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Supplementary Information

Ferrocene modified analogues of imatinib and nilotinib as potent anti-cancer agents

Irena Philipova, a Rositsa Mihaylova, Georgi Momekov, Rostislava Angelova and Georgi Stavrakov *ab

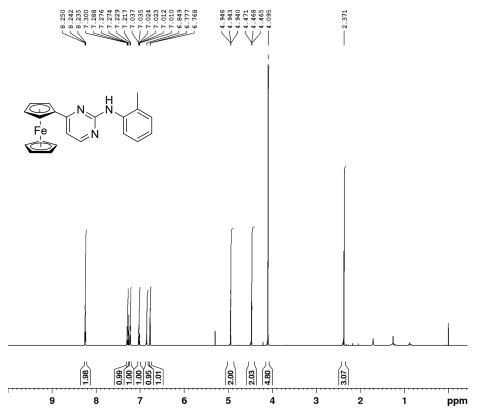
Copies of ¹H and ¹³C NMR spectra of the target compounds.

¹H NMR monitoring of 15a stability in DMSO-d₆ (80%) / PBS in D₂O (20%)

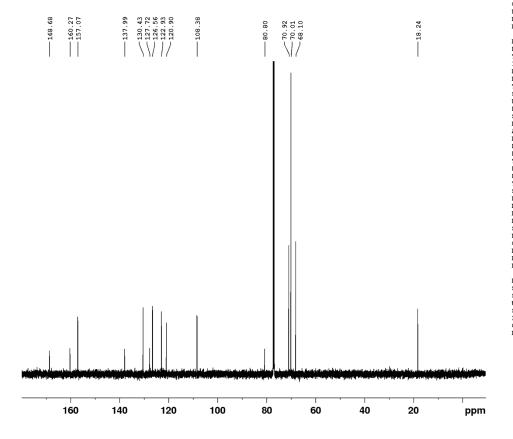
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Compound 3

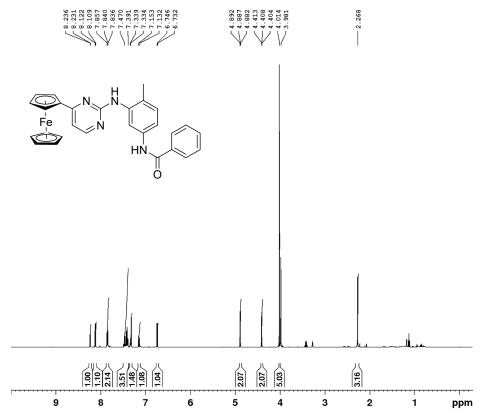


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PROBHD	Z847801_0047 (
PULPROG	zg30	
TD	65536	
SOLVENT	CDC13	
NS	16	
DS	0	
SWH	9615.385	Hz
FIDRES	0.293438	Hz
AQ	3.4078720	sec
RG	203	
DW	52.000	use
DE	14.38	use
TE	293.0	K
D1	2.00000000	sec
TDO	1	
SFO1	599.9845606	MHz
NUC1	1H	
P0	3.60	use
P1	10.80	use
PLW1	20.00000000	W
	ocessing paramete	ers
SI	65536	
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WDW	EM	
SSB	0	
LB	0	Ηz
GB	0	
PC	1.00	

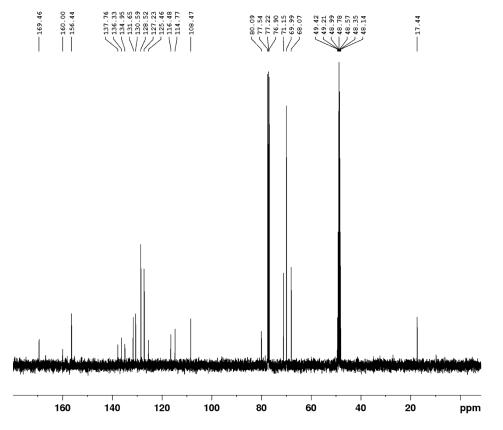


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PROCNO	1	
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Date	20220318	
Time	4.38	h
INSTRUM	spect	**
	7801 0047 (
PULPROG	zgdc30	
TD	32768	
SOLVENT	CDC13	
NS	128	
	128	
DS		
SWH	36057.691	Hz
FIDRES	2.200787	Hz
AQ		sec
RG	2050	
D₩	13.867	
DE		usec
TΕ	293.1	
D1	1.50000000	
D11	0.03000000	sec
TD0	1	
SFO1	150.8816889	MHz
NUC1	13C	
P0	3.27	usec
P1	9.80	usec
PLW1	40.00000000	W
SFO2	599.9824003	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	70.00	usec
PLW2	20.00000000	
PLW12	0.53044999	
LUNIE	0.55044555	
F2 - Process	ing paramete	re
SI	65536	113
SF	150.8650910	MU.
WDW	EM	MHZ
	EM.	
SSB	1.00	
LB		Hz
GB	0	
PC	1.40	

