The Diaza-Nazarov Cyclization Involving 2,3-Diaza-pentadienyl Cation for the Synthesis of Polysubstituted Pyrazoles

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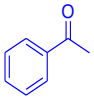
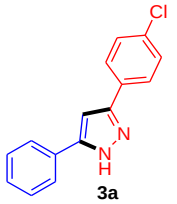
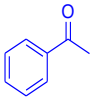
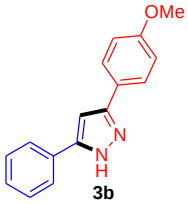
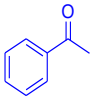
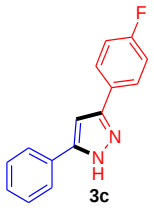
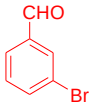
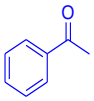
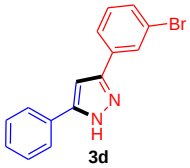
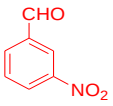
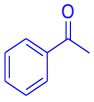
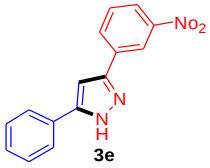
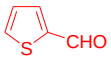
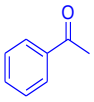
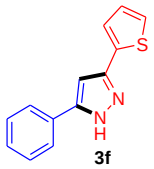
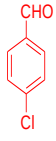
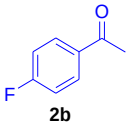
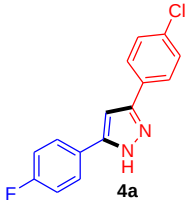
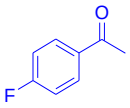
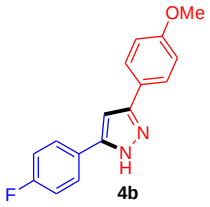
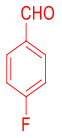
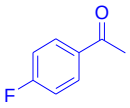
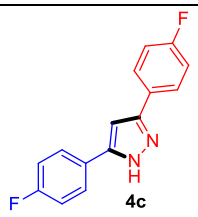
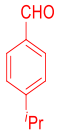
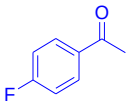
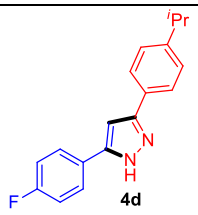
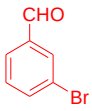
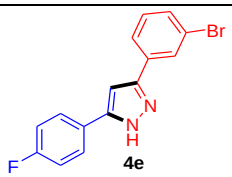
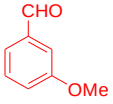
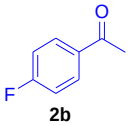
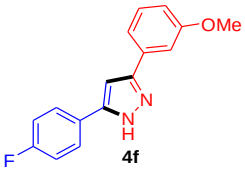
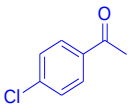
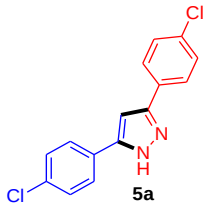
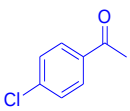
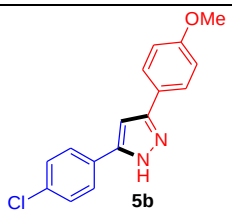
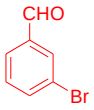
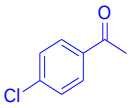
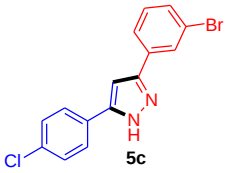
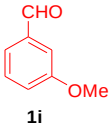
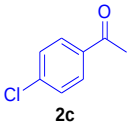
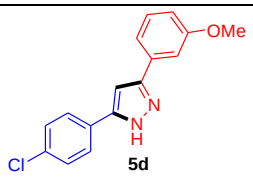
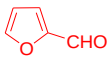
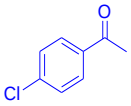
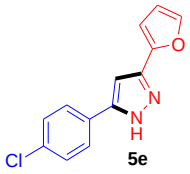
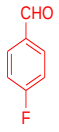
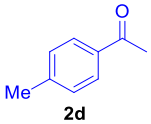
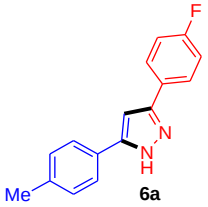
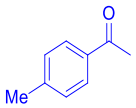
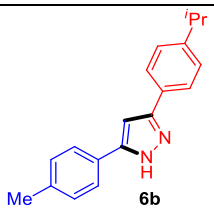
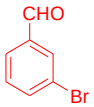
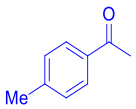
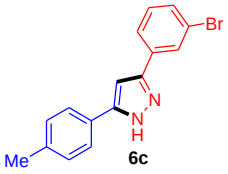
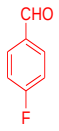
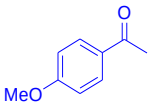
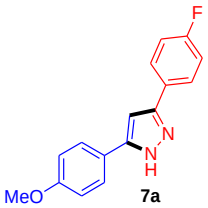
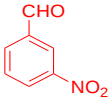
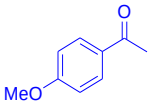
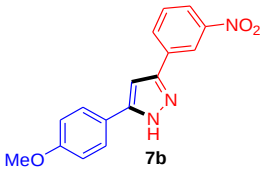
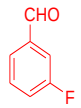
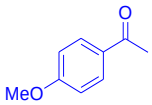
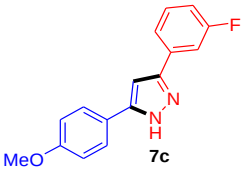
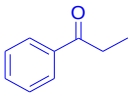
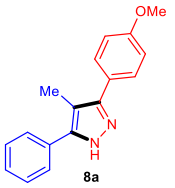
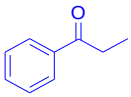
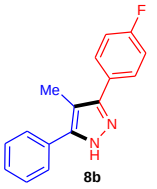
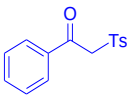
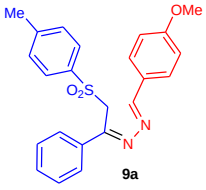
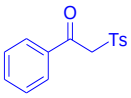
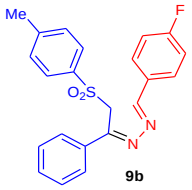
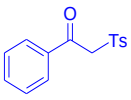
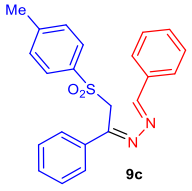
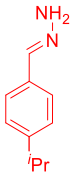
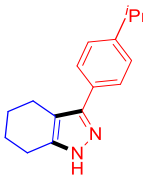
ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Iodine-mediated one-pot, three-component approach for the synthesis of substituted pyrazoles.

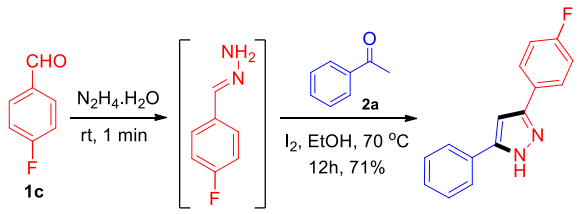
S. No.	Aldehyde/ Hydrazone	Acetophenone/ Derivative	Product	Yield (%)
1	 1a	 2a	 3a	71
2	 1b	 2a	 3b	70
3	 1c	 2a	 3c	71
4	 1d	 2a	 3d	67
5	 1e	 2a	 3e	82
6	 1f	 2a	 3f	58
7	 1a	 2b	 4a	70

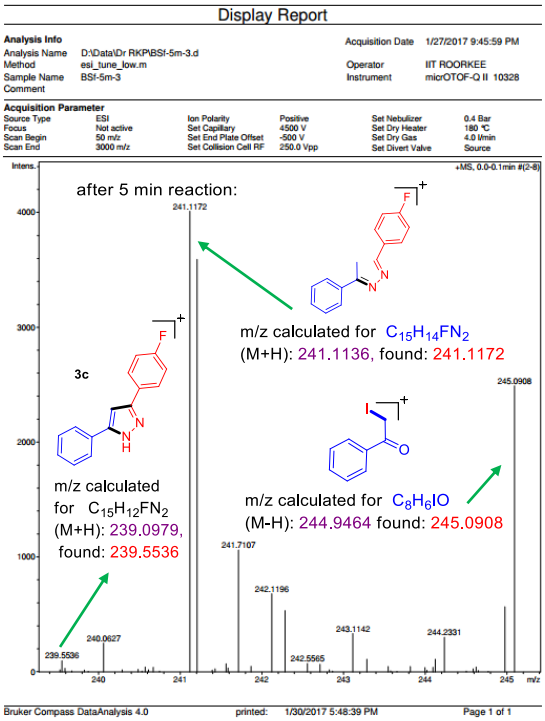
8	 1b	 2b	 4b	66
9	 1c	 2b	 4c	61
10	 1g	 2b	 4d	55
11	 1d	 2b	 4e	67
12	 1i	 2b	 4f	72
13	 1a	 2c	 5a	58
14	 1b	 2c	 5b	61

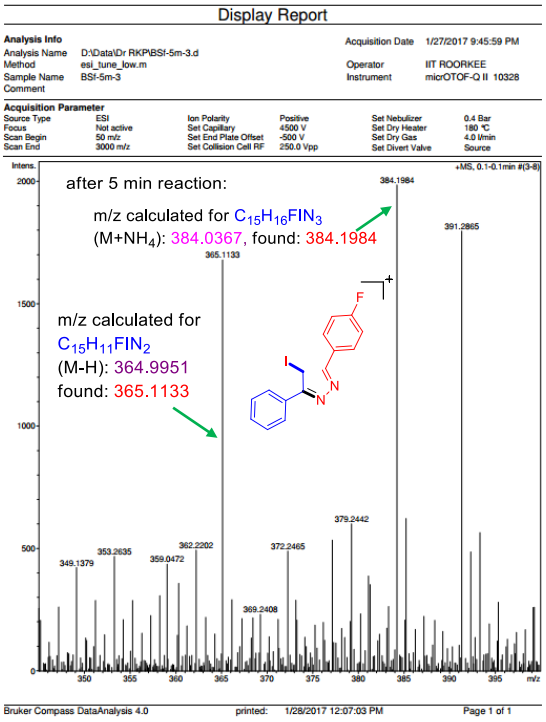
15	 1d	 2c	 5c	66
16	 1i	 2c	 5d	72
23	 1j	 2c	 5e	49
17	 1c	 2d	 6a	67
18	 1g	 2d	 6b	65
19	 1d	 2d	 6c	64
20	 1c	 2e	 7a	50
21	 1e	 2e	 7b	81

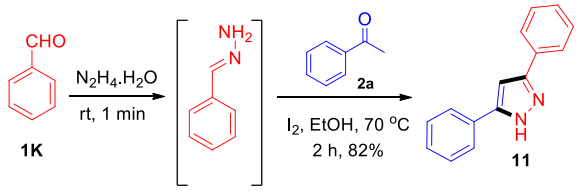
22	 1h	 2e	 7c	52
24	 1b	 2f	 8a	52
25	 1c	 2f	 8b	47
26	 1b	 2g	 9a	49
27	 1c	 2g	 9b	50
28		 2g	 9c	90
29	 1g'	 2h	 12	24

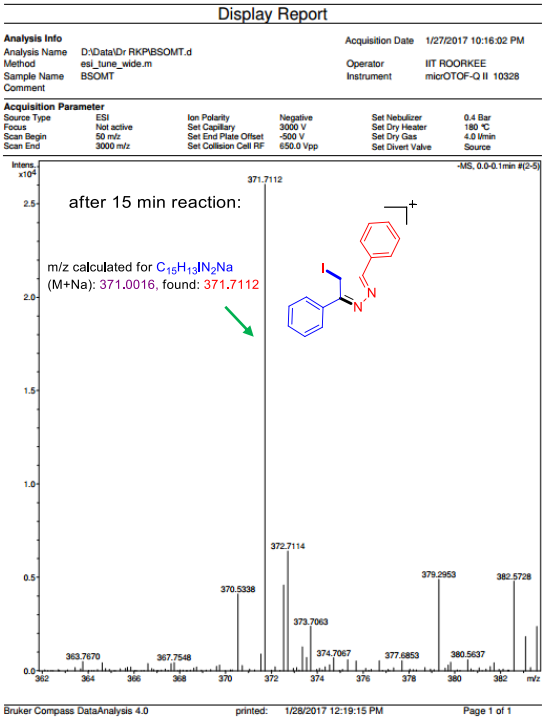
Monitoring reactions with mass spectral analysis








CHO
1K
$N_2H_4.H_2O$
rt, 1 min
NH2
N
O
2a
I_2, EtOH, 70 °C
2 h, 82%
N
N
H
11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Method esi_tune_wide.m
Sample Name BSOMT
Comment
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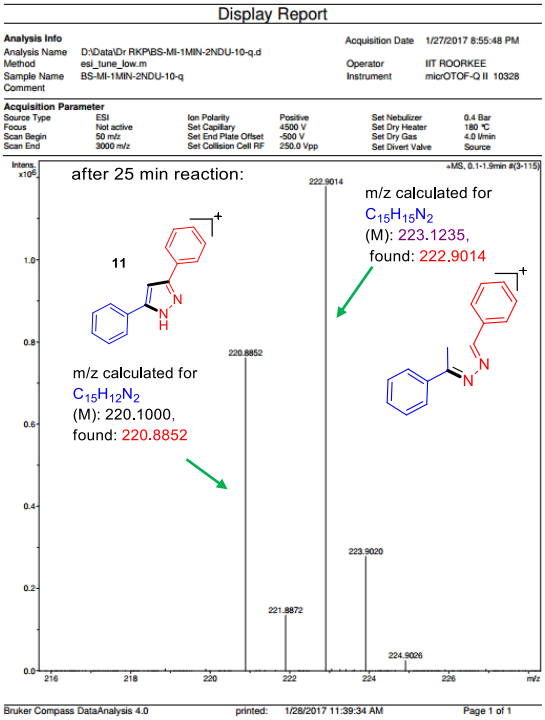
Operator IIT ROORKEE
Instrument micrOTOF-Q II 10328
Acquisition Parameter
Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 3000 m/z
Ion Polarity Negative
Set Capillary 3000 V
Set End Plate Offset -500 V
Set Collision Cell RF 650.0 Vpp
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Source
Intens.
x10^4
-MS, 0.0-0.1min #(2-5)
after 15 min reaction:
m/z calculated for C15H13IN2Na
(M+Na): 371.0016, found: 371.7112
371.7112
372.7114
370.5338
373.7063
374.7067
377.6853
379.2953
380.5637
382.5728
363.7670
367.7548
m/z
Bruker Compass DataAnalysis 4.0
printed: 1/28/2017 12:19:15 PM
Page 1 of 1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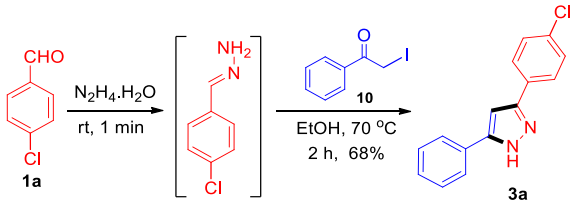
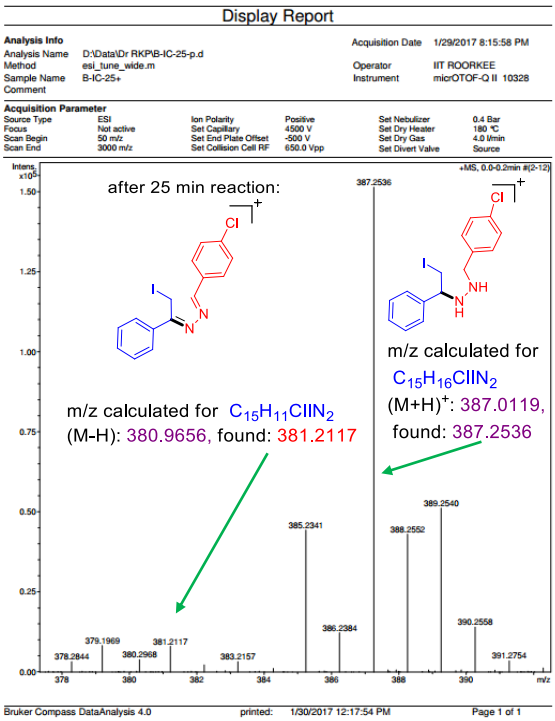
Method esi_tune_low.m
Sample Name BS-MI-1MIN-2NDU-10-q
Comment
Acquisition Date 1/27/2017 8:55:48 PM
Operator IIT ROORKEE
Instrument micrOTOF-Q II 10328
Acquisition Parameter
Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 3000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 250.0 Vpp
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
Intens.
x10^6
+MS, 0.1-1.9min #(3-115)
after 25 min reaction:
11
m/z calculated for
C15H12N2
(M): 220.1000,
found: 220.8852
m/z calculated for
C15H15N2
(M): 223.1235,
found: 222.9014
222.9014
220.8852
223.9020
221.8872
224.9026
m/z
Bruker Compass DataAnalysis 4.0
printed: 1/28/2017 11:39:34 AM
Page 1 of 1


CHO
Cl
1a
$N_2H_4.H_2O$
rt, 1 min
NH_2
N
Cl
O
I
10
EtOH, 70 °C
2 h, 68%
Cl
N
N
H
3a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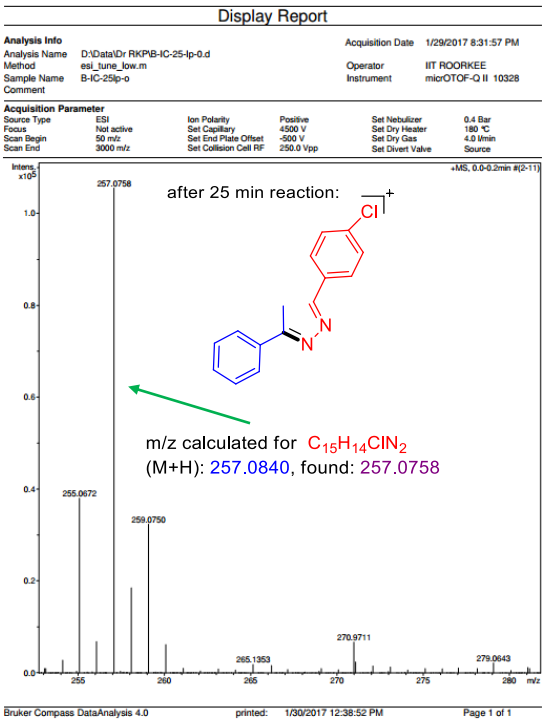
Method esi_tune_wide.m
Sample Name B-IC-25+
Comment
Acquisition Date 1/29/2017 8:15:58 PM
Operator IIT ROORKEE
Instrument micrOTOF-Q II 10328
Acquisition Parameter
Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 3000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 650.0 Vpp
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
after 25 min reaction:
m/z calculated for $C_{15}H_{11}ClIN_2$
(M-H): 380.9656, found: 381.2117
m/z calculated for
$C_{15}H_{16}ClIN_2$
$(M+H)^+$: 387.0119,
found: 387.2536
Bruker Compass DataAnalysis 4.0
printed: 1/30/2017 12:17:54 PM
Page 1 of 1


Display Report
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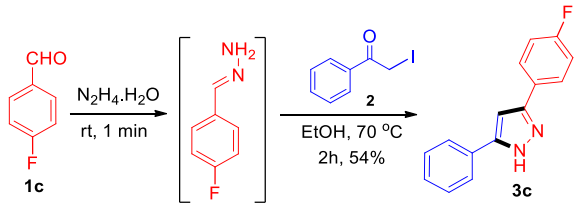
Method esi_tune_low.m
Sample Name B-IC-25lp-o
Comment
Acquisition Date 1/29/2017 8:31:57 PM
Operator IIT ROORKEE
Instrument micrOTOF-Q II 10328
Acquisition Parameter
Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 3000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 250.0 Vpp
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source
after 25 min reaction:
m/z calculated for $C_{15}H_{14}ClN_2$
(M+H): 257.0840, found: 257.0758
Bruker Compass DataAnalysis 4.0
printed: 1/30/2017 12:38:52 PM
Page 1 of 1



Display Report

Analysis Info

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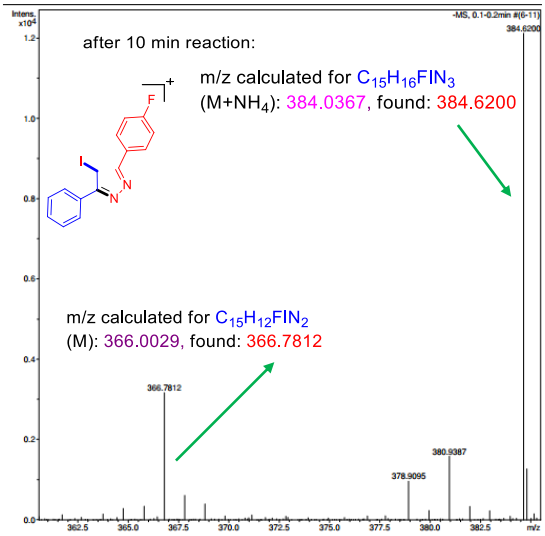
Method	esi_tune_wide.m	Operator	IIT ROORKEE
Sample Name	bfi-1-1-2	Instrument	micrOTOF-Q II 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Source



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Display Report

Analysis Info

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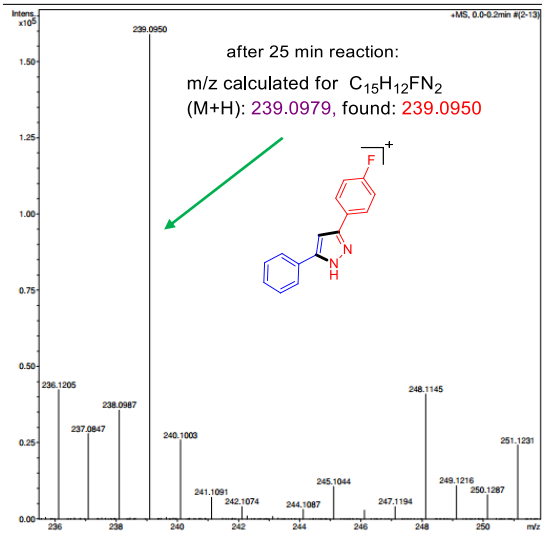
Method	esi_tune_low.m	Operator	IIT ROORKEE
Sample Name	bfi-25uoooj	Instrument	micrOTOF-Q II 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



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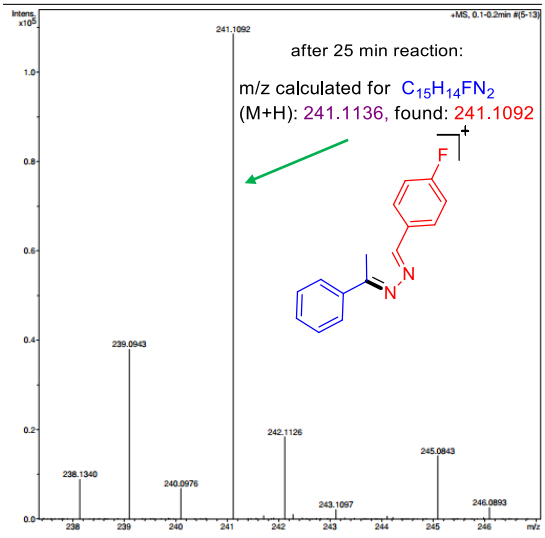
Display Report

Analysis Info

Analysis Name	D:\Data\Dr RKP\bfi-25hyhhh-f.d	Acquisition Date	1/29/2017 9:57:18 PM
Method	esi_tune_low.m	Operator	IIT ROORKEE
Sample Name	bfi-25uoooj-f	Instrument	micrOTOF-Q II 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



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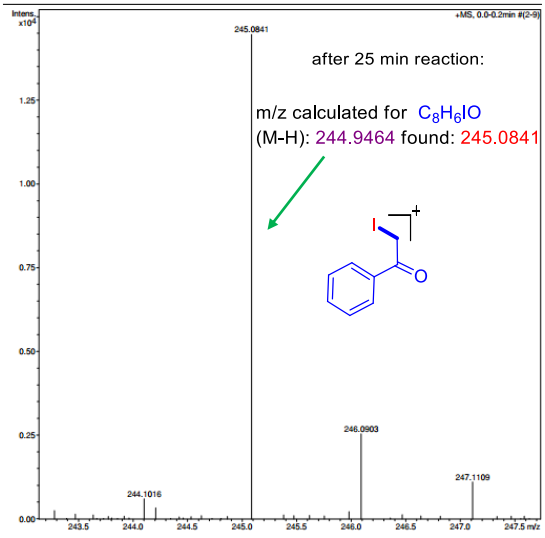
Display Report

Analysis Info

Analysis Name	D:\Data\Dr RKP\bfi-25hyhhh-f.d	Acquisition Date	1/29/2017 9:57:18 PM
Method	esi_tune_low.m	Operator	IIT ROORKEE
Sample Name	bfi-25uoooj-f	Instrument	micrOTOF-Q II 10328
Comment			

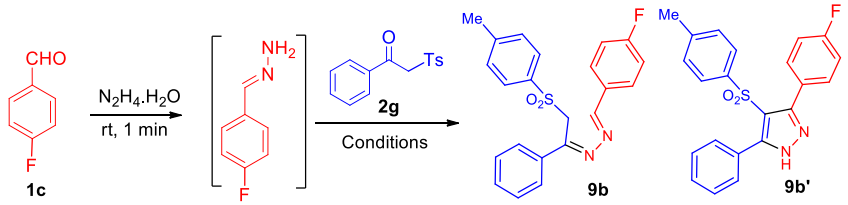
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Bruker Compass DataAnalysis 4.0 printed: 1/30/2017 3:59:36 PM Page 1 of 1

Table S2. Attempted cyclization of heterodienes.



Entry	Conditions	Product **9b** Yield (%)	Product **9b′** Yield (%)
1	I_2/TFA, EtOH, 80 °C, 12 h	52	Not observed
2	I_2/TFA, EtOH, 120 °C, 12 h	54	Not observed
3	$SnCl_4$, EtOH, 80 °C, 12 h	46	Not observed
4	$SnCl_4$, EtOH, 120 °C, 12 h	45	Not observed
5[a]	$FeCl_3$, EtOH, 80 °C, 12 h	0	Not observed
6[a]	$FeCl_3$, EtOH, 120 °C, 12 h	0	Not observed

Conditions: **1c** (0.5 mmol), Hydrazine hydrate (1 mmol), **2g** (0.6 mmol).
[a] Starting materials **1a** and **2g** were recovered as such.

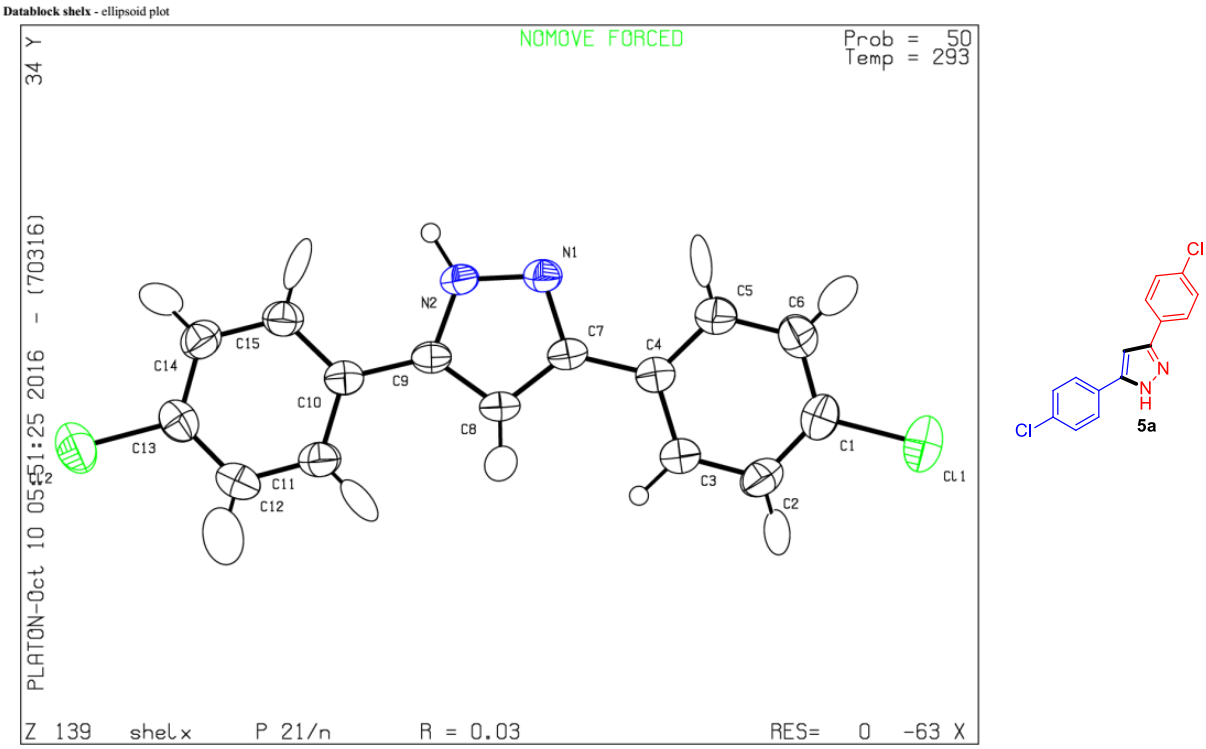
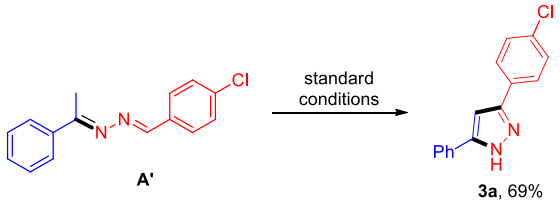
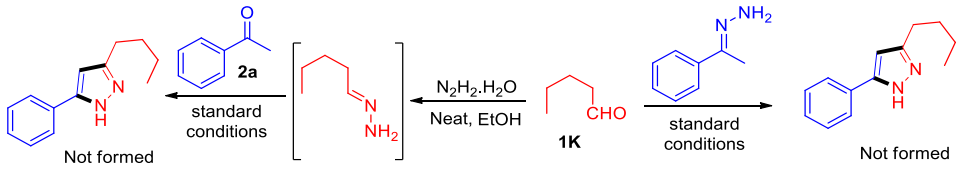


Figure S1. X-Ray crystal structure of the product **5a**.

Scheme S1. Substrate scope of DAN reaction.



Conditions: intermediate **A'** (0.5 mmol), iodine (0.6 mmol), EtOH (3 mL) at 70 °C for 12 h.



Conditions: **1k** (1.0 mmol), **2a** (1.0 mmol) iodine (0.6 mmol), EtOH (3 mL) at 70 °C for 12 h

Computational calculations

Table S3. Calculated electronic energies (in Hartree) for the B3LYP/6-311G** optimized structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction in gas phase.

Pathway	Energy	**R**	**TS**	**P**
	E	–688.76357468	–688.7450556	–688.7694985
1,5-	H	–688.508430	–688.491138	–688.513388
	G	–688.567734	–688.546576	–688.570101
	E	–688.7701048	–688.7371205	–688.737944
1,6-	H	–688.514615	–688.483234	–688.482915
	G	–688.573574	–688.537699	–688.538274
	E	–688.7632717	–688.7207741	–688.7466207
1,7-	H	–688.508123	–688.466286	–688.490507
	G	–688.567709	–688.520559	–688.544822

Table S4. Calculated relative electronic energies (in kcal/mol) for the B3LYP/6-311G** optimized structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction in gas phase.

Pathway	Energy	R	TS	P
	ΔE	0	11.62	–3.72
1,5-	ΔH	0	10.85	–3.11
	ΔG	0	13.28	–1.49
	ΔE	0	20.70	20.18
1,6-	ΔH	0	19.69	19.89
	ΔG	0	22.51	22.15
	ΔE	0	26.67	10.45
1,7-	ΔH	0	26.25	11.05
	ΔG	0	29.59	14.36

Table S5. Calculated electronic energies (in Hartree) for the structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction optimized at B3LYP/6-311G** level of theory using CPCM solvation model, with Ethanol solvent.

Pathway	Energy	**R**	**TS**	**P**
	E	–688.7635747	–688.7450556	–688.7694985
1,5-	H	–688.508430	–688.491138	–688.513388
	G	–688.567734	–688.546576	–688.570101
	E	–688.7701048	–688.7371204	–688.737944
1,6-	H	–688.514615	–688.483234	–688.482915
	G	–688.573574	–688.537700	–688.538274
	E	–688.7632717	–688.7207743	–688.7466207
1,7-	H	–688.508123	–688.466288	–688.490507
	G	–688.567709	–688.520560	–688.544822

Table S6. Calculated electronic energies (in kcal/mol) for the structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction optimized at B3LYP/6-311G** level of theory using CPCM solvation model, with Ethanol solvent.

