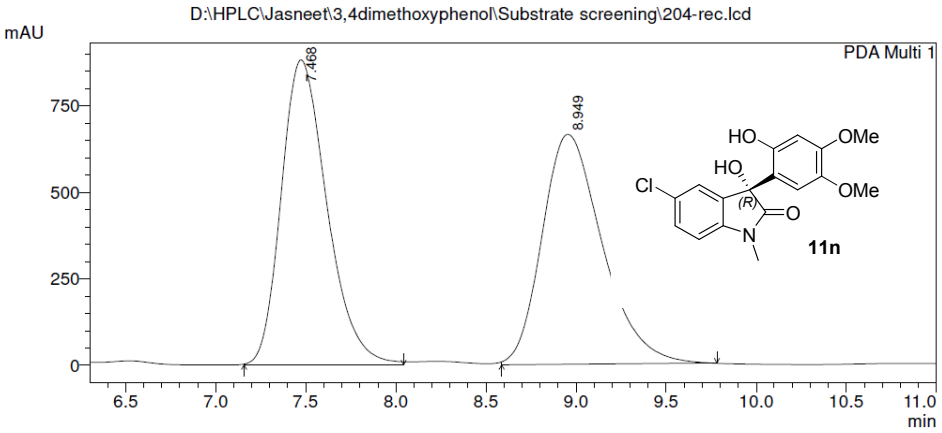


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.082	4142038	320925	91.677	89.396
2	7.013	376017	38068	8.323	10.604
Total		4518055	358994	100.000	100.000

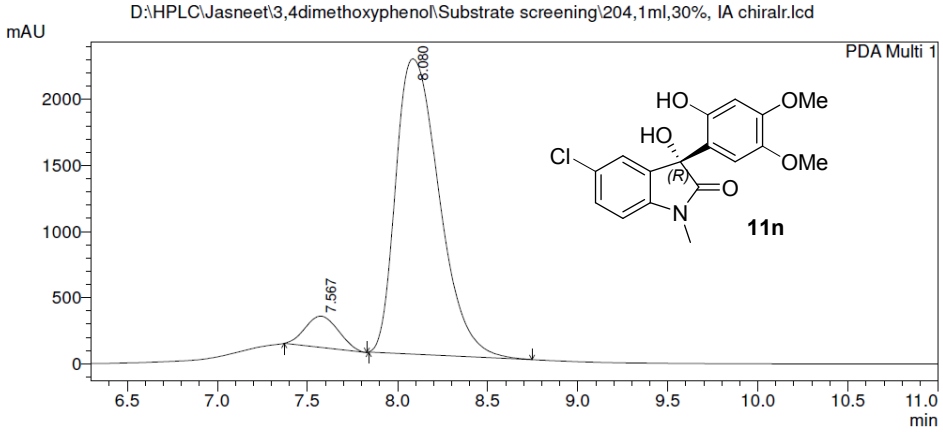


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.468	15559147	881164	50.158	57.004
2	8.949	15461263	664626	49.842	42.996
Total		31020410	1545790	100.000	100.000

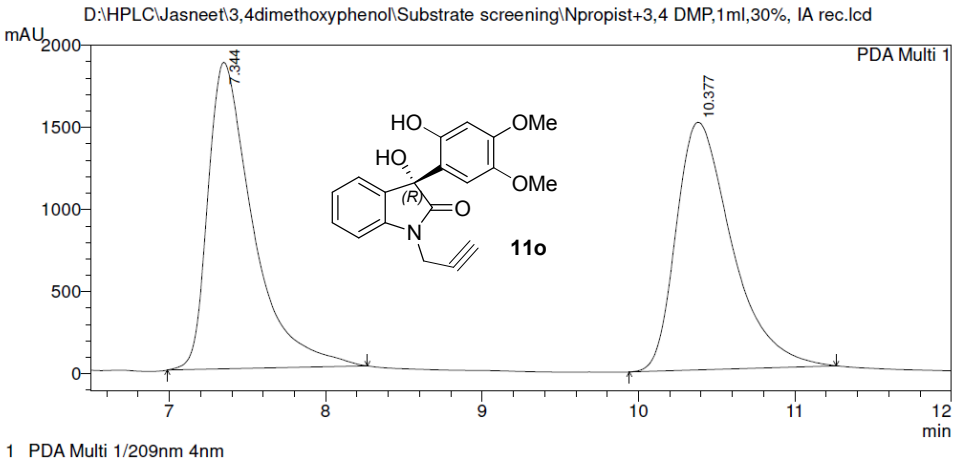


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.567	2998904	235534	7.396	9.537
2	8.080	37546402	2234119	92.604	90.463
Total		40545305	2469653	100.000	100.000

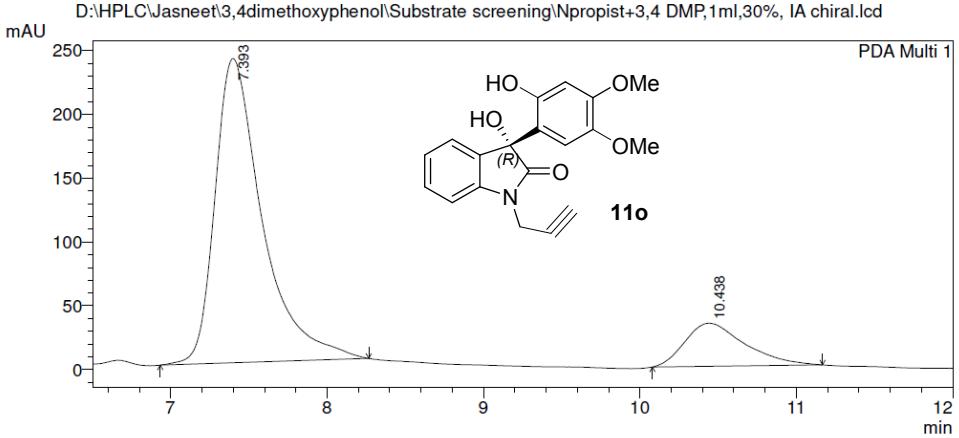


1 PDA Multi 1/209nm 4nm

PeakTable

PDA Ch1 209nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.344	37329065	1866231	49.907	55.319
2	10.377	37467925	1507347	50.093	44.681
Total		74796990	3373579	100.000	100.000



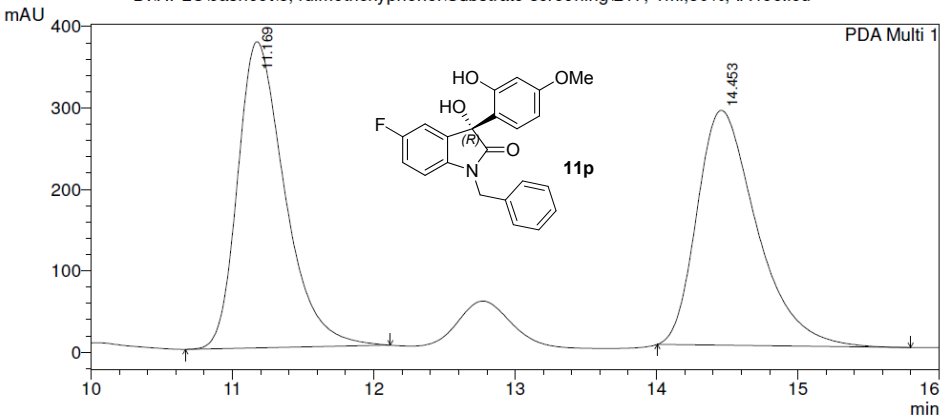
1 PDA Multi 1/209nm 4nm

PeakTable

PDA Ch1 209nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.393	5013143	238422	84.770	87.588
2	10.438	900667	33786	15.230	12.412
Total		5913810	272208	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\217, 1ml,30%, IA rec.lcd



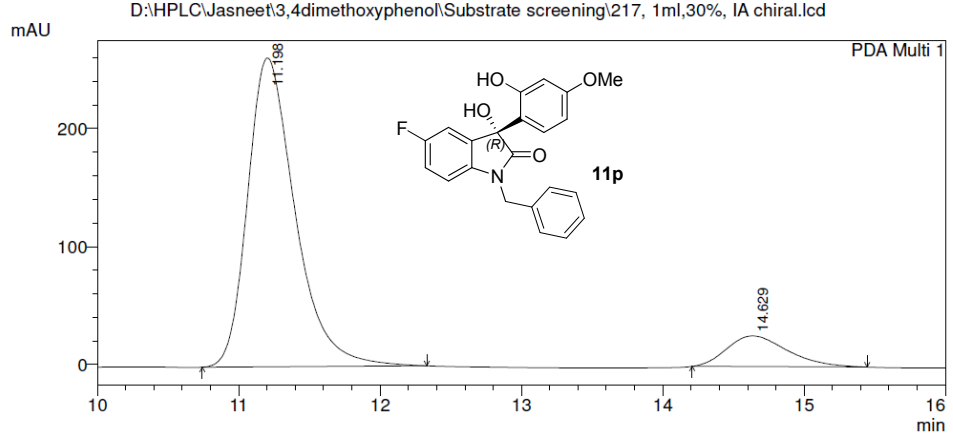
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.169	8719758	376111	50.689	56.590
2	14.453	8482799	288517	49.311	43.410
Total		17202557	664628	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\217, 1ml,30%, IA chiral.lcd



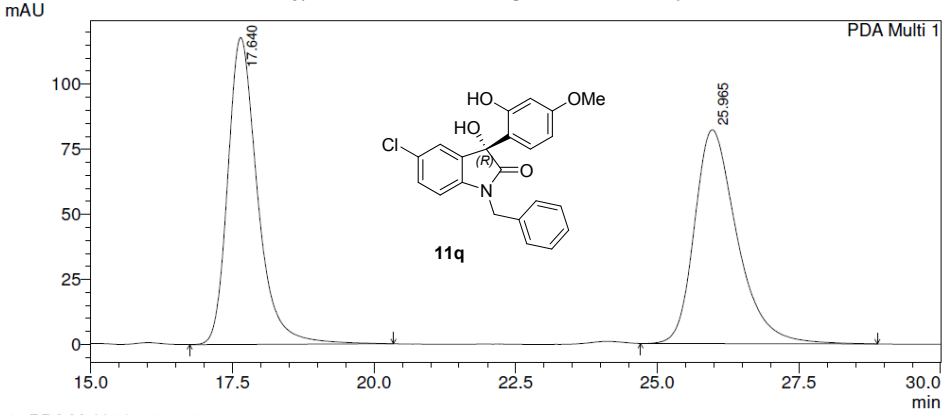
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.198	6118524	262034	88.744	90.964
2	14.629	776080	26030	11.256	9.036
Total		6894605	288065	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\Cl-Nbenzist+3-metphenol, 1ml,20%, IA rec.lcd



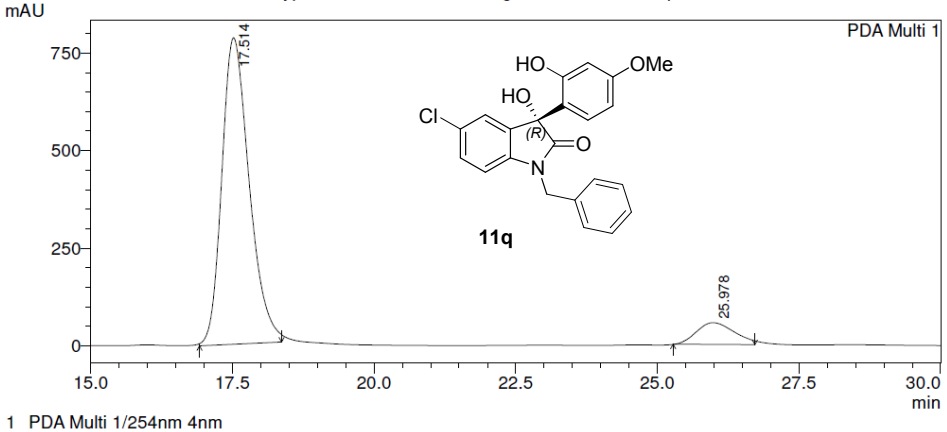
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.640	4315332	117835	50.058	58.923
2	25.965	4305328	82145	49.942	41.077
Total		8620660	199980	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\Cl-Nbenzist+3-metphenol, 1ml,20%, IA chiral.lcd

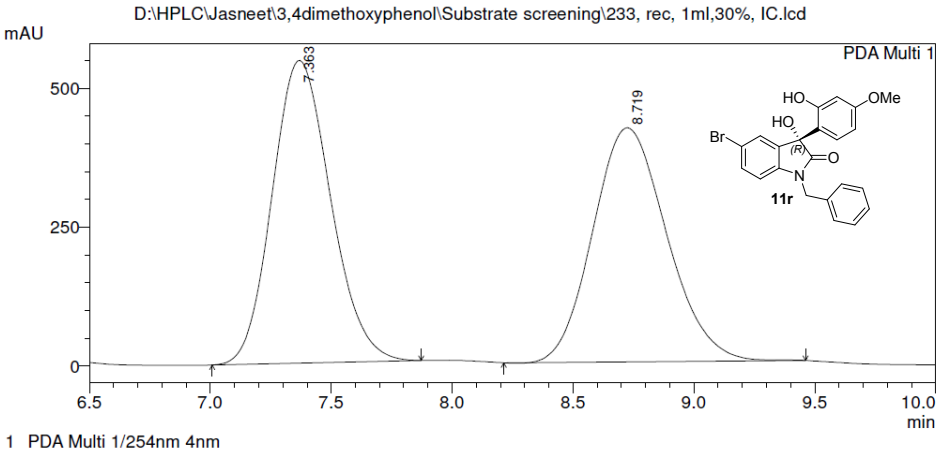


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.514	26384127	784666	91.071	93.372
2	25.978	2586898	55699	8.929	6.628
Total		28971025	840365	100.000	100.000

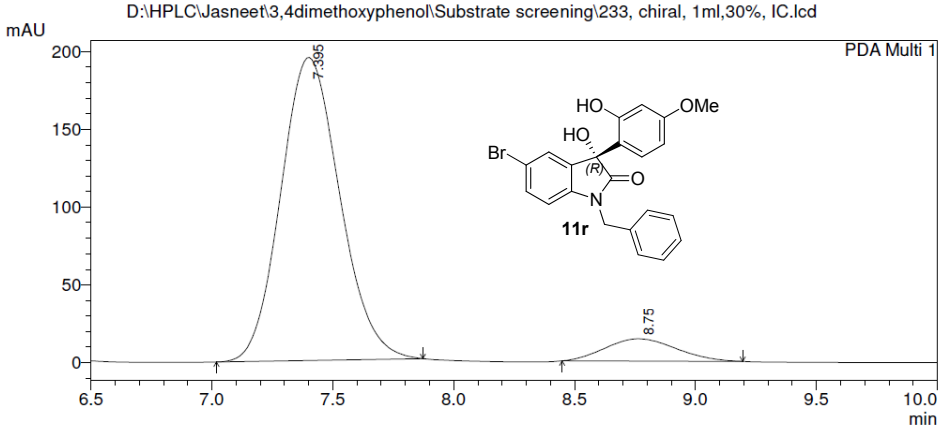


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.363	9170894	545216	50.589	56.387
2	8.719	8957485	421696	49.411	43.613
Total		18128379	966912	100.000	100.000

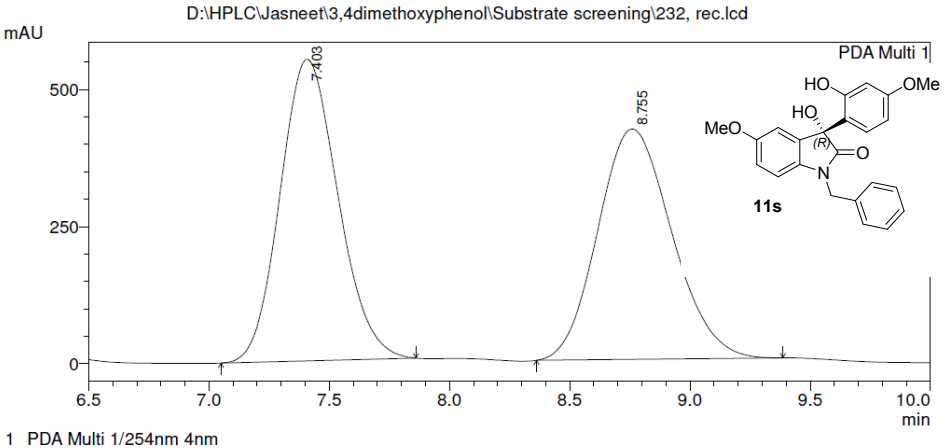


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.395	3311031	194844	91.846	93.136
2	8.758	293933	14360	8.154	6.864
Total		3604964	209204	100.000	100.000

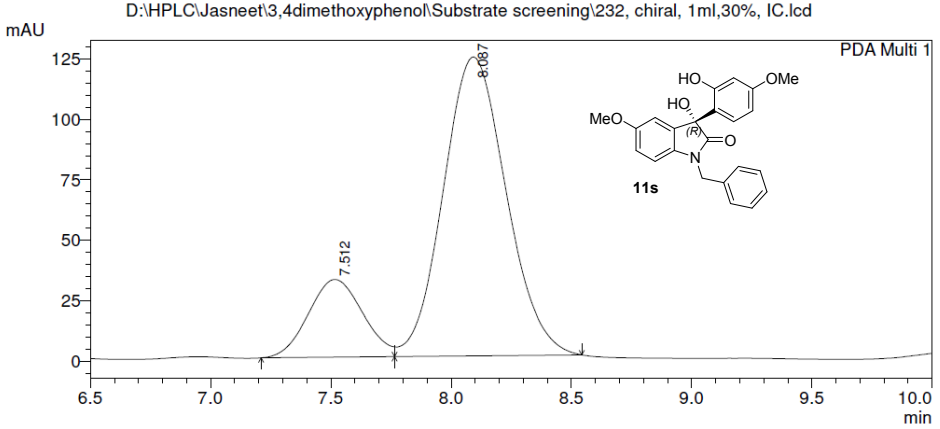


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.403	9201371	549656	50.591	56.682
2	8.755	8986491	420060	49.409	43.318
Total		18187863	969716	100.000	100.000

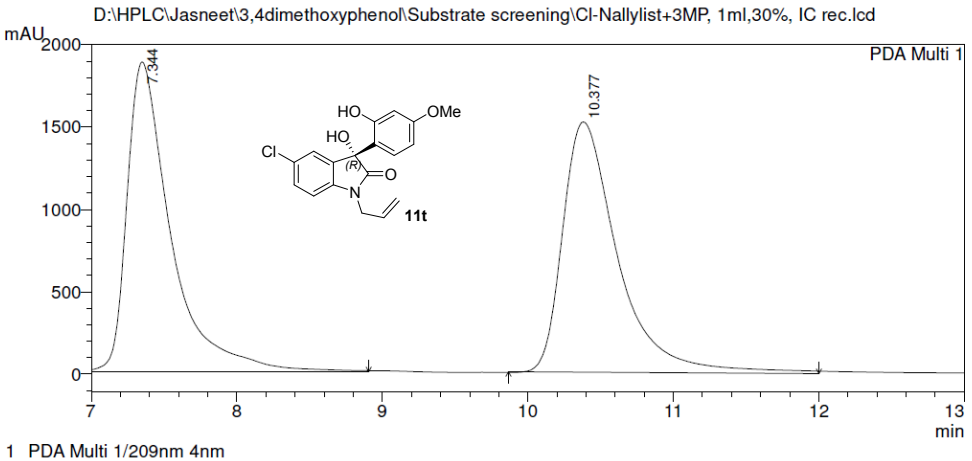


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.512	503909	32094	18.328	20.625
2	8.087	2245541	123513	81.672	79.375
Total		2749450	155608	100.000	100.000

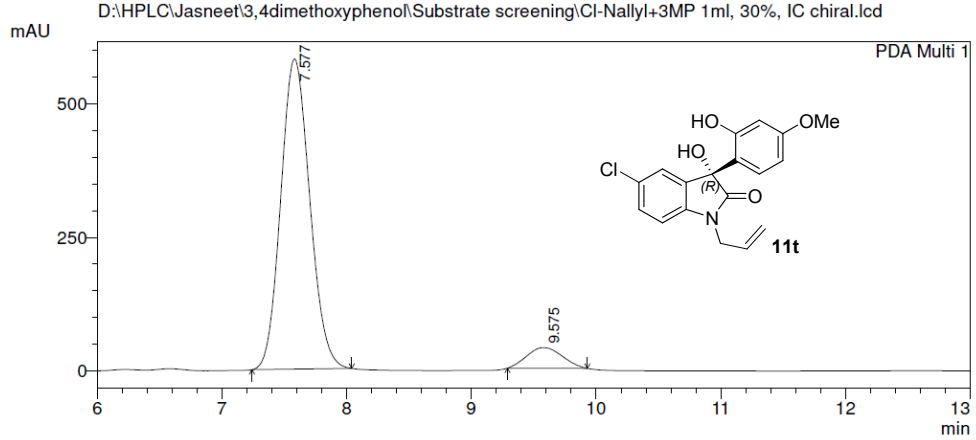


1 PDA Multi 1/209nm 4nm

PeakTable

PDA Ch1 209nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.344	39534485	1881713	49.663	55.327
2	10.377	40070939	1519338	50.337	44.673
Total		79605424	3401051	100.000	100.000



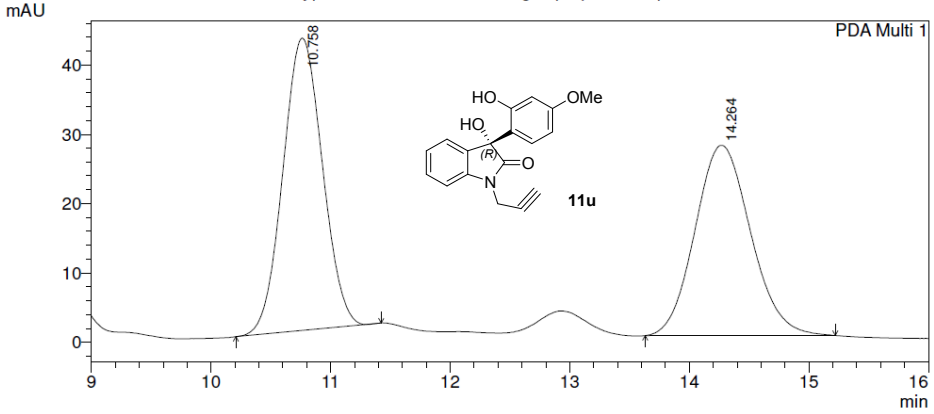
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.577	9372977	580727	92.503	93.764
2	9.575	759685	38622	7.497	6.236
Total		10132662	619349	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\N-propt+,3-Metphenol,1ml,30%, IC rec.lcd



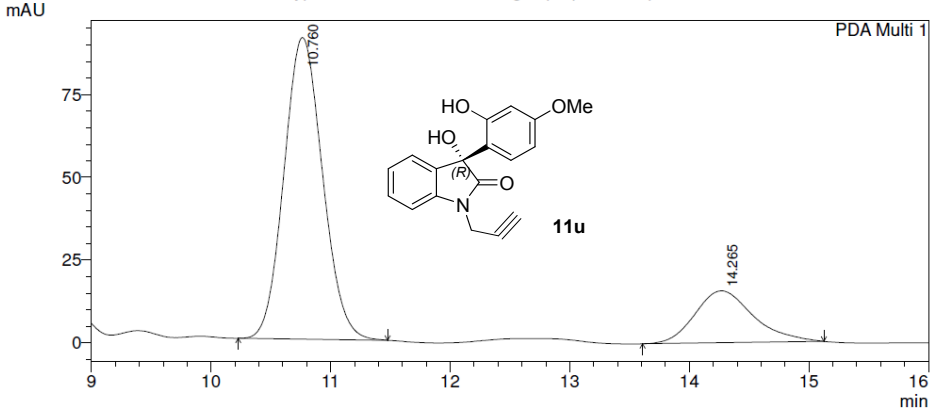
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.758	967728	42177	52.188	60.584
2	14.264	886567	27441	47.812	39.416
Total		1854295	69617	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\N-propt+,3-Metphenol,1ml,30%, IC chiral.lcd



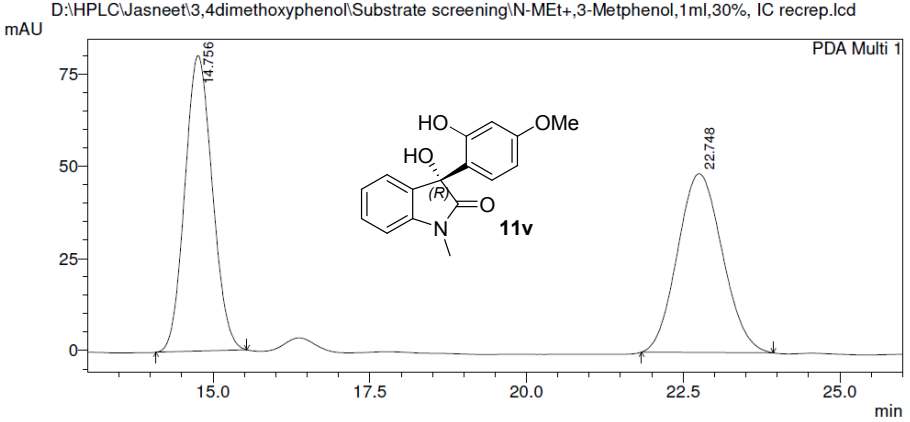
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.760	2047657	91204	79.340	85.320
2	14.265	533212	15693	20.660	14.680
Total		2580869	106896	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\N-MEt+,3-Metphenol,1ml,30%, IC recrep.lcd



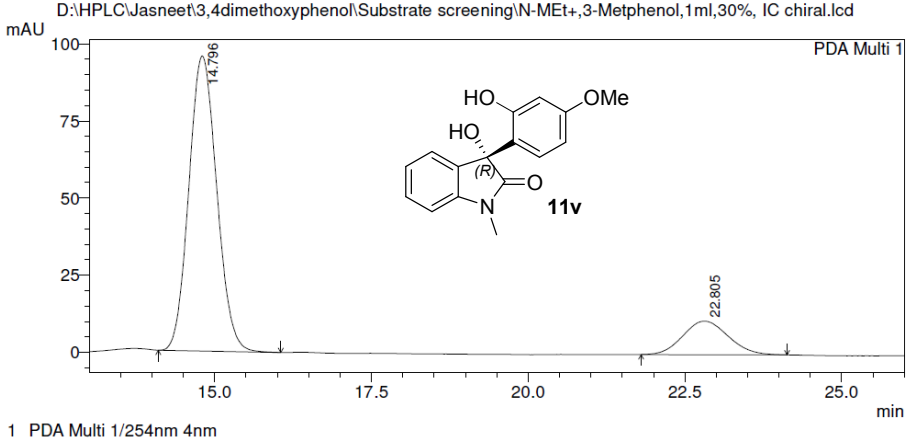
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.756	2451532	80244	50.384	62.322
2	22.748	2414133	48514	49.616	37.678
Total		4865665	128758	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\N-MEt+,3-Metphenol,1ml,30%, IC chiral.lcd

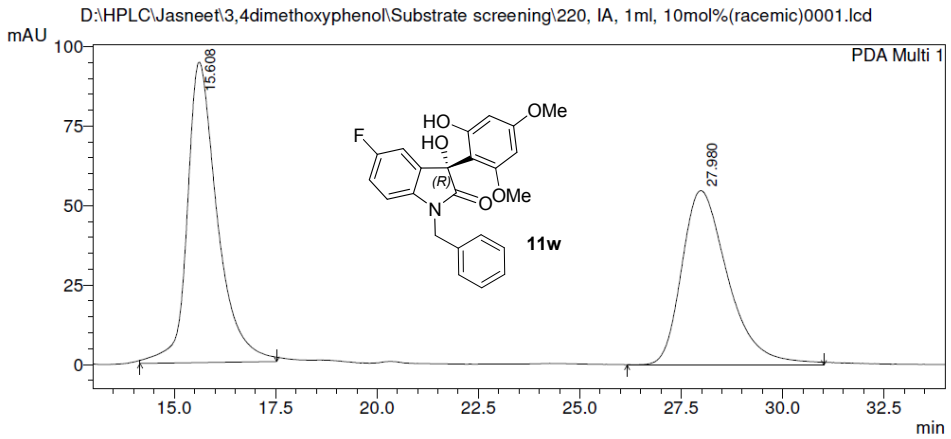


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.796	2959141	95618	84.339	89.766
2	22.805	549480	10901	15.661	10.234
Total		3508621	106519	100.000	100.000

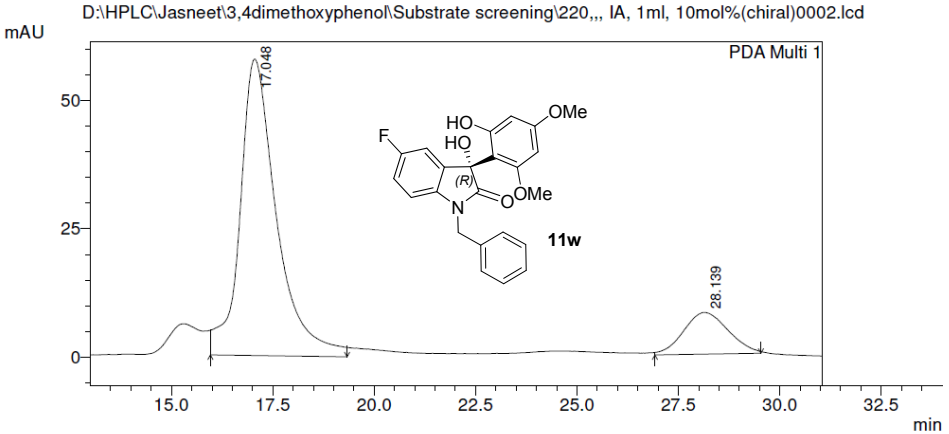


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.608	4888271	94563	52.736	63.256
2	27.980	4381015	54929	47.264	36.744
Total		9269287	149492	100.000	100.000

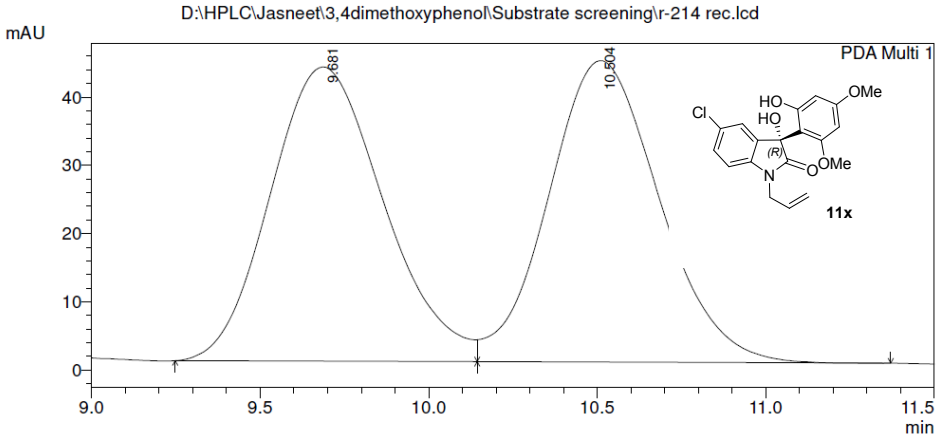


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.048	3616132	57731	85.301	87.690
2	28.139	623152	8104	14.699	12.310
Total		4239283	65835	100.000	100.000

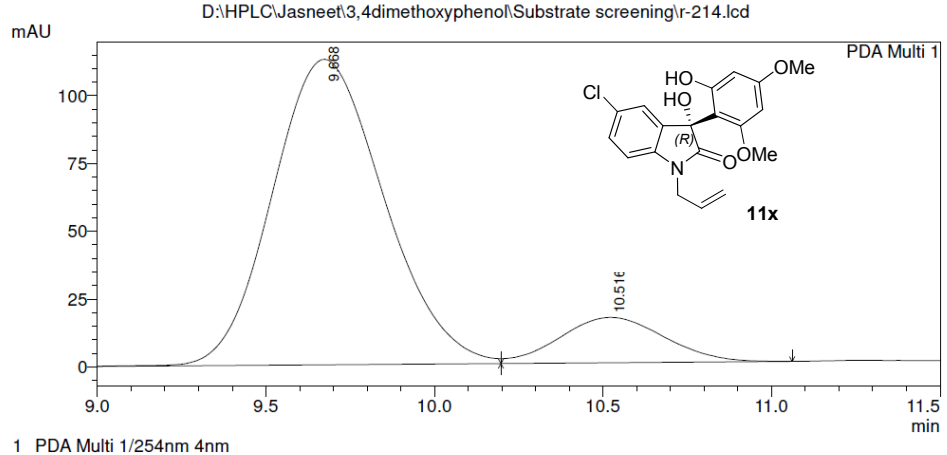


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.681	1007418	43122	50.012	49.398
2	10.504	1006944	44173	49.988	50.602
Total		2014361	87295	100.000	100.000

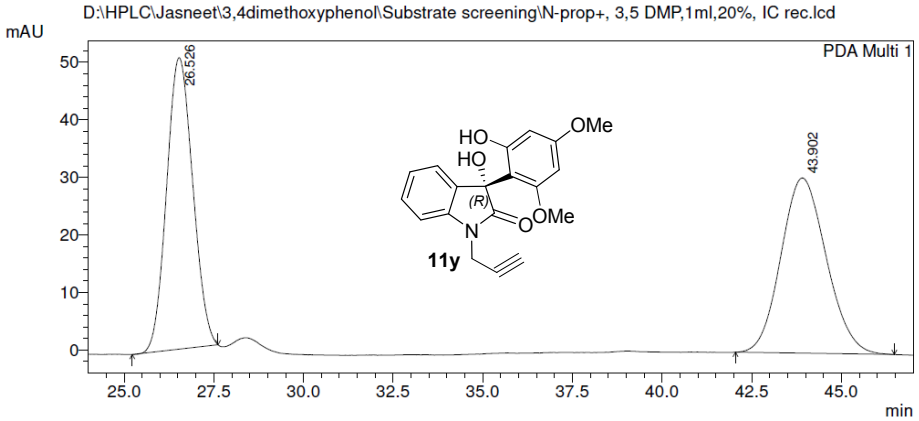


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.668	2588111	112605	87.746	87.070
2	10.516	361424	16721	12.254	12.930
Total		2949535	129327	100.000	100.000

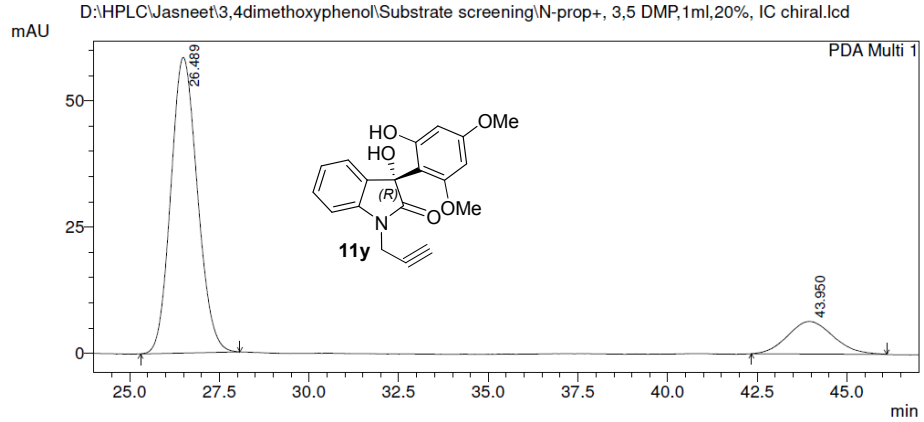


1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.526	2572176	50679	49.017	62.473
2	43.902	2675352	30442	50.983	37.527
Total		5247528	81121	100.000	100.000



1 PDA Multi 1/254nm 4nm

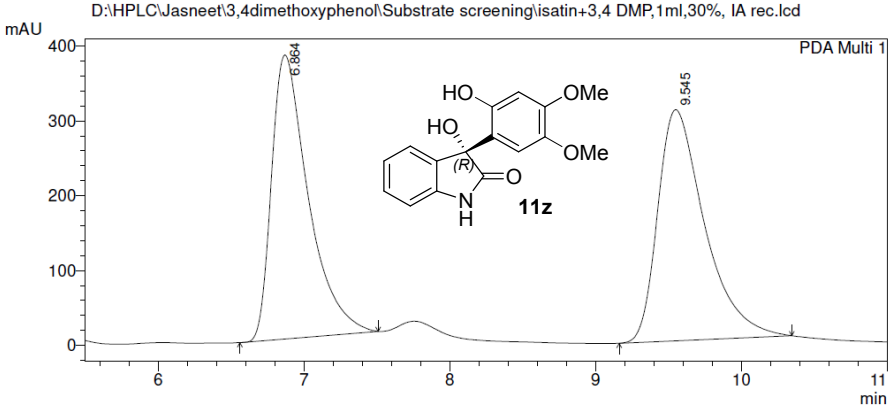
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.489	3024689	58522	84.063	90.049
2	43.950	573429	6467	15.937	9.951
Total		3598118	64989	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\isatin+3,4 DMP,1ml,30%, IA rec.lcd



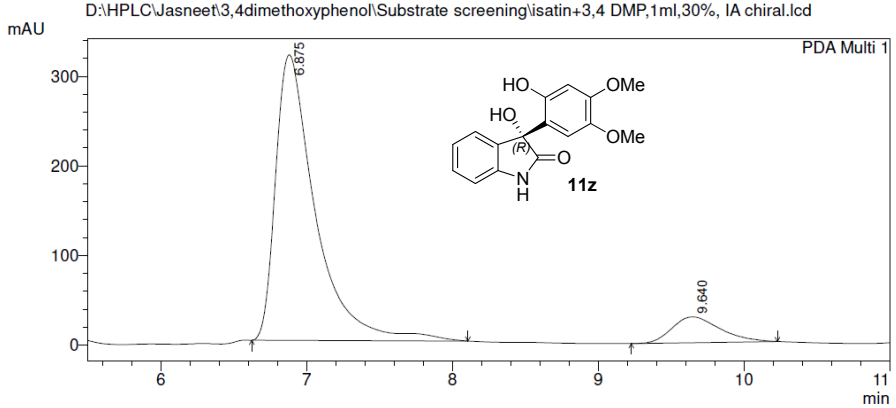
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.864	6659271	380054	49.059	55.138
2	9.545	6914647	309223	50.941	44.862
Total		13573918	689276	100.000	100.000

D:\HPLC\Jasneet\3,4dimethoxyphenol\Substrate screening\isatin+3,4 DMP,1ml,30%, IA chiral.lcd

