Supplementary Material

A facile and rapid one-step synthesis of 8-substituted xanthine derivatives *via* tandem ring closure at room temperature

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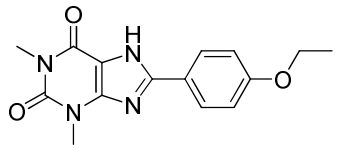
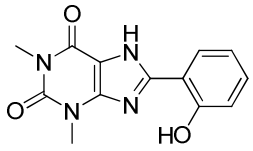
All the synthesized 8-substituted xanthine derivatives are fully characterized by five independent characterization techniques (Melting point, FT-IR, ^{1}H-NMR, HPLC and ESI-MS) as follows:



6a

8-(4-ethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6a) [1]

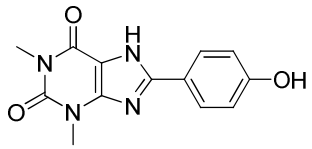
Light brown solid; Yield: 0.615 g, 82%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3170, 1691, 1652, 1613, 1249; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 1.35 (t, J = 6.8 Hz, 3H, CH_3), 3.26 (s, 3H, CH_3), 3.49 (s, 3H, CH_3), 4.09 (q, J = 6.8 Hz, 2H, CH_2), 7.02-7.04 (m, 2H), 8.05-8.07 (m, 2H), 13.59 (s, br, 1H, NH); HPLC RT (min) 3.325; ESI-MS: *m/z* 301 $[M+H]^+$.



6b

8-(2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6b) [1]

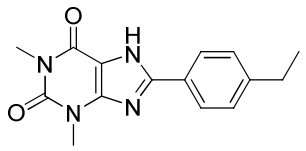
Light brown solid; Yield: 0.470 g, 69%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3460, 3149, 1703, 1661; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.49 (s, 3H, CH_3), 6.94-6.98 (m, 1H), 6.99-7.01 (m, 1H), 7.34-7.38 (m, 1H), 8.07-8.09 (m, 1H), 11.62 (s, br, 1H, OH), 13.77 (s, br, 1H, NH); HPLC RT (min) 3.302; ESI-MS: *m/z* 273 $[M+H]^+$.



6c

8-(4-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6c) [1]

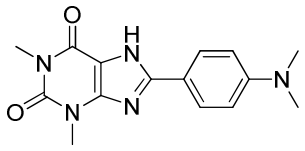
Light yellow solid; Yield: 0.537 g, 79%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3343, 3187, 1687, 1645, 1618; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.26 (s, 3H, CH_3), 3.48 (s, 3H, CH_3), 6.85-6.87 (m, 2H), 7.96-7.98 (m, 2H), 10.02 (s, br, 1H, OH), 13.50 (s, br, 1H, NH); HPLC RT (min) 2.948; ESI-MS: *m/z* 273 $[M+H]^+$.



6d

8-(4-ethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6d) [1]

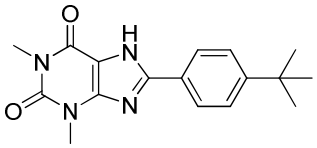
Milky white solid; Yield: 0.540 g, 76%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3173, 1705, 1667; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 1.21 (t, J = 7.6 Hz, 3H, CH_3), 2.66 (q, J = 7.6 Hz, 2H, CH_2), 3.27 (s, 3H, CH_3), 3.50 (s, 3H, CH_3), 7.34-7.36 (m, 2H), 8.04-8.06 (m, 2H), 13.75 (s, br, 1H, NH); HPLC RT (min) 3.503; ESI-MS: *m/z* 285 $[M+H]^+$.



6e

8-(4-(dimethylamino)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6e) [1]

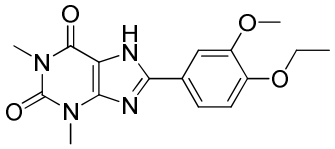
Light brown solid; Yield: 0.508 g, 68%; m.p >300 °C; FT-IR (KBr, cm^{-1}): 3174, 1699, 1652, 1609; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 2.99 (s, 6H, $2CH_3$), 3.26 (s, 3H, CH_3), 3.49 (s, 3H, CH_3), 6.77-6.79 (m, 2H), 7.96-7.98 (m, 2H), 13.33 (s, br, 1H, NH); HPLC RT (min) 3.354; ESI-MS: *m/z* 300 $[M+H]^+$.



6f

8-(4-*tert*-butylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6f) [2]

Off white solid; Yield: 0.515 g, 66%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3154, 1701, 1650; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 1.31 (s, 9H, $3CH_3$), 3.27 (s, 3H, CH_3), 3.50 (s, 3H, CH_3), 7.52-7.54 (m, 2H), 8.06-8.08 (m, 2H), 13.75 (s, br, 1H, NH); HPLC RT (min) 3.675; ESI-MS: *m/z* 313 $[M+H]^+$.

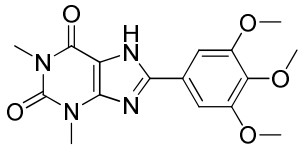


6g

8-(4-ethoxy-3-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6g) [3]

Off white solid; Yield: 0.619 g, 75%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3182, 1703, 1646, 1594, 1274; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 1.35 (t, J = 6.8 Hz, 3H,

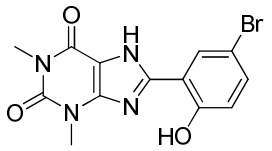
CH_3), 3.26 (s, 3H, CH_3), 3.49 (s, 3H, CH_3), 3.84 (s, 3H, OCH_3), 4.07 (q, J = 6.8 Hz, 2H, CH_2), 7.04-7.06 (m, 1H), 7.69-7.71 (m, 1H), 7.73 (s, 1H), 13.59 (s, br, 1H, NH); HPLC RT (min) 3.232; ESI-MS: *m/z* 331 $[M+H]^+$.



6h

8-(3,4,5-trimethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6h) [4]

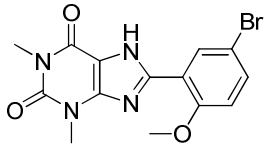
Light brown solid; Yield: 0.623 g, 72%; m.p. >300 °C; FTIR (KBr): 3156, 1708, 1665, 1226 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.51 (s, 3H, CH_3), 3.72 (s, 3H, OCH_3), 3.87 (s, 6H, $2OCH_3$), 7.48 (s, 2H), 13.74 (s, br, 1H, NH); HPLC RT (min) 3.112; ESI-MS: *m/z* 347 $[M+H]^+$.



6i

8-(5-bromo-2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6i) [3]

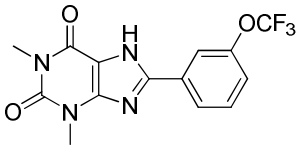
Light brown solid; Yield: 0.650 g, 74%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3453, 3183, 1705, 1645, 1605, 1257, 728; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.26 (s, 3H, CH_3), 3.47 (s, 3H, CH_3), 6.94-6.96 (m, 1H), 7.46-7.48 (m, 1H), 8.26 (s, 1H), 11.67 (s, br, 1H, OH), 13.80 (s, br, 1H, NH); HPLC RT (min) 3.658; ESI-MS: *m/z* 352 $[M+H]^+$.



6j

8-(5-bromo-2-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6j) [3]

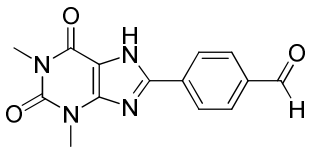
Light brown solid; Yield: 0.712 g, 78%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3166, 1693, 1657, 1277, 760; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.26 (s, 3H, CH_3), 3.50 (s, 3H, CH_3), 3.93 (s, 3H, OCH_3), 7.17-7.19 (m, 1H), 7.63-7.65 (m, 1H), 8.10 (s, 1H), 13.01 (s, br, 1H, NH); HPLC RT (min) 4.031; ESI-MS: *m/z* 366 $[M+H]^+$.



6k

8-(3-(trifluoromethoxy)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6k) [3]

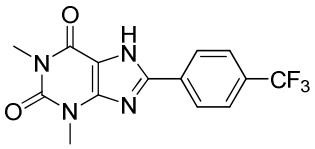
Off white solid; Yield: 0.672 g, 79%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3170, 1699, 1668, 1596, 1295, 984; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.50 (s, 3H, CH_3), 7.48-7.50 (m, 1H), 7.64-7.68 (m, 1H), 8.10 (s, 1H), 8.16-8.18 (m, 1H), 14.09 (s, br, 1H, NH); HPLC RT (min) 3.322; ESI-MS: *m/z* 341 $[M+H]^+$.



6l

4-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzaldehyde (6l) [5]

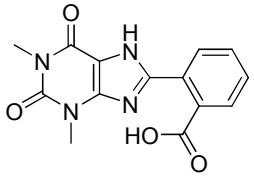
Yellow solid; Yield: 0.511 g, 72%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3157, 1699, 1648, 1603, 1530, 1212; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.51 (s, 3H, CH_3), 8.01-8.03 (m, 2H), 8.32-8.34 (m, 2H), 10.05 (s, 1H, CHO), 14.15 (s, br, 1H, NH); HPLC RT (min) 3.153; ESI-MS: *m/z* 285 $[M+H]^+$.



6m

8-(4-(trifluoromethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6m) [6]

Off white solid; Yield: 0.656 g, 81%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3143, 1714, 1647, 1602, 1119; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.51 (s, 3H, CH_3), 7.88-7.90 (m, 2H), 8.33-8.35 (m, 2H), 14.17 (s, br, 1H, NH); HPLC RT (min) 3.336; ESI-MS: *m/z* 325 $[M+H]^+$.

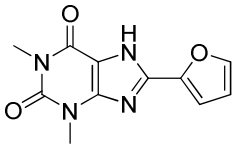


6n

2-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzoic acid (6n) [1]

Light brown solid; Yield: 0.480 g, 64%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3463, 3185, 1696, 1660, 1605; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.46 (s,

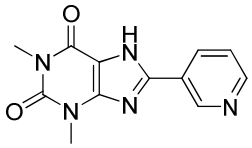
3H, CH_3), 7.58-7.62 (m, 1H), 7.64-7.67 (m, 1H), 7.70-7.72 (m, 1H), 7.82-7.84 (m, 1H), 12.98 (s, br, 1H, COOH), 13.75 (s, br, 1H, NH); HPLC RT (min) 3.958; ESI-MS: *m/z* 301 $[M+H]^+$.



6o

8-(furan-2-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6o) [7]

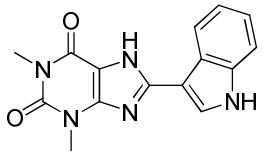
Dark brown solid; Yield: 0.382 g, 62%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3126, 1707, 1648, 1601, 1253; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.25 (s, 3H, CH_3), 3.46 (s, 3H, CH_3), 6.81-6.82 (m, 1H), 7.22-7.23 (m, 1H), 7.89-7.90 (m, 1H), 13.98 (s, br, 1H, NH); HPLC RT (min) 3.196; ESI-MS: *m/z* 247 $[M+H]^+$.



6p

8-(pyridin-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6p) [8]

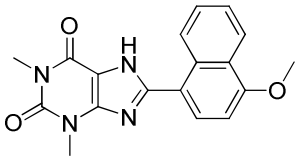
Light brown solid; Yield: 0.502 g, 78%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3146, 1695, 1645, 1607; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.50 (s, 3H, CH_3), 7.53-7.56 (m, 1H), 8.42-8.45 (m, 1H), 7.65-7.66 (m, 1H), 9.27 (s, 1H), 14.09 (s, br, 1H, NH); HPLC RT (min) 3.047; ESI-MS: *m/z* 258 $[M+H]^+$.



6q

8-(1*H*-indol-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6q) [9]

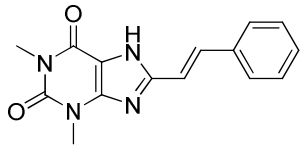
Green solid; Yield: 0.546 g, 74%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3294, 1688, 1648, 1586; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.27 (s, 3H, CH_3), 3.57 (s, 3H, CH_3), 7.17-7.21 (m, 2H), 7.46-7.48 (m, 1H), 8.22 (s, 1H), 8.40-8.42 (m, 1H), 11.70 (s, br, 1H, NH of indole), 13.27 (s, br, 1H, NH); HPLC RT (min) 3.399; ESI-MS: *m/z* 296 $[M+H]^+$.



6r

8-(4-methoxynaphthalen-1-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6r) [3]

Dark green solid; Yield: 0.546 g, 65%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3202, 1697, 1648, 1252; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.25 (s, 3H, CH_3), 3.55 (s, 3H, CH_3), 4.06 (s, 3H, OCH_3), 7.11-7.13 (m, 1H), 7.57-7.61 (m, 1H), 7.63-7.65 (m, 1H), 7.92-7.94 (m, 1H), 8.25-8.27 (m, 1H), 8.88-8.90 (m, 1H), 13.71 (s, br, 1H, NH); HPLC RT (min) 3.303; ESI-MS: *m/z* 337 $[M+H]^+$.



6s

8-styryl-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6s) [10]

Pale yellow solid; Yield: 0.536 g, 76%; m.p. >300 °C; FT-IR (KBr, cm^{-1}): 3152, 1694, 1645, 1601; ^1H NMR (400 MHz, DMSO-d_6): δ (ppm) 3.25 (s, 3H, CH_3), 3.48 (s, 3H, CH_3), 7.01-7.05 (m, 1H), 7.36-7.38 (m, 2H), 7.41-7.44 (m, 1H), 7.61-7.63 (m, 2H), 7.67 (s, 1H), 13.59 (s, br, 1H, NH); HPLC RT (min) 3.303; ESI-MS: *m/z* 283 $[M+H]^+$.