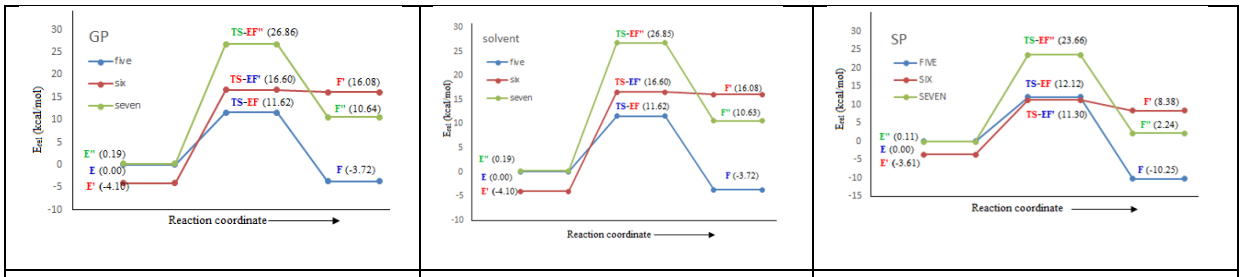
Pathway	Energy	R	TS	P
	ΔE	0	11.62	–3.72
1,5-	ΔH	0	10.85	–3.11
	ΔG	0	13.28	–1.49
	ΔE	0	20.69	20.18
1,6-	ΔH	0	19.69	19.89
	ΔG	0	22.51	22.15
	ΔE	0	26.67	10.45
1,7-	ΔH	0	26.44	11.25
	ΔG	0	29.60	14.37

Table S7. Single point electronic energy, E (in Hartree) for the structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction calculated at M06/6-311+G(d,p)//B3LYP/6-311G** level of theory using CPCM solvation model, with Ethanol solvent

Pathway	Energy	R	TS	P
1,5-	E	–688.2902521	–688.2709314	–688.3065877
1,6-	E	–688.2960064	–688.2722362	–688.2768907
1,7-	E	–688.290431	–688.2525481	–688.2866835

Table S8. Single point electronic energy, E (in kcal/mol) for the structures of 1,5-, 1,6- and 1,7-cyclization pathways for electro-cyclization step of diaza-Nazarov reaction calculated at M06/6-311+G(d,p)//B3LYP/6-311G** level of theory using CPCM solvation model, with Ethanol solvent.

Pathway	Energy	R	TS	P
1,5-	ΔE	0	12.12	–10.25
1,6-	ΔE	0	14.91	11.99
1,7-	ΔE	0	23.77	2.35



(a) Gas phase | (b) Solution phase | (c) Single point energies

Figure S2. A comparative energy profile diagrams for the 1,5-, 1,6- and 1,7-cyclization pathways of electro-cyclization step of diaza-Nazarov reaction for (a) gas phase (optimized at B3LYP/6-311G** level), (b) Solution phase (optimized at B3LYP/6-311G** level using Ethanol solvent with CPCM model) and (c) Single point energies (at M06/6-311+G(d,p)//B3LYP/6-311G** level using Ethanol solvent with CPCM model).

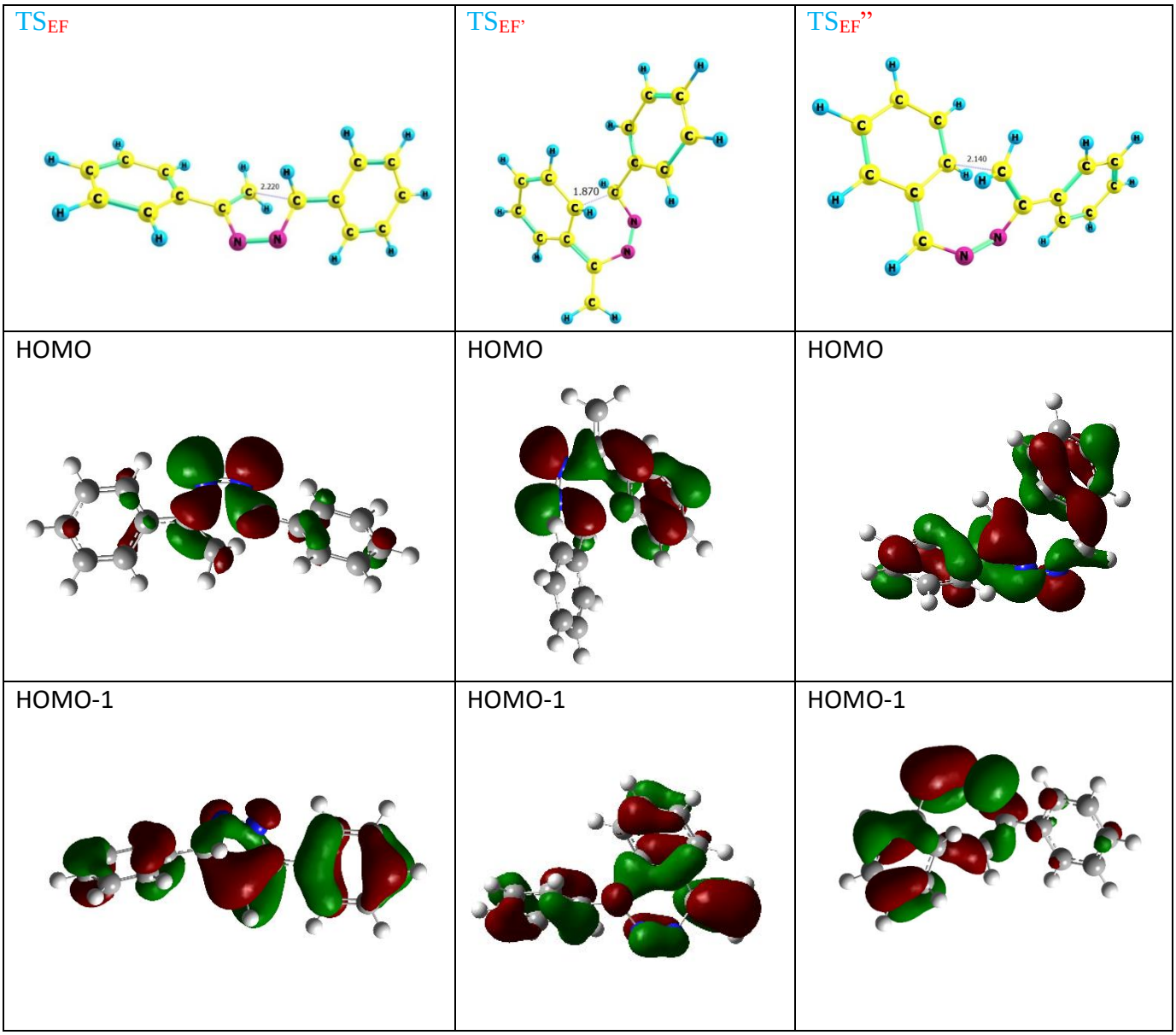
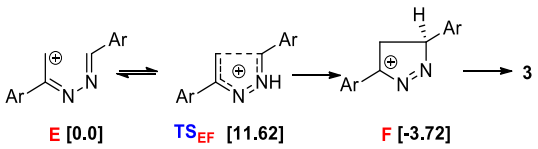


Figure S3. Optimised structures of TSs with HOMO and HOMO-1 molecular diagrams of each TS of the 1,5-, 1,6- and 1,7-cyclization pathways of electrocyclization step of diaza-Nazarov reaction at B3LYP/6-311G** level of theory in gas phase.

Table S9. Cartesian coordinates of B3LYP/6-311G** optimized structures of 1,5-, 1,6- and 1,7-electro-cyclization pathways of electro-cyclization step of Nazarov reaction in gas phase.



E

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6	1.492683000	1.113699000	0.290877000
1	0.411261000	2.671369000	1.258871000
6	2.681876000	0.263654000	0.092479000
6	3.492128000	-0.060118000	1.190302000
6	3.021871000	-0.217982000	-1.180715000
6	4.634754000	-0.829825000	1.011829000
6	4.168175000	-0.986202000	-1.351445000
6	4.976961000	-1.291861000	-0.259043000
1	3.219745000	0.270614000	2.185863000
1	2.402647000	0.019589000	-2.036499000
1	5.253411000	-1.077979000	1.865684000
1	4.430364000	-1.344758000	-2.339402000
1	5.866566000	-1.895121000	-0.394561000
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6	-2.586679000	-0.966879000	0.215197000
6	-4.287170000	0.691688000	-0.344080000
6	-3.585891000	-1.870684000	0.532819000
6	-5.279258000	-0.223372000	-0.021810000
6	-4.930038000	-1.500474000	0.415967000
1	-1.546415000	-1.257048000	0.307692000
1	-4.552612000	1.685183000	-0.687565000
1	-3.325656000	-2.865162000	0.873180000
1	-6.321401000	0.056345000	-0.111592000
1	-5.706004000	-2.213157000	0.668636000
7	0.462904000	0.861022000	-0.676388000
7	-0.681684000	1.165296000	-0.485837000
1	-2.258418000	2.280445000	-0.978539000
1	2.139313000	2.383031000	1.849080000

TS$_{EF}$

6	-0.210895000	0.694356000	-0.927639000
6	1.172753000	-0.294893000	0.501336000
6	-1.155794000	-0.227086000	-0.477394000
1	0.563292000	0.380923000	-1.615495000
6	-2.557123000	-0.006542000	-0.220394000
6	-3.206177000	1.157327000	-0.690454000
6	-3.298104000	-0.961533000	0.513276000
6	-4.544374000	1.369438000	-0.409323000
6	-4.638203000	-0.741774000	0.784301000
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1	-6.311095000	0.588529000	0.539068000
6	2.573895000	-0.058937000	0.303250000
6	3.328976000	-0.839786000	-0.599631000
6	3.199097000	0.985130000	1.017680000
6	4.675657000	-0.576414000	-0.775684000
6	4.546673000	1.245825000	0.827936000
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1	2.622922000	1.580829000	1.717389000
1	5.261546000	-1.180906000	-1.456839000
1	5.028533000	2.044663000	1.377528000
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1	-0.421886000	1.756964000	-0.918302000

F

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6	1.153756000	-0.350475000	0.982287000
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1	0.232535000	1.342925000	-0.053284000
6	-2.436561000	-0.016743000	0.039907000
6	-2.983532000	1.292225000	0.201651000
6	-3.282595000	-1.083760000	-0.399453000
6	-4.314346000	1.517271000	-0.063099000
6	-4.614825000	-0.839439000	-0.657628000
6	-5.128437000	0.453060000	-0.491159000
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1	-6.176532000	0.639449000	-0.697609000
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6	2.889182000	1.290430000	0.124791000
6	4.608486000	-0.780383000	-0.582178000
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6	4.994834000	0.542134000	-0.787699000
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1	4.434017000	2.608322000	-0.569607000
1	5.962383000	0.765578000	-1.220696000

7	-0.577891000	-1.578876000	0.134266000
7	0.629678000	-1.636196000	0.475847000
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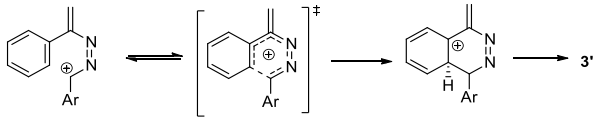

E' [-4.1] $TS_{EF'}$ [16.6] F' [16.08]

E′

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6	2.317521000	0.217013000	0.544808000
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1	5.489600000	-1.071800000	-1.247508000
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6	-1.578446000	-0.833816000	-0.711852000
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6	-2.035282000	-2.146292000	-0.656012000
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1	-1.444681000	-2.940369000	-1.096695000
1	-3.608995000	-3.460584000	-0.006562000
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1	-2.203915000	3.656530000	-0.675446000
1	-3.593209000	2.505533000	-1.140403000
1	-0.643746000	-0.618277000	-1.218254000
1	1.121553000	0.577208000	2.357466000

$TS_{EF'}$

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6	-2.432593000	0.889029000	0.825035000
6	-2.216635000	-1.125008000	-0.507134000
6	-3.772524000	0.983514000	0.463159000
6	-3.554400000	-1.026759000	-0.864180000
6	-4.332604000	0.028529000	-0.382903000
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1	-1.626090000	-1.960534000	-0.866860000
1	-4.379170000	1.794329000	0.847379000
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6	0.828438000	0.413454000	-0.660635000
6	2.807082000	2.237057000	0.144031000
6	0.594343000	1.832481000	-0.718536000
6	1.558731000	2.716324000	-0.299131000
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1	3.234301000	-3.343009000	-0.272613000
1	4.057520000	-1.946294000	-1.193463000
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1	0.016930000	0.403823000	1.592758000

F′

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6	2.826940000	2.250564000	0.060683000
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6	1.546289000	2.717635000	-0.309424000
1	4.101965000	0.561171000	0.457936000
1	3.603888000	2.970908000	0.292048000
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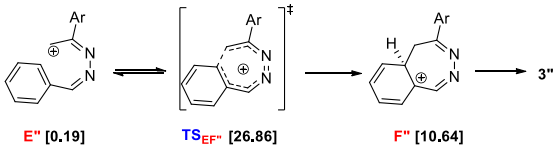

E″

6	0.999620000	-1.576083000	1.196294000
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6	2.802681000	-0.156958000	0.125295000
6	3.887893000	-0.999424000	0.407910000
6	3.045455000	1.149955000	-0.323927000
6	5.188879000	-0.533505000	0.269097000
6	4.350742000	1.609770000	-0.459136000
6	5.423438000	0.772660000	-0.161259000
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1	2.218350000	1.809197000	-0.554995000
1	6.020864000	-1.192660000	0.485031000
1	4.529310000	2.623139000	-0.797548000
1	6.439410000	1.131714000	-0.273367000
6	-3.001058000	-0.155578000	-0.466275000
6	-2.949069000	0.645951000	0.689836000
6	-4.242156000	-0.539533000	-1.005528000
6	-4.127460000	1.057717000	1.288481000
6	-5.416441000	-0.121499000	-0.395125000
6	-5.359808000	0.673979000	0.748651000
1	-1.996243000	0.948233000	1.109350000
1	-4.280626000	-1.155646000	-1.896792000
1	-4.094192000	1.678161000	2.175366000
1	-6.373297000	-0.412910000	-0.809747000
1	-6.277641000	0.999185000	1.223684000
7	0.472277000	0.023754000	-0.517334000
7	-0.614062000	-0.427839000	-0.748748000
1	-1.895364000	-1.164937000	-2.083582000
1	1.685285000	-2.017068000	1.906650000

TS$_{EF"}$

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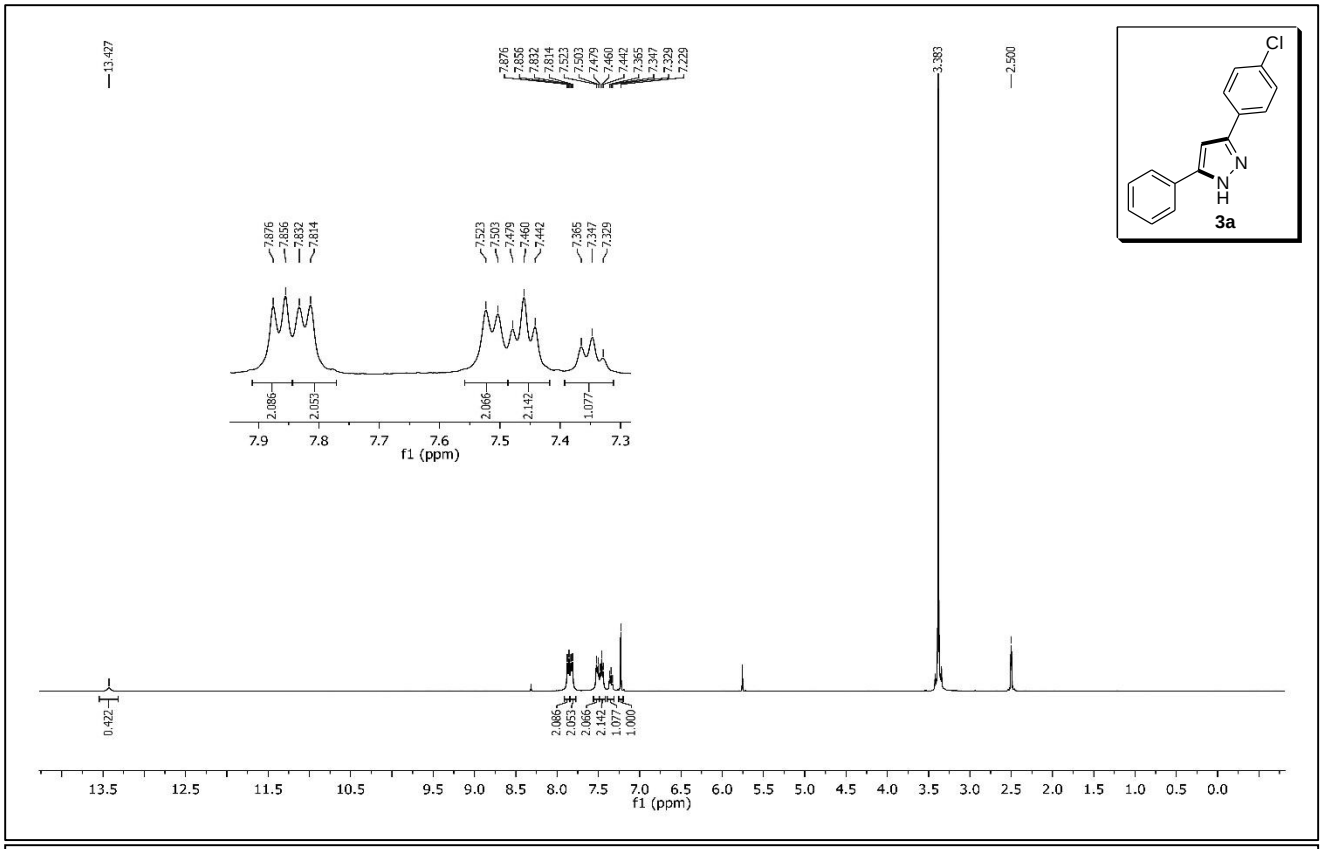
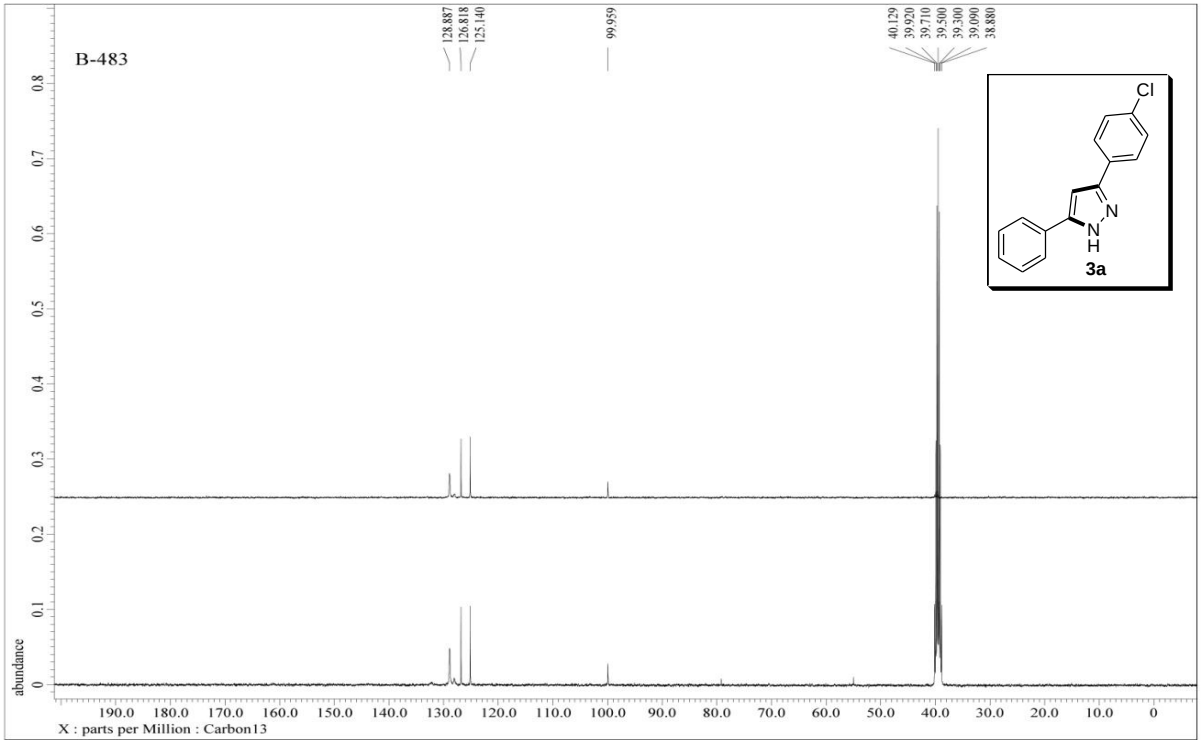
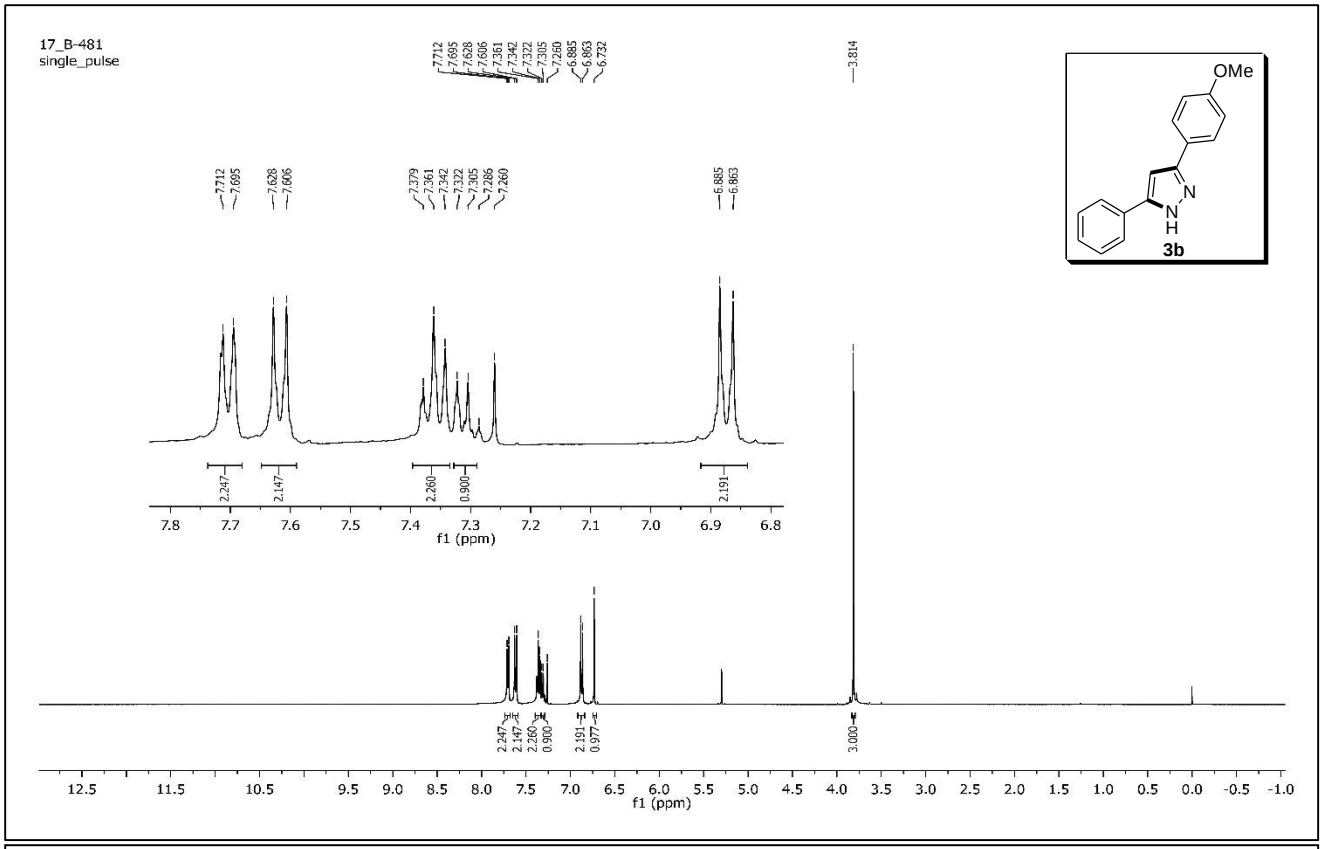
1	1.063489000	0.041441000	1.734906000
6	-2.070508000	0.110659000	0.233413000
6	-2.606288000	-1.041783000	0.830216000
6	-2.875102000	0.872002000	-0.631286000
6	-3.910157000	-1.435516000	0.551453000
6	-4.174125000	0.472298000	-0.907274000
6	-4.694098000	-0.683440000	-0.320225000
1	-2.022863000	-1.622691000	1.535404000
1	-2.475708000	1.772561000	-1.081439000
1	-4.316743000	-2.321962000	1.022606000
1	-4.786616000	1.062416000	-1.578026000
1	-5.711247000	-0.988887000	-0.534479000
6	2.522327000	0.675039000	-0.267363000
6	1.631832000	-0.396339000	-0.658975000
6	3.832714000	0.352268000	0.112939000
6	2.153781000	-1.724109000	-0.749463000
6	4.288083000	-0.957514000	0.050781000
6	3.442452000	-2.005377000	-0.366055000
1	0.792129000	-0.168080000	-1.298533000
1	4.501081000	1.138635000	0.443755000
1	1.507138000	-2.508650000	-1.125123000
1	5.317708000	-1.174087000	0.311043000
1	3.824401000	-3.017271000	-0.418893000
7	-0.248949000	1.671343000	0.028212000
7	0.831648000	2.276334000	0.341359000
1	2.783530000	2.780551000	0.306220000
1	0.111664000	-1.392412000	1.105273000

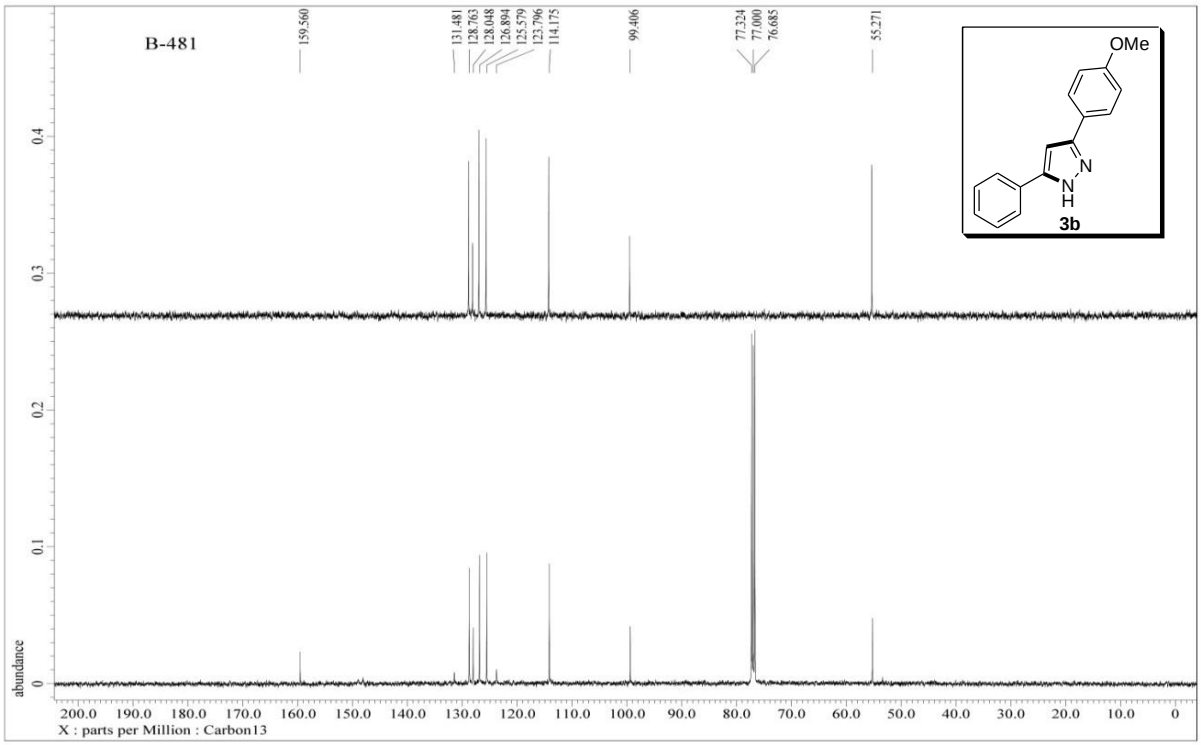
F″

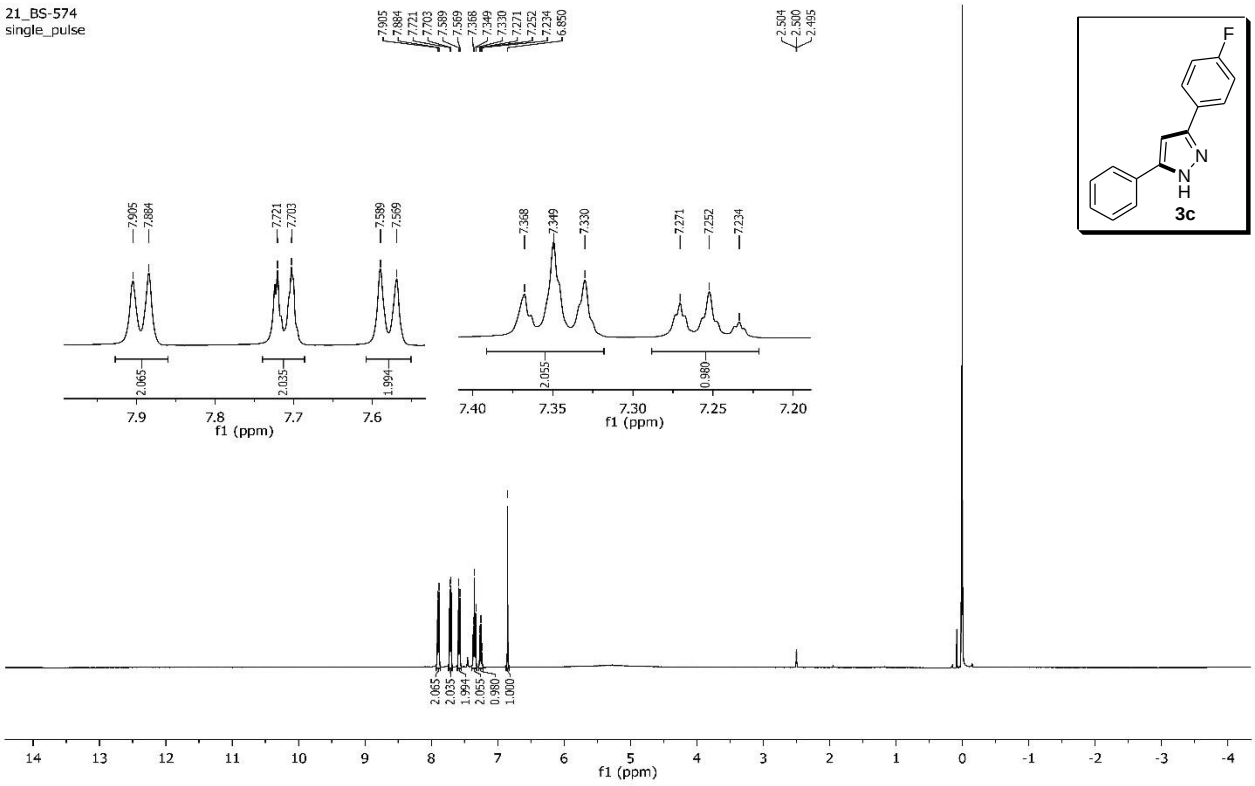
6	0.402692000	-0.294518000	1.109497000
6	1.927279000	2.006996000	-0.035670000
6	-0.674673000	0.564695000	0.481699000
1	0.823207000	0.208544000	1.984551000
6	-2.020962000	0.082274000	0.184753000
6	-2.360995000	-1.281371000	0.269859000
6	-3.009392000	1.005190000	-0.219927000
6	-3.639636000	-1.709120000	-0.060555000
6	-4.281984000	0.570583000	-0.550730000
6	-4.601767000	-0.786610000	-0.471921000
1	-1.632650000	-2.020951000	0.577355000
1	-2.763779000	2.058981000	-0.244389000
1	-3.888721000	-2.761228000	0.003120000
1	-5.034275000	1.288731000	-0.853105000
1	-5.601705000	-1.122911000	-0.718993000
6	2.377491000	0.669861000	-0.213697000
6	1.509104000	-0.528172000	0.046089000
6	3.732866000	0.465861000	-0.533519000
6	2.232252000	-1.829889000	0.157159000
6	4.289548000	-0.796292000	-0.523833000
6	3.541597000	-1.955808000	-0.158029000
1	0.972736000	-0.664304000	-0.922951000
1	4.353353000	1.324059000	-0.763150000
1	1.643011000	-2.697055000	0.435180000
1	5.336693000	-0.911026000	-0.782298000
1	4.034190000	-2.919097000	-0.118297000
7	-0.371385000	1.778050000	0.138700000
7	0.732062000	2.447684000	0.308457000
1	2.686627000	2.782685000	-0.059887000
1	0.006064000	-1.248643000	1.445723000

