

Supplementary document

The synthesis and investigation of novel 3-benzoylbenzofurans and pyrazole derivatives for anti-HIV activity

Sinothile S. Khuzwayo¹, Mamoalosi A. Selepe², Debra Meyer³ and Ntombenhle H. Gama¹

¹ *Biochemistry Department, University of Pretoria, 2 Lynnwood road, Pretoria, 0002, South Africa.*

² *Chemistry Department, University of Pretoria, 2 Lynnwood road, Pretoria, 0002, South Africa.*

³ *School of Natural and Applied Sciences, Sol Plaatje University, Kimberley, 8300, South Africa.*

*Correspondence to:

Ms Sinothile Khuzwayo: snothilesementha81@gmail.com

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1.1 Results

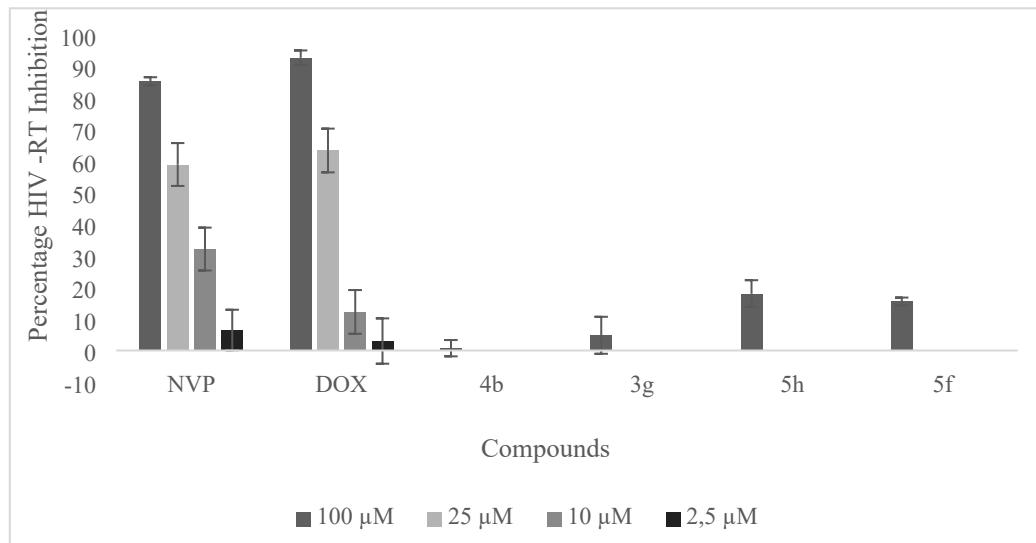


Fig. S1: Inhibition of HIV-1 RT by active compounds. Doxorubicin (DOX) and nevirapine (NVP) were used as controls in four decreasing concentrations to test the validity of the kit. The bars represent the mean \pm SEM obtained from three independent experiments.

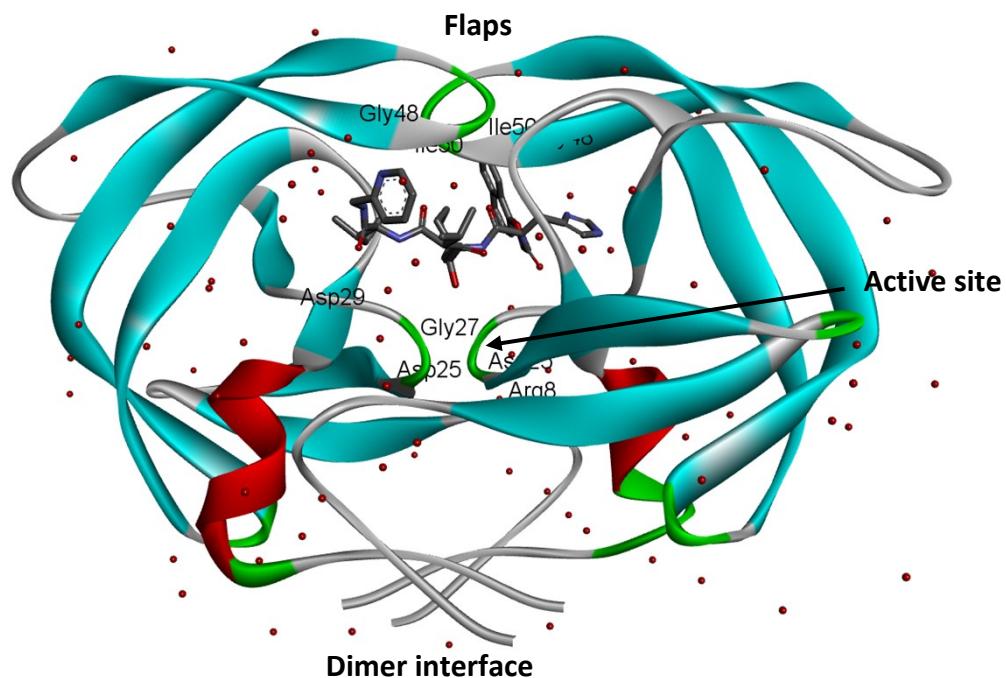


Fig. S2: Crystal structure of HIV-1 PR with an inhibitor. The catalytic site of HIV-1 protease showing a ligand and the amino acid residues that make up the active site. Created using Discovery Studio 2024.

Table S1: Analysis of drug-likeness of 3-benzoylbenzofurans and pyrazole derivatives according to the Lipinski and Pfizer rule.

Compound	MW (g/mol)	MLogP	nHA	nHD	TPSA Å ²	Lipinski rule	Pfizer rule	PAINS alerts
4b	340.37	1.75	5	0	57.90	Yes	No	0
5b	354.40	1.78	5	2	76.60	Yes	Yes	0
4d	411.25	2.94	4	0	48.67	Yes	No	0
5d	425.28	2.96	4	2	67.37	Yes	No	0
3f	286.25	1.76	5	1	59.67	Yes	No	0
5f	300.28	1.78	5	3	78.37	Yes	Yes	0
3g	328.32	0.74	6	1	78.13	Yes	Yes	0
5g	342.35	0.79	6	3	96.83	Yes	Yes	0
3h	298.29	1.05	5	1	68.90	Yes	No	0
5h	312.32	1.08	5	3	87.60	Yes	Yes	0
Saquenavir	670.84	1.40	7	5	166.75	No	Yes	0
Lenacapavir	968.30	4.86	12	2	174.70	No	Yes	0

Molecular weight; MW; g/mol, Lipophilicity; MlogP, Number of hydrogen bond acceptors; nHA, Number of hydrogen bond donors; nHD.

1.2 Spectra and analysis of chromatograms

1.2.1 NMR Spectra

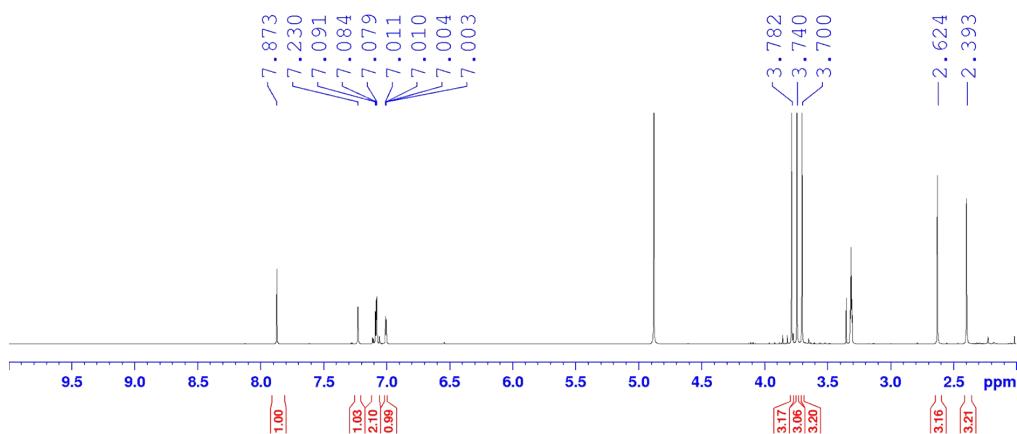


Plate 1a: The ¹H NMR (400 MHz, Methanol-d₄) spectrum for (2,5-dimethoxyphenyl)(5-methoxy-4,7-dimethyl-1-benzofuran-3-yl)methanone (**4a**).

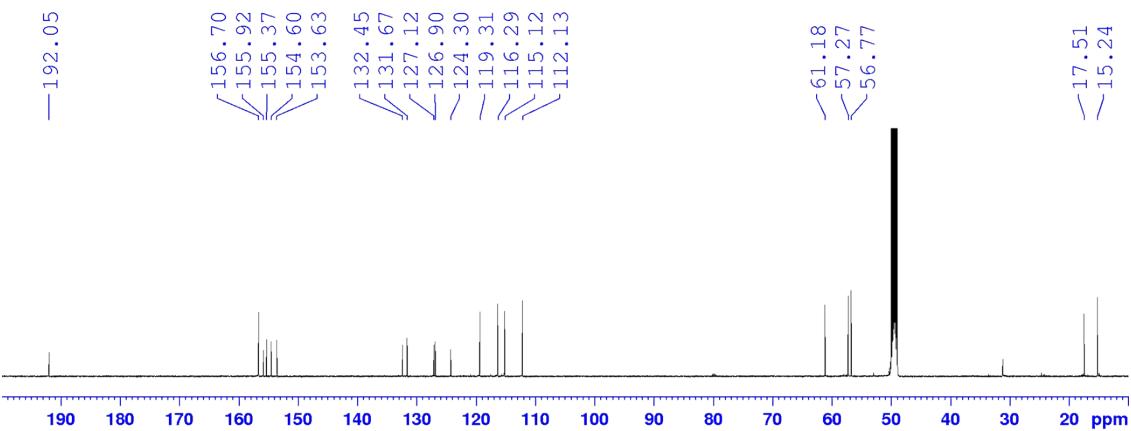


Plate 1b: The ^{13}C NMR (125 MHz, Methanol- d_4) spectrum for (2,5-dimethoxyphenyl)(5-methoxy-4,7-dimethyl-1-benzofuran-3-yl)methanone (**4a**).

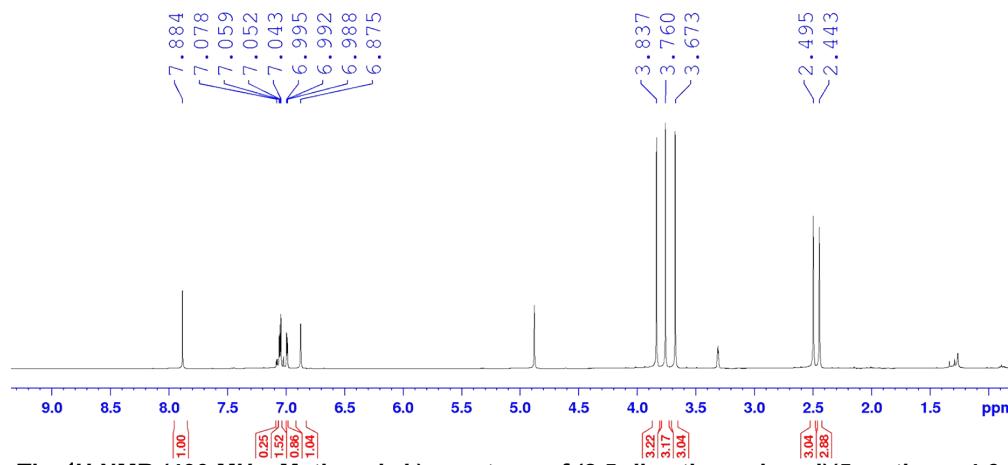


Plate 2a: The ^1H NMR (400 MHz, Methanol- d_4) spectrum of (2,5-dimethoxyphenyl)(5-methoxy-4,6-dimethyl-1-benzofuran-3-yl)methanone (**4b**).