References

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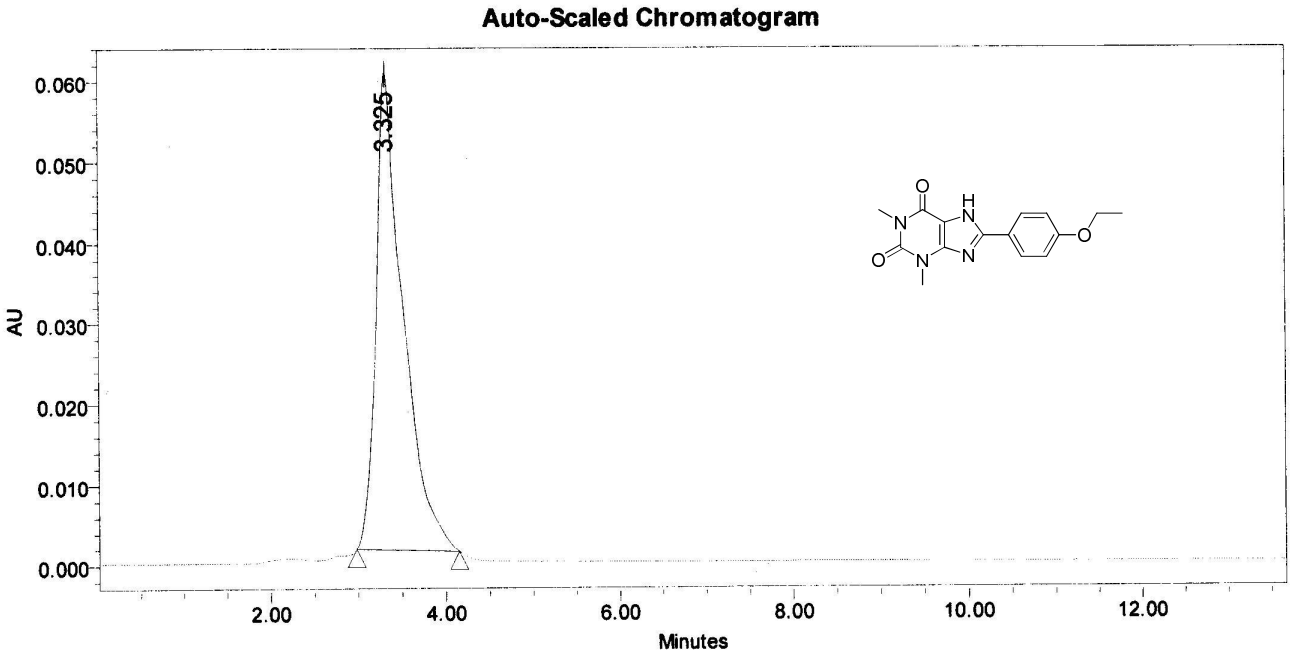
HPLC Chromatogram and ^{1}H-NMR spectra for all the synthesized 8-substituted xanthine derivatives are given below as evidence of purity:

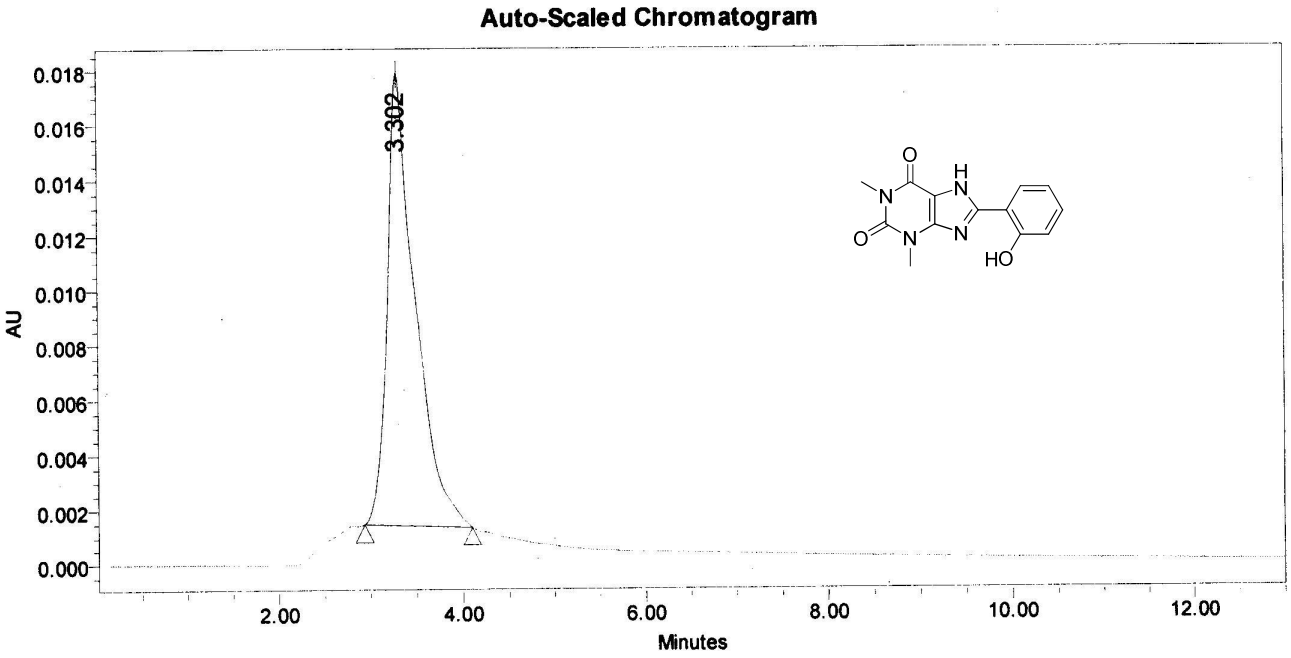
HPLC Chromatogram of 8-(4-ethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6a)



Peak Results

	RT	Area	Height
1	3.325	1272159	59265

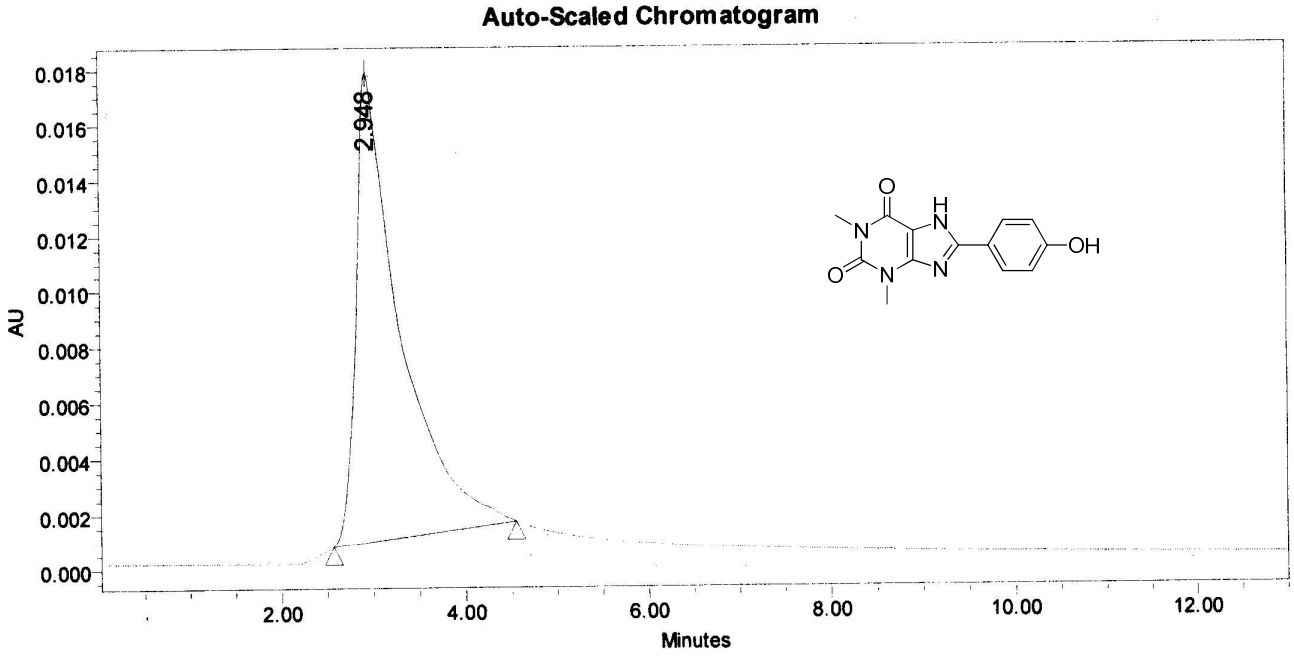
HPLC Chromatogram of 8-(2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6b)



Peak Results

	RT	Area	Height
1	3.302	344677	16446

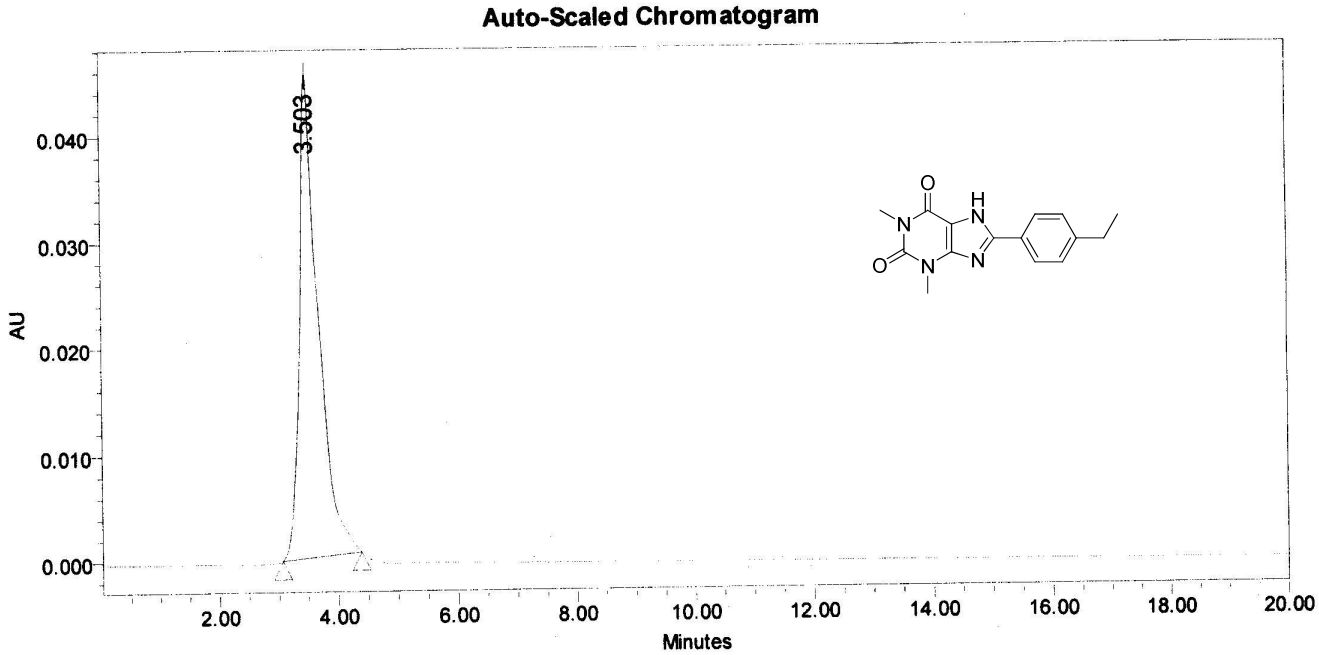
HPLC Chromatogram of 8-(4-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6c)



Peak Results

	RT	Area	Height
1	2.948	559666	16903

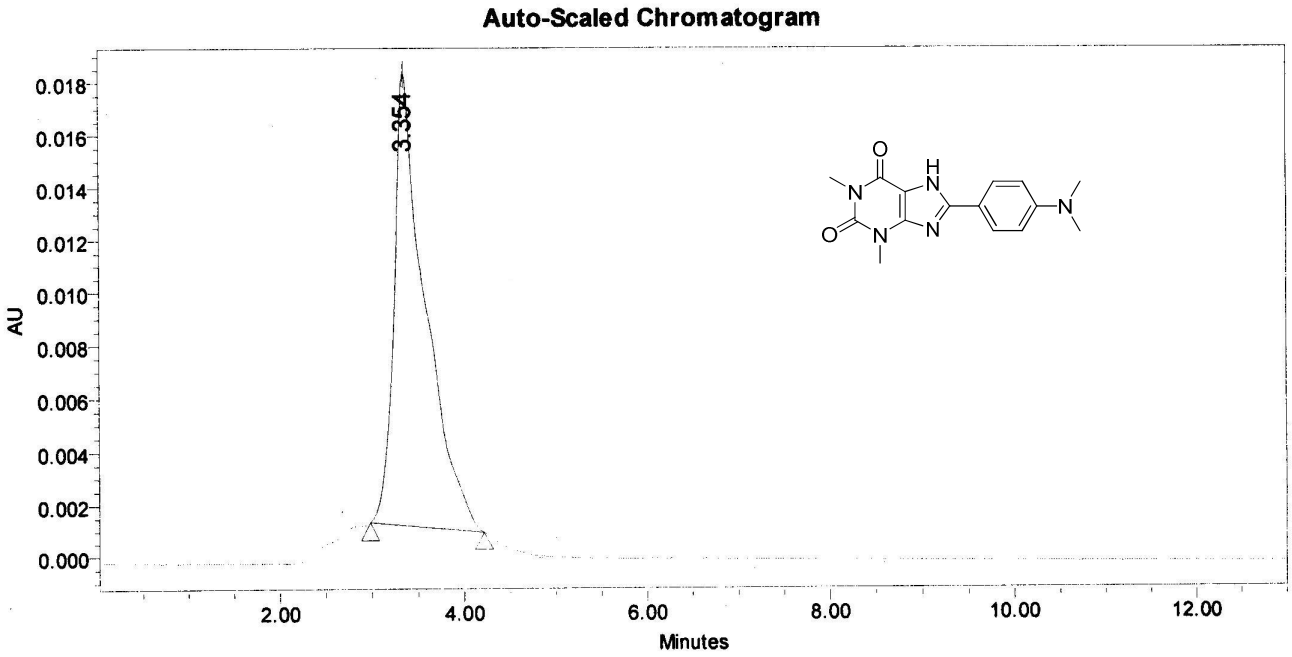
HPLC Chromatogram of 8-(4-ethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6d)