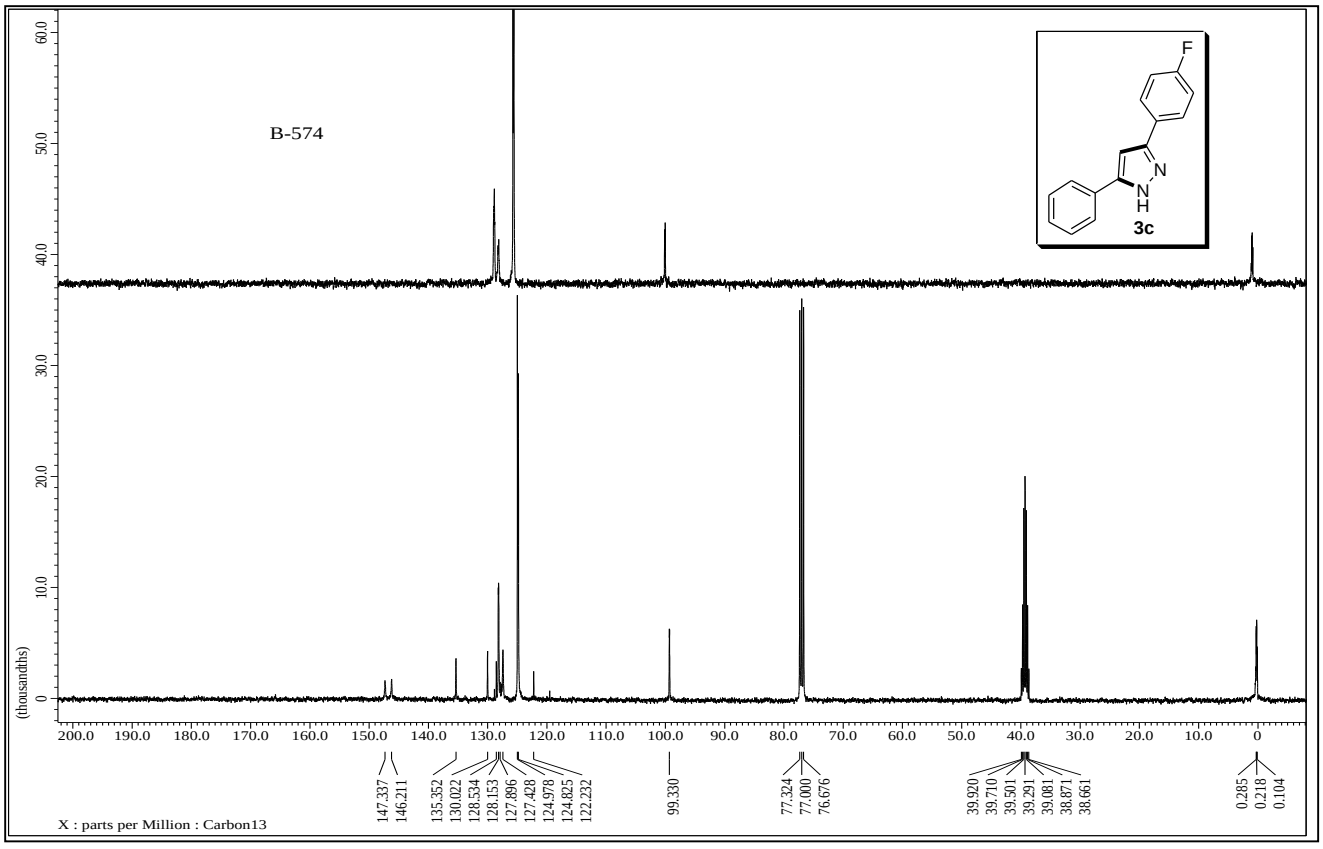

13.427
7.876
7.856
7.832
7.814
7.523
7.503
7.479
7.460
7.442
7.365
7.347
7.329
7.229
3.383
2.500
Cl
N
N
H
3a
2.086
2.053
2.066
2.142
1.077
1.000
0.422
f1 (ppm)

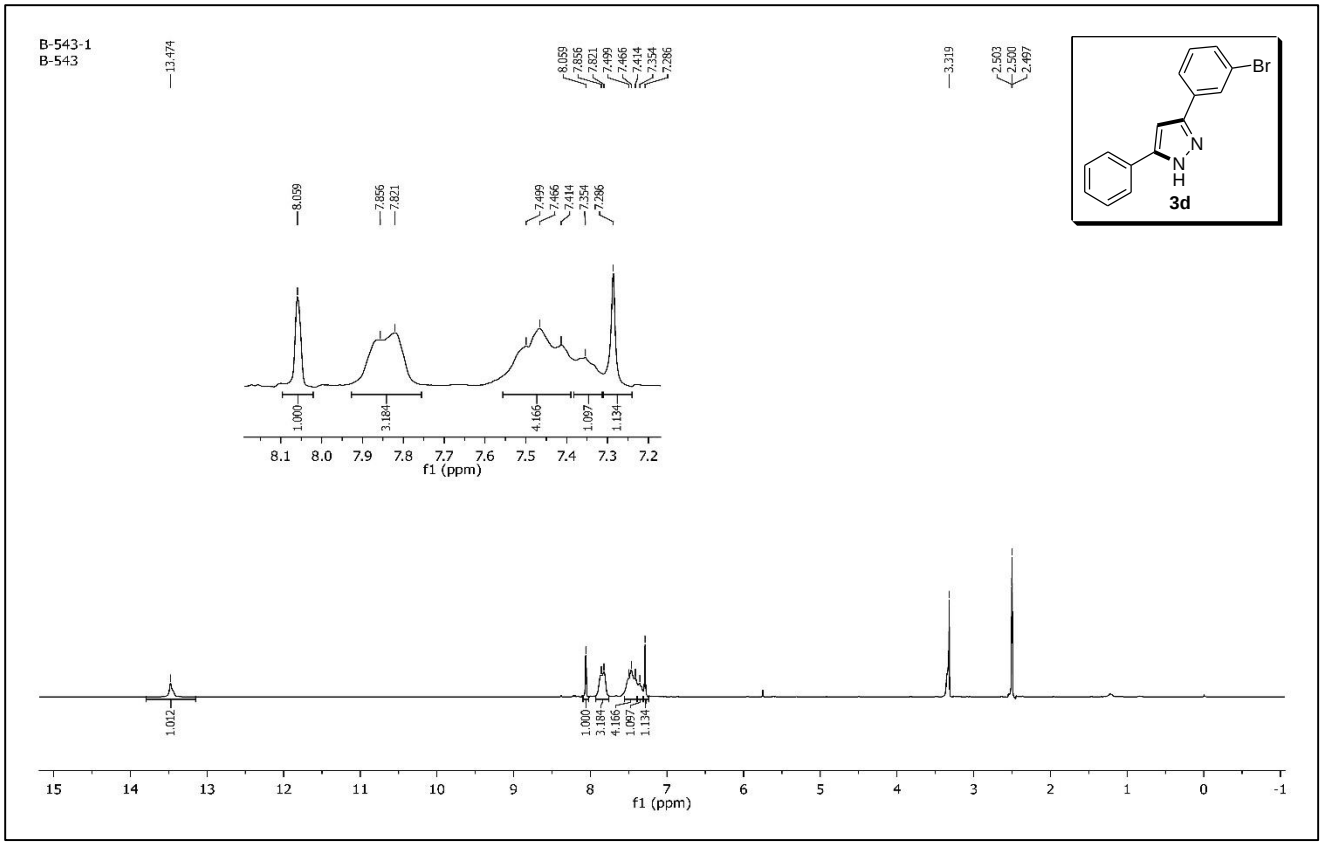

B-483
128.887
126.818
125.140
99.959
40.129
39.920
39.710
39.500
39.300
39.090
38.880
Cl
N
N
H
3a
abundance
X : parts per Million : Carbon13

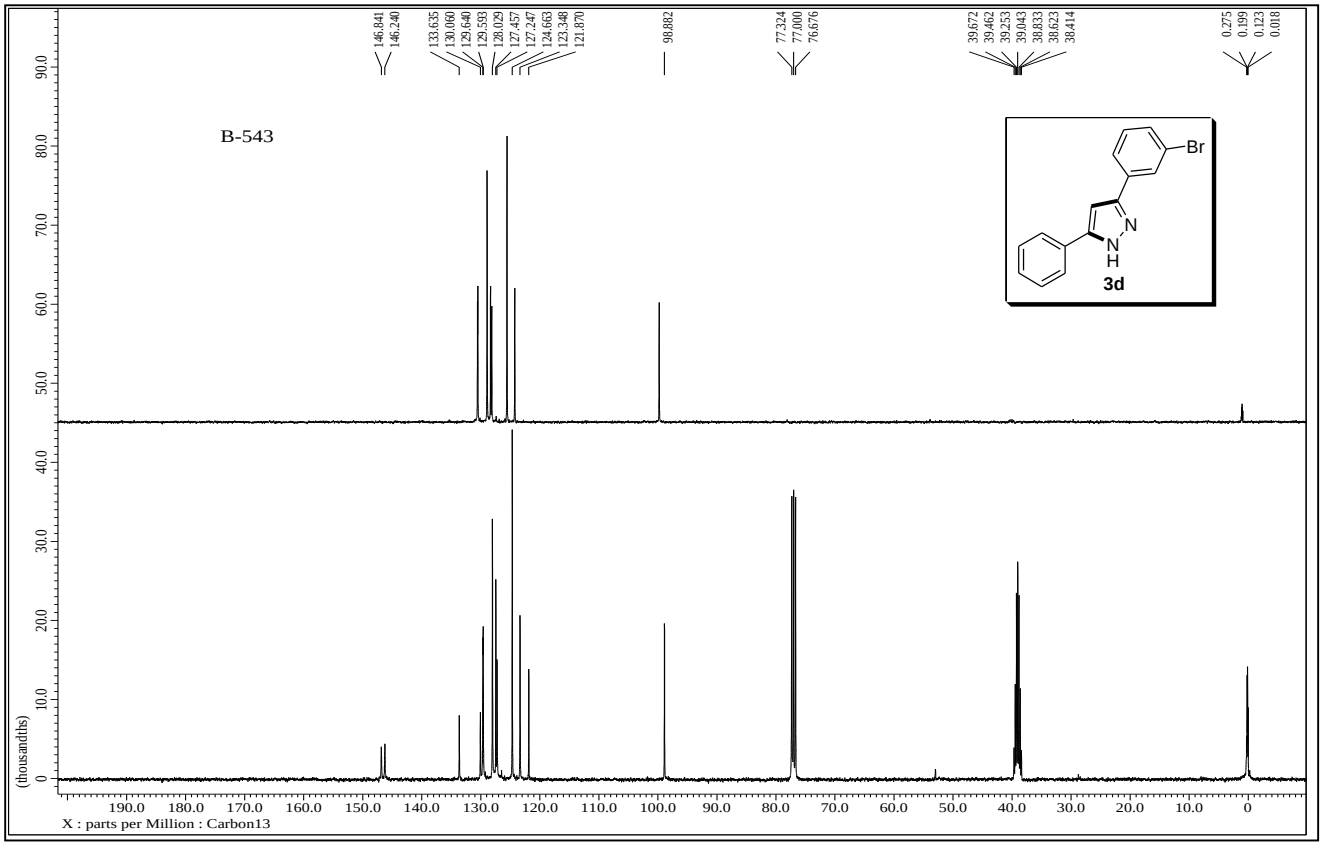

17_B-481
single_pulse
7.712
7.695
7.628
7.606
7.379
7.361
7.342
7.322
7.305
7.286
7.260
6.885
6.863
6.732
3.814
OMe
N
N
H
3b
2.247
2.147
2.260
0.900
2.191
3.000
f1 (ppm)

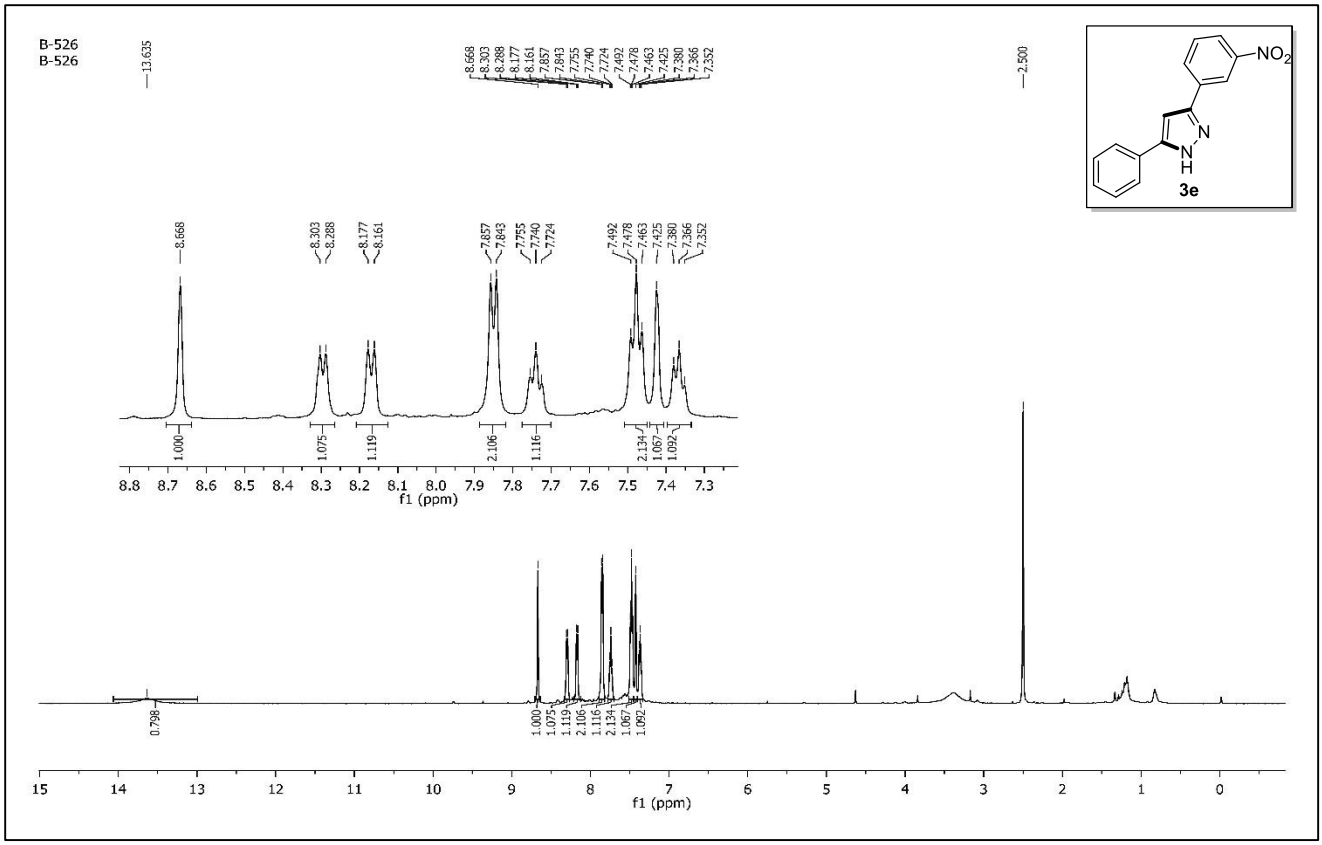

B-481
159.560
131.481
128.763
128.048
126.894
125.579
123.796
114.175
99.406
77.324
77.000
76.685
55.271
OMe
N
N
H
3b
abundance
X : parts per Million : Carbon13

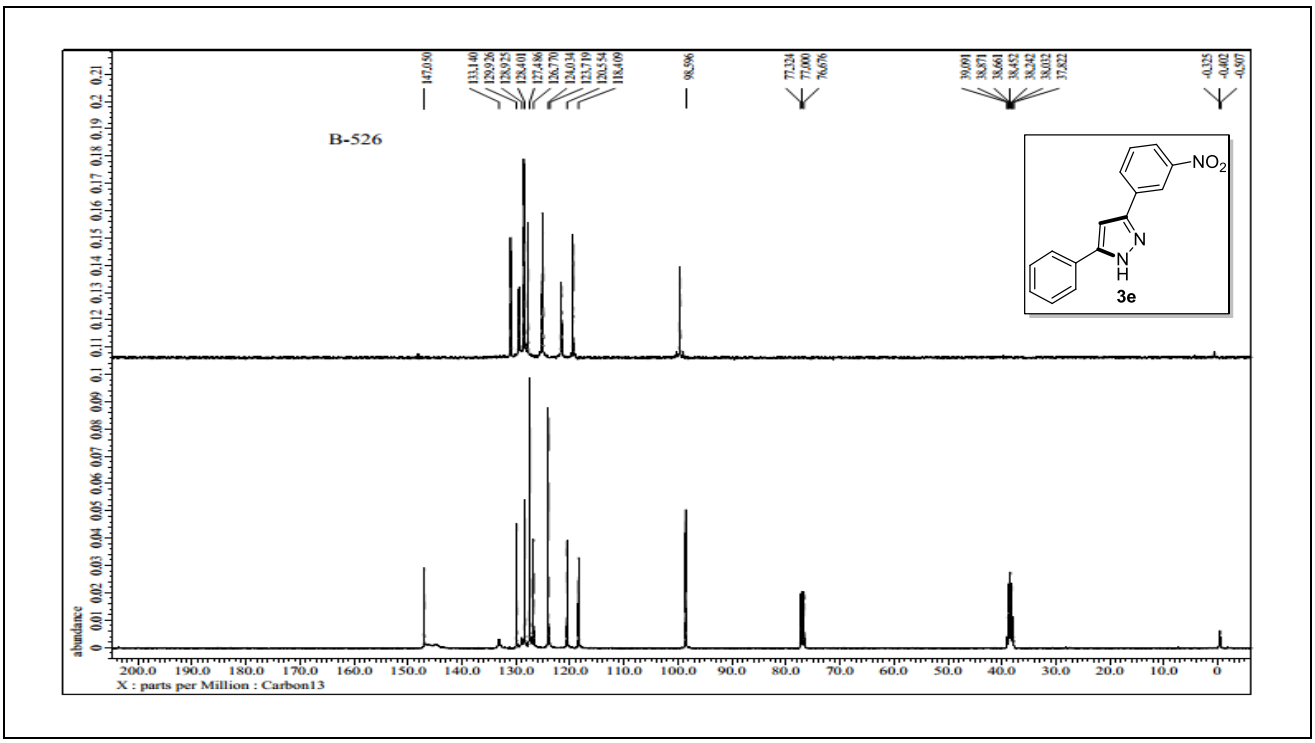

21_BS-574
single_pulse
7.905
7.884
7.721
7.703
7.589
7.569
7.368
7.349
7.330
7.271
7.252
7.234
6.850
2.504
2.500
2.495
2.065
2.035
1.994
2.055
0.980
1.000
f1 (ppm)
F
N
N
H
3c

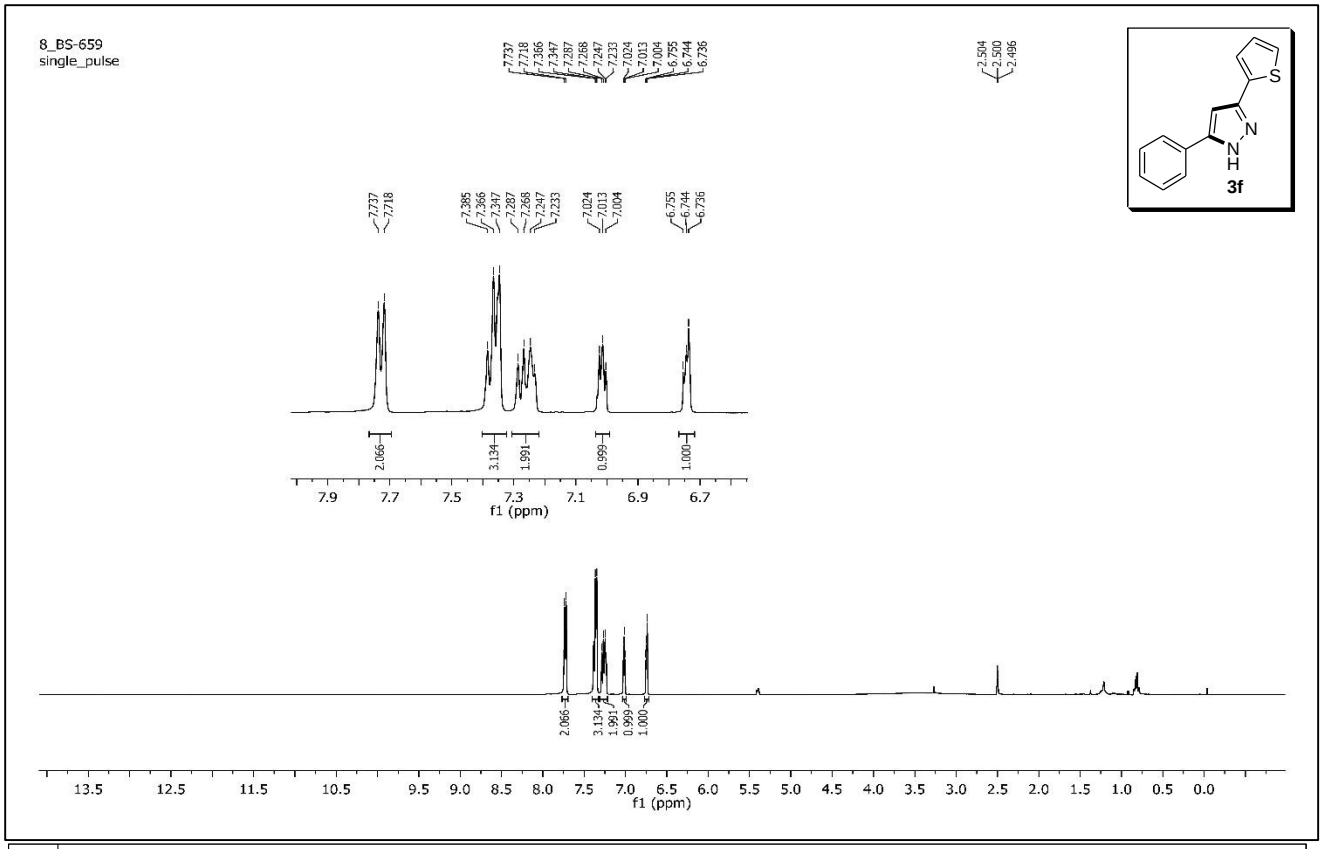

B-574
F
N
N
H
3c
(thousandths)
X : parts per Million : Carbon13
147.337
146.211
135.352
130.022
128.534
128.153
127.896
127.428
124.978
124.825
122.232
99.330
77.324
77.000
76.676
39.920
39.710
39.501
39.291
39.081
38.871
38.661
0.285
0.218
0.104

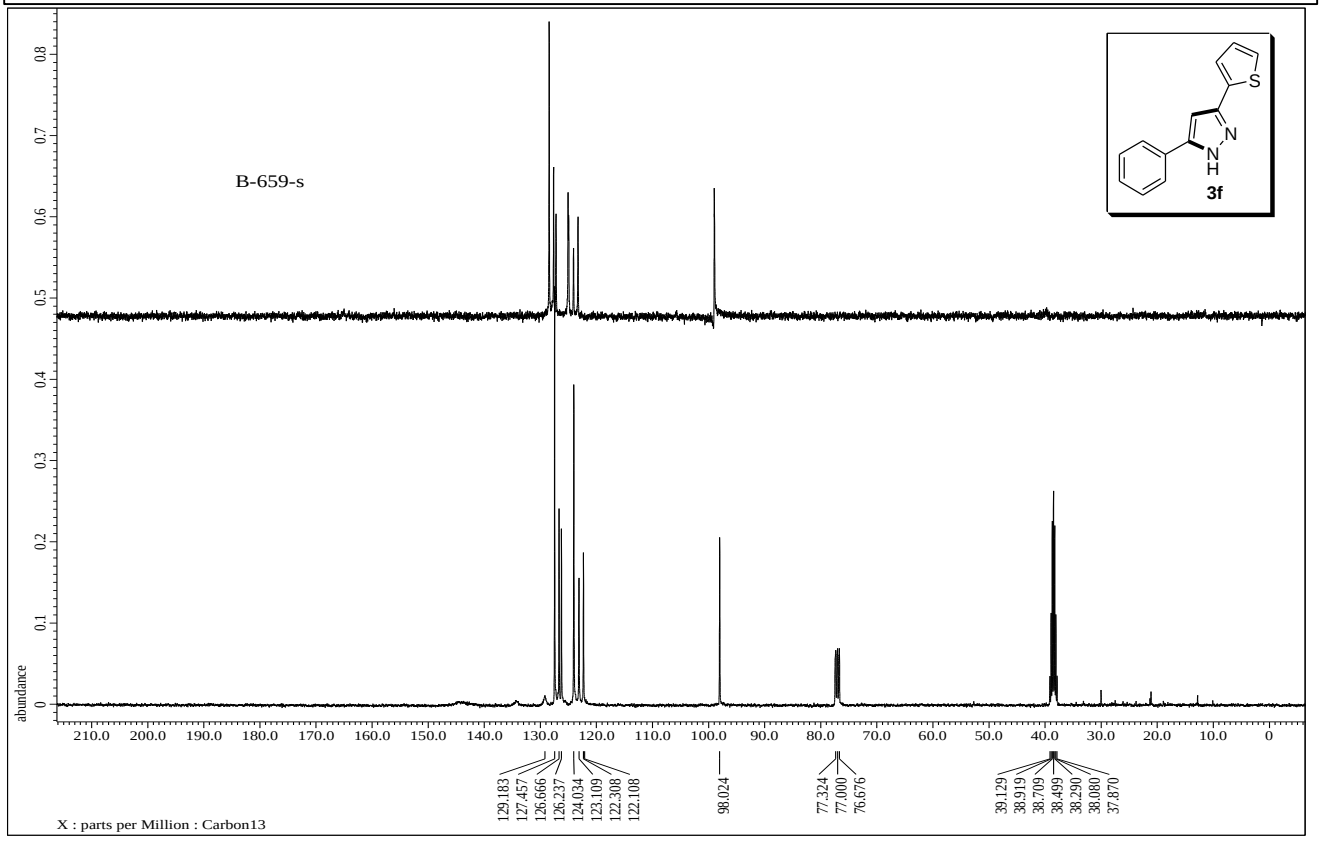

B-543-1
B-543
13.474
8.059
7.856
7.821
7.499
7.466
7.414
7.354
7.286
3.319
2.503
2.500
2.497
Br
N
N
H
3d
1.000
3.184
4.166
1.097
1.134
1.012
f1 (ppm)

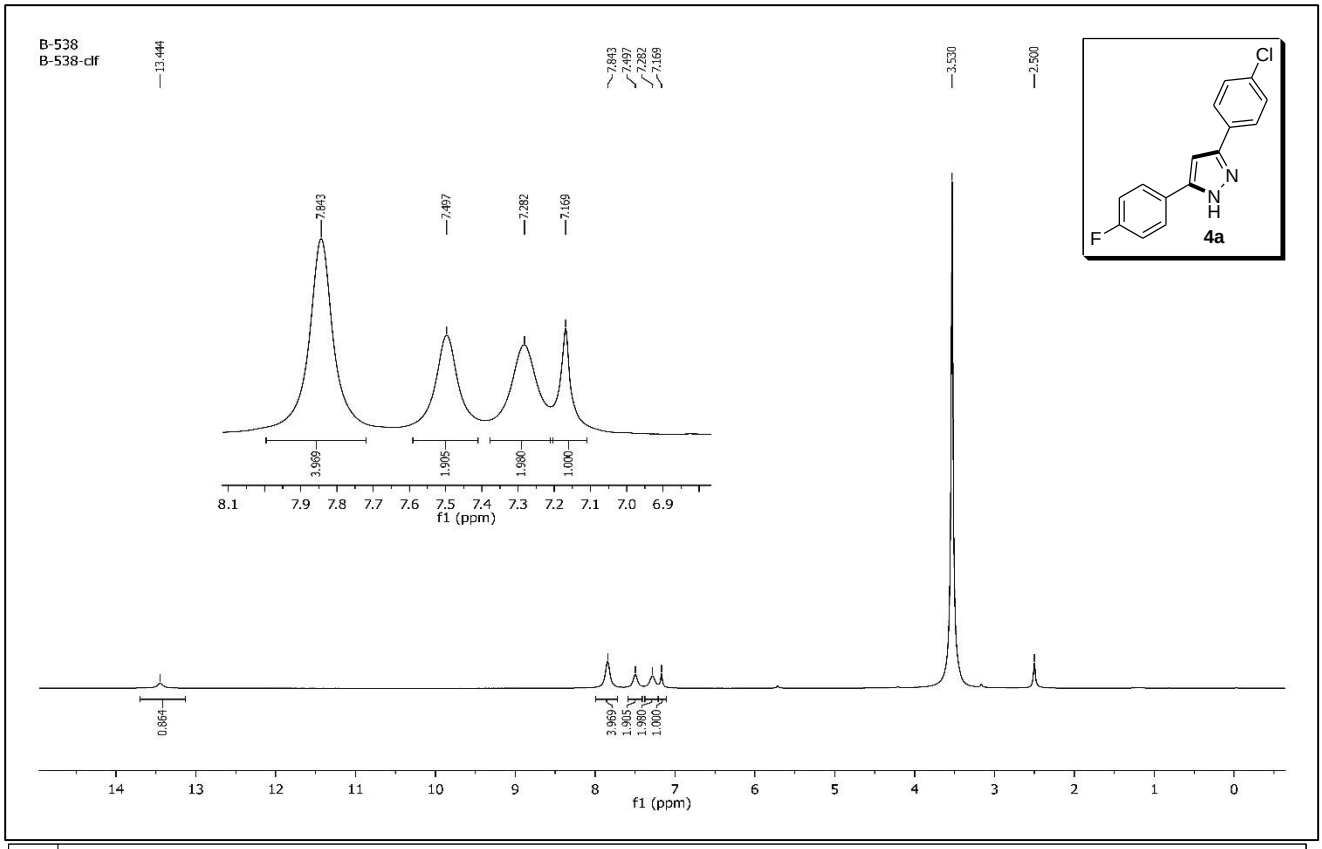

B-543
146.841
146.240
133.635
130.060
129.640
129.593
128.029
127.457
127.247
124.663
123.348
121.870
98.882
77.324
77.000
76.676
39.672
39.462
39.253
39.043
38.833
38.623
38.414
0.275
0.199
0.123
0.018
Br
N
N
H
3d
(thousandths)
X : parts per Million : Carbon13

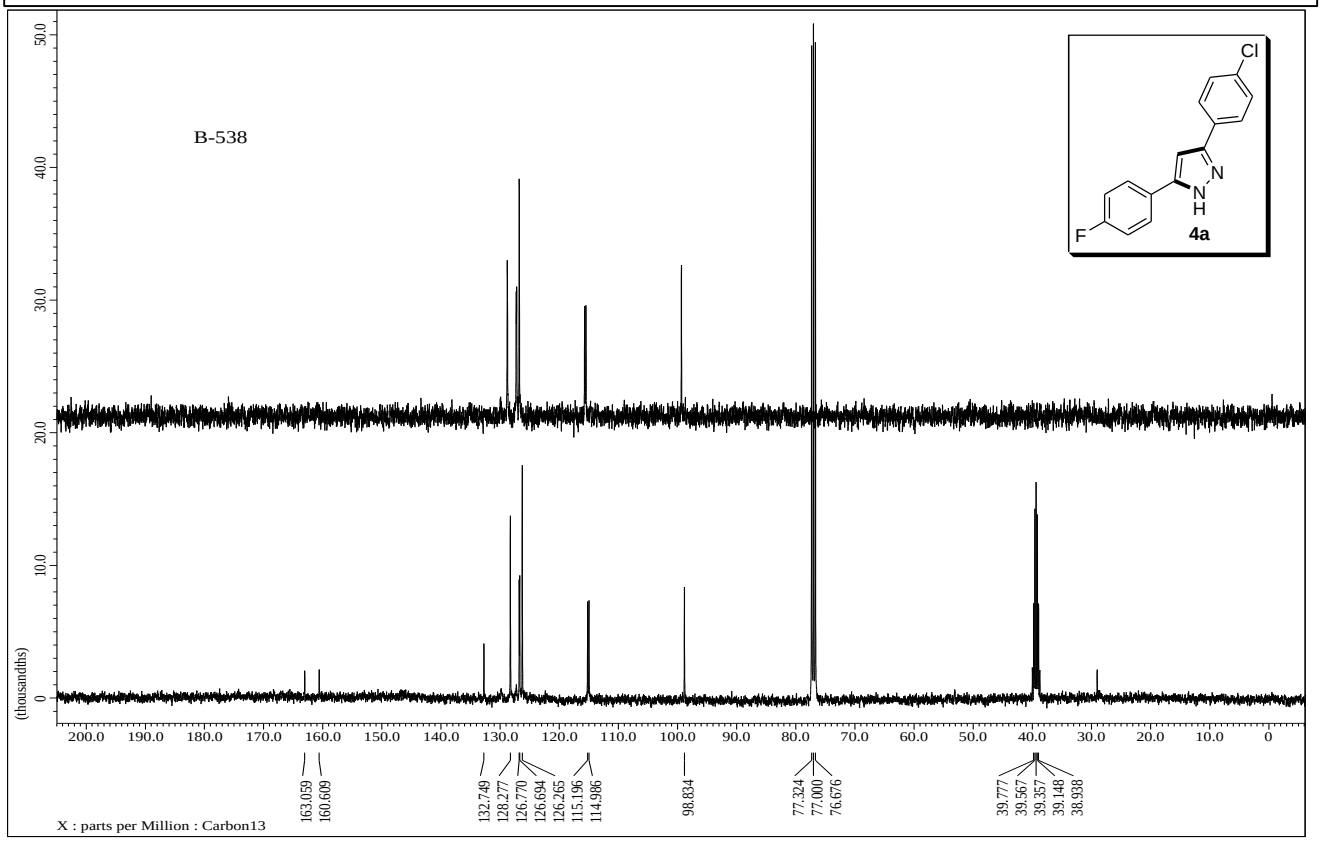

B-526
B-526
13.635
8.668
8.303
8.288
8.177
8.161
7.857
7.843
7.755
7.740
7.724
7.492
7.478
7.463
7.425
7.380
7.366
7.352
2.500
NO2
N
N
H
3e
1.000
1.075
1.119
2.106
1.116
2.134
1.067
1.092
f1 (ppm)
0.798