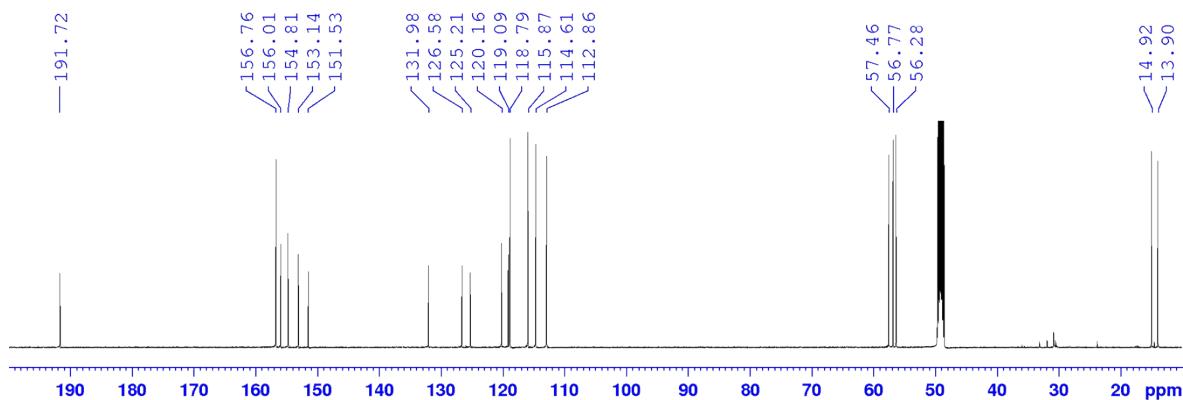


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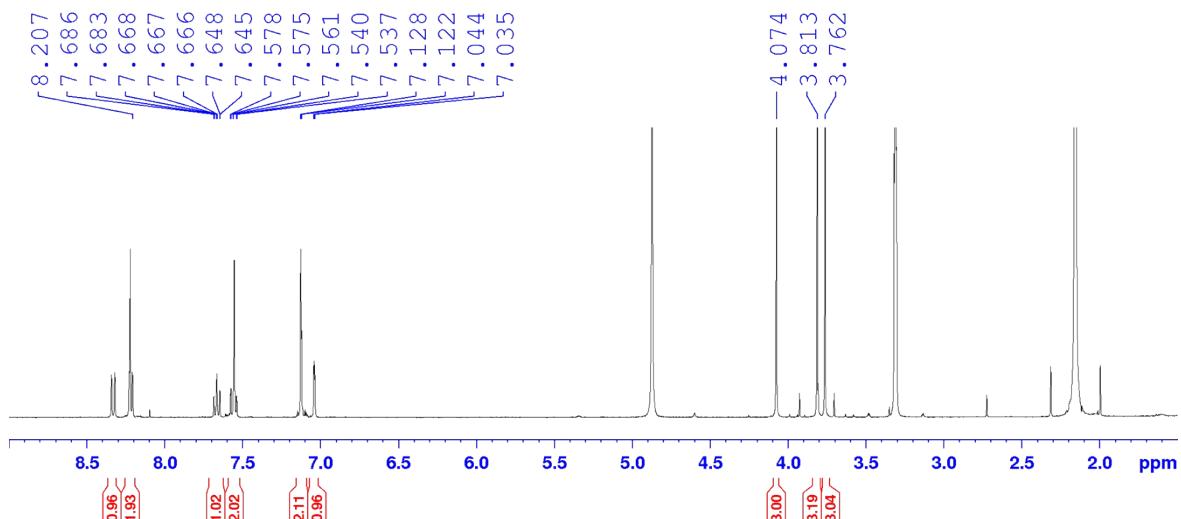


Plate 3a: The ¹H NMR (400 MHz, Methanol-*d*₄) spectrum of (2,5-dimethoxyphenyl)(5-methoxynaphtho[1,2-*b*]furan-3-yl)methanone (4c).

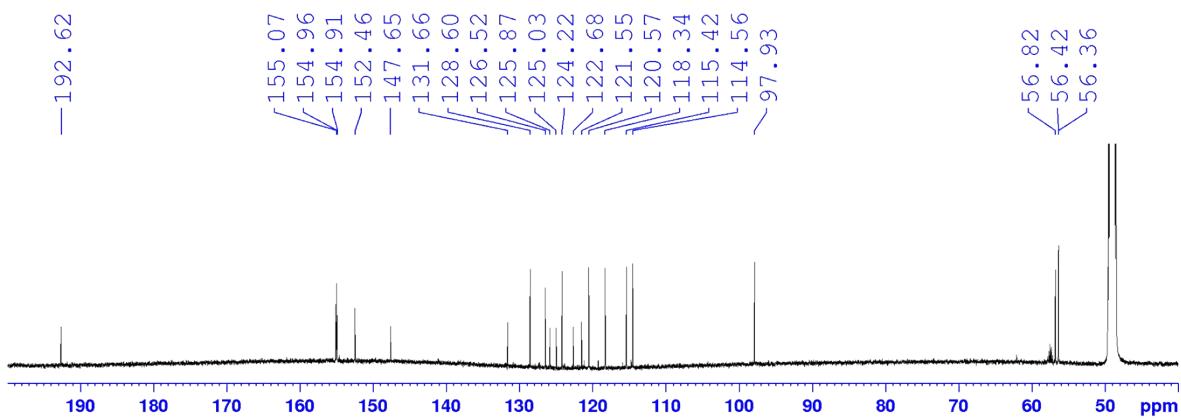


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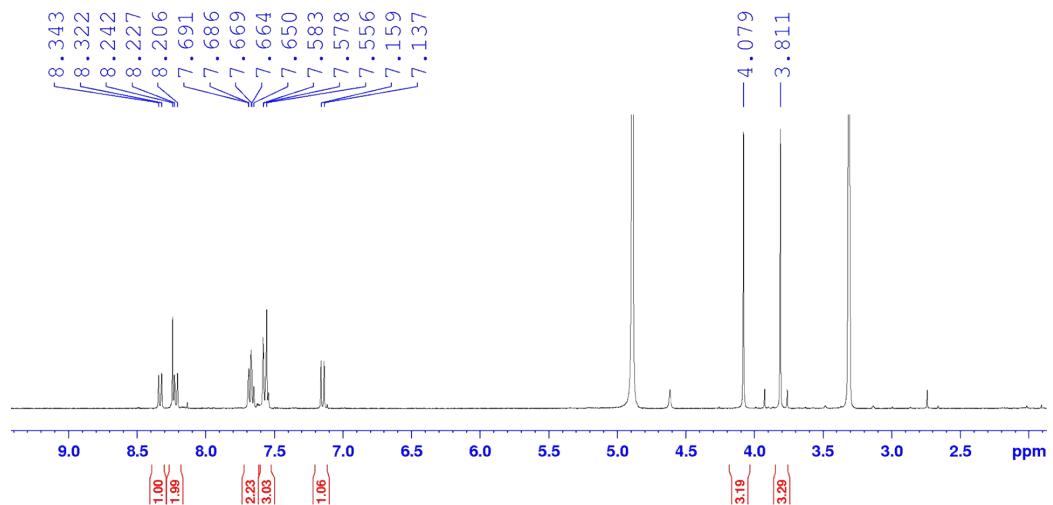


Plate 4a: The ¹H NMR (400 MHz, Methanol-*d*₄) spectrum for (5-bromo-2-methoxyphenyl)(5-methoxynaphtho[1,2-*b*]furan-3-yl)methanone (4d).

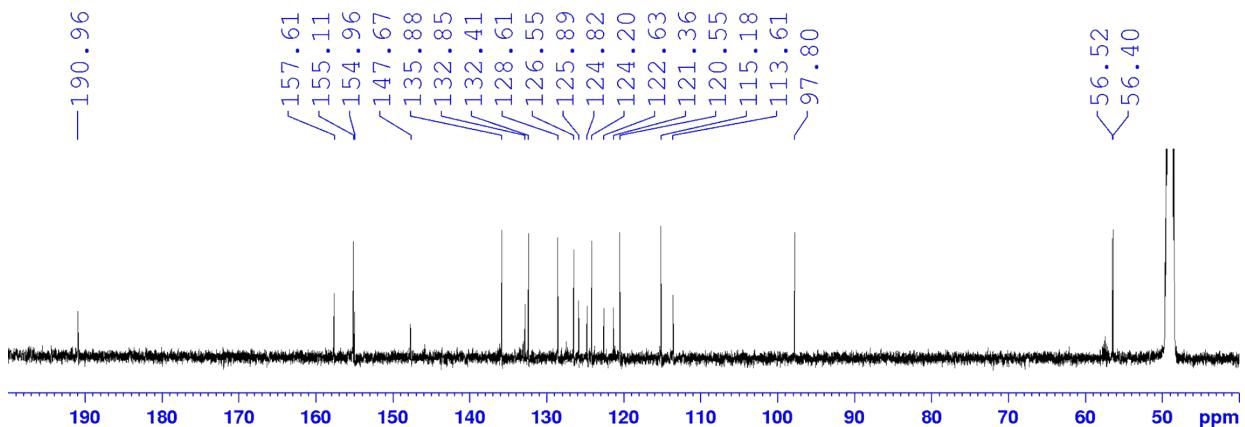


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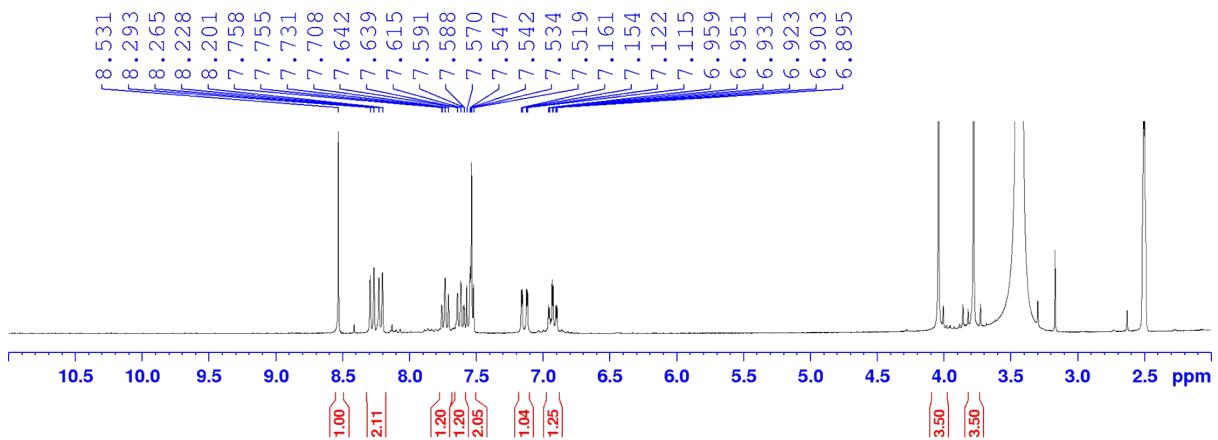


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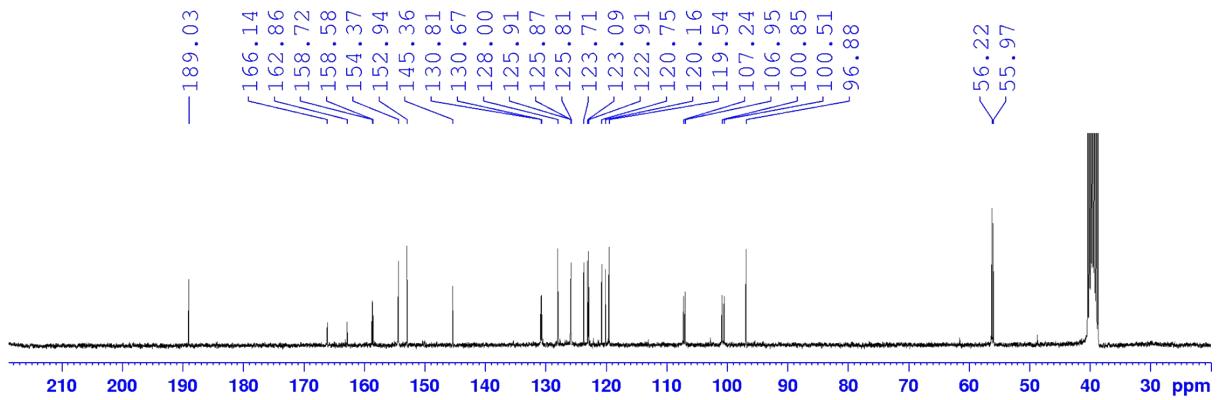


Plate 5b: The ^{13}C NMR (75 MHz, Methanol- d_4) spectrum for (4-fluoro-2-methoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4e).

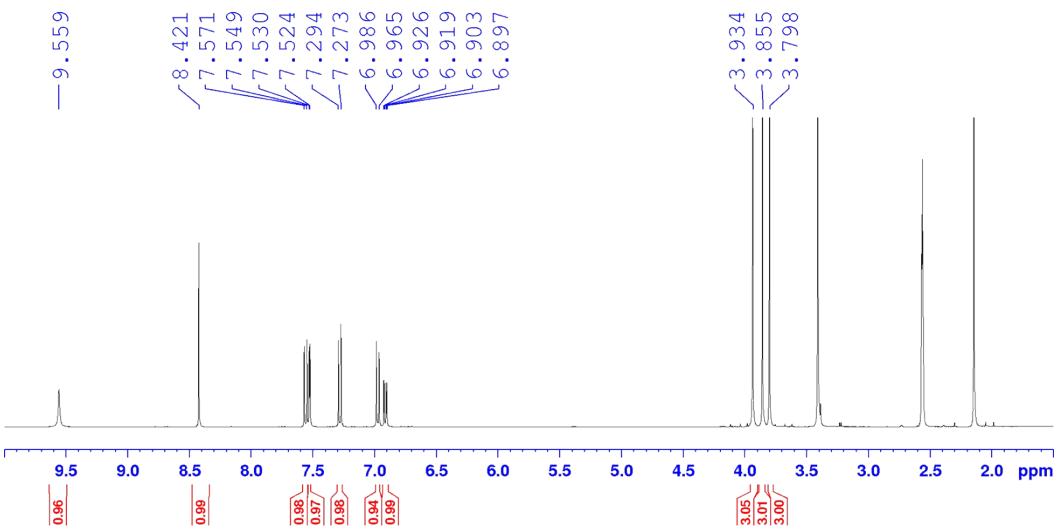


Plate 6a: The ^1H NMR (400 MHz, DMSO- d_6) spectrum of (5-hydroxy-1-benzofuran-3-yl)(2,3,4-trimethoxyphenyl)methanone (3g).