Compound 9

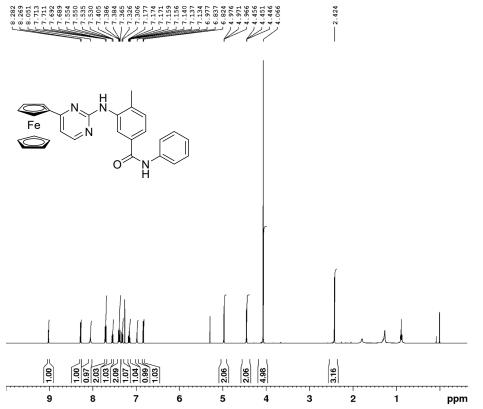


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PULPROG	zg30	
TD	65536	
SOLVENT	MeOD	
NS	32	
DS	0	
SWH	6578.947	
FIDRES	0.200774	
AQ	4.9807358	sec
RG	101	
DW	76.000	
DE	7.79	
TE	298.0	
D1	2.00000000	sec
TD0	1	
SFO1	400.1330415	MHz
NUC1	1H	
P0	3.33	
P1	10.00	usec
PLW1	20.07200050	W
F2 - Pro	cessing paramete	ers
SI	65536	
SF	400.1300230	MHz
WDW	EM	
SSB	0	
LB	0	Hz
GB	0	
PC	1.00	



Current Dat	ta Parameters	
NAME	FL09402	
EXPNO	18	
PROCNO	1	
F2 - Acqui:	sition Paramet	ters
Date_	20220517	
Time	14.06	h
INSTRUM A	vance Neo 400	
PROBHD Z:	175272_0007 (
PULPROG	zgdc30	
TD	32768	
SOLVENT	MeOD	
NS	128	
DS	0	
SWH	23809.523	
FIDRES	1.453218	
AQ	0.6881280	sec
RG	32	
D ₩	21.000	
DE	6.50	
TE	298.0	
D1	1.50000000	
D11	0.03000000	sec
TD0	1	
SF01	100.6238383	MHz
NUC1	13C	
P0		usec
P1	10.00	
PLW1	58.46900177	
SFO2	400.1316008	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	
PLW2	20.07200050	
PLW12	0.24781001	W
	ssing paramete	ers
SI	65536 100.6127690	
SF	100.612/690 EM	
WDW		
SSB	0	TT-
LB GB	1.00	nz
PC PC	1.40	
FC	1.40	

Compound 15a

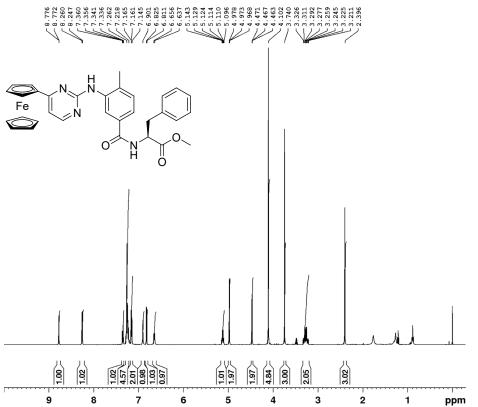


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PROBHD	Z175272 0007 (
PULPROG	zg30	
TD	32768	
SOLVENT	CDC13	
NS	32	
DS	0	
SWH	6578.947	u-
FIDRES	0.401547	
AQ.	2.4903679	
RG	2.4903679	sec
DW	76.000	
	76.000	
DE	7.79 298.0	
TE		
D1	2.00000000	sec
TD0	1	
SFO1	400.1330415	
NUC1	1H	
P0	3.33	
P1	10.00	
PLW1	20.07200050	W
	cessing paramete	ers
SI	65536	
SF	400.1300102	MHz
WDW	EM	
SSB	0	
LB	0	Hz
GB	0	
PC	1.00	