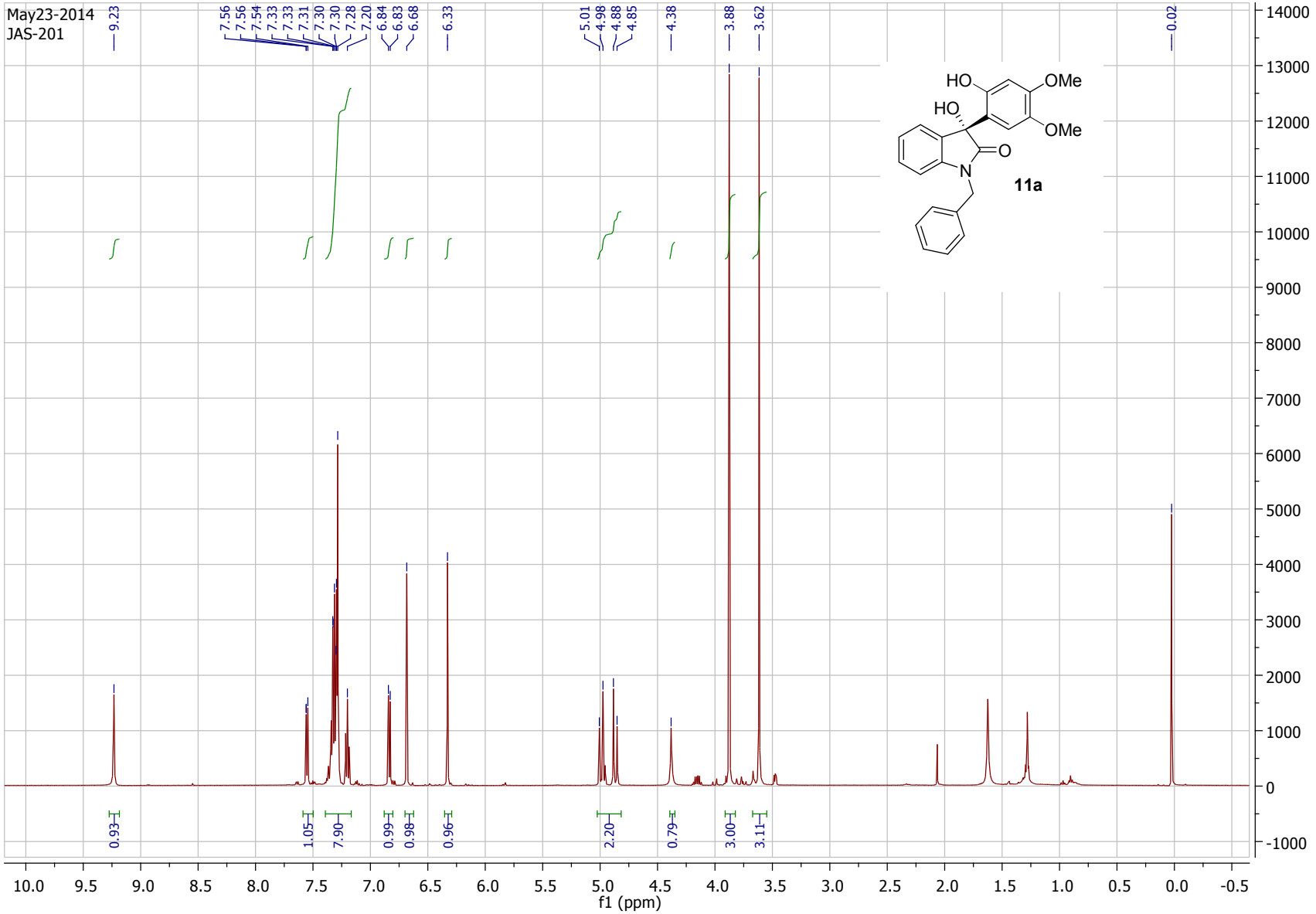


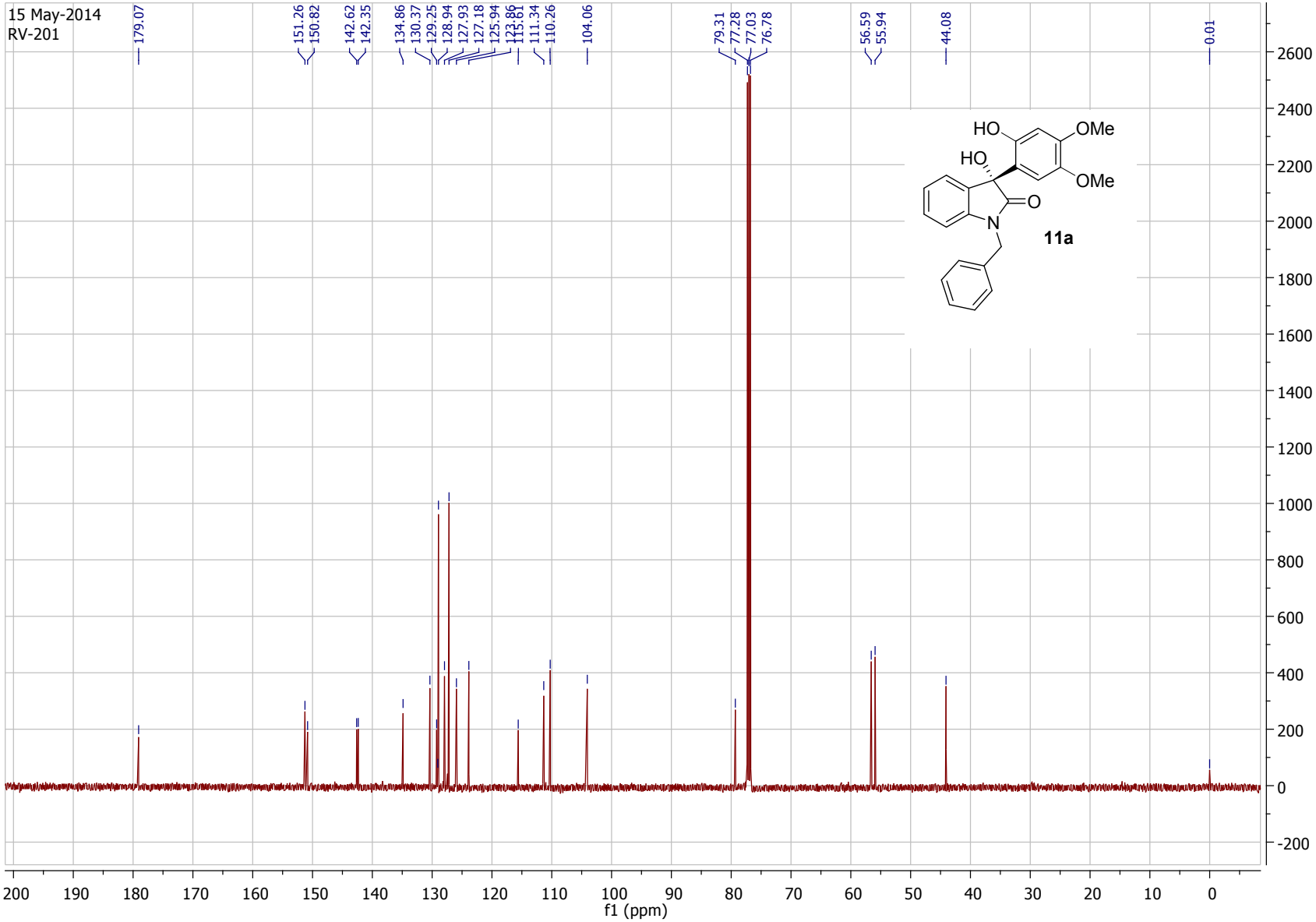
1 PDA Multi 1/254nm 4nm

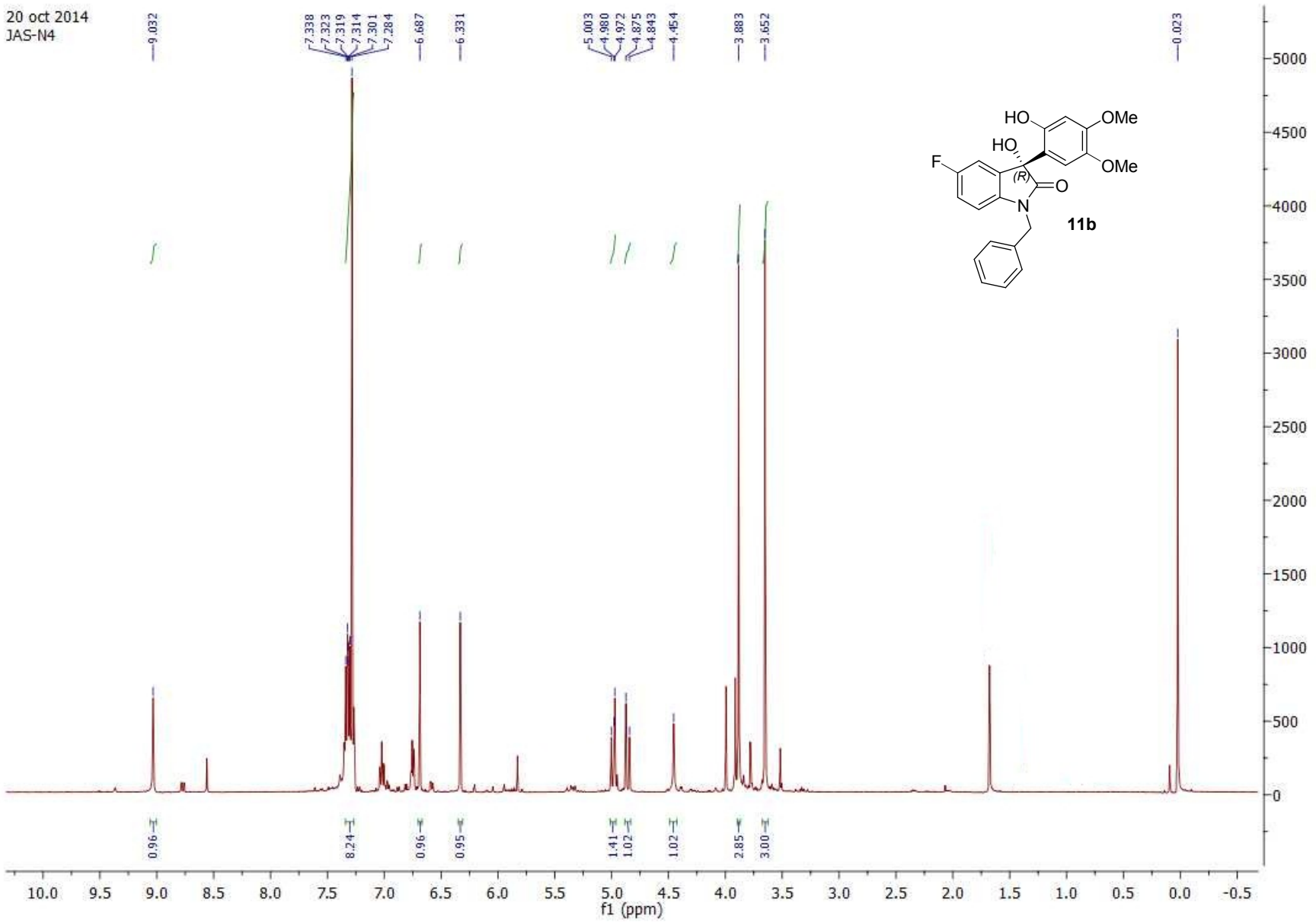
PeakTable

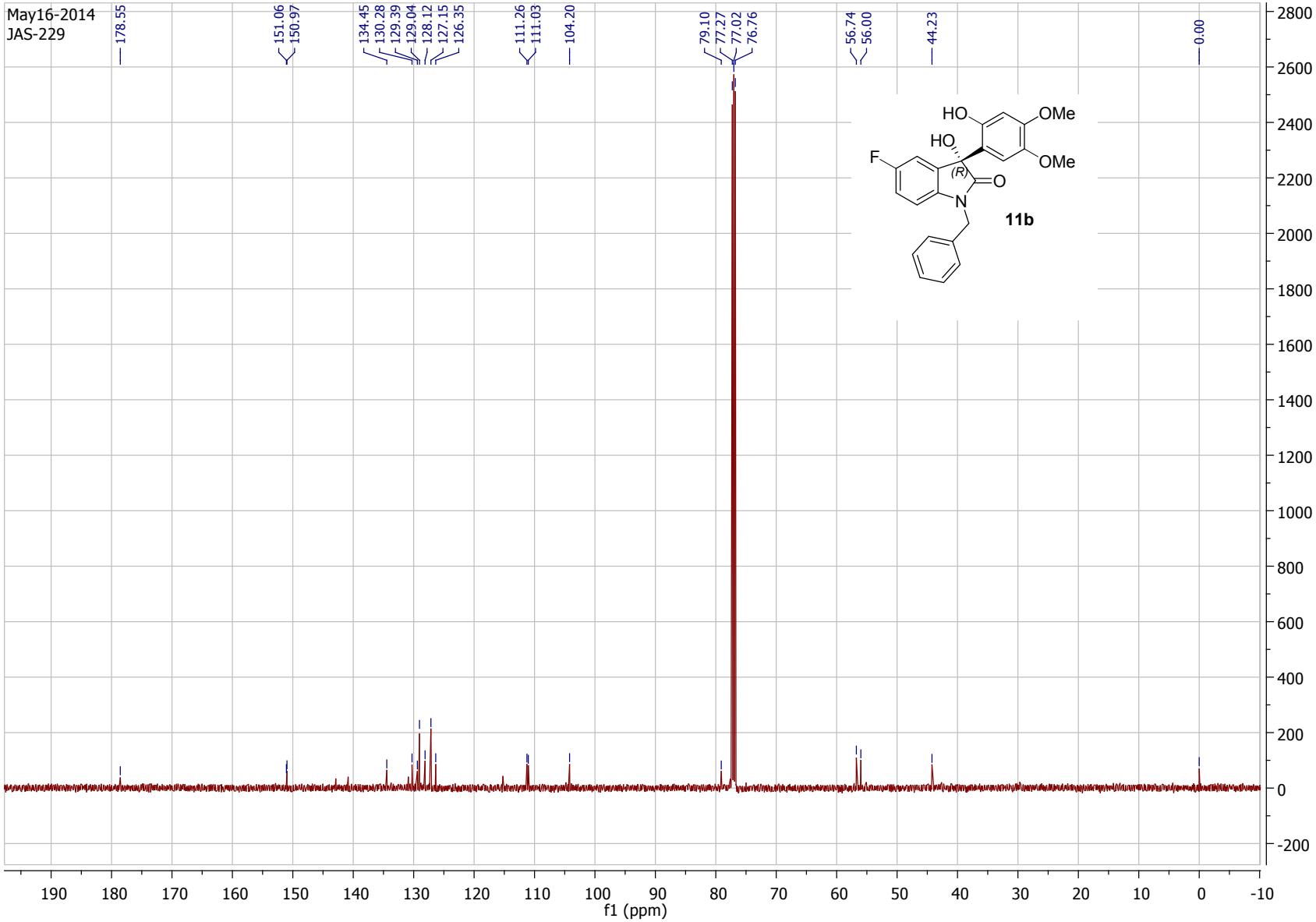
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.875	6048064	319080	90.089	91.692
2	9.640	665378	28912	9.911	8.308
Total		6713442	347992	100.000	100.000

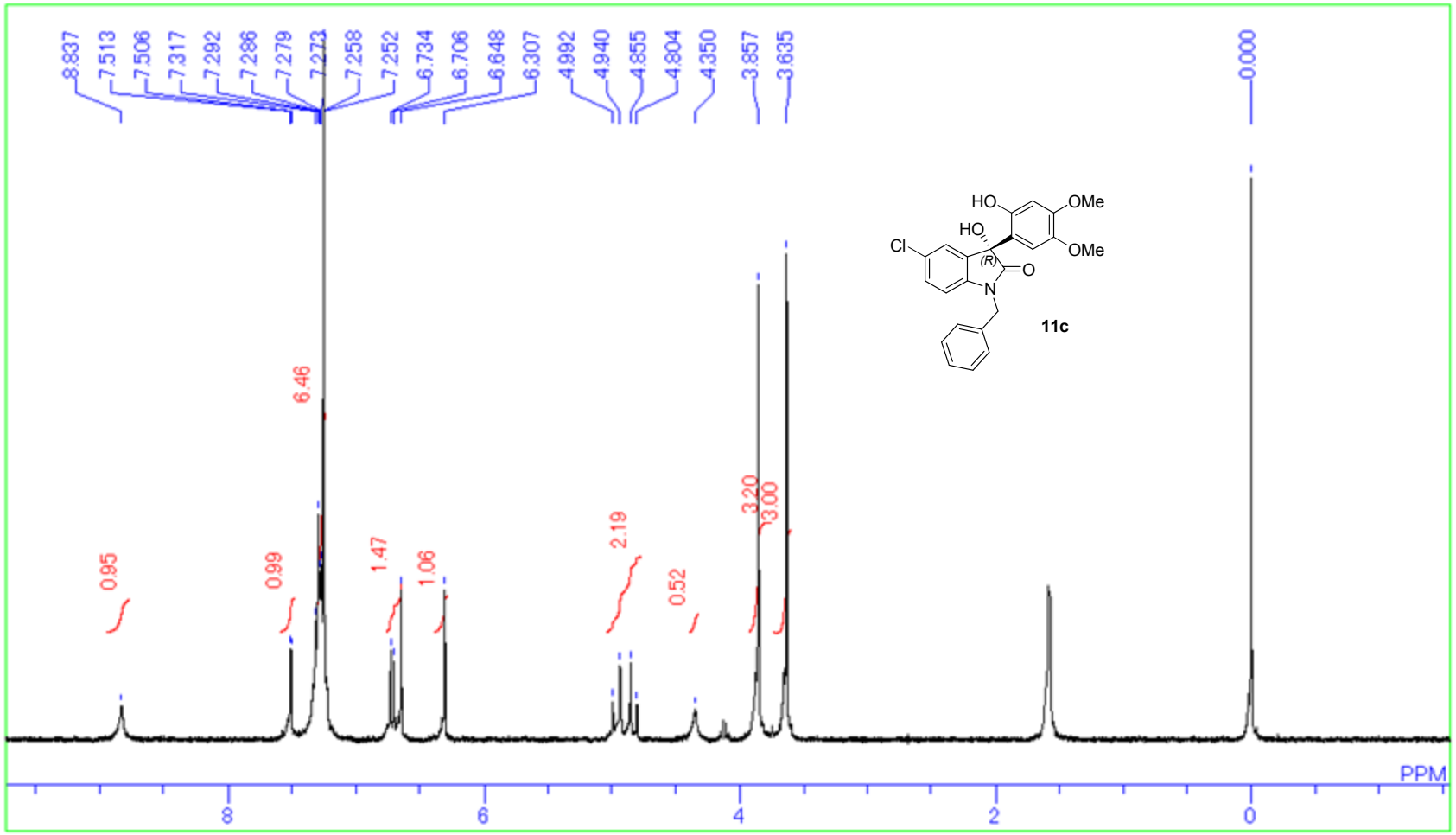

May23-2014
JAS-201
9.23
7.56
7.56
7.54
7.33
7.33
7.31
7.30
7.30
7.28
7.20
6.84
6.83
6.68
6.33
5.01
4.98
4.88
4.85
4.38
3.88
3.62
0.02
HO
HO
OMe
OMe
O
N
11a
0.93
1.05
7.90
0.99
0.98
0.96
2.20
0.79
3.00
3.11
f1 (ppm)

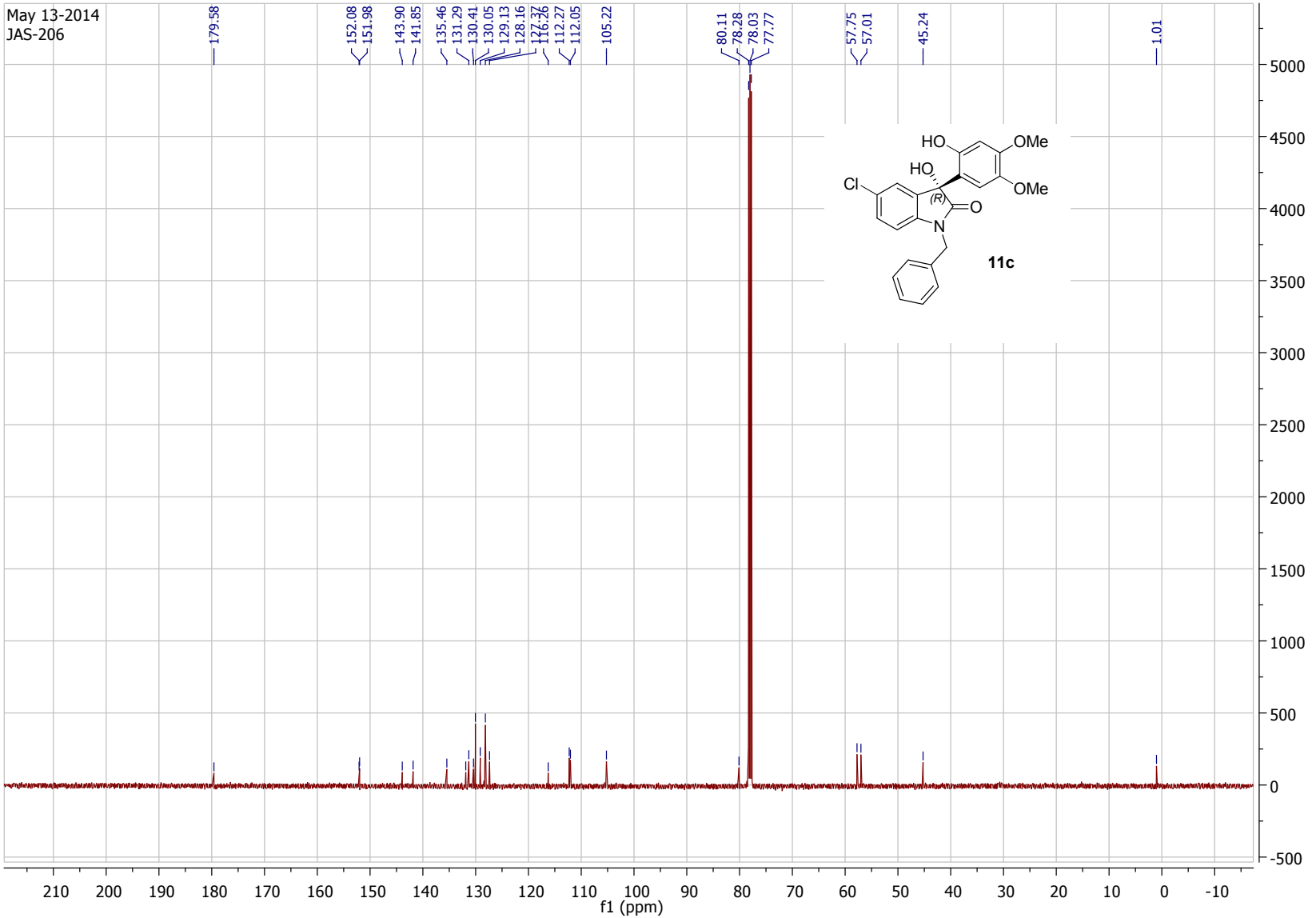

15 May-2014
RV-201
179.07
151.26
150.82
142.62
142.35
134.86
130.37
129.25
128.94
127.93
127.18
125.94
123.86
123.61
115.01
111.34
110.26
104.06
79.31
77.28
77.03
76.78
56.59
55.94
44.08
0.01
HO
OMe
HO
OMe
O
N
11a
f1 (ppm)


20 oct 2014
JAS-N4
9.032
7.338
7.323
7.319
7.314
7.301
7.284
6.687
6.331
5.003
4.980
4.972
4.875
4.843
4.454
3.883
3.652
0.023
HO
OMe
HO
F
OMe
(R)
O
N
11b
0.96
8.24
0.96
0.95
1.41
1.02
1.02
2.85
3.00
f1 (ppm)

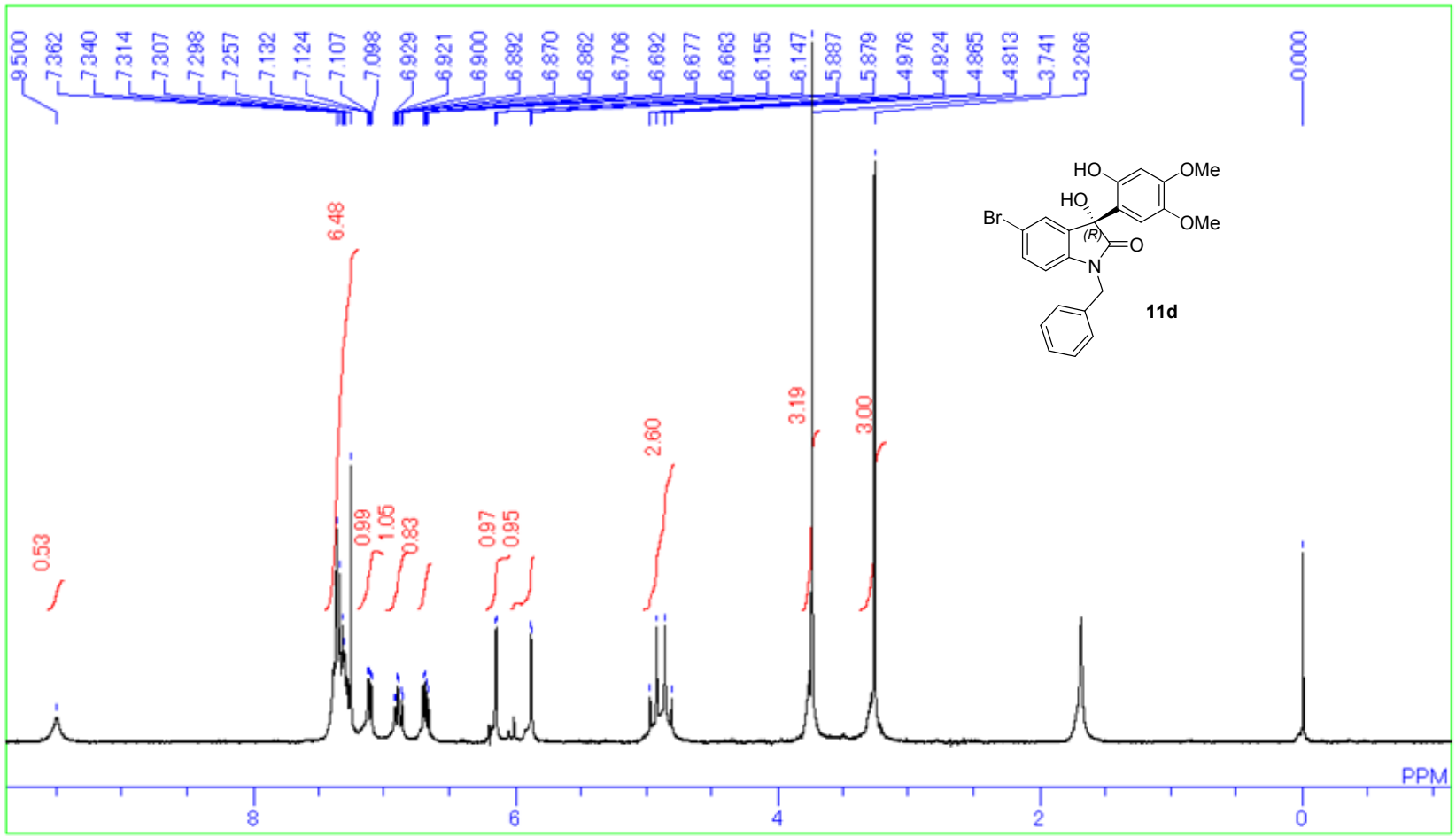

May16-2014
JAS-229
178.55
151.06
150.97
134.45
130.28
129.39
129.04
128.12
127.15
126.35
111.26
111.03
104.20
79.10
77.27
77.02
76.76
56.74
56.00
44.23
0.00
HO
OMe
HO
OMe
F
(R)
O
N
11b
f1 (ppm)

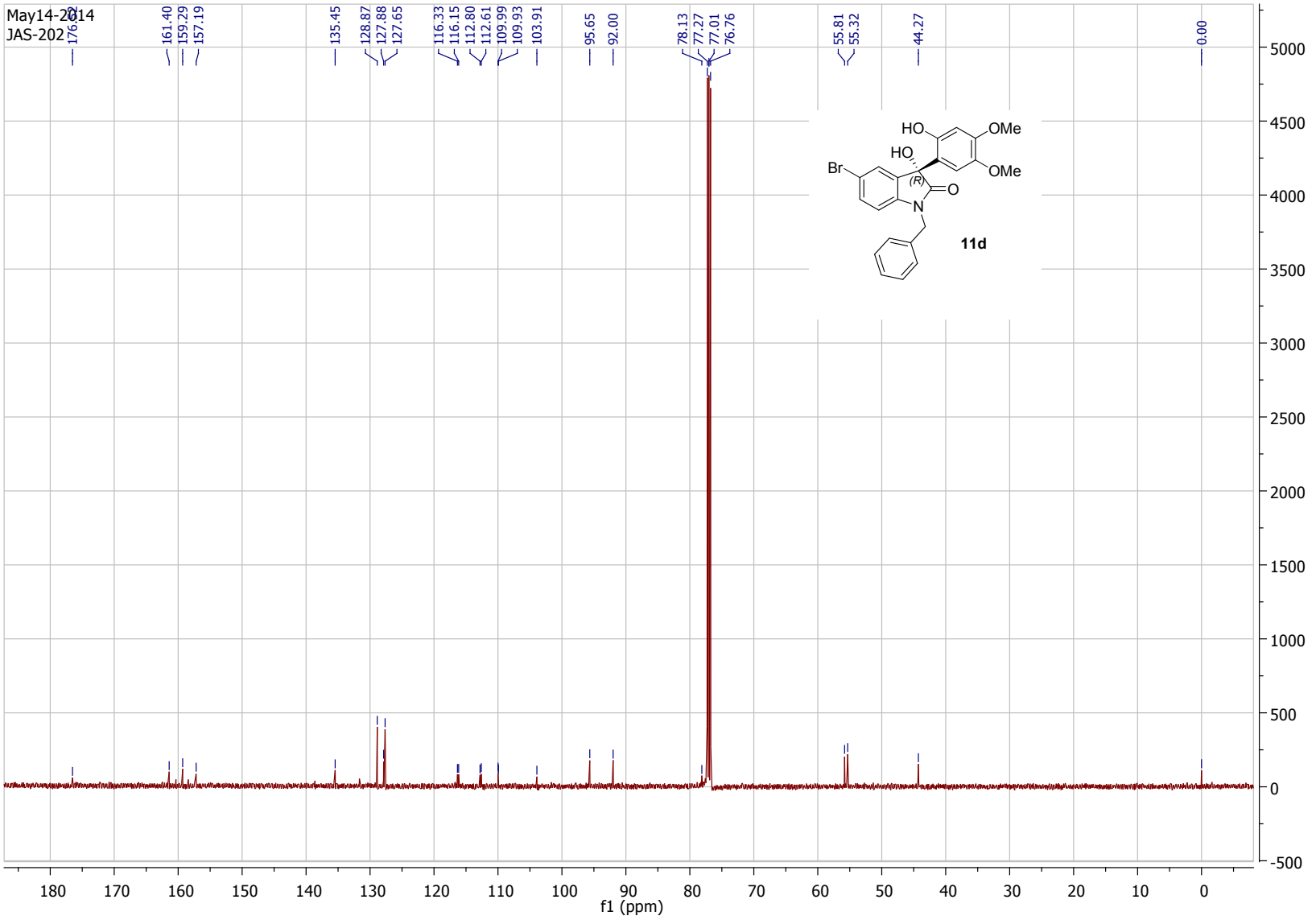
C:¥Users¥technologies¥Desktop¥nmrs¥Dr_Chimni¥C-SB2061NON_E2_FT.als

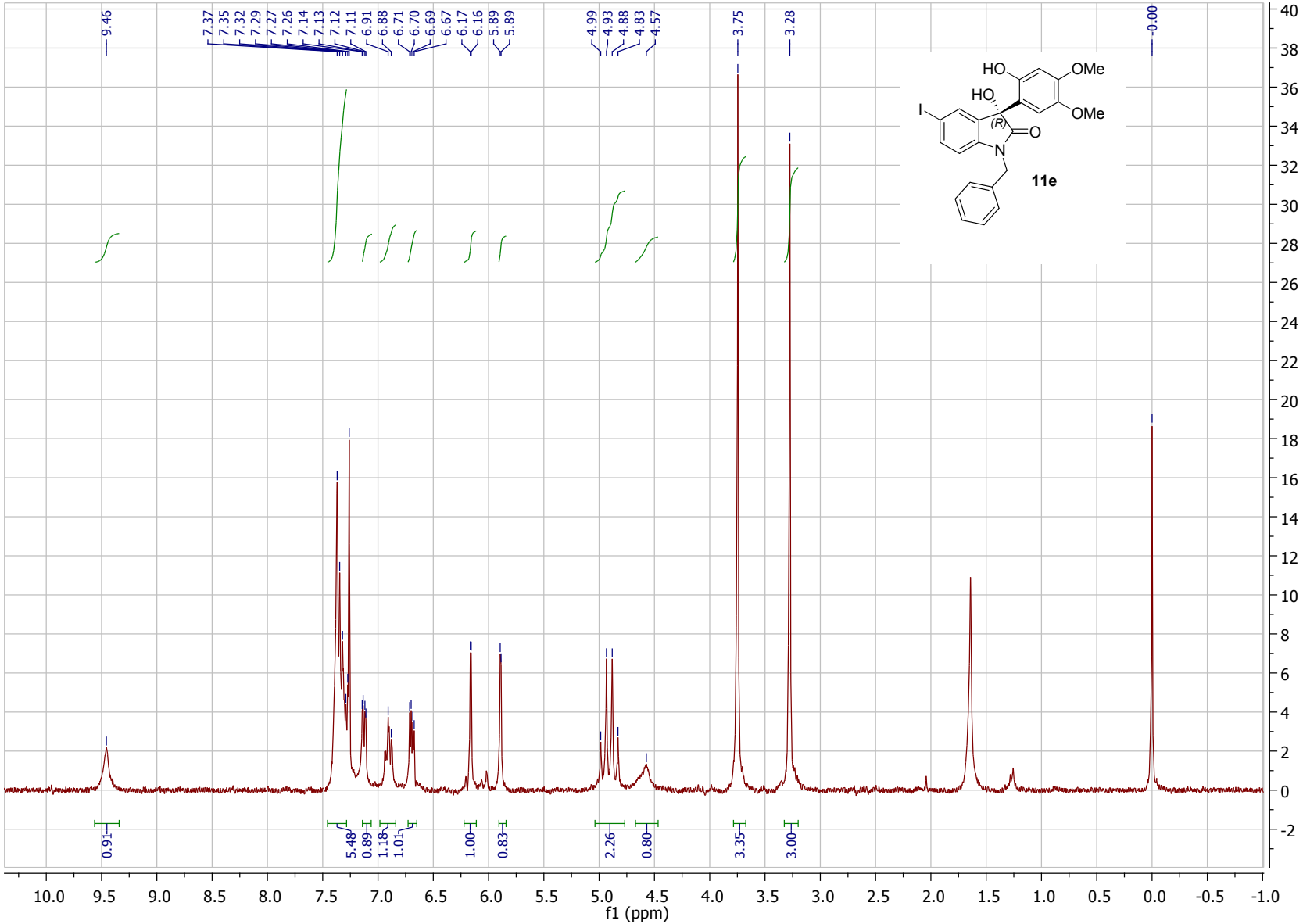


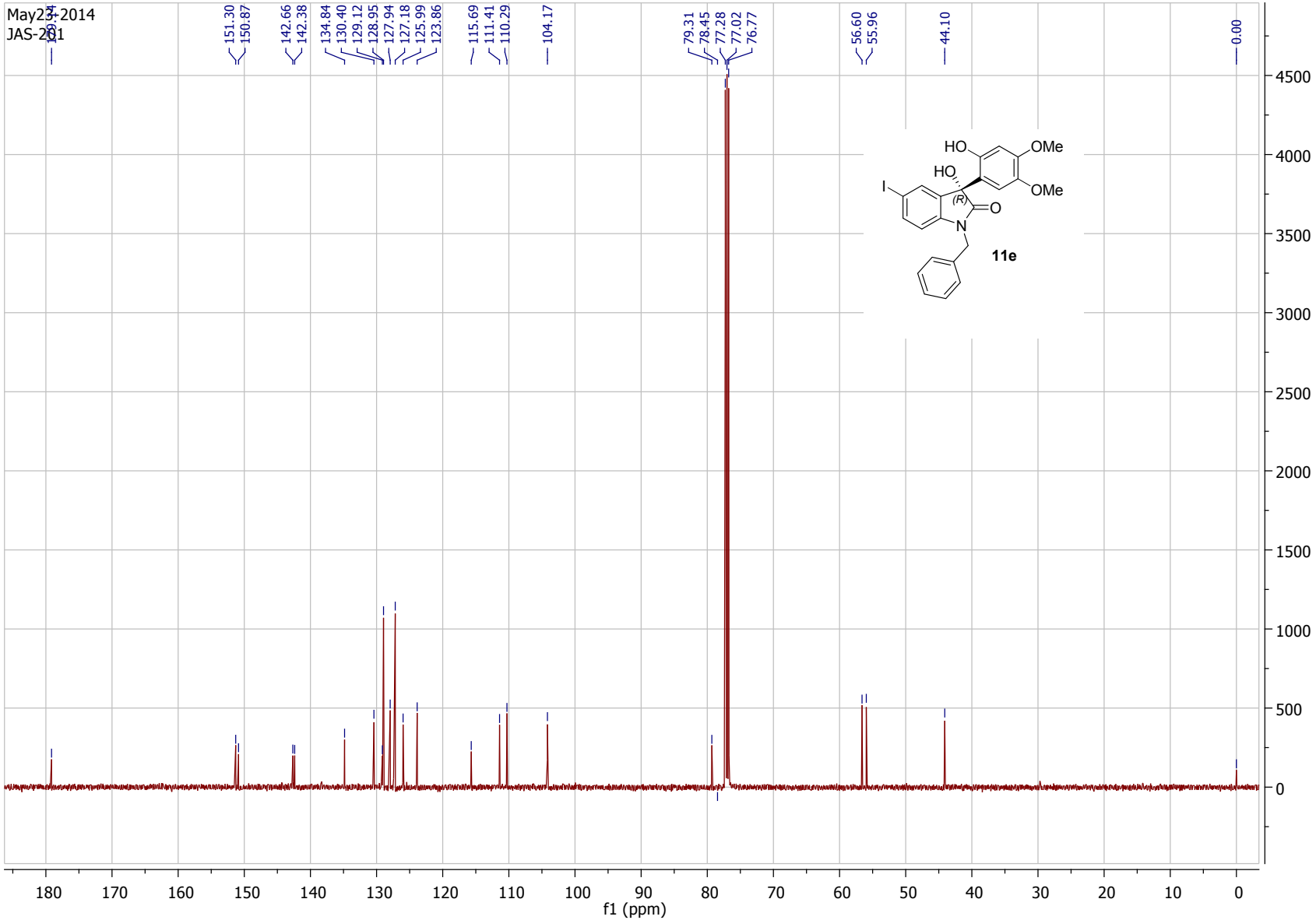

May 13-2014
JAS-206
179.58
152.08
151.98
143.90
141.85
135.46
131.29
130.41
130.05
129.13
128.16
127.37
116.26
112.27
112.05
105.22
80.11
78.28
78.03
77.77
57.75
57.01
45.24
1.01
HO
OMe
HO
Cl
(R)
O
N
OMe
11c
f1 (ppm)

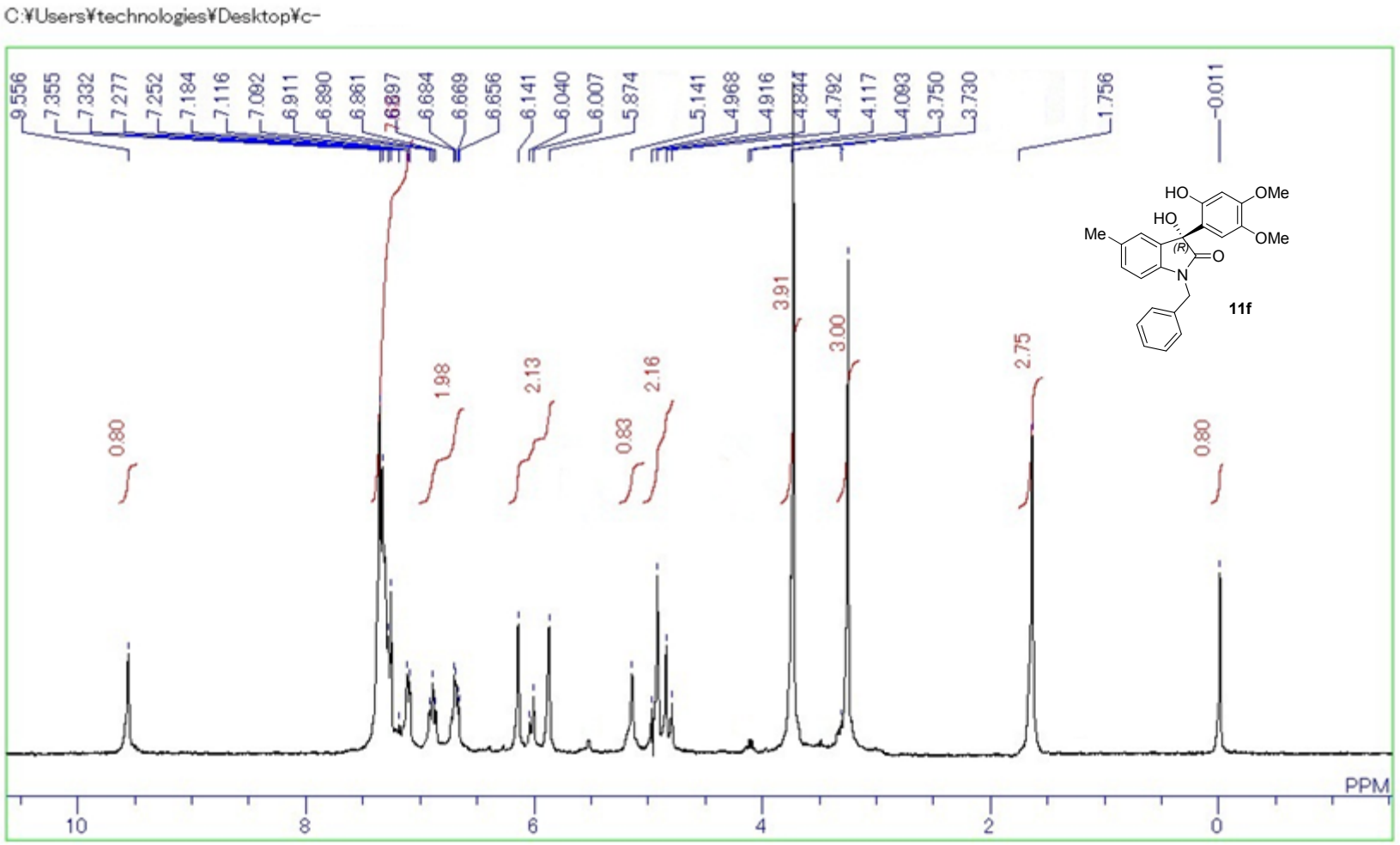
C:¥Users¥technologies¥Desktop¥nmrs¥Dr_Chimni¥C-JAS2021NON_E4_FT.als