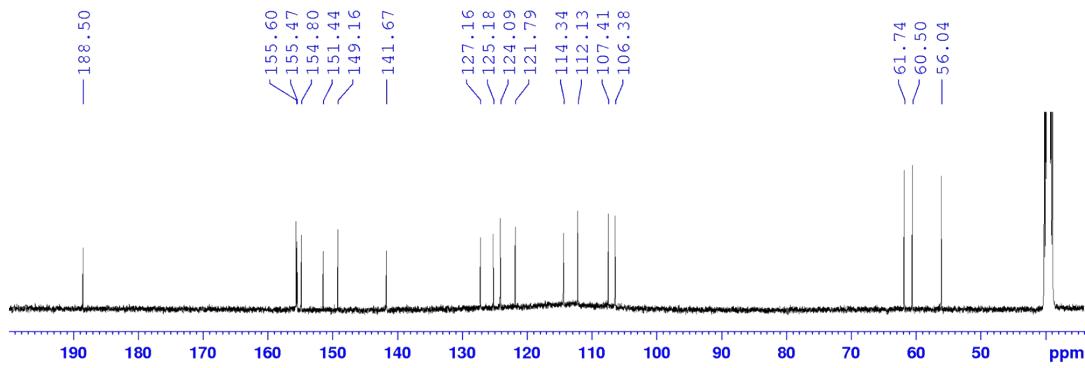


Plate 6b: The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of (5-hydroxy-1-benzofuran-3-yl)(2,3,4-trimethoxyphenyl)methanone (3g).

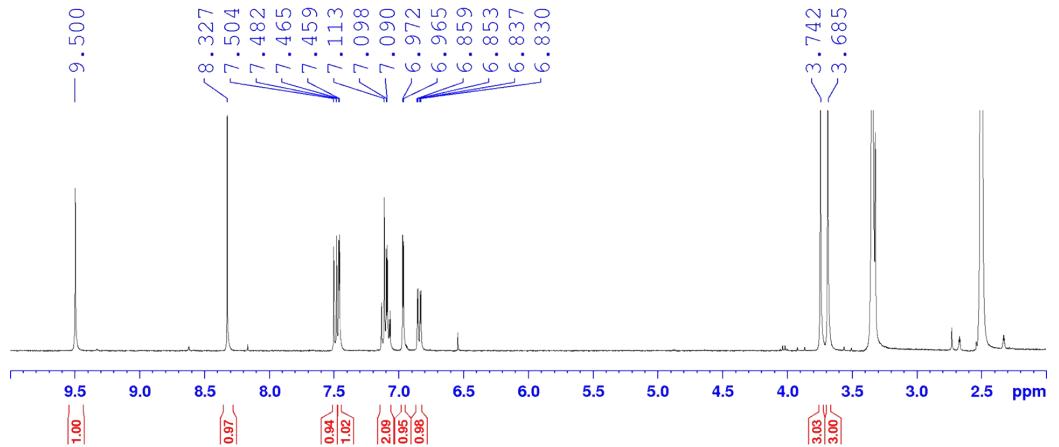


Plate 7a: The ^1H NMR (400 MHz, DMSO- d_6) spectrum of (2,5-dimethoxyphenyl)(5-hydroxy-1-benzofuran-3-yl)methanone (3h).

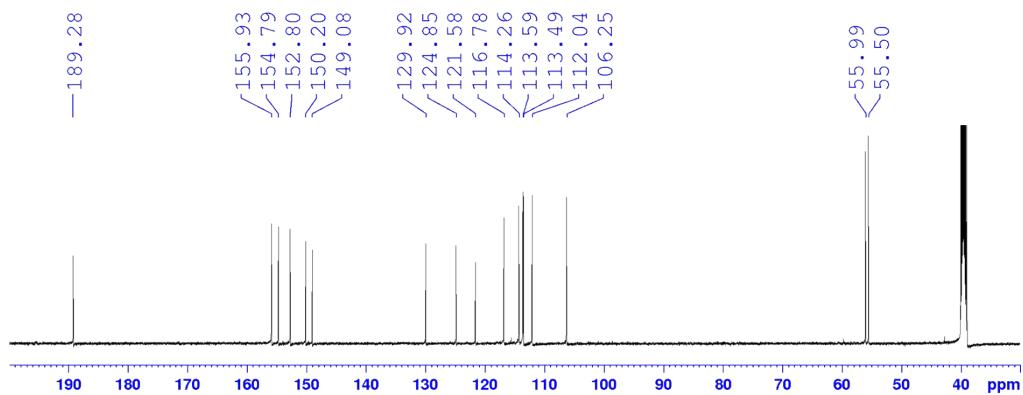


Plate 7b: The ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of (2,5-dimethoxyphenyl)(5-hydroxy-1-benzofuran-3-yl)methanone (3h).

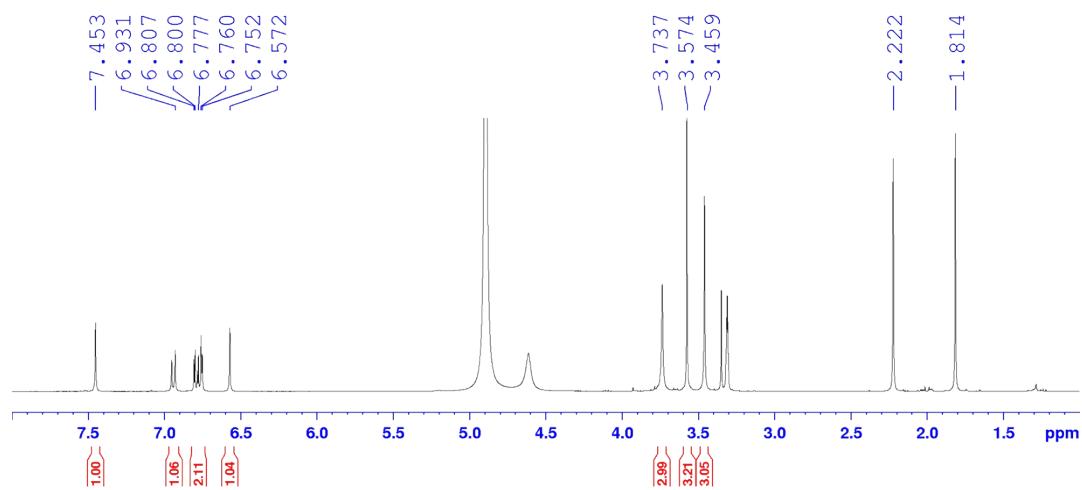


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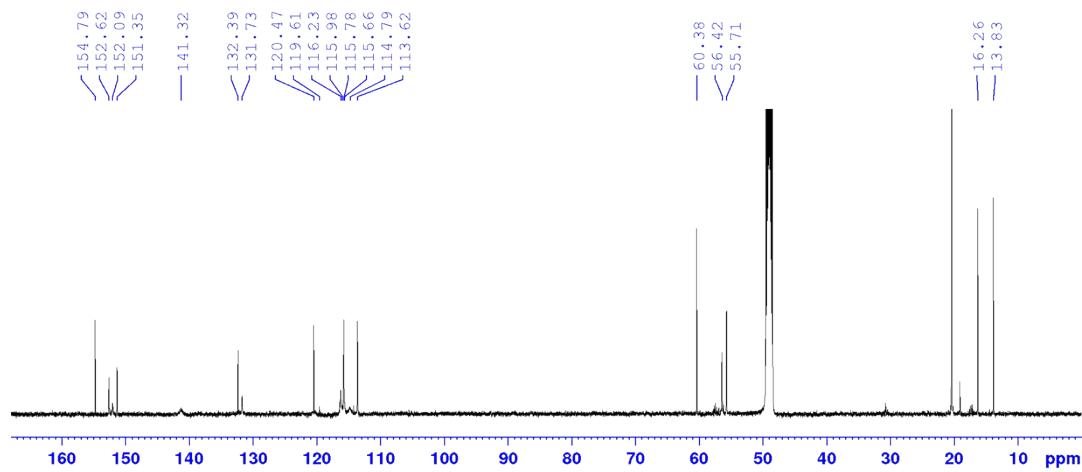


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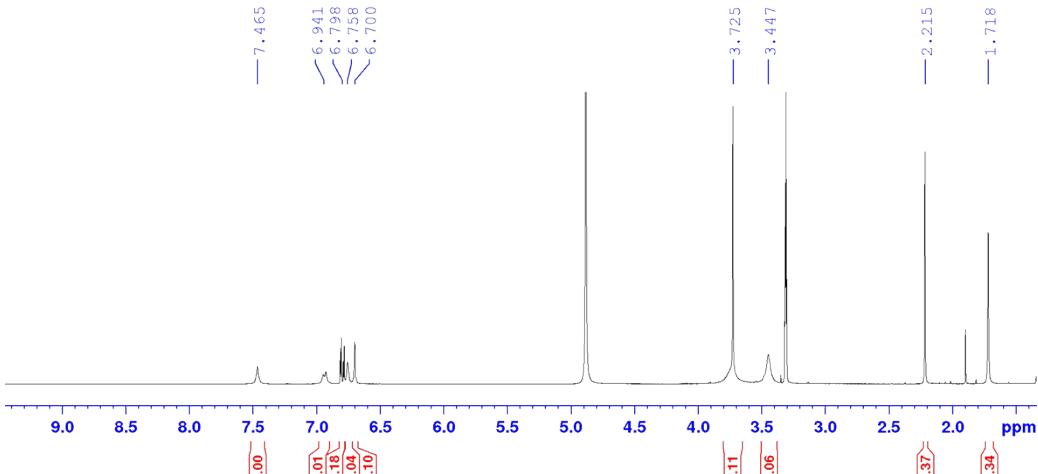


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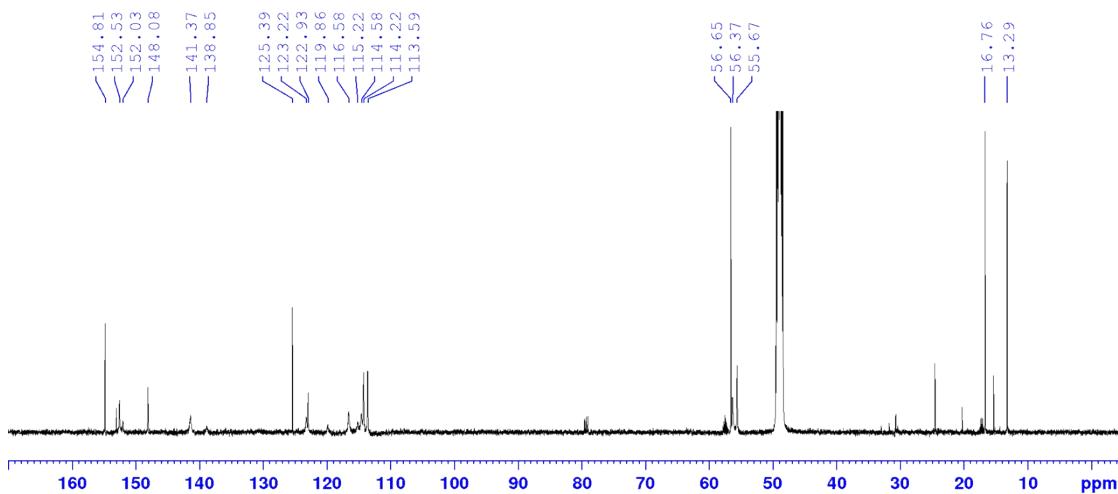


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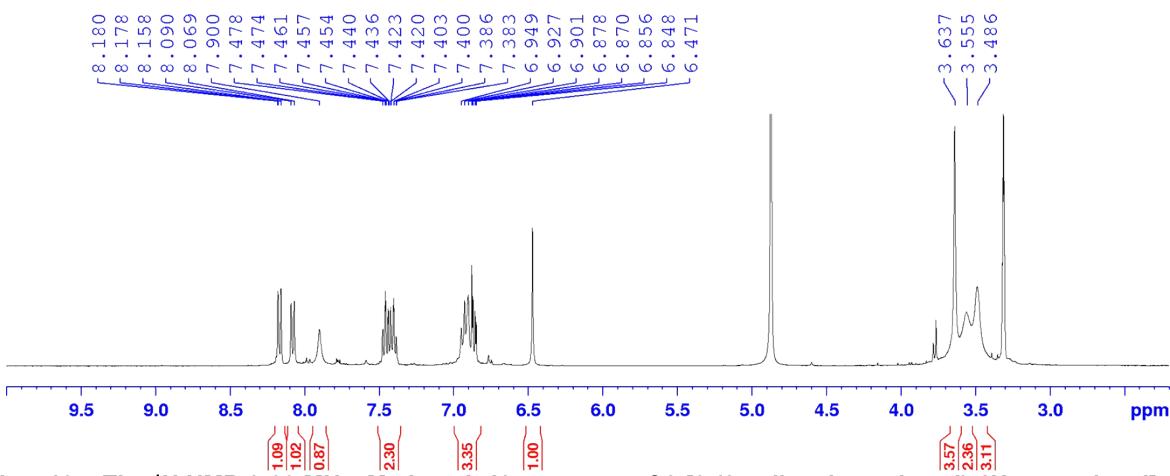