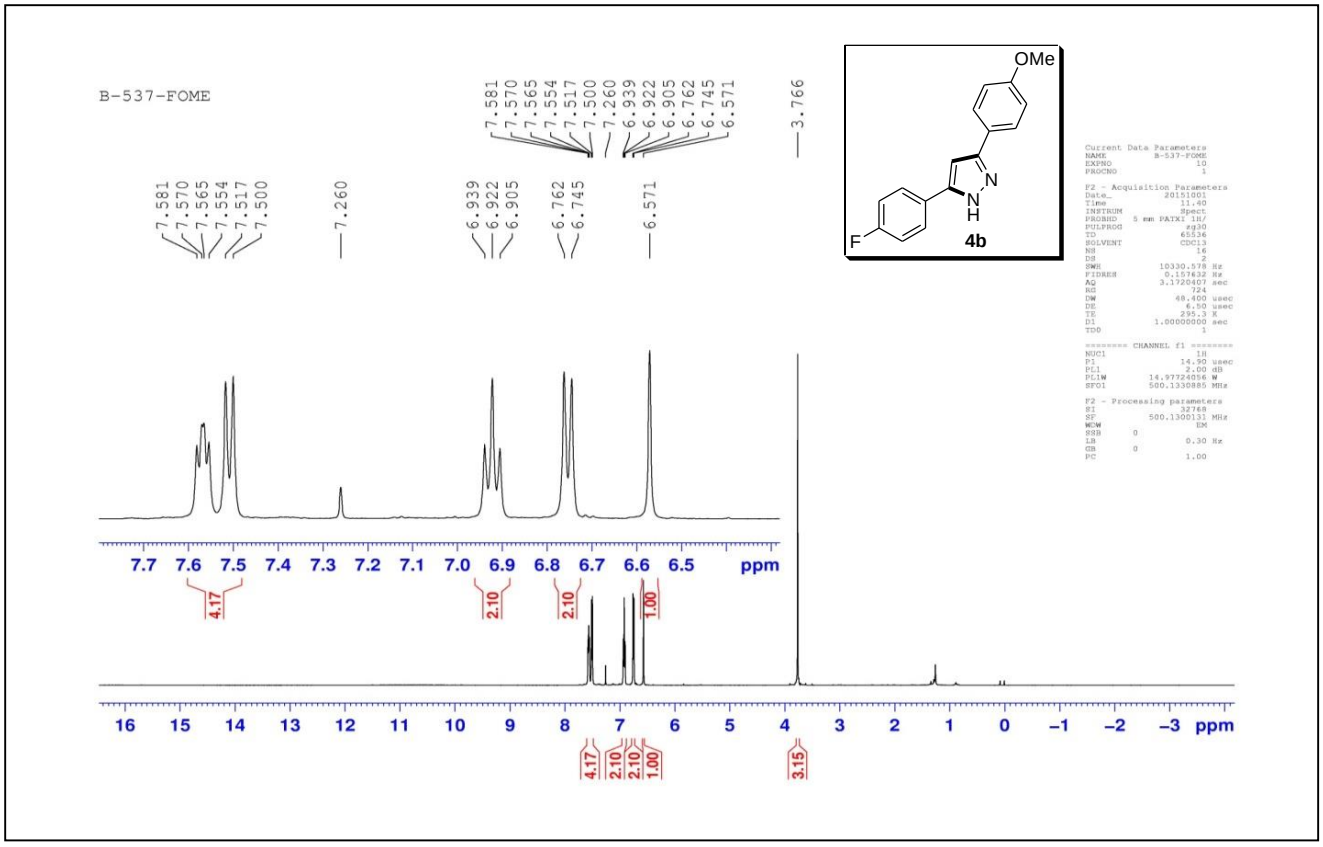

147.050
133.140
129.926
129.925
128.401
127.486
126.770
124.034
123.719
120.554
118.409
90.596
77.324
77.000
76.676
39.091
38.871
38.661
38.452
38.242
38.032
37.822
-0.325
-0.402
-0.507
B-526
NO2
N
N
H
3e
abundance
X : parts per Million : Carbon13

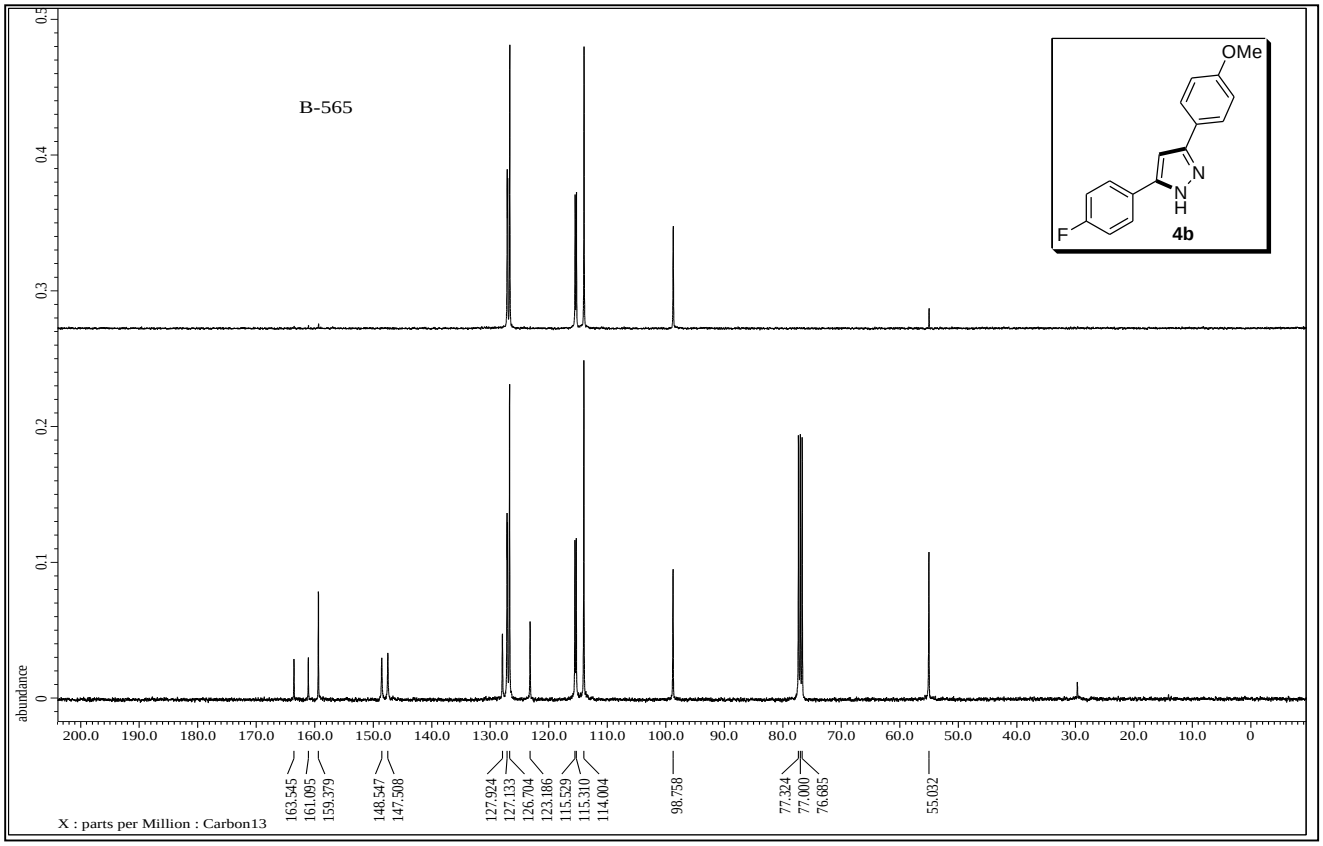

8_BS-659
single_pulse
3f
f1 (ppm)

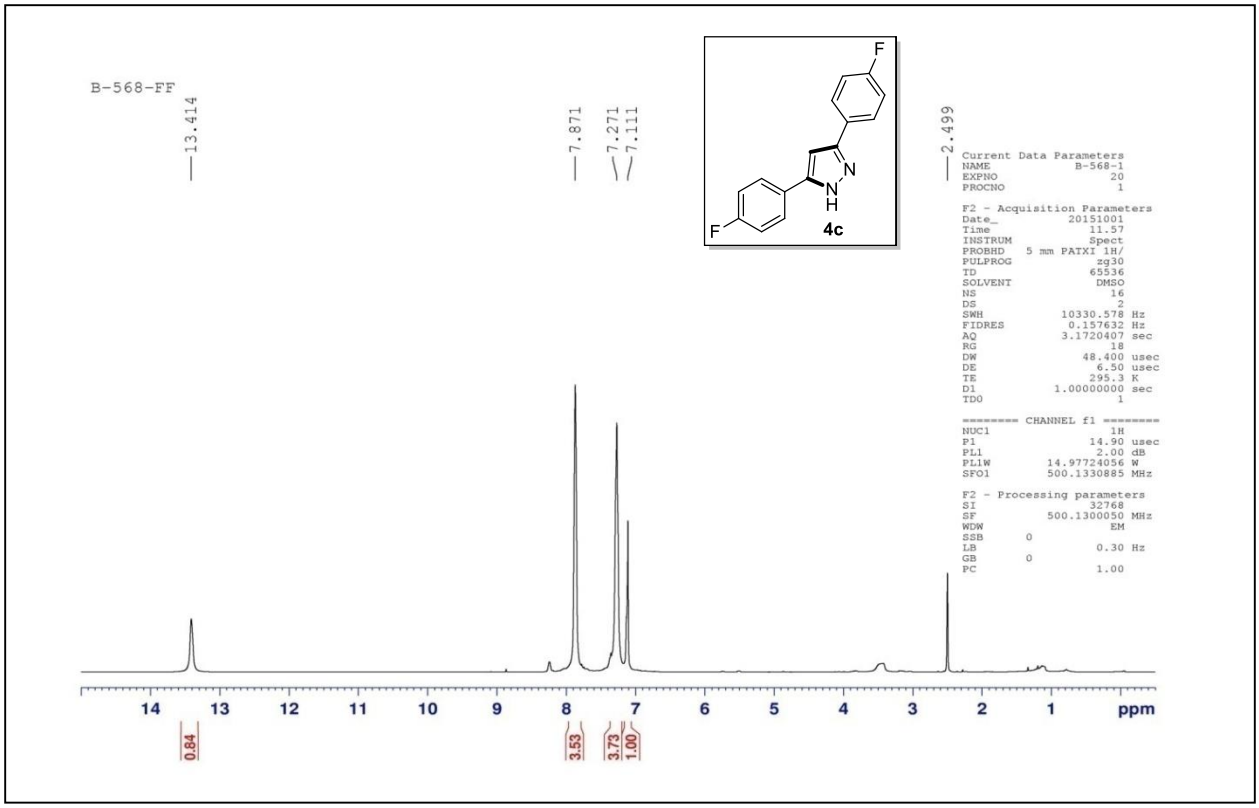

B-659-s
3f
abundance
X : parts per Million : Carbon13

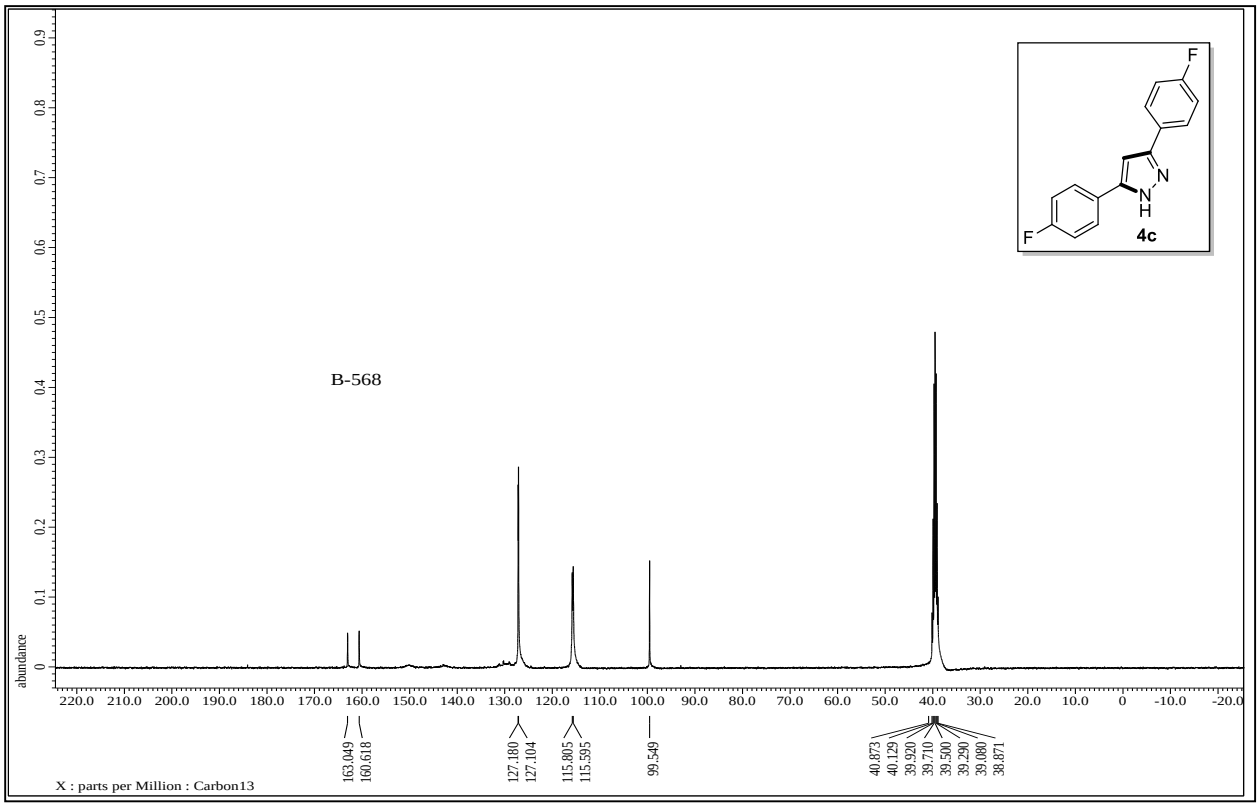

B-538
B-538-dif
13.444
7.843
7.497
7.282
7.169
3.530
2.500
3.969
1.905
1.980
1.000
0.864
f1 (ppm)
Cl
N
N
H
F
4a

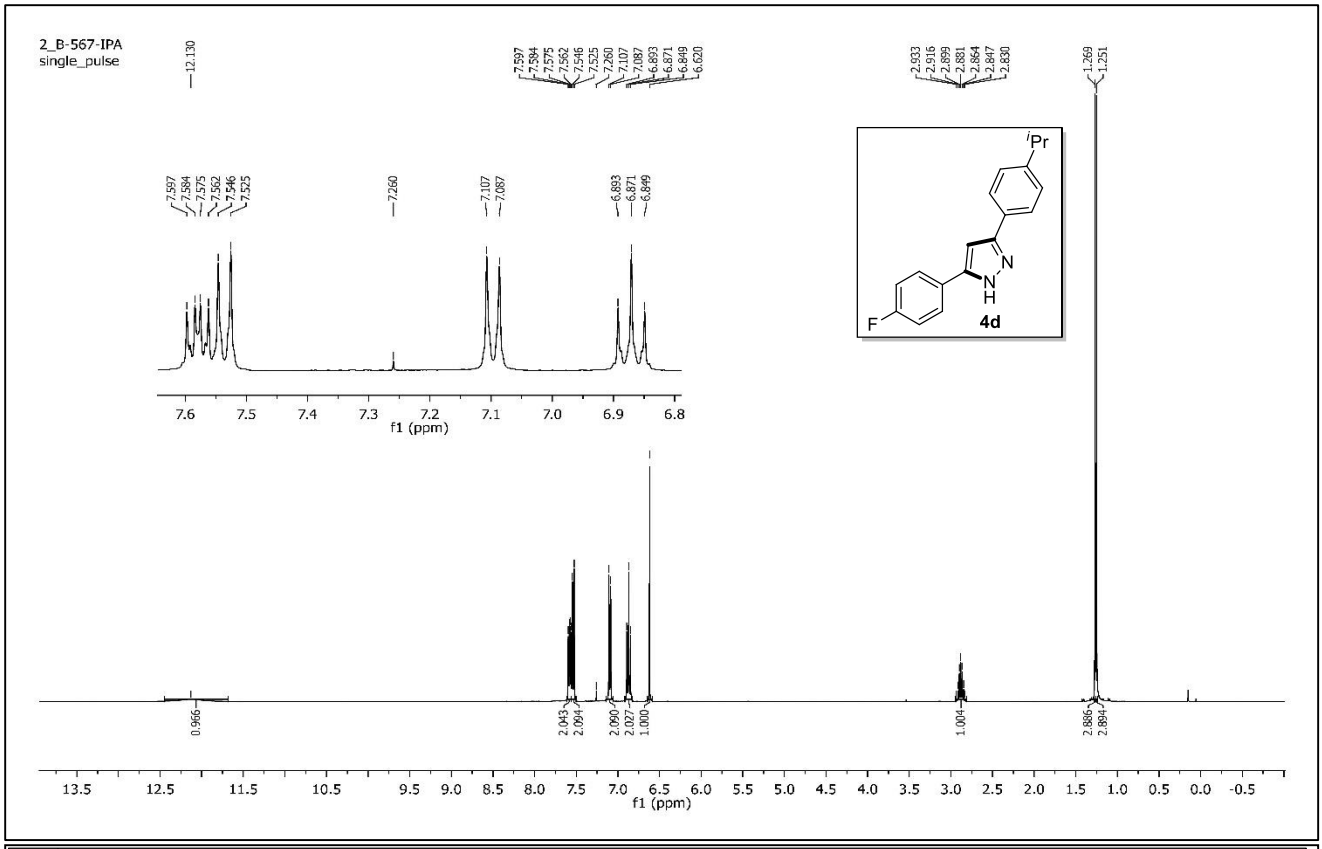

B-538
(thousandths)
163.059
160.609
132.749
128.277
126.770
126.694
126.265
115.196
114.986
98.834
77.324
77.000
76.676
39.777
39.567
39.357
39.148
38.938
X : parts per Million : Carbon13
Cl
N
N
H
F
4a

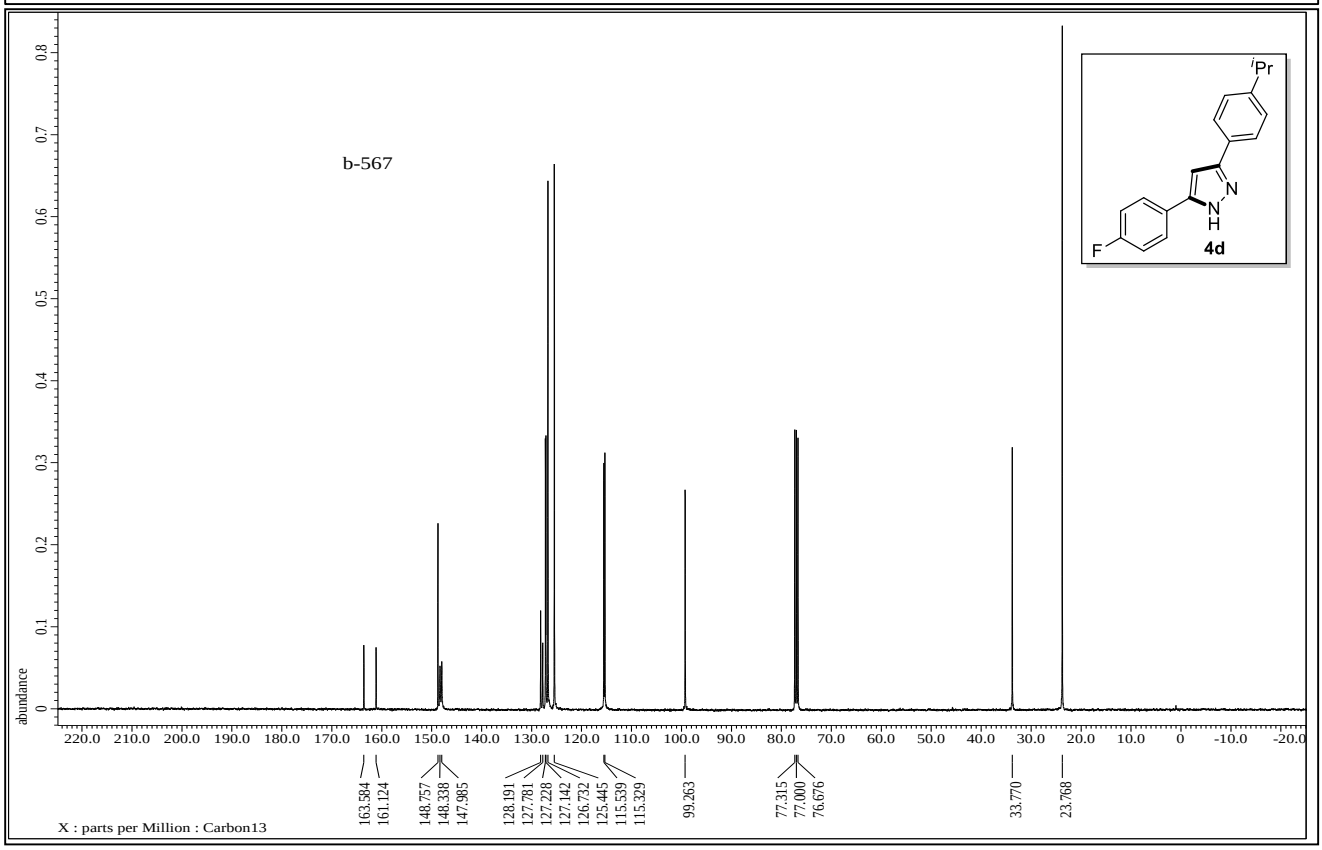

B-537-FOME
7.581
7.570
7.565
7.554
7.517
7.500
7.260
6.939
6.922
6.905
6.762
6.745
6.571
3.766
OMe
N
N
H
F
4b
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 ppm
4.17
2.10
2.10
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 ppm
4.17
2.10
2.10
1.00
3.15

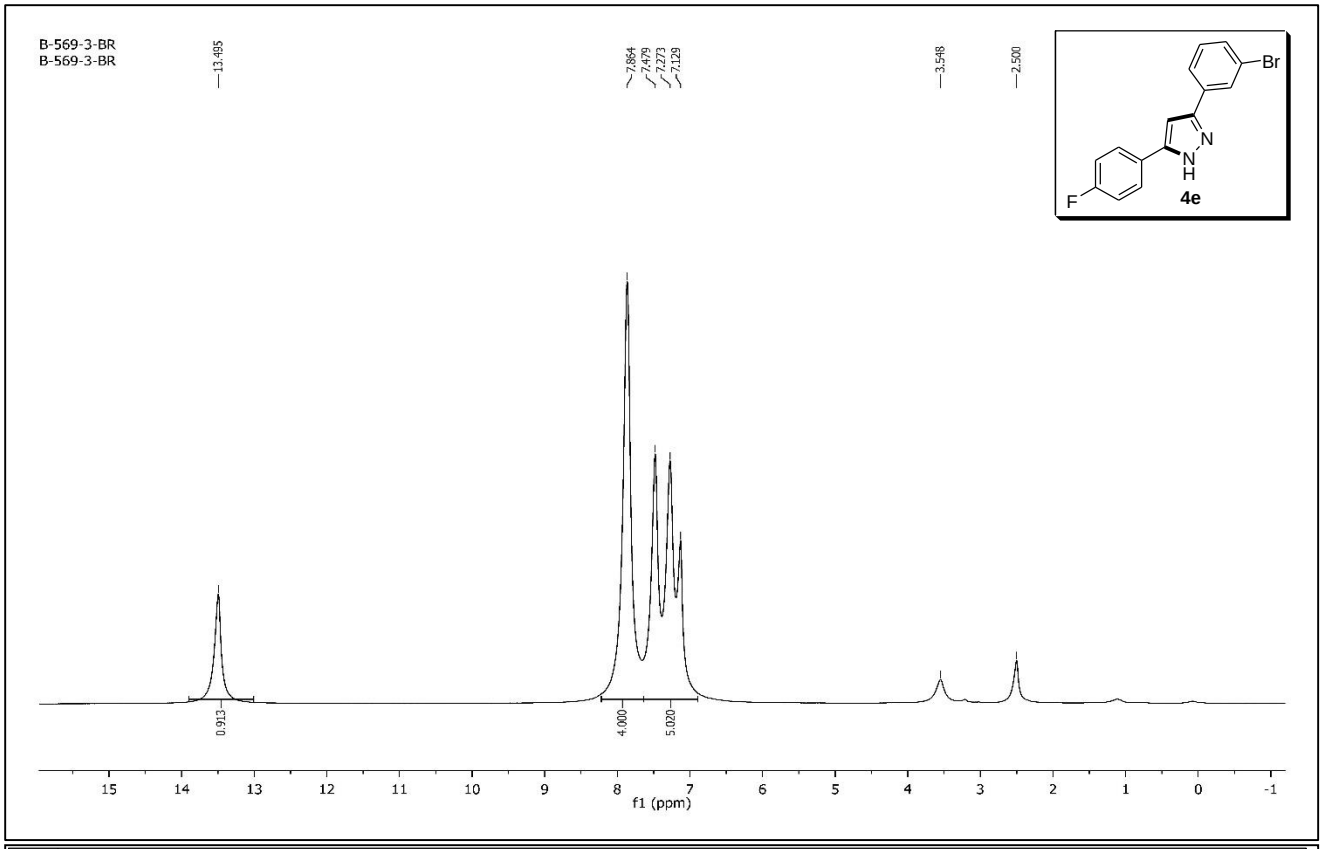

B-565
OMe
N
N
H
F
4b
abundance
0.5
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
163.545
161.095
159.379
148.547
147.508
127.924
127.133
126.704
123.186
115.529
115.310
114.004
98.758
77.324
77.000
76.685
55.032
X : parts per Million : Carbon13

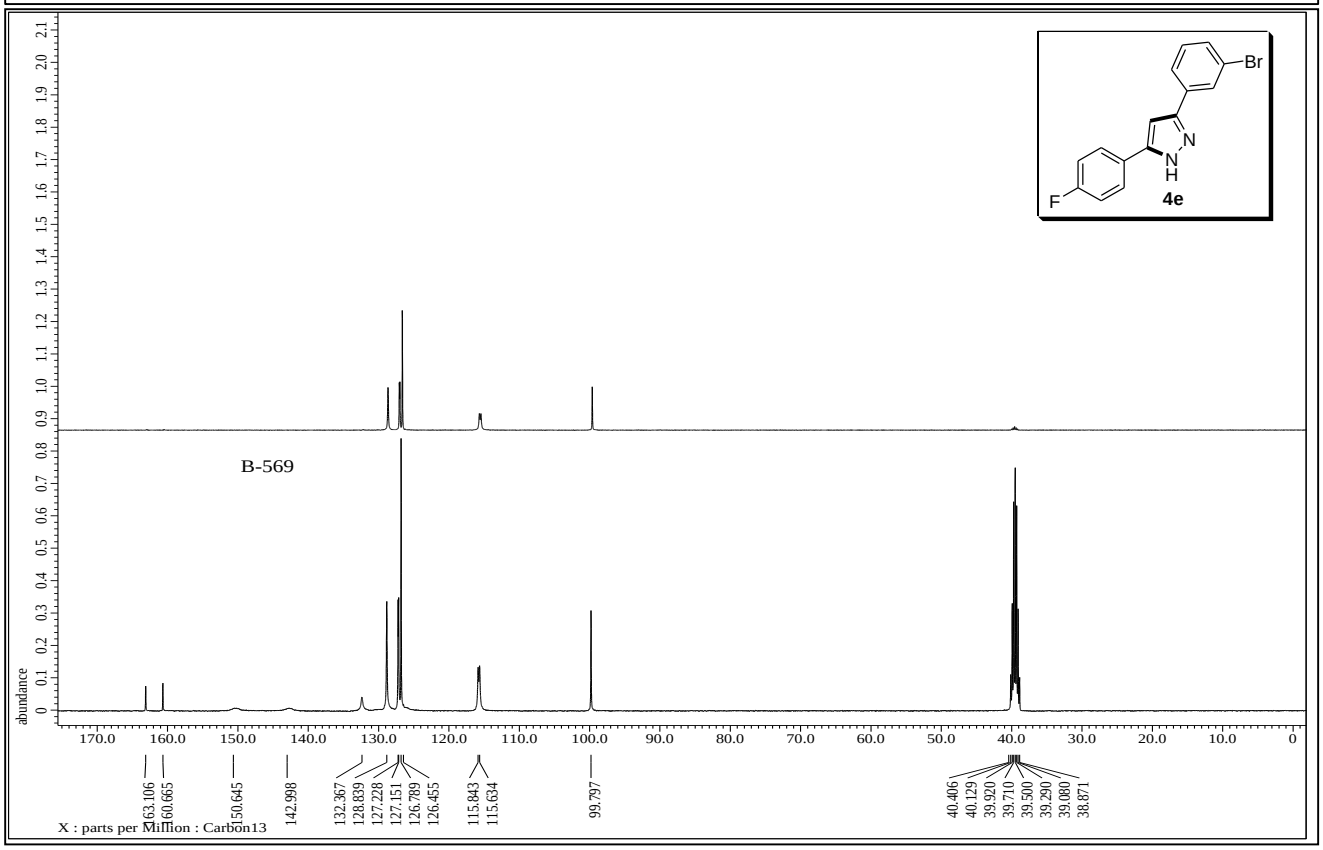

B-568-FF
13.414
7.871
7.271
7.111
2.499
4c
Current Data Parameters
NAME B-568-1
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151001
Time 11.57
INSTRUM Spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 18
DW 48.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 14.97724056 W
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.84
3.53
3.73
1.00

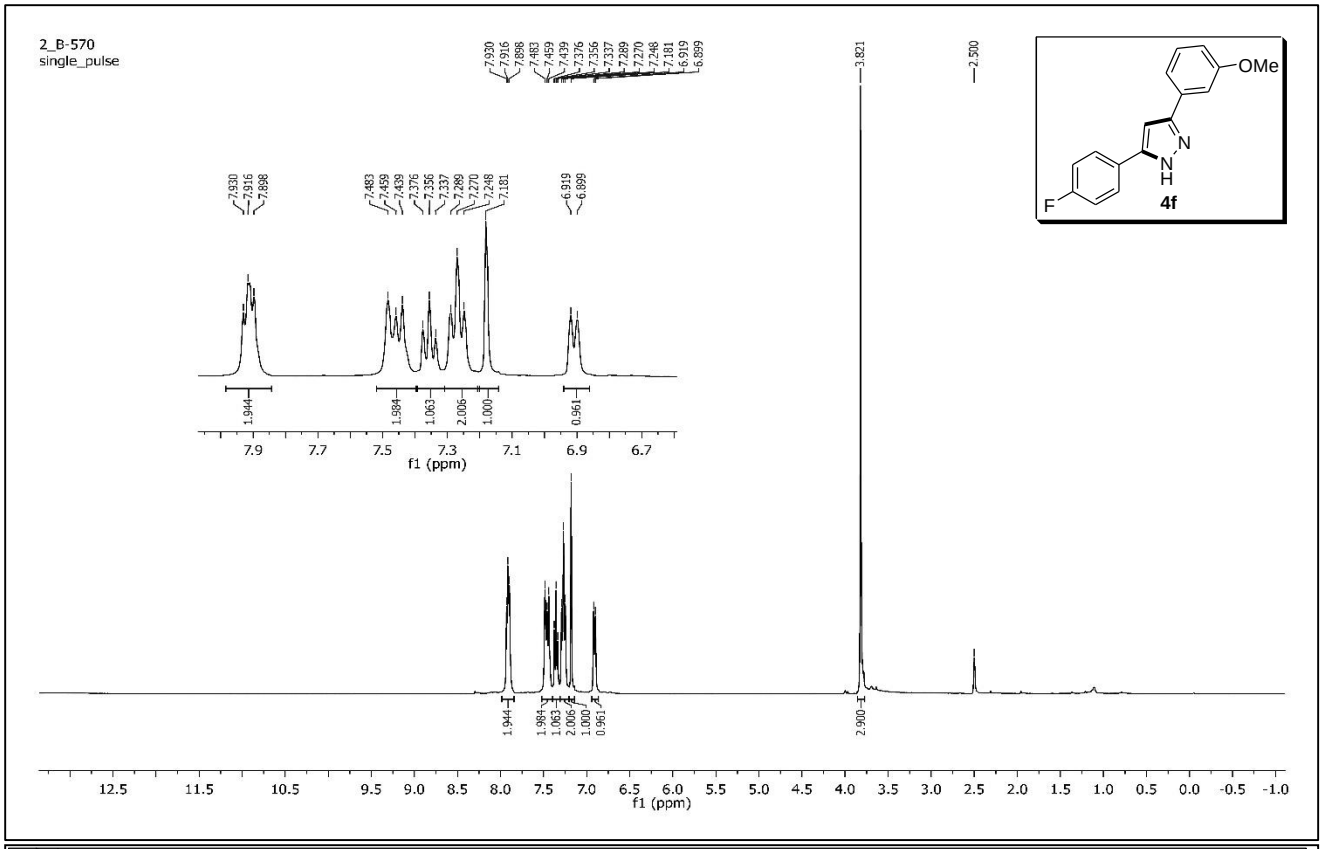

B-568
4c
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.049
160.618
127.180
127.104
115.805
115.595
99.549
40.873
40.129
39.920
39.710
39.500
39.290
39.080
38.871
X : parts per Million : Carbon13