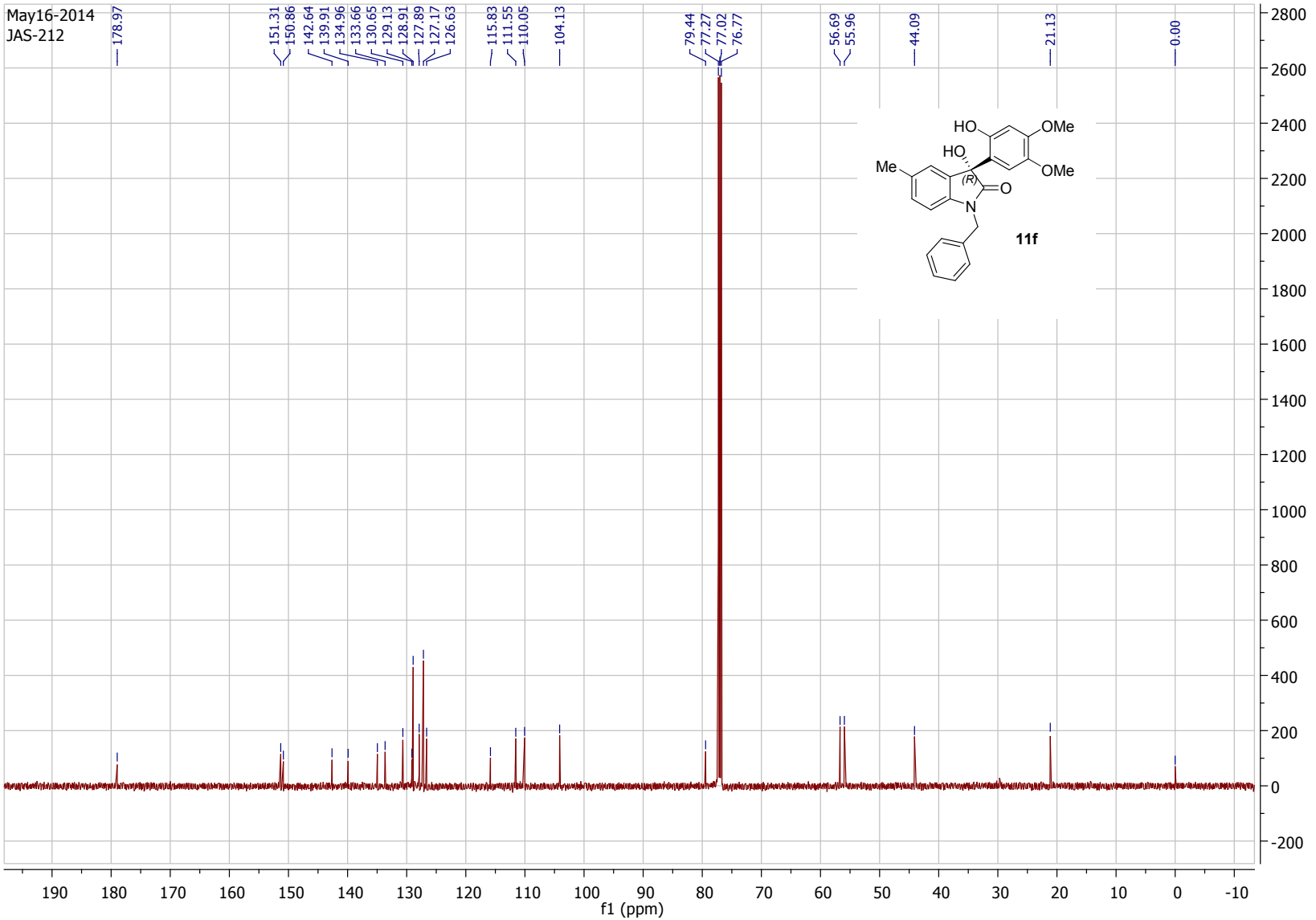



May14-2014
JAS-202
176.
161.40
159.29
157.19
135.45
128.87
127.88
127.65
116.33
116.15
112.80
112.61
109.99
109.93
103.91
95.65
92.00
78.13
77.27
77.01
76.76
55.81
55.32
44.27
0.00
HO
OMe
HO
Br
(R)
O
N
OMe
11d
f1 (ppm)

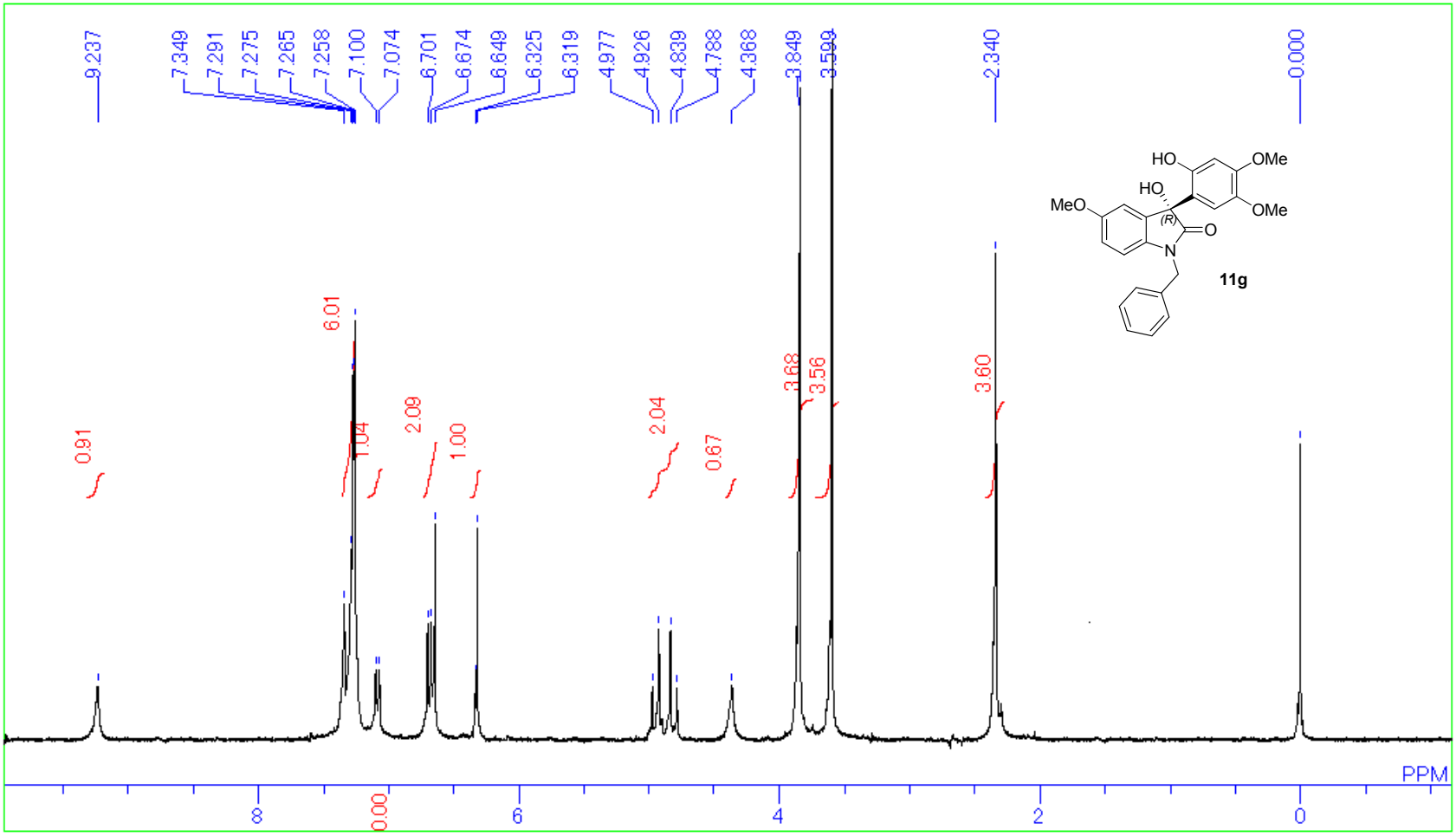

9.46
7.37
7.35
7.32
7.29
7.27
7.26
7.14
7.13
7.12
7.11
6.91
6.88
6.71
6.70
6.69
6.67
6.17
6.16
5.89
5.89
4.99
4.93
4.88
4.83
4.57
3.75
3.28
-0.00
HO
OMe
HO
OMe
I
(R)
O
N
11e
0.91
5.48
0.89
1.18
1.01
1.00
0.83
2.26
0.80
3.35
3.00
f1 (ppm)

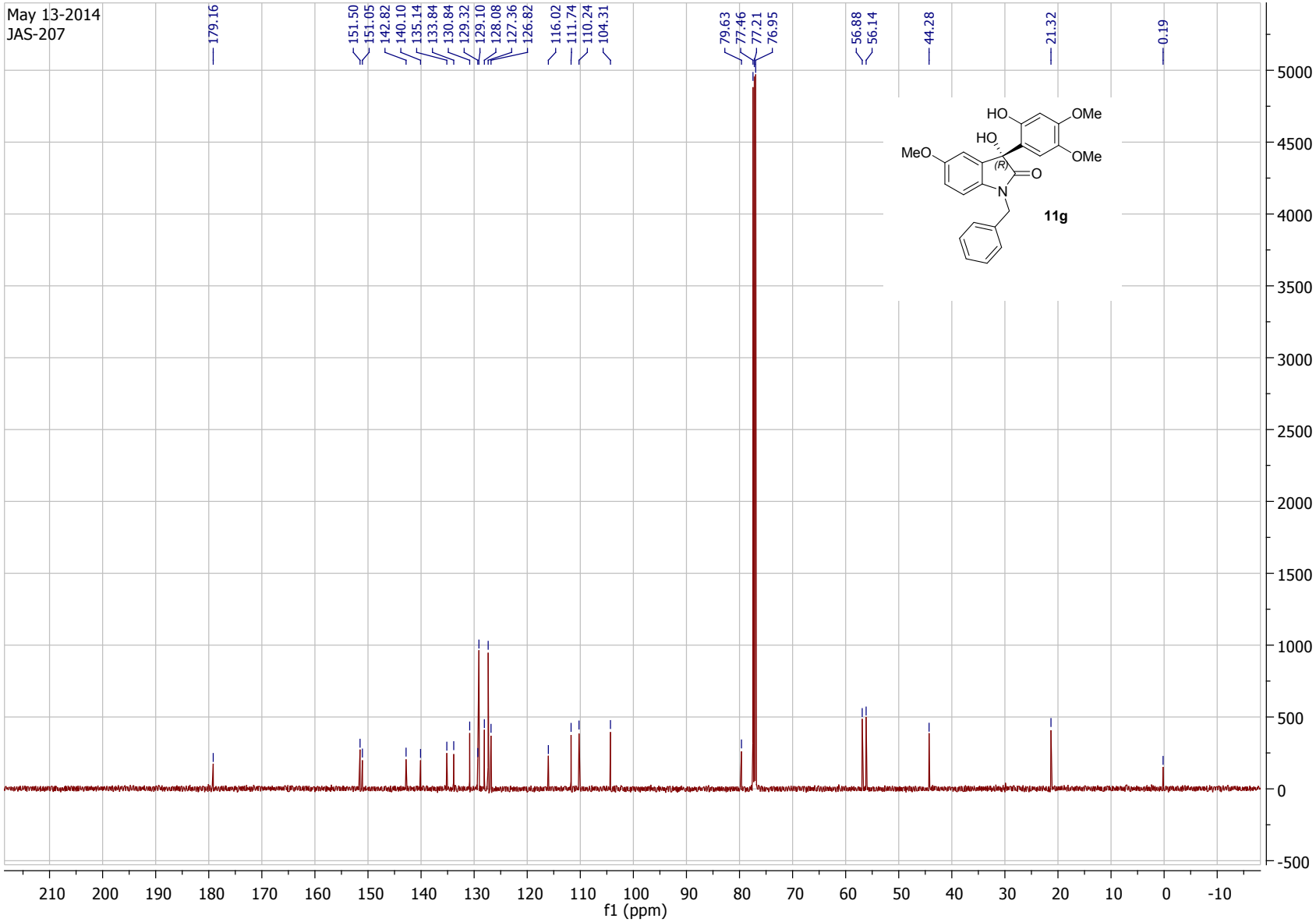

May23-2014
JAS-231
151.30
150.87
142.66
142.38
134.84
130.40
129.12
128.95
127.94
127.18
125.99
123.86
115.69
111.41
110.29
104.17
79.31
78.45
77.28
77.02
76.77
56.60
55.96
44.10
0.00
HO
OMe
HO
OMe
I
(R)
O
N
11e
f1 (ppm)

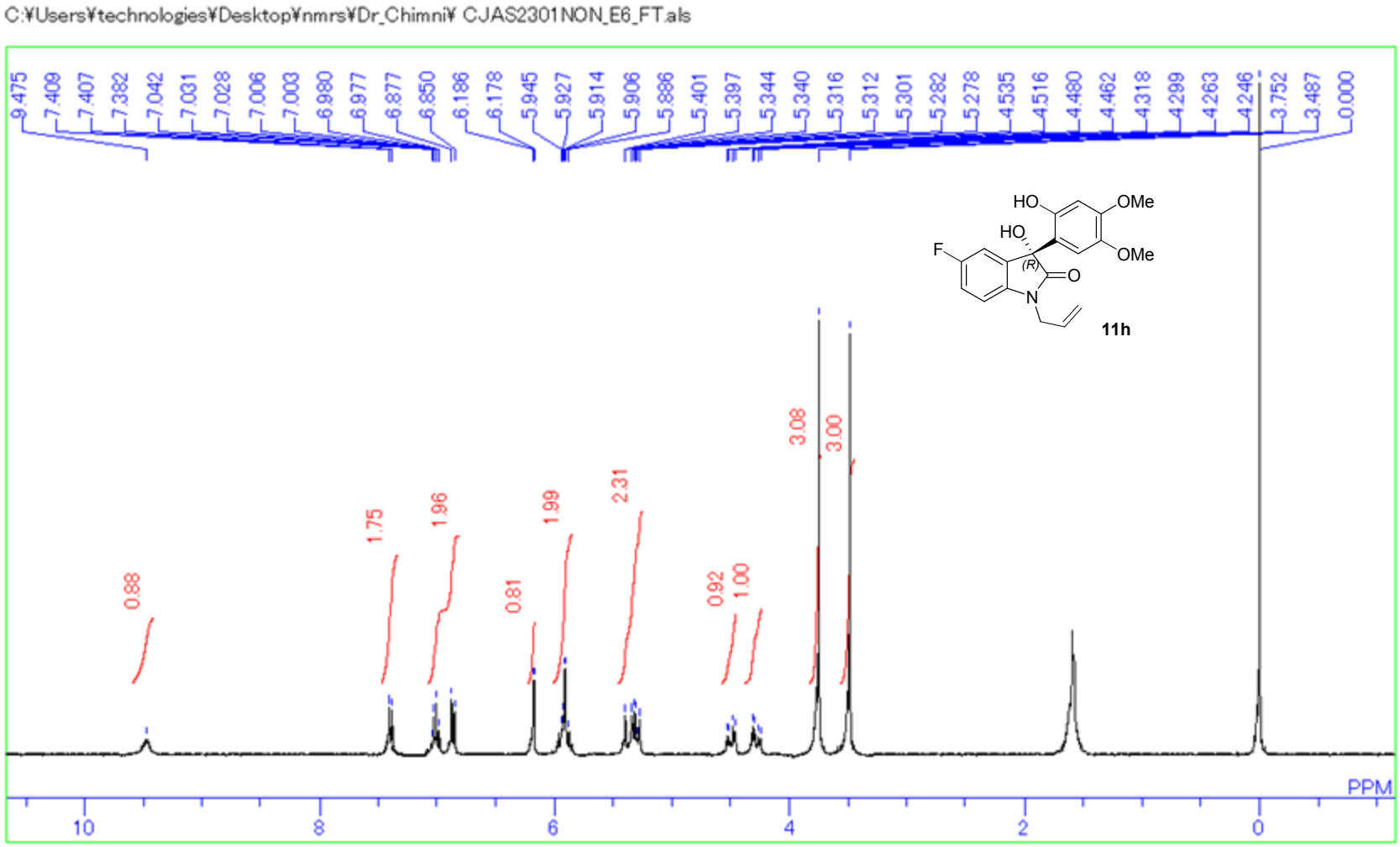

C:¥Users¥technologies¥Desktop¥c-
9.556
7.355
7.332
7.277
7.252
7.184
7.116
7.092
6.911
6.890
6.861
6.684
6.669
6.656
6.141
6.040
6.007
5.874
5.141
4.968
4.916
4.844
4.792
4.117
4.093
3.750
3.730
1.756
0.011
0.80
1.98
2.13
0.83
2.16
3.91
3.00
2.75
0.80
HO
OMe
HO
Me
(R)
O
N
OMe
11f
PPM
10
8
6
4
2
0

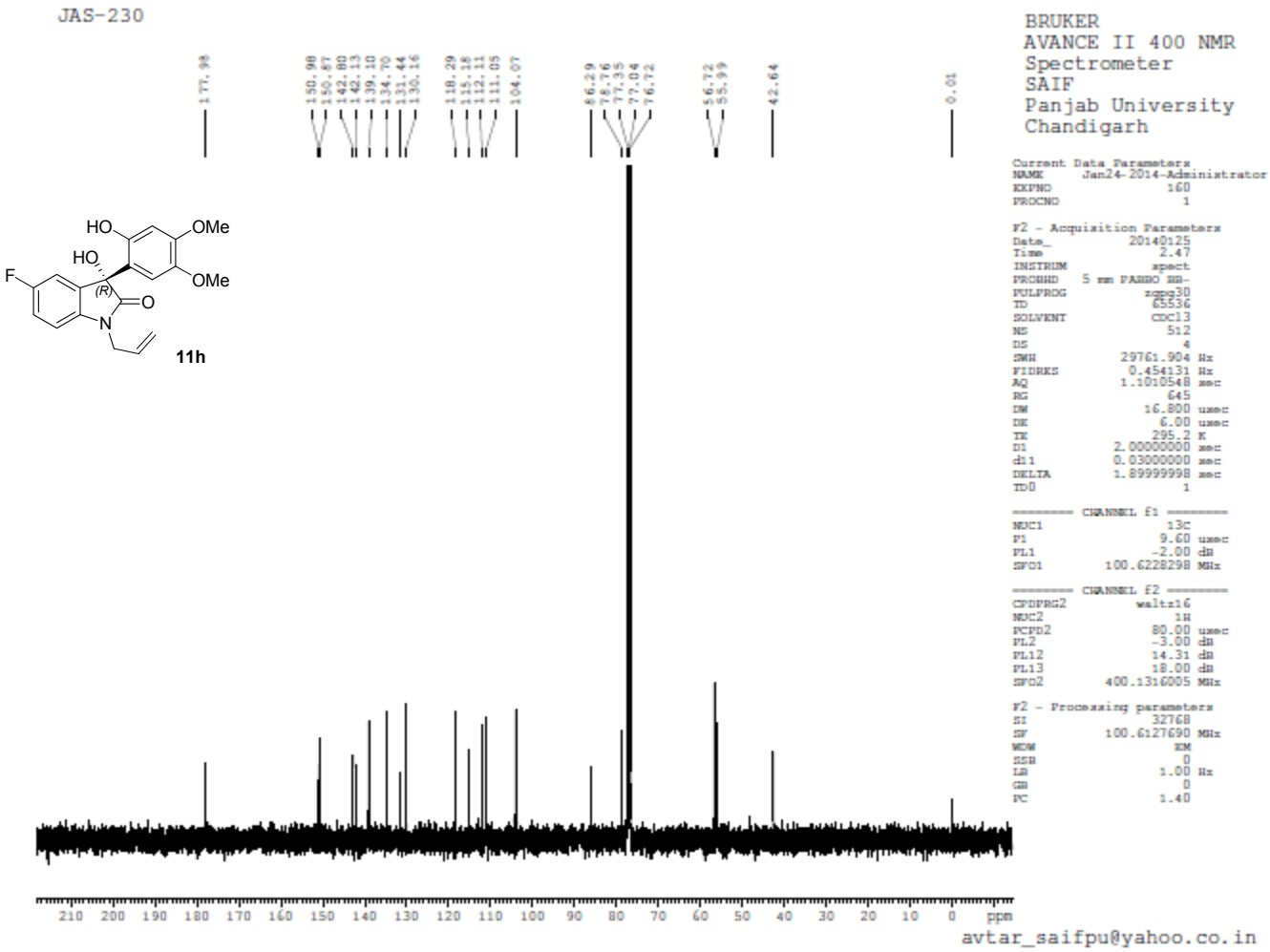

May16-2014
JAS-212
178.97
151.31
150.86
142.64
139.91
134.96
133.66
130.65
129.13
128.91
127.89
127.17
126.63
115.83
111.55
110.05
104.13
79.44
77.27
77.02
76.77
56.69
55.96
44.09
21.13
0.00
HO
OMe
HO
Me
OMe
(R)
O
N
11f
f1 (ppm)

C:¥Users¥technologies¥Desktop¥nmrs¥Dr_Chimni¥C-JAS2071NON_E3_FT.als

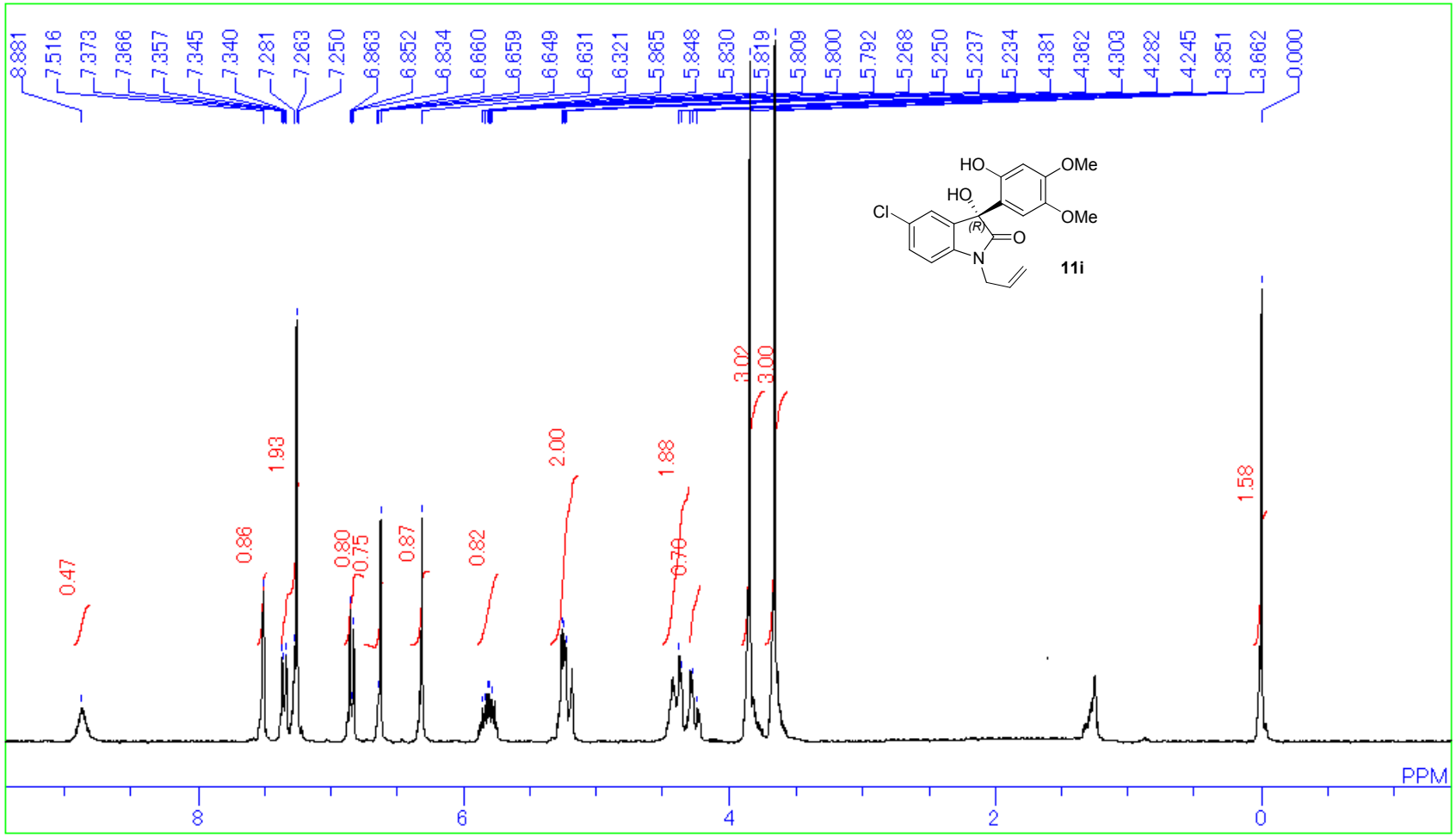


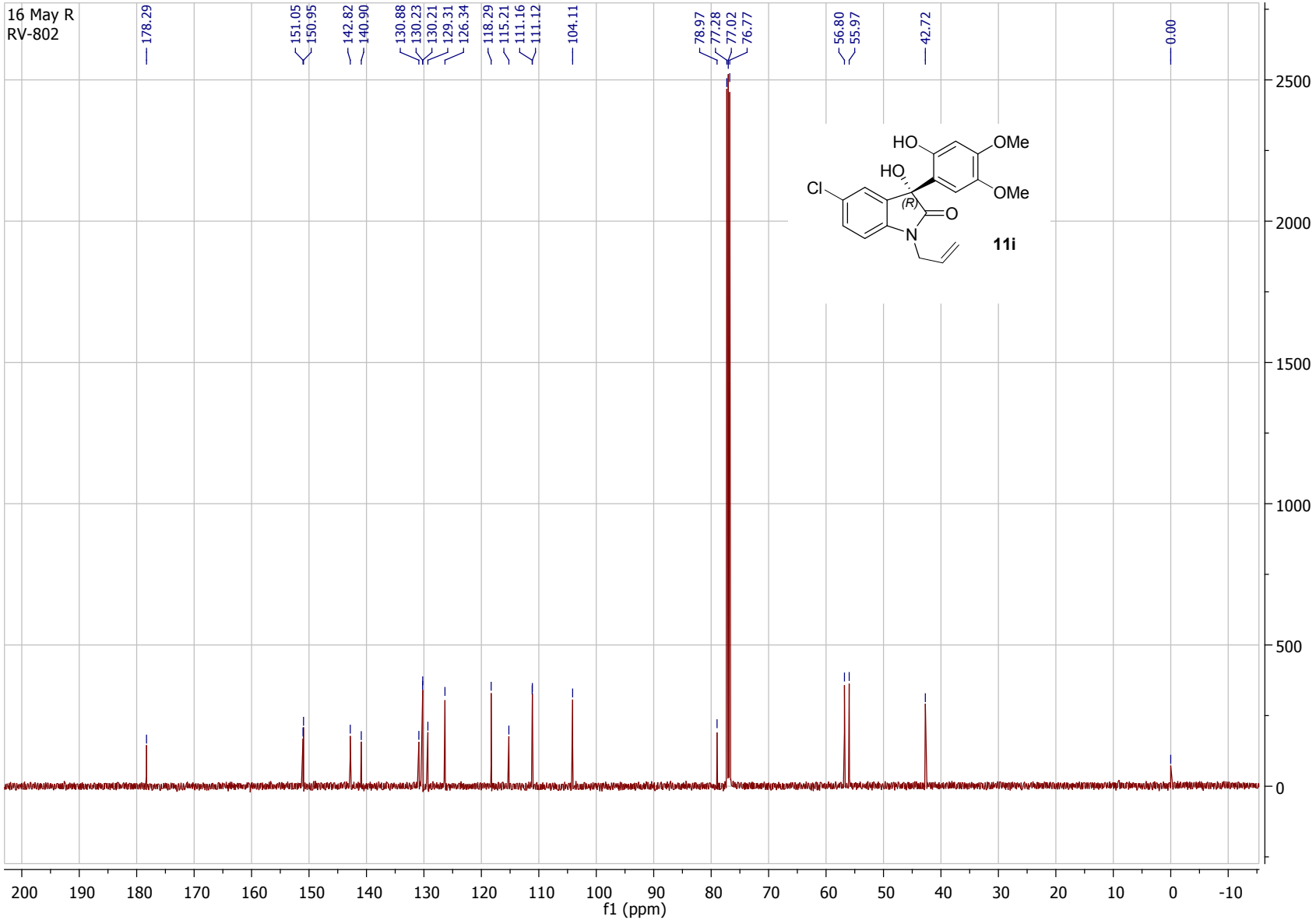

May 13-2014
JAS-207
179.16
151.50
151.05
142.82
140.10
135.14
133.84
130.84
129.32
129.10
128.08
127.36
126.82
116.02
111.74
110.24
104.31
79.63
77.46
77.21
76.95
56.88
56.14
44.28
21.32
0.19
HO
OMe
HO
MeO
OMe
(R)
O
N
11g
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


C:¥Users¥technologies¥Desktop¥nmrs¥Dr_Chimni¥ CJAS2301NON_E6_FT.als
9.475
7.409
7.407
7.382
7.042
7.031
7.028
7.006
7.003
6.980
6.977
6.877
6.850
6.186
6.178
5.945
5.927
5.914
5.906
5.886
5.401
5.397
5.344
5.340
5.316
5.312
5.301
5.282
5.278
4.535
4.516
4.480
4.462
4.318
4.299
4.263
4.246
3.752
3.487
0.000
HO
OMe
HO
F
OMe
(R)
O
N
11h
0.88
1.75
1.96
0.81
1.99
2.31
0.92
1.00
3.08
3.00
PPM
10
8
6
4
2
0

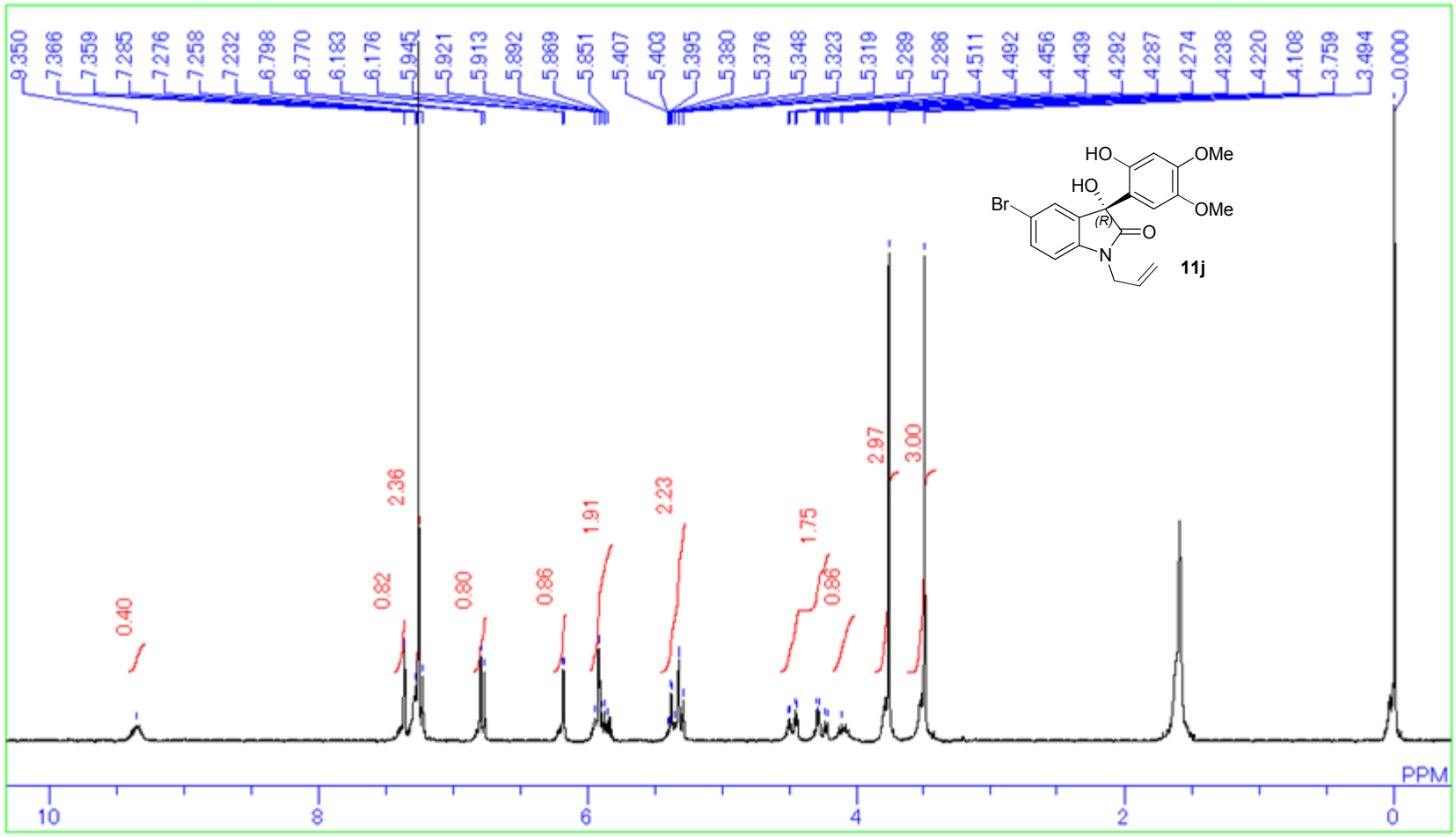

JAS-230
177.98
150.98
150.87
142.80
142.13
139.10
134.70
131.44
130.16
118.29
115.18
112.11
111.05
104.07
86.29
86.16
77.35
77.04
76.72
56.72
55.99
42.64
0.01
HO
OMe
HO
OMe
F
(R)
O
N
11h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Jan24-2014-Administrator
EXPNO 160
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140125
Time 2.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 645
DW 16.800 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
avtar_saifpu@yahoo.co.in

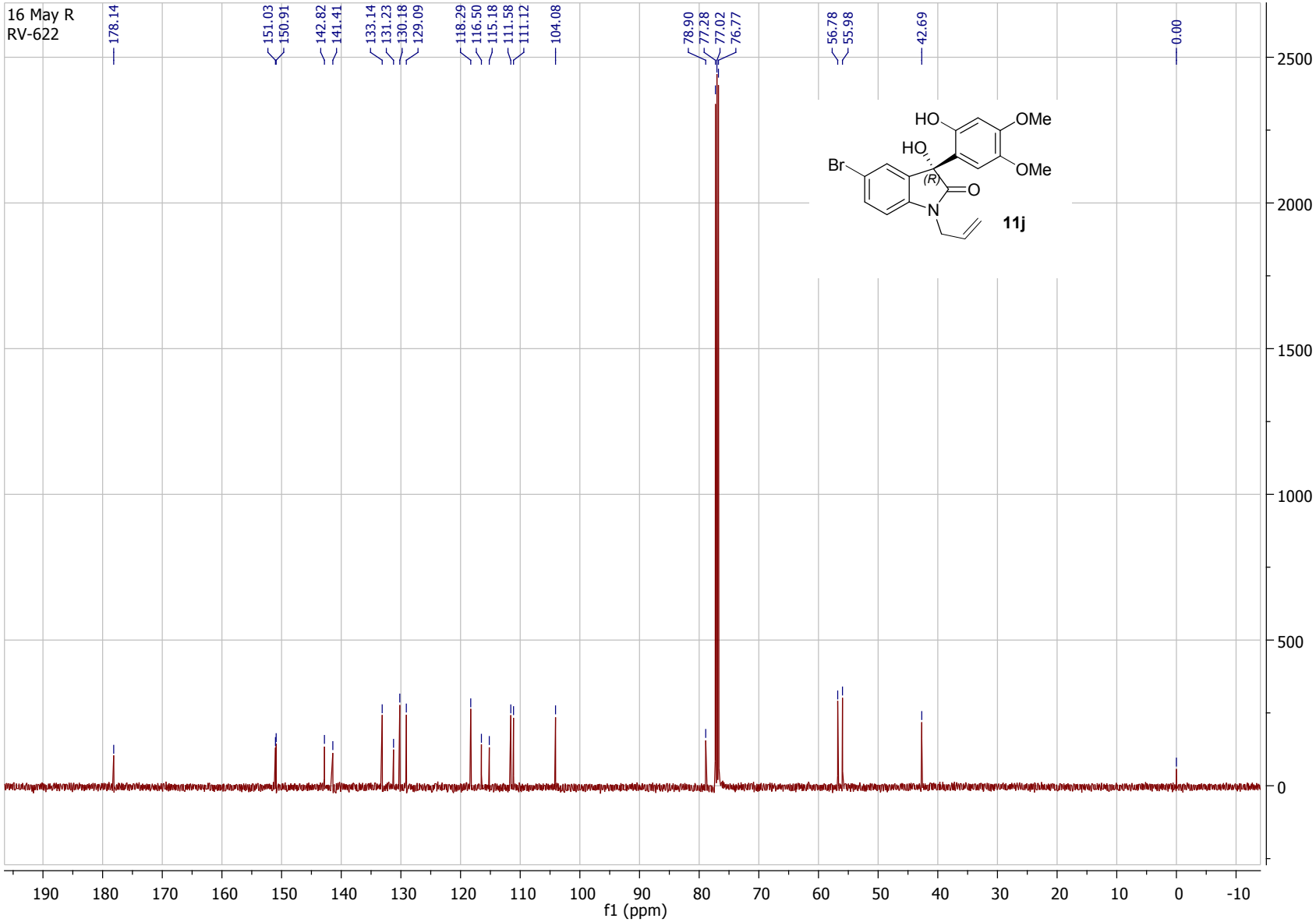
C:¥Users¥technologies¥Desktop¥C



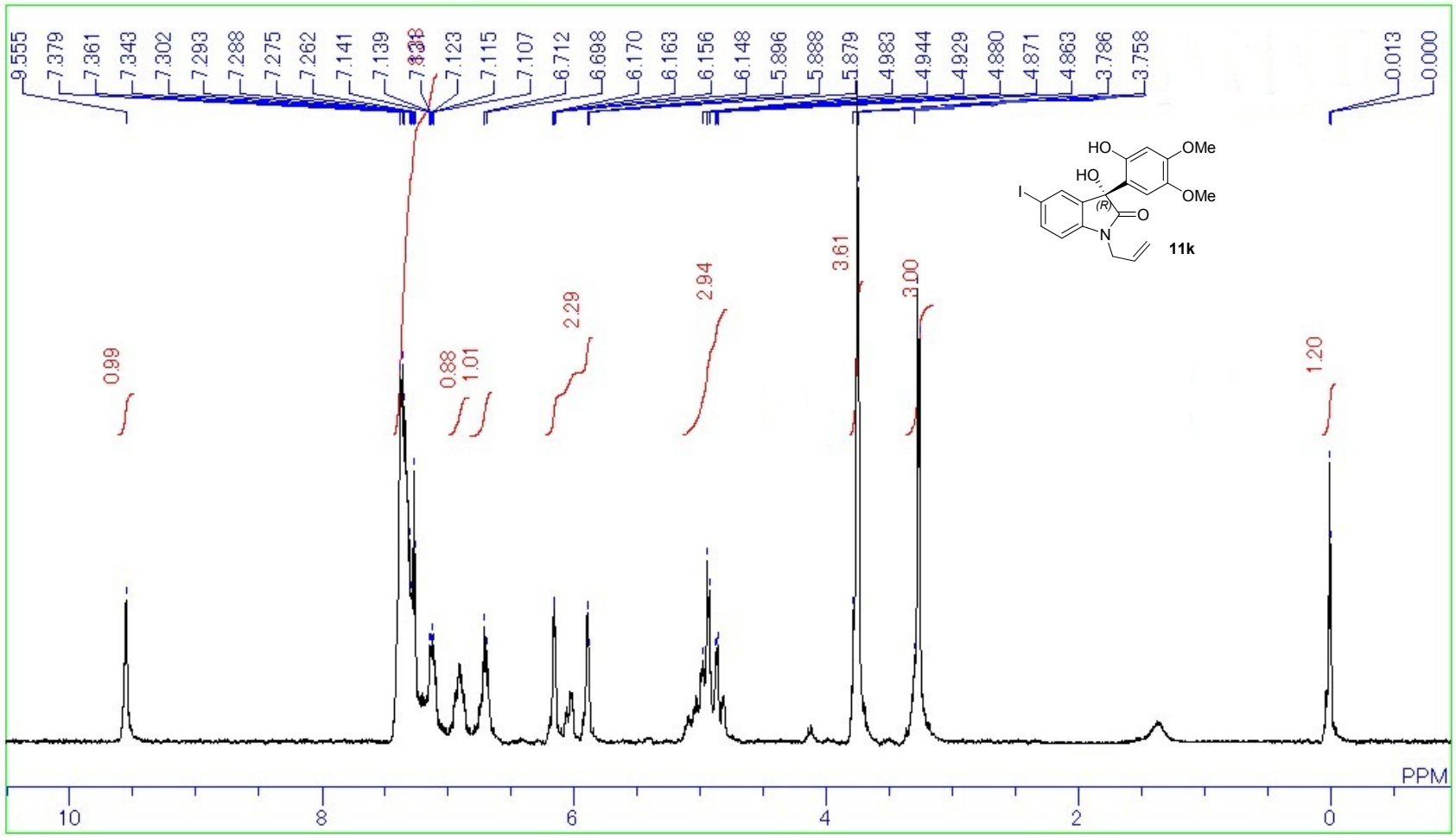

16 May R
RV-802
178.29
151.05
150.95
142.82
140.90
130.88
130.23
130.21
129.31
126.34
118.29
115.21
111.16
111.12
104.11
78.97
77.28
77.02
76.77
56.80
55.97
42.72
0.00
HO
OMe
HO
Cl
(R)
O
OMe
N
11i
2500
2000
1500
1000
500
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