Peak Results

	RT	Area	Height
1	3.503	996913	45475

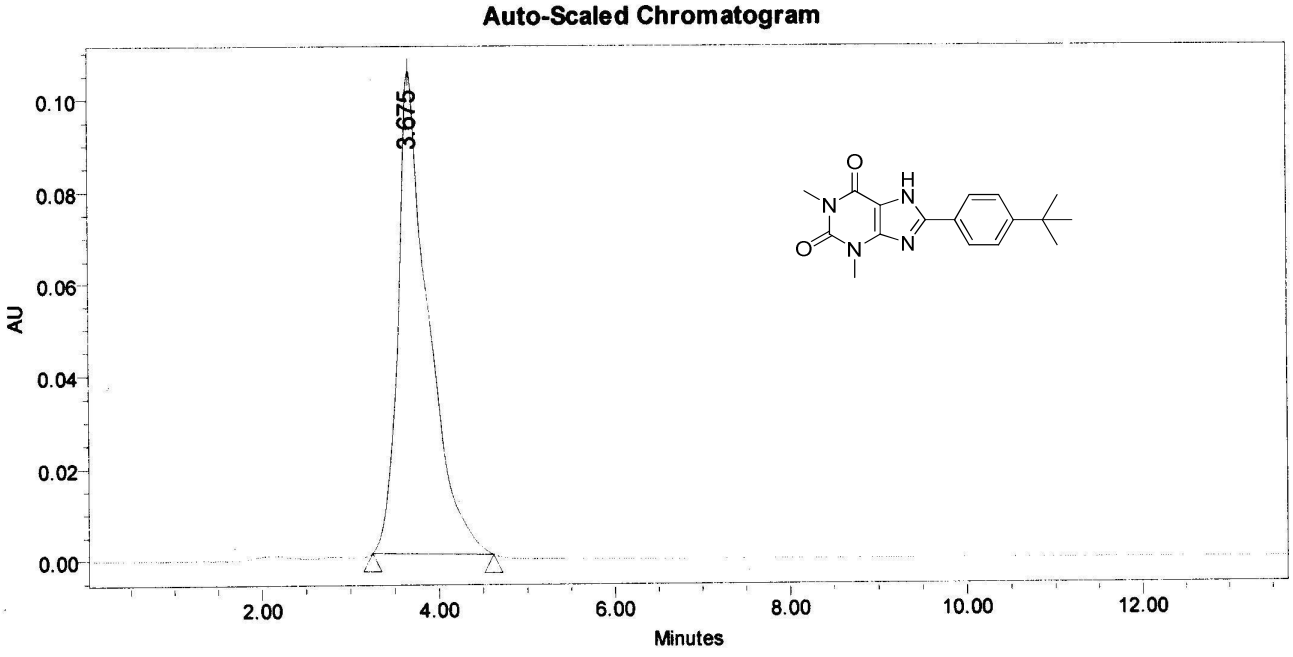
HPLC Chromatogram of 8-(4-(dimethylamino)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6e)



Peak Results

	RT	Area	Height
1	3.354	401406	17171

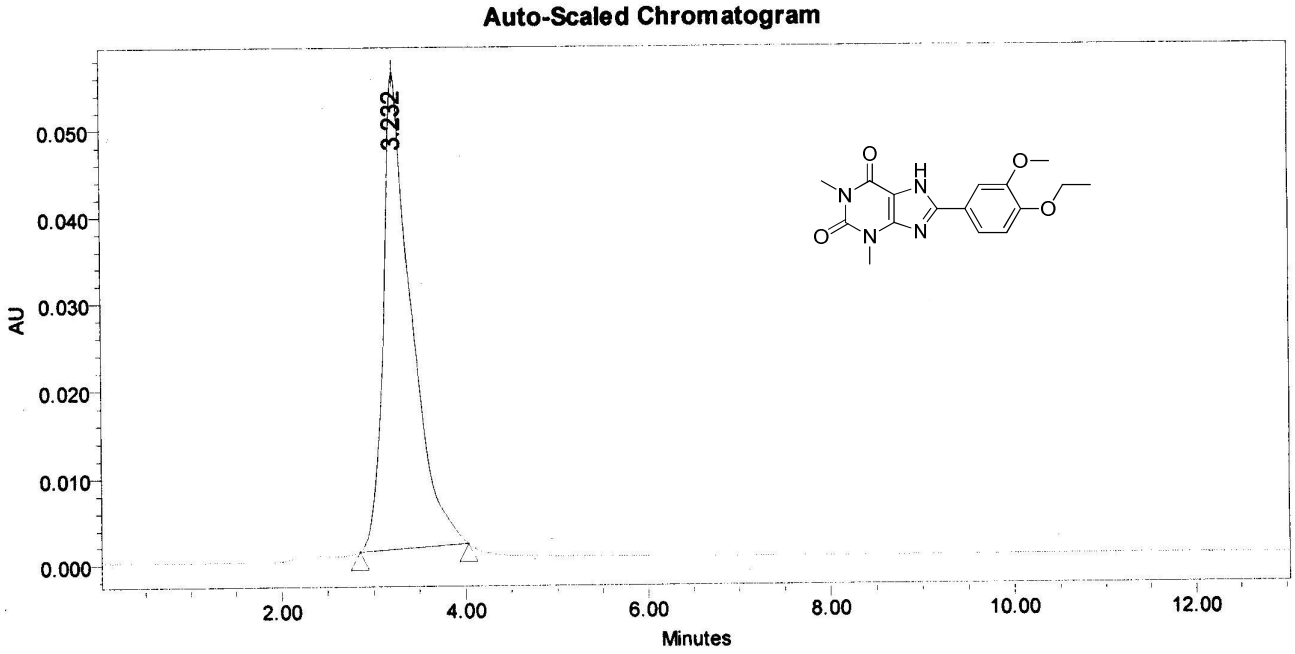
HPLC Chromatogram of 8-(4-*tert*-butylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6f)



Peak Results

	RT	Area	Height
1	3.675	2486390	105124

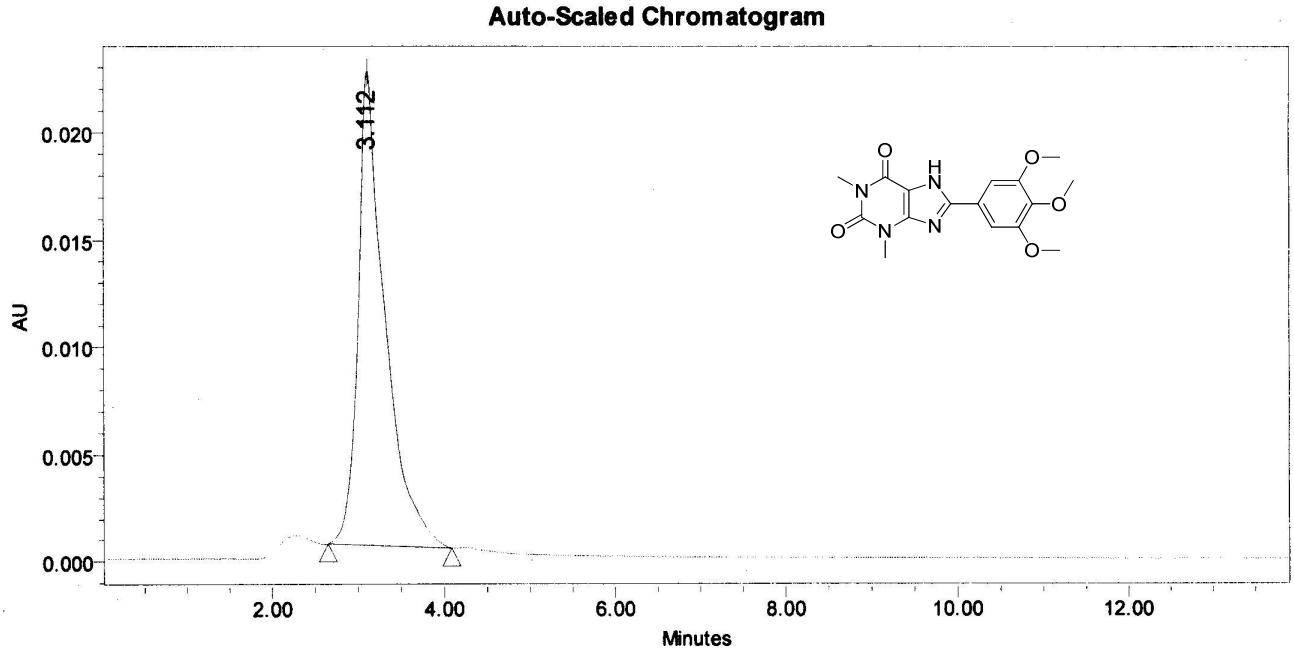
HPLC Chromatogram of 8-(4-ethoxy-3-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6g)



Peak Results

	RT	Area	Height
1	3.232	1150961	54960

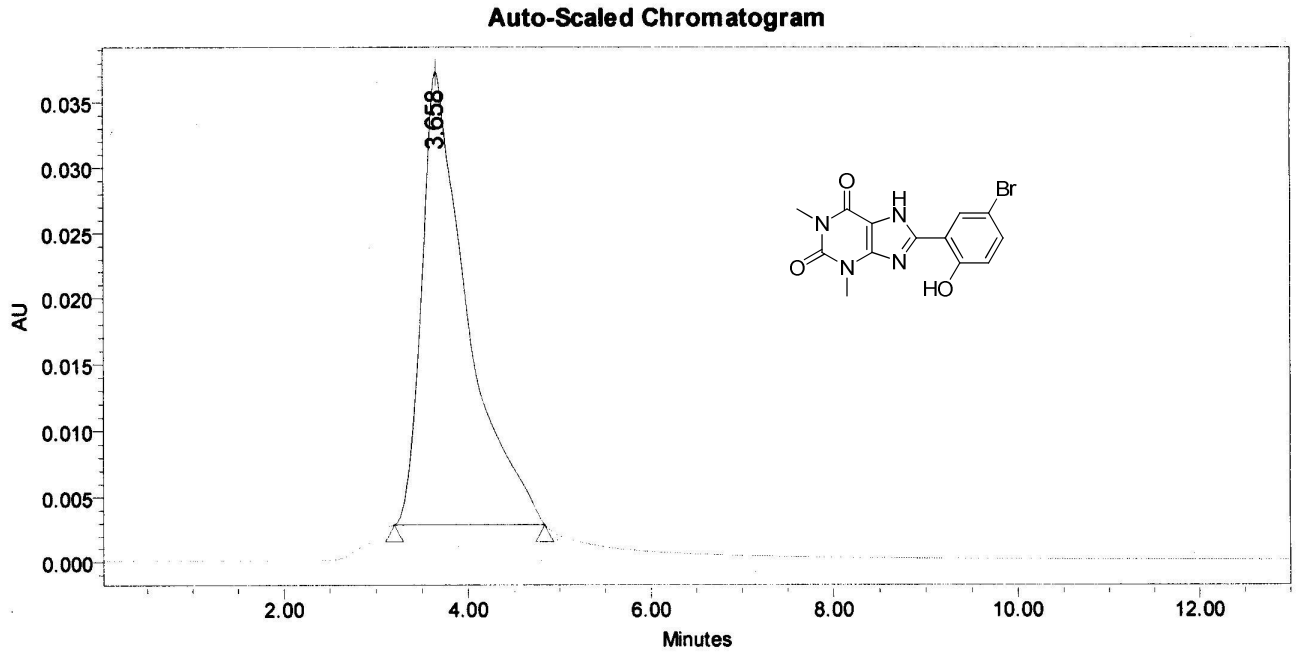
HPLC Chromatogram of 8-(3,4,5-trimethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6h)



Peak Results

	RT	Area	Height
1	3.112	481690	22094

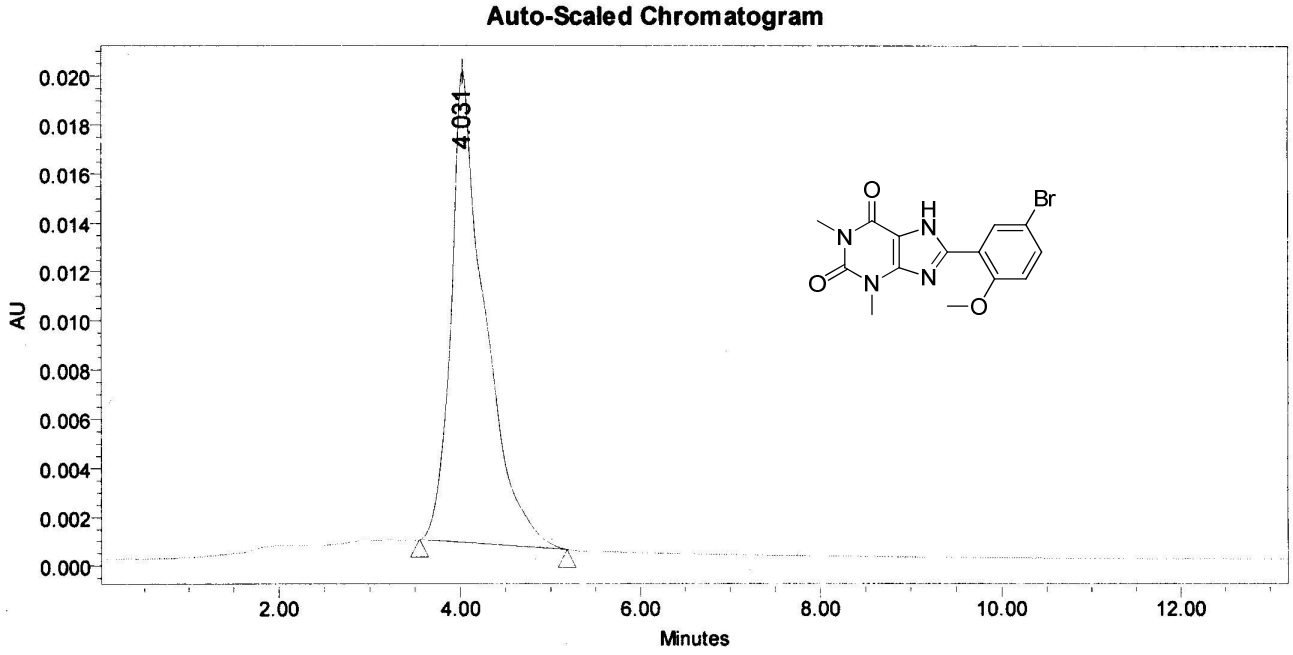
HPLC Chromatogram of 8-(5-bromo-2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6i)