168.97 —— 165.98 —— 159.86		138.44	130.83	124.34	117.91			80.45	71.22					18.23	
 المادية المادية	addille buses	دار دار در در				وروا المراوات المراوا	المتلا في المتلا ا	Medie	11 h. (1)	سهامة الخاد الماميد	ماند و رود	mt. al l 181	مالا المالية		والمراجعة

	a Parameters	
NAME	FL08402	
EXPNO	12	
PROCNO	1	
	ition Parame	ters
Date_	20220411	
Time	18.02	h
INSTRUM Av	ance Neo 400	
	75272_0007 (
PULPROG	zgdc30	
TD	32768	
SOLVENT	CDC13	
NS	128	
DS	0	
SWH	23809.523	Hz
FIDRES	1.453218	
AQ	0.6881280	sec
RG	22.6	
D W	21.000	
DE	6.50	usec
TE	298.0	K
D1	1.50000000	
D11	0.03000000	sec
TD0	1	
SFO1	100.6238383	
NUC1	13C	
P0		usec
P1	10.00	
PLW1	58.46900177	
SFO2	400.1316008	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	
PLW2	20.07200050	
PLW12	0.24781001	W
	sing paramet	ers
SI	65536	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

Compound 15b

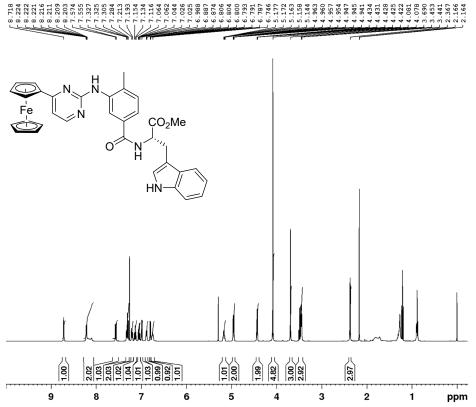


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PROCNO	1	
PROCNO	-	
F2 - Acc	quisition Paramet	ers
Date_	20220418	
Time	16.56	h
INSTRUM	Avance Neo 400	
PROBHD	Z175272_0007 (
PULPROG	zg30	
TD	32768	
SOLVENT	CDC13	
NS	32	
DS	0	
SWH	6578.947	Ηz
FIDRES	0.401547	Hz
AQ.	2.4903679	sec
RG	101	
DW	76,000	use
DE	7.79	use
TE	298.0	K
D1	2.00000000	sec
TD0	1	
SFO1	400.1330415	MHz
NUC1	1H	
P0	3.33	use
P1	10.00	use
PLW1	20.07200050	W
E0 D		
	cessing paramete 65536	ers
SI		M77 -
SF	400.1300103 EM	MHZ
WDW		
SSB	0	**-
LB	0	Hz
GB	0	
PC	1.00	

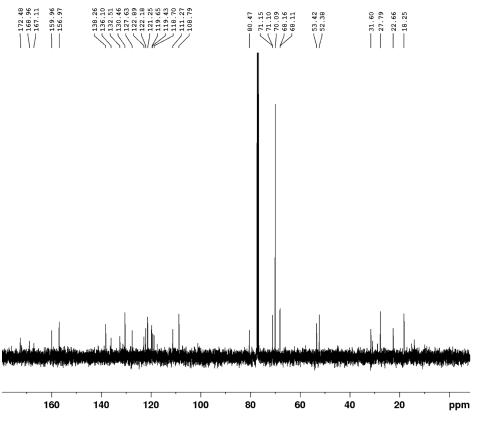
172.11	159.97 156.98	138.36 136.01 132.52 131.24 130.52	128.60		80.46 71.13 70.08 68.15	52.34	38.09	18.27
Li								
ساز بدو اود زاد خارد الاحطر إن الامورد وي سور سواس چاران موجد چارارا و کاچه	, 1 (1 (1 (1 (1 (1 (1 (1 (1 (1 (1 (1 (1 (1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-	i k danily i i i k dayada	en eta erregia elipto-sosta eli		and tracking of the second	1	Activity of the control to the contr
180	160	140	120	100	80	60	40	20 ppm

Current Dat	a Parameters	
NAME	FL08802	
EXPNO	12	
PROCNO	1	
22100110	-	
F2 - Acquis	ition Paramet	ters
Date_	20220418	
Time	17.02	h
	ance Neo 400	
	75272 0007 (
PULPROG	zgdc30	
TD	32768	
SOLVENT	CDC13	
NS	128	
DS	0	
SWH	23809.523	u-
FIDRES	1.453218	
AO	0.6881280	
RG	22.6	
DW	21.000	
DE	6.50	
	298.0	
TE D1	1.50000000	
	0.03000000	
D11 TD0	0.03000000	sec
	100.6238383	
SFO1 NUC1	100.6238383 13C	MHZ
	3.33	
P0		
P1	10.00	
PLW1	58.46900177	
SFO2	400.1316008	
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	
PLW2	20.07200050	
PLW12	0.24781001	W
	sing paramete	ers
SI	65536	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