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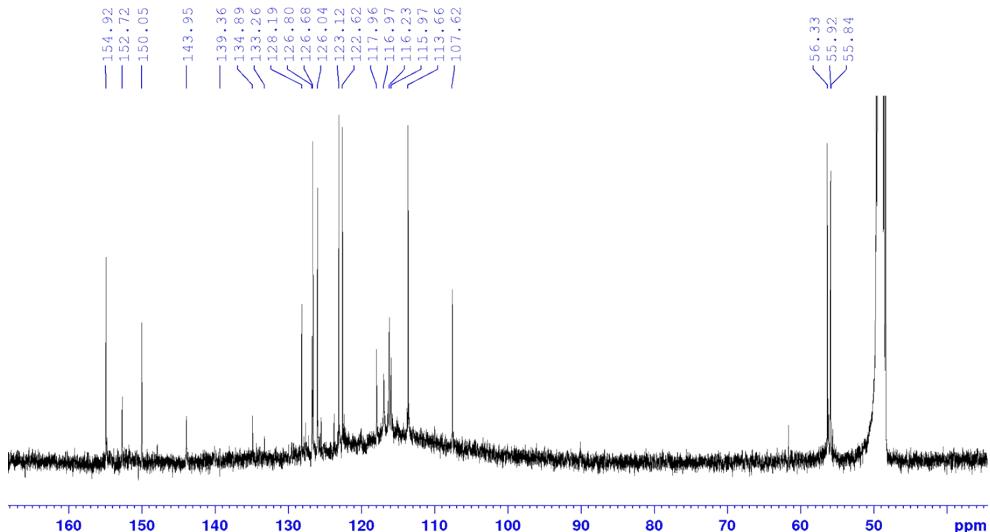


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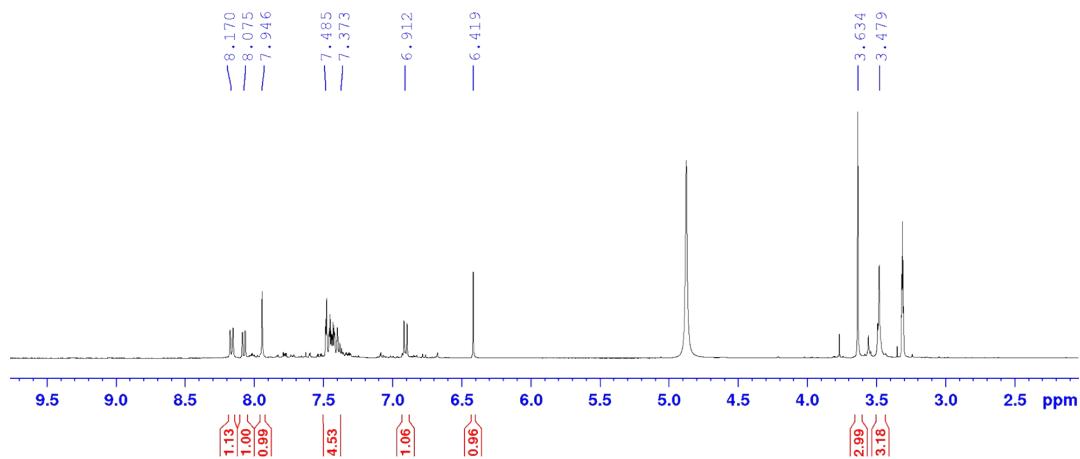


Plate 11a: The ¹H NMR (400 MHz, Methanol-*d*₄) spectrum of 2-[3-(5-bromo-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5d).

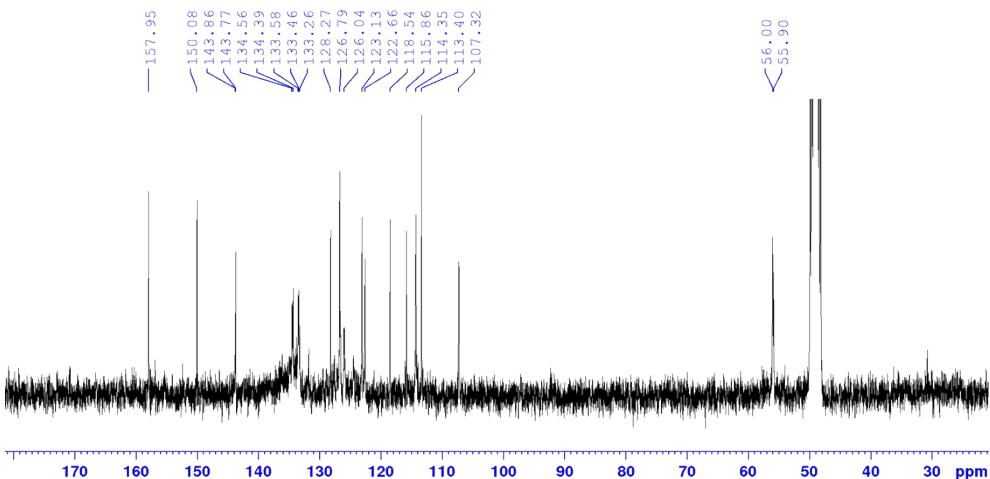


Plate 11b: The ¹³C NMR (75 MHz, Methanol-*d*₄) spectrum of 2-[3-(5-bromo-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5d).

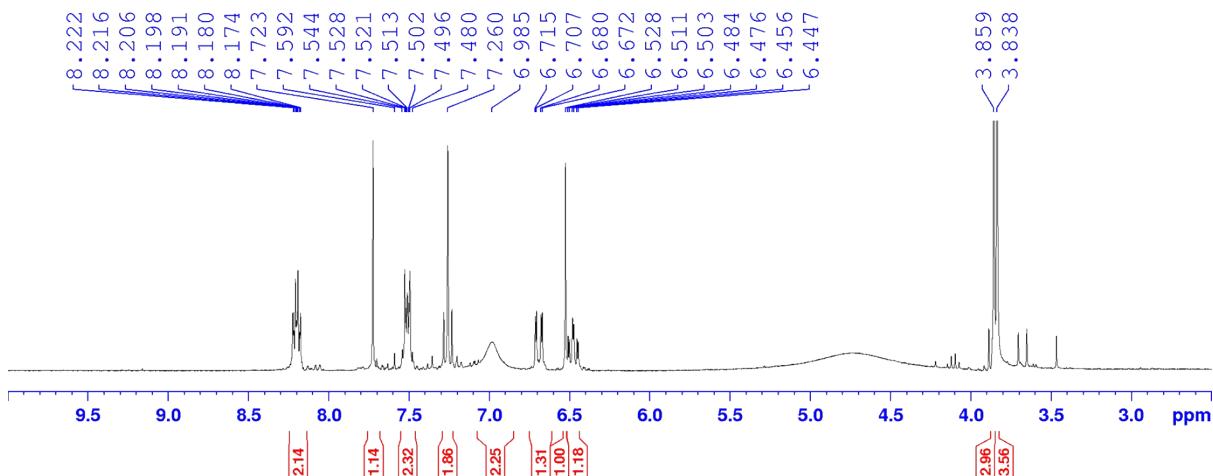


Plate 12a: The ¹H NMR (300 MHz, Chloroform-d₁) spectrum of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (**5e**).

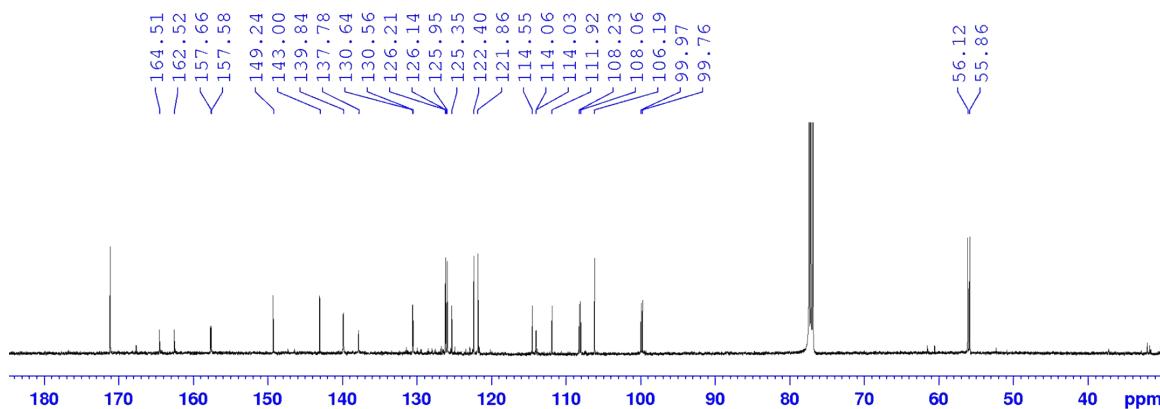


Plate 12b: The ¹³C NMR (125 MHz, Chloroform-d₁) spectrum of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (**5e**).

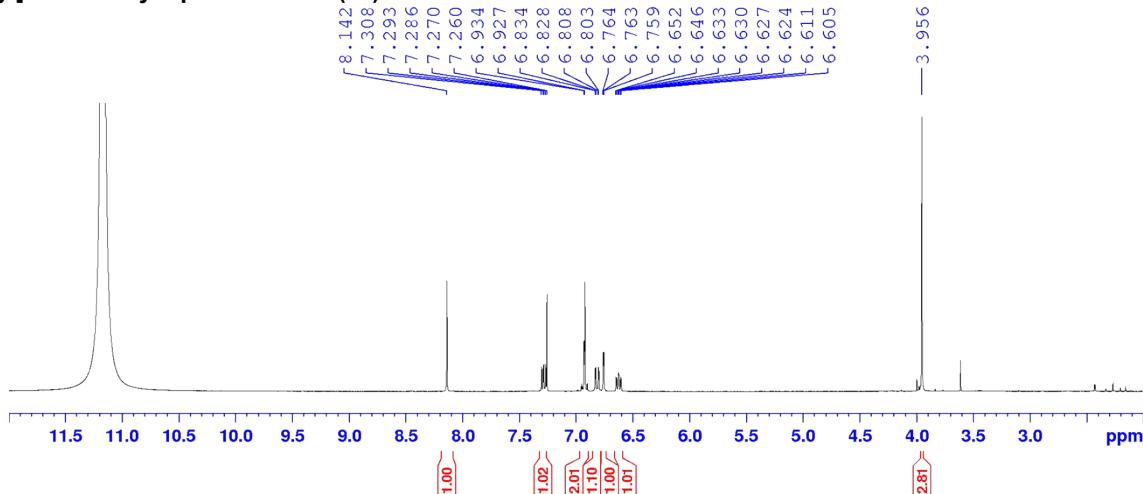


Plate 13a: The ¹H NMR (400 MHz, Chloroform-d₁) spectrum for 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]benzene-1,4-diol (**5f**).

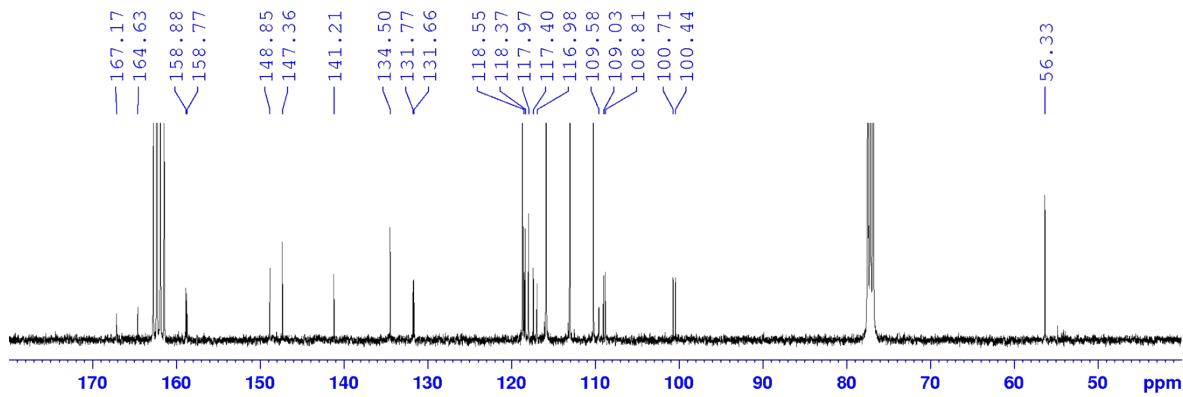


Plate 13b: The ^{13}C NMR (100 MHz, Chloroform- d_1) spectrum for 2-[3-(4-fluoro-2-methoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5f).