Peak Results

	RT	Area	Height
1	3.658	1175091	34491

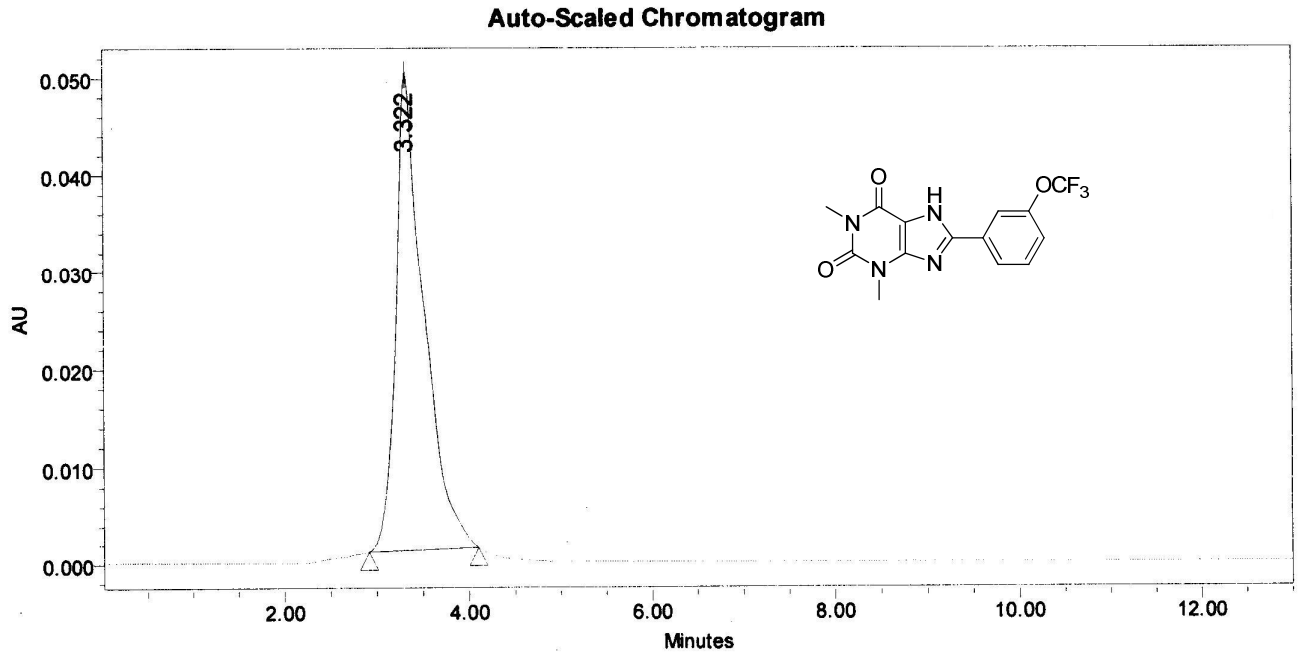
HPLC Chromatogram of 8-(5-bromo-2-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6j)



Peak Results

	RT	Area	Height
1	4.031	498964	19267

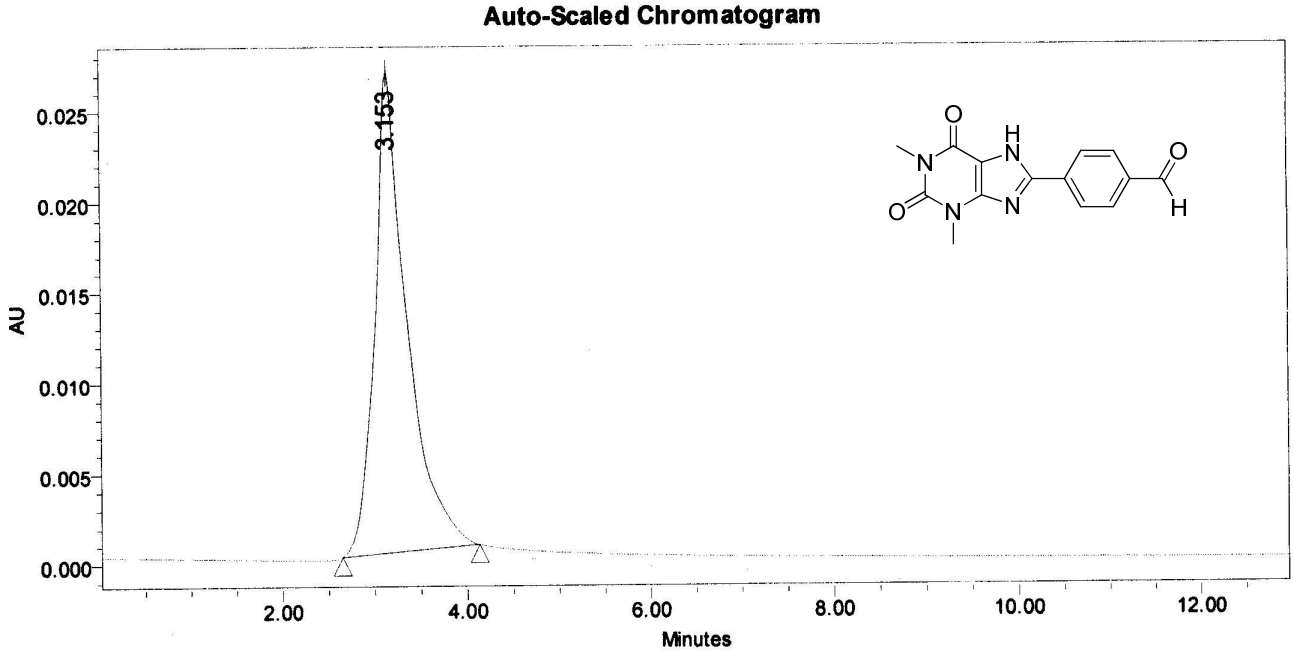
HPLC Chromatogram of 8-(3-(trifluoromethoxy)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6k)



Peak Results

	RT	Area	Height
1	3.322	1035365	49160

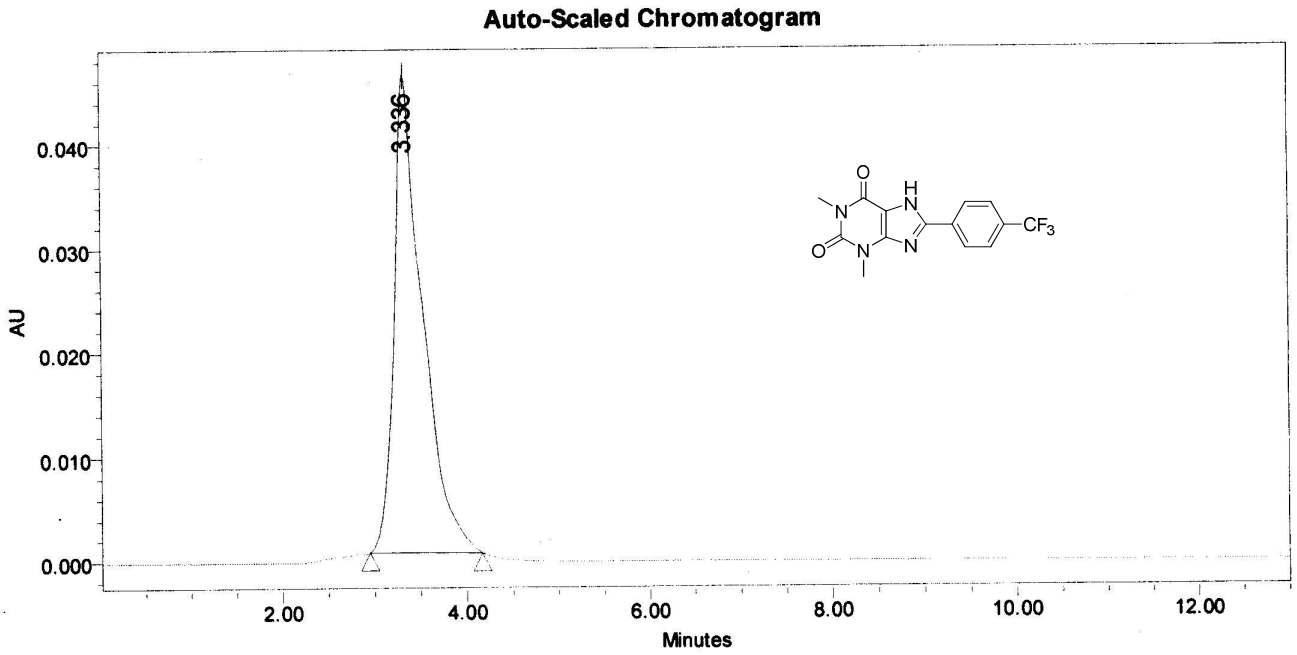
HPLC Chromatogram of 4-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzaldehyde (6l)



Peak Results

	RT	Area	Height
1	3.153	643433	26582

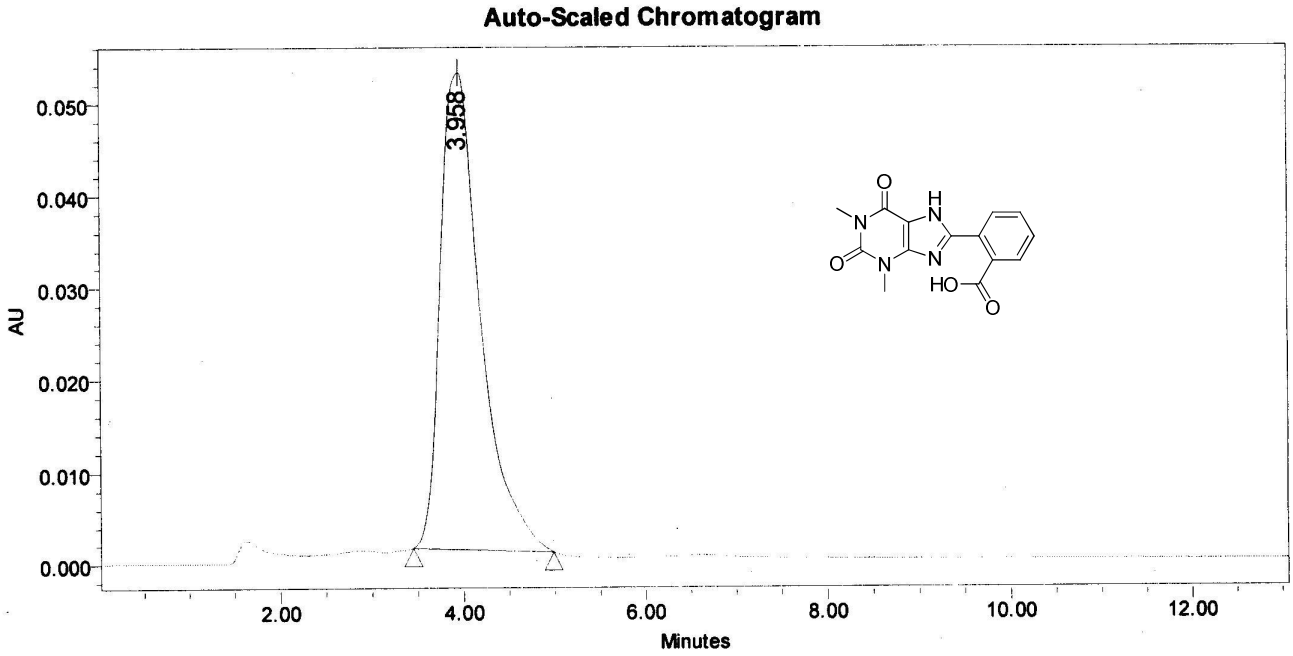
HPLC Chromatogram of 8-(4-(trifluoromethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6m)