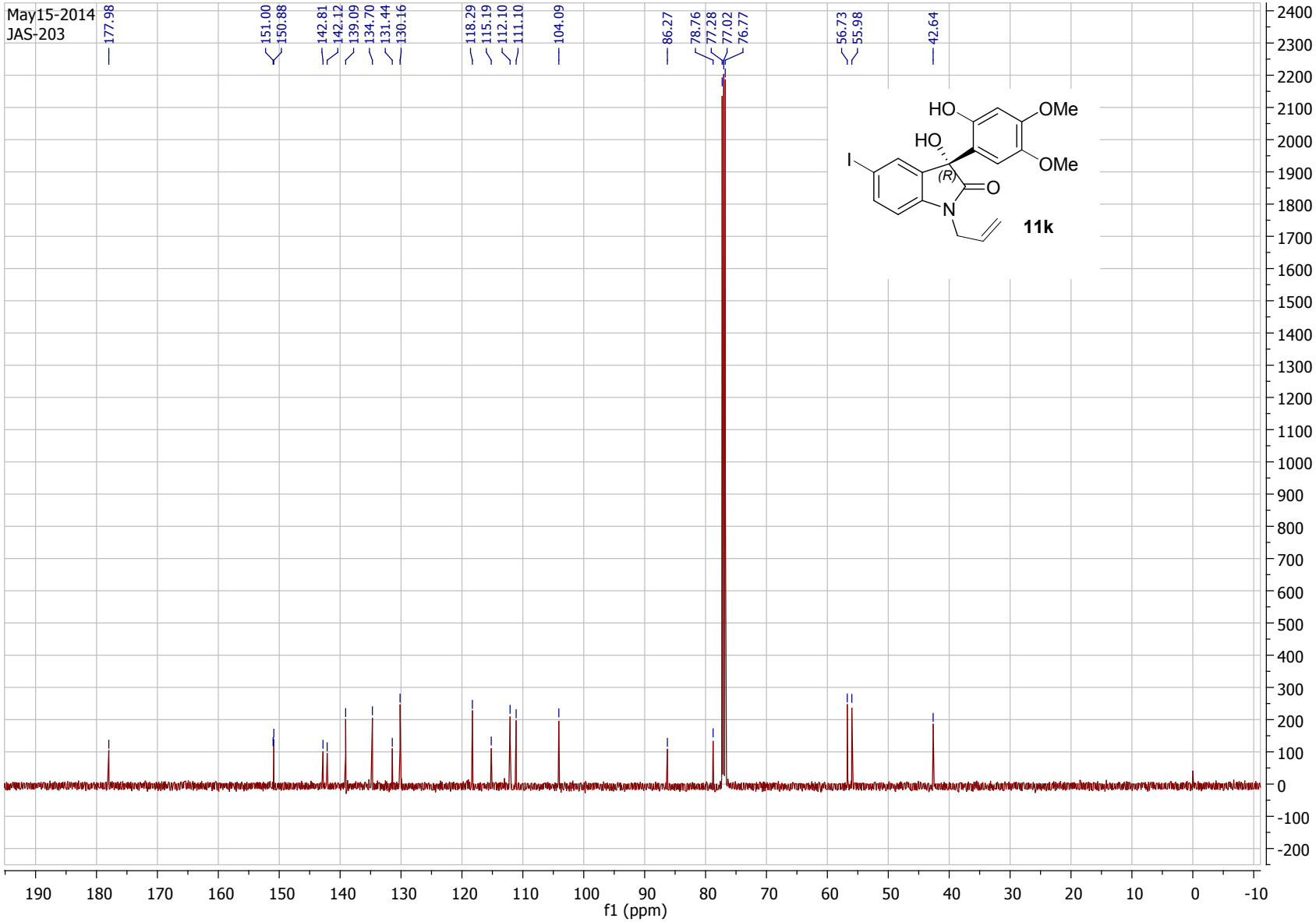
C:¥Users¥technologies¥Desktop¥nmrs¥Dr_Chimni¥ CJAS2261NON_E7_FT.als

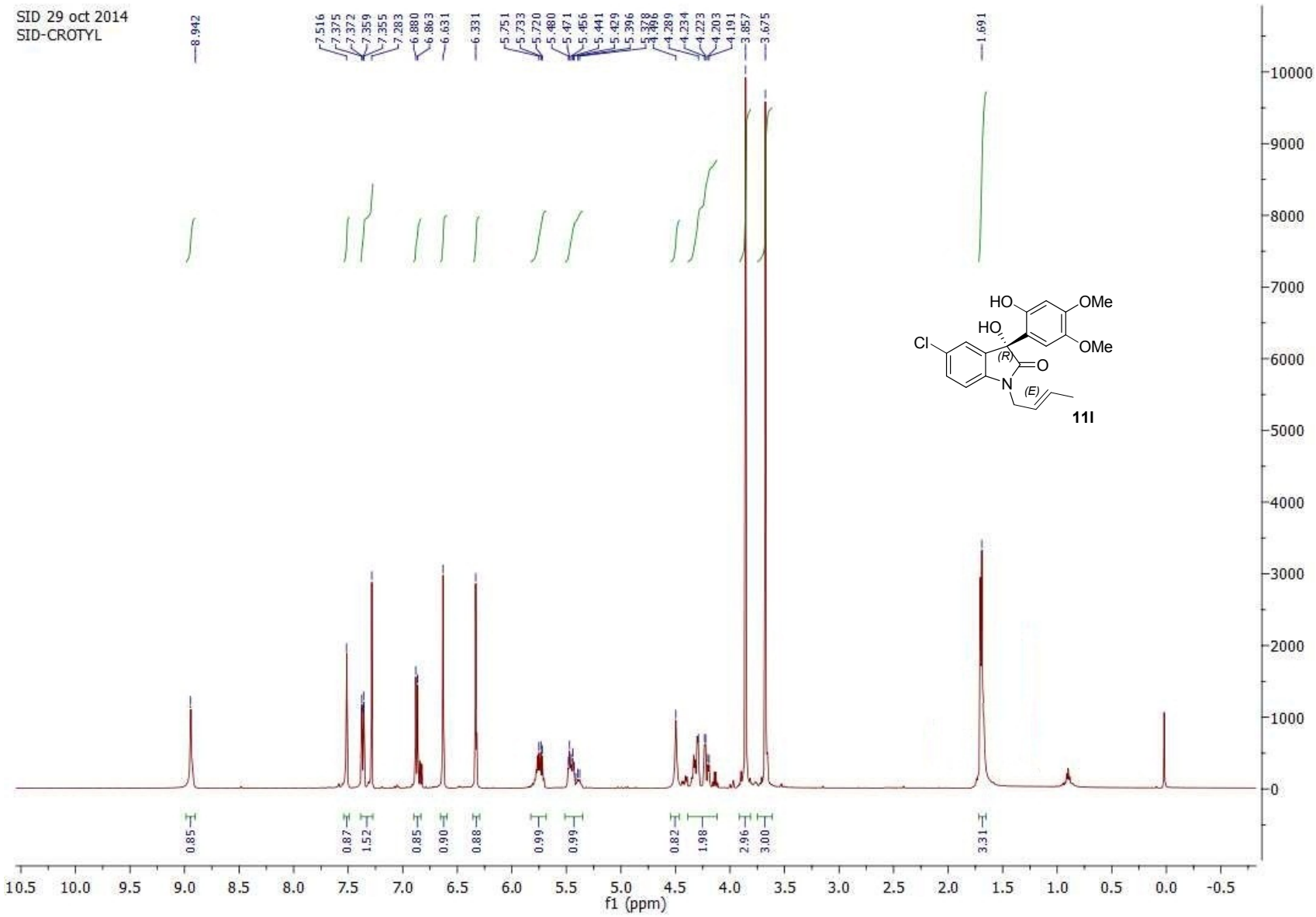


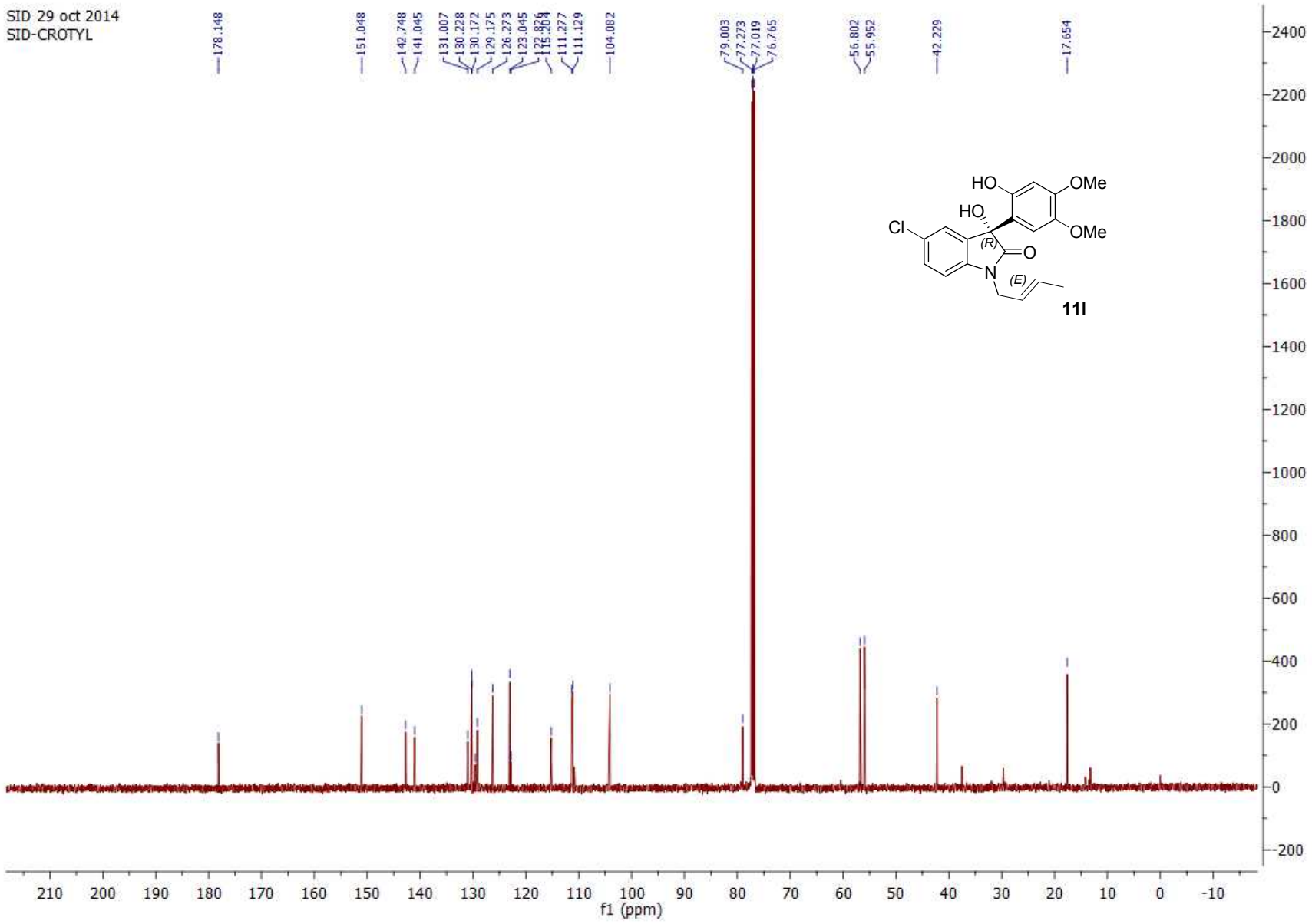

16 May R
RV-622
178.14
151.03
150.91
142.82
141.41
133.14
131.23
130.18
129.09
118.29
116.50
115.18
111.58
111.12
104.08
78.90
77.28
77.02
76.77
56.78
55.98
42.69
0.00
HO
OMe
HO
Br
(R)
O
N
OMe
11j
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

C:¥Users¥technologies¥Desktop¥C

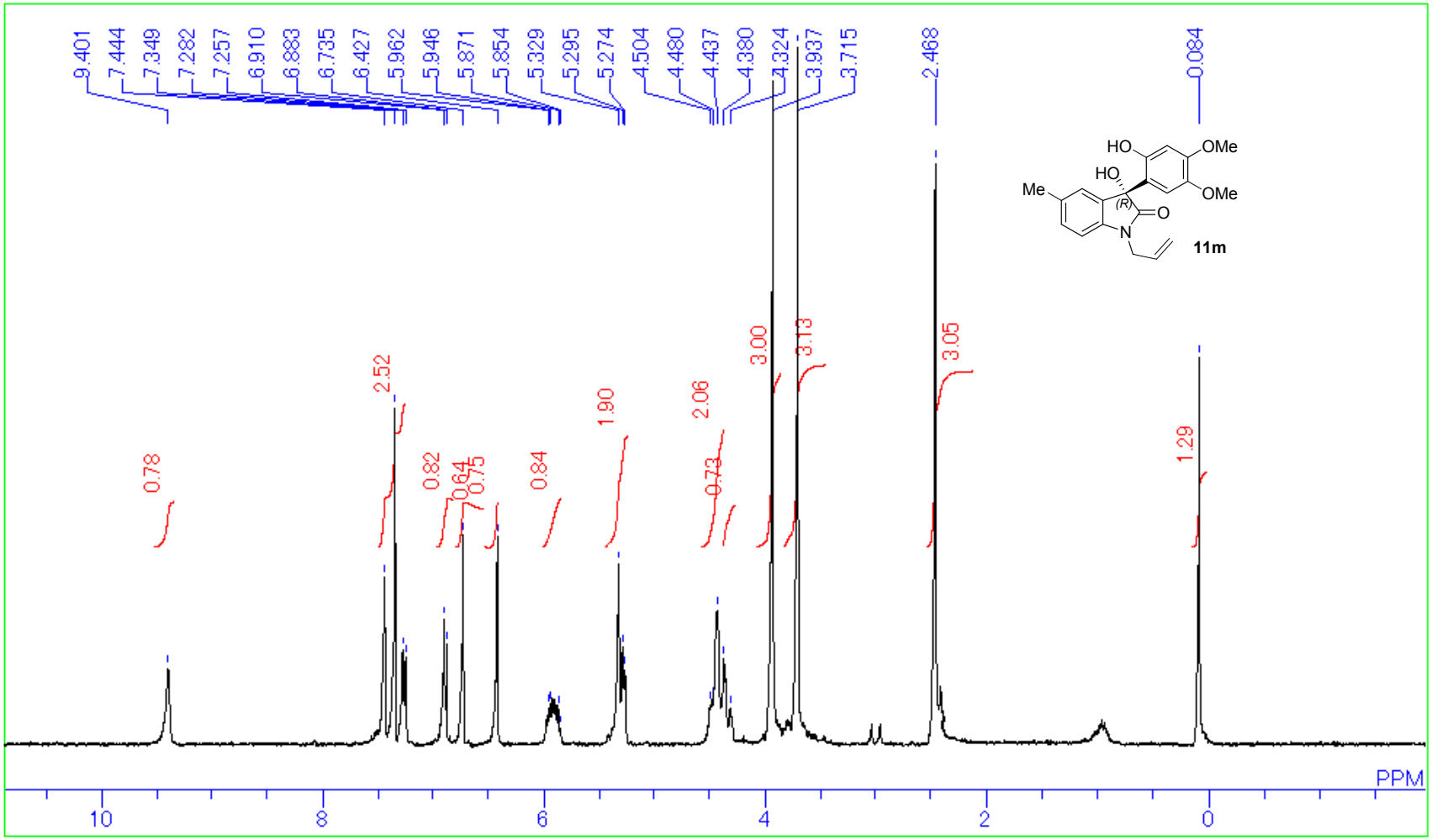


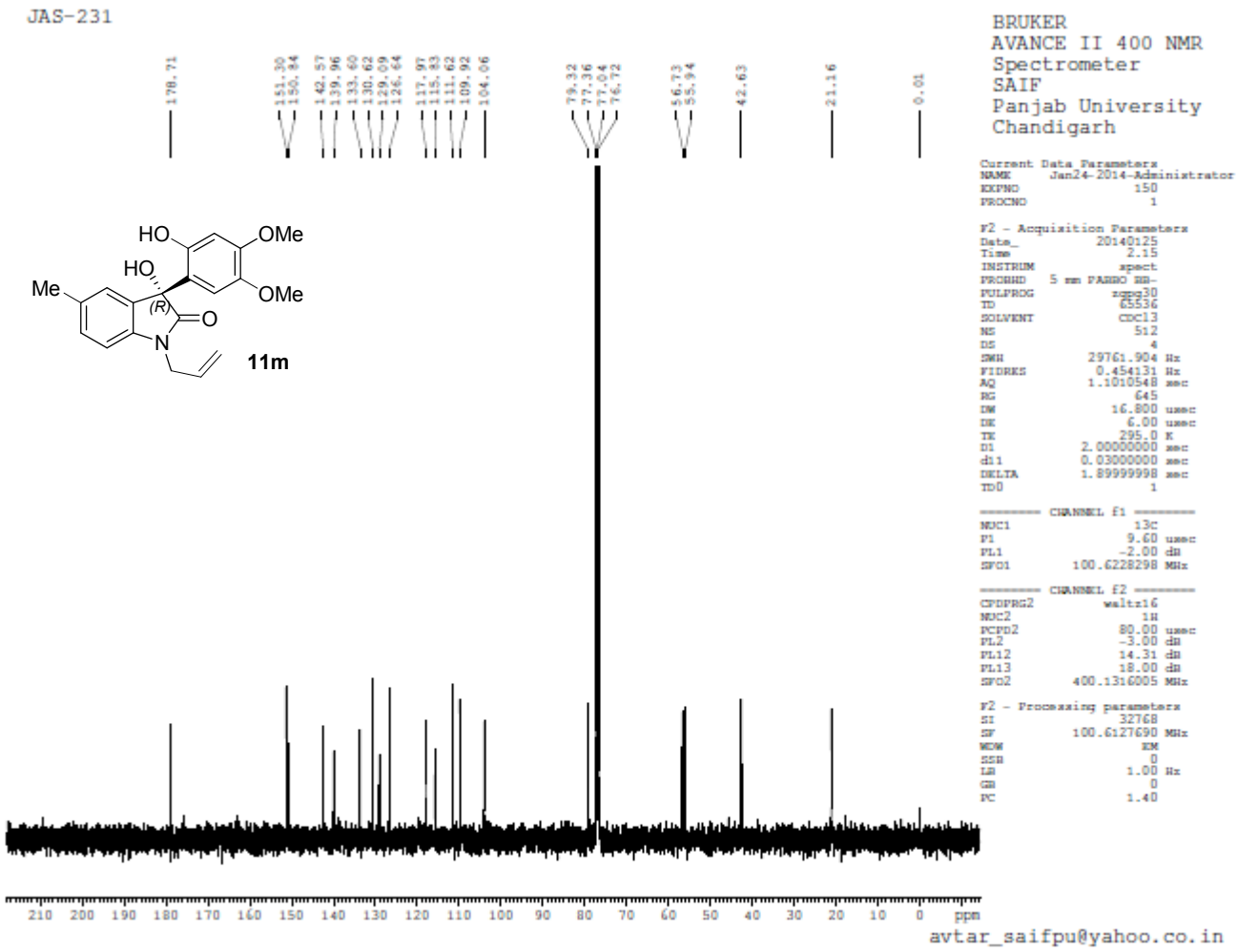

May15-2014
JAS-203
177.98
151.00
150.88
142.81
142.12
139.09
134.70
131.44
130.16
118.29
115.19
112.10
111.10
104.09
86.27
78.76
77.28
77.02
76.77
56.73
55.98
42.64
HO
OMe
HO
OMe
I
(R)
O
N
11k
f1 (ppm)


SID 29 oct 2014
SID-CROTYL
8.942
7.516
7.375
7.372
7.359
7.355
7.283
6.880
6.863
6.631
6.331
5.751
5.733
5.720
5.480
5.471
5.456
5.441
5.429
5.396
4.289
4.234
4.223
4.203
4.191
3.857
3.675
1.691
HO
OMe
HO
Cl
OMe
(R)
O
N
(E)
11l
0.85
0.87
1.52
0.85
0.90
0.88
0.99
0.99
0.82
1.98
2.96
3.00
3.31
f1 (ppm)


SID 29 oct 2014
SID-CROTYL
178.148
151.048
142.748
141.045
131.007
130.228
130.172
129.175
126.273
123.045
111.277
111.129
104.082
79.003
77.273
77.019
76.765
56.802
55.952
42.229
17.654
HO
OMe
HO
Cl
OMe
(R)
O
N
(E)
11l
f1 (ppm)

C:¥Users¥technologies¥Desktop¥indoles¥all DMP data¥New folder¥nmr dmphenols¥Dr_Chimni¥JAS231.als





BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

```
Current Data Parameters
NAME       Jan24-2014-Administrator
EXPNO                 150
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140125
Time               2.15
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG                 645
DW              16.800 usec
DE               6.00 usec
TE              295.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

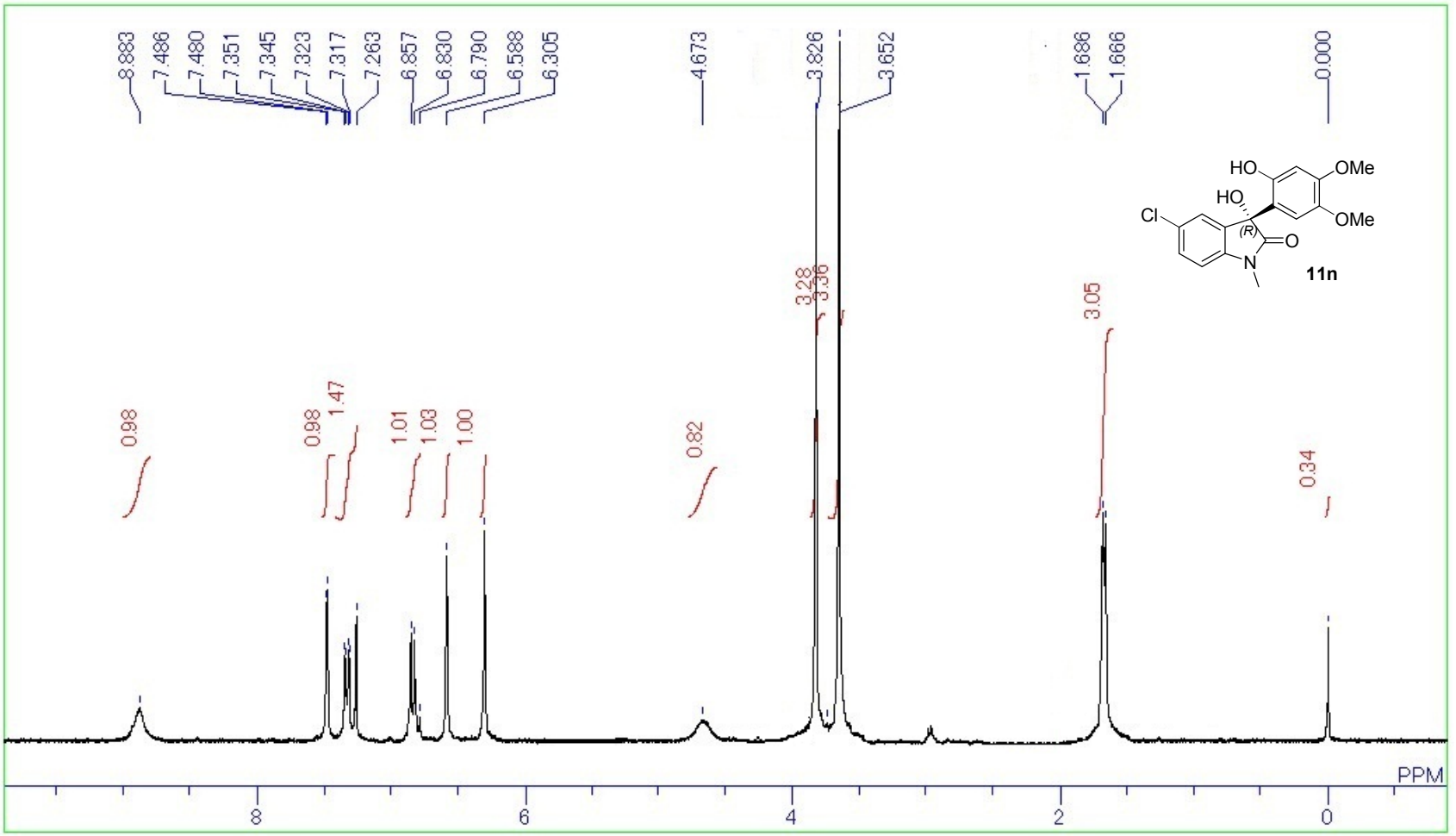
======== CHANNEL f1 ========
NUC1               13C
P1               9.60 usec
PL1             -2.00 dB
SFO1       100.6228298 MHz

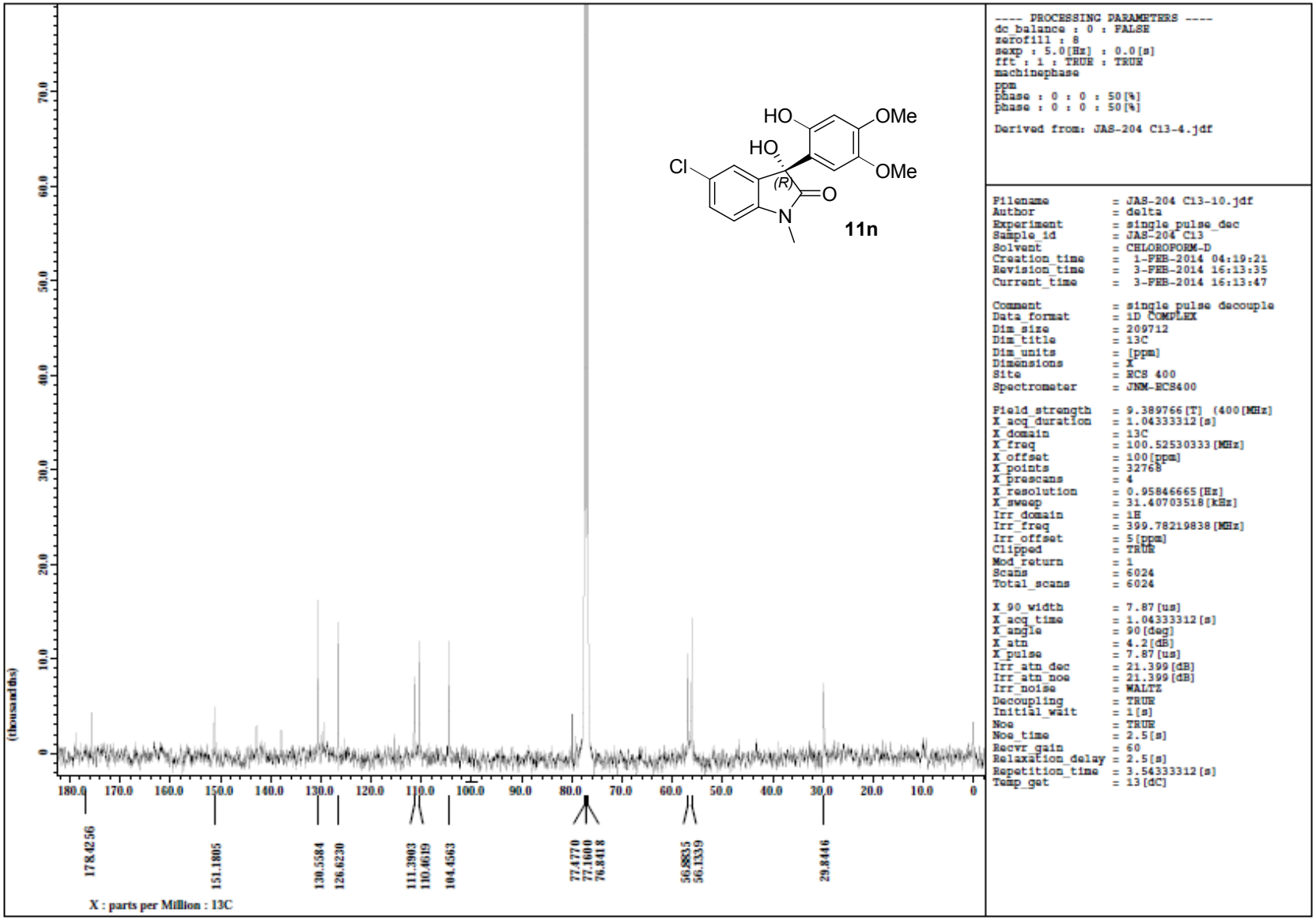
======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2               1H
PCPD2           80.00 usec
PL2             -3.00 dB
PL12            14.31 dB
PL13            18.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC                1.40
```

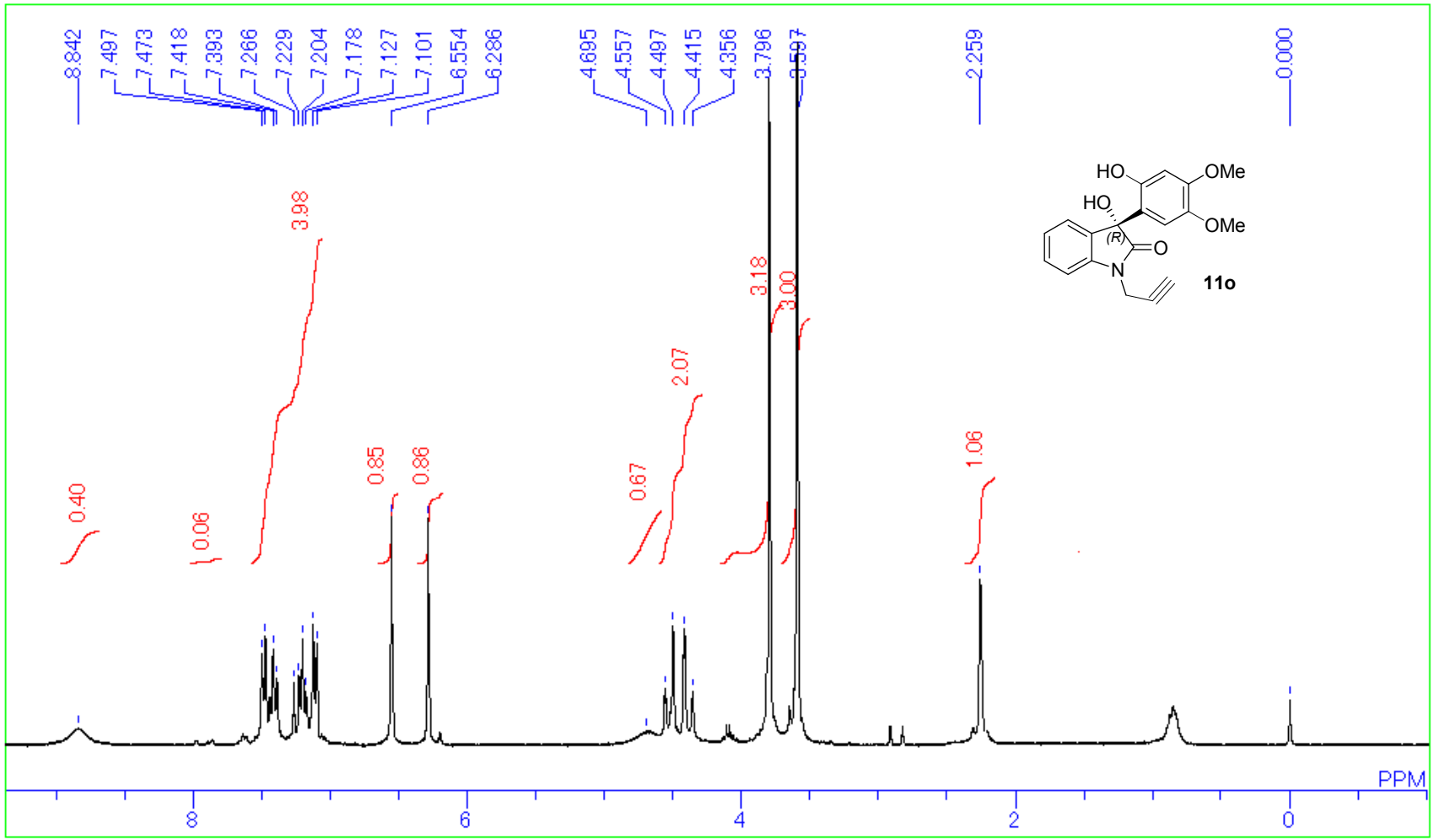
avtar_saifpu@yahoo.co.in

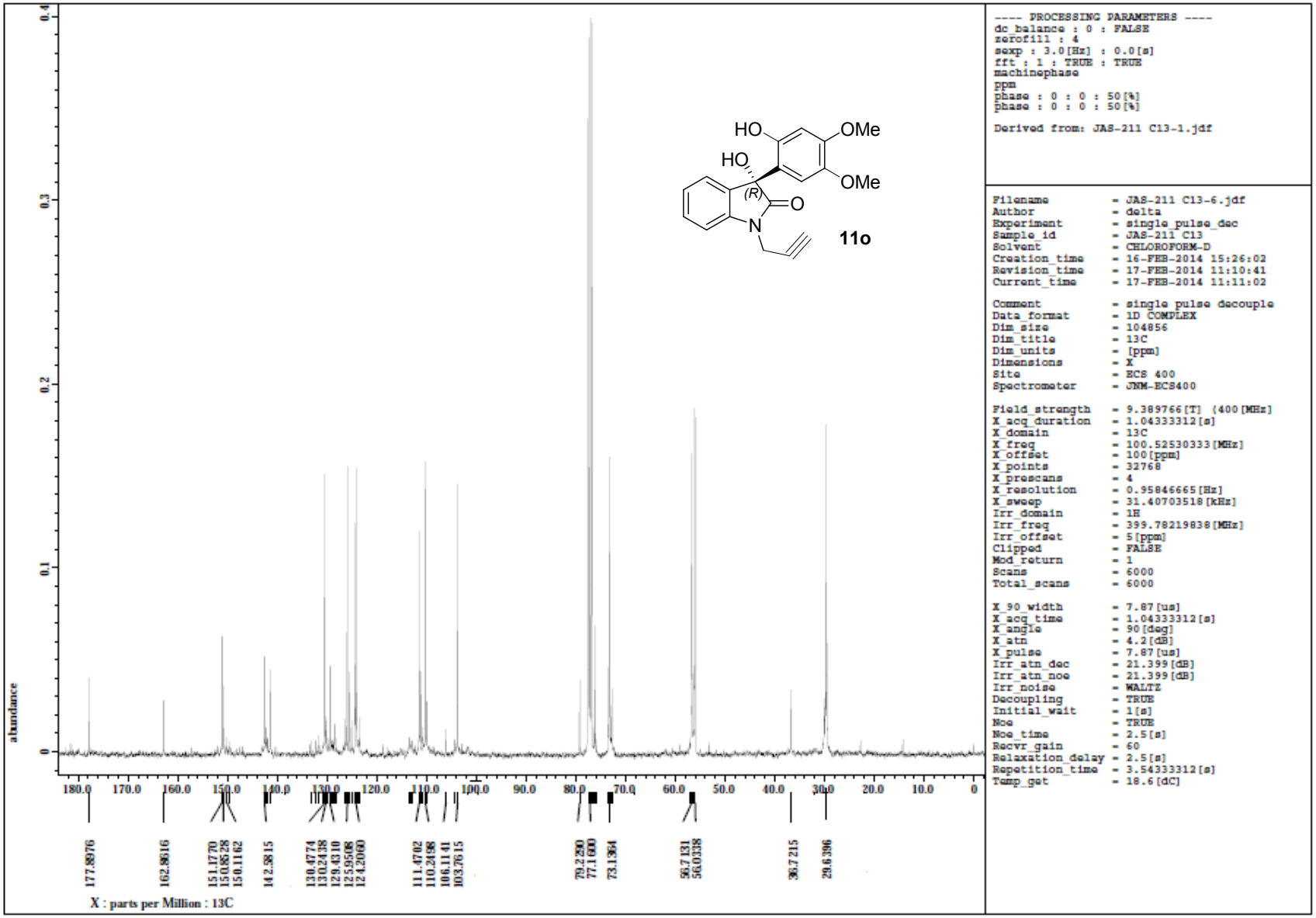
C:¥Users¥technologies¥Desktop¥C




HO
OMe
HO
Cl
(R)
O
OMe
N
11n
(thousandths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
178.4256
151.1805
130.5584
126.6230
111.3903
110.4619
104.4563
77.4770
77.1600
76.8418
56.8835
56.1339
29.8446
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 8
sexp : 5.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]
Derived from: JAS-204 C13-4.jdf
Filename = JAS-204 C13-10.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = JAS-204 C13
Solvent = CHLOROFORM-D
Creation_time = 1-FEB-2014 04:19:21
Revision_time = 3-FEB-2014 16:13:35
Current_time = 3-FEB-2014 16:13:47
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 209712
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = NCS 400
Spectrometer = JNM-NCS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 6024
Total_scans = 6024
X_90_width = 7.87[us]
X_acq_time = 1.04333312[s]
X_angle = 90[deg]
X_atn = 4.2[dB]
X_pulse = 7.87[us]
Irr_atn_dec = 21.399[dB]
Irr_atn_noe = 21.399[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2.5[s]
Recvr_gain = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.54333312[s]
Temp_get = 13[dC]