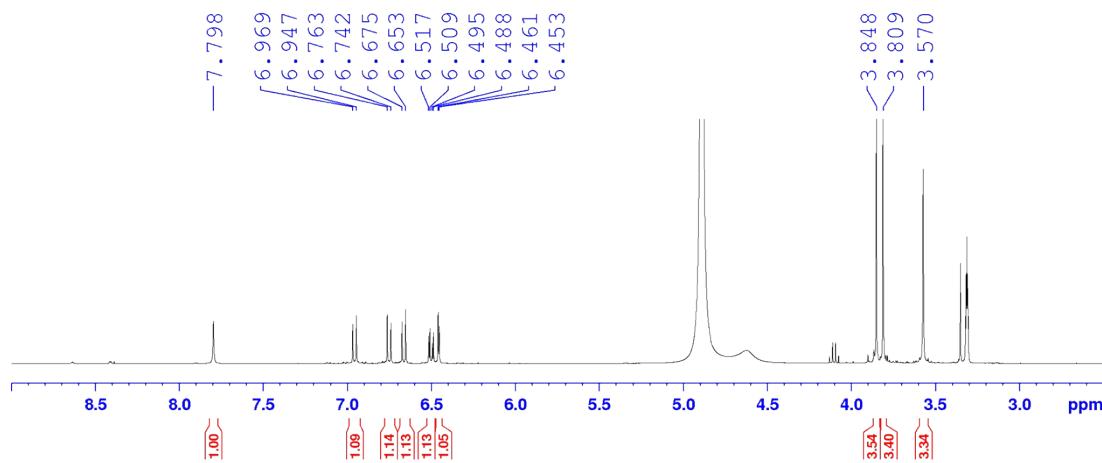


Plate 14a: The ^1H NMR (400 MHz, Methanol- d_4) spectrum for 2-[3-(2,3,4-trimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5g).

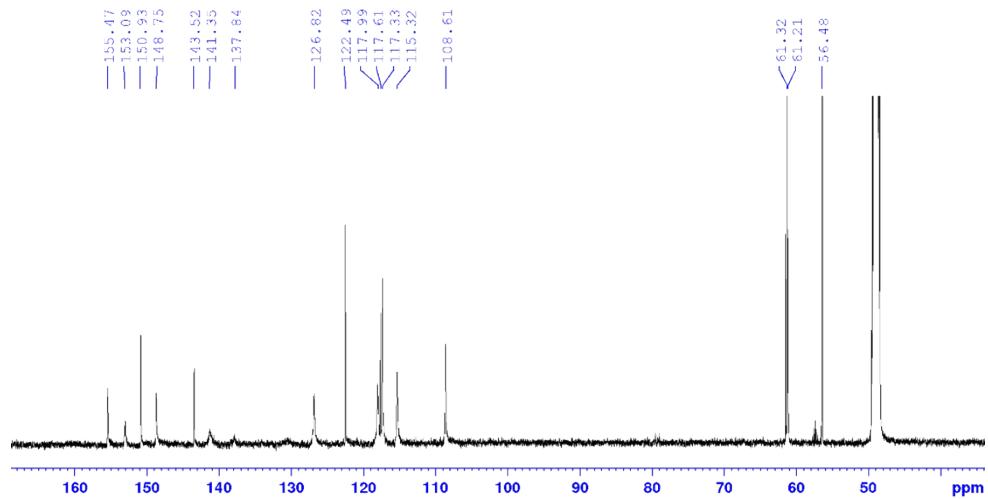


Plate 14b: The ^{13}C NMR (100 MHz, Methanol- d_4) spectrum for 2-[3-(2,3,4-trimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5g).

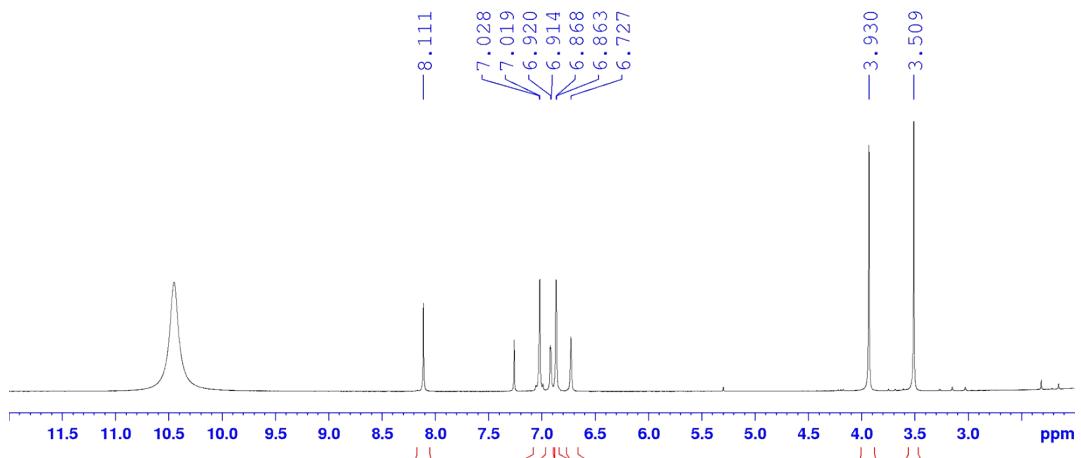


Plate 15a: The ^1H NMR (300 MHz, Chloroform- d_1) spectrum for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5h).

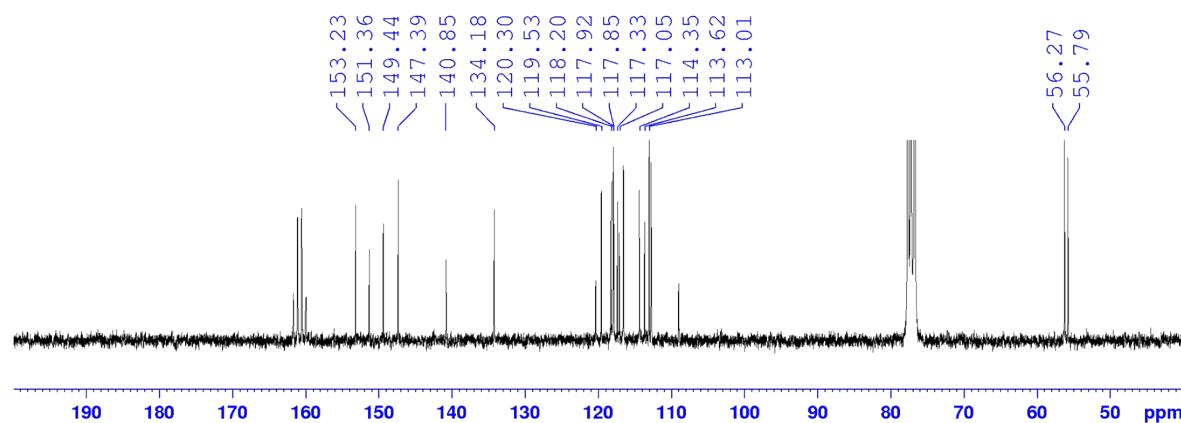


Plate 15b: The ^{13}C NMR (75 MHz, Chloroform- d_1) spectrum for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5h).

1.2.2 Chromatograms

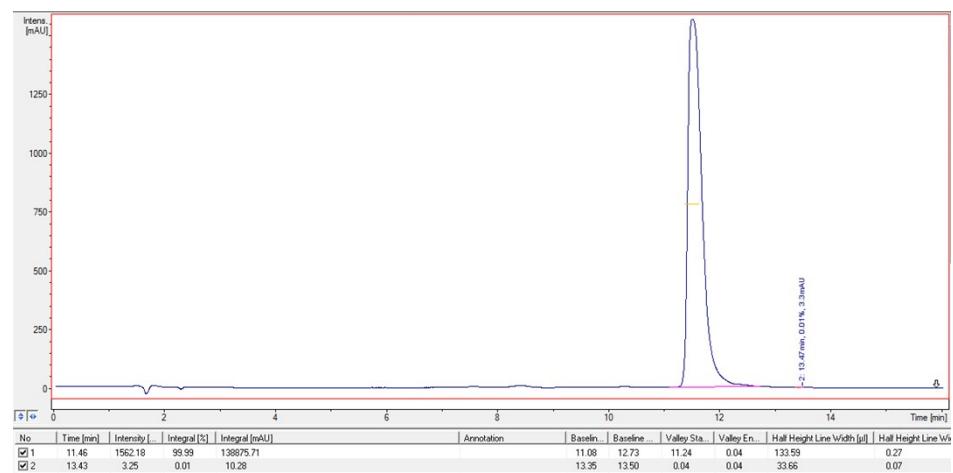


Plate 1c: UV chromatogram of (2,5-dimethoxyphenyl)(5-methoxy-4,7-dimethyl-1-benzofuran-3-yl)methanone (4a) measured at 280 nm.

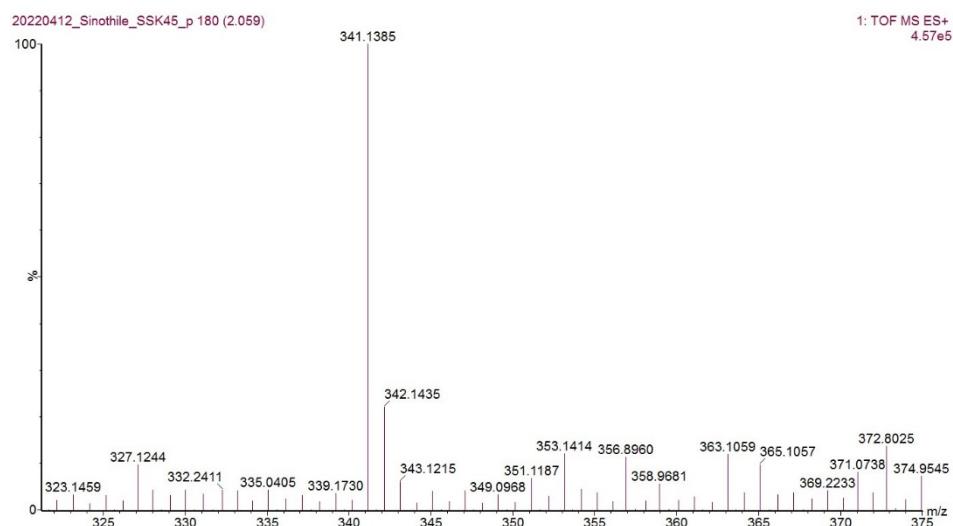


Plate 1d: HR-MS spectrum of (2,5-dimethoxyphenyl)(5-methoxy-4,7-dimethyl-1-benzofuran-3-yl)methanone (4a).

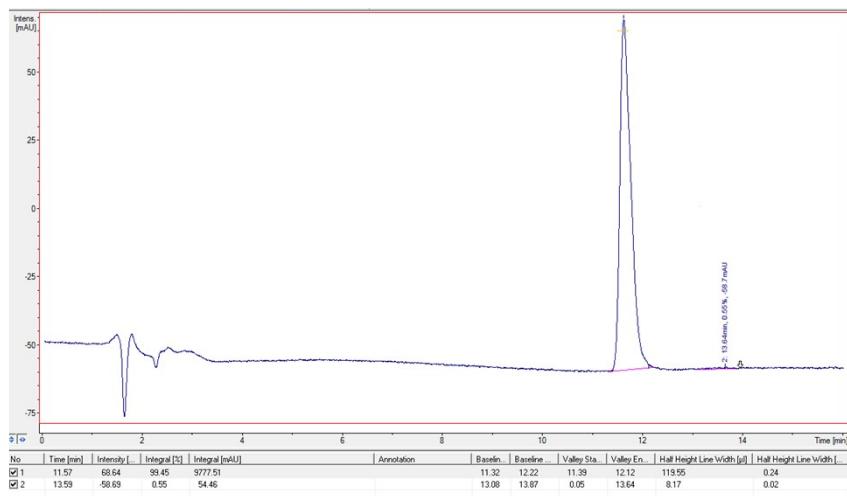


Plate 2c: UV chromatogram of (2,5-dimethoxyphenyl)(5-methoxy-4,6-dimethyl-1-benzofuran-3-yl)methanone (4b) measured at 280 nm.