Peak Results

	RT	Area	Height
1	3.336	981864	45928

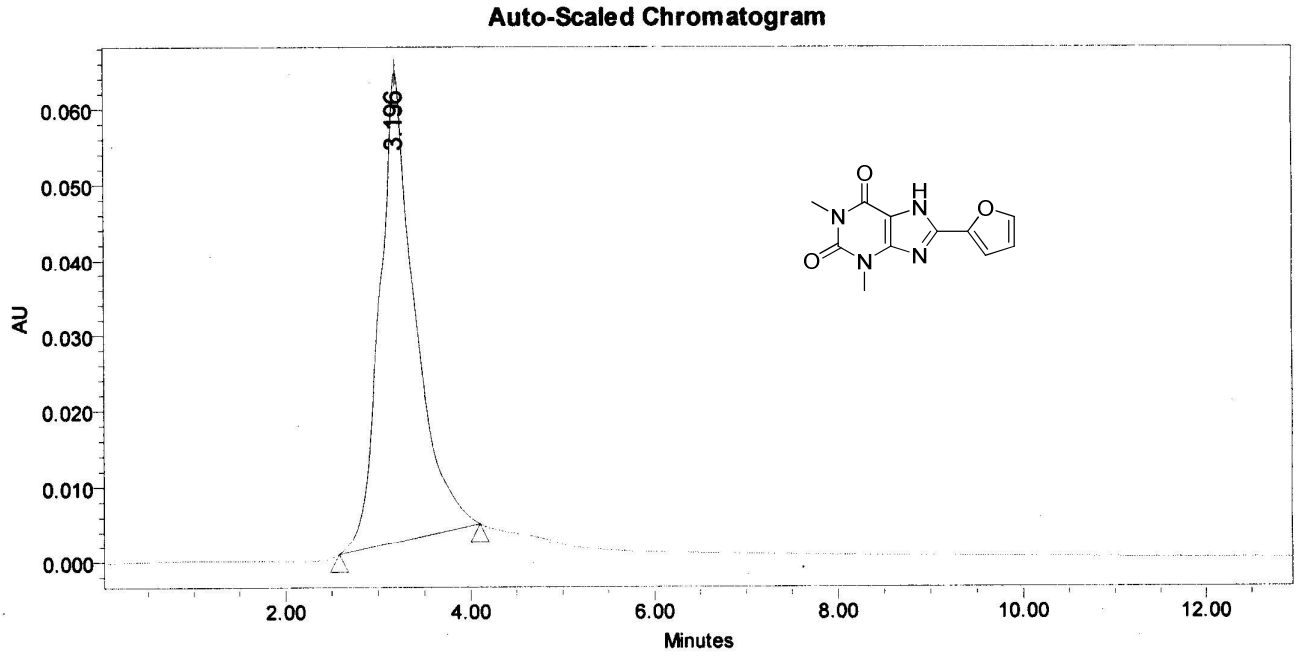
HPLC Chromatogram of 2-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzoic acid (6n)



Peak Results

	RT	Area	Height
1	3.958	1587345	51877

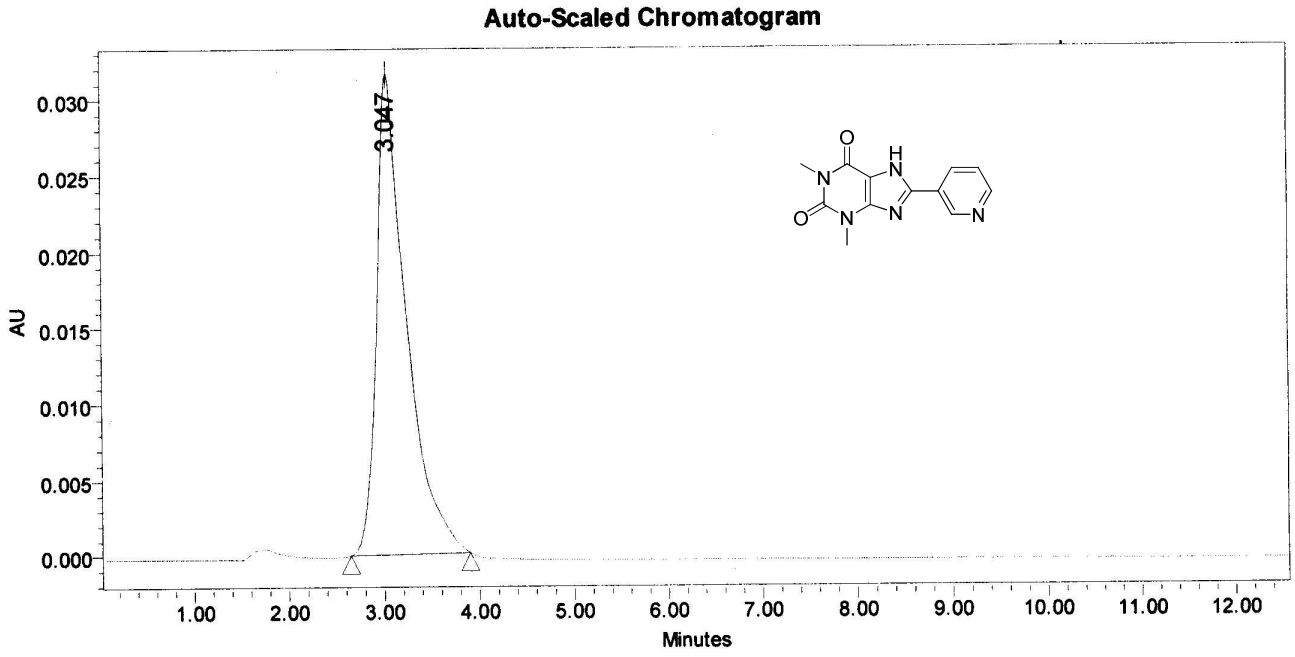
HPLC Chromatogram of 8-(furan-2-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6o)



Peak Results

	RT	Area	Height
1	3.196	1636320	62289

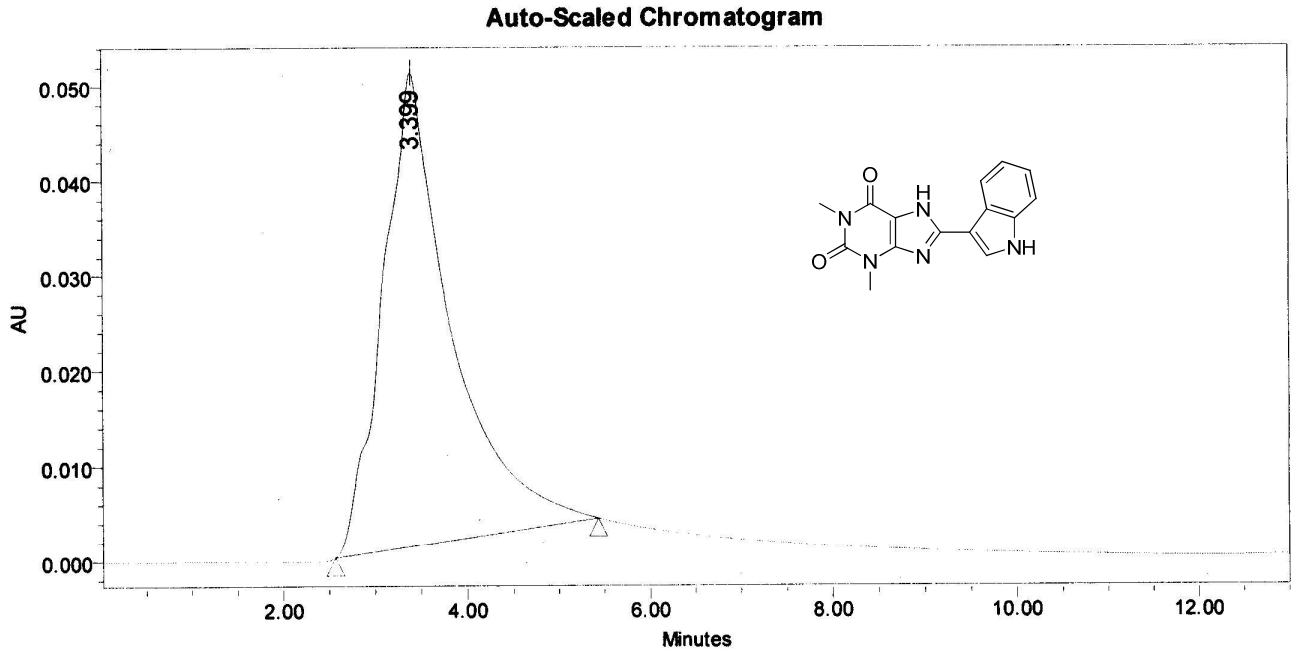
HPLC Chromatogram of 8-(pyridin-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6p)



Peak Results

	RT	Area	Height
1	3.047	687740	31654

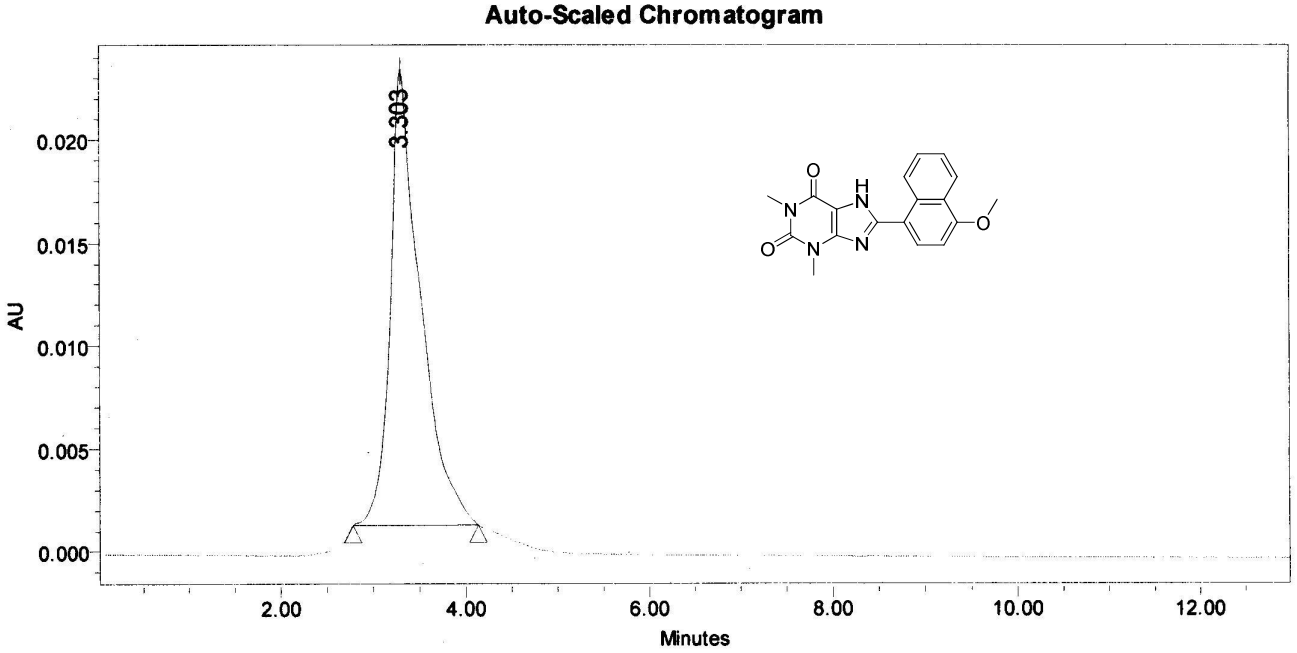
HPLC Chromatogram of 8-(1*H*-indol-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6q)



Peak Results

	RT	Area	Height
1	3.399	2569197	49861

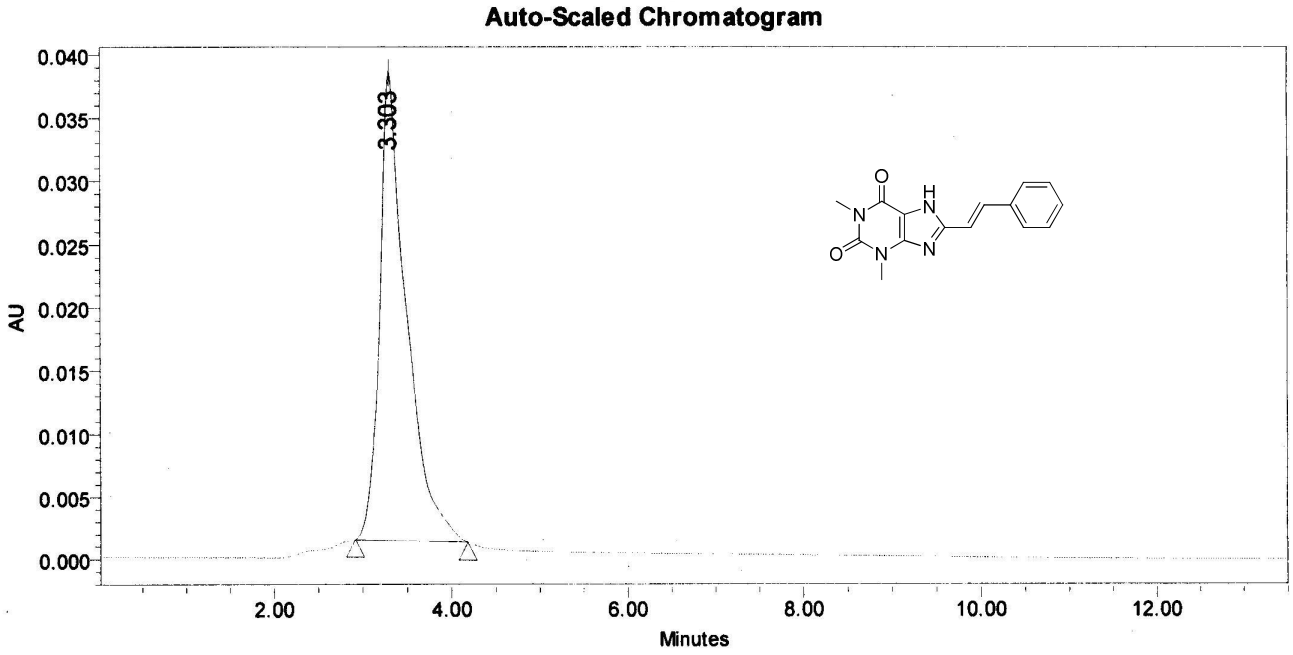
HPLC Chromatogram of 8-(4-methoxynaphthalen-1-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6r)