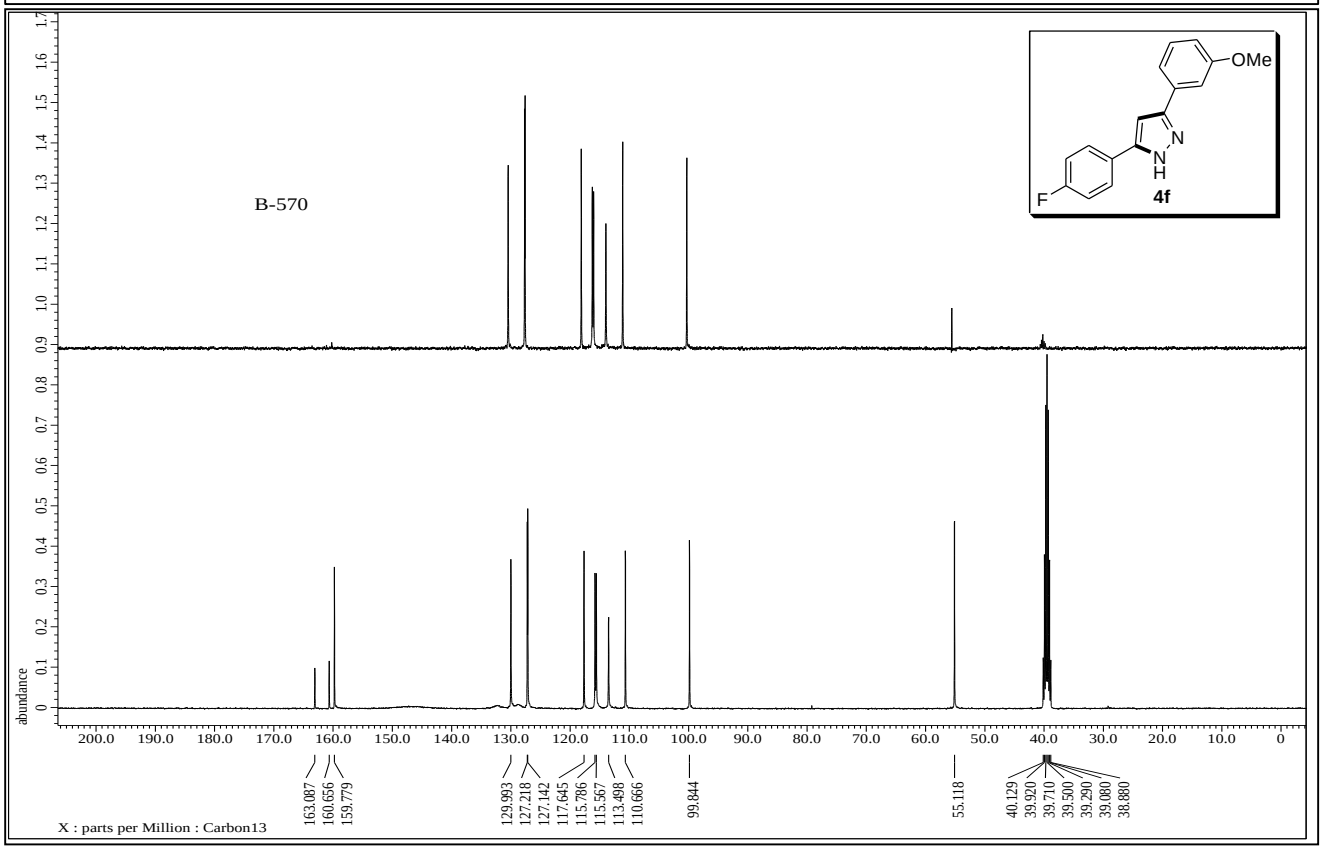

2_B-567-IPA
single_pulse
4d
f1 (ppm)

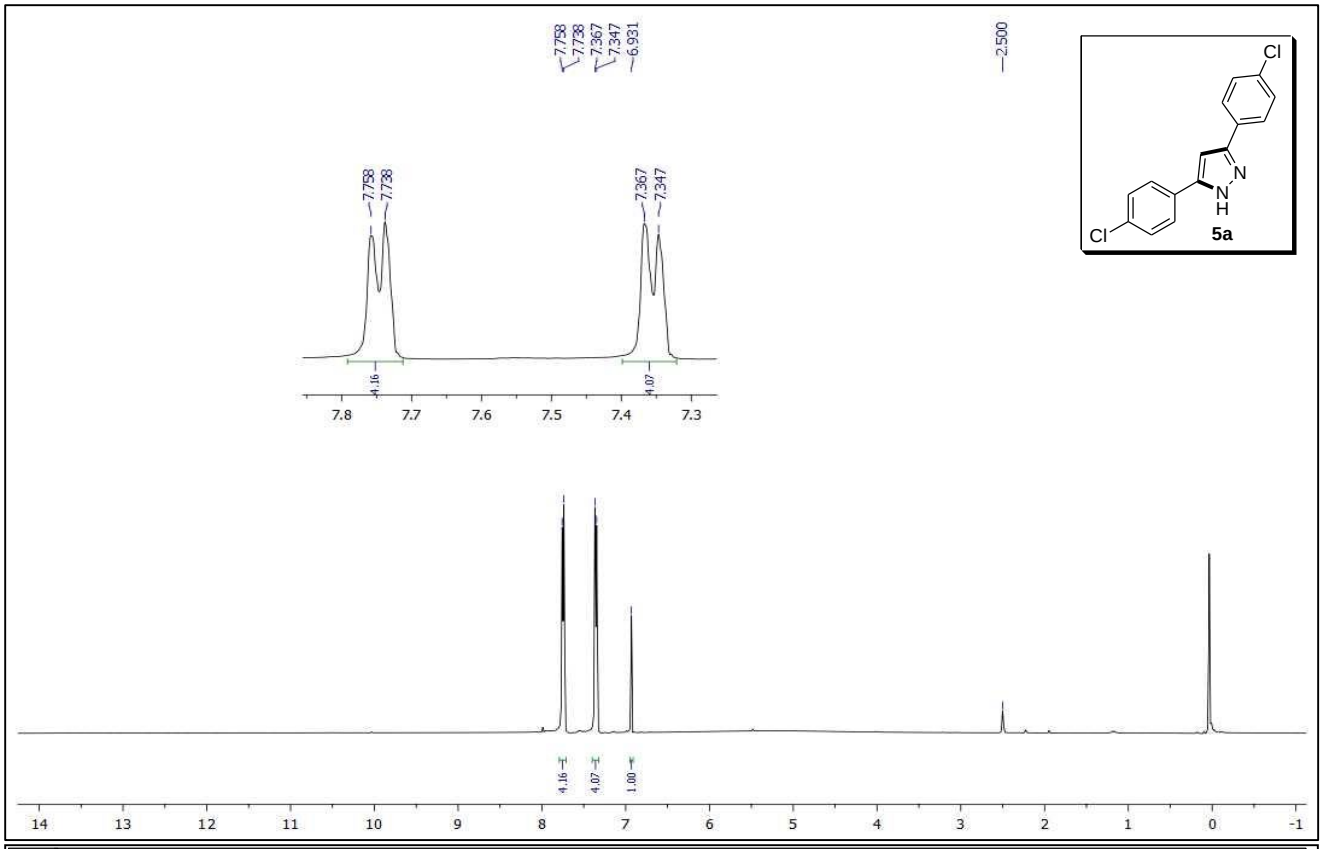

b-567
4d
abundance
X : parts per Million : Carbon13

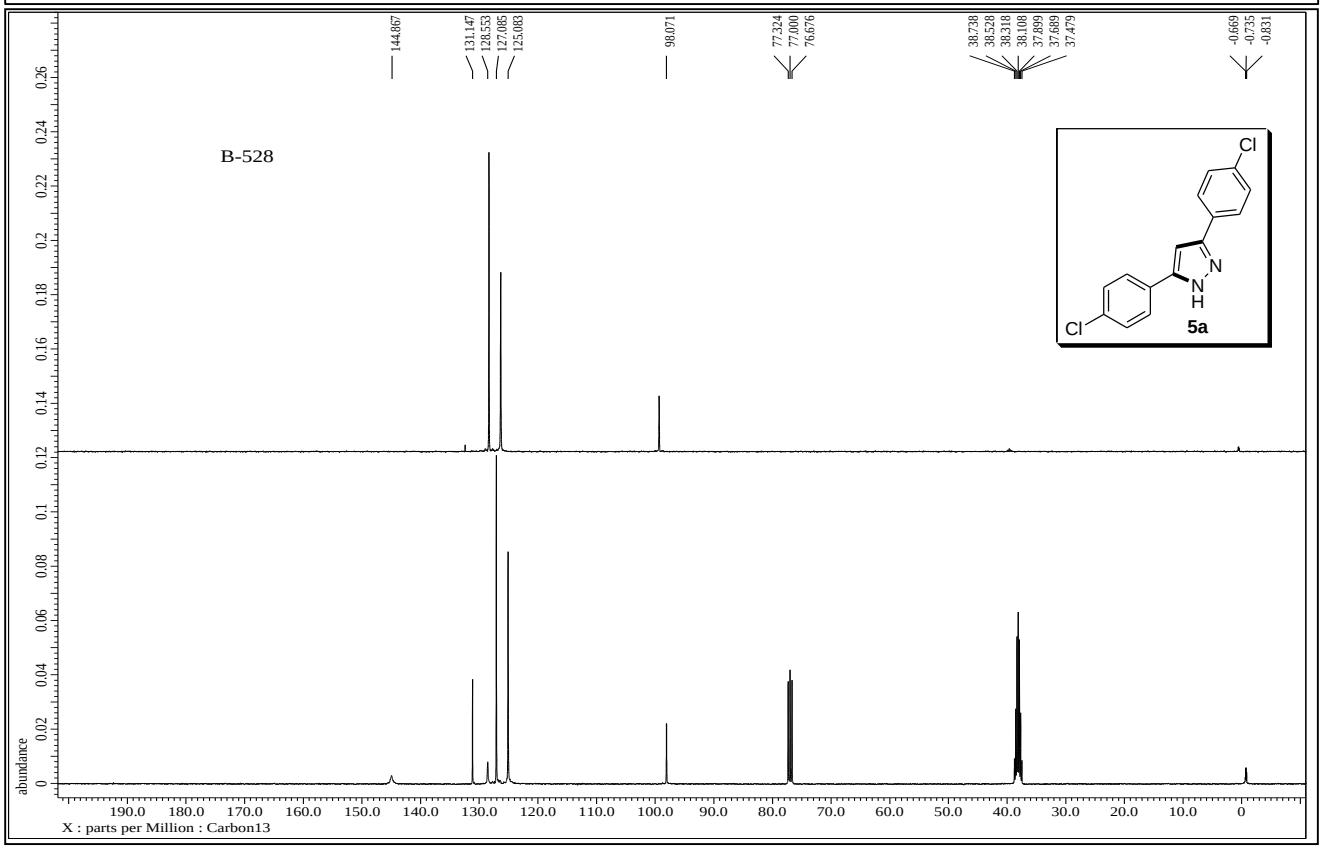

B-569-3-BR
B-569-3-BR
13.495
7.864
7.479
7.273
7.129
3.548
2.500
Br
N
N
H
F
4e
0.913
4.000
5.020
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

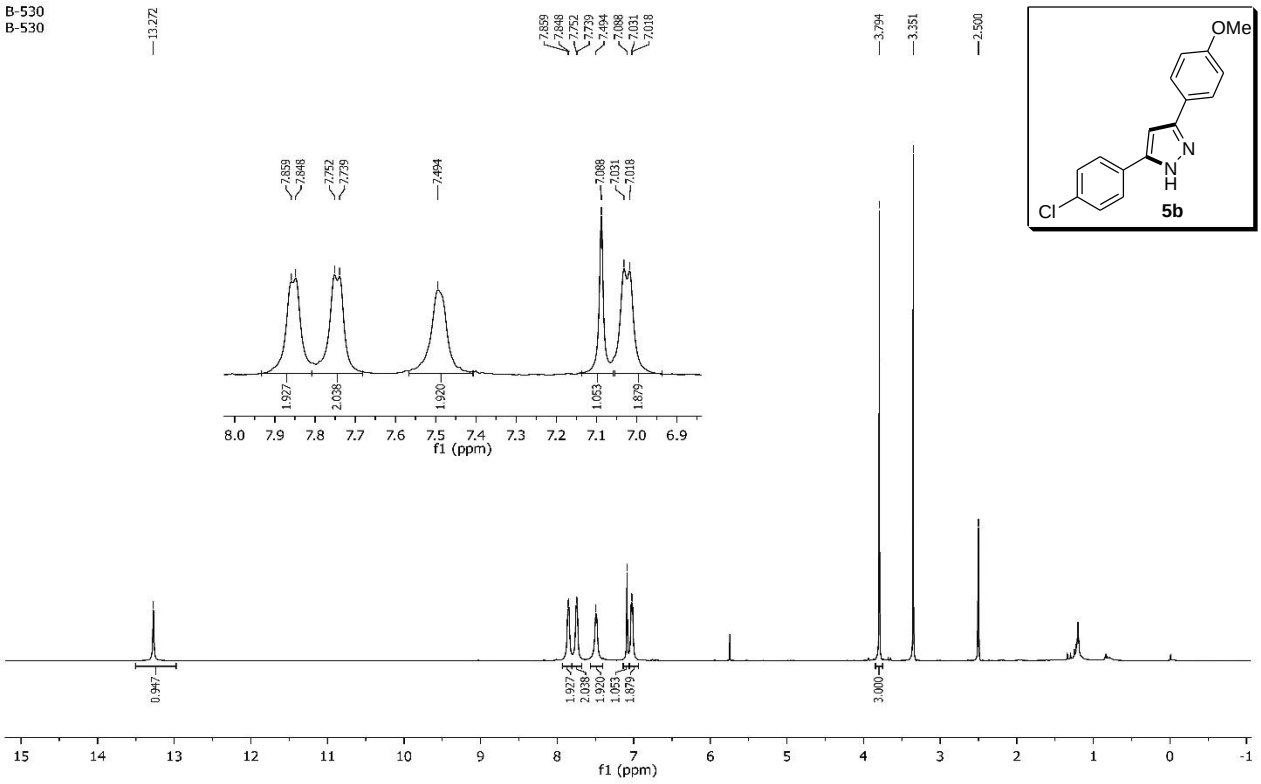

Br
N
N
H
F
4e
B-569
abundance
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
63.106
60.665
50.645
142.998
132.367
128.839
127.228
127.151
126.789
126.455
115.843
115.634
99.797
40.406
40.129
39.920
39.710
39.500
39.290
39.080
38.871
X : parts per Million : Carbon13

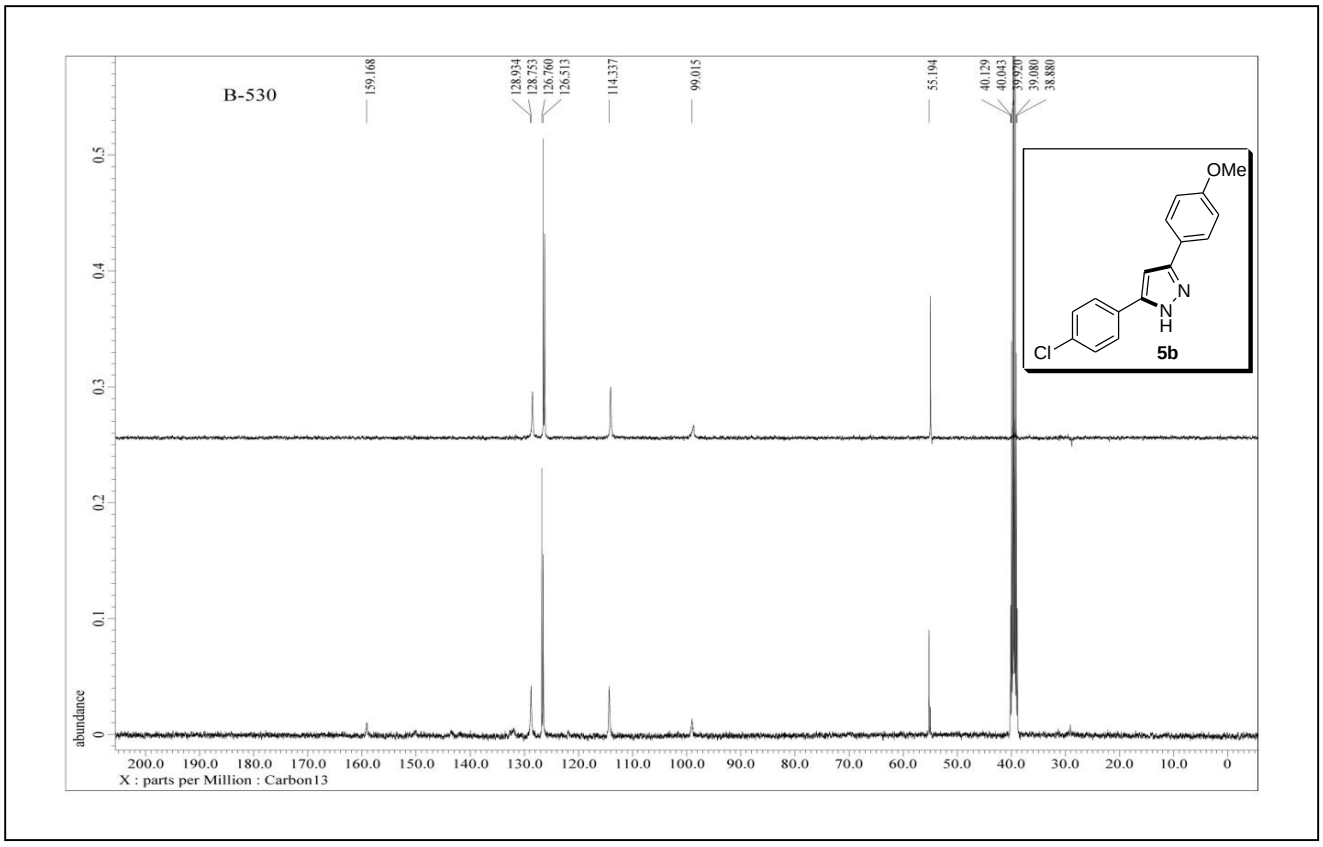

2_B-570
single_pulse
OMe
N
N
H
F
4f
f1 (ppm)

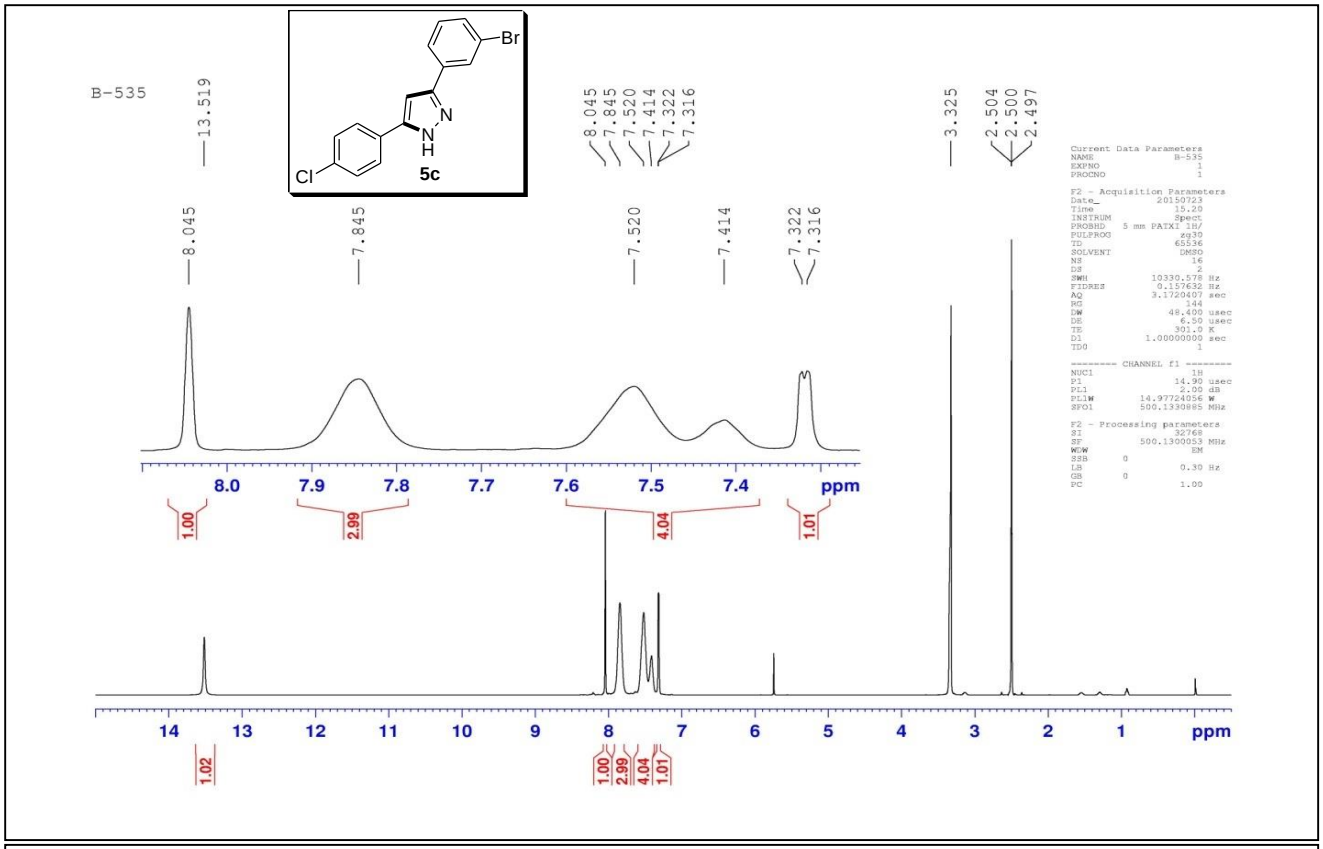

B-570
OMe
N
N
H
F
4f
abundance
X : parts per Million : Carbon13

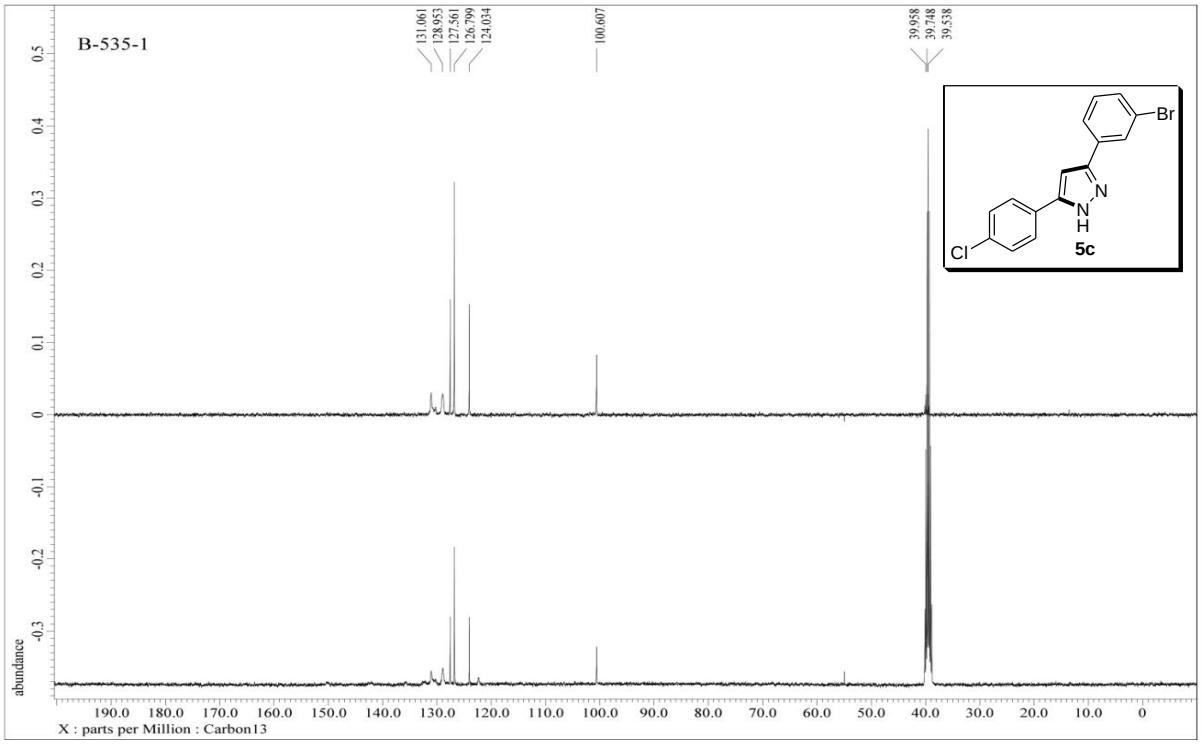

7.758
7.738
7.367
7.347
6.931
2.500
Cl
N
N
H
Cl
5a
4.16
4.07
1.00

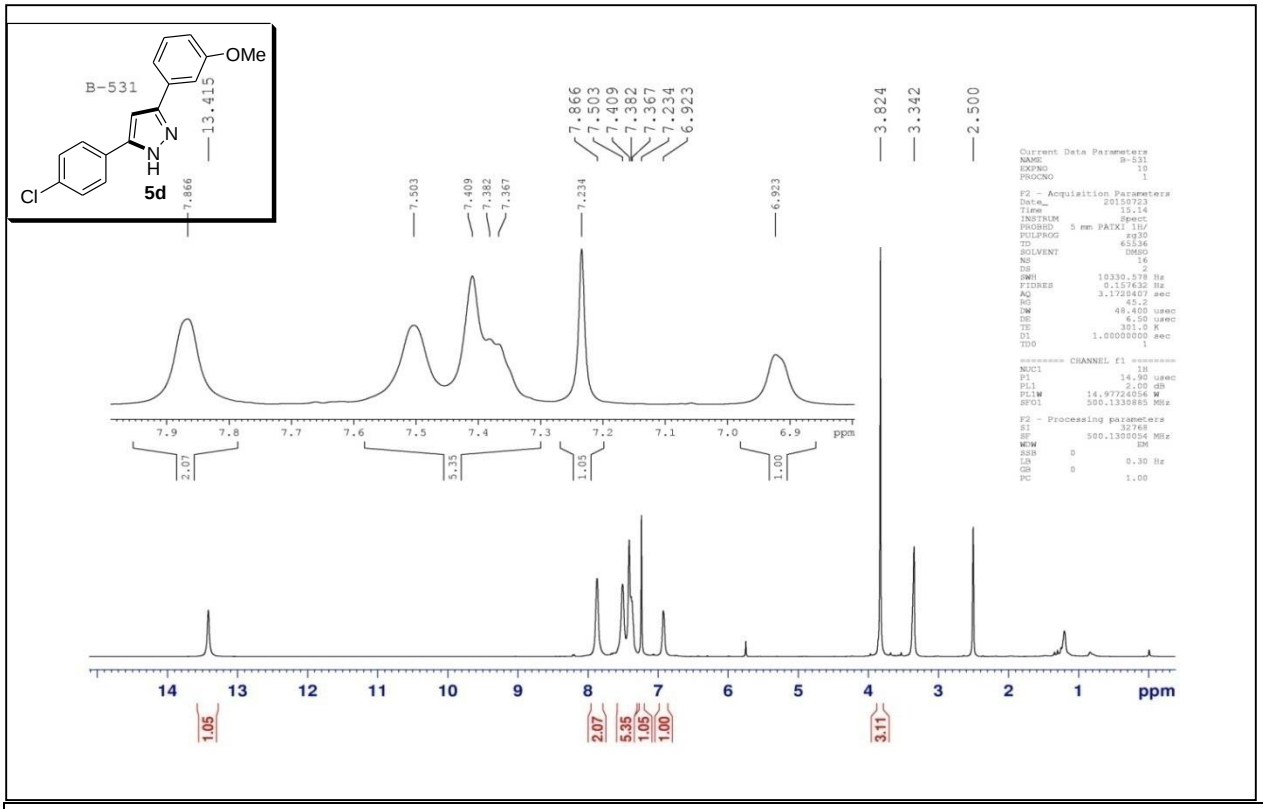

144.867
131.147
128.553
127.085
125.083
98.071
77.324
77.000
76.676
38.738
38.528
38.318
38.108
37.899
37.689
37.479
-0.669
-0.735
-0.831
B-528
Cl
N
N
H
Cl
5a
abundance
X : parts per Million : Carbon13

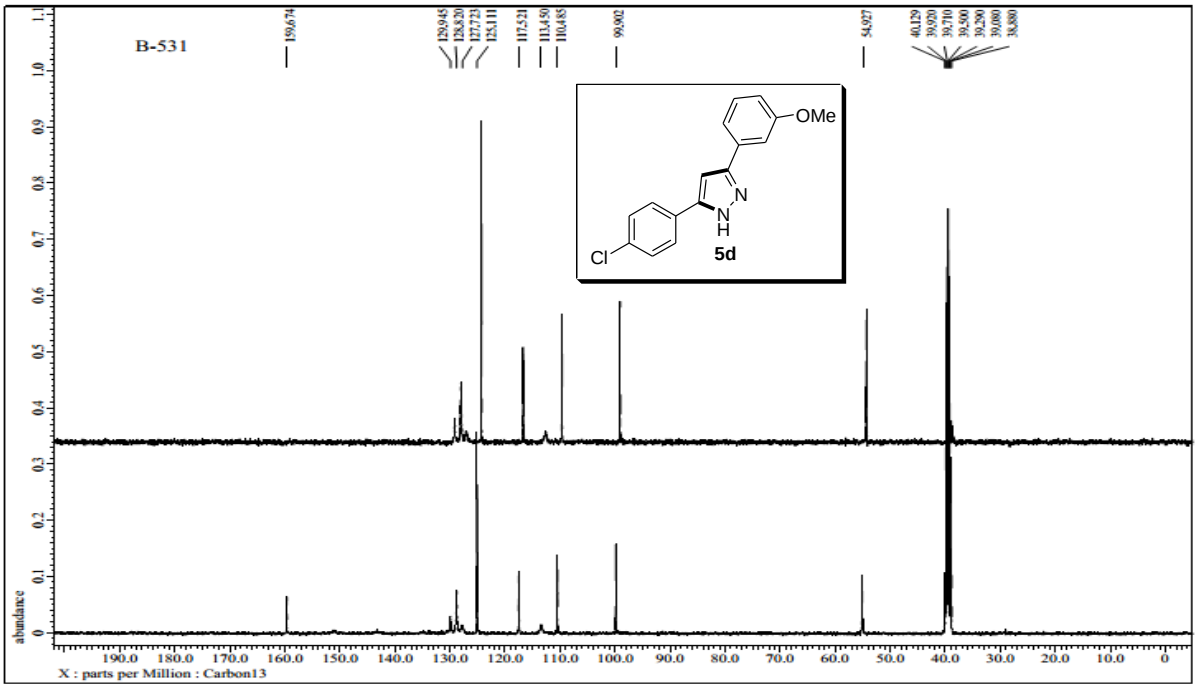

B-530
B-530
13.272
7.859
7.848
7.752
7.739
7.494
7.088
7.031
7.018
3.794
3.351
2.500
OMe
N
N
H
Cl
5b
1.927
2.038
1.920
1.053
1.879
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
0.947
3.000
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

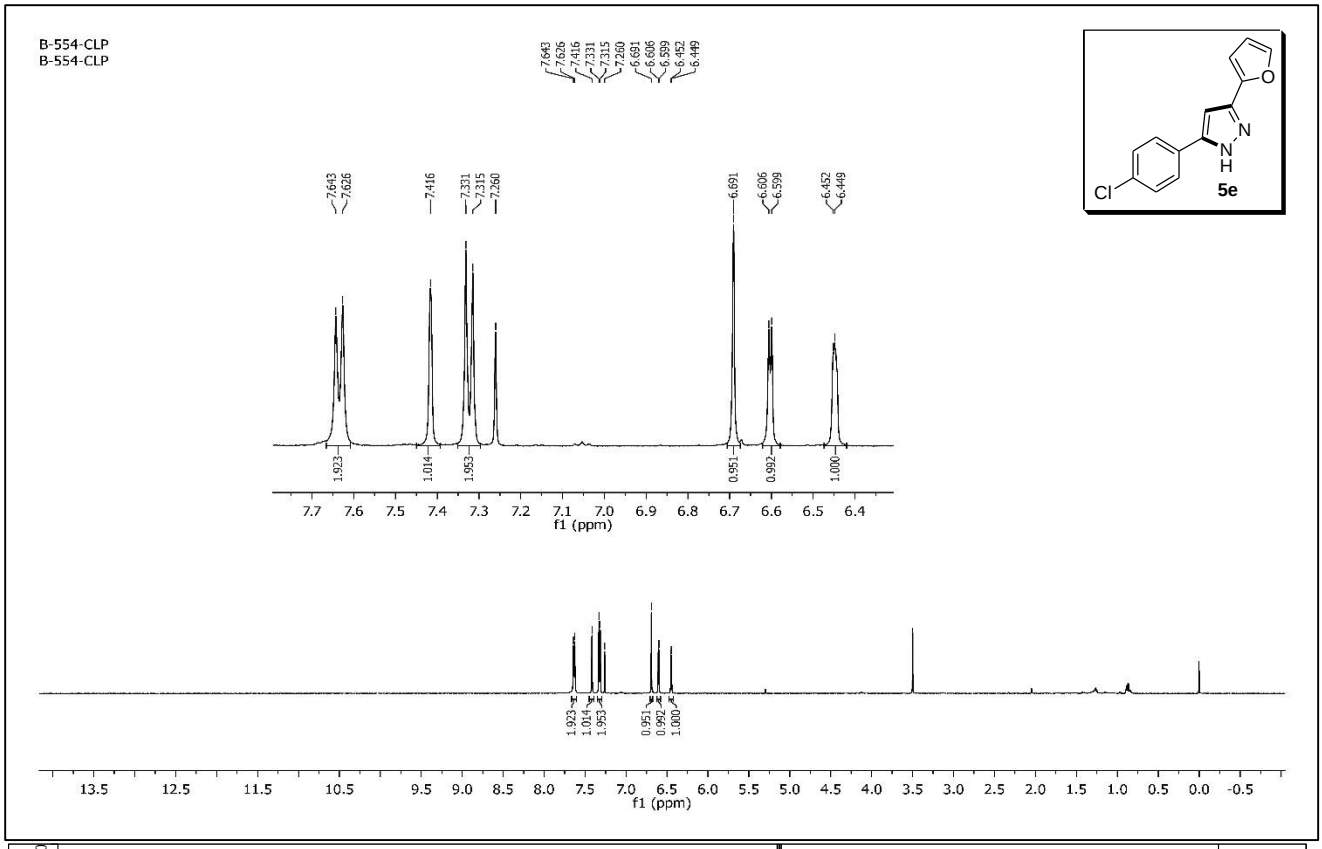

B-530
159.168
128.934
128.753
126.760
126.513
114.337
99.015
55.194
40.129
40.043
39.920
39.080
38.880
OMe
N
N
H
Cl
5b
abundance
0 0.1 0.2 0.3 0.4 0.5
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : Carbon13