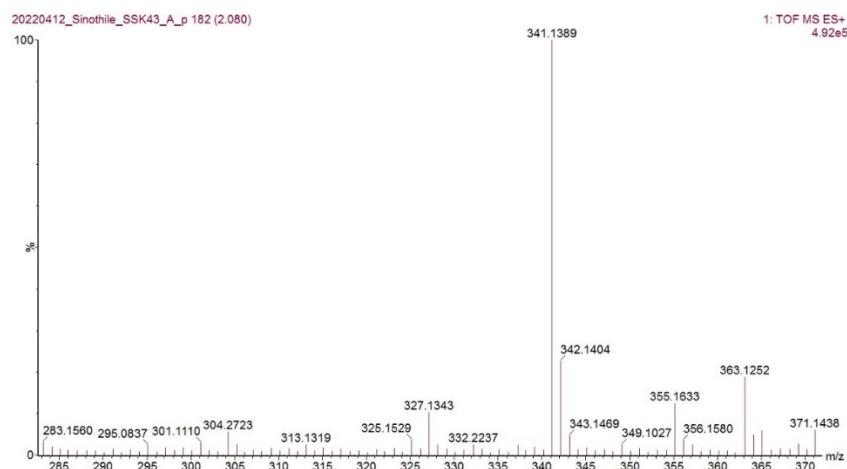


Plate 2d: HR-MS spectrum of (2,5-dimethoxyphenyl)(5-methoxy-4,6-dimethyl-1-benzofuran-3-yl)methanone (4b).

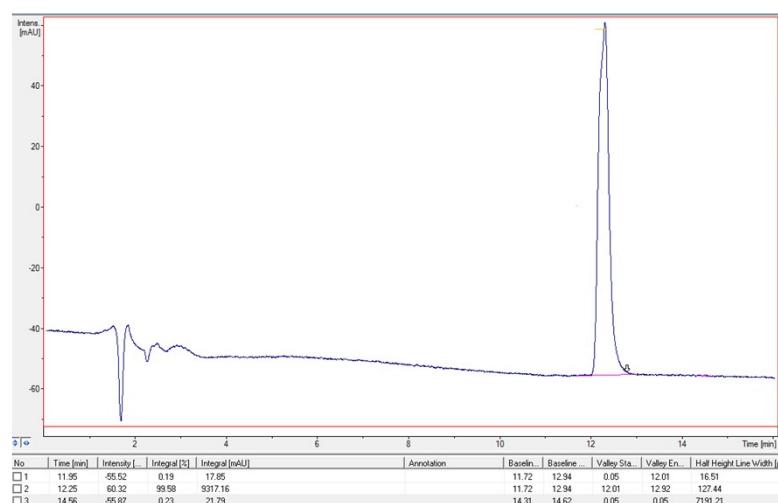


Plate 3c: UV chromatogram of (2,5-dimethoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4c).

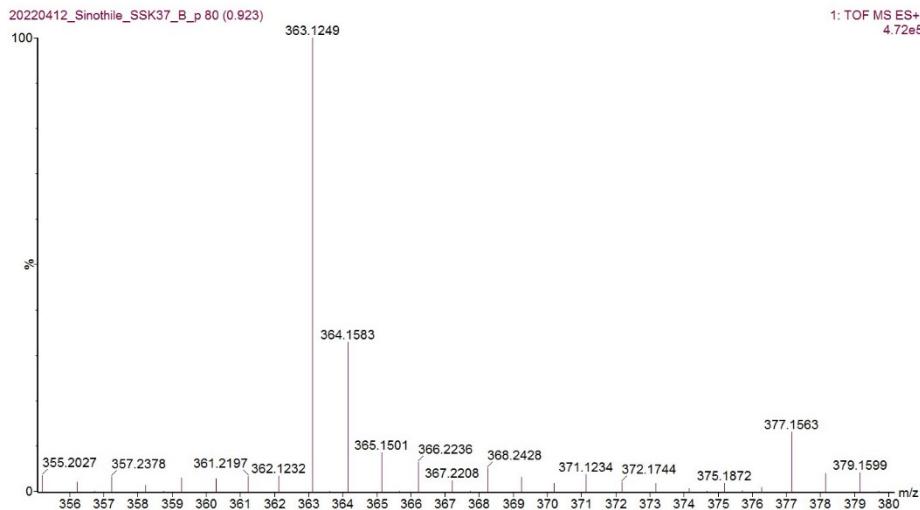


Plate 3d: HR-MS spectrum of (2,5-dimethoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4c).

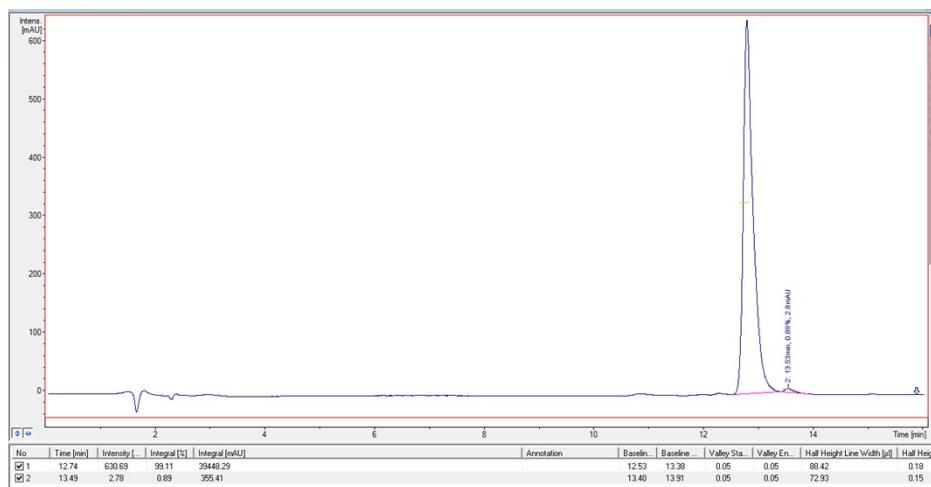


Plate 4c: UV chromatogram of (5-bromo-2-methoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4d) measured at 280 nm.

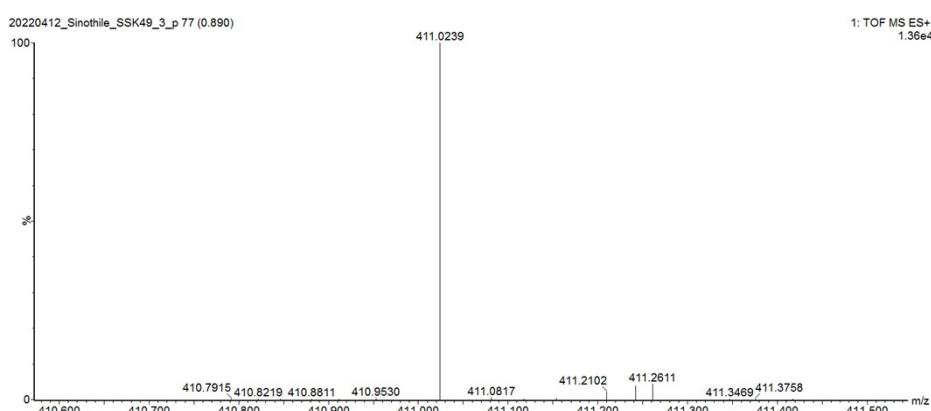


Plate 4d: HR-MS spectrum of (5-bromo-2-methoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4d).

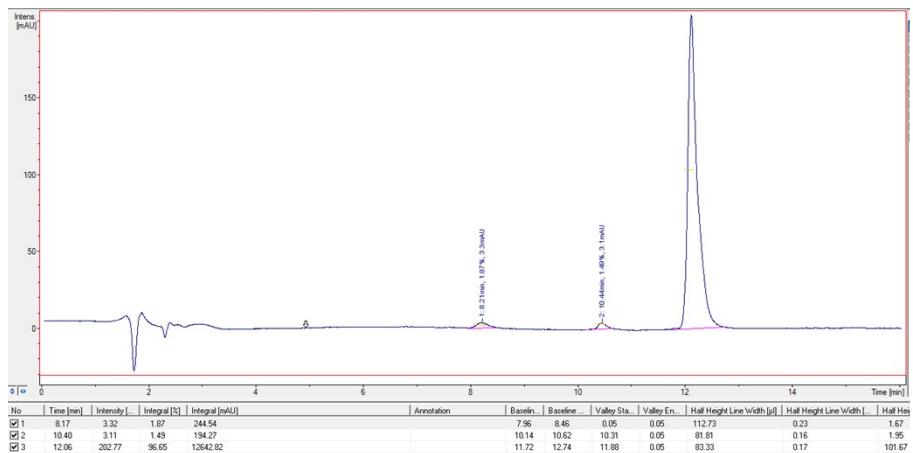


Plate 5c: UV chromatogram of (4-fluoro-2-methoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4e) measured at 280 nm.

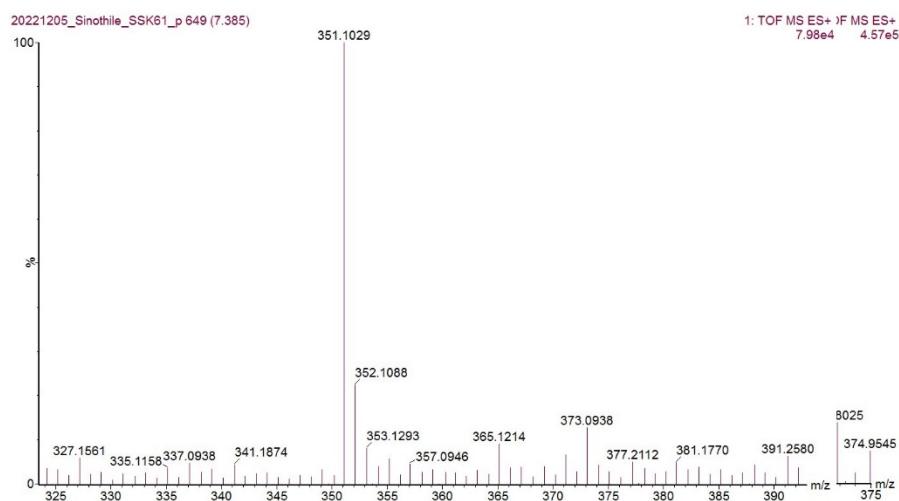


Plate 5d: HR-MS spectrum of (4-fluoro-2-methoxyphenyl)(5-methoxynaphtho[1,2-b]furan-3-yl)methanone (4e).

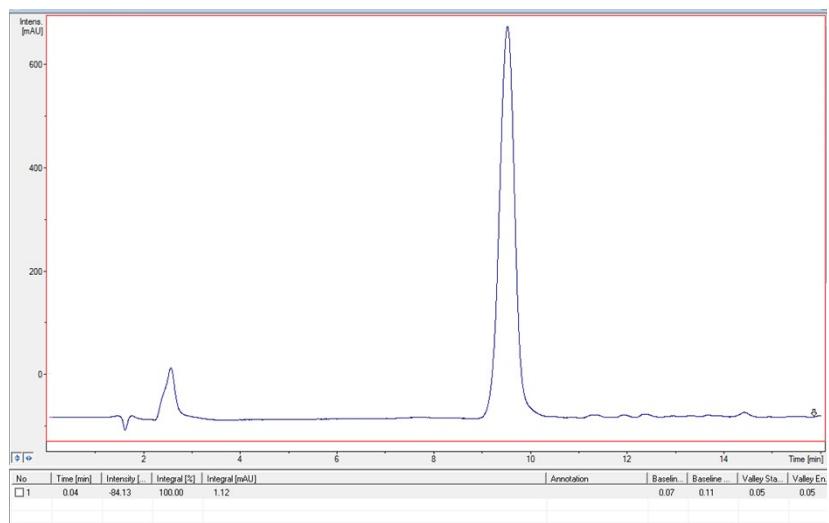


Plate 6c: UV chromatogram of (5-hydroxy-1-benzofuran-3-yl)(2,3,4-trimethoxyphenyl)methanone (3g) measured at 280 nm.

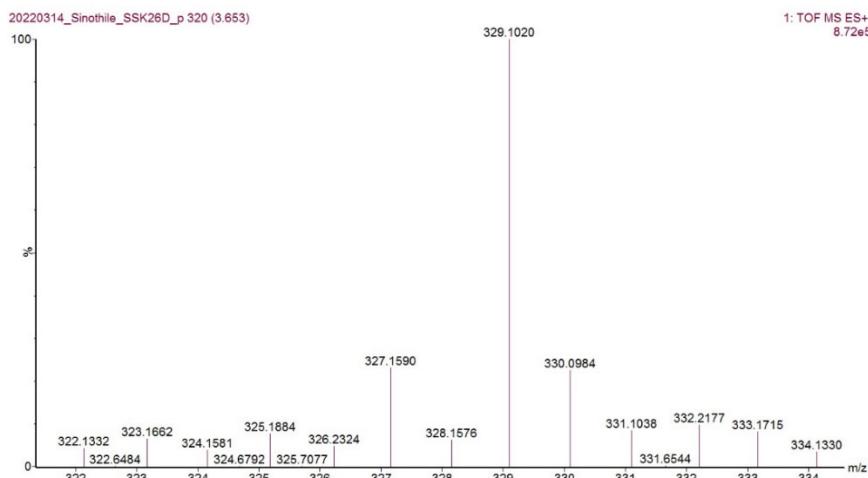


Plate 6d: HR-MS spectrum of (5-hydroxy-1-benzofuran-3-yl)(2,3,4-trimethoxyphenyl)methanone (3g).