Peak Results

	RT	Area	Height
1	3.303	500954	22119

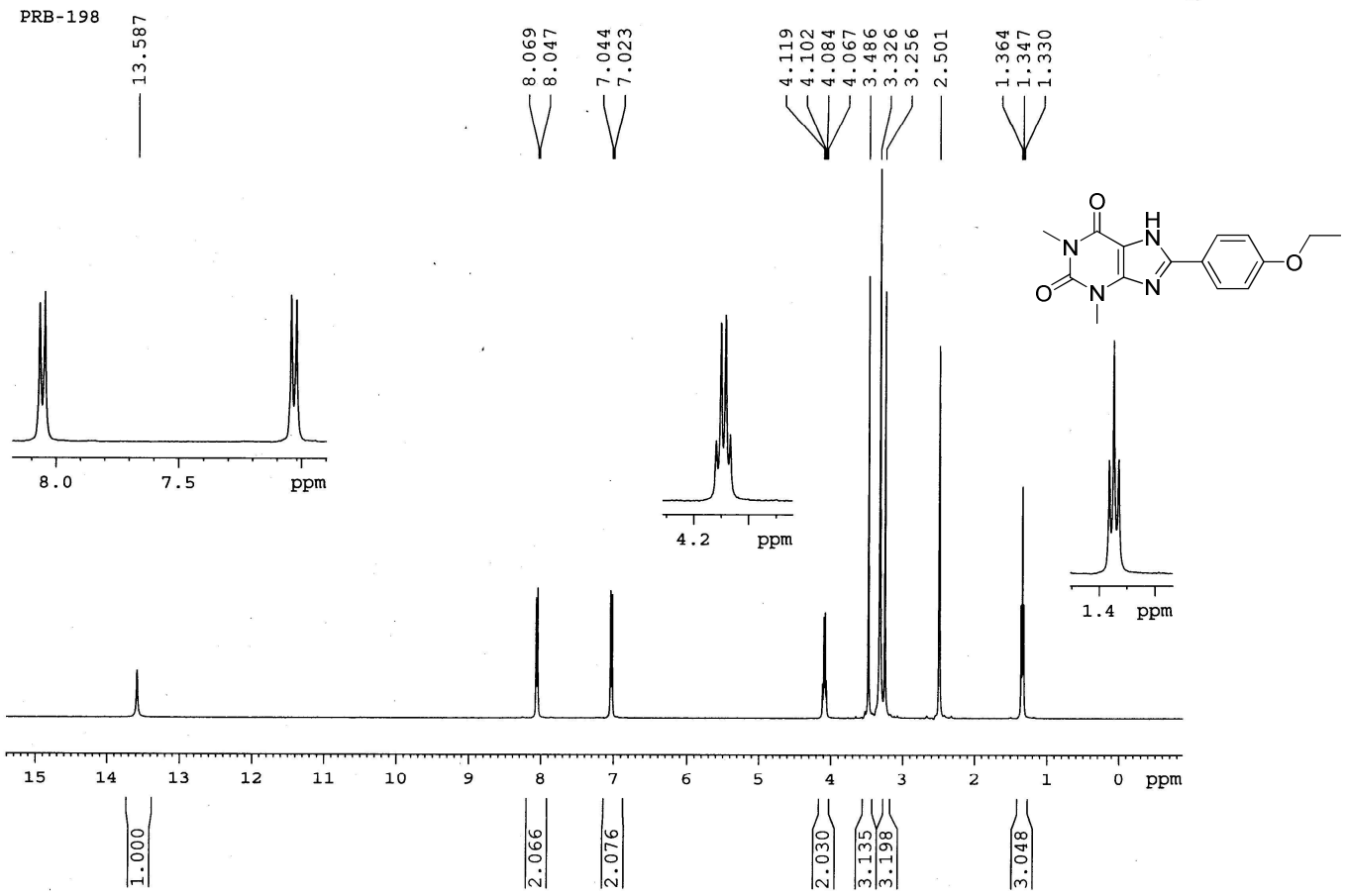
HPLC Chromatogram of 8-styryl-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6s)



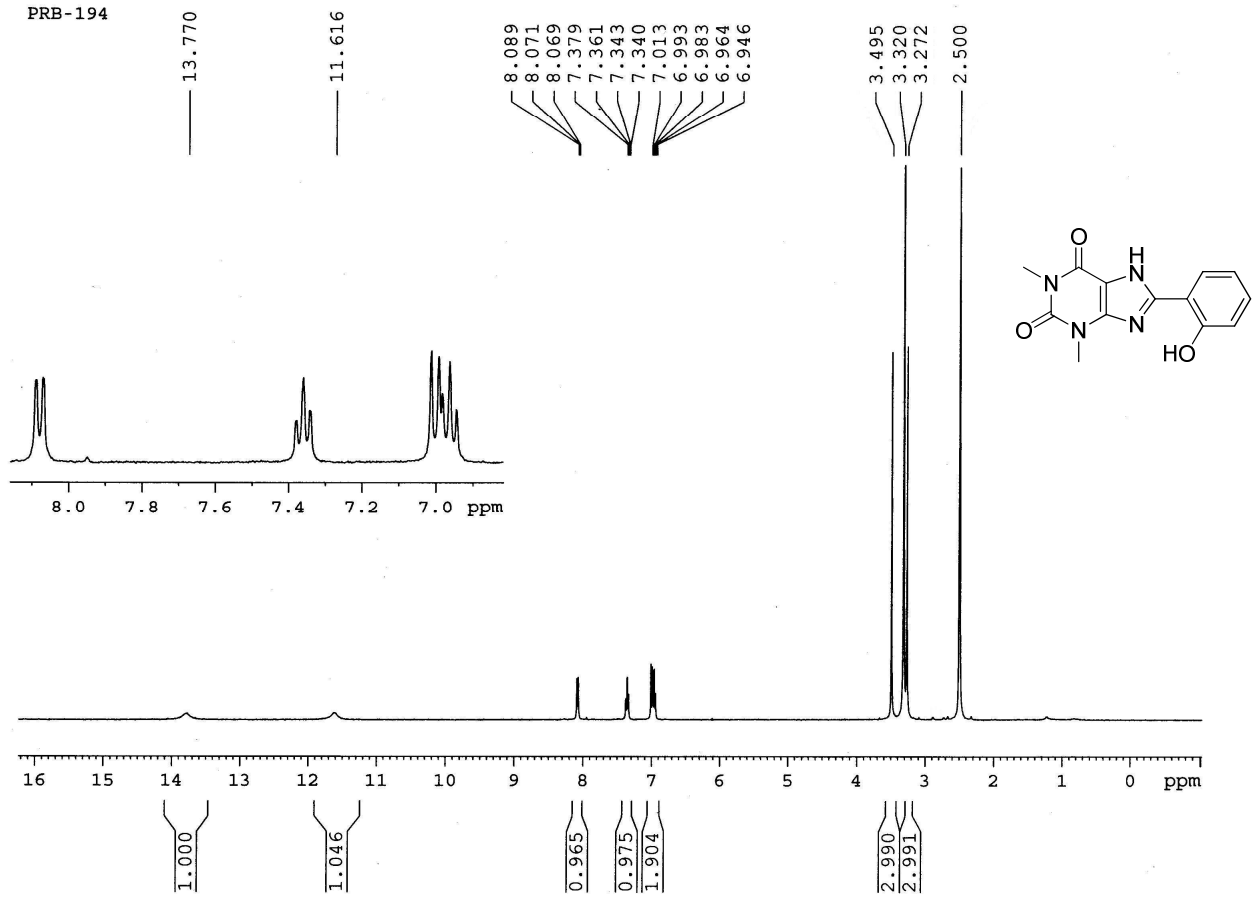
Peak Results

	RT	Area	Height
1	3.303	778521	37167

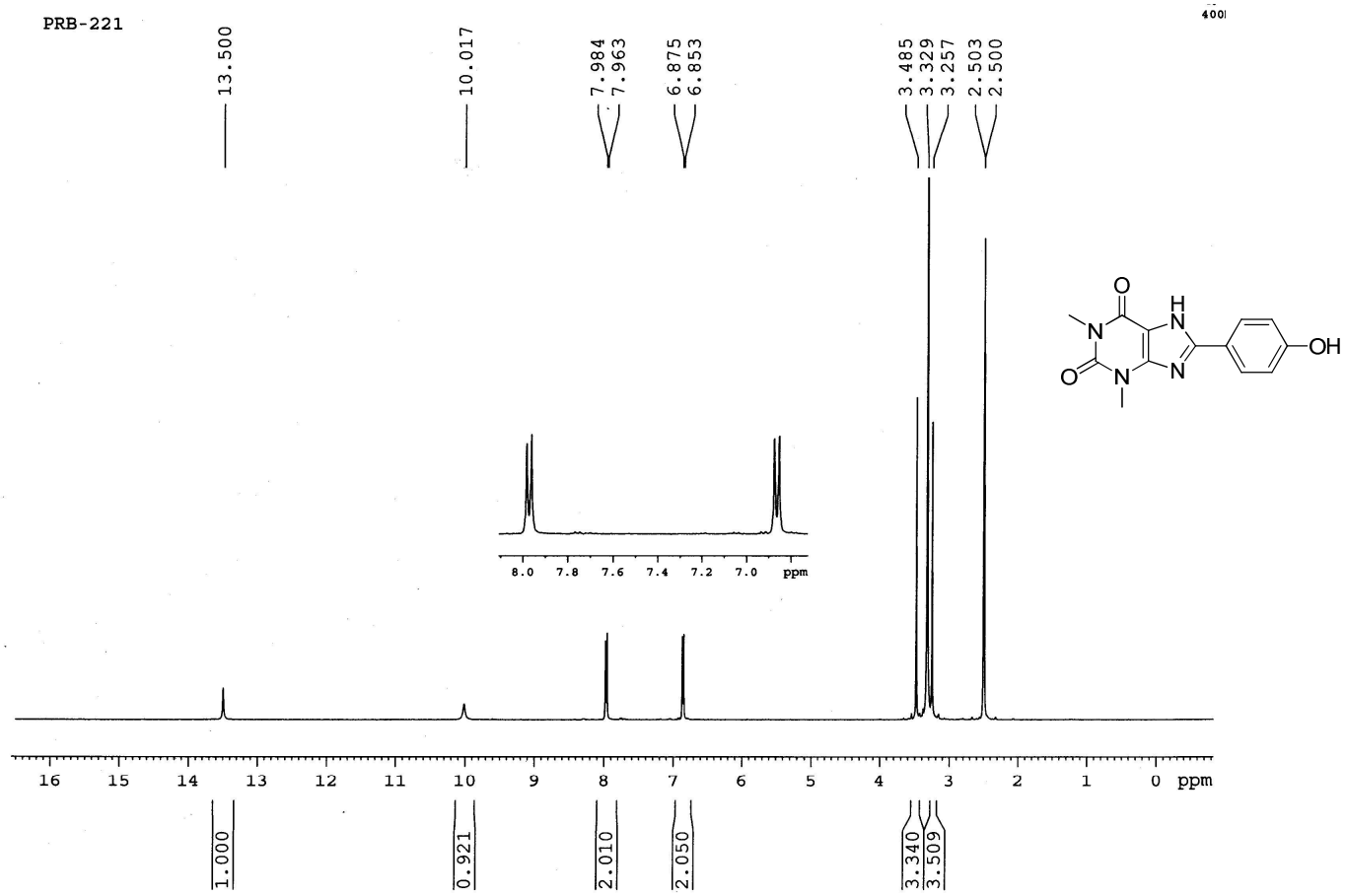
^{1}H-NMR spectrum of 8-(4-ethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6a) (DMSO-d_6)



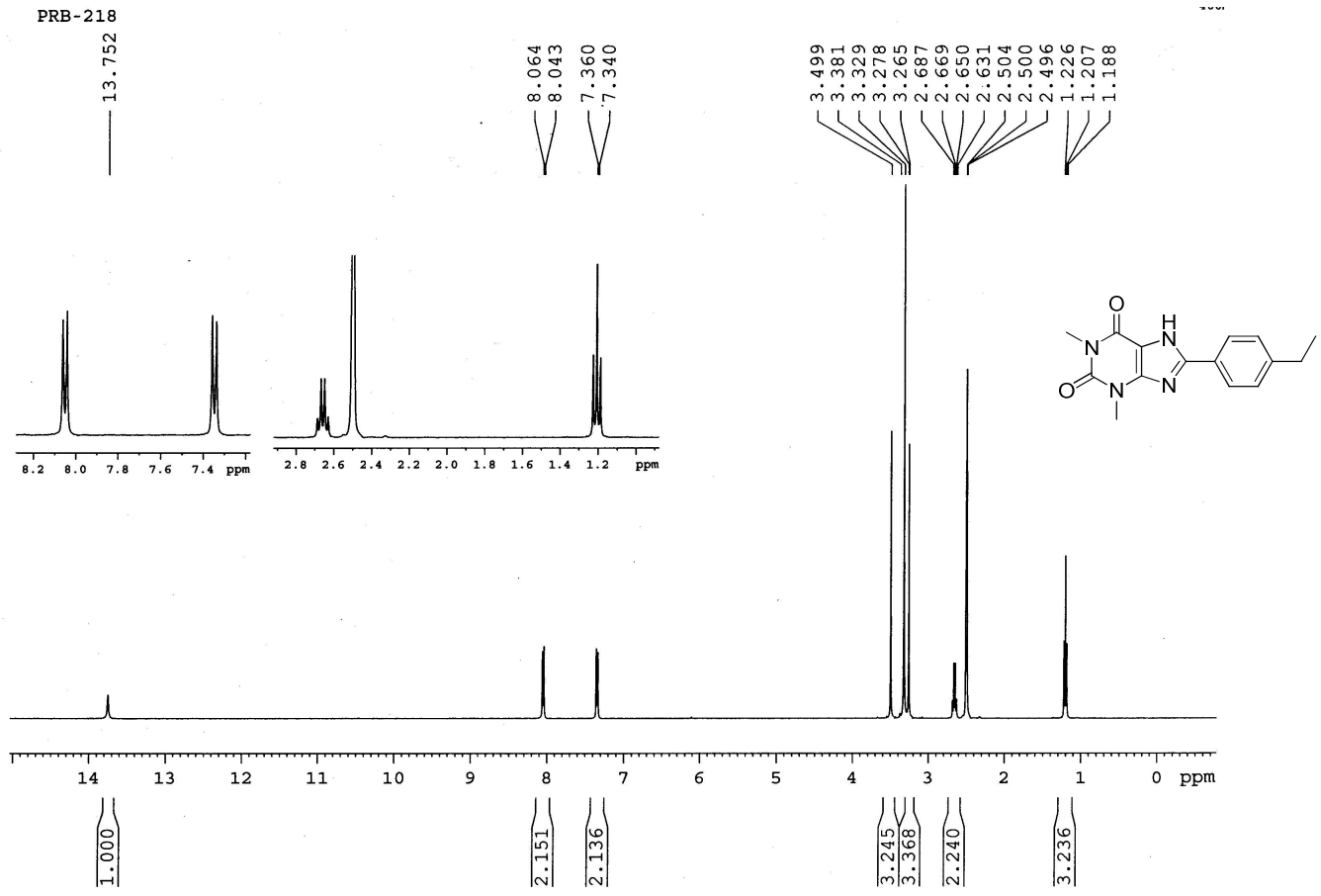
^{1}H-NMR spectrum of 8-(2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6b) (DMSO-d_6)