C:¥Users¥technologies¥Desktop¥C-JAS2111NON_E6_FT.als

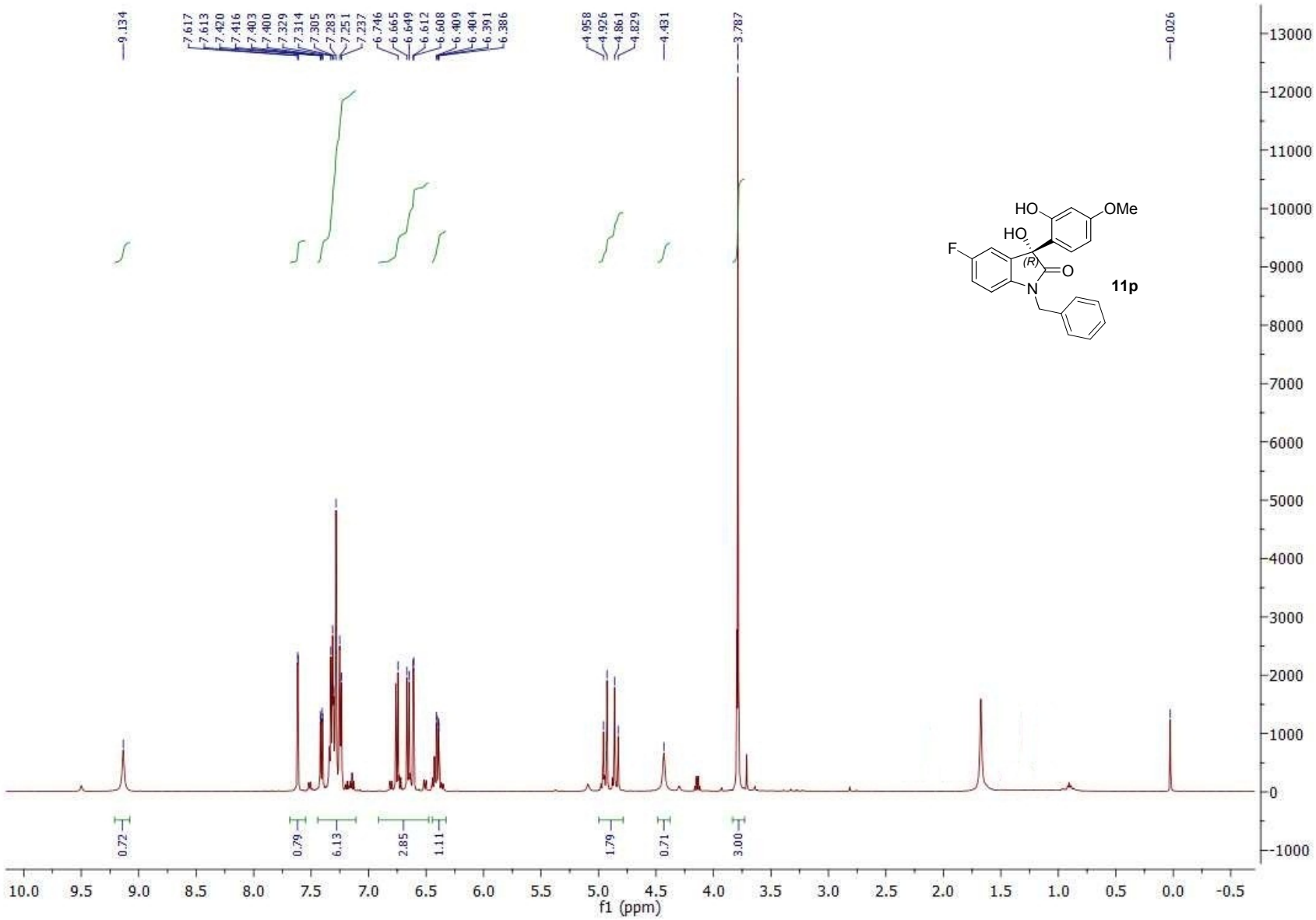


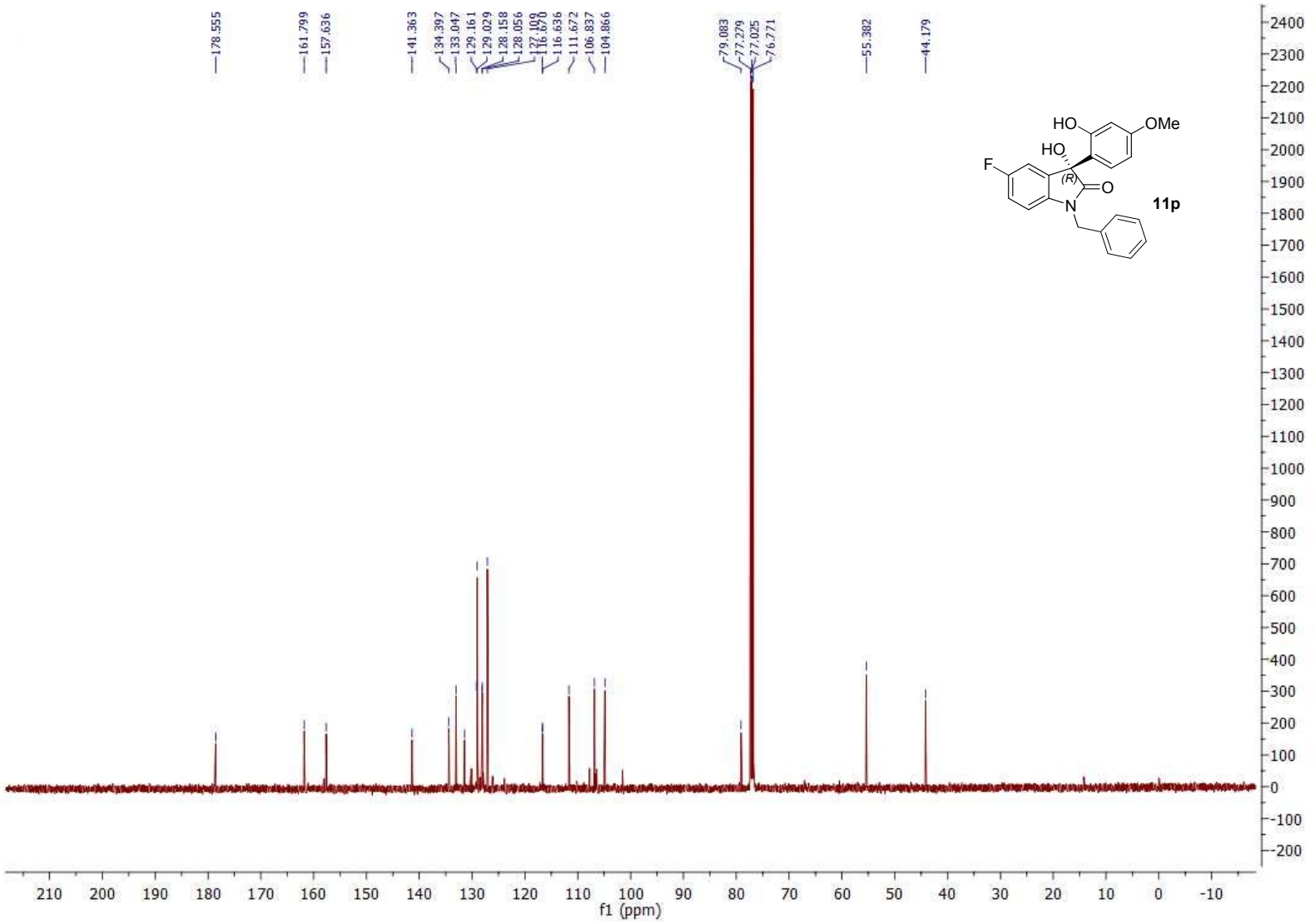


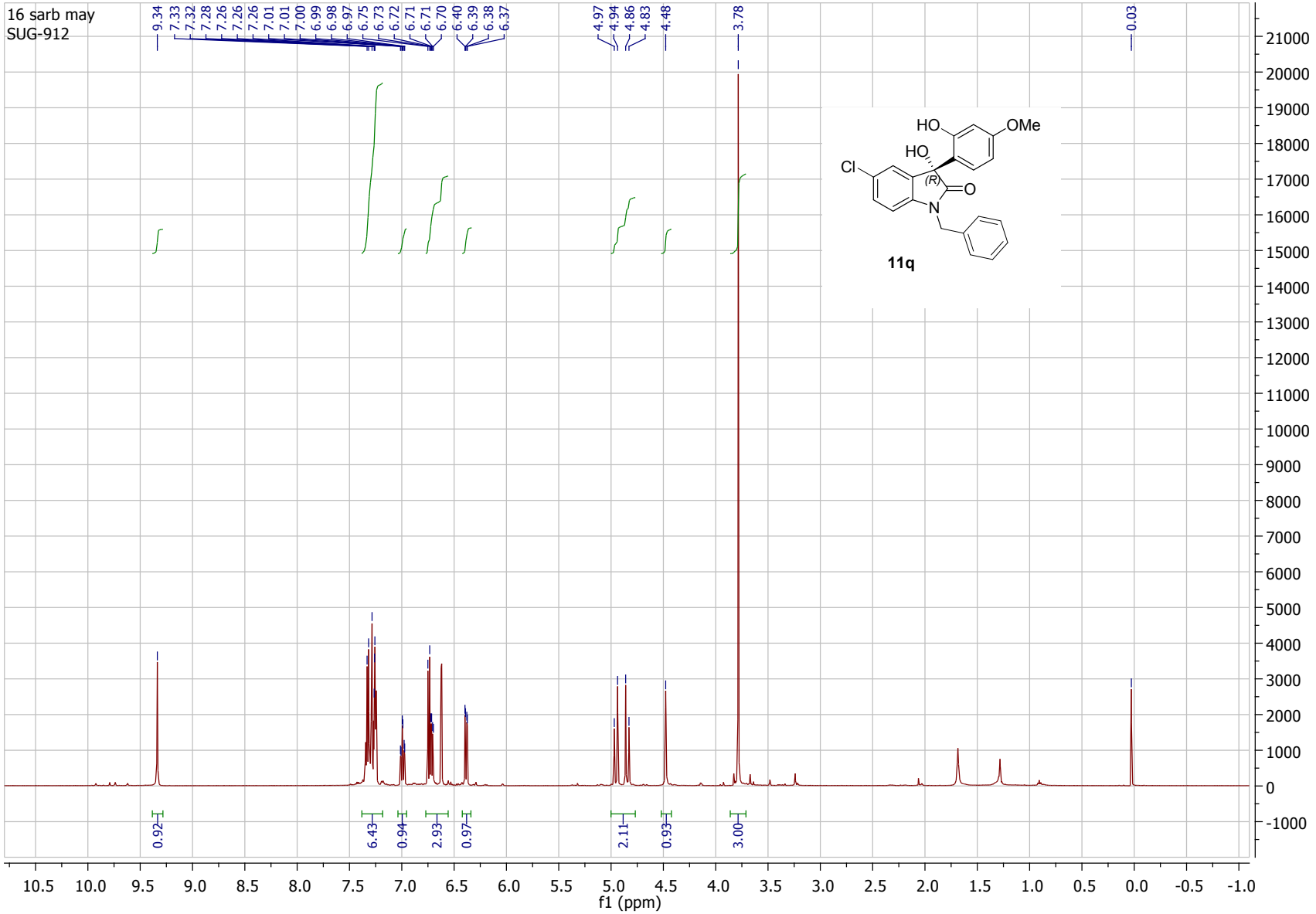

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 4
sexp : 3.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]

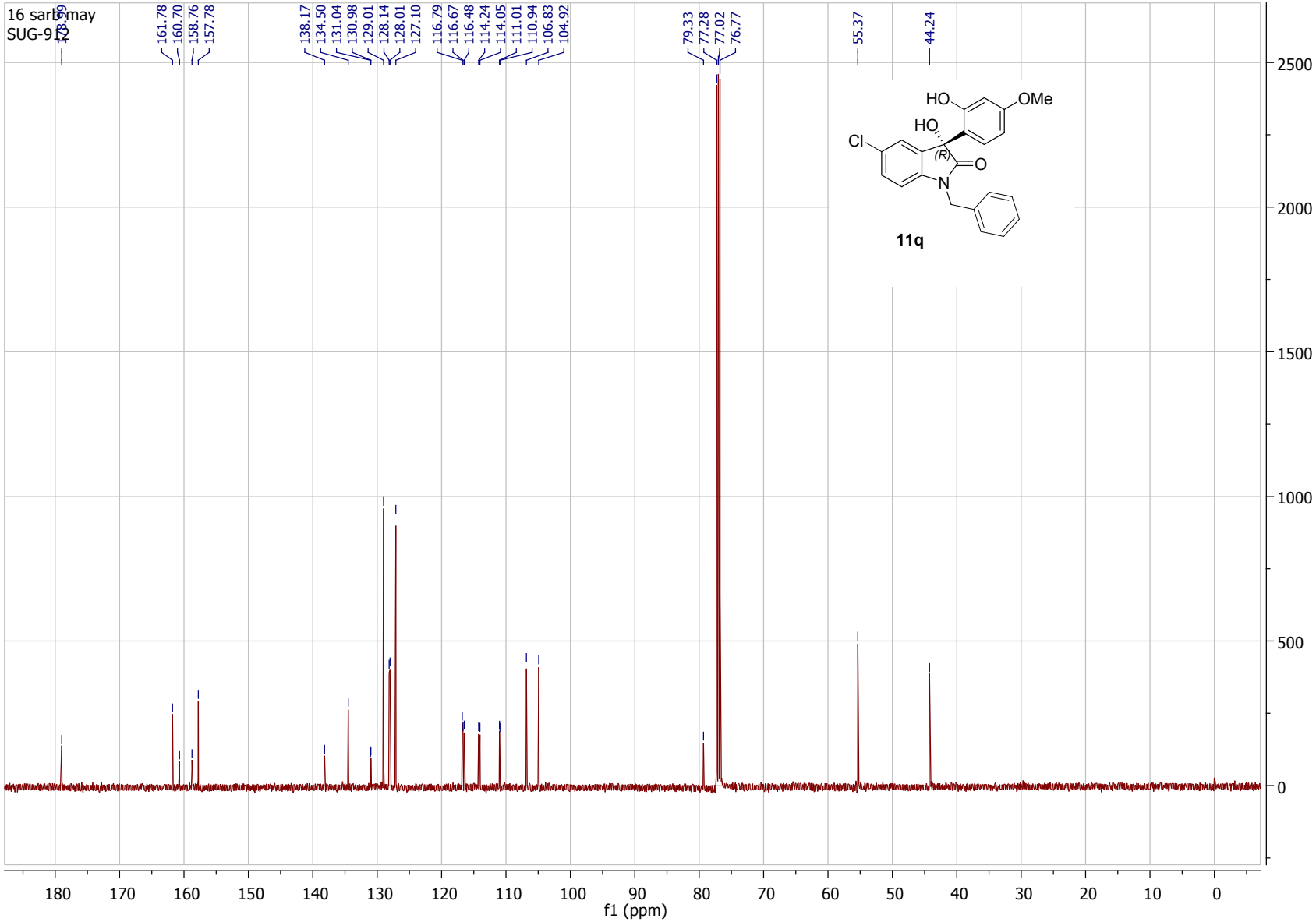
Derived from: JAS-211 C13-1.jdf
```

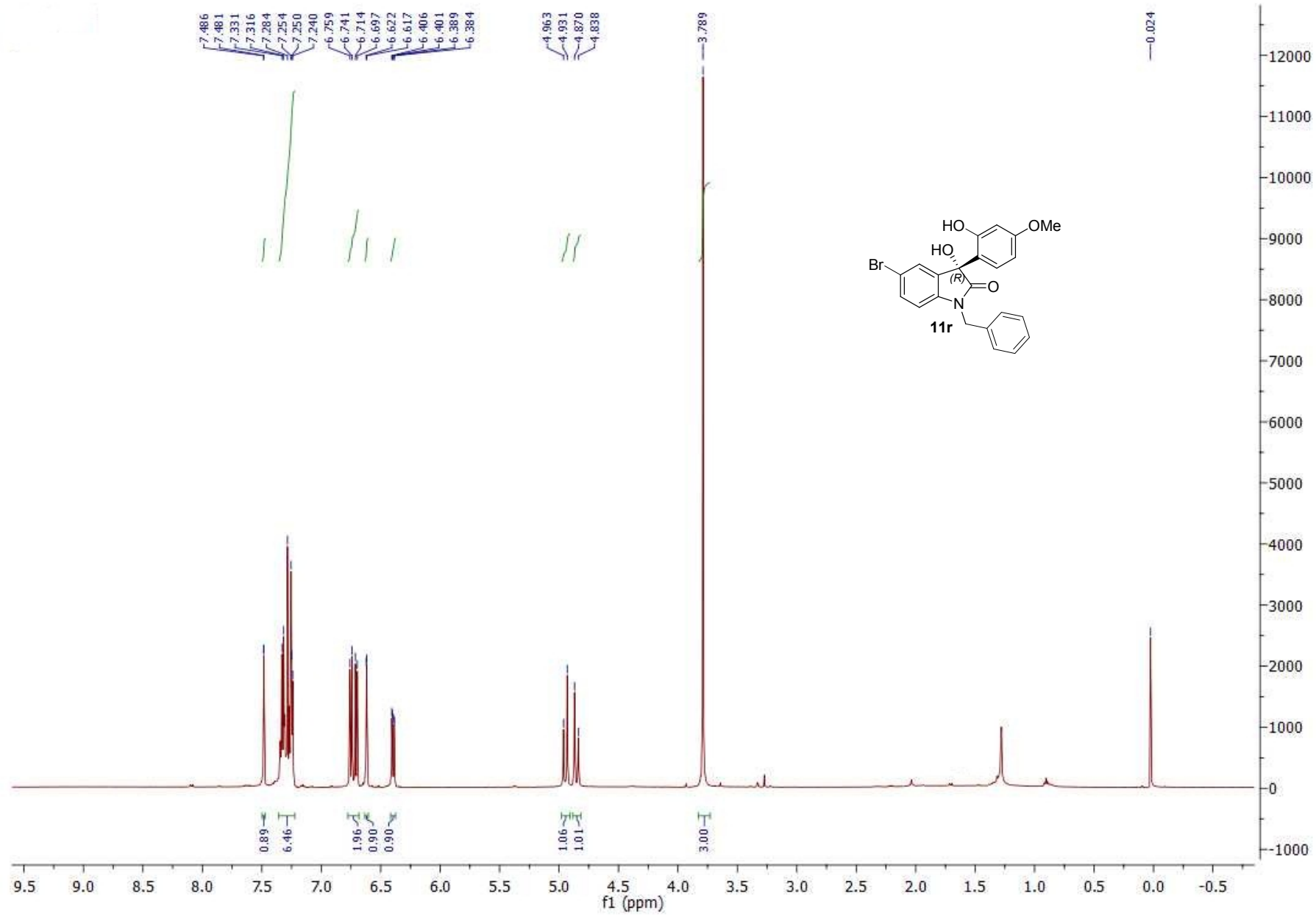
Filename	= JAS-211 C13-6.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= JAS-211 C13
Solvent	= CHLOROFORM-D
Creation_time	= 16-FEB-2014 15:26:02
Revision_time	= 17-FEB-2014 11:10:41
Current_time	= 17-FEB-2014 11:11:02
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 104856
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.04333312[s]
X_domain	= 13C
X_freq	= 100.52530333[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95846665[Hz]
X_sweep	= 31.40703518[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 6000
Total_scans	= 6000
X_90_width	= 7.87[us]
X_acq_time	= 1.04333312[s]
X_angle	= 90[deg]
X_atn	= 4.2[dB]
X_pulse	= 7.87[us]
Irr_atn_dec	= 21.399[dB]
Irr_atn_noe	= 21.399[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2.5[s]
Recvr_gain	= 60
Relaxation_delay	= 2.5[s]
Repetition_time	= 3.54333312[s]
Temp_get	= 18.6[dC]

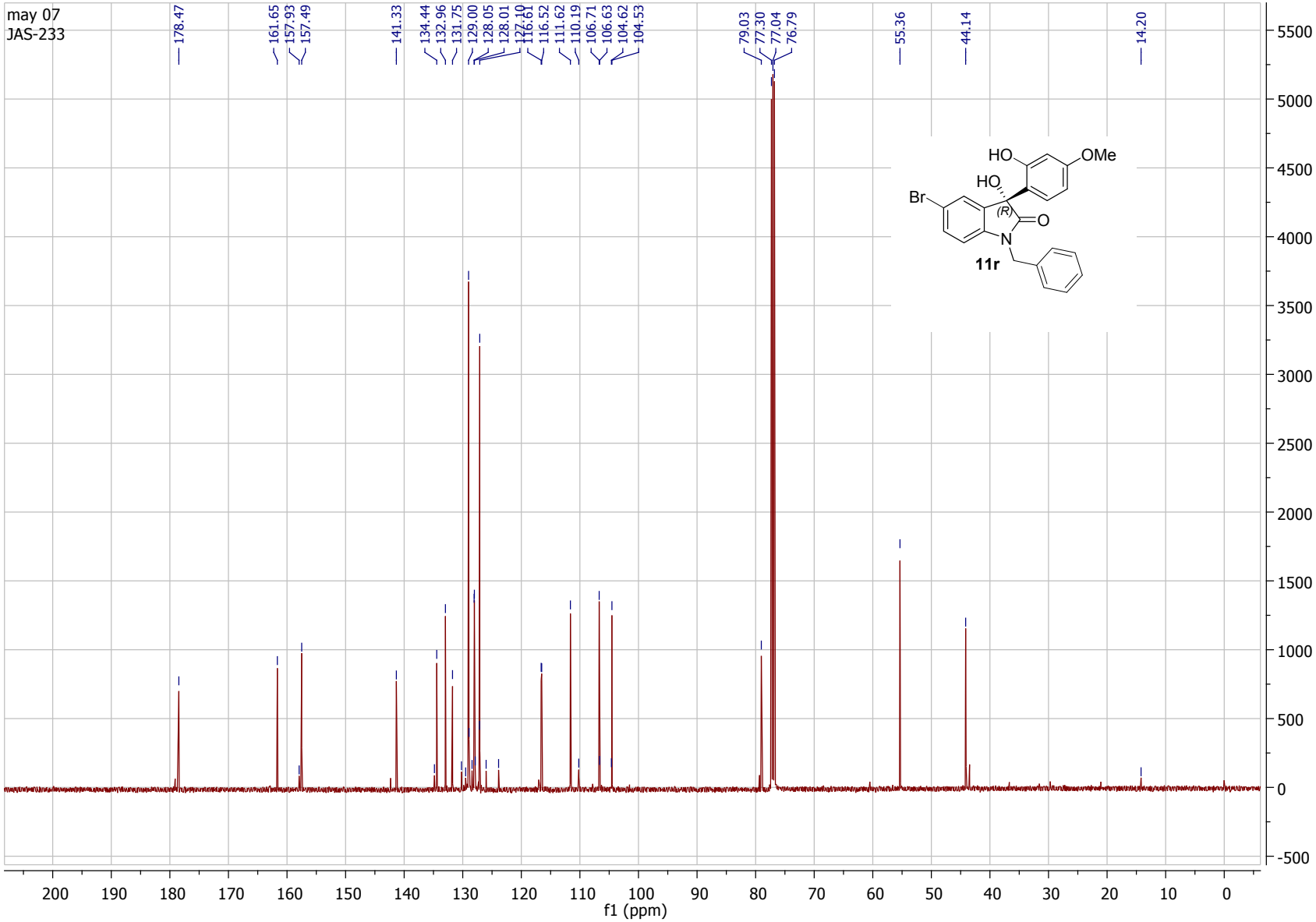

9.134
7.617
7.613
7.420
7.416
7.403
7.400
7.329
7.314
7.305
7.283
7.251
7.237
6.746
6.665
6.649
6.612
6.608
6.409
6.404
6.391
6.386
4.958
4.926
4.861
4.829
4.431
3.787
0.026
HO
OMe
HO
F
(R)
O
N
11p
0.72
0.79
6.13
2.85
1.11
1.79
0.71
3.00
f1 (ppm)

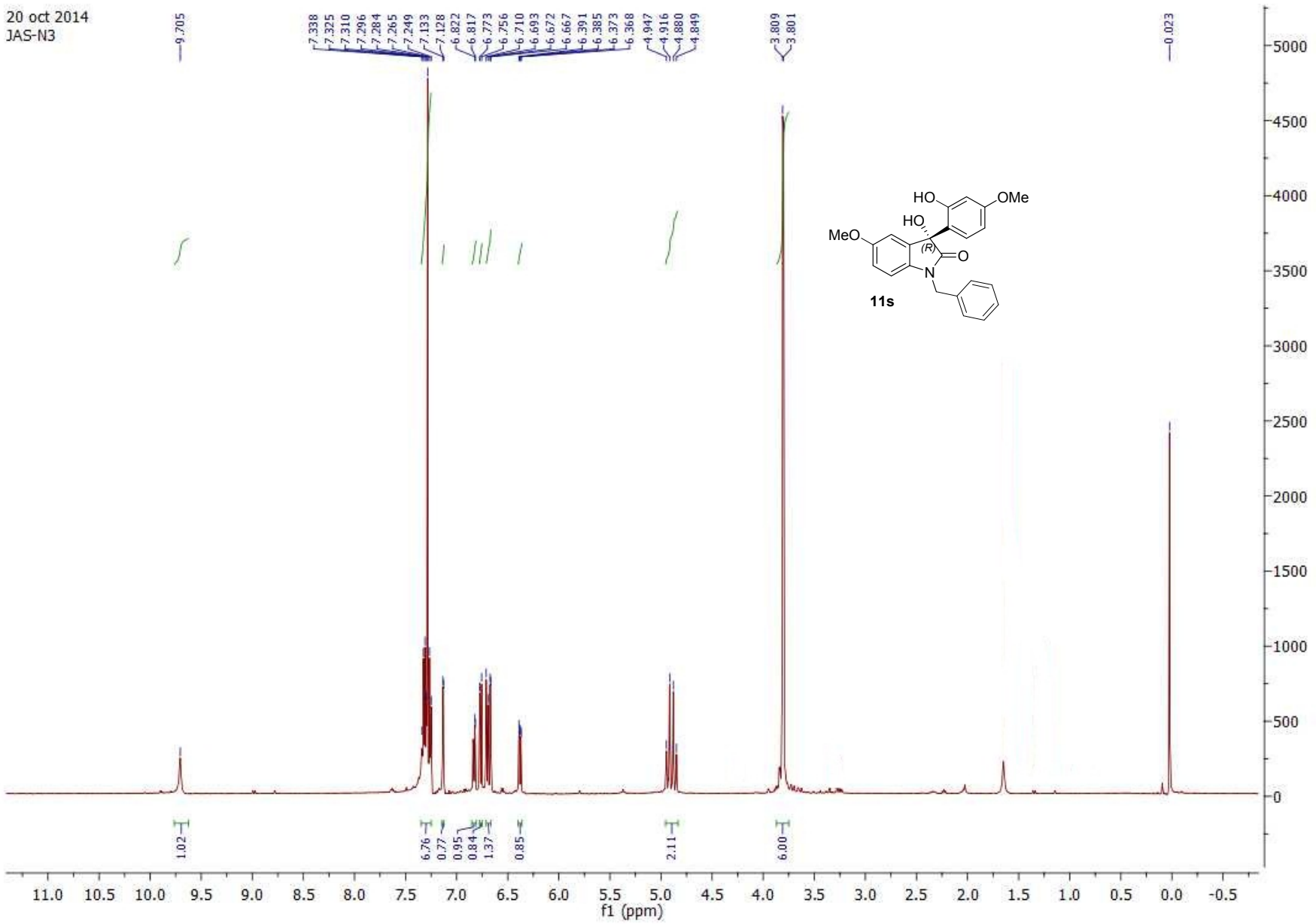

178.555
161.799
157.636
141.363
134.397
133.047
129.161
129.029
128.158
128.056
116.636
111.672
106.837
104.866
79.083
77.279
77.025
76.771
55.382
44.179
HO
OMe
HO
F
(R)
O
N
11p
f1 (ppm)

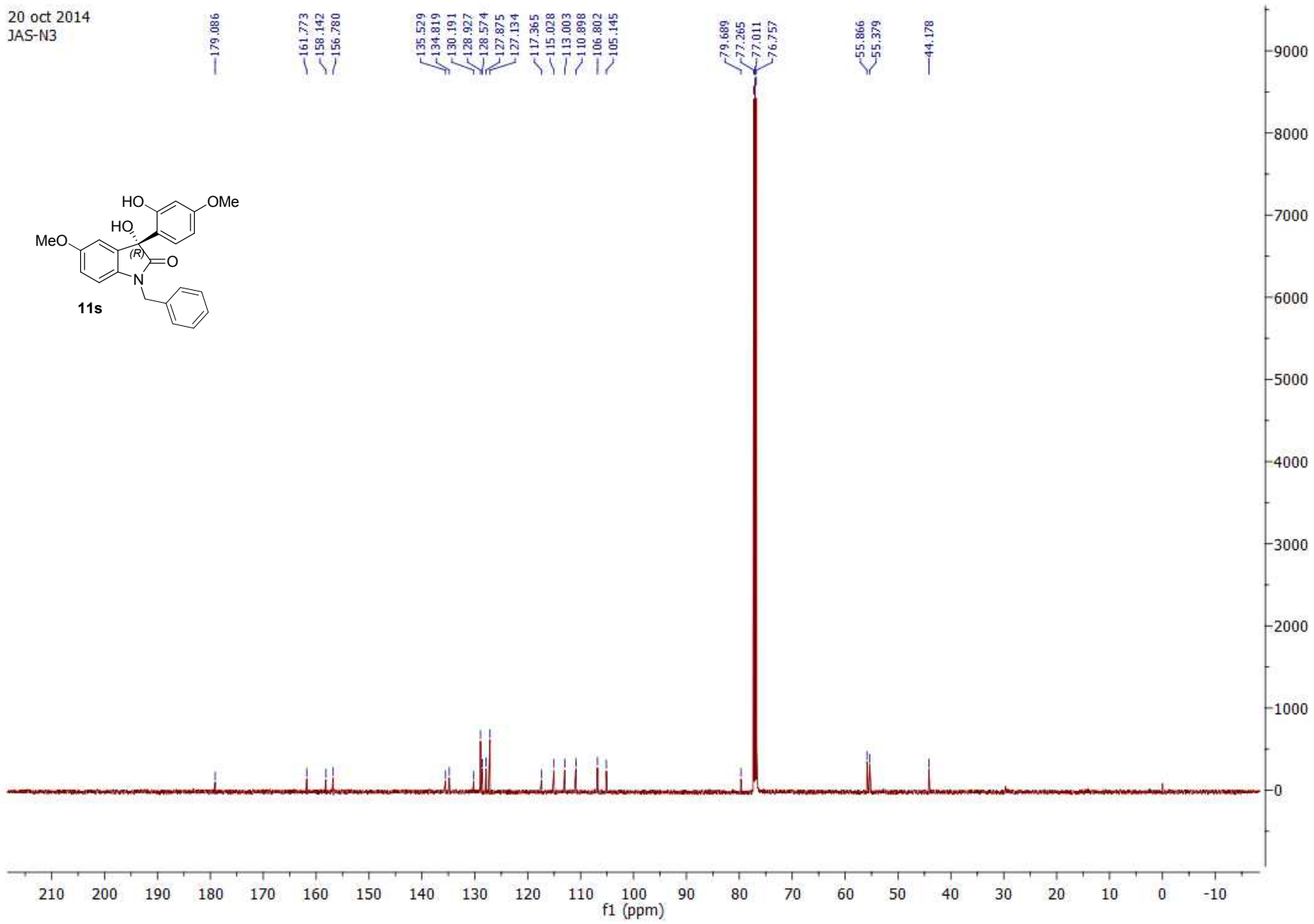

16 sarb may
SUG-912
9.34
7.33
7.32
7.28
7.26
7.26
7.26
7.01
7.01
7.00
6.99
6.98
6.97
6.75
6.73
6.72
6.71
6.71
6.70
6.40
6.39
6.38
6.37
4.97
4.94
4.86
4.83
4.48
3.78
0.03
HO
OMe
HO
Cl
(R)
O
N
11q
0.92
6.43
0.94
2.93
0.97
2.11
0.93
3.00
f1 (ppm)

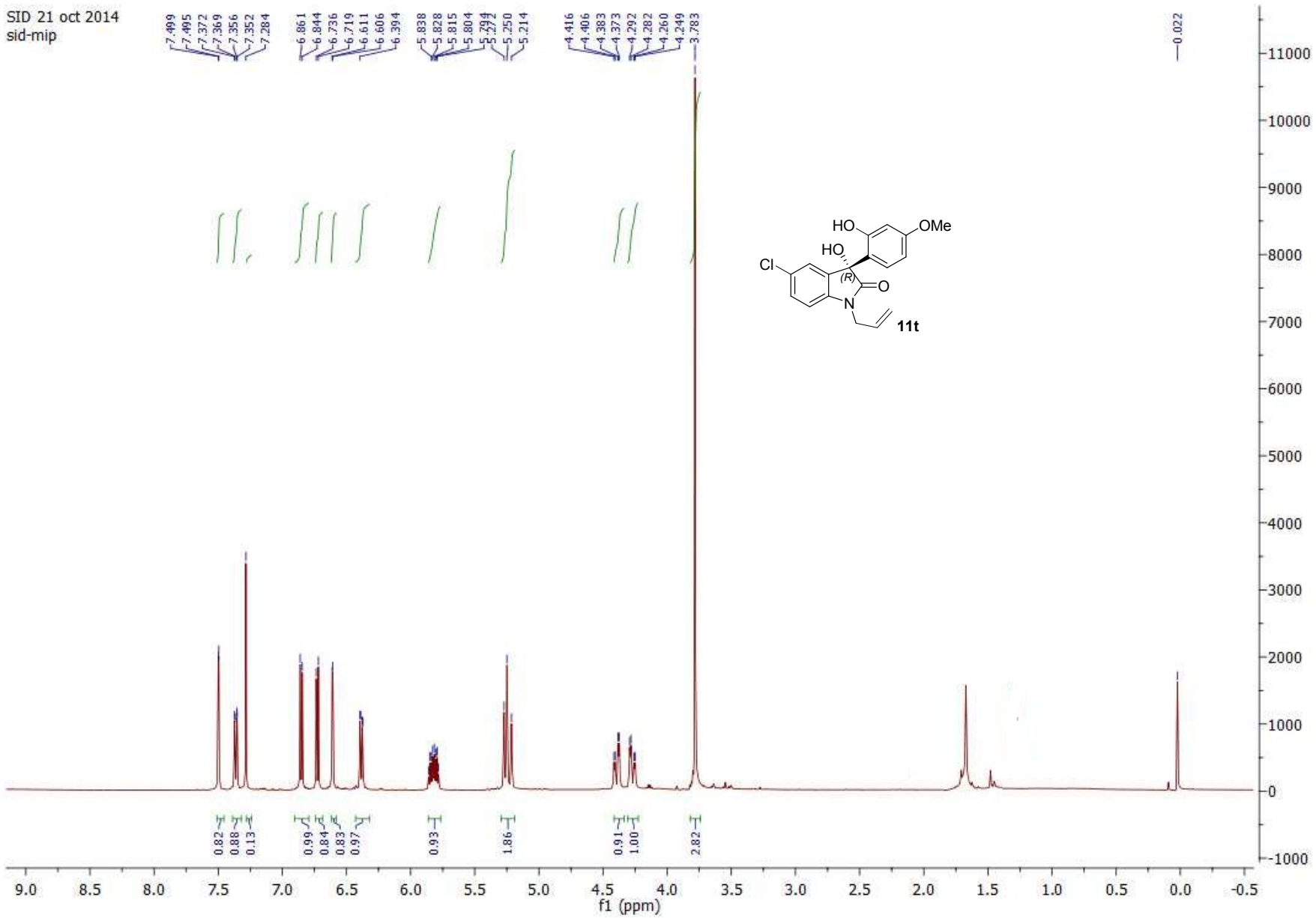

16 sarbmay
SUG-912
179.89
161.78
160.70
158.76
157.78
138.17
134.50
131.04
130.98
129.01
128.14
128.01
127.10
116.79
116.67
116.48
114.24
114.05
111.01
110.94
106.83
104.92
79.33
77.28
77.02
76.77
55.37
44.24
HO
OMe
HO
Cl
(R)
O
N
11q
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

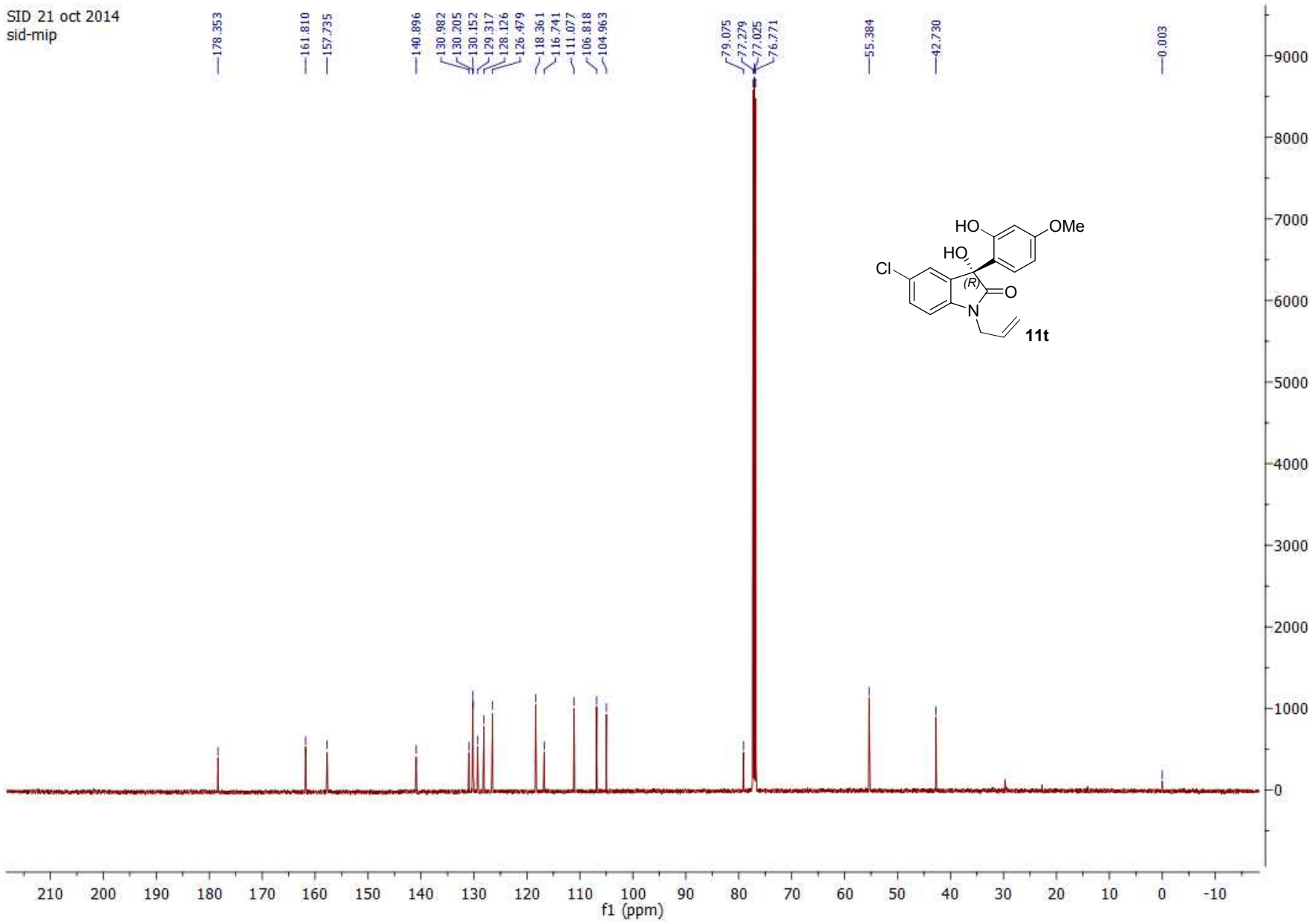

7.486
7.481
7.331
7.316
7.284
7.254
7.250
7.240
6.759
6.741
6.714
6.697
6.622
6.617
6.406
6.401
6.389
6.384
4.963
4.931
4.870
4.838
3.789
0.024
HO
OMe
HO
Br
(R)
O
N
11r
0.89
6.46
1.96
0.90
0.90
1.06
1.01
3.00
f1 (ppm)


may 07
JAS-233
178.47
161.65
157.93
157.49
141.33
134.44
132.96
131.75
129.00
128.05
128.01
127.10
116.61
116.52
111.62
110.19
106.71
106.63
104.62
104.53
79.03
77.30
77.04
76.79
55.36
44.14
14.20
HO
OMe
HO
Br
(R)
O
N
11r
f1 (ppm)

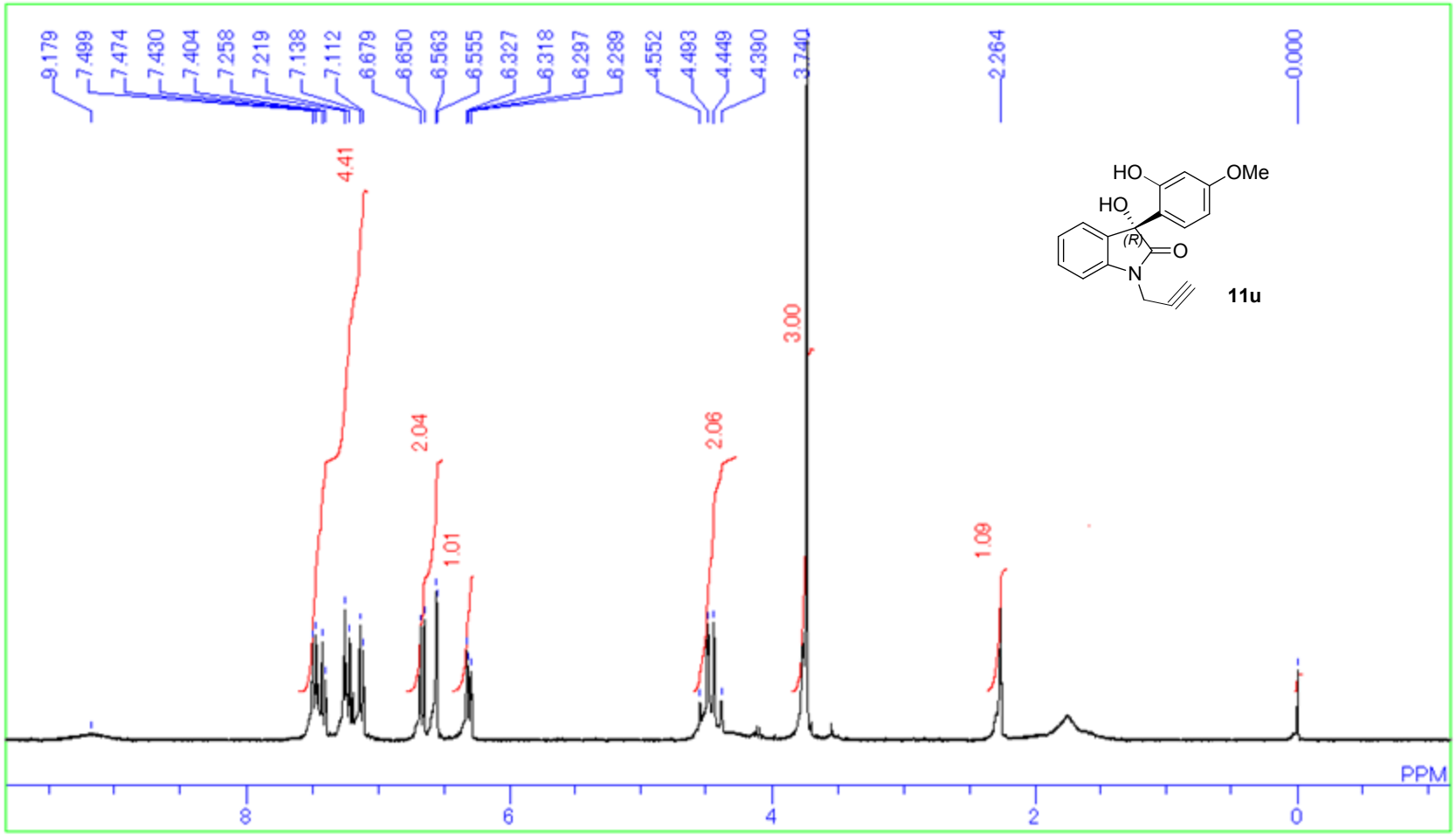

20 oct 2014
JAS-N3
9.705
7.338
7.325
7.310
7.296
7.284
7.265
7.249
7.133
7.128
6.822
6.817
6.773
6.756
6.710
6.693
6.672
6.667
6.391
6.385
6.373
6.368
4.947
4.916
4.880
4.849
3.809
3.801
0.023
HO
OMe
HO
MeO
(R)
O
N
11s
1.02
6.76
0.77
0.95
0.84
1.37
0.85
2.11
6.00
f1 (ppm)

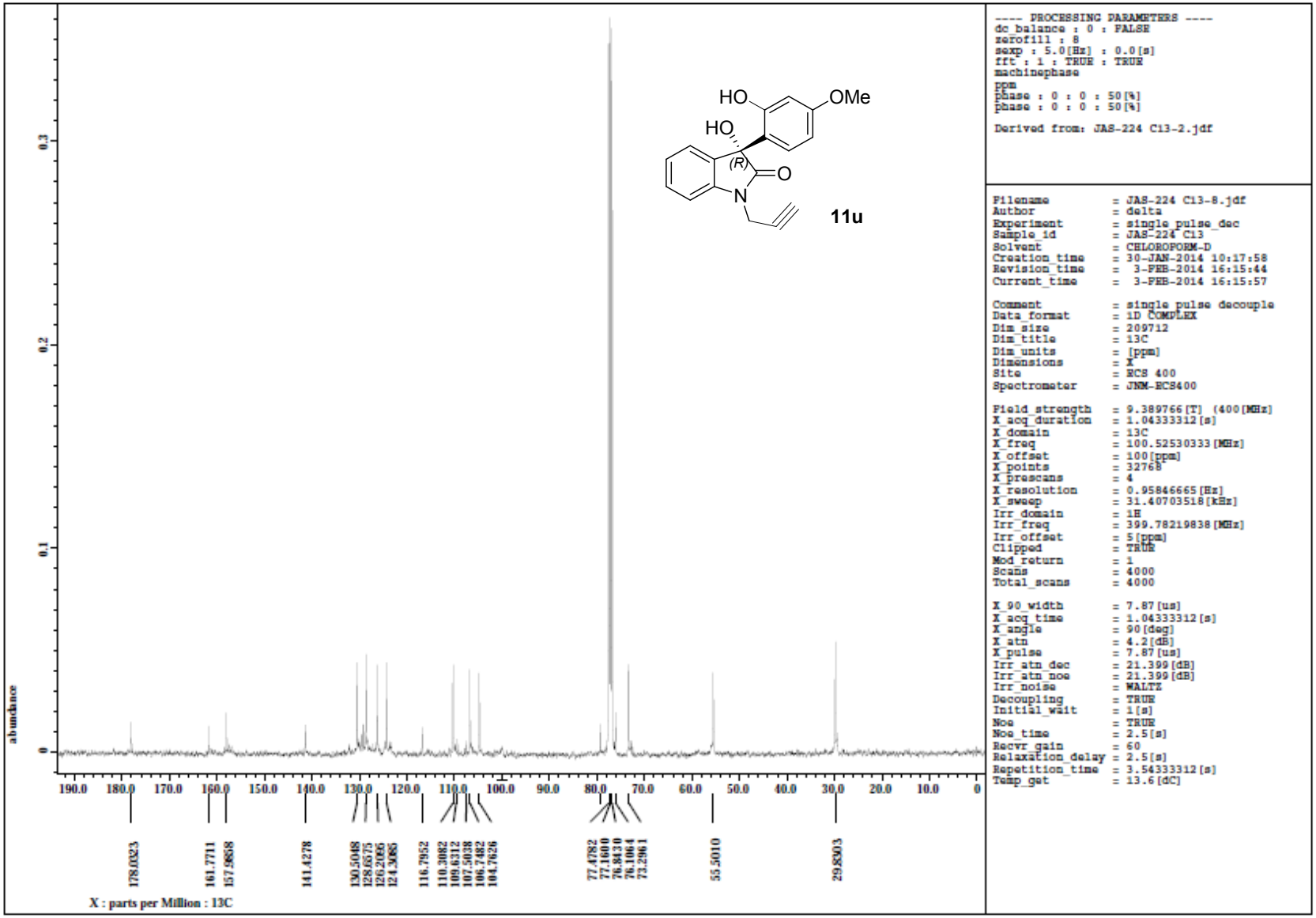

20 oct 2014
JAS-N3
179.086
161.773
158.142
156.780
135.529
134.819
130.191
128.927
128.574
127.875
127.134
117.365
115.028
113.003
110.898
106.802
105.145
79.689
77.265
77.011
76.757
55.866
55.379
44.178
HO
OMe
HO
MeO
(R)
O
N
11s
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

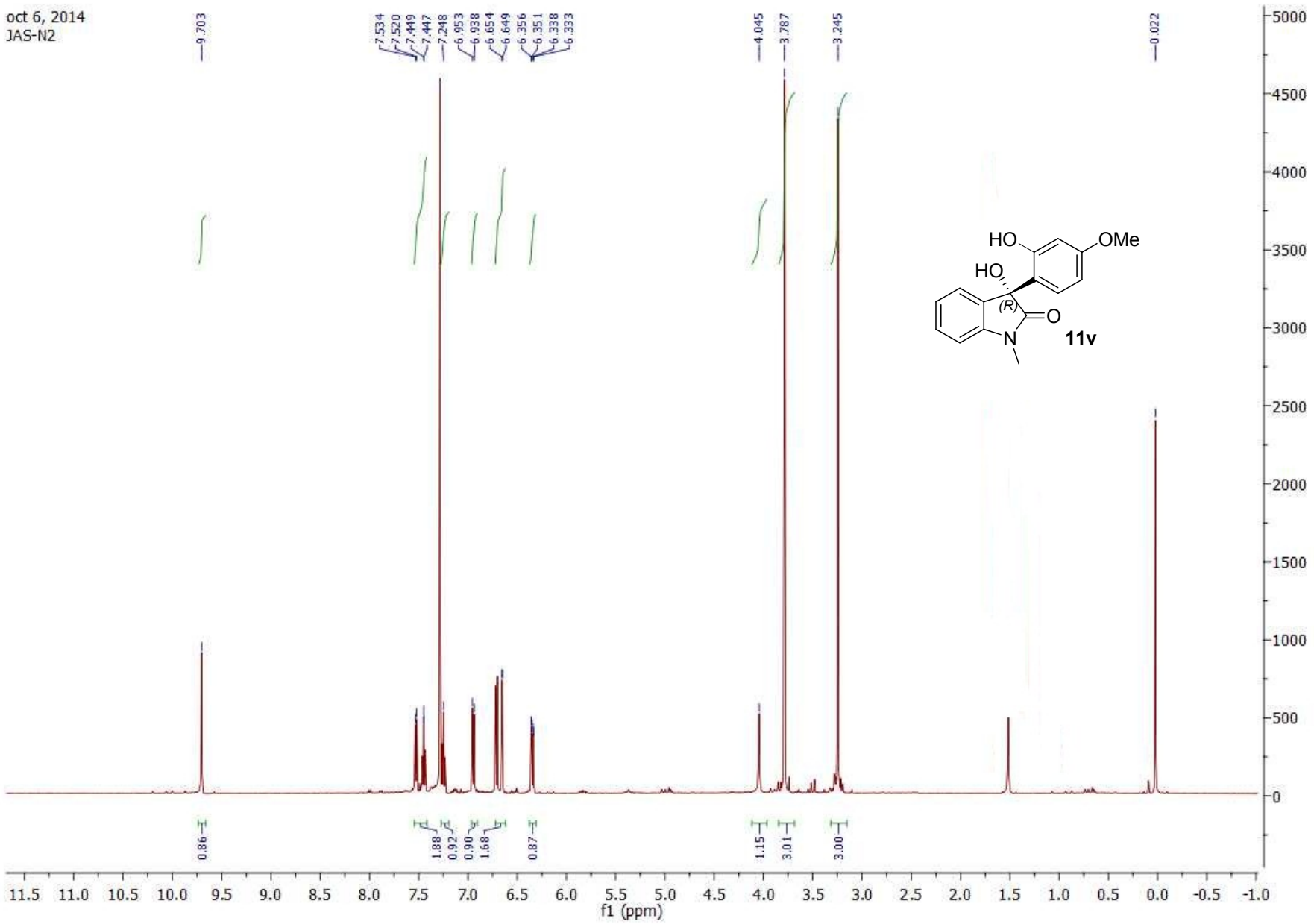

SID 21 oct 2014
sid-mip
7.499
7.495
7.372
7.369
7.356
7.352
7.284
6.861
6.844
6.736
6.719
6.611
6.606
6.394
5.838
5.828
5.815
5.804
5.250
5.214
4.416
4.406
4.383
4.373
4.292
4.282
4.260
4.249
3.783
0.022
HO
OMe
HO
Cl
(R)
O
N
11t
0.82
0.88
0.13
0.99
0.84
0.83
0.97
0.93
1.86
0.91
1.00
2.82
f1 (ppm)

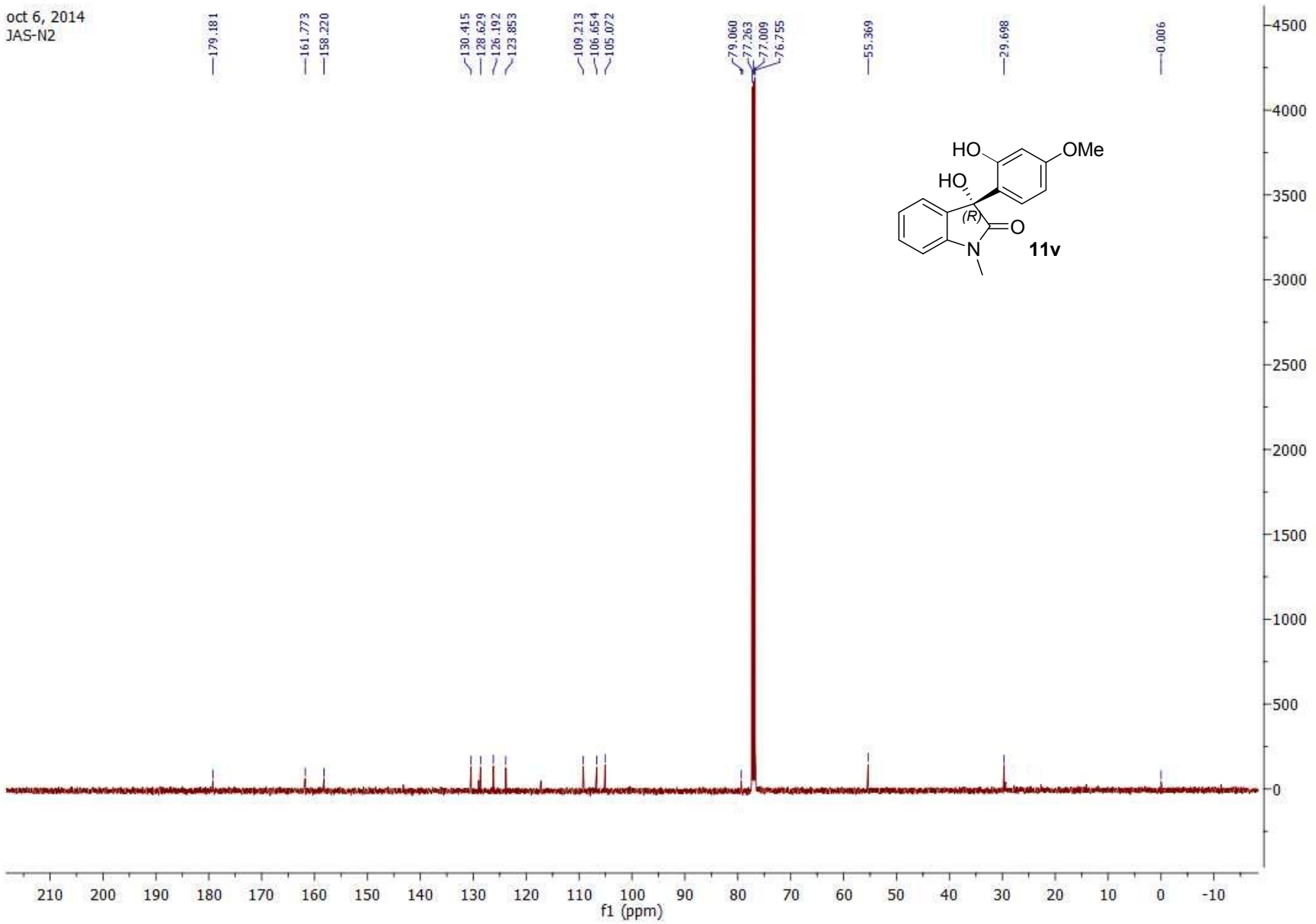

SID 21 oct 2014
sid-mip
178.353
161.810
157.735
140.896
130.982
130.205
130.152
129.317
128.126
126.479
118.361
116.741
111.077
106.818
104.963
79.075
77.279
77.025
76.771
55.384
42.730
0.003
HO
OMe
HO
Cl
(R)
O
N
11t
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

C:¥Users¥technologies¥Desktop¥C-JAS2241NON_E2_FT - Copy.als

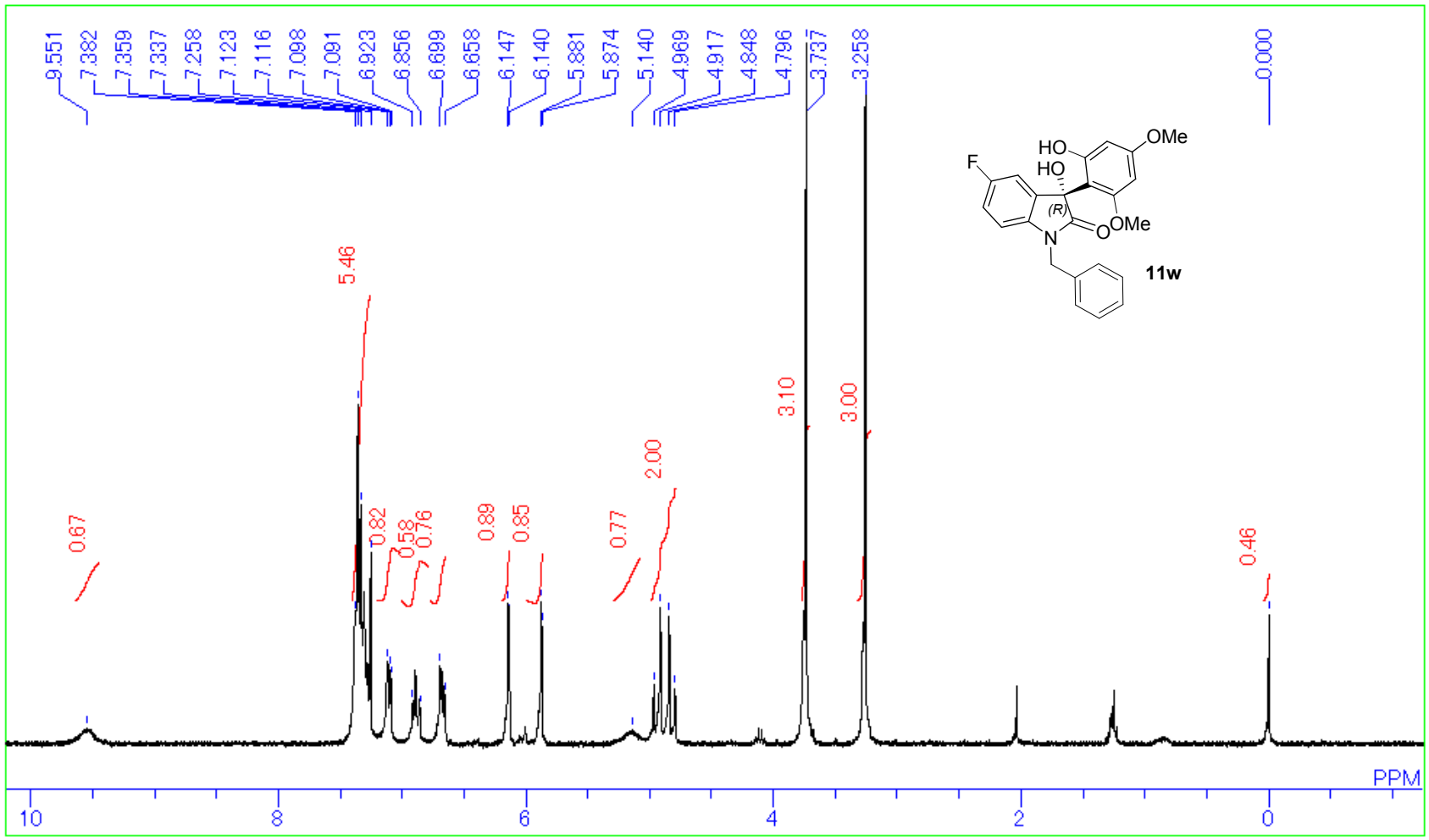


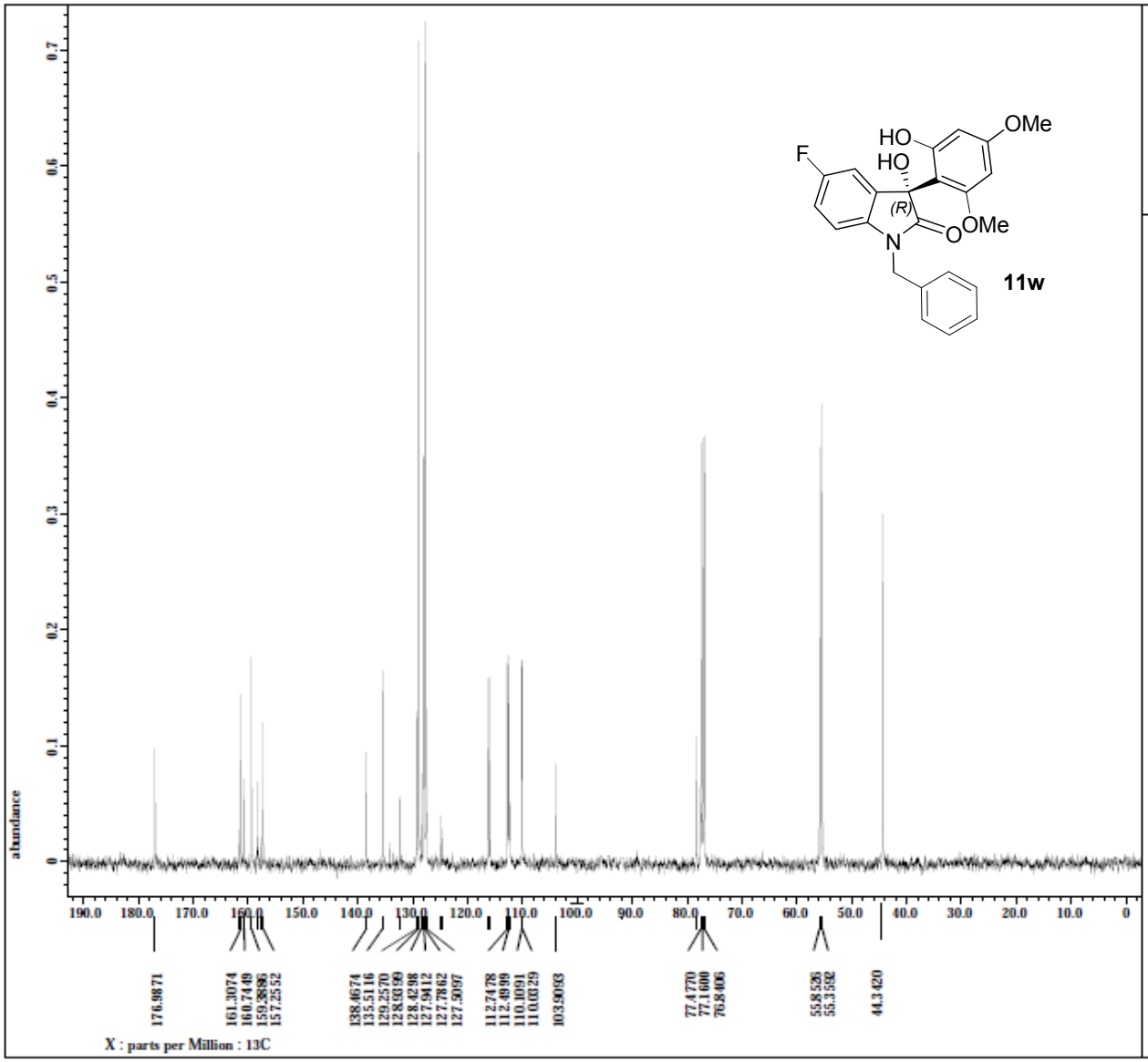

HO
OMe
HO
(R)
O
N
11u
abundance
0
0.1
0.2
0.3
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
178.0323
161.7711
157.9858
141.4278
130.5048
128.6575
126.2006
124.3085
116.7952
110.3082
109.6312
107.5038
106.7482
104.7626
77.4782
77.1600
76.8430
76.1064
73.2961
55.5010
29.8303
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 8
sexp : 5.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]
Derived from: JAS-224 C13-2.jdf
Filename = JAS-224 C13-8.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = JAS-224 C13
Solvent = CHLOROFORM-D
Creation_time = 30-JAN-2014 10:17:58
Revision_time = 3-FEB-2014 16:15:44
Current_time = 3-FEB-2014 16:15:57
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 209712
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = RCS 400
Spectrometer = JNM-RCS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 4000
Total_scans = 4000
X_90_width = 7.87[us]
X_acq_time = 1.04333312[s]
X_angle = 90[deg]
X_atn = 4.2[dB]
X_pulse = 7.87[us]
Irr_atn_dec = 21.399[dB]
Irr_atn_noe = 21.399[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2.5[s]
Recvr_gain = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.54333312[s]
Temp_get = 13.6[dC]


oct 6, 2014
JAS-N2
9.703
7.534
7.520
7.449
7.447
7.248
6.953
6.938
6.654
6.649
6.356
6.351
6.338
6.333
4.045
3.787
3.245
0.022
HO
OMe
HO
(R)
O
N
11v
0.86
1.88
0.92
0.90
1.68
0.87
1.15
3.01
3.00
f1 (ppm)


oct 6, 2014
JAS-N2
179.181
161.773
158.220
130.415
128.629
126.192
123.853
109.213
106.654
105.072
79.060
77.263
77.009
76.755
55.369
29.698
0.006
HO
OMe
HO
(R)
O
N
11v
f1 (ppm)

C:¥Users¥technologies¥Desktop¥indoles¥all DMP data¥New folder¥nmr dmphenols¥Dr_Chimni¥C-JAS2201NON_E4_FT.als






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 4
sexp : 3.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]

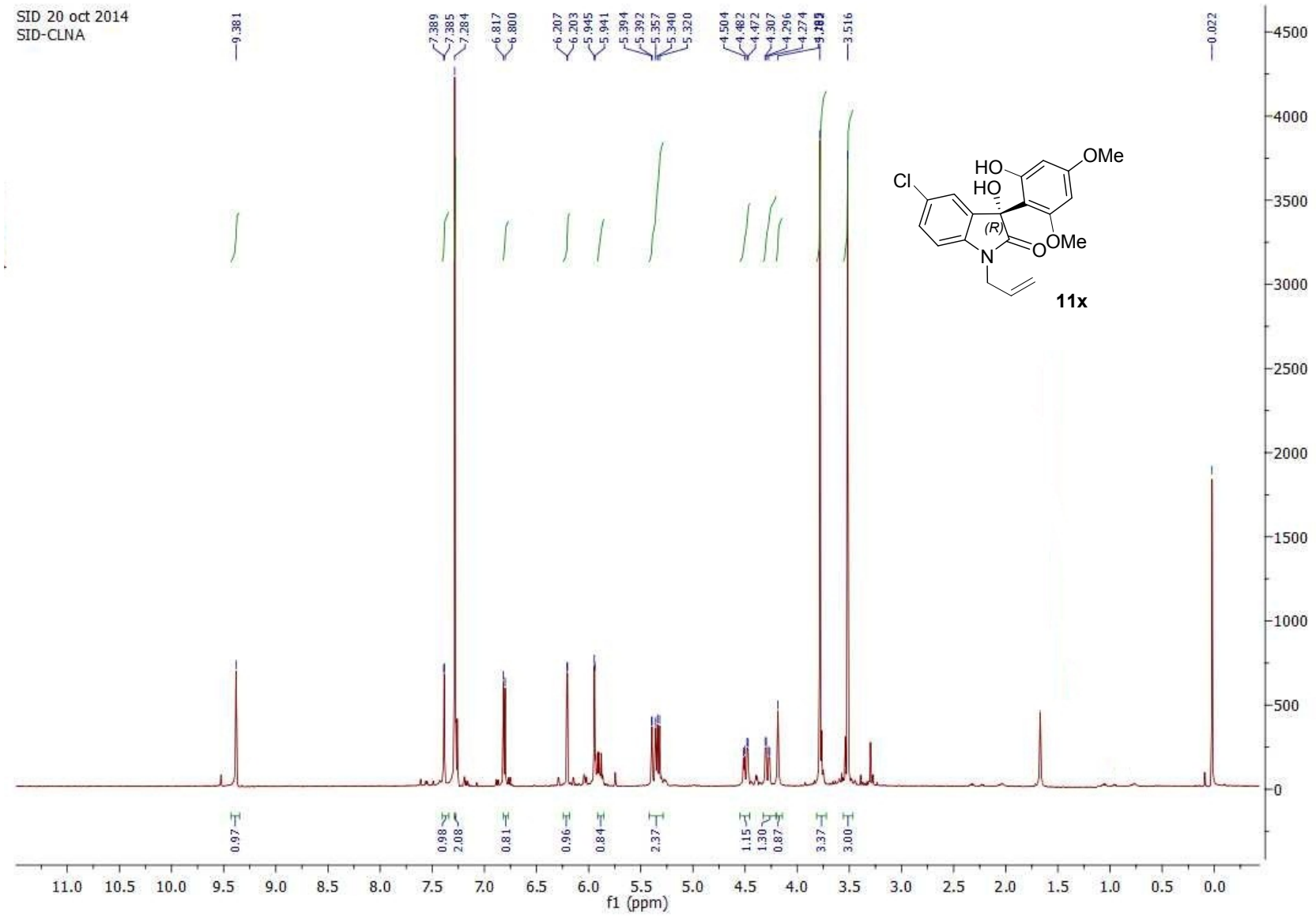
Derived from: JAS-220 C13-1.jdf
```