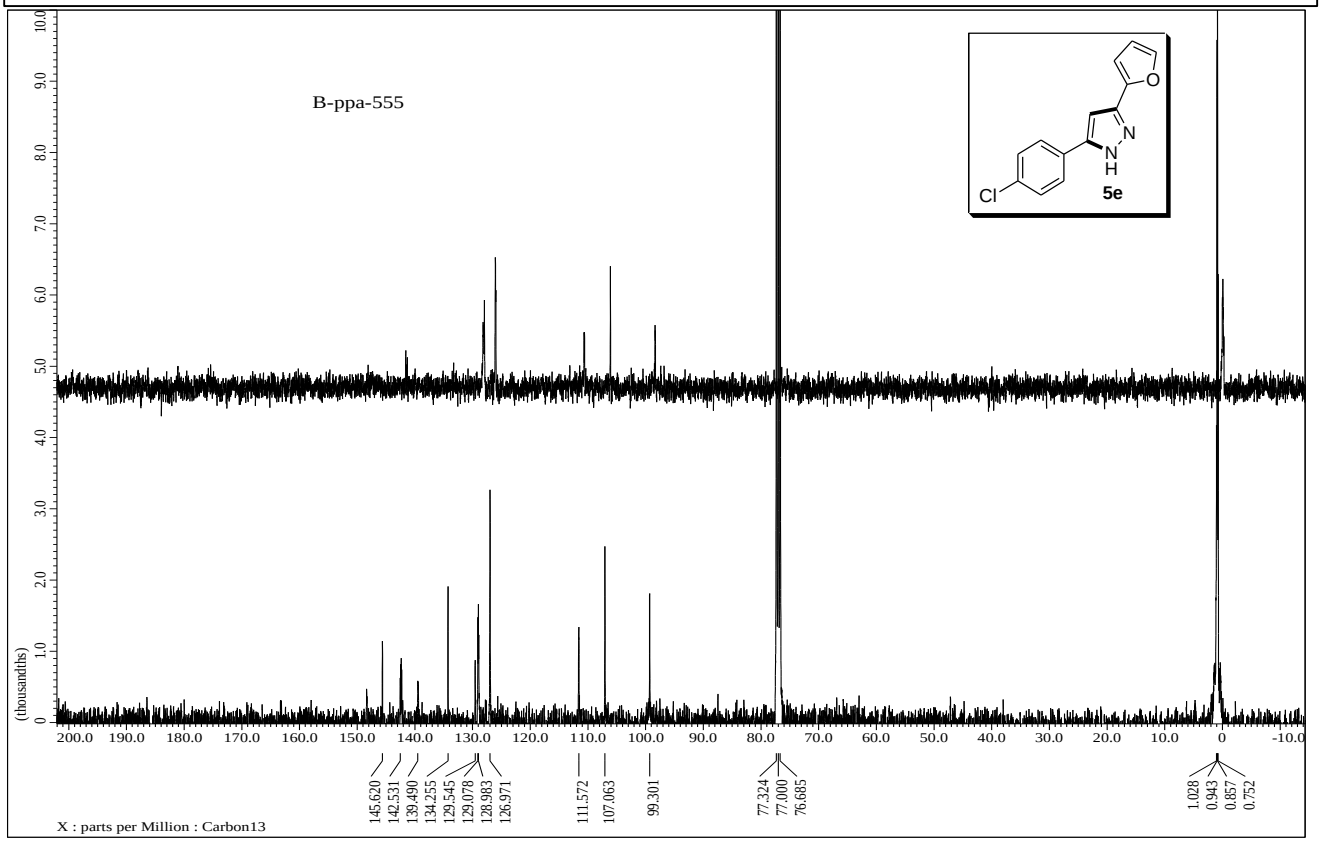

B-535
13.519
8.045
7.845
7.520
7.414
7.322
7.316
3.325
2.504
2.500
2.497
Br
Cl
N
N
H
5c
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
1.00
2.99
4.04
1.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.00
2.99
4.04
1.01

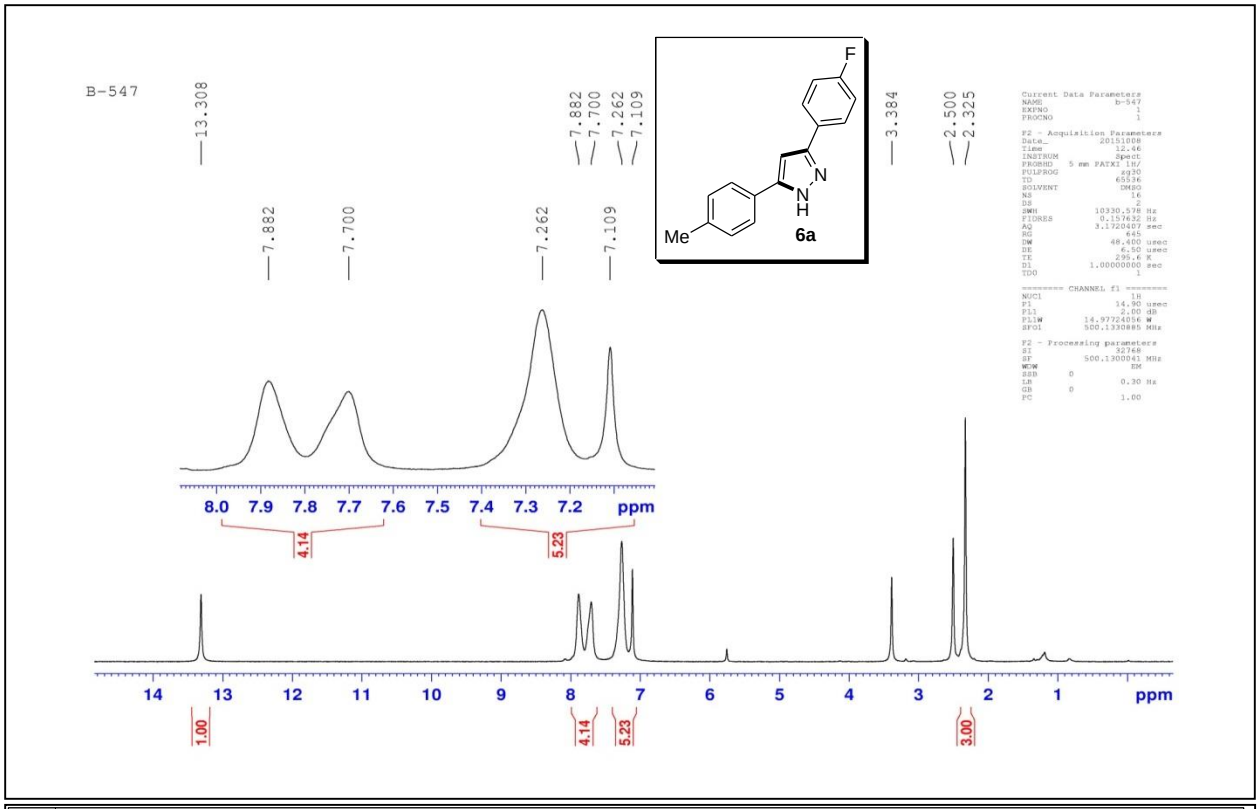

B-535-1
131.061
128.953
127.561
126.799
124.034
100.607
39.958
39.748
39.538
Br
Cl
N
N
H
5c
abundance
X : parts per Million : Carbon13

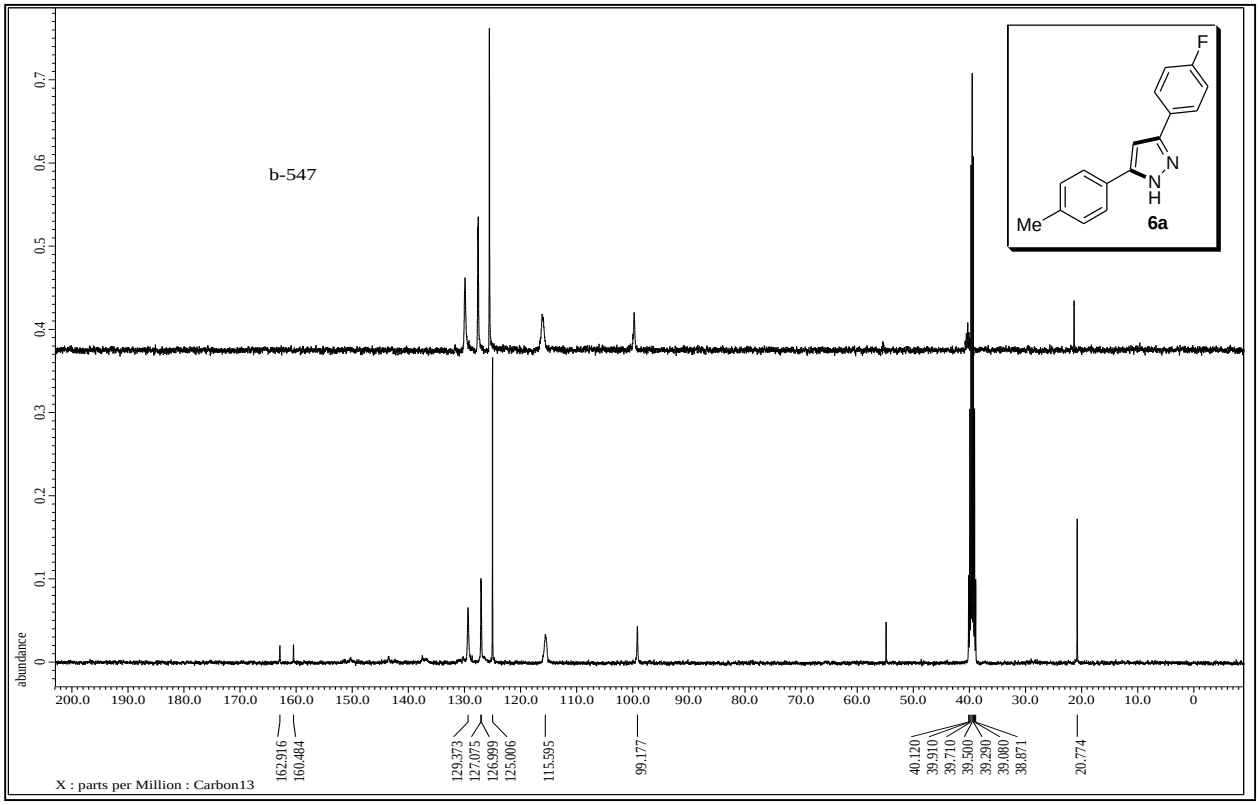

B-531
OMe
Cl
N
N
H
5d
13.415
7.866
7.503
7.409
7.382
7.367
7.234
6.923
3.824
3.342
2.500
ppm

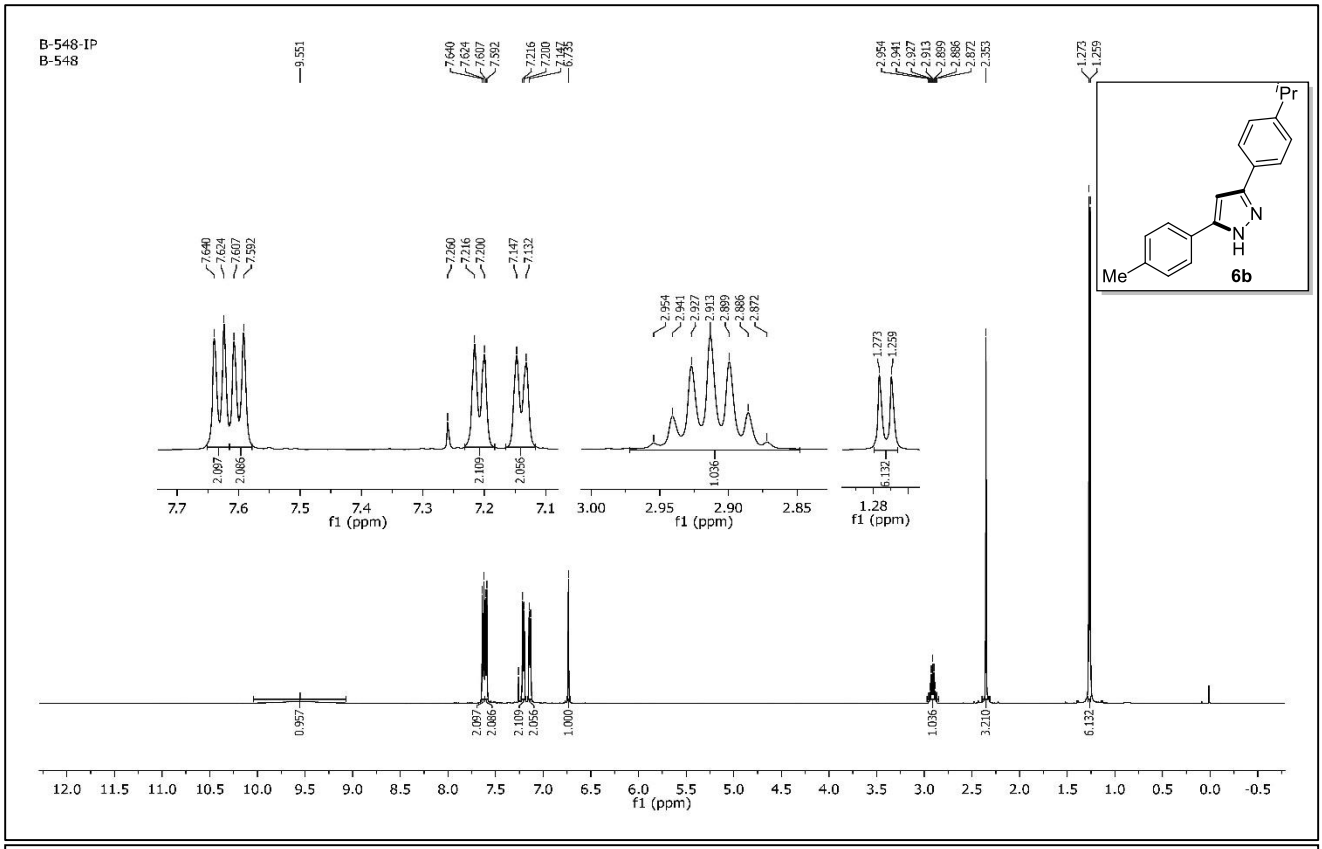

B-531
159.674
129.945
128.820
127.723
125.111
117.521
113.450
110.485
99.902
54.927
40.129
39.920
39.710
39.500
39.290
39.080
38.880
OMe
Cl
N
N
H
5d
abundance
X : parts per Million : Carbon13

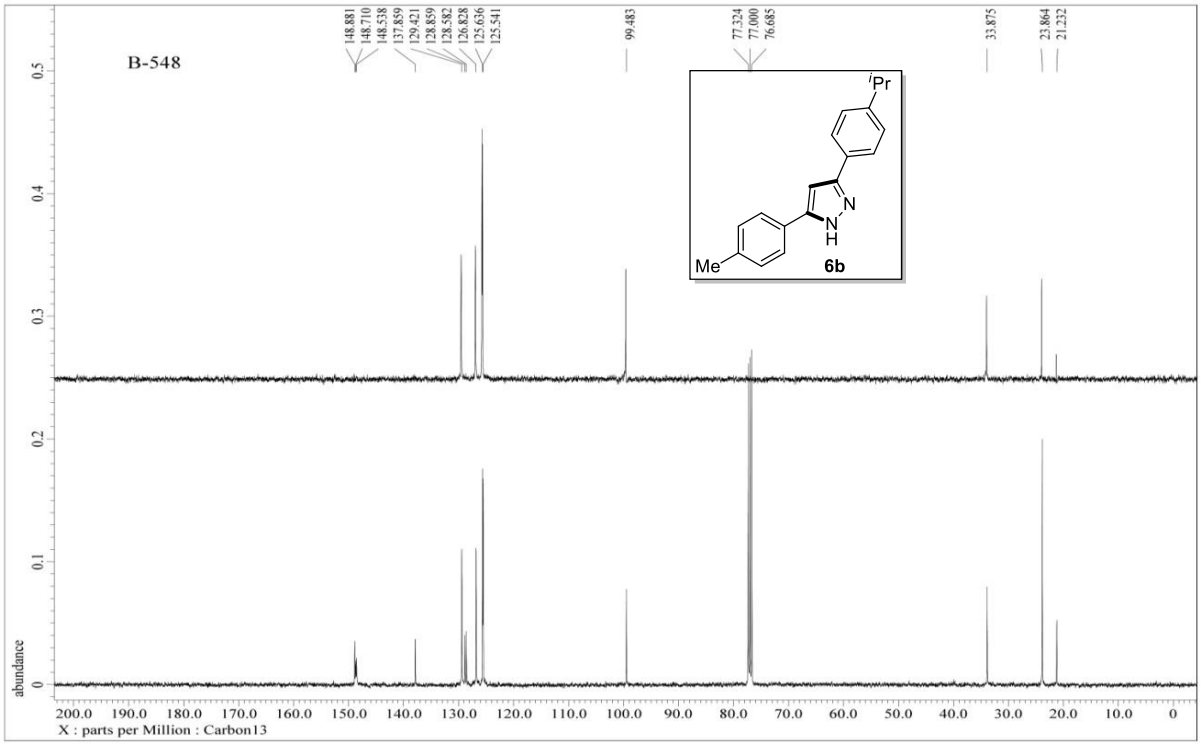

B-554-CLP
B-554-CLP
7.643
7.626
7.416
7.331
7.315
7.260
6.691
6.606
6.599
6.452
6.449
1.923
1.014
1.953
0.951
0.992
1.000
f1 (ppm)
Cl
5e

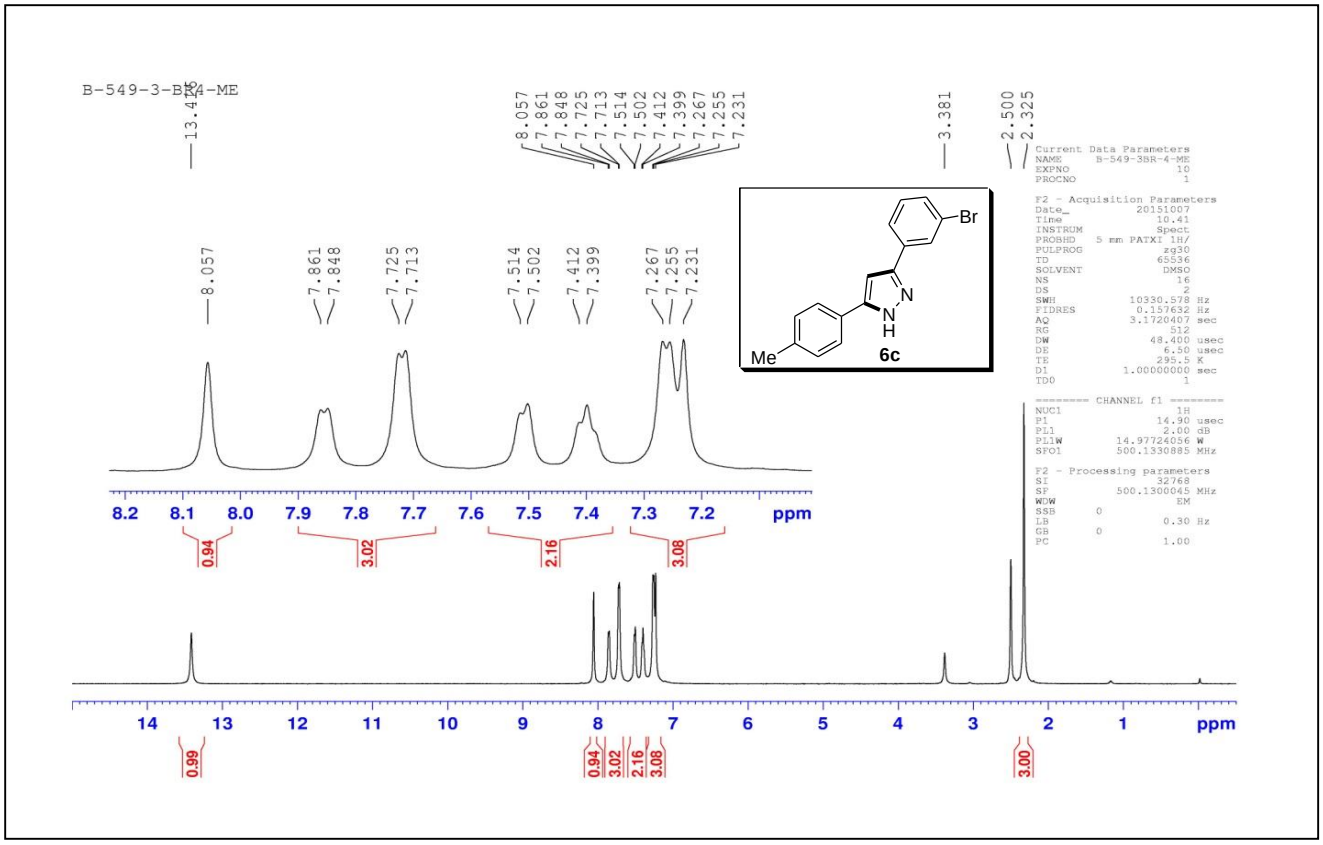

B-ppa-555
Cl
5e
(thousandths)
145.620
142.531
139.490
134.255
129.545
129.078
128.983
126.971
111.572
107.063
99.301
77.324
77.000
76.685
1.028
0.943
0.857
0.752
X : parts per Million : Carbon13

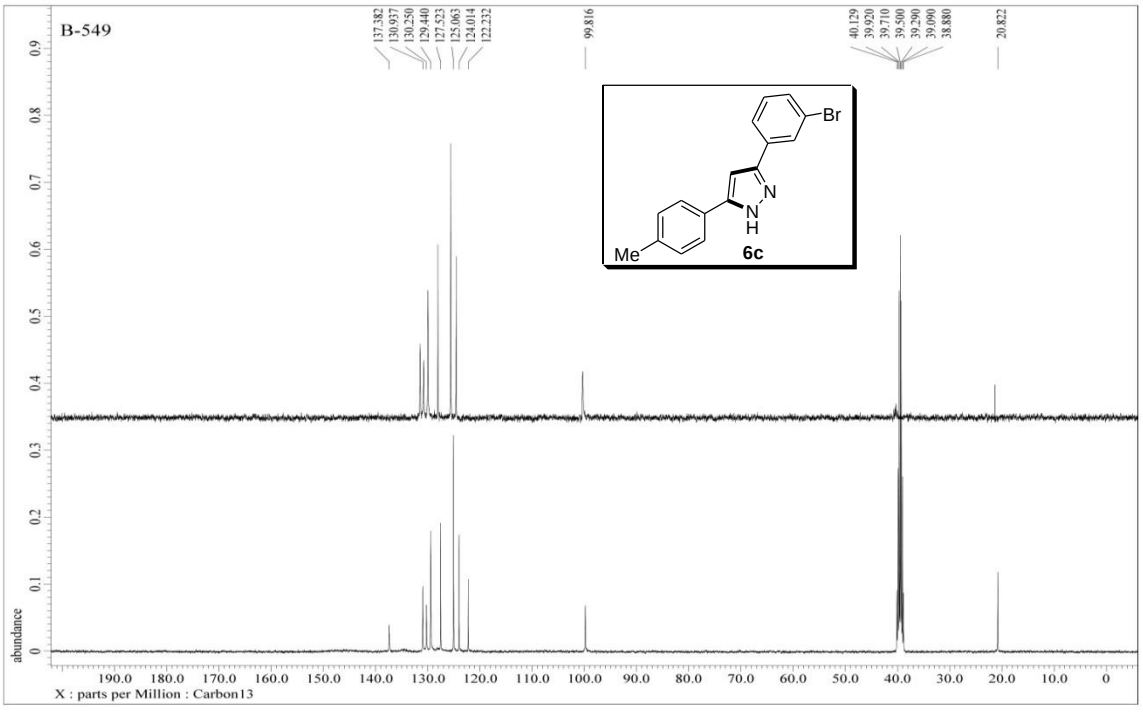

B-547
13.308
7.882
7.700
7.262
7.109
3.384
2.500
2.325
F
Me
N
N
H
6a
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
4.14
5.23
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
4.14
5.23
3.00

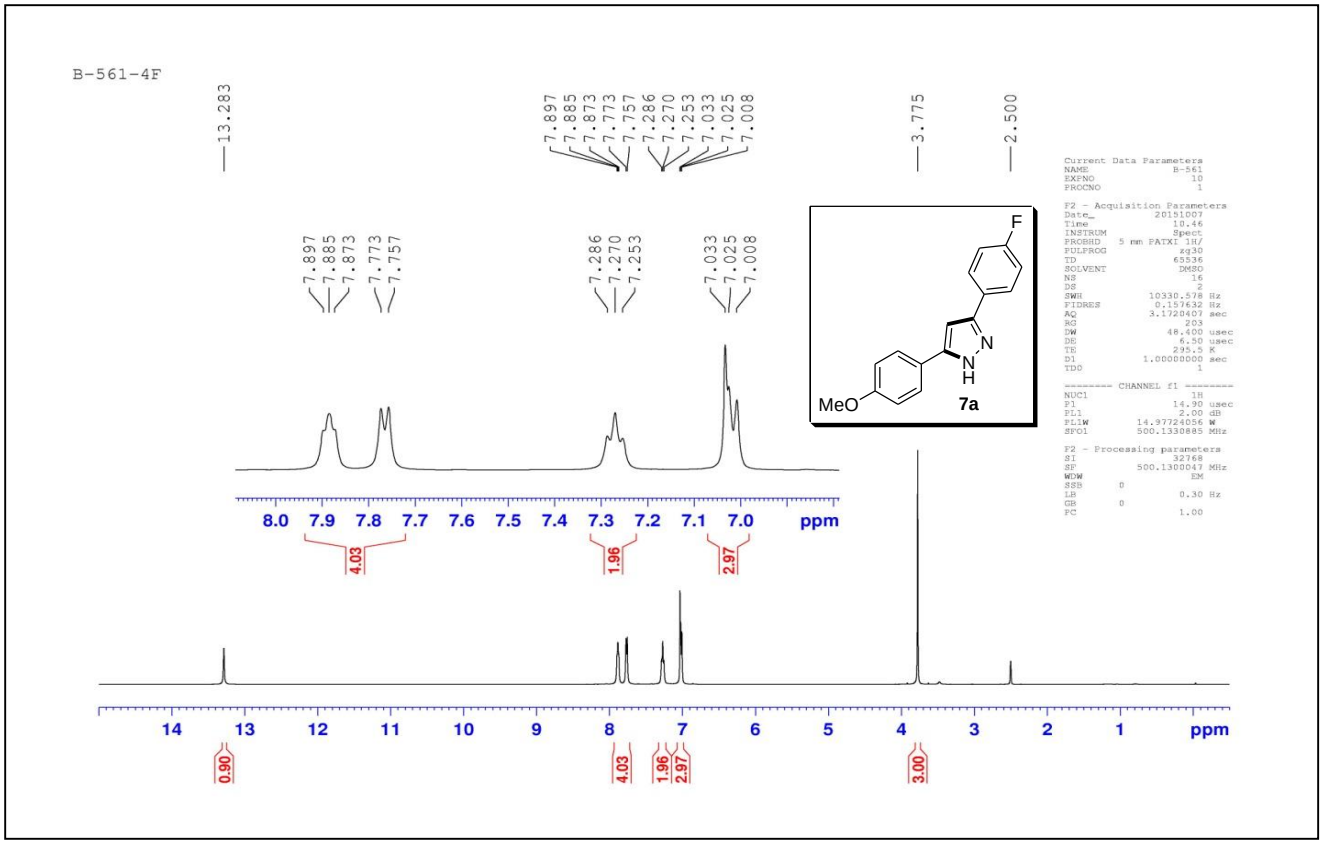

b-547
F
Me
N
N
H
6a
abundance
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
162.916
160.484
129.373
127.075
126.999
125.006
115.595
99.177
40.120
39.910
39.710
39.500
39.290
39.080
38.871
20.774
X : parts per Million : Carbon13

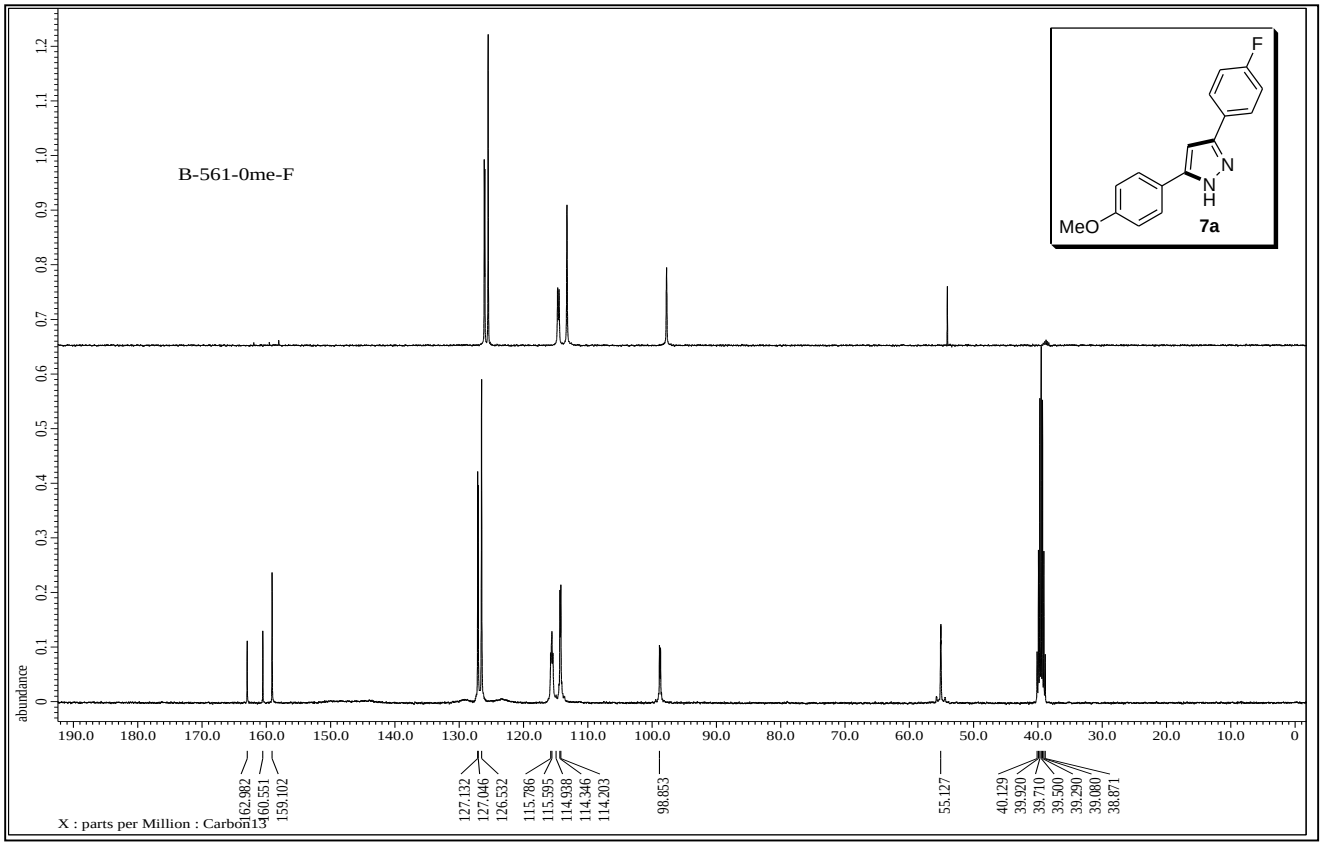

B-548-IP
B-548
9.551
7.640
7.624
7.607
7.592
7.260
7.216
7.200
7.147
7.132
2.954
2.941
2.927
2.913
2.899
2.886
2.872
1.273
1.259
2.097
2.085
2.109
2.056
1.036
6.132
0.957
1.000
3.210
f1 (ppm)
iPr
Me
6b