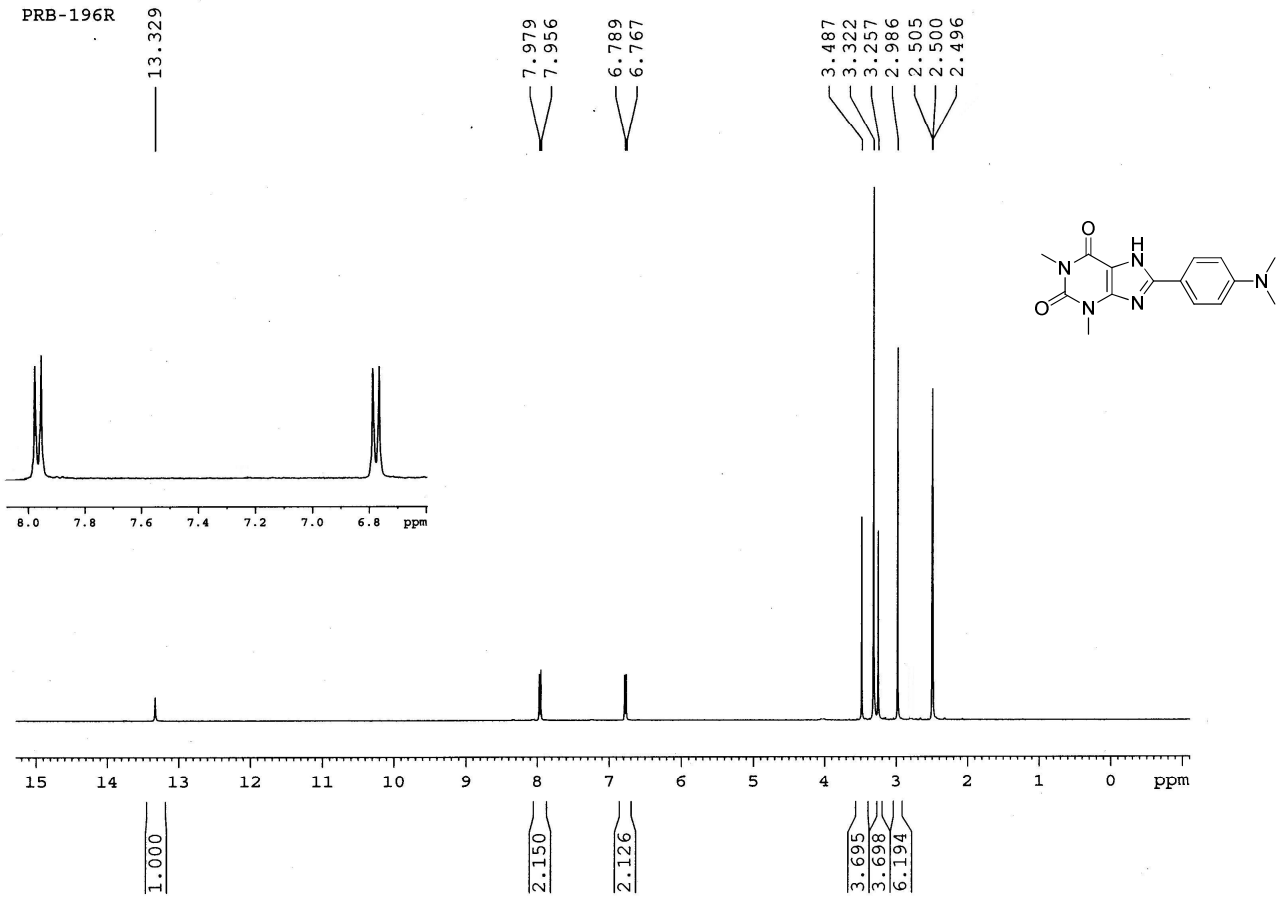
^{1}H-NMR spectrum of 8-(4-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6c) (DMSO-d_6)



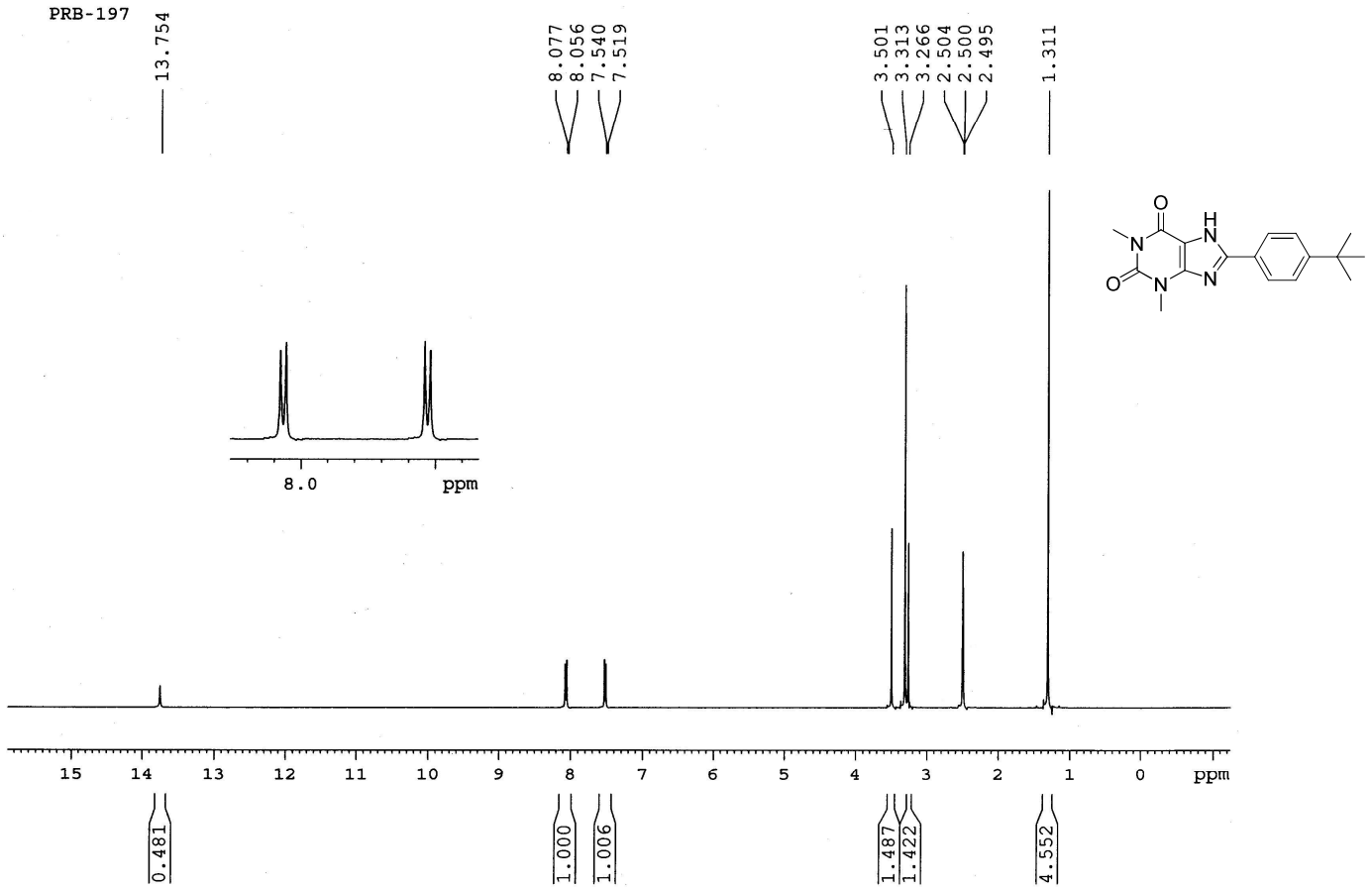
^{1}H-NMR spectrum of 8-(4-ethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6d) (DMSO-d_6)



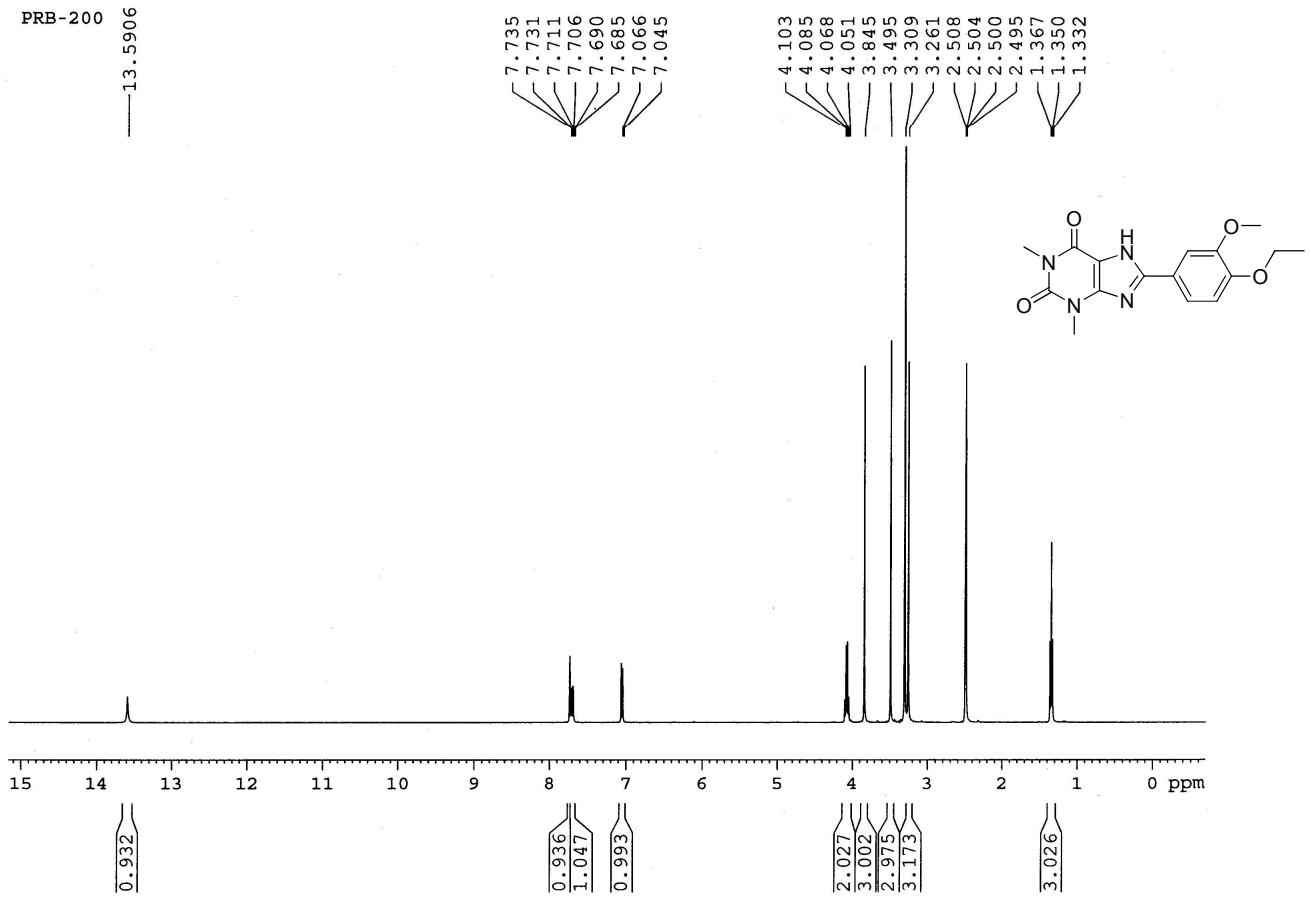
^{1}H-NMR spectrum of 8-(4-(dimethylamino)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6e) (DMSO-d_6)