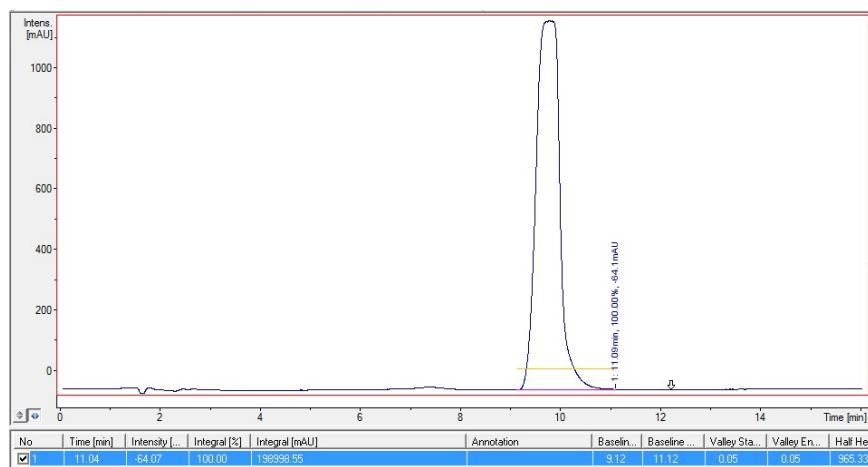


Plate 7c: UV chromatogram of (2,5-dimethoxyphenyl)(5-hydroxy-1-benzofuran-3-yl)methanone (3h) measured at 280 nm.

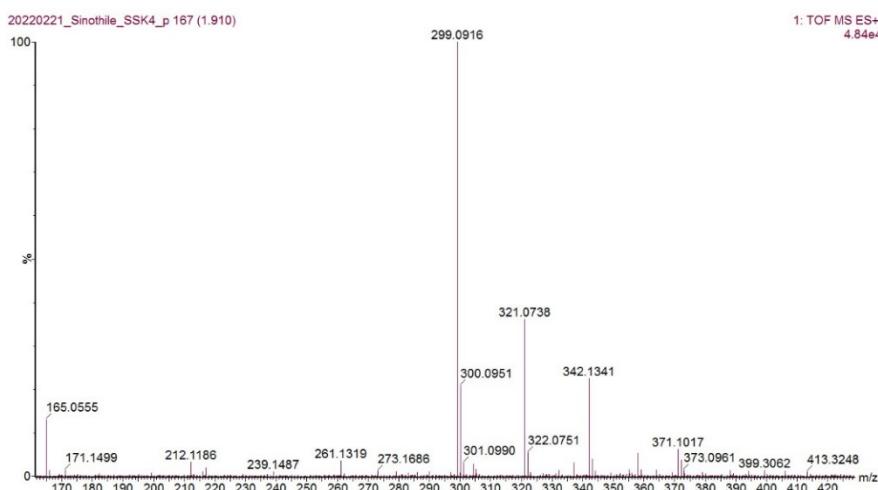


Plate 7d: HR-MS spectrum of (2,5-dimethoxyphenyl)(5-hydroxy-1-benzofuran-3-yl)methanone (3h).

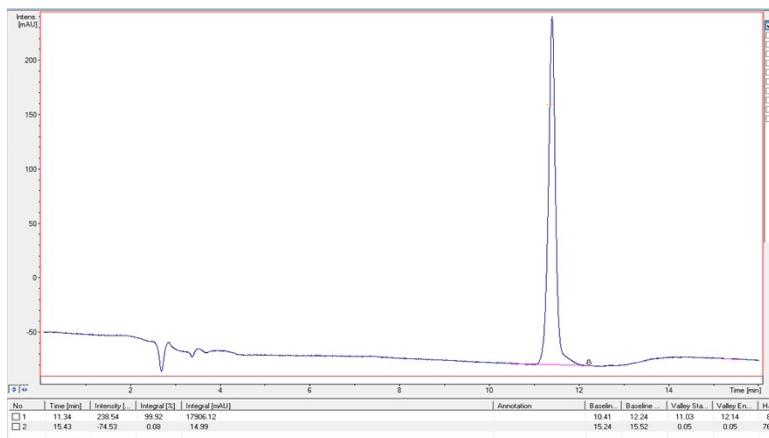


Plate 8c: UV chromatogram of 2-[3-(2,5-dimethoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxy-3,6-dimethylphenol (**5a**) measured at 280 nm.

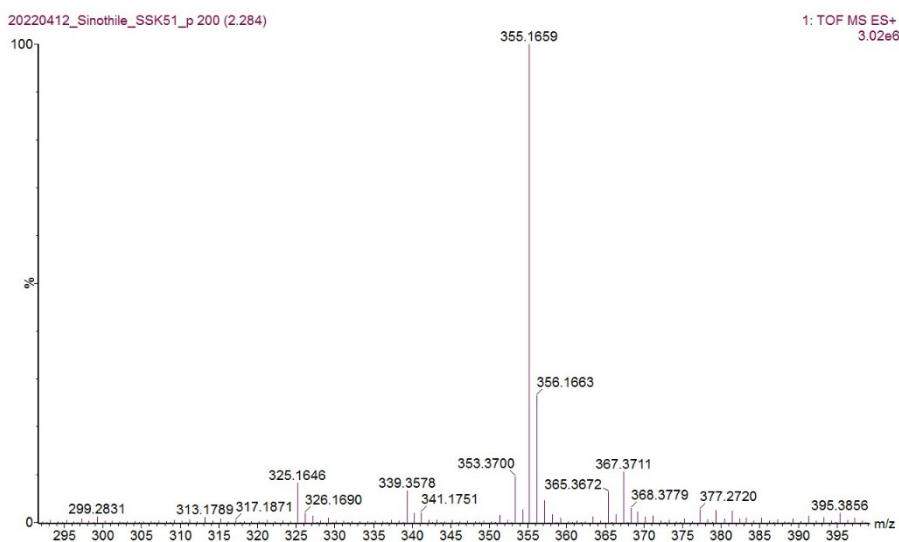


Plate 8d: HR-MS spectrum of 2-[3-(2,5-dimethoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxy-3,6-dimethylphenol (**5a**).

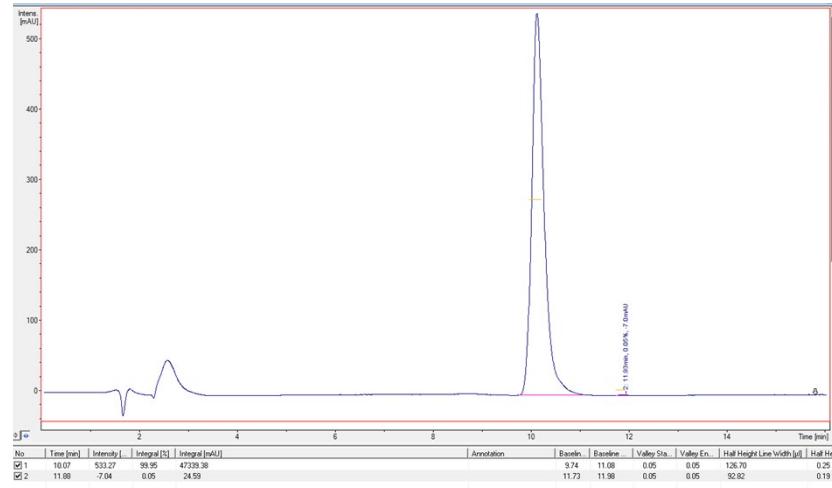


Plate 9c: UV chromatogram of 2-[3-(2,5-dimethoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxy-3,5-dimethylphenol (**5b**) measured at 280 nm.

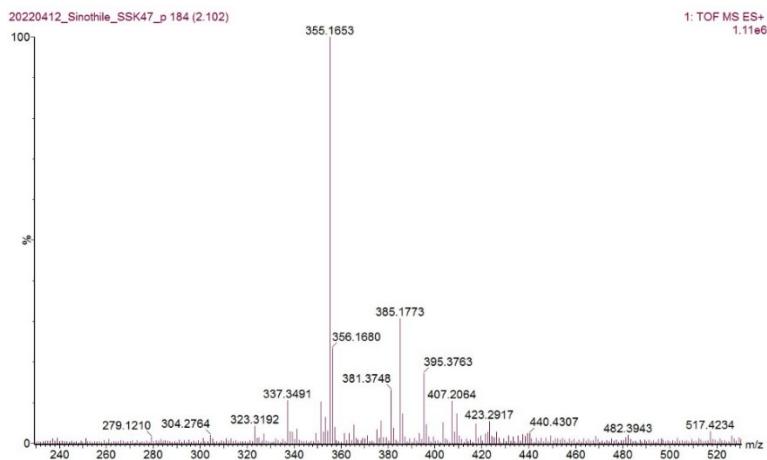


Plate 9d: HR-MS spectrum for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]-4-methoxy-3,5 dimethylphenol (5b).

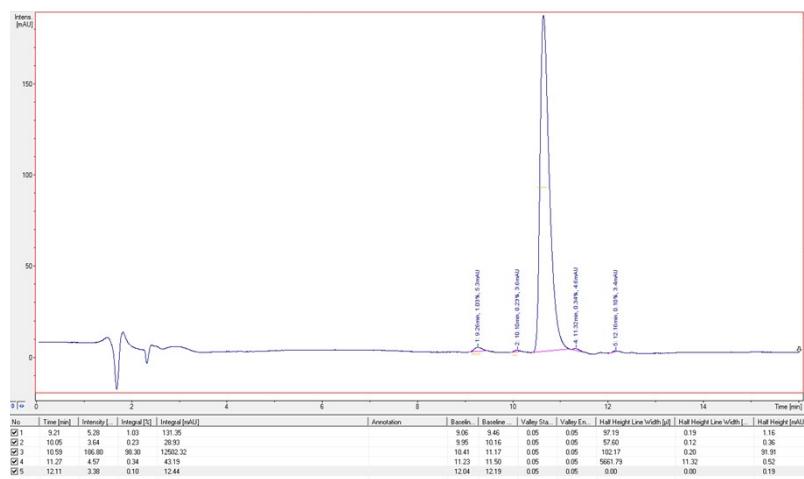


Plate 10c: UV chromatogram of 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5c) measured at 260 nm.

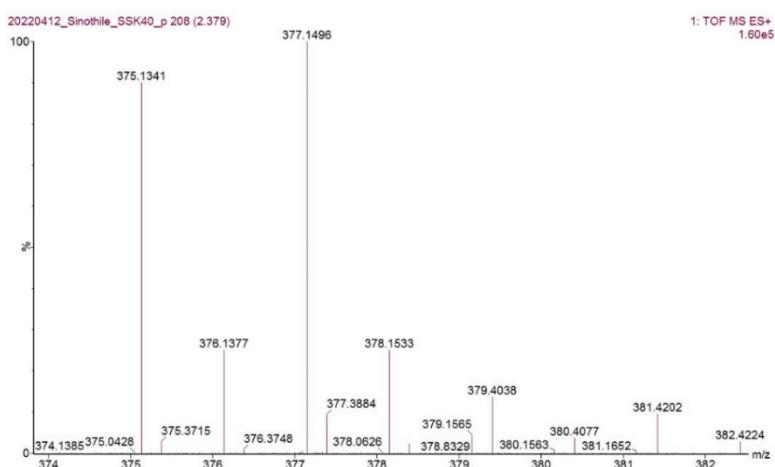


Plate 10d: HR-MS spectrum for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5c).

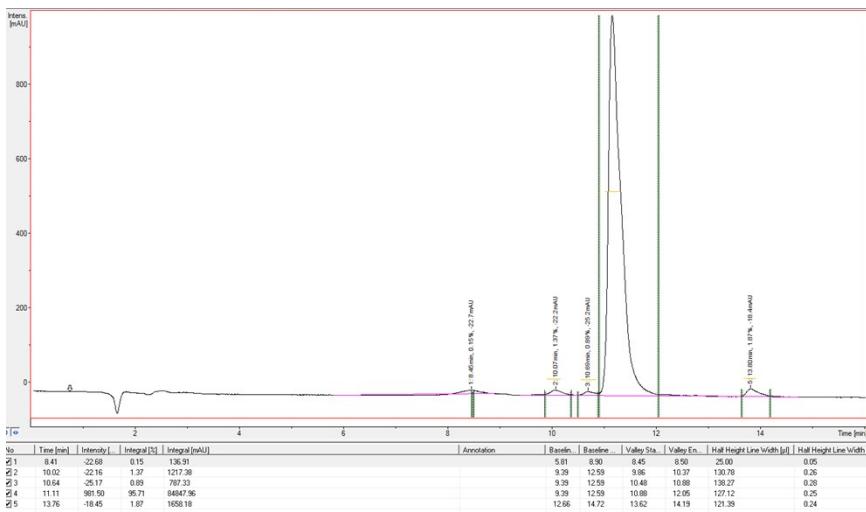


Plate 11c: UV chromatogram of 2-[3-(5-bromo-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5d) measured at 260 nm.