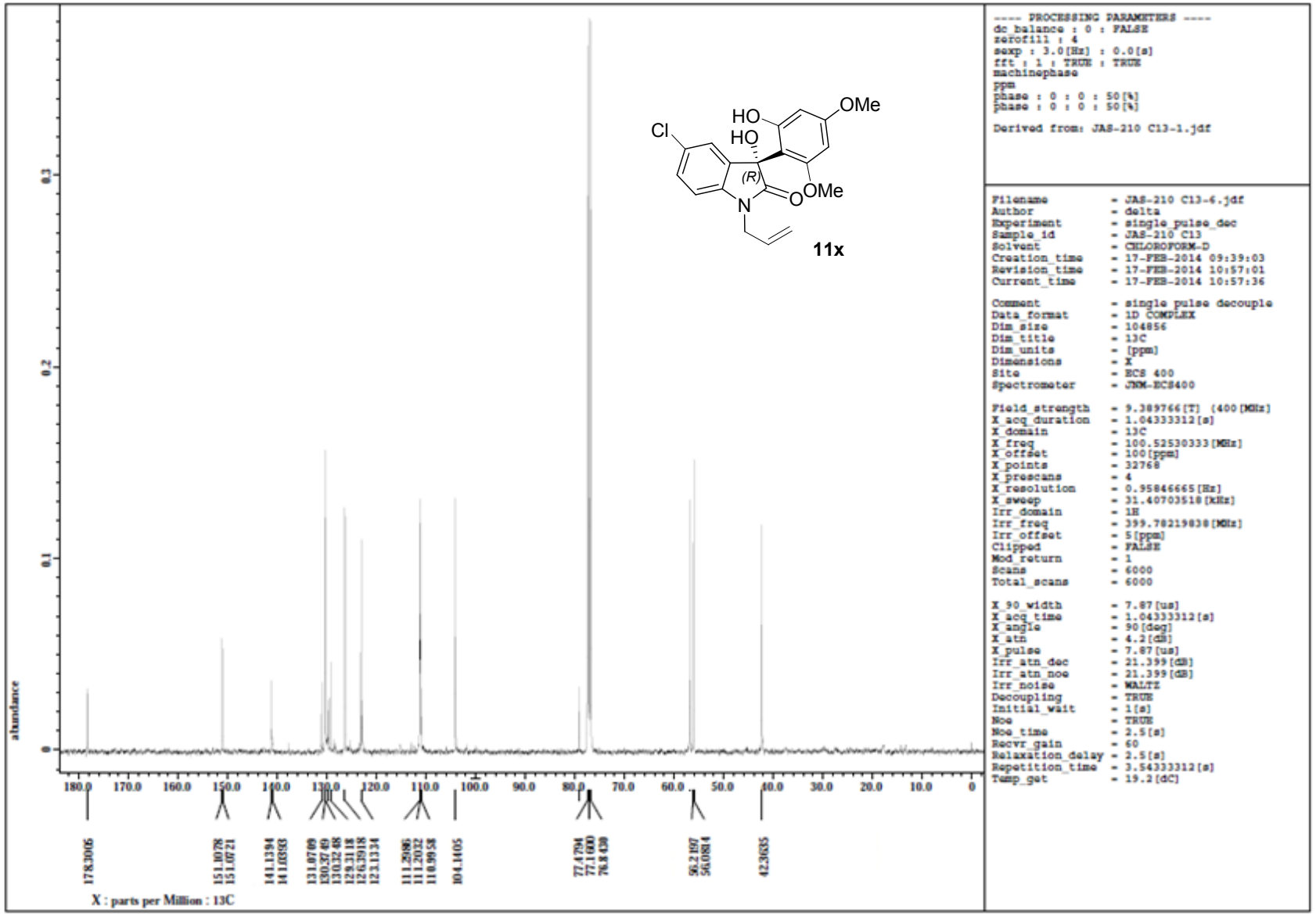
```
Filename          = JAS-220 C13-6.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = JAS-220 C13
Solvent           = CHLOROFORM-D
Creation_time     = 17-FEB-2014 14:24:04
Revision_time     = 17-FEB-2014 10:50:19
Current_time      = 17-FEB-2014 10:51:00

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 104856
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 380
Total_scans       = 380

X_90_width        = 7.87[us]
X_acq_time        = 1.04333312[s]
X_angle           = 90[deg]
X_atn             = 4.2[dB]
X_pulse           = 7.87[us]
Irr_atn_dec       = 21.399[dB]
Irr_atn_noe       = 21.399[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2.5[s]
Recvr_gain        = 60
Relaxation_delay  = 2.5[s]
Repetition_time   = 3.54333312[s]
Temp_get          = 19.1[dC]
```


SID 20 oct 2014
SID-CLNA
9.381
7.389
7.385
7.284
6.817
6.800
6.207
6.203
5.945
5.941
5.394
5.392
5.357
5.340
5.320
4.504
4.482
4.472
4.307
4.296
4.274
3.516
0.022
HO
HO
OMe
Cl
(R)
OMe
O
N
11x
0.97
0.98
2.08
0.81
0.96
0.84
2.37
1.15
1.30
0.87
3.37
3.00
f1 (ppm)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 4
sexp : 3.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]

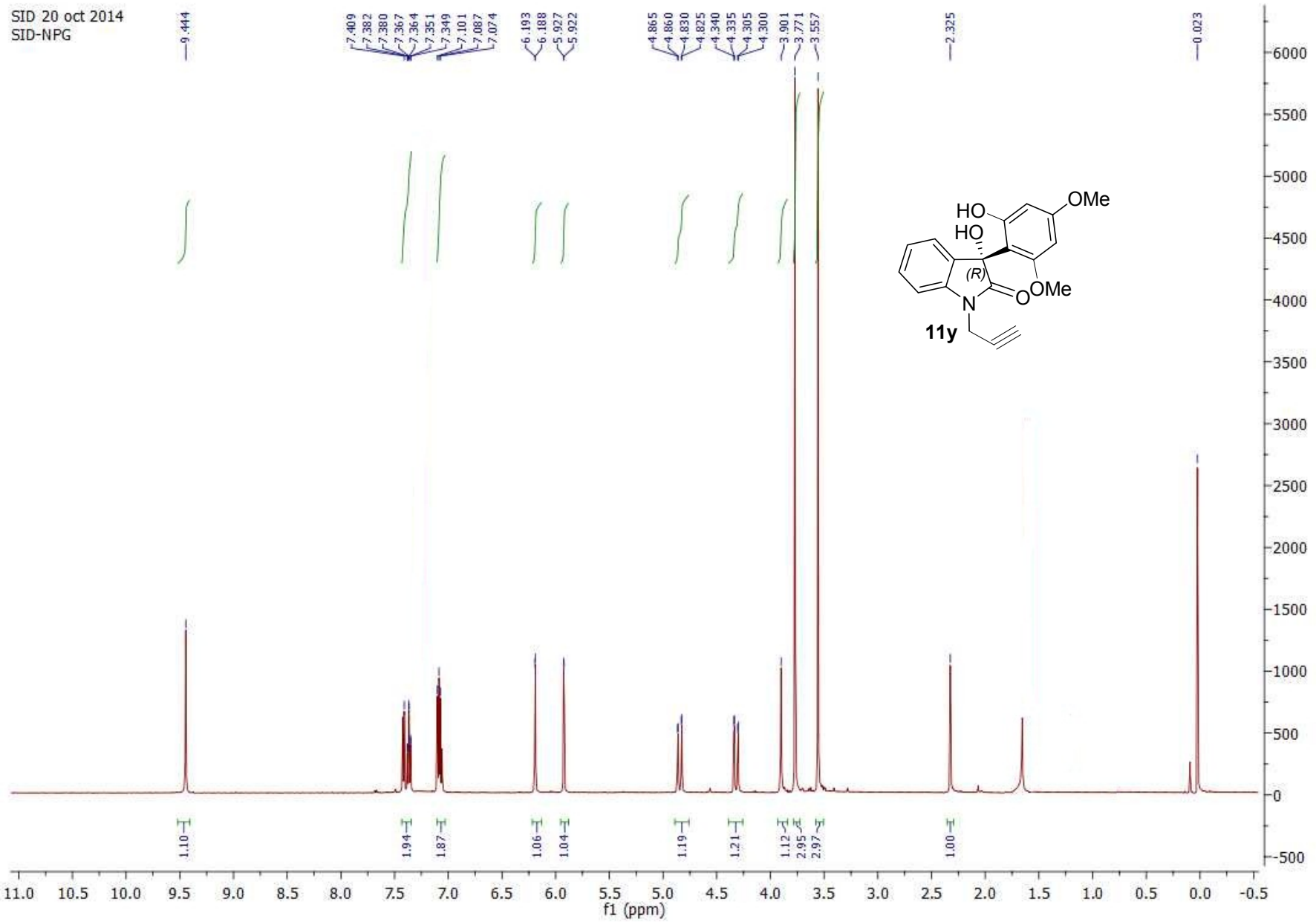
Derived from: JAS-210 C13-1.jdf
```

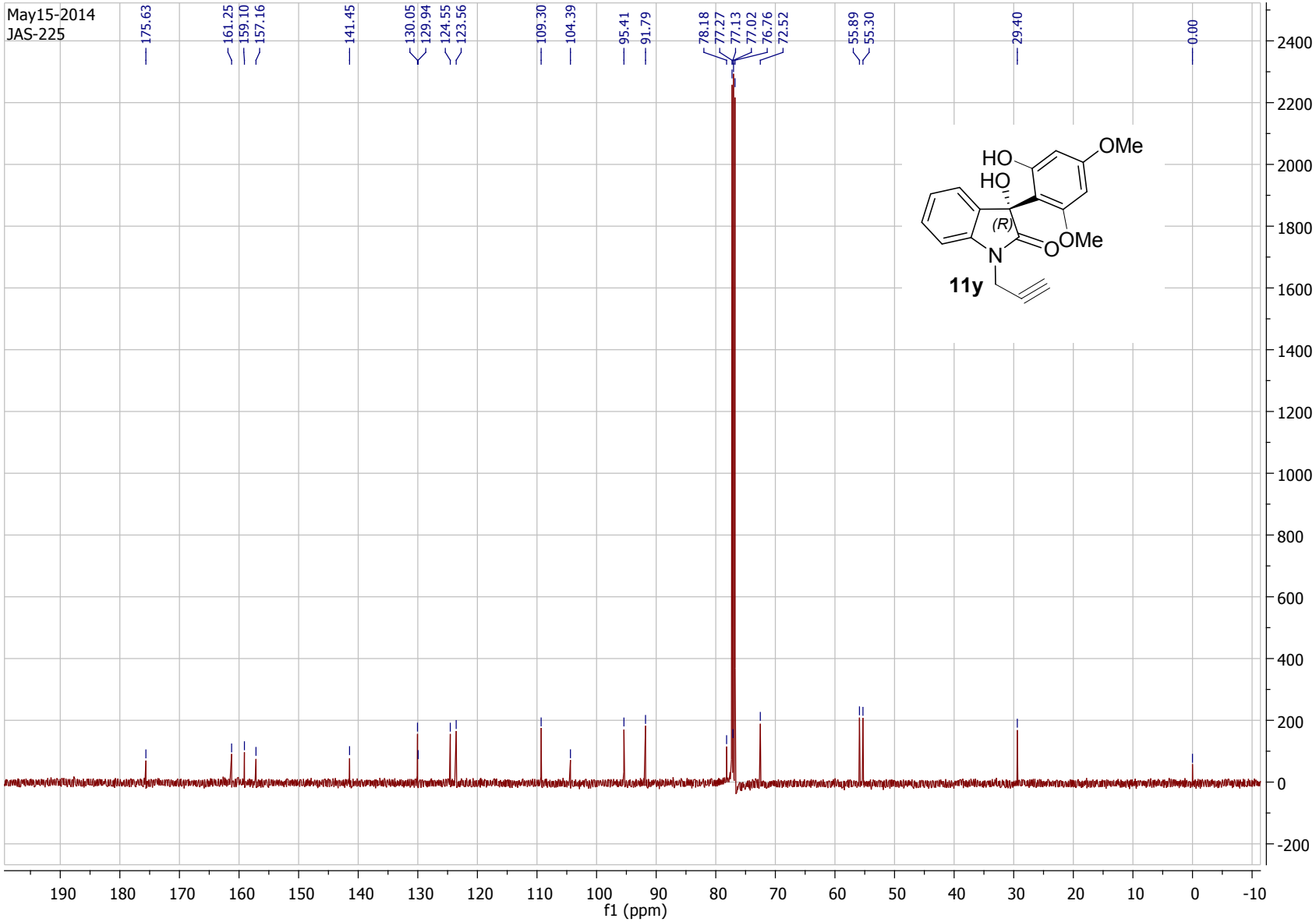
```
Filename            = JAS-210 C13-6.jdf
Author              = delta
Experiment          = single_pulse_dec
Sample_id           = JAS-210 C13
Solvent             = CHLOROFORM-D
Creation_time       = 17-FEB-2014 09:39:03
Revision_time       = 17-FEB-2014 10:57:01
Current_time        = 17-FEB-2014 10:57:36

Comment             = single pulse decouple
Data_format         = 1D COMPLEX
Dim_size            = 104856
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

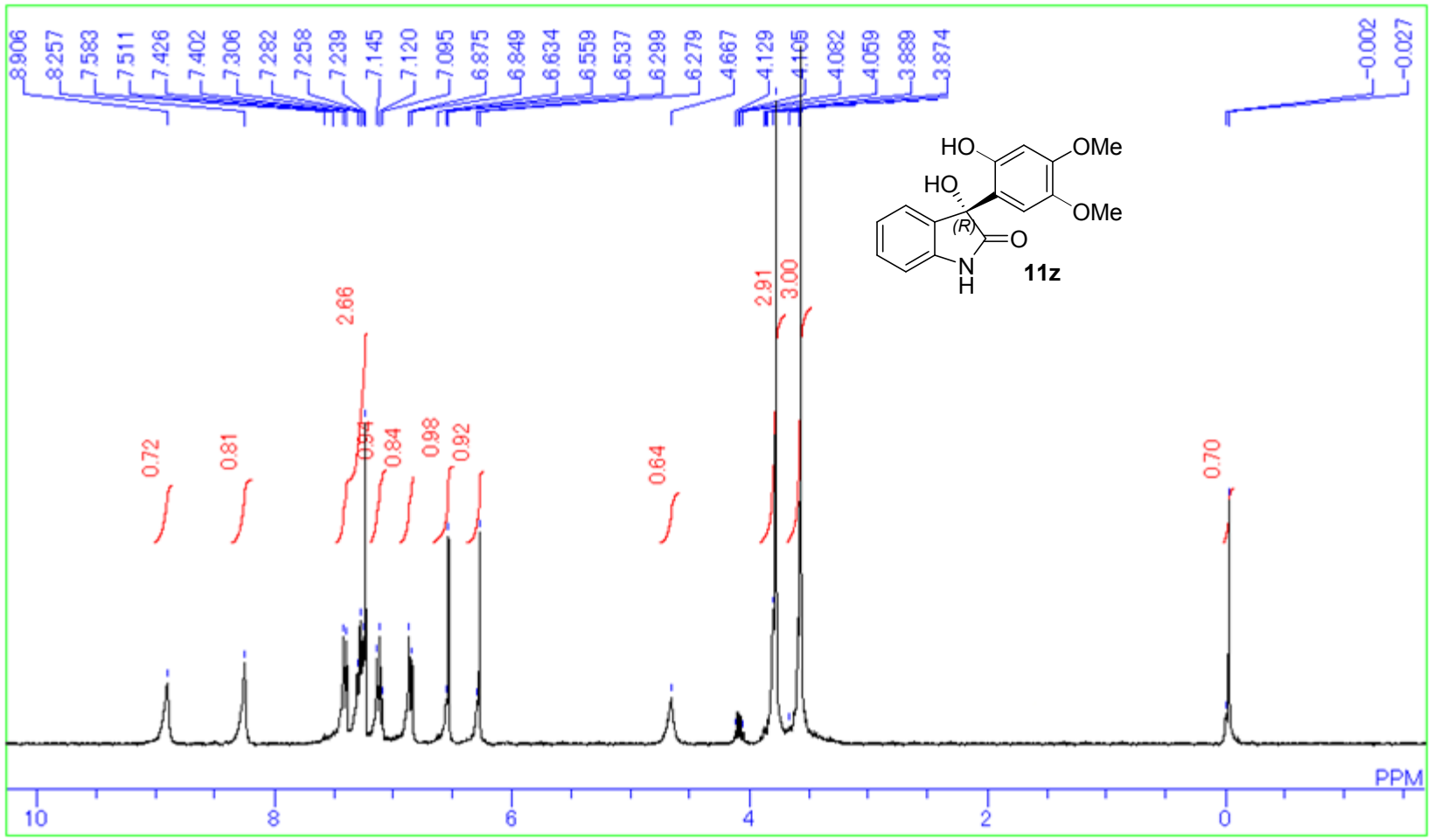
Field_strength      = 9.389766[T] (400[MHz]
X_acq_duration      = 1.04333312[s]
X_domain            = 13C
X_freq              = 100.52530333[MHz]
X_offset            = 100[ppm]
X_points            = 32768
X_prescans          = 4
X_resolution        = 0.95846665[Hz]
X_sweep             = 31.40703518[kHz]
Irr_domain          = 1H
Irr_freq            = 399.78219838[MHz]
Irr_offset          = 5[ppm]
Clipped             = FALSE
Mod_return          = 1
Scans               = 6000
Total_scans         = 6000