Compound 15c

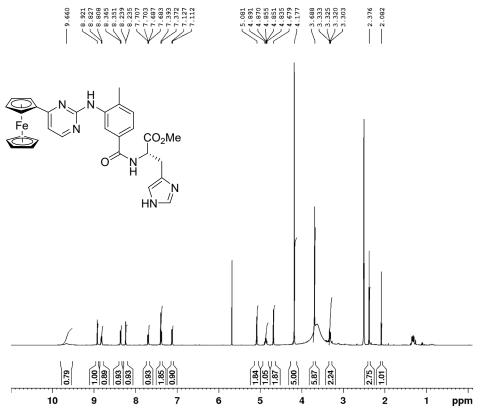


NAME	Data Parameters FL08902	
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PROCNO	1	
	quisition Paramet	ters
Date_	20220419	
Time	16.40	h
	Avance Neo 400	
PROBHD	Z175272_0007 (
PULPROG	zg30	
TD	32768	
SOLVENT	CDC13	
NS	32	
DS	0	
SWH	6578.947	
FIDRES	0.401547	
AQ	2.4903679	
RG	101	
DW DE	76.000 7.79	
DE TE	7.79 298.0	
D1	2,00000000	
TD0	2.00000000	sec
SFO1	400.1330415	MII.
NUC1	400.1330415 1H	
PO	3.33	
P1	10.00	
PLW1	20.07200050	
F2 - Pro	cessing paramete 65536	ers
SF	400.1300107	мна
WDW	EM	
SSB	0	
LB	0	Hz
GB	0	
	1.00	

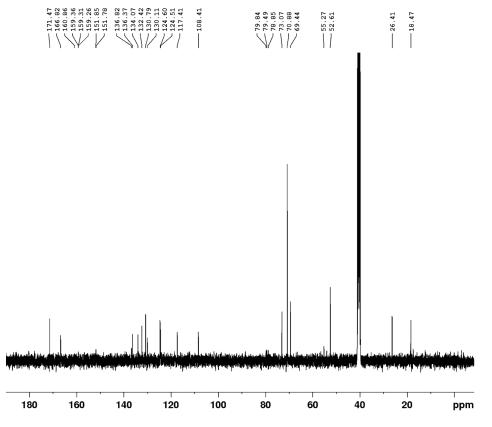


	a Parameters	
NAME	FL08902	
EXPNO	12	
PROCNO	1	
F2 - Acmis	ition Paramet	ers
Date_	20220419	
Time	16.45	h
	ance Neo 400	
	75272 0007 (
PULPROG	zadc30	
TD	32768	
SOLVENT	CDC13	
NS	128	
DS	0	
SWH	23809.523	Hz
FIDRES	1.453218	Hz
AQ	0.6881280	sec
RG	22.6	
D W	21.000	usec
DE	6.50	usec
TE	298.0	K
D1	1.50000000	sec
D11	0.03000000	sec
TD0	1	
SF01	100.6238383	MHz
NUC1	13C	
P0	3.33	
P1	10.00	
PLW1	58.46900177	
SFO2	400.1316008	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	
PLW2	20.07200050	
PLW12	0.24781001	W
F2 - Proces	sing paramete	ers
SI	65536	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	0.50	