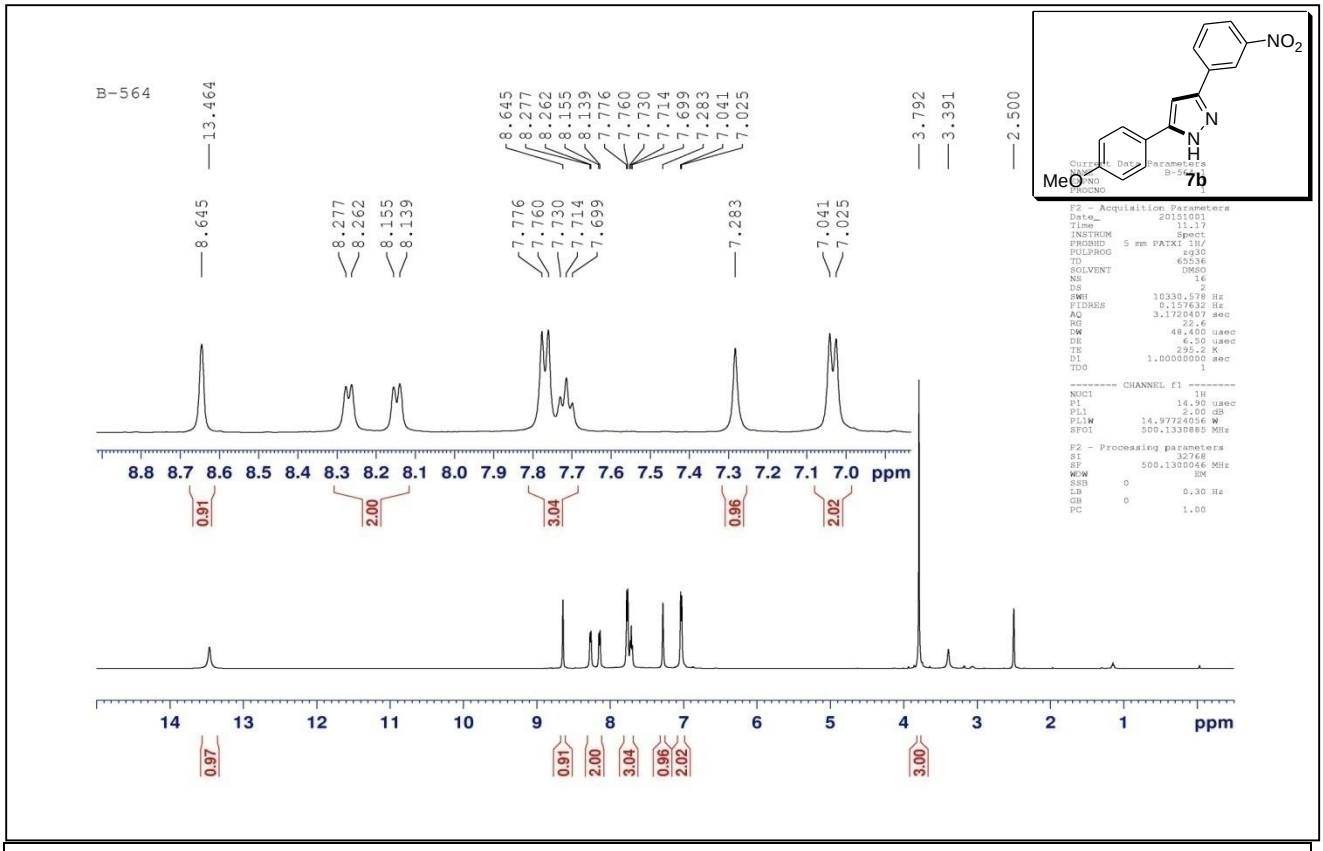

B-548
148.881
148.710
148.538
137.859
129.421
128.859
128.582
126.828
125.636
125.541
99.483
77.324
77.000
76.685
33.875
23.864
21.232
abundance
X : parts per Million : Carbon13
iPr
Me
6b

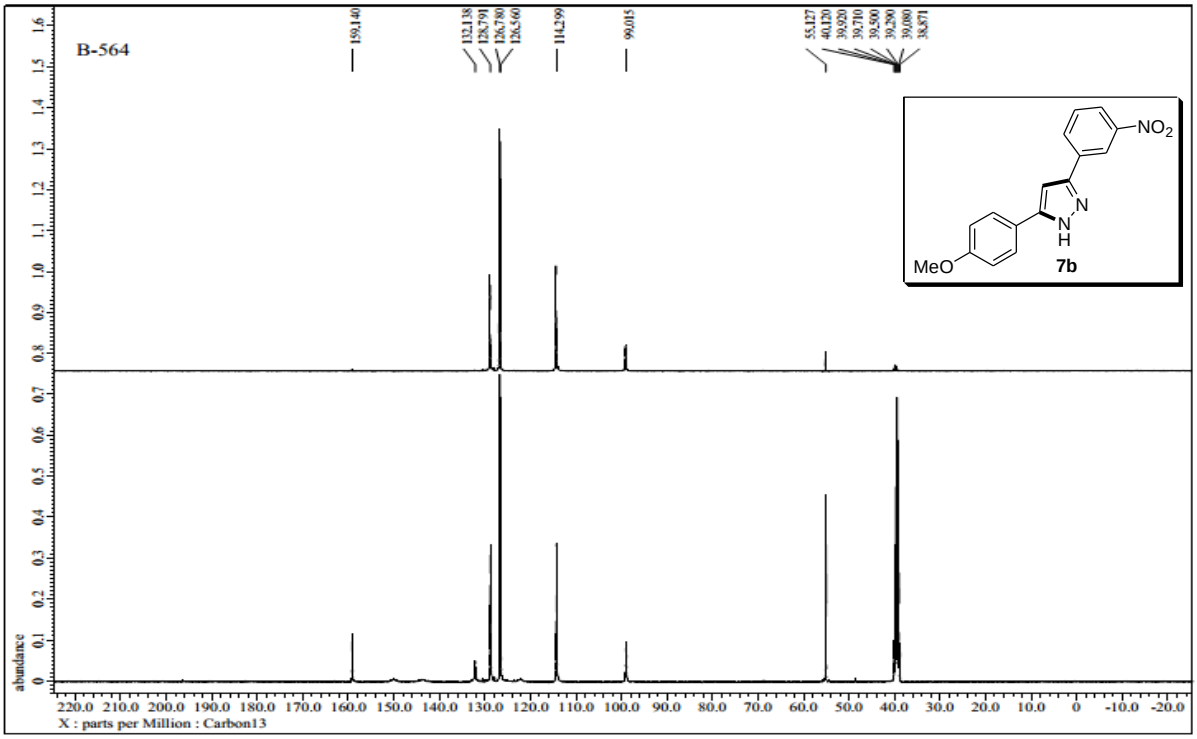

B-549-3-BR-4-ME
13.414
8.057
7.861
7.848
7.725
7.713
7.514
7.502
7.412
7.399
7.267
7.255
7.231
3.381
2.500
2.325
Br
N
N
H
Me
6c
ppm
0.94
3.02
2.16
3.08
0.99
3.00

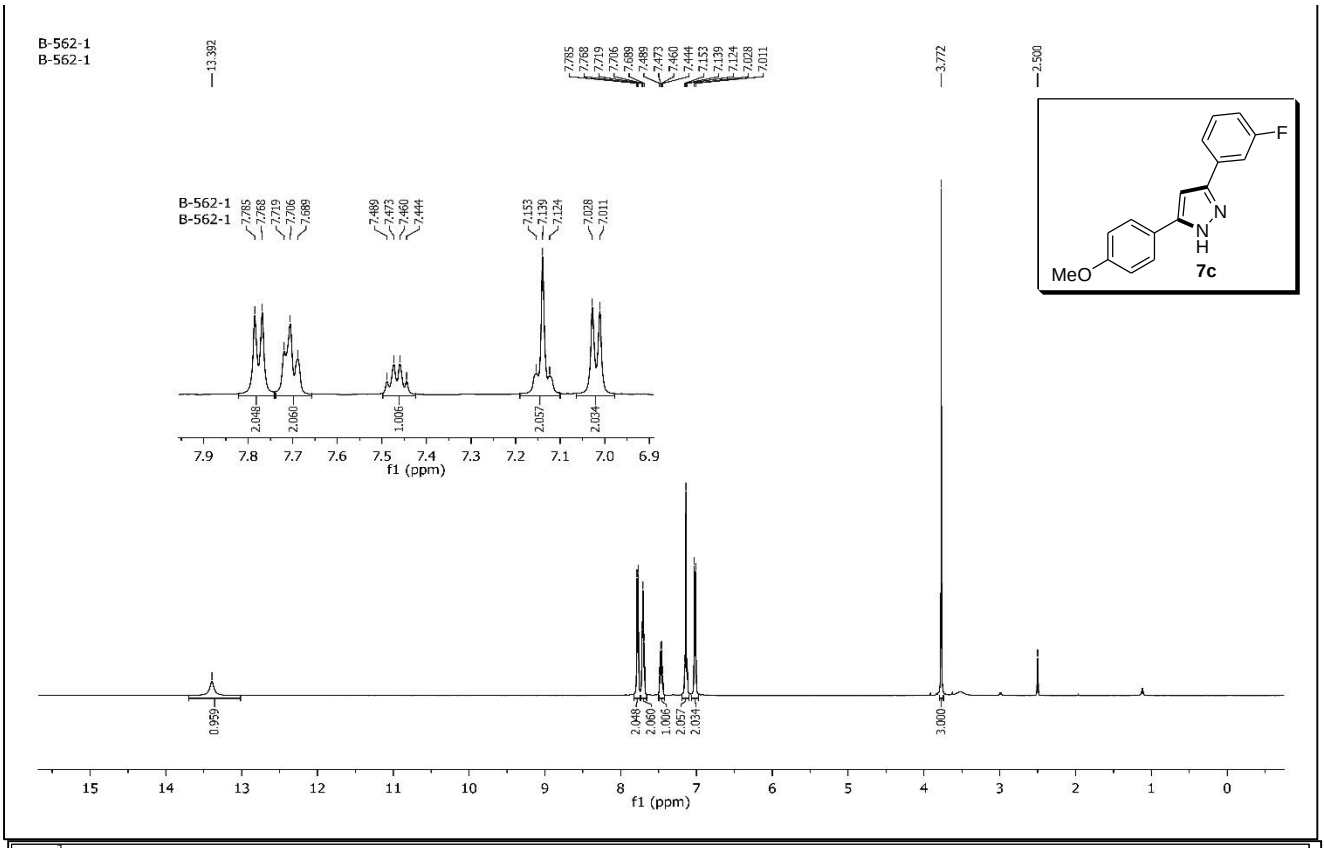

B-549
137.382
130.937
130.250
129.440
127.523
125.063
124.014
122.232
99.816
40.129
39.920
39.710
39.500
39.290
39.090
38.880
20.822
Br
N
N
H
Me
6c
abundance
X : parts per Million : Carbon13

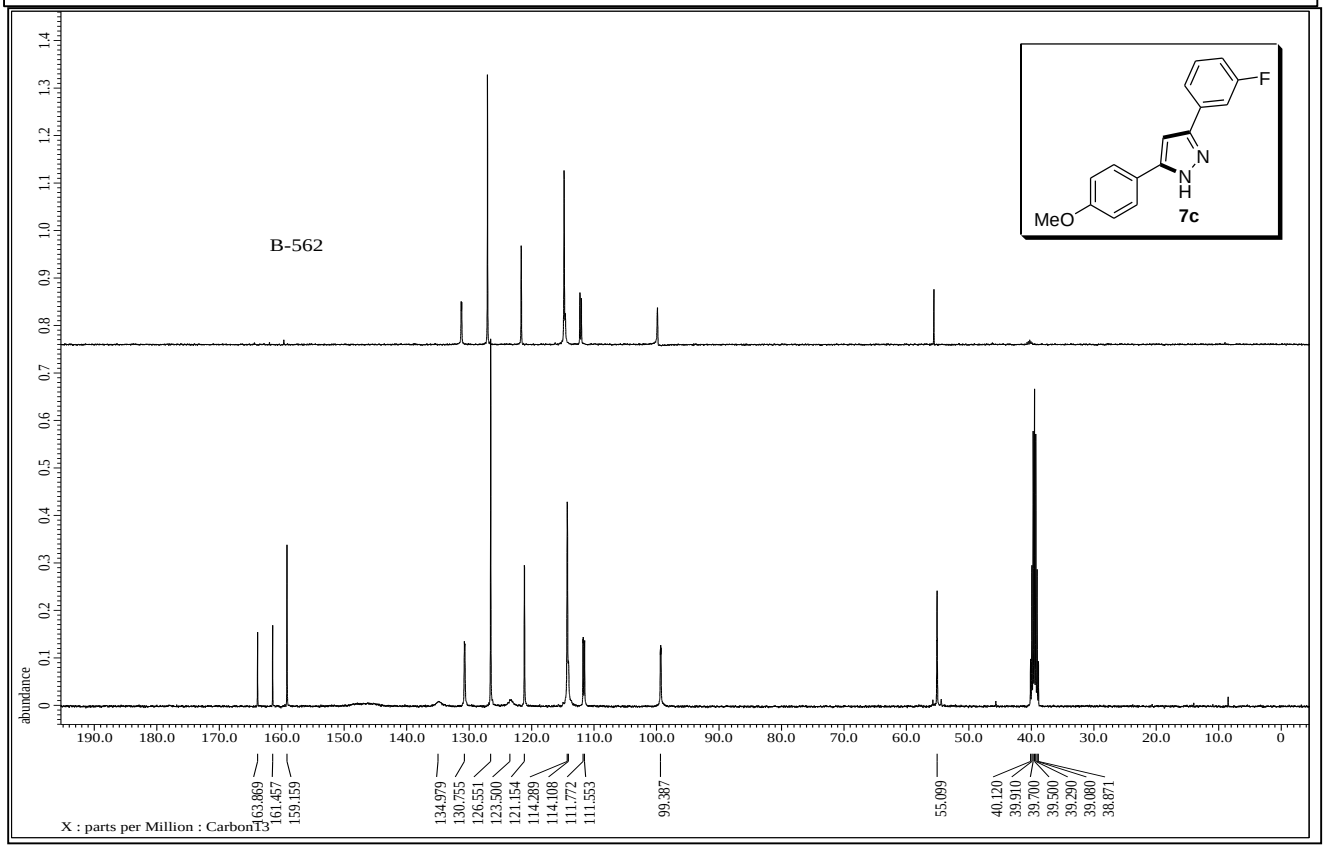

B-561-4F
13.283
7.897
7.885
7.873
7.773
7.757
7.286
7.270
7.253
7.033
7.025
7.008
3.775
2.500
F
N
N
H
MeO
7a
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
4.03
1.96
2.97
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.90
4.03
1.96
2.97
3.00

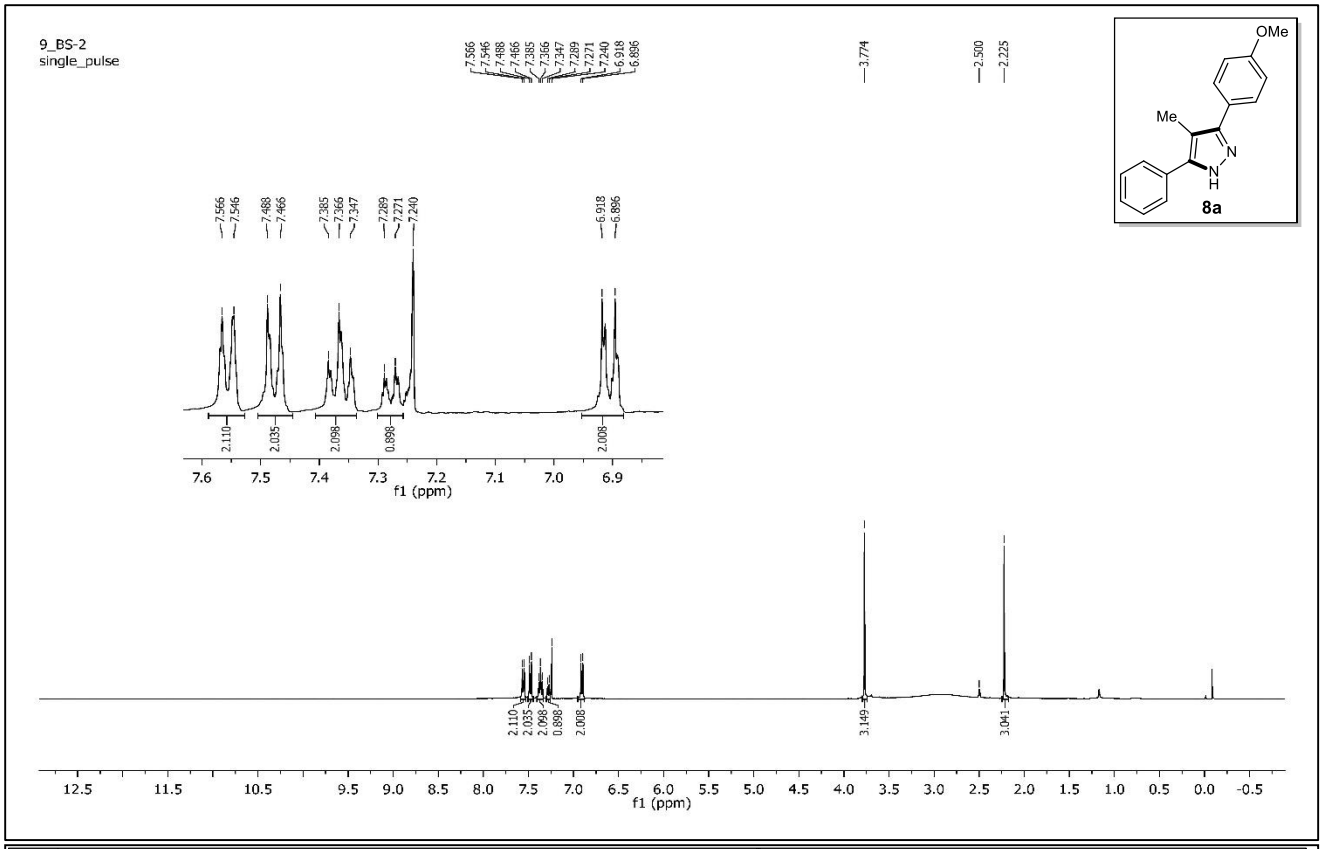

B-561-0me-F
F
N
N
H
MeO
7a
abundance
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
162.982
160.551
159.102
127.132
127.046
126.532
115.786
115.595
114.938
114.346
114.203
98.853
55.127
40.129
39.920
39.710
39.500
39.290
39.080
38.871
X : parts per Million : Carbon13

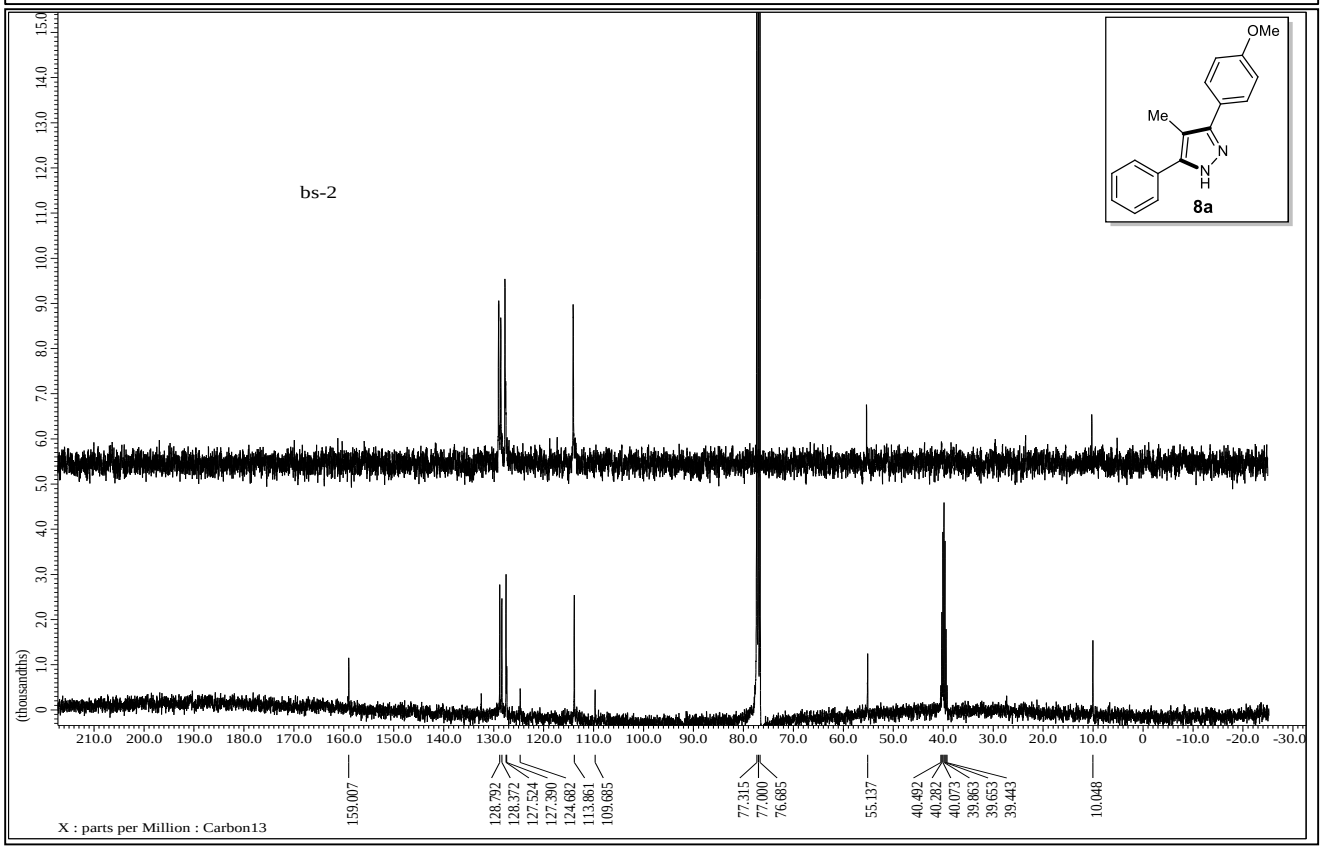

B-564
13.464
8.645
8.277
8.262
8.155
8.139
7.776
7.760
7.730
7.714
7.699
7.283
7.041
7.025
3.792
3.391
2.500
MeO
7b
0.91
2.00
3.04
0.96
2.02
0.97
3.00
ppm

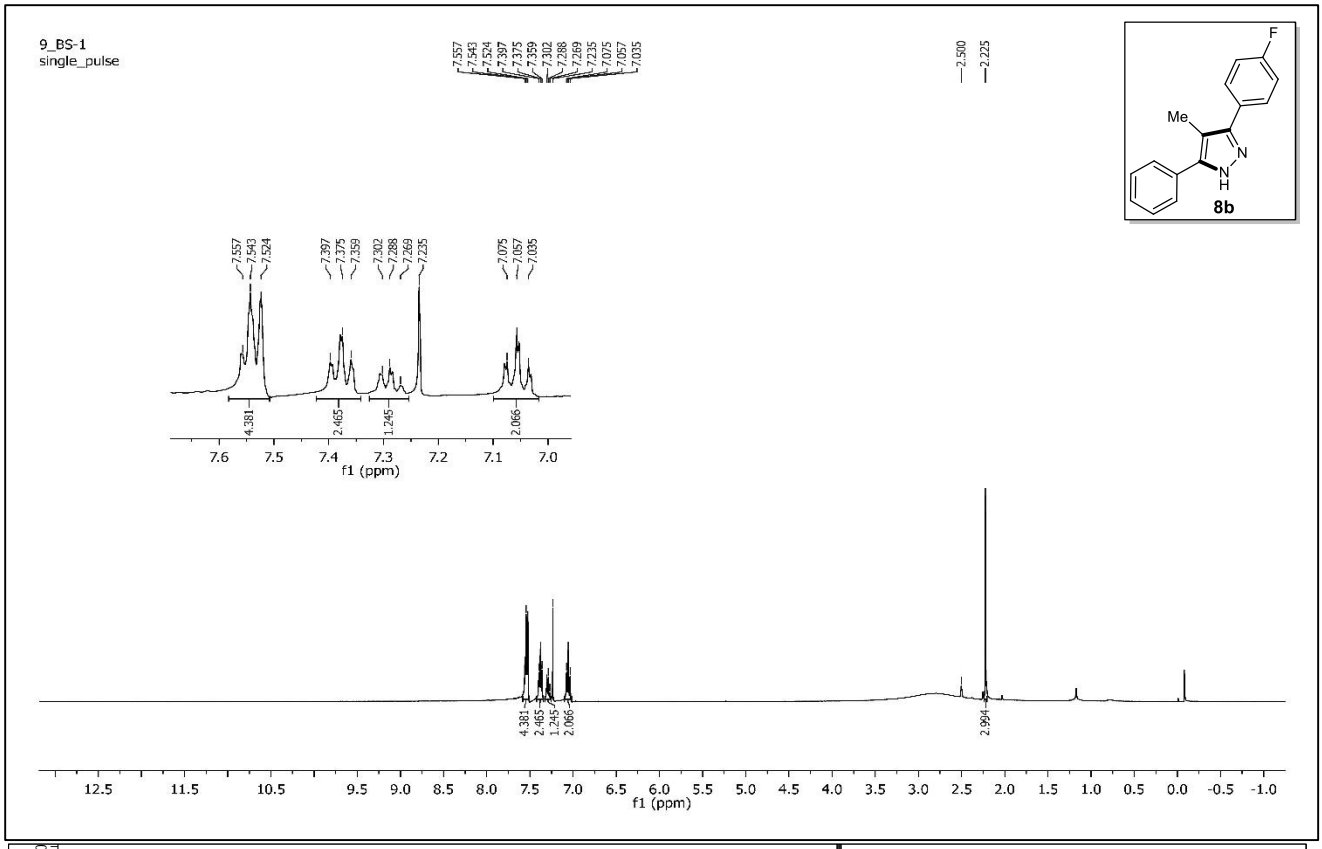

B-564
159.140
132.138
126.791
126.780
126.560
114.299
99.015
55.127
40.120
39.920
39.710
39.500
39.290
39.080
38.871
MeO
7b
abundance
X : parts per Million : Carbon13

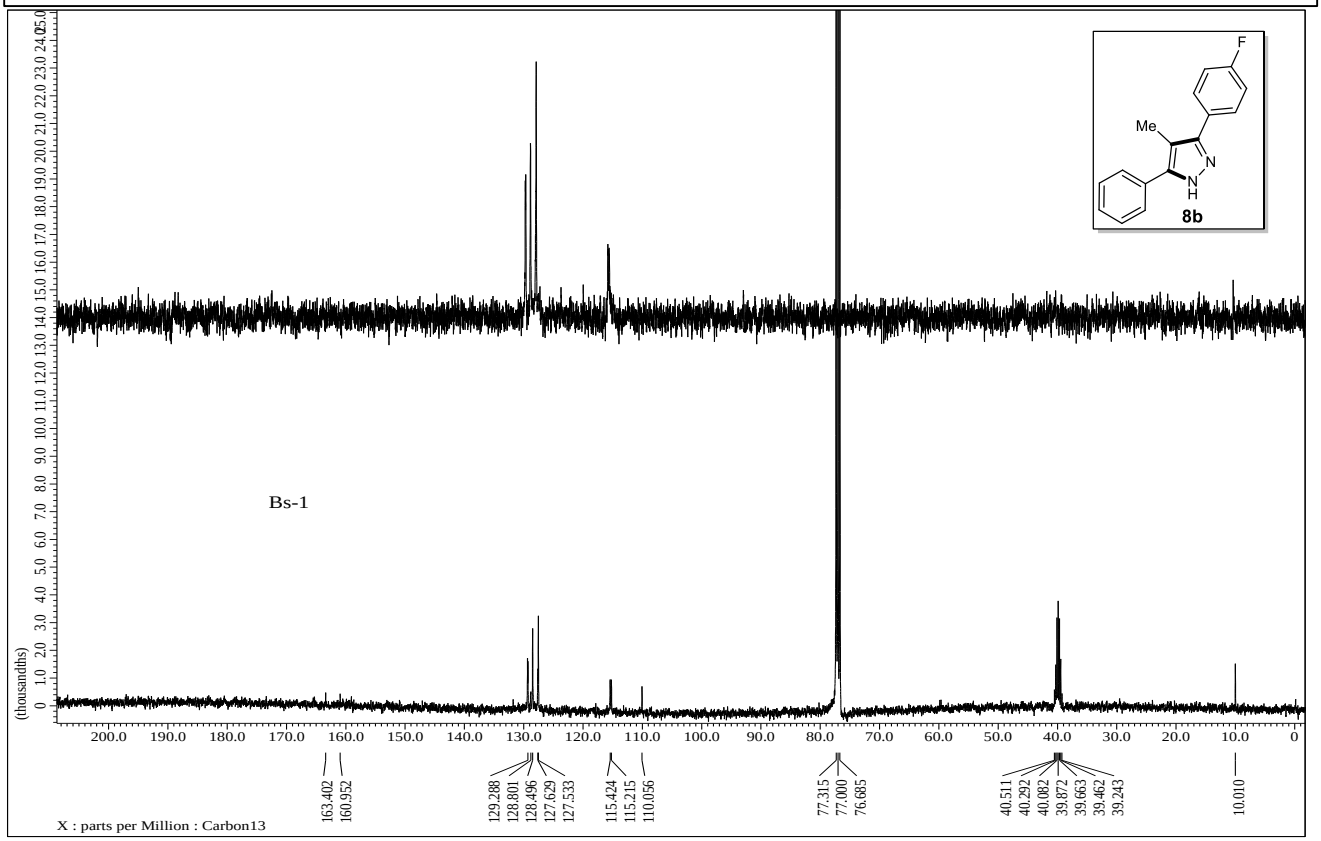

B-562-1
B-562-1
13.392
7.785
7.768
7.719
7.706
7.689
7.489
7.473
7.460
7.444
7.153
7.139
7.124
7.028
7.011
3.772
2.500
F
N
N
H
MeO
7c
f1 (ppm)
0.959
2.048
2.060
1.006
2.057
2.034
3.000

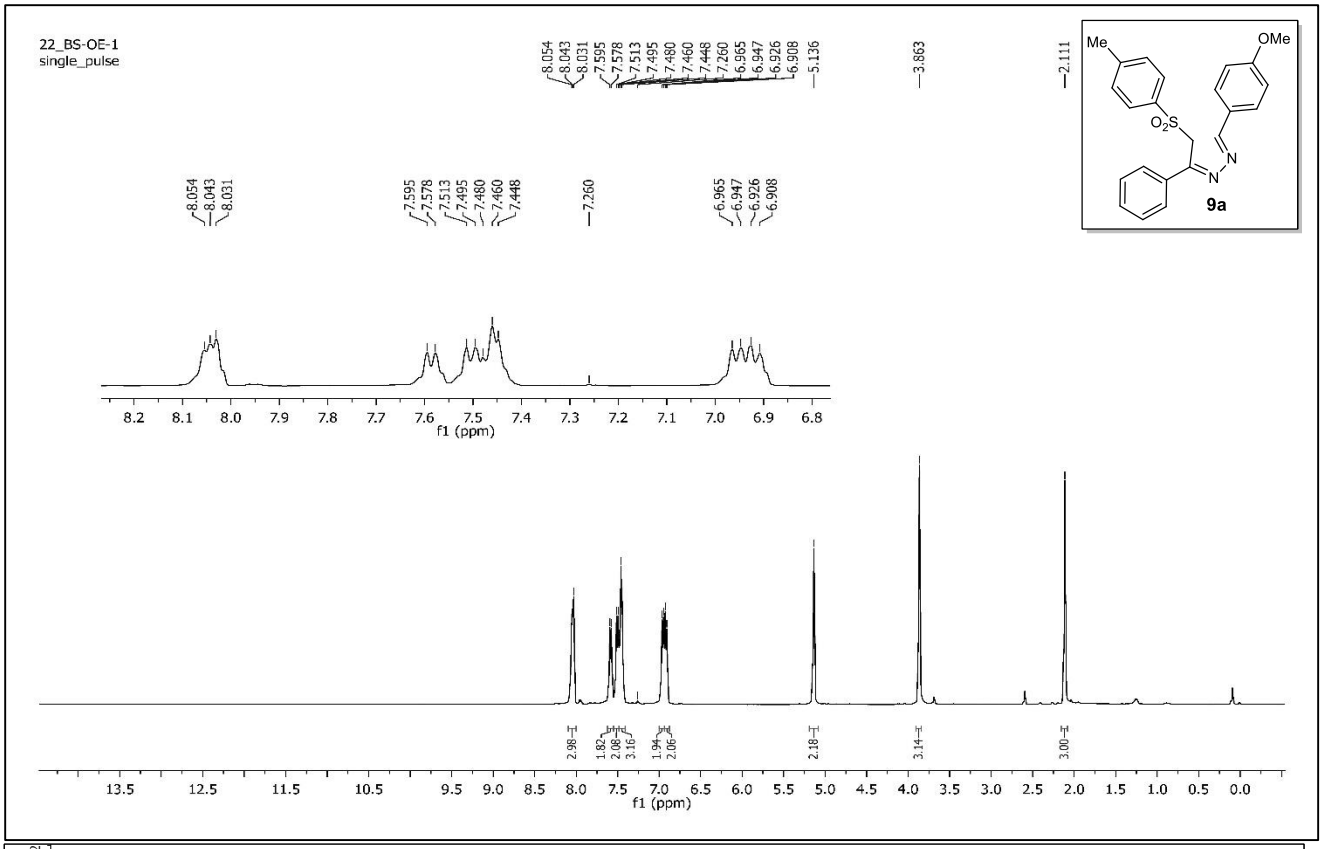

B-562
F
N
N
H
MeO
7c
abundance
X : parts per Million : Carbon13
163.869
161.457
159.159
134.979
130.755
126.551
123.500
121.154
114.289
114.108
111.772
111.553
99.387
55.099
40.120
39.910
39.700
39.500
39.290
39.080
38.871