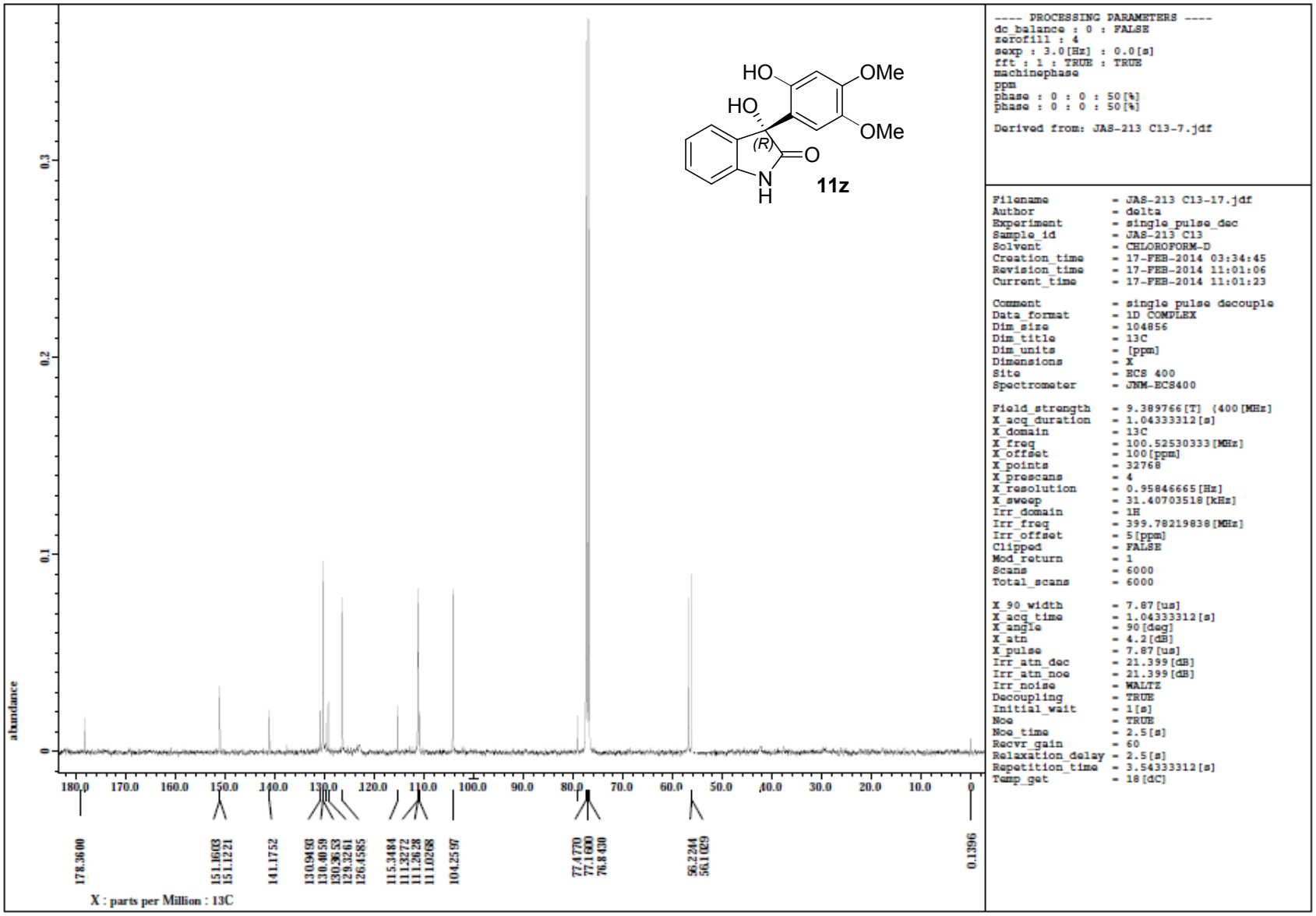
X_90_width          = 7.87[us]
X_acq_time          = 1.04333312[s]
X_angle             = 90[deg]
X_atn               = 4.2[dB]
X_pulse             = 7.87[us]
Irr_atn_dec         = 21.399[dB]
Irr_atn_noe         = 21.399[dB]
Irr_noise           = WALTZ
Decoupling          = TRUE
Initial_wait        = 1[s]
Noe                 = TRUE
Noe_time            = 2.5[s]
Recvr_gain          = 60
Relaxation_delay    = 2.5[s]
Repetition_time     = 3.54333312[s]
Temp_get            = 19.2[dC]
```

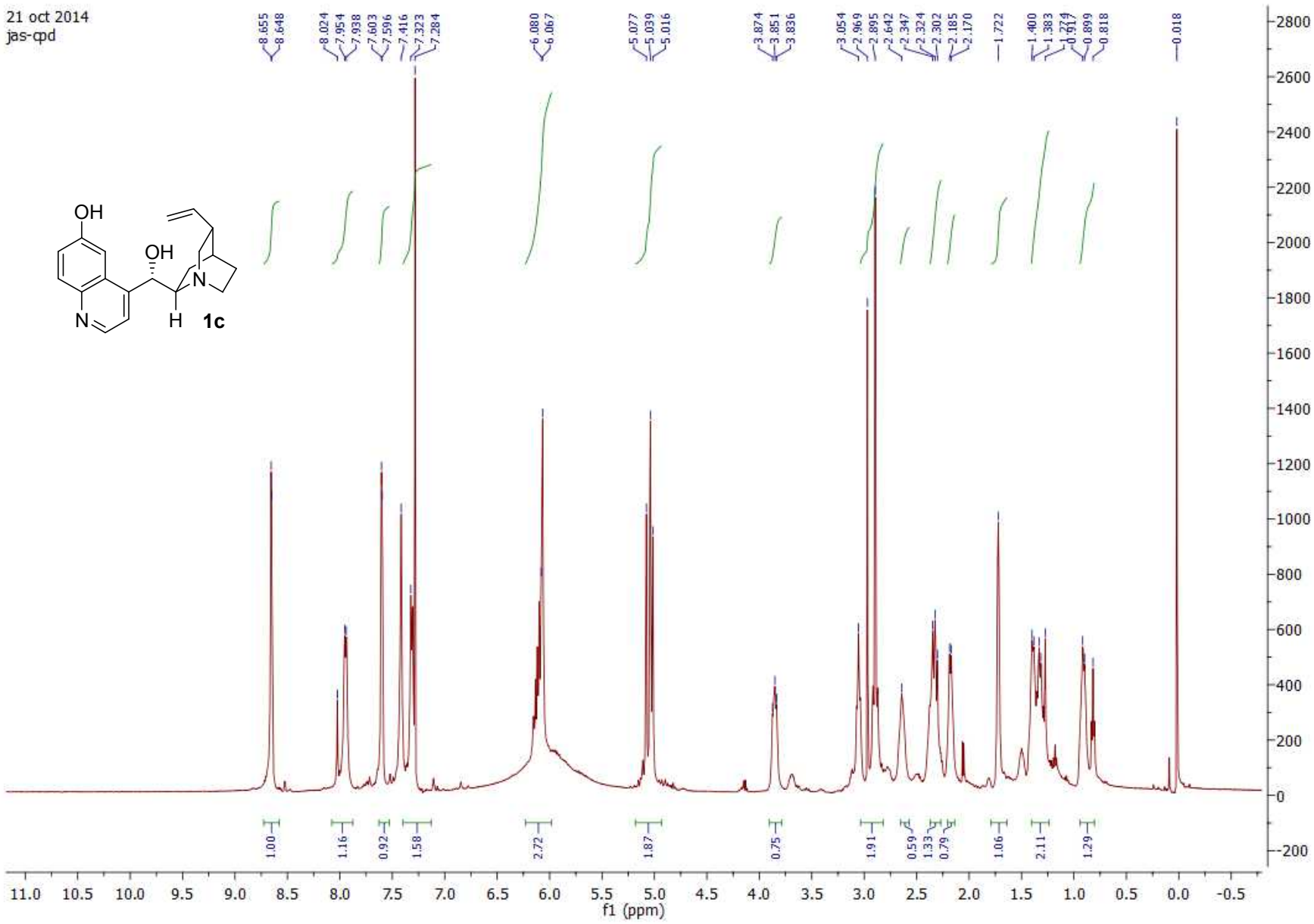

SID 20 oct 2014
SID-NPG
9.444
7.409
7.382
7.380
7.367
7.364
7.351
7.349
7.101
7.087
7.074
6.193
6.188
5.927
5.922
4.865
4.860
4.830
4.825
4.340
4.335
4.305
4.300
3.901
3.771
3.557
2.325
0.023
HO
HO
OMe
(R)
OMe
O
N
11y
1.10
1.94
1.87
1.06
1.04
1.19
1.21
1.12
2.95
2.97
1.00
f1 (ppm)

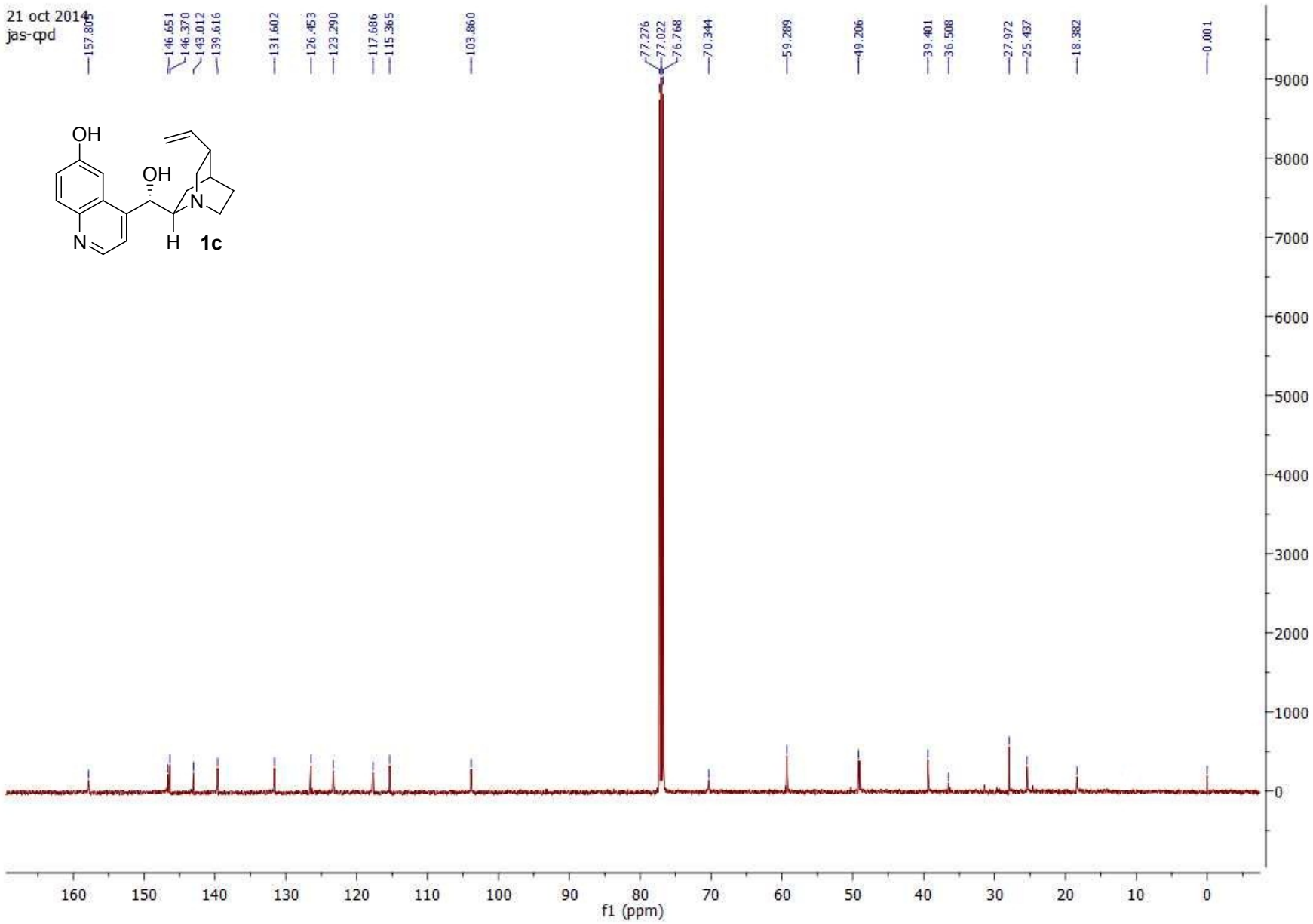

May15-2014
JAS-225
175.63
161.25
159.10
157.16
141.45
130.05
129.94
124.55
123.56
109.30
104.39
95.41
91.79
78.18
77.27
77.13
77.02
76.76
72.52
55.89
55.30
29.40
0.00
HO
HO
OMe
(R)
N
O
OMe
11y
f1 (ppm)

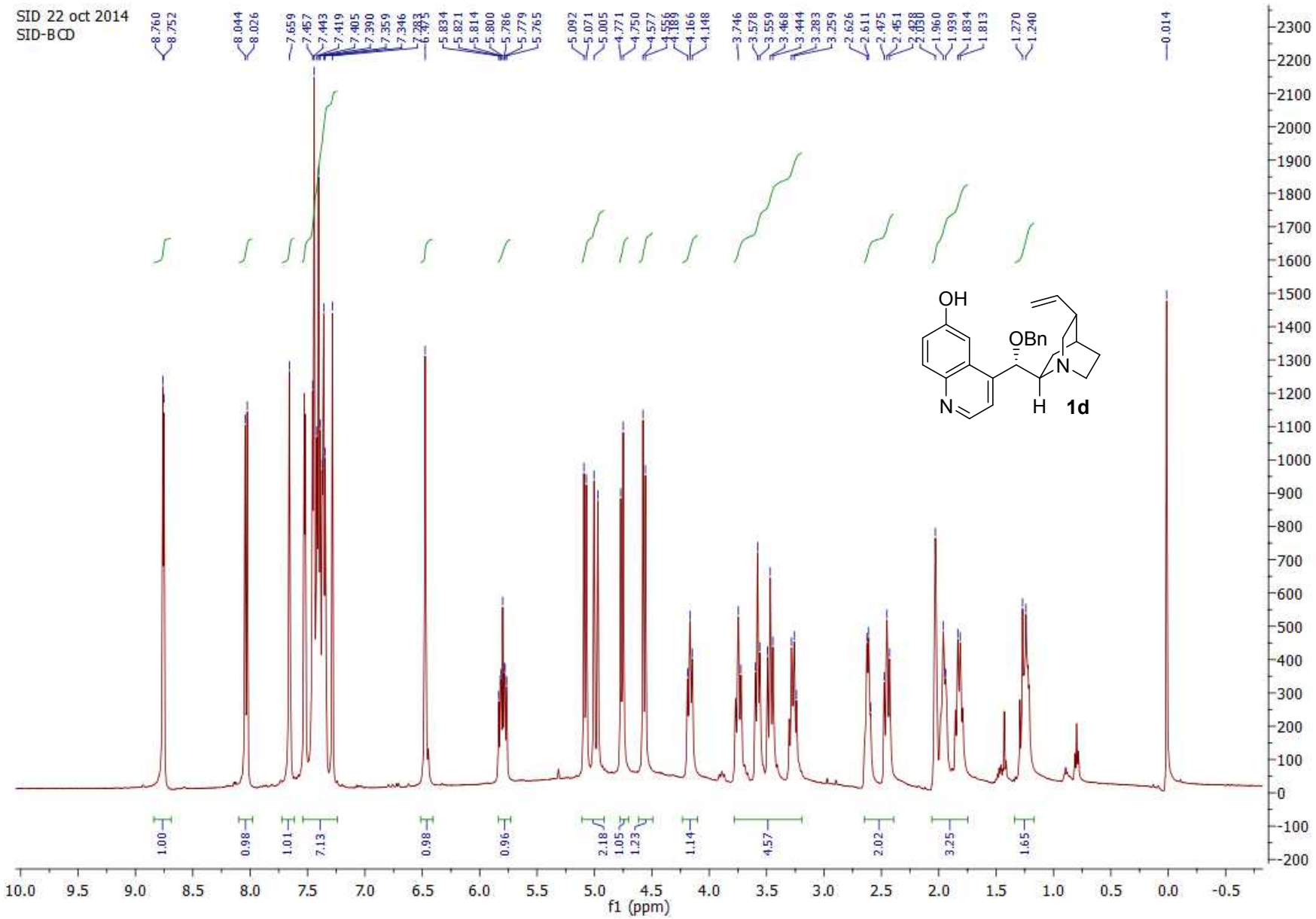
C:¥Users¥technologies¥Desktop¥malemide nmrs¥Dr_Chimni¥cjas500.als

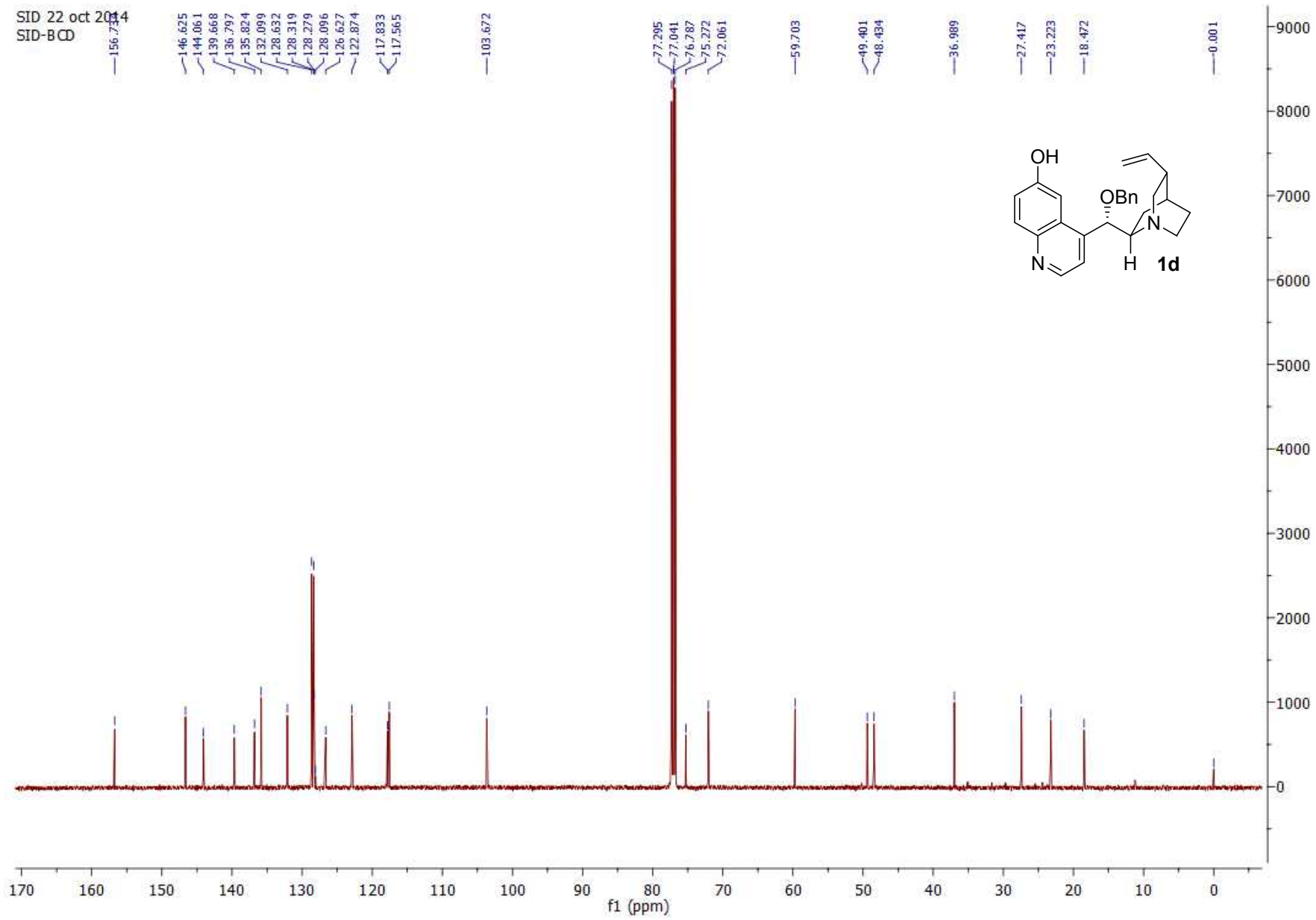



HO
OMe
HO
OMe
(R)
O
N
H
11z
abundance
0.3
0.2
0.1
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
178.3600
151.4603
151.1221
141.1752
130.0493
130.4059
130.3653
129.3261
126.4585
115.3484
111.3272
111.2628
111.0208
104.2597
77.4770
77.1600
76.8430
56.2244
56.1029
0.1396
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
zerofill : 4
sexp : 3.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]
Derived from: JAS-213 C13-7.jdf
Filename = JAS-213 C13-17.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = JAS-213 C13
Solvent = CHLOROFORM-D
Creation_time = 17-FEB-2014 03:34:45
Revision_time = 17-FEB-2014 11:01:06
Current_time = 17-FEB-2014 11:01:23
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 104856
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 6000
Total_scans = 6000
X_90_width = 7.87[us]
X_acq_time = 1.04333312[s]
X_angle = 90[deg]
X_atn = 4.2[dB]
X_pulse = 7.87[us]
Irr_atn_dec = 21.399[dB]
Irr_atn_noe = 21.399[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2.5[s]
Recvr_gain = 60
Relaxation_delay = 2.5[s]
Repetition_time = 3.54333312[s]
Temp_get = 18[dC]


21 oct 2014
jas-cpd
OH
OH
N
N
H
1c
f1 (ppm)

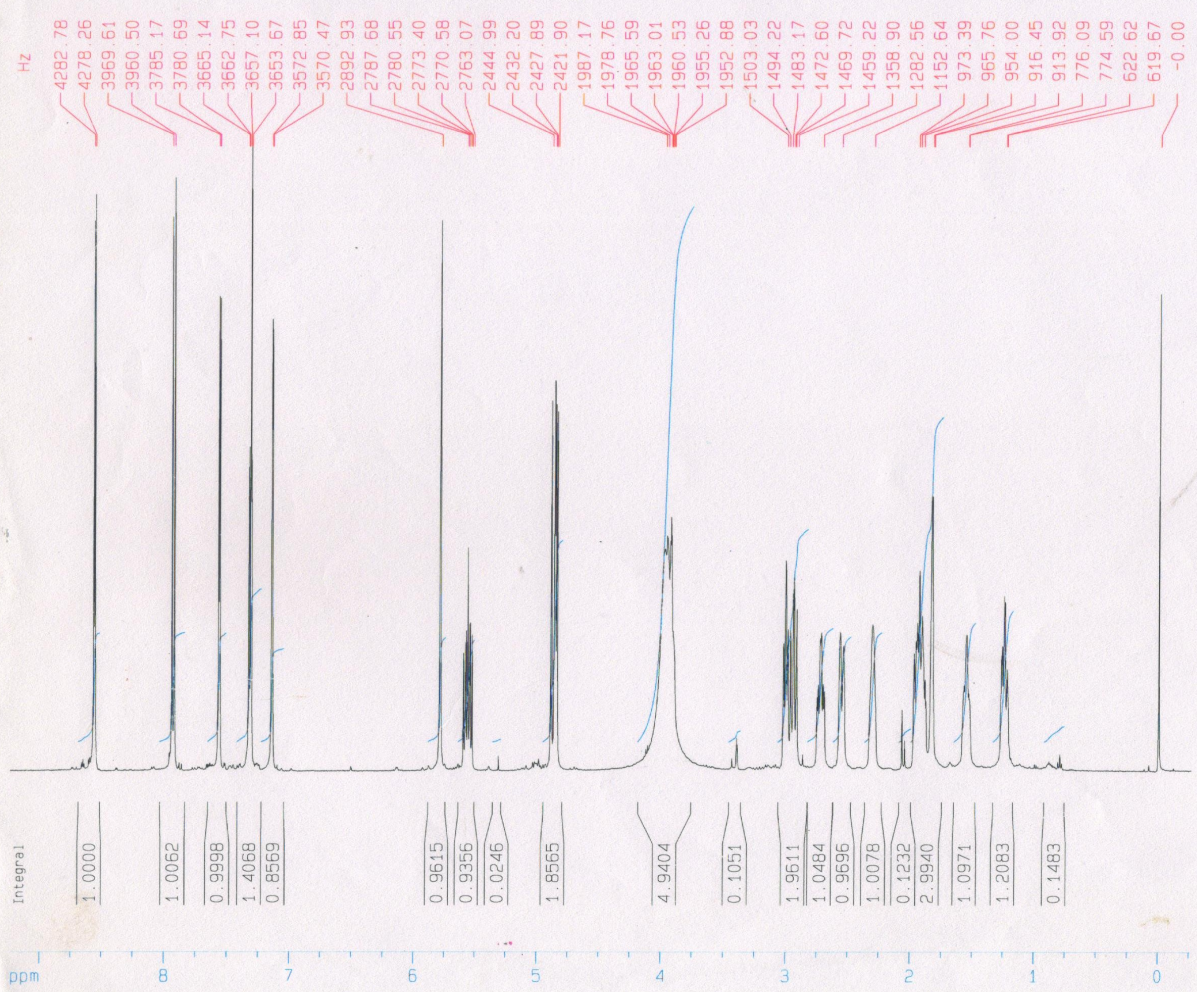

21 oct 2014
jas-cpd
157.805
146.651
146.370
143.012
139.616
131.602
126.453
123.290
117.686
115.365
103.860
77.276
77.022
76.768
70.344
59.289
49.206
39.401
36.508
27.972
25.437
18.382
0.001
OH
OH
N
N
H
1c
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

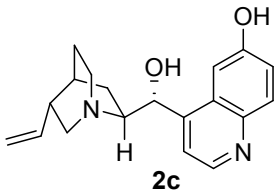

SID 22 oct 2014
SID-BCD
OH
OBn
N
N
H
1d
f1 (ppm)


SID 22 oct 2014
SID-BCD
156.734
146.625
144.061
139.668
136.797
135.824
132.099
128.632
128.319
128.279
128.096
126.627
122.874
117.833
117.565
103.672
77.295
77.041
76.787
75.272
72.061
59.703
49.401
48.434
36.989
27.417
23.223
18.472
0.001
OH
OBn
N
N
H
1d
f1 (ppm)

GAL-6-OH-Q

CPN



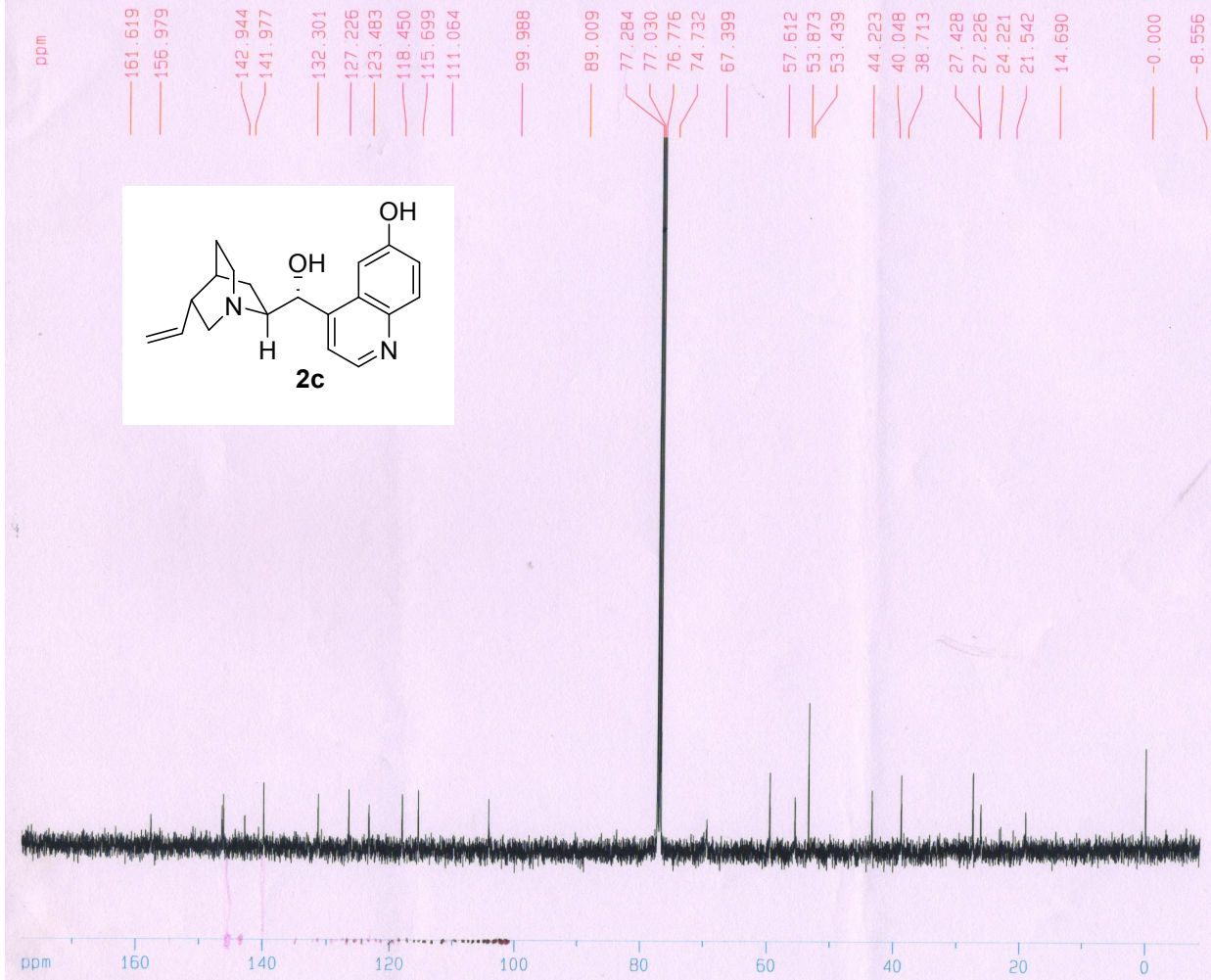


2c

NS	16
DS	2
SWH	12531.328 Hz
FIDRES	0.191213 Hz
AQ	2.6149764 sec
RG	181
DW	39.900 usec
DE	6.00 usec
TE	683.6 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	9.00 usec
PL1	-2.00 dB
SF01	500.1324719 MHz
F2 - Processing parameters	
SI	32768
SF	500.1299871 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	0.30
1D NMR plot parameters	
CX	20.00 cm
CY	10.00 cm
F1P	9.237 ppm
F1	4619.89 Hz
F2P	-0.263 ppm
F2	-131.76 Hz
PPMCM	0.47504 ppm/cm
HZCM	237.58279 Hz/cm

CPN

R-CPN



2c

Current Data Parameters
NAME Apr09-2010-purnima
EXPNO 12
PROCNO 1

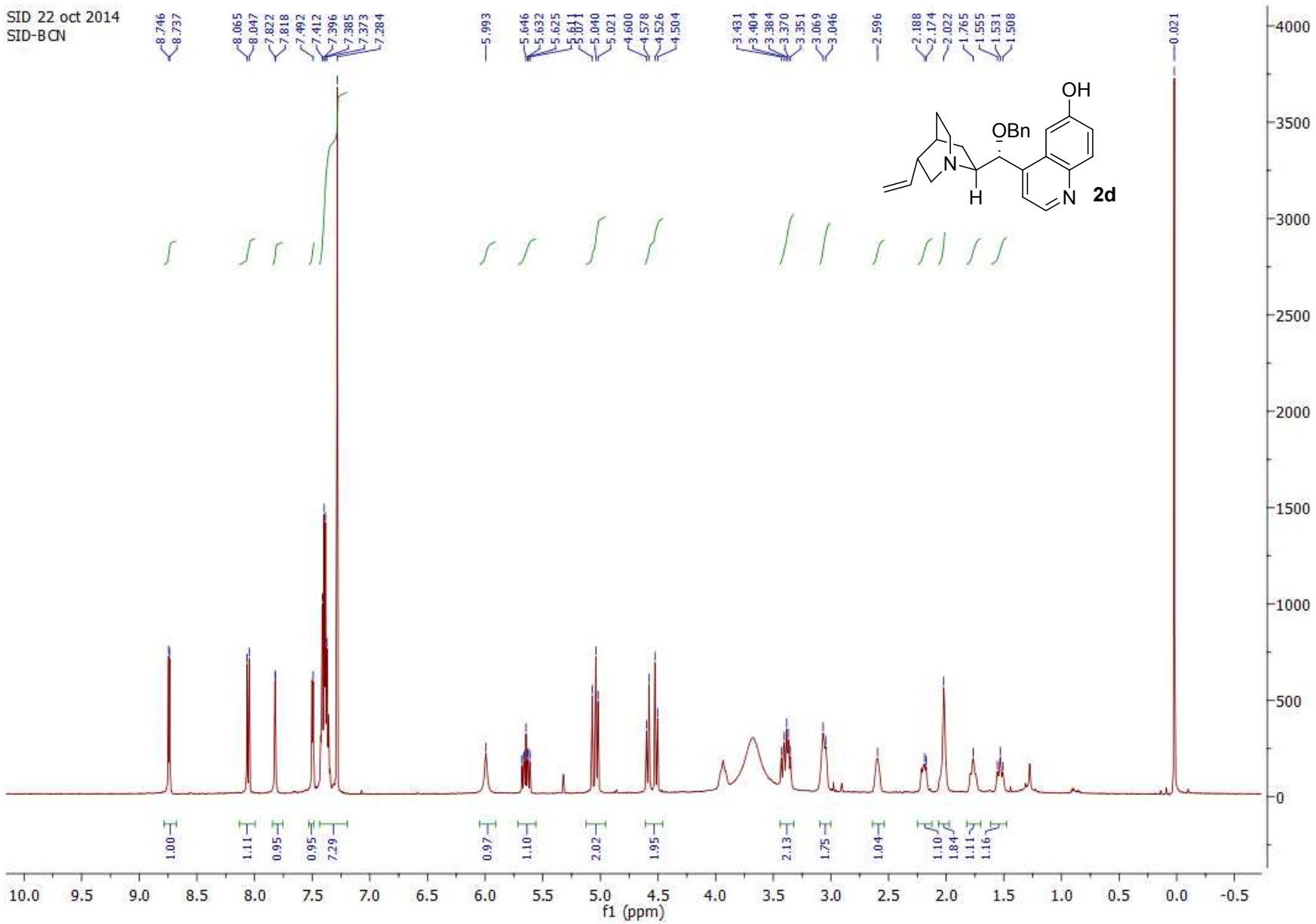
F2 - Acquisition Parameters
Date_ 20100409
Time 13.35
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 3251
DW 15.900 usec
DE 6.00 usec
TE 683.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 0.00 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 21.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577899 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.80

1D NMR plot parameters
CX 20.00 cm
CY 2.00 cm
F1P 178.055 ppm
F1 22391.77 Hz
F2P -8.720 ppm
F2 -1096.56 Hz
PPMCM 9.33872 ppm/cm
HZCM 1174.41626 Hz/cm


SID 22 oct 2014
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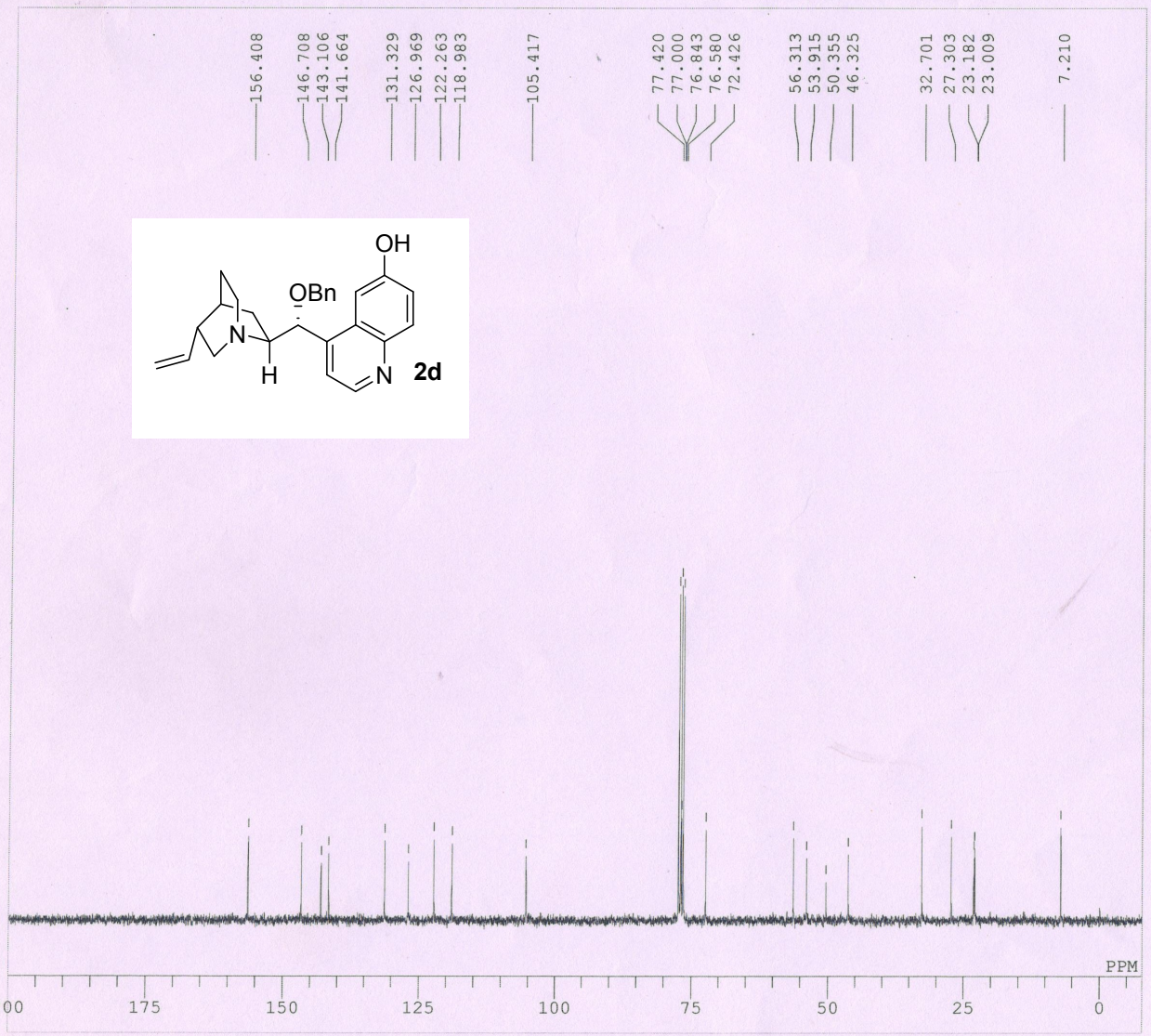
8.737
8.065
8.047
7.822
7.818
7.492
7.412
7.396
7.385
7.373
7.284
5.993
5.646
5.632
5.625
5.611
5.040
5.021
4.600
4.578
4.526
4.504
3.431
3.404
3.384
3.370
3.351
3.069
3.046
2.596
2.188
2.174
2.022
1.765
1.555
1.531
1.508
0.021
OH
OBn
N
H
N
2d
1.00
1.11
0.95
0.95
7.29
0.97
1.10
2.02
1.95
2.13
1.75
1.04
1.10
1.84
1.11
1.16
f1 (ppm)

C:\WINNMR98\Z_JASBIR\nbbcd.als

Bn CPN

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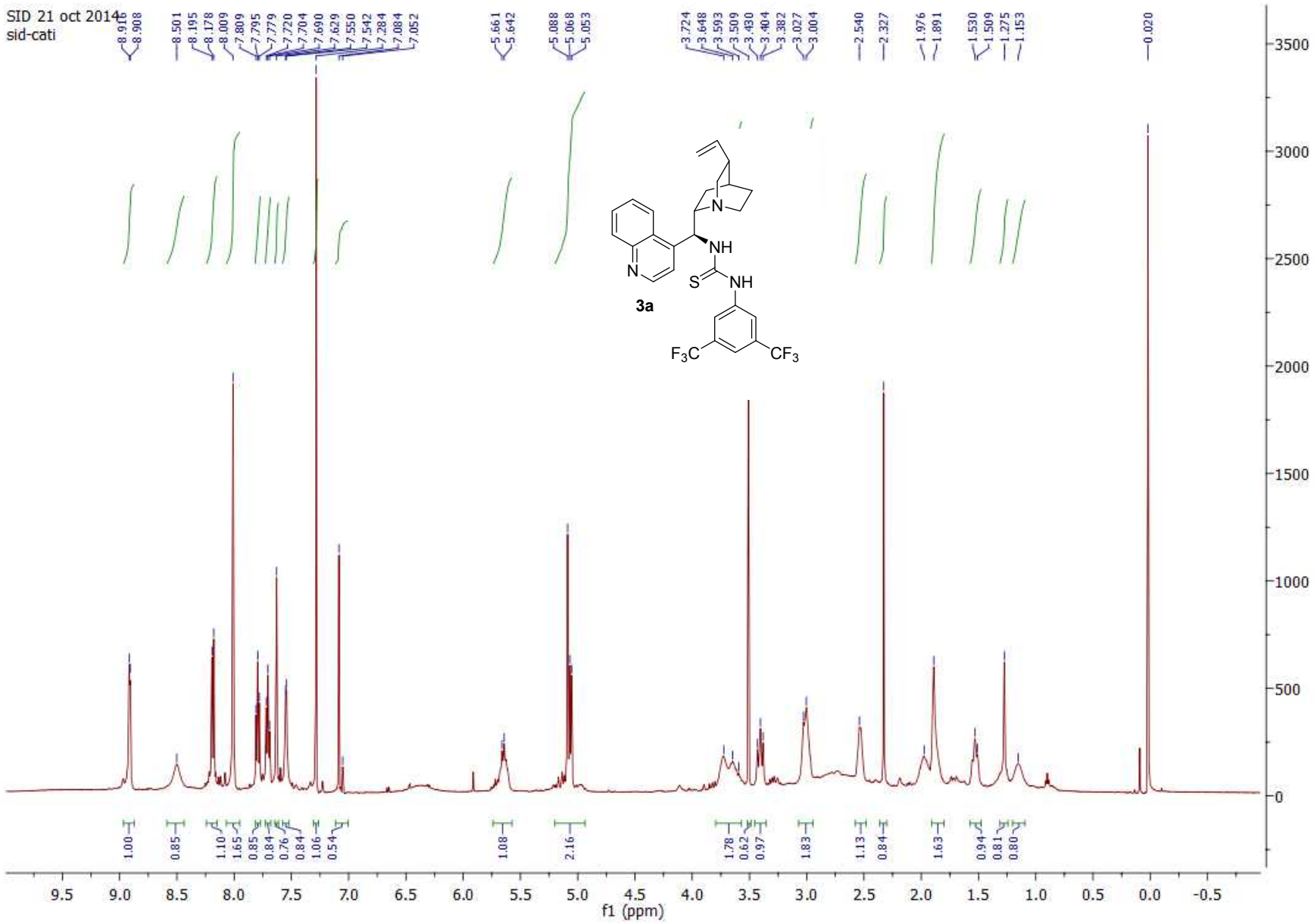
OBNUC   13C
EXMOD   BCM
OFR          75.45 MHz
OBSET       124.00 KHz
OBFIN      1840.0 Hz
POINT       32768
FREQU      20408.1 Hz
SCANS          260
ACQTM        1.606 sec
PD           3.000 sec
PW1            5.5 us
IRN
CTEMP       -204.8 c
SLVNT   CDCL3
EXREF        77.00 ppm
BF            1.20 Hz
RGAIN           24
```