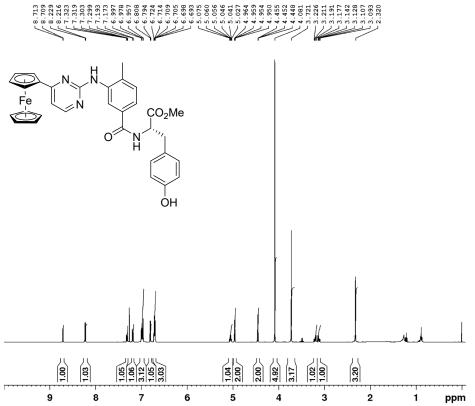
Compound 15d



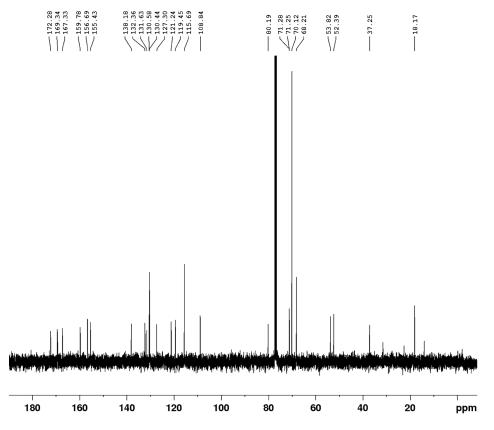
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EXPNO	24	
PROCNO	1	
11100110	-	
F2 - Acqu	isition Paramet	ters
Date_	20220513	
Time	14.58	h
INSTRUM	Avance Neo 400	
	Z175272 0007 (
PULPROG	zg30	
TD	32768	
SOLVENT	DMSO	
NS	32	
DS	0	
SWH	6578.947	U-
FIDRES	0.401547	
AO	2.4903679	
RG	101	
DW	76.000	
DE		usec
TE	353.0	
D1	2.00000000	
TD0	2.00000000	sec
SFO1	400.1330415	M77 -
NUC1	400.1330413 1H	
PO		usec
P0 P1	10.00	
PLW1	20.07200050	
PLIMI	20.07200050	W
F2 - Proc	essing paramete	ars
si	65536	
SF	400.1300037	
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SSB	0	
LB		Hz
GB	0	112
PC PC	1.00	
	1.00	



Compound 15e

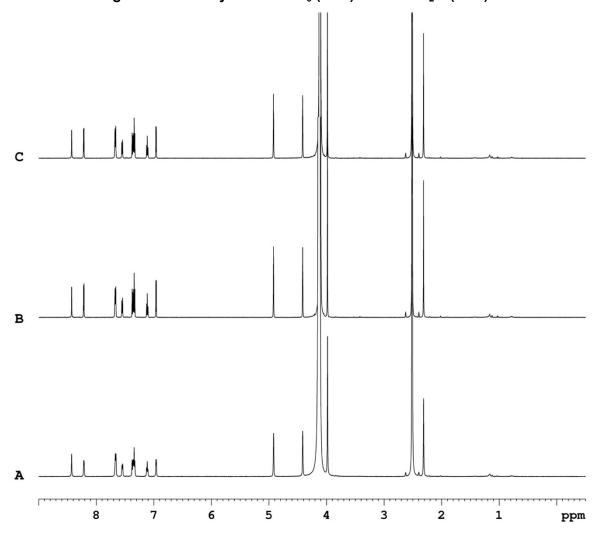


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PROBHD	Z175272_0007 (
PULPROG	zg30	
TD	32768	
SOLVENT	CDC13	
NS	32	
DS	0	
SWH	6578.947	
FIDRES	0.401547	
AQ	2.4903679	se
RG	101	
DW	76.000	
DE	7.79	
TE	298.0	
D1	2.00000000	se
TD0	1	
SFO1	400.1330415	MH
NUC1	1H	
P0	3.33	us
P1	10.00	us
PLW1	20.07200050	W
F2 - Pro	cessing paramete	ers
SI	65536	
SF	400.1300098	MH
WDW	EM	
SSB	0	
LB	0	Ηz
GB	0	
	1.00	



NAME	FL09302	
EXPNO	12	
PROCNO	1	
LICOMO	-	
F2 - Acmi	sition Paramet	ers
Date_	20220510	-615
Time	18.38	h
	vance Neo 400	**
	175272 0007 (
PULPROG	zgdc30	
TD	32768	
SOLVENT	CDC13	
	128	
NS		
DS	0	
SWH	23809.523	
FIDRES	1.453218	
AQ	0.6881280	sec
RG	22.6	
D₩	21.000	
DE	6.50	
TE	298.0	
D1	1.50000000	
D11	0.03000000	sec
TD0	1	
SF01	100.6238383	MHz
NUC1	13C	
P0	3.33	
P1	10.00	
PLW1	58.46900177	
SFO2	400.1316008	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	
PLW2	20.07200050	
PLW12	0.24781001	W
	ssing paramete	ers
SI	65536	
SF	100.6127690	MHZ
WDW	EM	
SSB	0	
LB	1.00	Hz
GB		
PC	1.40	

1 H NMR monitoring of 15a stability in DMSO- d_{6} (80%) / PBS in D₂O (20%)



Spectra recorded at: \mathbf{A} t = 0 min; \mathbf{B} t = 24 h; \mathbf{C} t = 4 d.