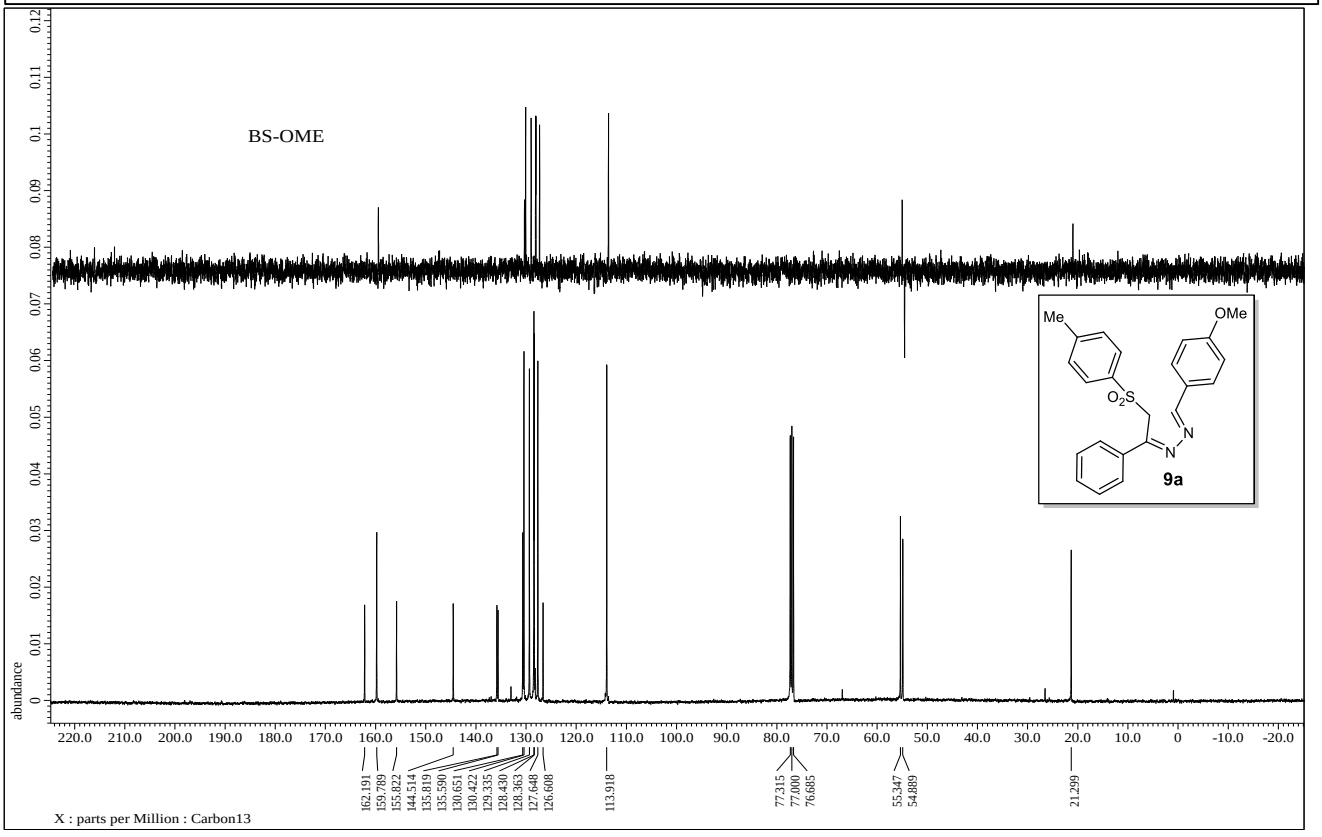

9_BS-2
single_pulse
OMe
Me
N
N
H
8a
f1 (ppm)

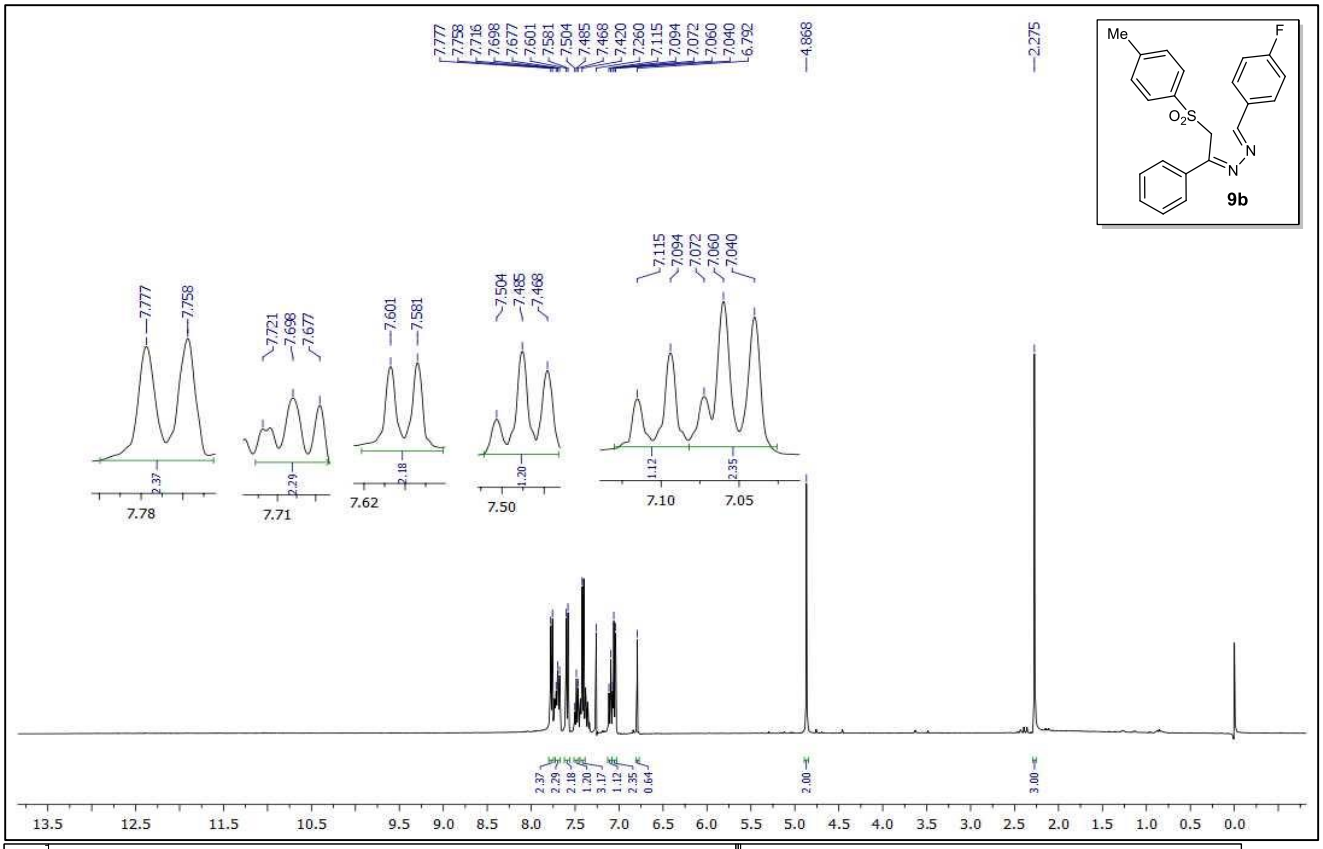

bs-2
OMe
Me
N
N
H
8a
(thousandths)
X : parts per Million : Carbon13

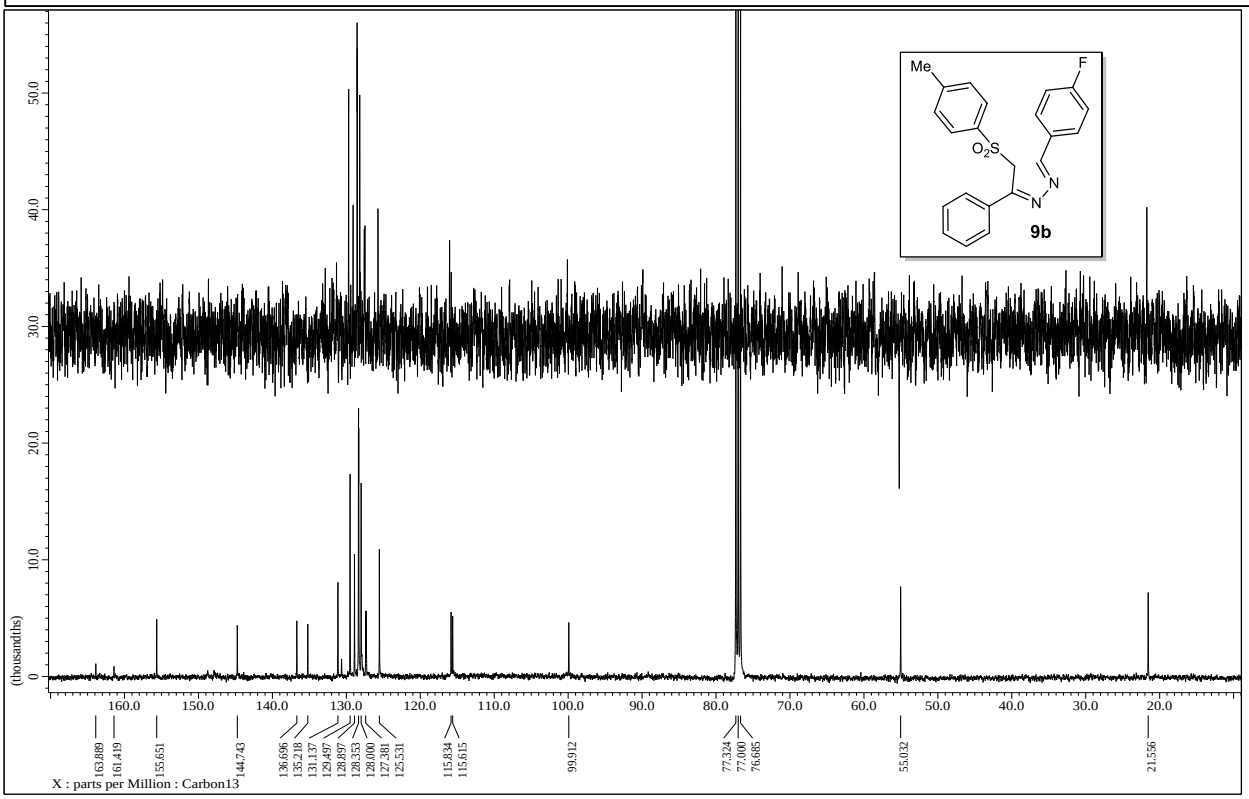

9_BS-1
single_pulse
7.557
7.543
7.524
7.397
7.375
7.359
7.302
7.288
7.269
7.235
7.075
7.057
7.035
2.500
2.225
F
Me
N
N
H
8b
4.381
2.465
1.245
2.066
2.994
f1 (ppm)

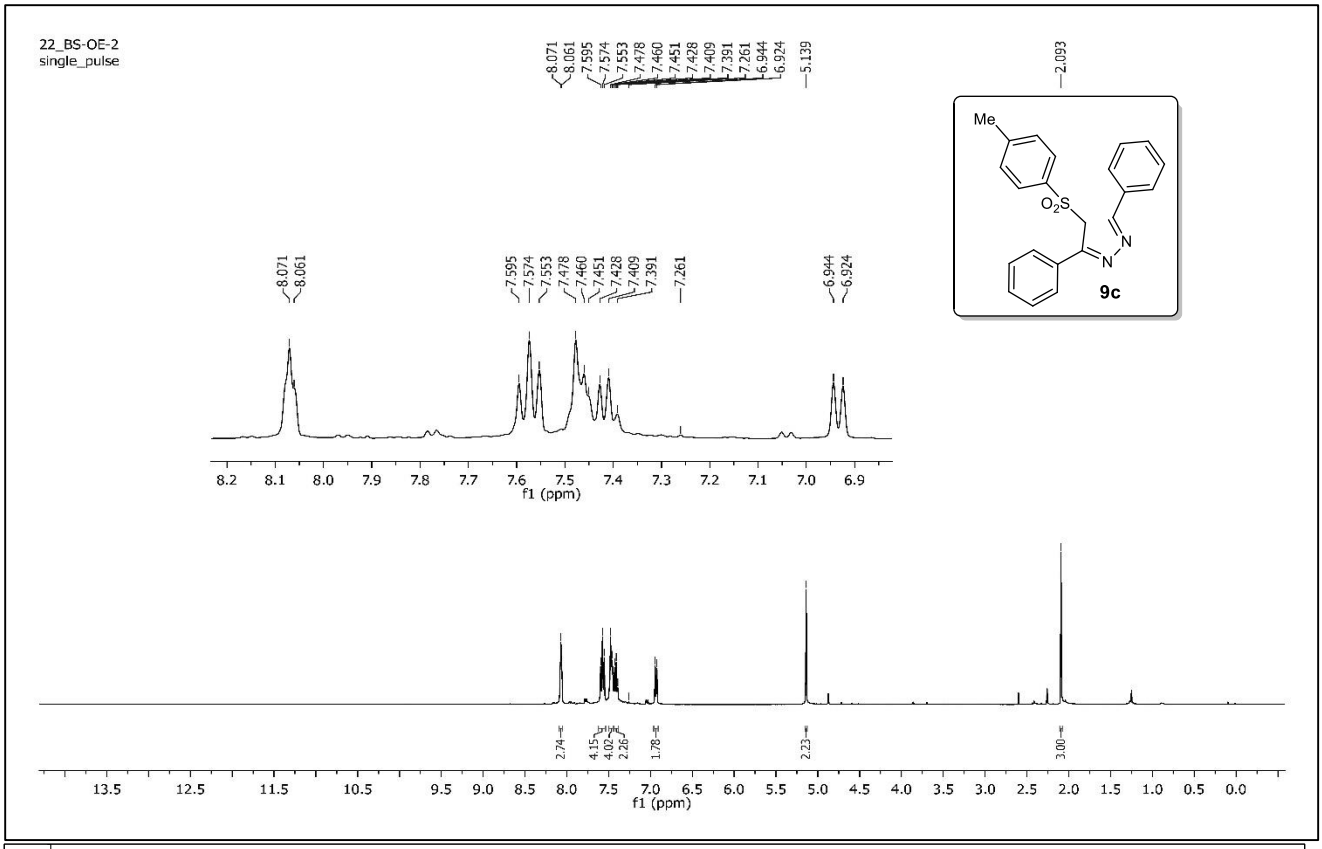

F
Me
N
N
H
8b
Bs-1
(thousandths)
163.402
160.952
129.288
128.801
128.496
127.629
127.533
115.424
115.215
110.056
77.315
77.000
76.685
40.511
40.292
40.082
39.872
39.663
39.462
39.243
10.010
X : parts per Million : Carbon13

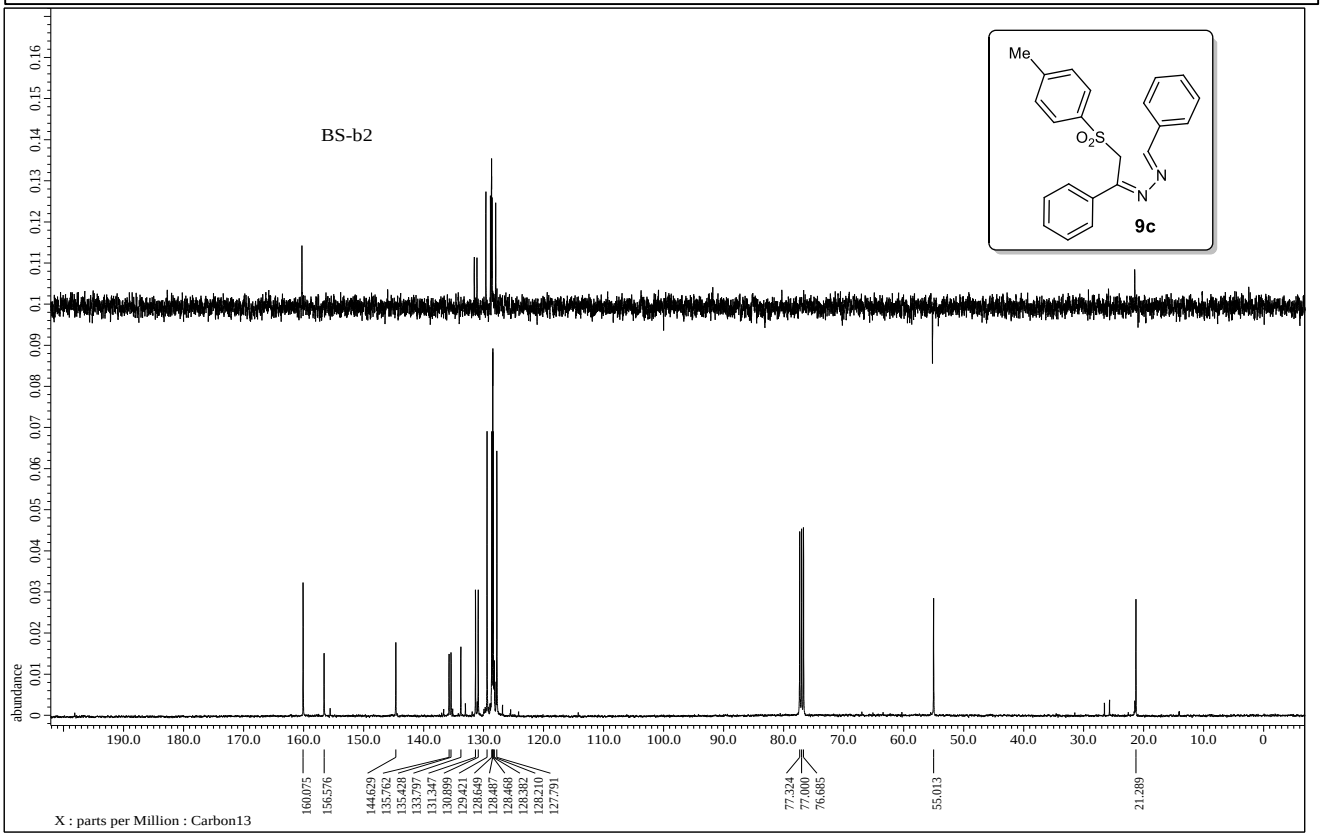

22_BS-OE-1
single_pulse
8.054
8.043
8.031
7.595
7.578
7.513
7.495
7.480
7.460
7.448
7.260
6.965
6.947
6.926
6.908
5.136
3.863
2.111
Me
OMe
O2S
N
N
9a
f1 (ppm)
2.98
1.82
2.08
3.16
1.94
2.06
2.18
3.14
3.00

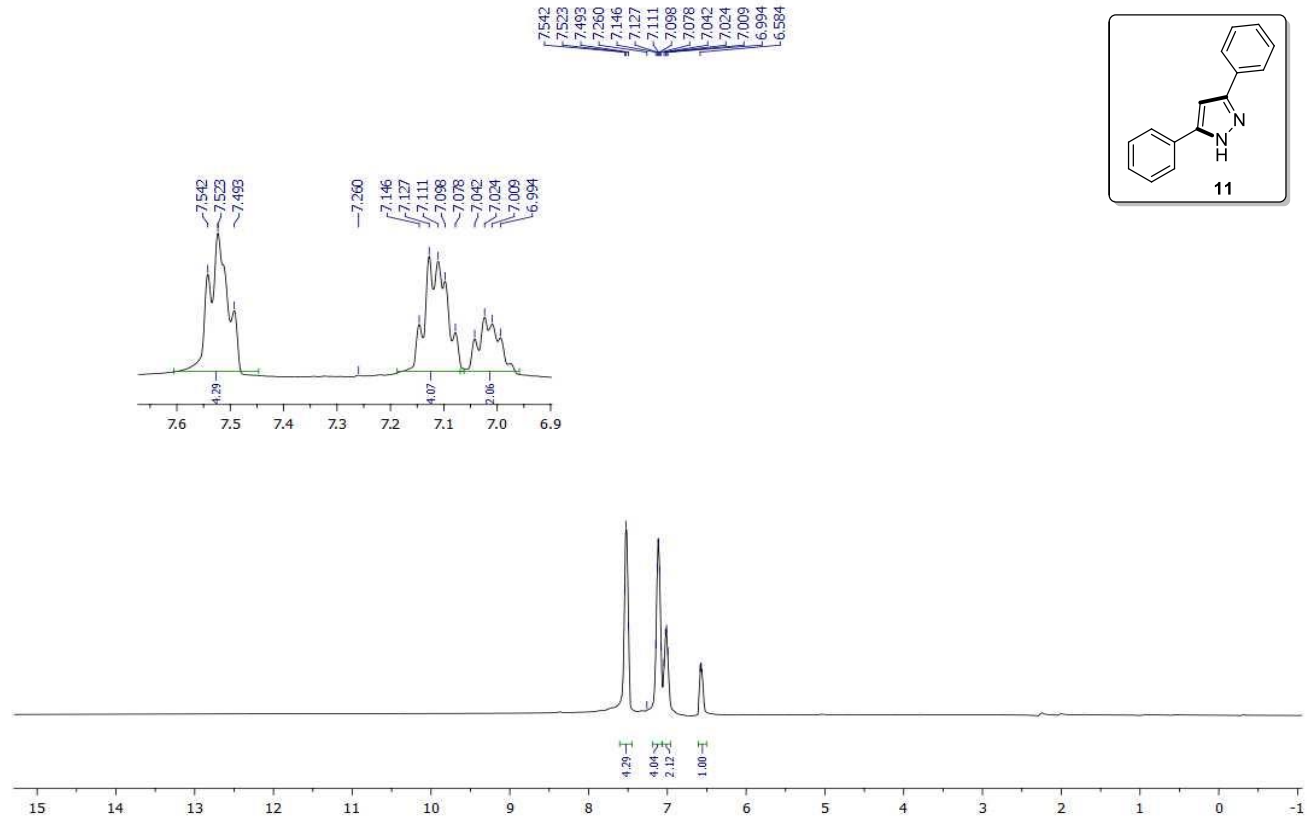

BS-OME
abundance
Me
OMe
O2S
N
N
9a
162.191
159.789
155.822
144.514
135.819
135.590
130.651
130.422
129.335
128.430
128.363
127.648
126.608
113.918
77.315
77.000
76.685
55.347
54.889
21.299
X : parts per Million : Carbon13

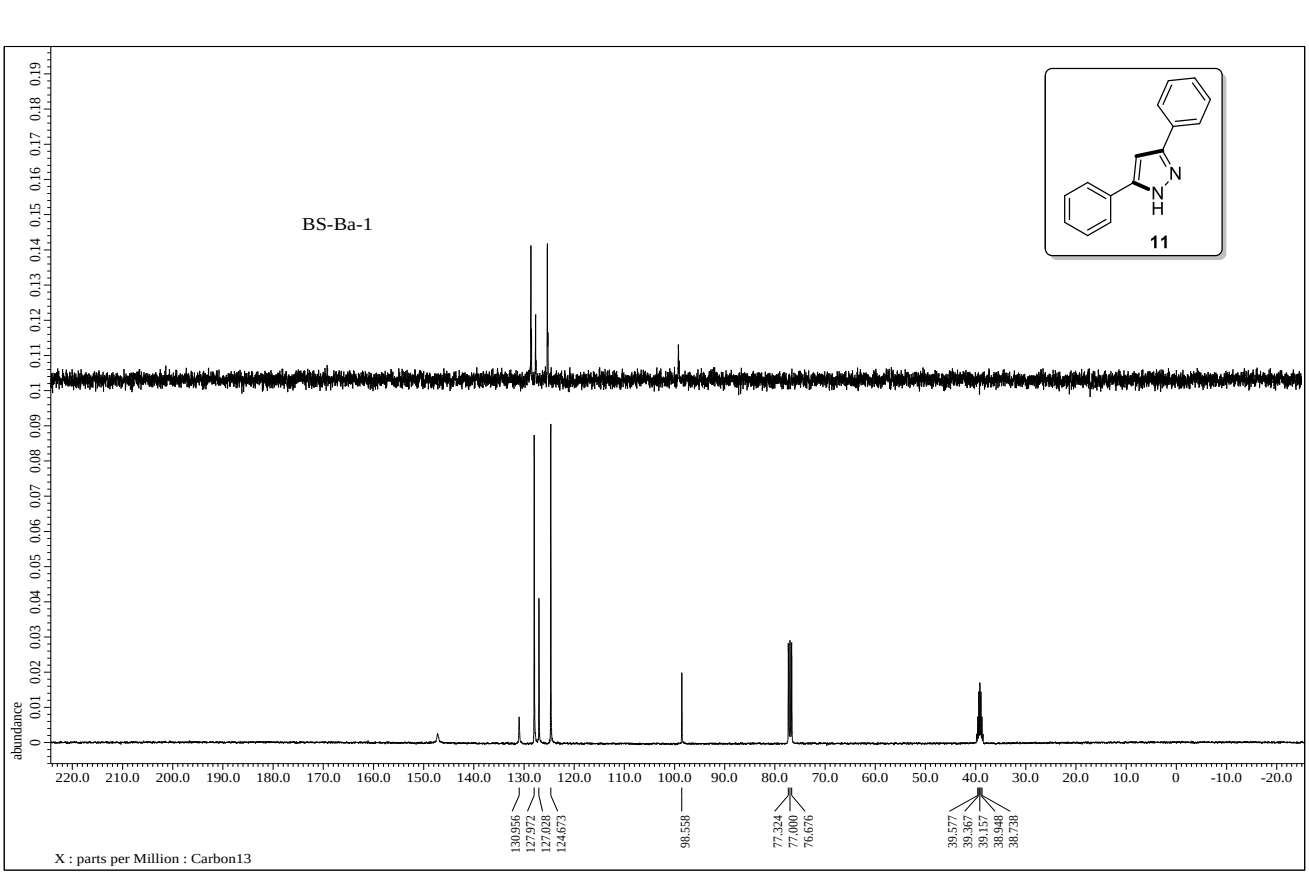

7.777
7.758
7.716
7.698
7.677
7.601
7.581
7.504
7.485
7.468
7.420
7.260
7.115
7.094
7.072
7.060
7.040
6.792
4.868
2.275
Me
F
O2S
N
N
9b
7.78
7.71
7.62
7.50
7.10
7.05
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

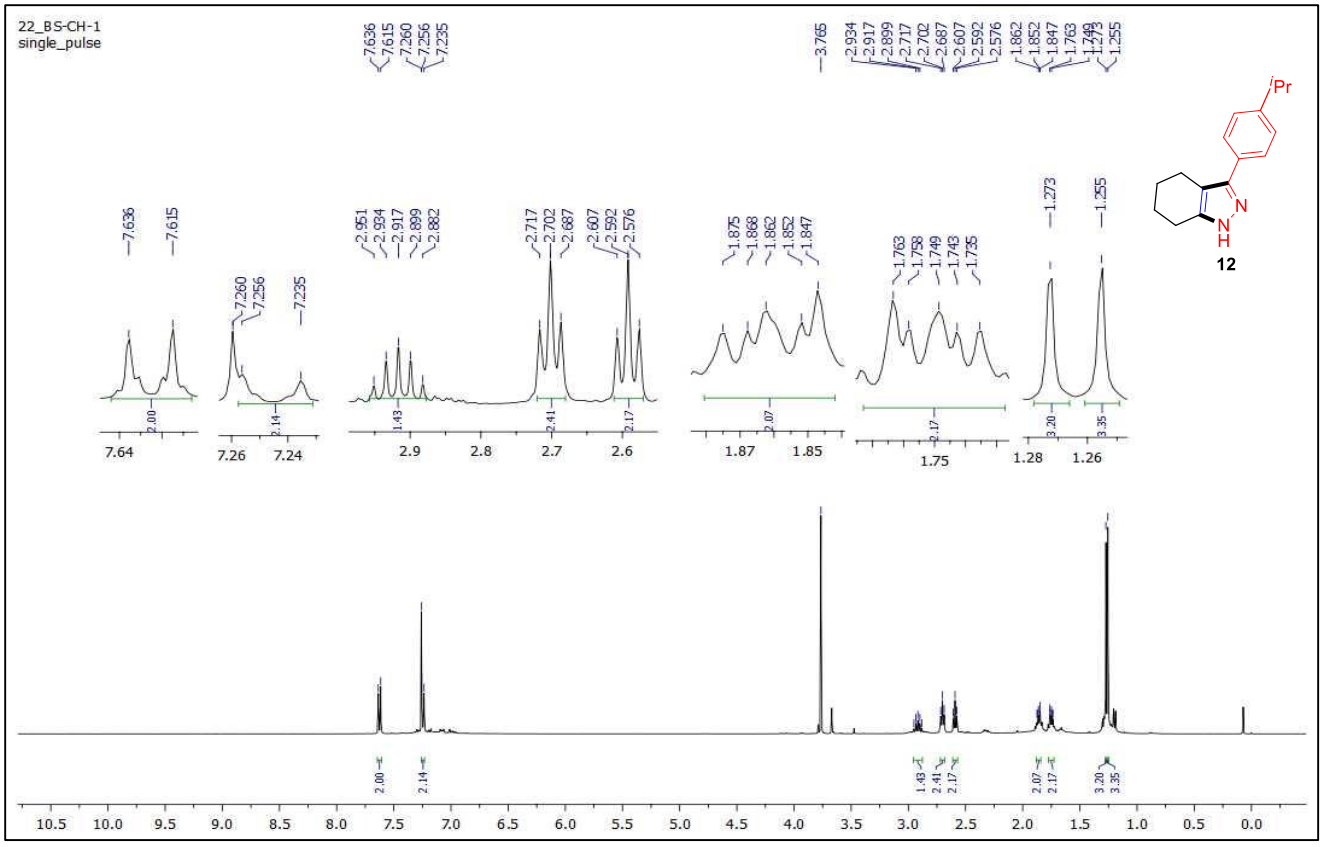

Me
F
O2S
N
N
9b
(thousandths)
50.0
40.0
30.0
20.0
10.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
163.889
161.419
155.651
144.743
136.696
135.218
131.137
129.497
128.897
128.353
128.000
127.581
125.531
115.834
115.615
99.912
77.324
77.000
76.685
55.032
21.556
X : parts per Million : Carbon13

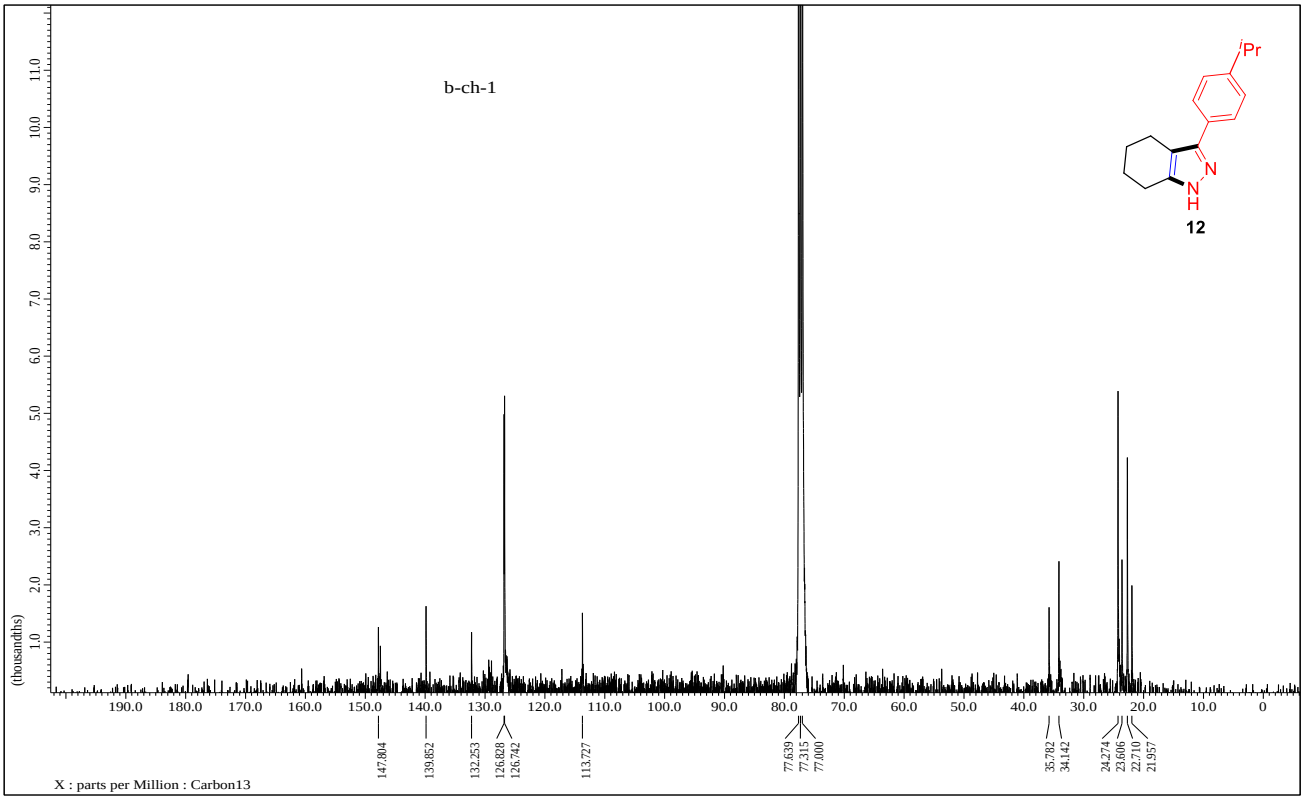

22_BS-OE-2
single_pulse
8.071
8.061
7.595
7.574
7.553
7.478
7.460
7.451
7.428
7.409
7.391
7.261
6.944
6.924
5.139
2.093
Me
O2S
N
N
9c
f1 (ppm)
2.74
4.15
4.02
2.26
1.78
2.23
3.00


BS-b2
Me
O2S
N
N
9c
abundance
f1 (ppm)
160.075
156.576
144.629
135.762
135.428
133.797
131.347
130.899
129.421
128.649
128.487
128.468
128.382
128.210
127.791
77.324
77.000
76.685
55.013
21.289
X : parts per Million : Carbon13


7.542
7.523
7.493
7.260
7.146
7.127
7.111
7.098
7.078
7.042
7.024
7.009
6.994
6.584
11


BS-Ba-1
11
abundance
130.956
127.972
127.028
124.673
98.558
77.324
77.000
76.676
39.577
39.367
39.157
38.948
38.738
X : parts per Million : Carbon13


22_BS-CH-1
single_pulse
12


b-ch-1
12
(thousandths)
X : parts per Million : Carbon13