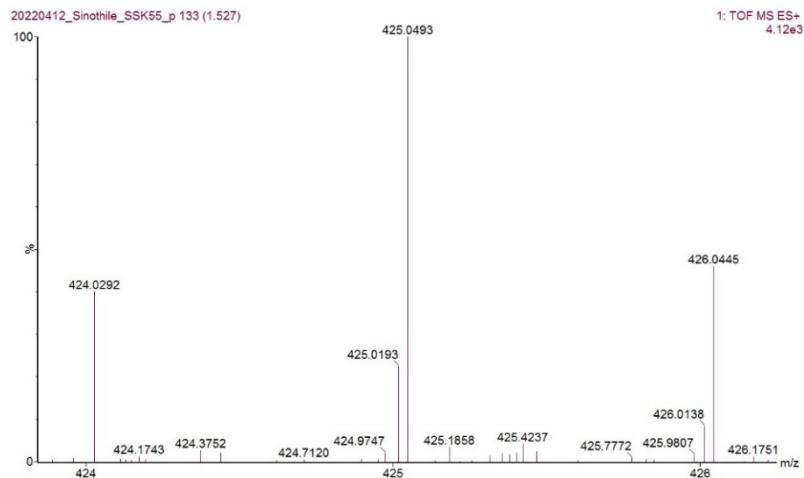


Plate 11d: HR-MS spectrum of 2-[3-(5-bromo-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5d).

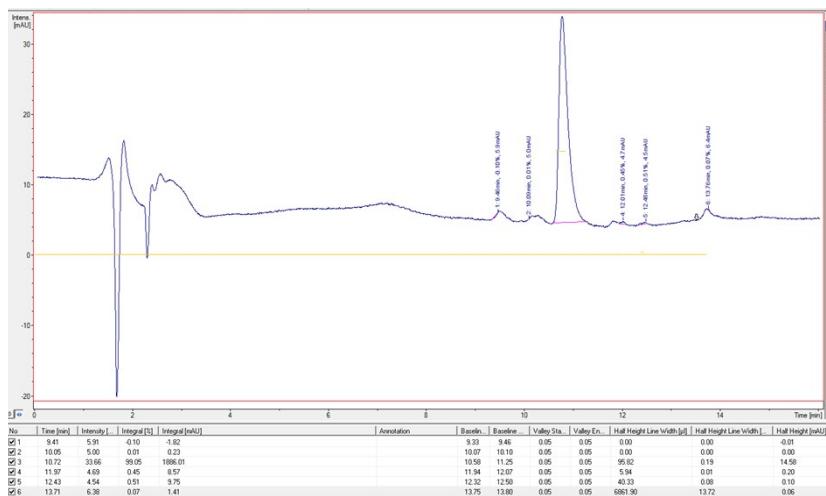


Plate 12c: UV chromatogram of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (5e).

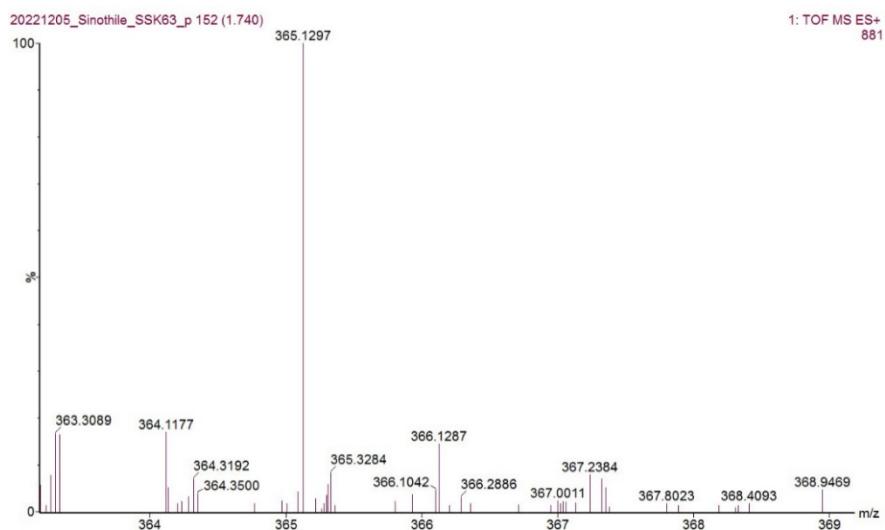


Plate 12d: HR-MS spectrum of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]-4-methoxynaphthalen-1-ol (**5e**).

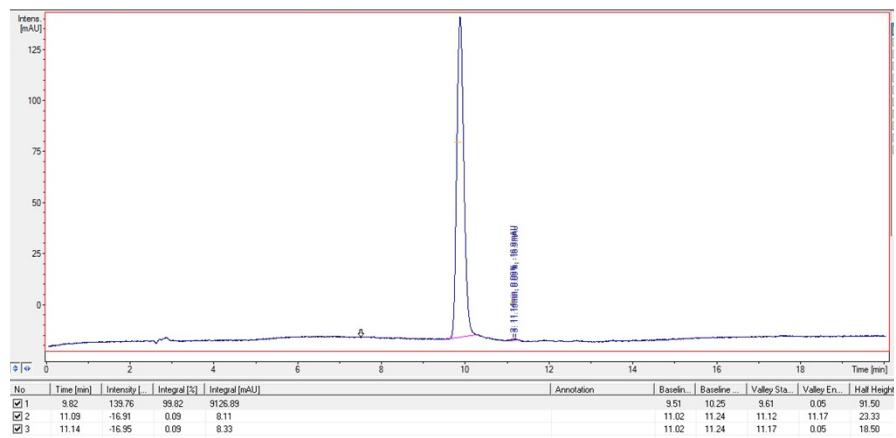


Plate 13c: UV chromatogram of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]benzene-1,4-diol (**5f**) measured at 280 nm.

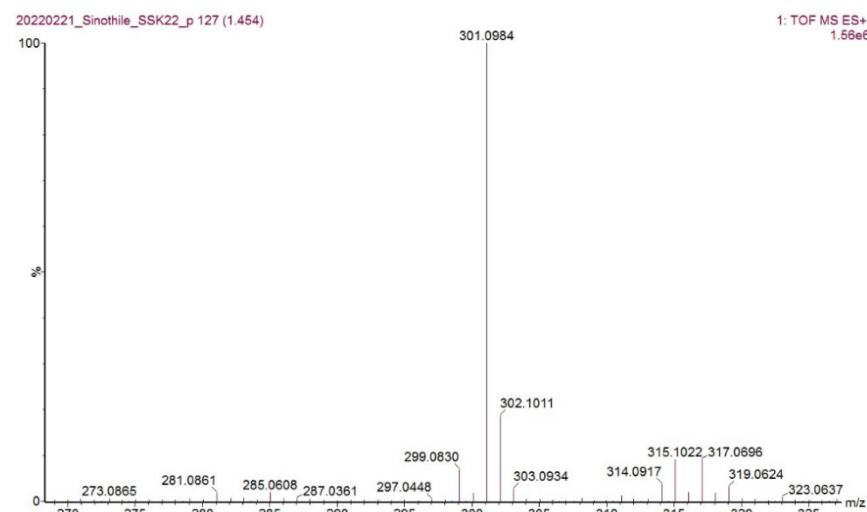


Plate 13d: HR-MS spectrum of 2-[3-(4-fluoro-2-methoxyphenyl)-1*H*-pyrazol-4-yl]benzene-1,4-diol (**5f**).

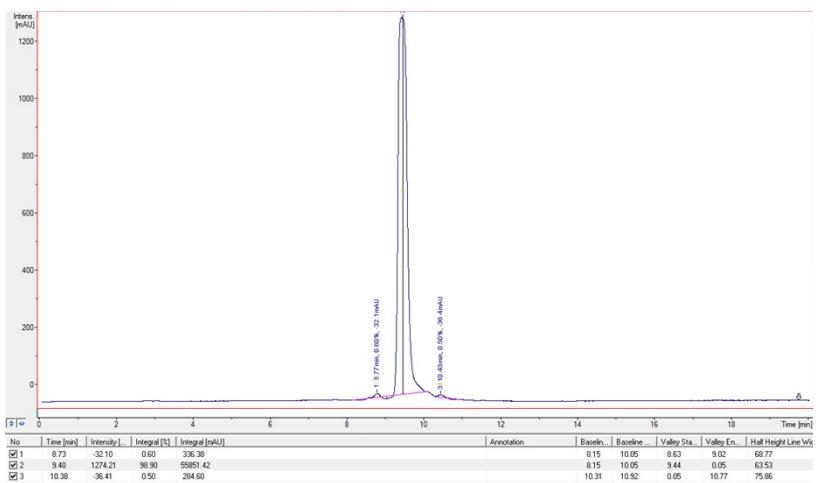


Plate 14c: UV chromatogram of 2-[3-(2,3,4-trimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5g) at 280 nm.

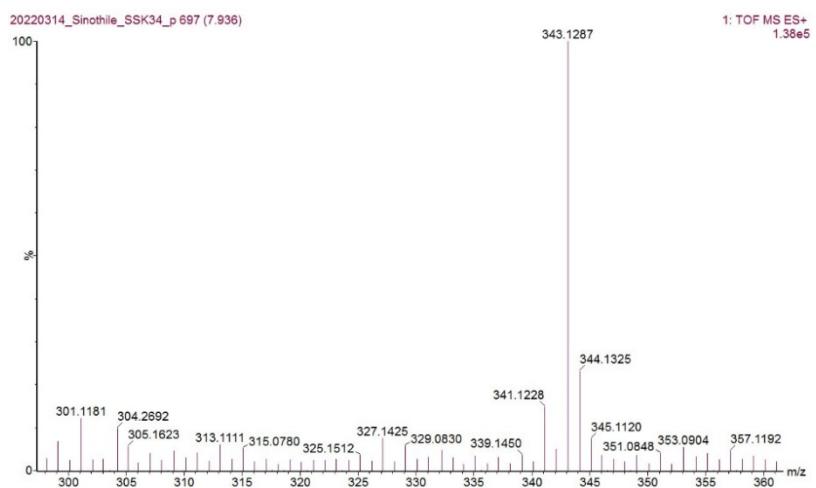


Plate 14d: HR-MS spectrum of 2-[3-(2,3,4-trimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5g).

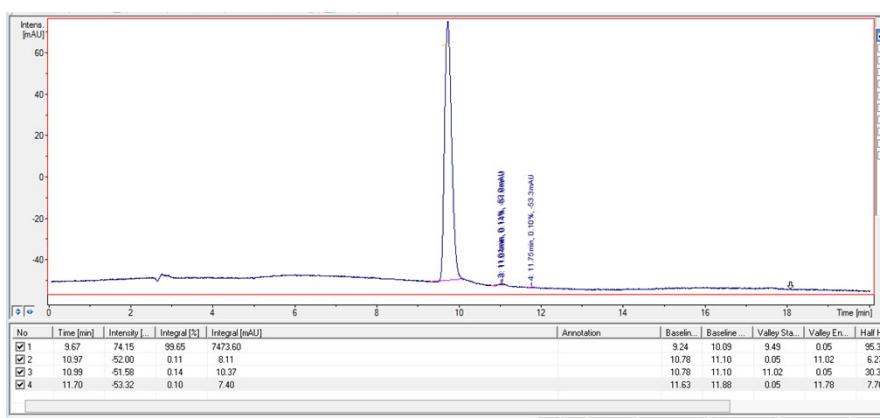


Plate 15c: UV chromatogram for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5h) measured at 280 nm.

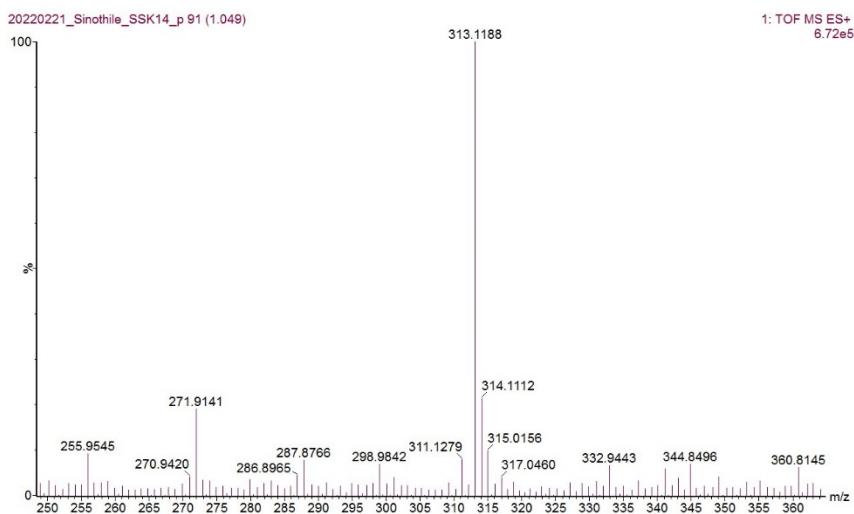


Plate 15d: HR-MS spectrum for 2-[3-(2,5-dimethoxyphenyl)-1H-pyrazol-4-yl]benzene-1,4-diol (5h) measured at 280 nm.