SID 21 oct 2014
sid-cati
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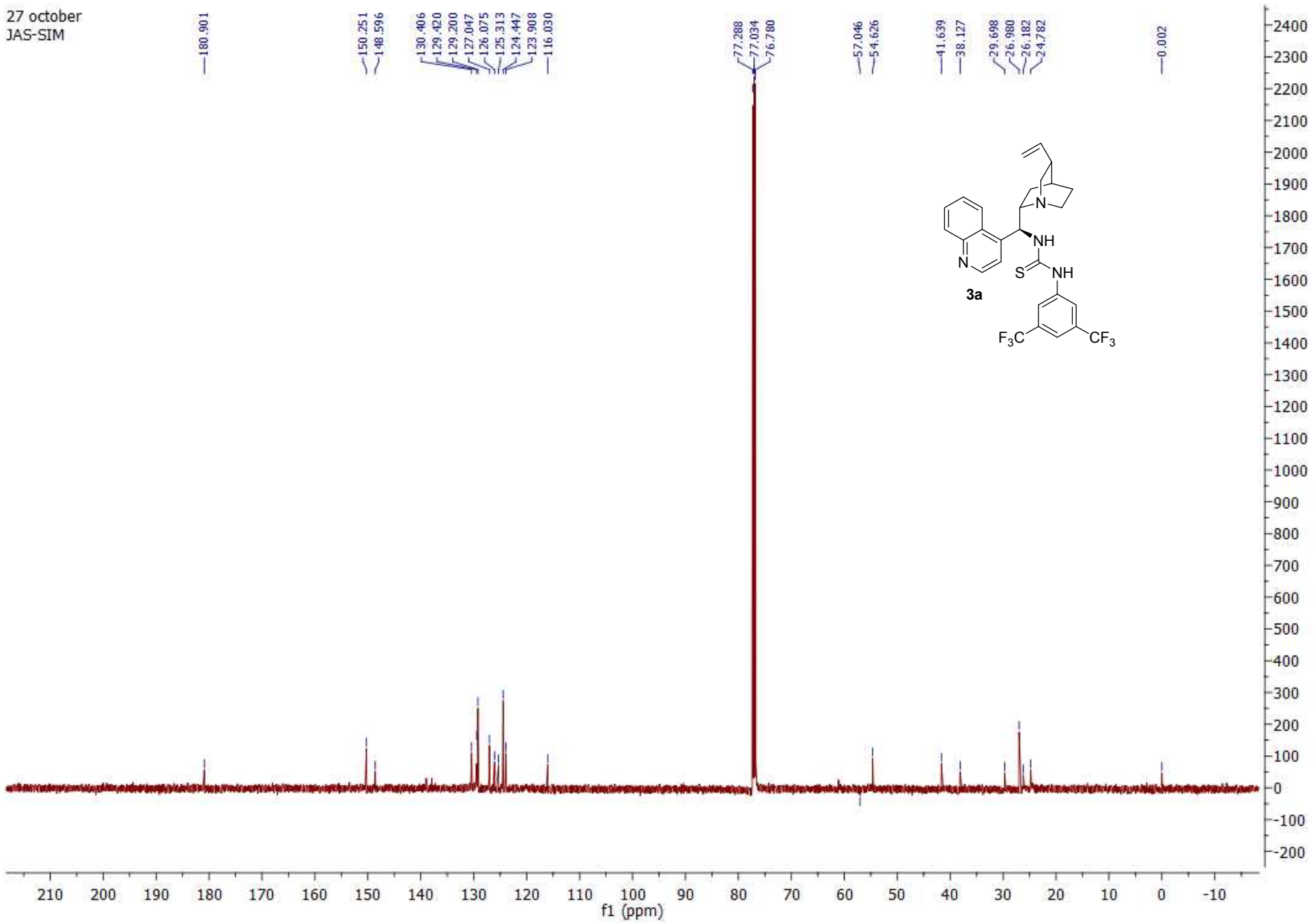
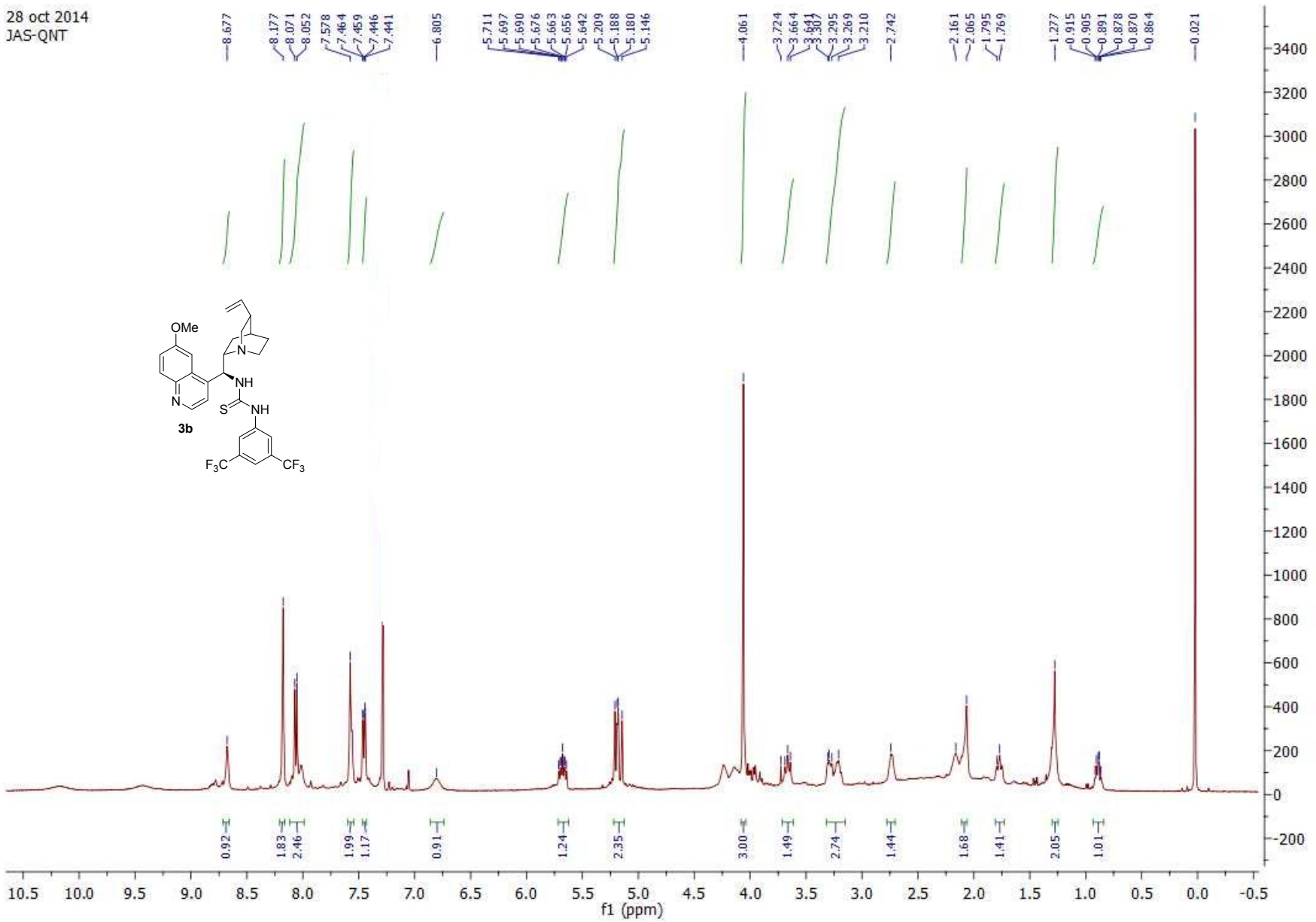
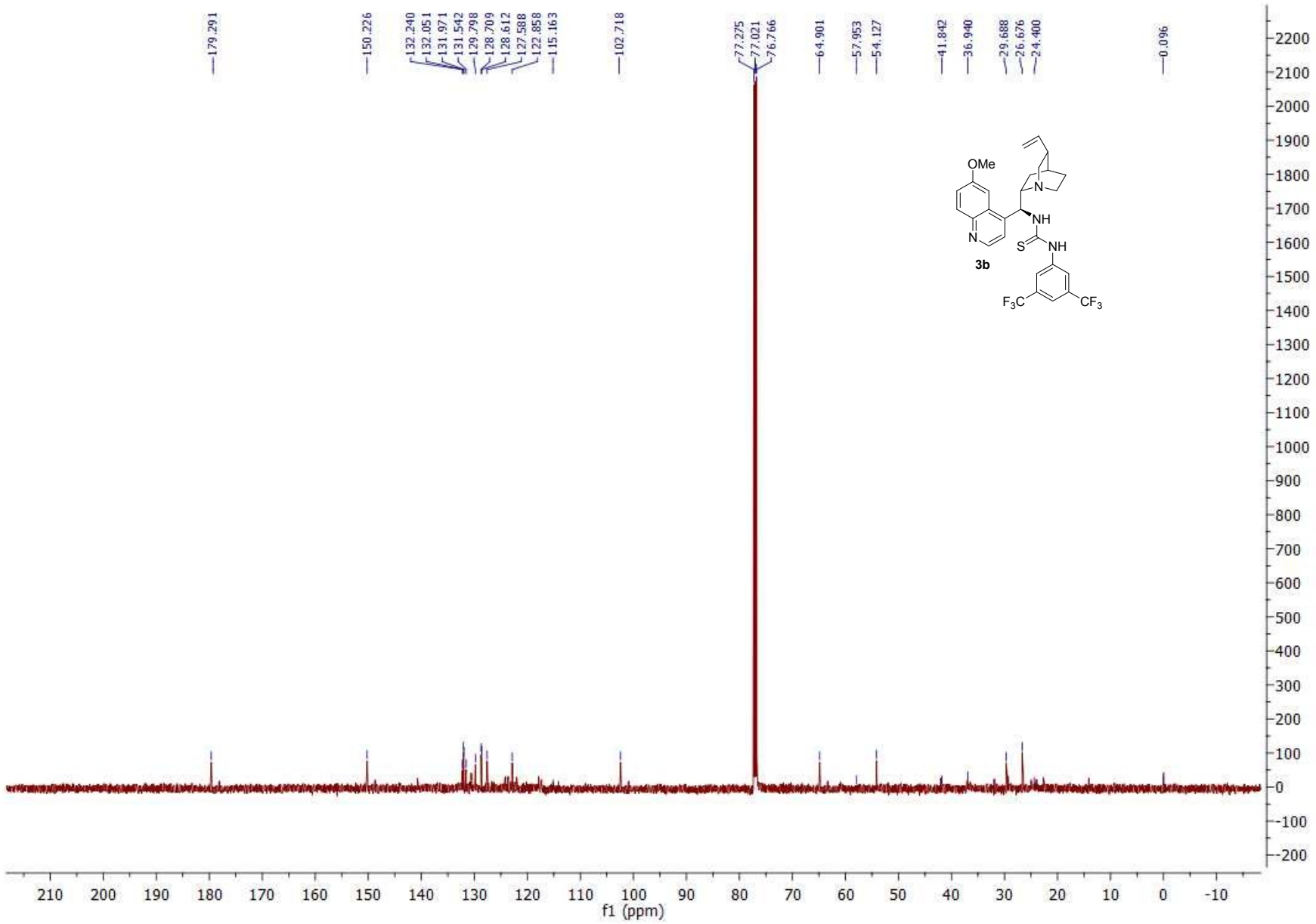
8.908
8.501
8.195
8.178
8.009
7.809
7.795
7.779
7.720
7.704
7.690
7.629
7.550
7.542
7.284
7.084
7.052
5.661
5.642
5.088
5.068
5.053
3.724
3.648
3.593
3.509
3.430
3.404
3.382
3.027
3.004
2.540
2.327
1.976
1.891
1.530
1.509
1.275
1.153
0.020
3a
F3C
CF3
NH
NH
S
N
N
1.00
0.85
1.10
1.65
0.85
0.84
0.76
0.84
1.06
0.54
1.08
2.16
1.78
0.62
0.97
1.83
1.13
0.84
1.63
0.94
0.81
0.80
f1 (ppm)


27 october
JAS-SIM
180.901
150.251
148.596
130.406
129.420
129.200
127.047
126.075
125.313
124.447
123.908
116.030
77.288
77.034
76.780
57.046
54.626
41.639
38.127
29.698
26.980
26.182
24.782
0.002
3a
f1 (ppm)


28 oct 2014
JAS-QNT
8.677
8.177
8.071
8.052
7.578
7.464
7.459
7.446
7.441
6.805
5.711
5.697
5.690
5.676
5.663
5.656
5.642
5.209
5.188
5.180
5.146
4.061
3.724
3.664
3.641
3.307
3.295
3.269
3.210
2.742
2.161
2.065
1.795
1.769
1.277
0.915
0.905
0.891
0.878
0.870
0.864
0.021
OMe
N
NH
S
NH
3b
F3C
CF3
0.92
1.83
2.46
1.99
1.17
0.91
1.24
2.35
3.00
1.49
2.74
1.44
1.68
1.41
2.05
1.01
f1 (ppm)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132.051
131.971
131.542
129.798
128.709
128.612
127.588
122.858
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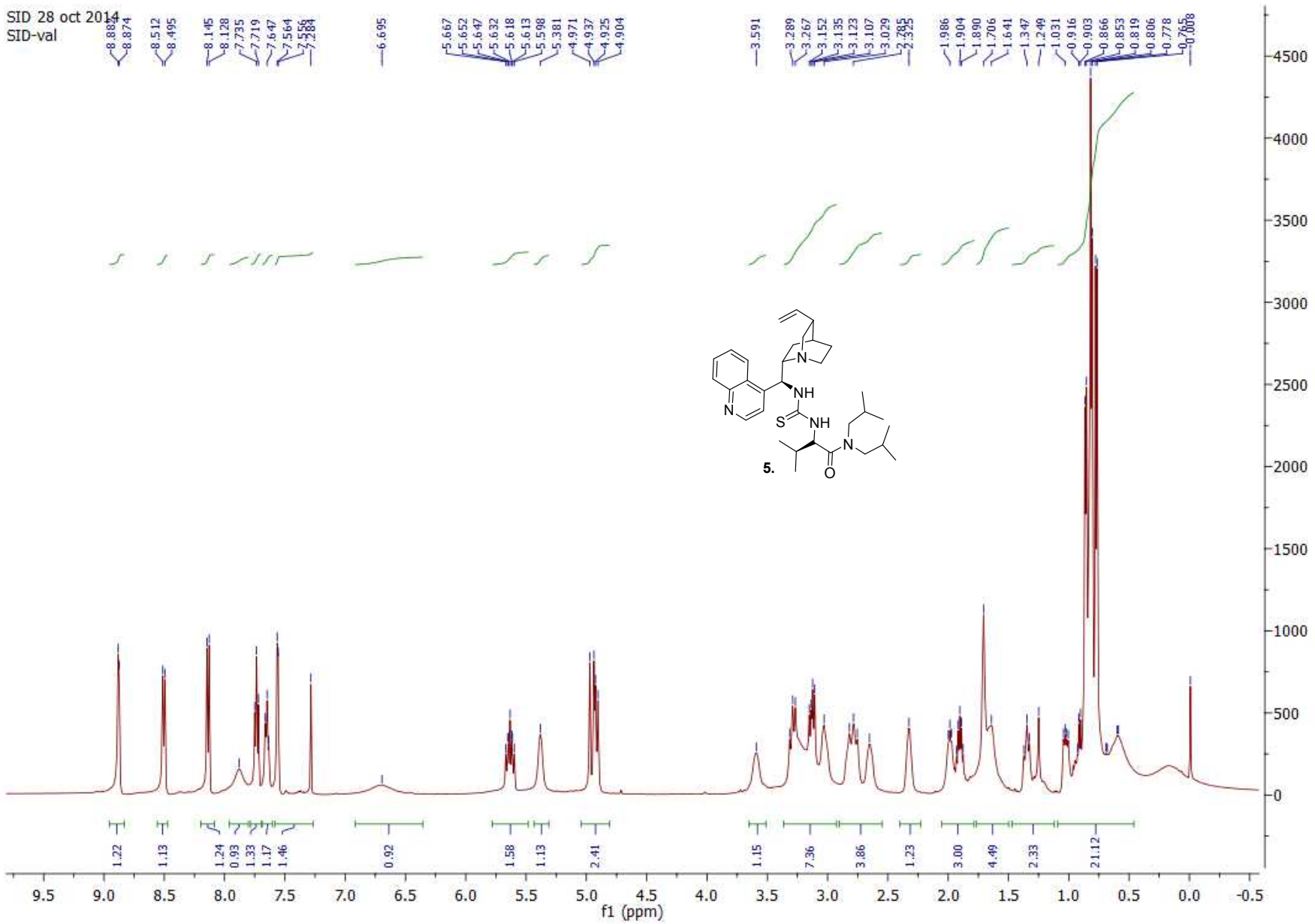
102.718
77.275
77.021
76.766
64.901
57.953
54.127
41.842
36.940
29.688
26.676
24.400
0.096
OMe
N
NH
S
NH
F3C
CF3
3b
f1 (ppm)


SID 28 oct 2014
SID-val
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8.512
8.495
8.145
8.128
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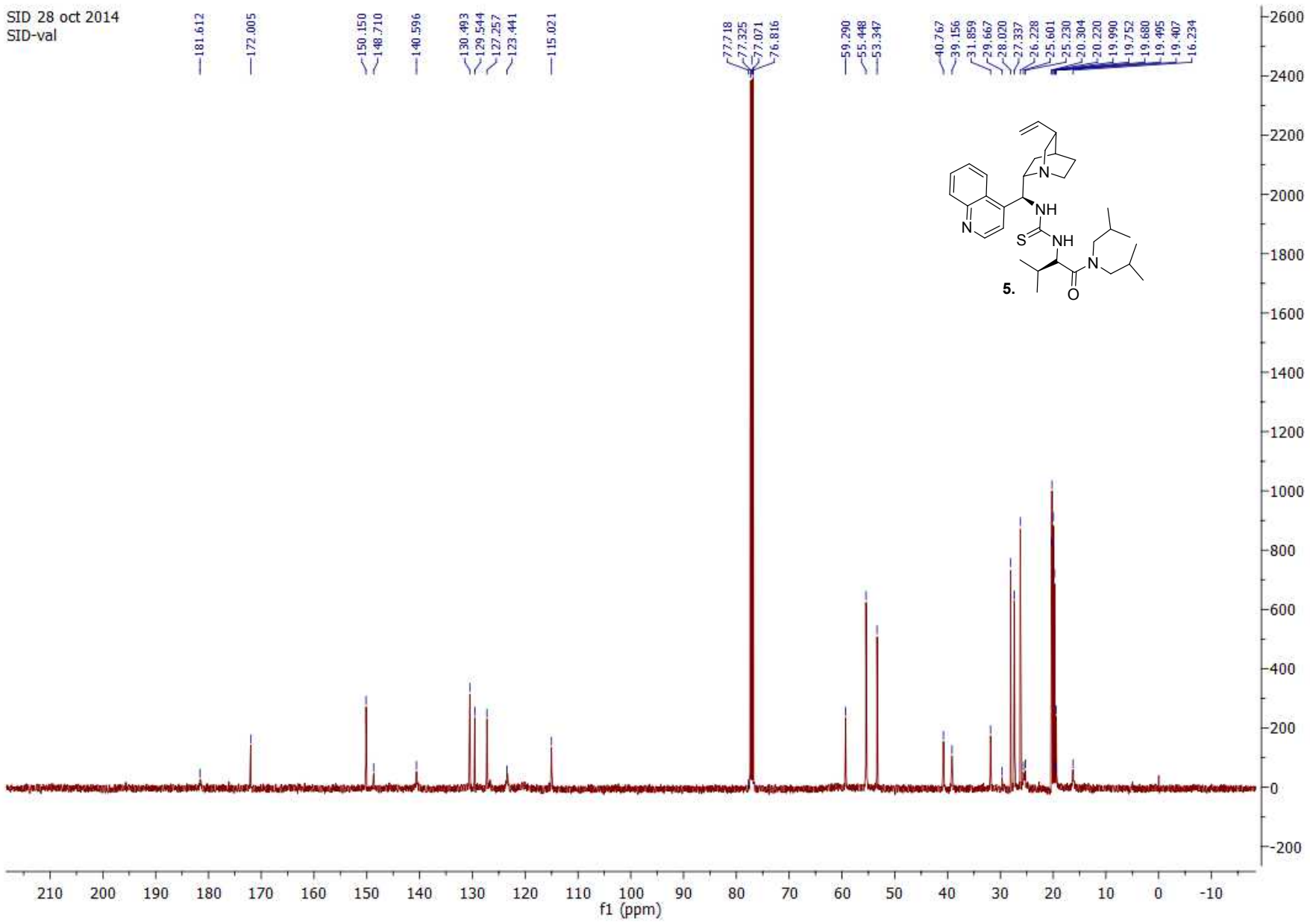
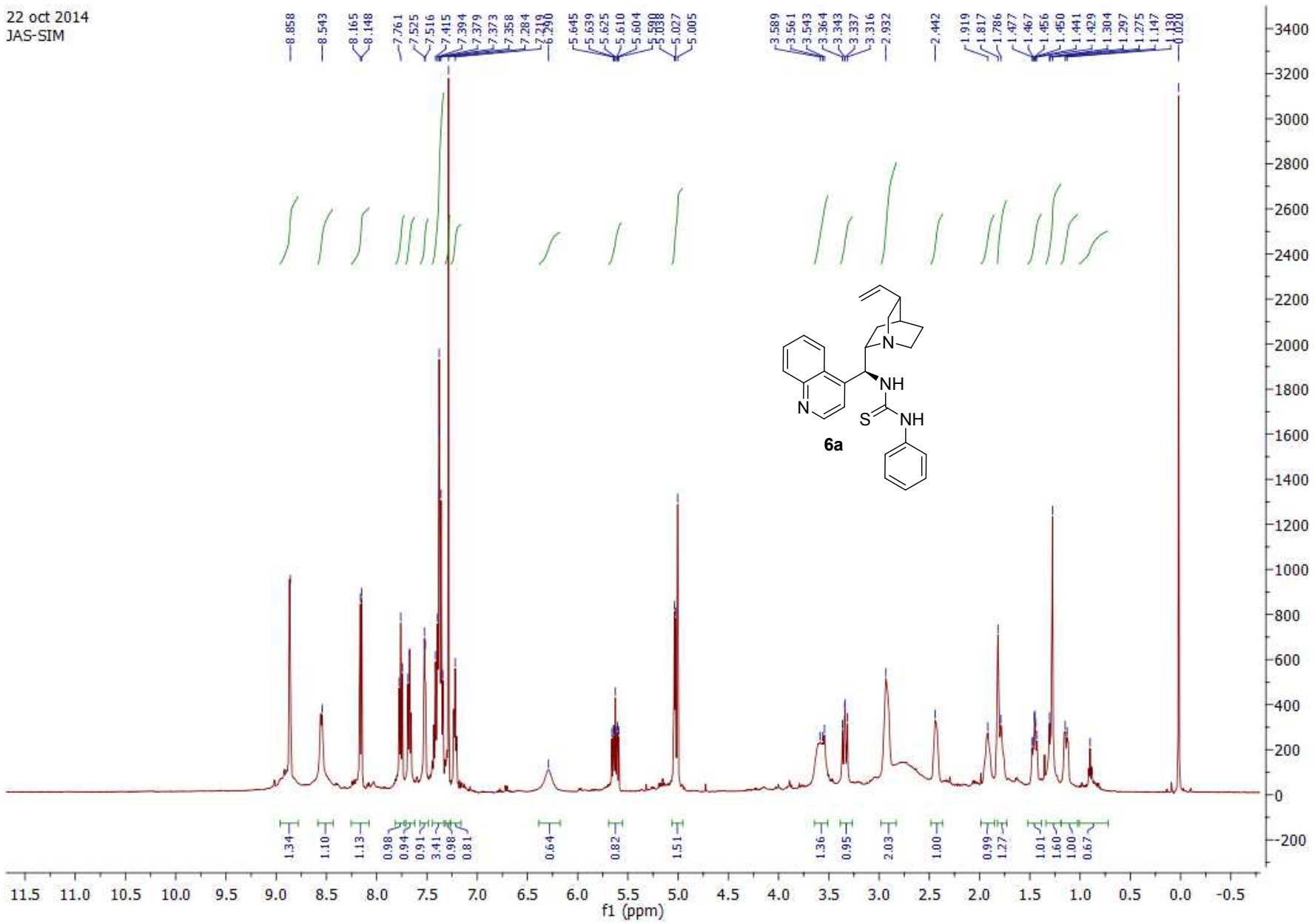
7.719
7.647
7.564
7.556
7.284
6.695
5.667
5.652
5.647
5.632
5.618
5.613
5.598
5.381
4.971
4.937
4.925
4.904
3.591
3.289
3.267
3.152
3.135
3.123
3.107
3.029
2.785
2.325
1.986
1.904
1.890
1.706
1.641
1.347
1.249
1.031
0.916
0.903
0.866
0.853
0.819
0.806
0.778
0.765
0.008
5.
N
NH
S
NH
N
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.22
1.13
1.24
0.93
1.33
1.17
1.46
0.92
1.58
1.13
2.41
1.15
7.36
3.86
1.23
3.00
4.49
2.33
21.12
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


SID 28 oct 2014
SID-val
181.612
172.005
150.150
148.710
140.596
130.493
129.544
127.257
123.441
115.021
77.718
77.325
77.071
76.816
59.290
55.448
53.347
40.767
39.156
31.859
29.667
28.020
27.337
26.228
25.601
25.230
20.304
20.220
19.990
19.752
19.680
19.495
19.407
16.234
N
NH
S
NH
N
O
5.
f1 (ppm)


22 oct 2014
JAS-SIM
8.858
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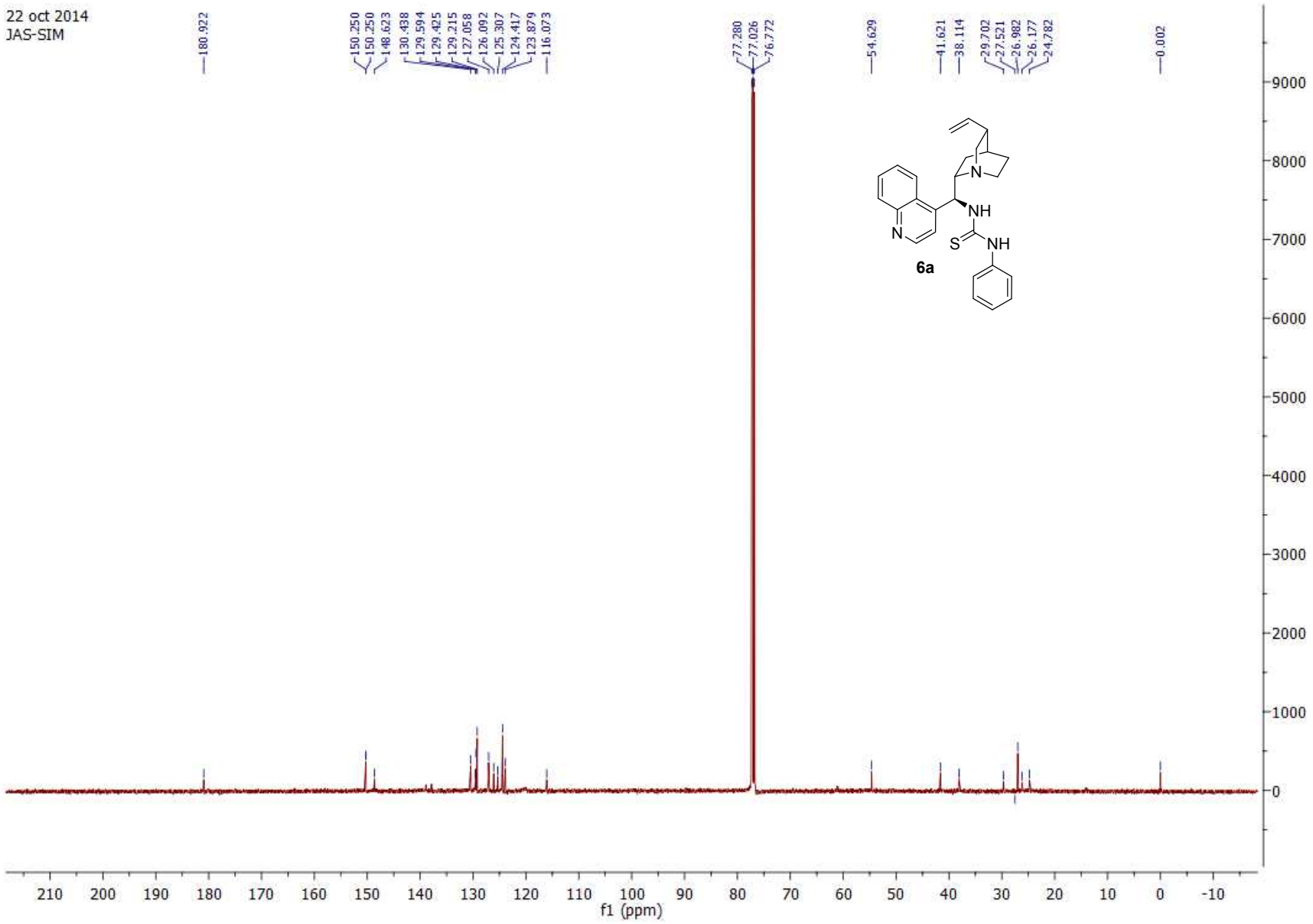
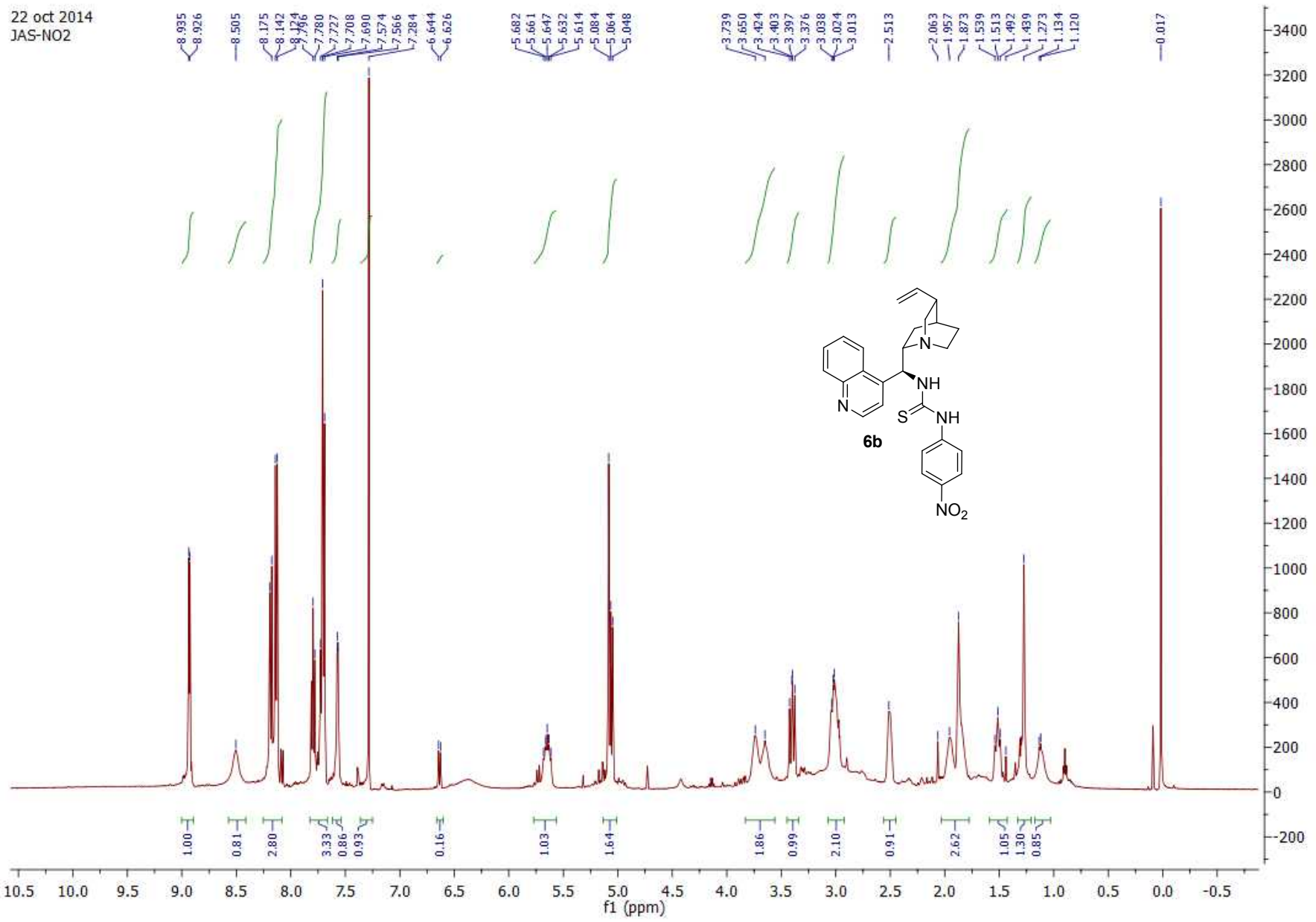
8.148
7.761
7.525
7.516
7.415
7.394
7.379
7.373
7.358
7.284
7.219
6.290
5.645
5.639
5.625
5.610
5.604
5.027
5.005
3.589
3.561
3.543
3.364
3.343
3.337
3.316
2.932
2.442
1.919
1.817
1.786
1.477
1.467
1.456
1.450
1.441
1.429
1.304
1.297
1.275
1.147
0.020
N
NH
S
NH
6a
1.34
1.10
1.13
0.98
0.94
0.91
3.41
0.98
0.81
0.64
0.82
1.51
1.36
0.95
2.03
1.00
0.99
1.27
1.01
1.60
1.00
0.67
f1 (ppm)


22 oct 2014
JAS-SIM
180.922
150.250
150.250
148.623
130.438
129.594
129.425
129.215
127.058
126.092
125.307
124.417
123.879
116.073
77.280
77.026
76.772
54.629
41.621
38.114
29.702
27.521
26.982
26.177
24.782
0.002
6a
f1 (ppm)


22 oct 2014
JAS-NO2
8.935
8.926
8.505
8.175
8.142
7.796
7.780
7.727
7.708
7.690
7.574
7.566
7.284
6.644
6.626
5.682
5.661
5.647
5.632
5.614
5.084
5.064
5.048
3.739
3.650
3.424
3.403
3.397
3.376
3.038
3.024
3.013
2.513
2.063
1.957
1.873
1.539
1.513
1.492
1.439
1.273
1.134
1.120
0.017
6b
NH
NH
S
N
N
NO2
1.00
0.81
2.80
3.33
0.86
0.93
0.16
1.03
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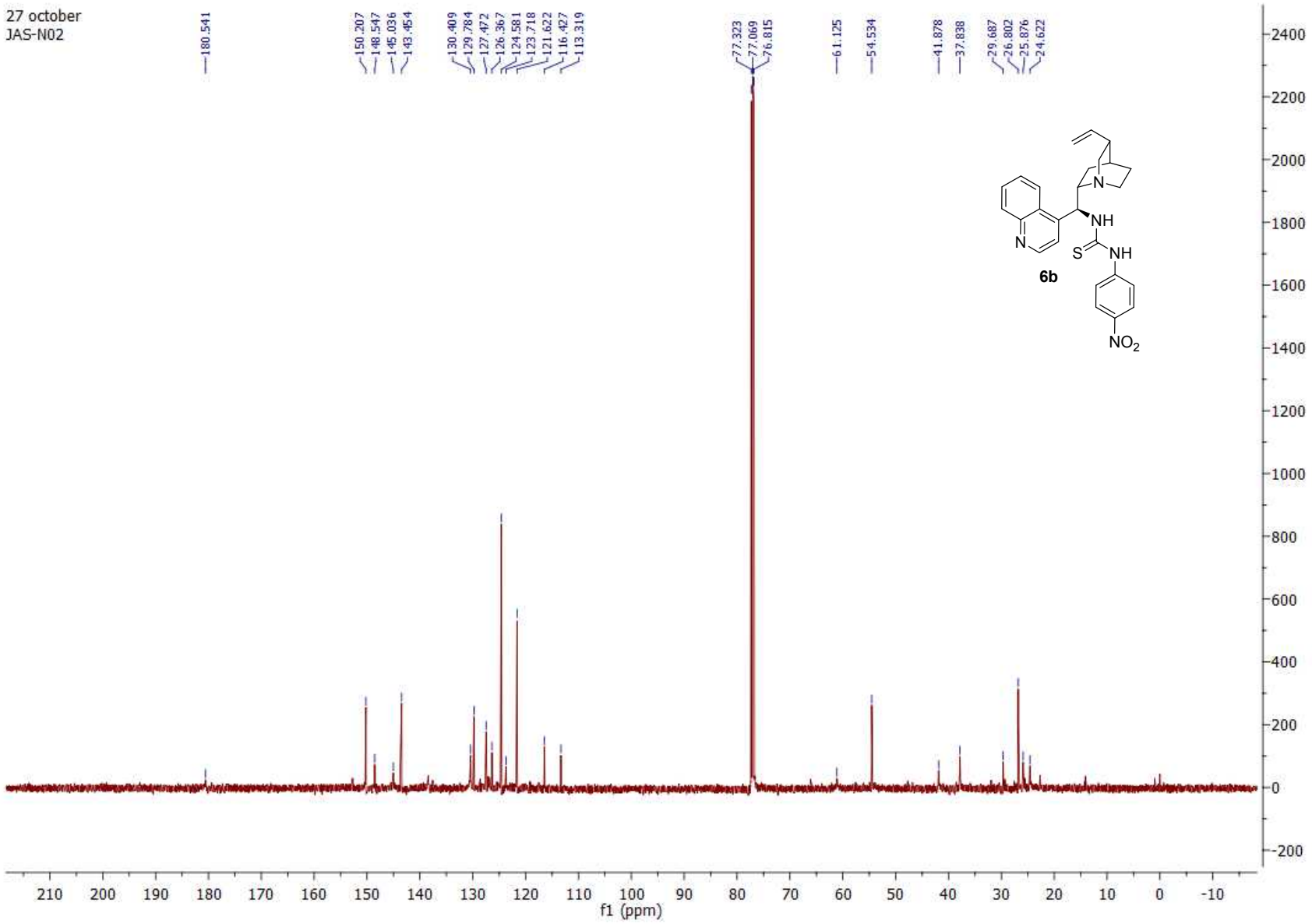
1.86
0.99
2.10
0.91
2.62
1.05
1.30
0.85
f1 (ppm)


27 october
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180.541
150.207
148.547
145.036
143.454
130.409
129.784
127.472
126.367
124.581
123.718
121.622
116.427
113.319
77.323
77.069
76.815
61.125
54.534
41.878
37.838
29.687
26.802
25.876
24.622
6b
f1 (ppm)