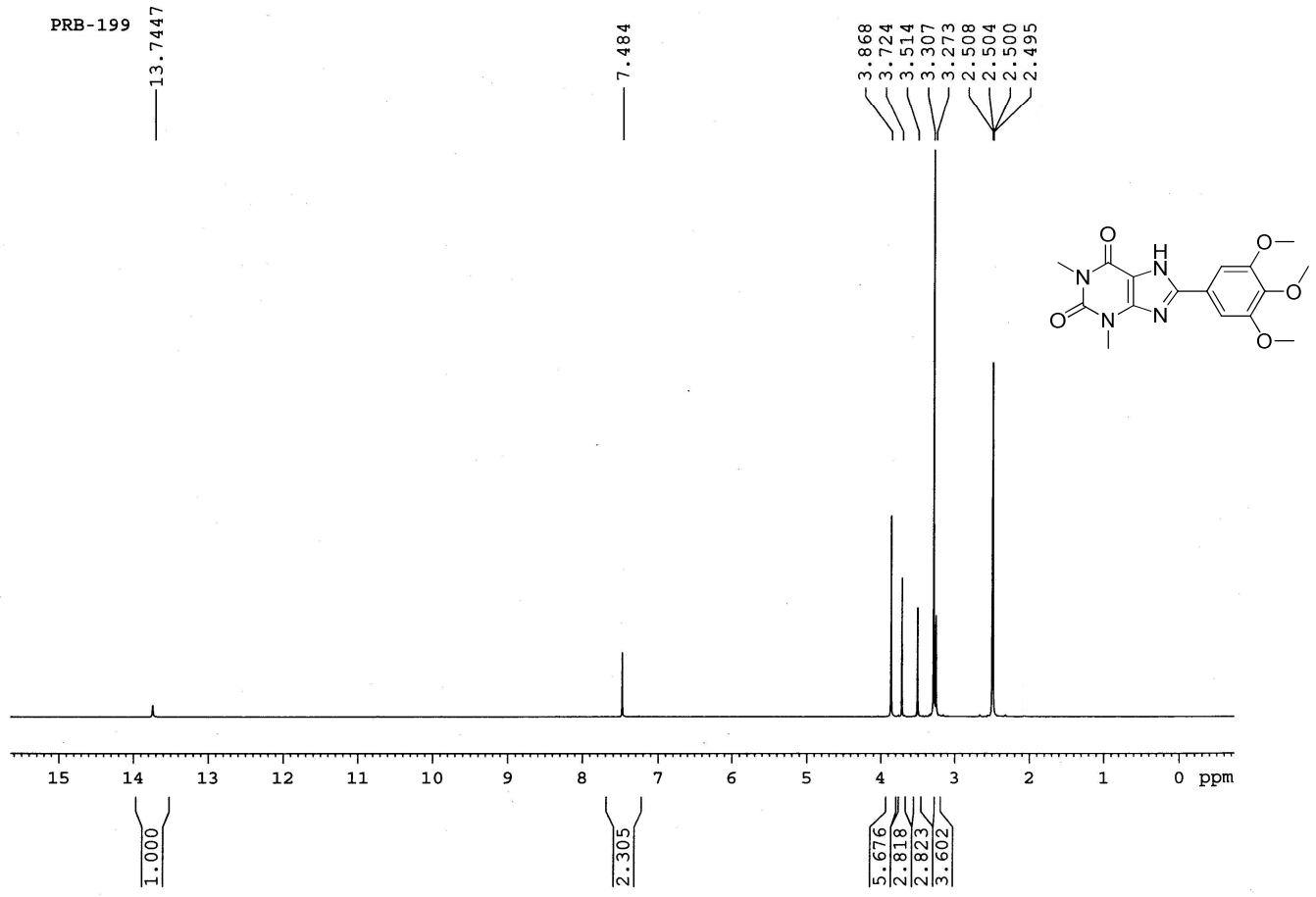
^{1}H-NMR spectrum of 8-(4-*tert*-butylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6f) (DMSO-d_6)



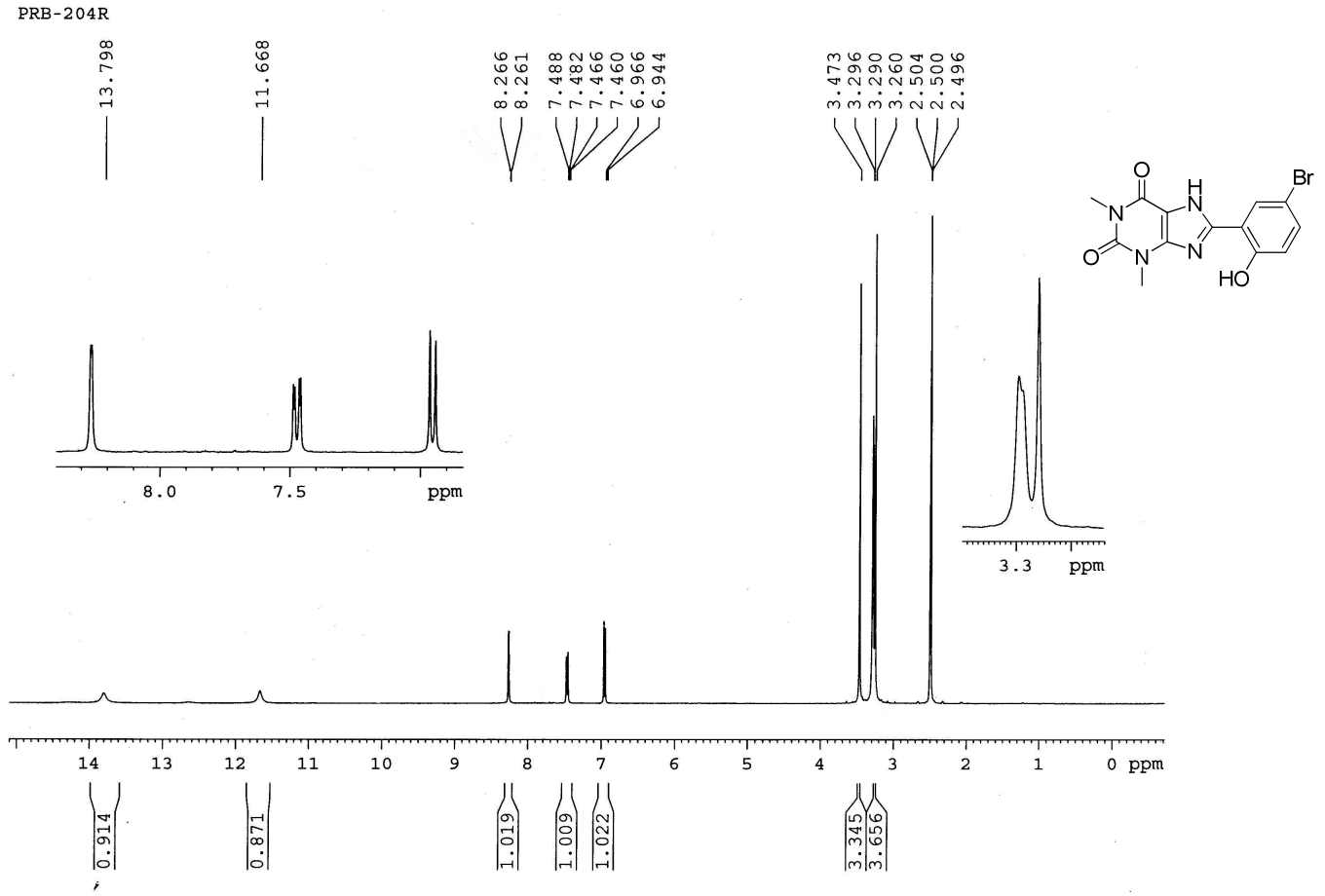
^{1}H-NMR spectrum of 8-(4-ethoxy-3-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6g) (DMSO-d$_6$)



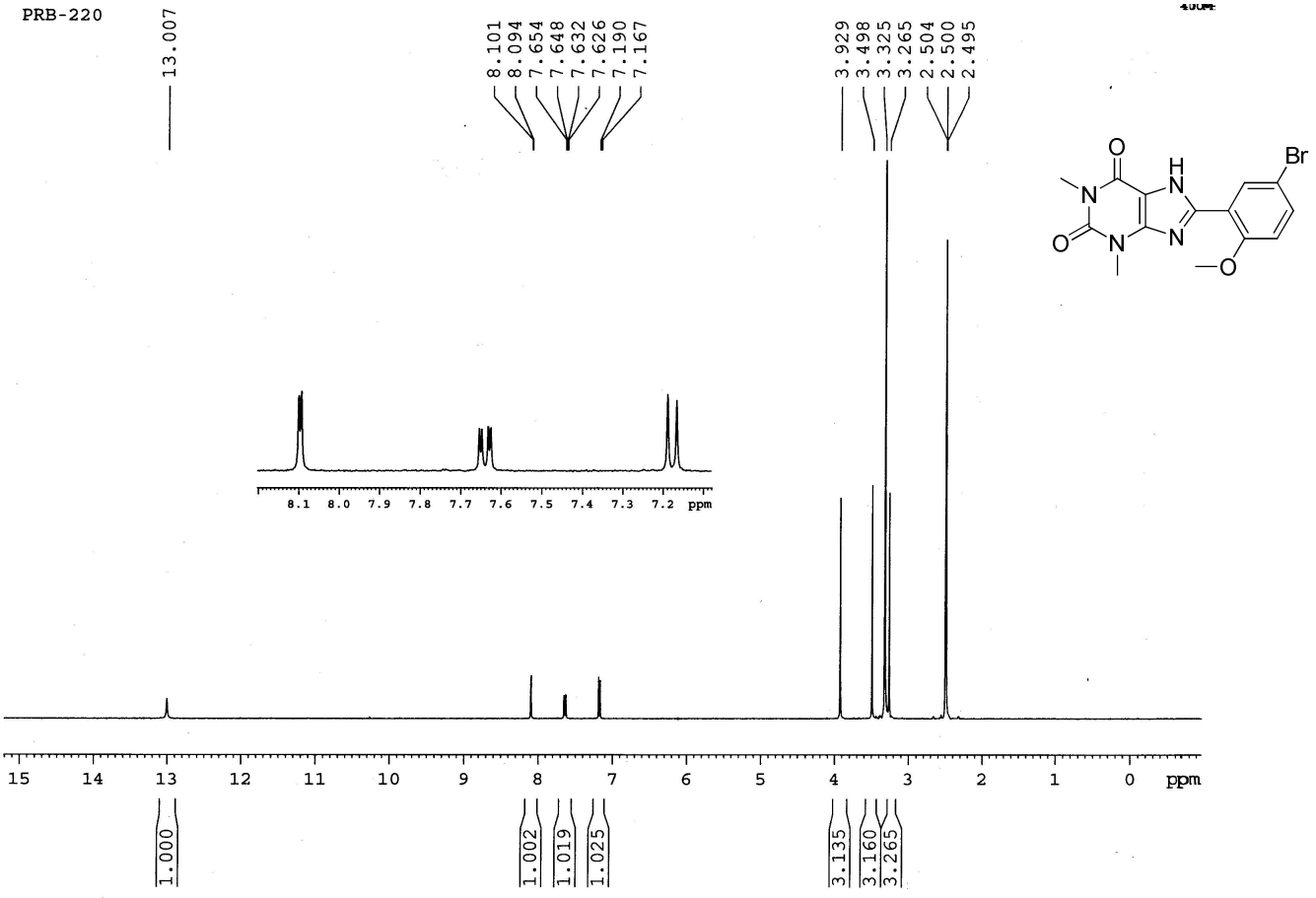
^{1}H-NMR spectrum of 8-(3,4,5-trimethoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6h) (DMSO-d$_6$)



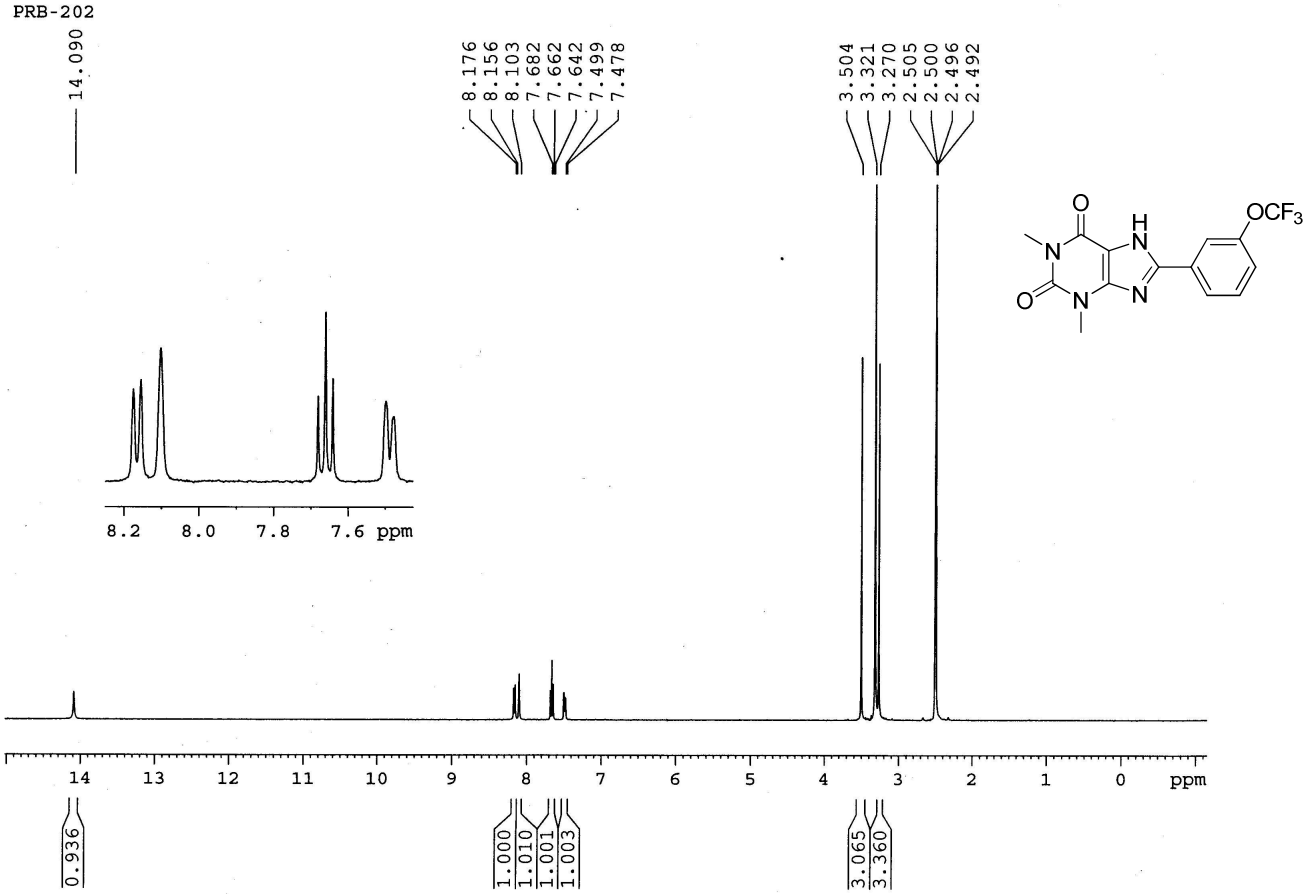
^{1}H-NMR spectrum of 8-(5-bromo-2-hydroxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6i) (DMSO-d$_6$)



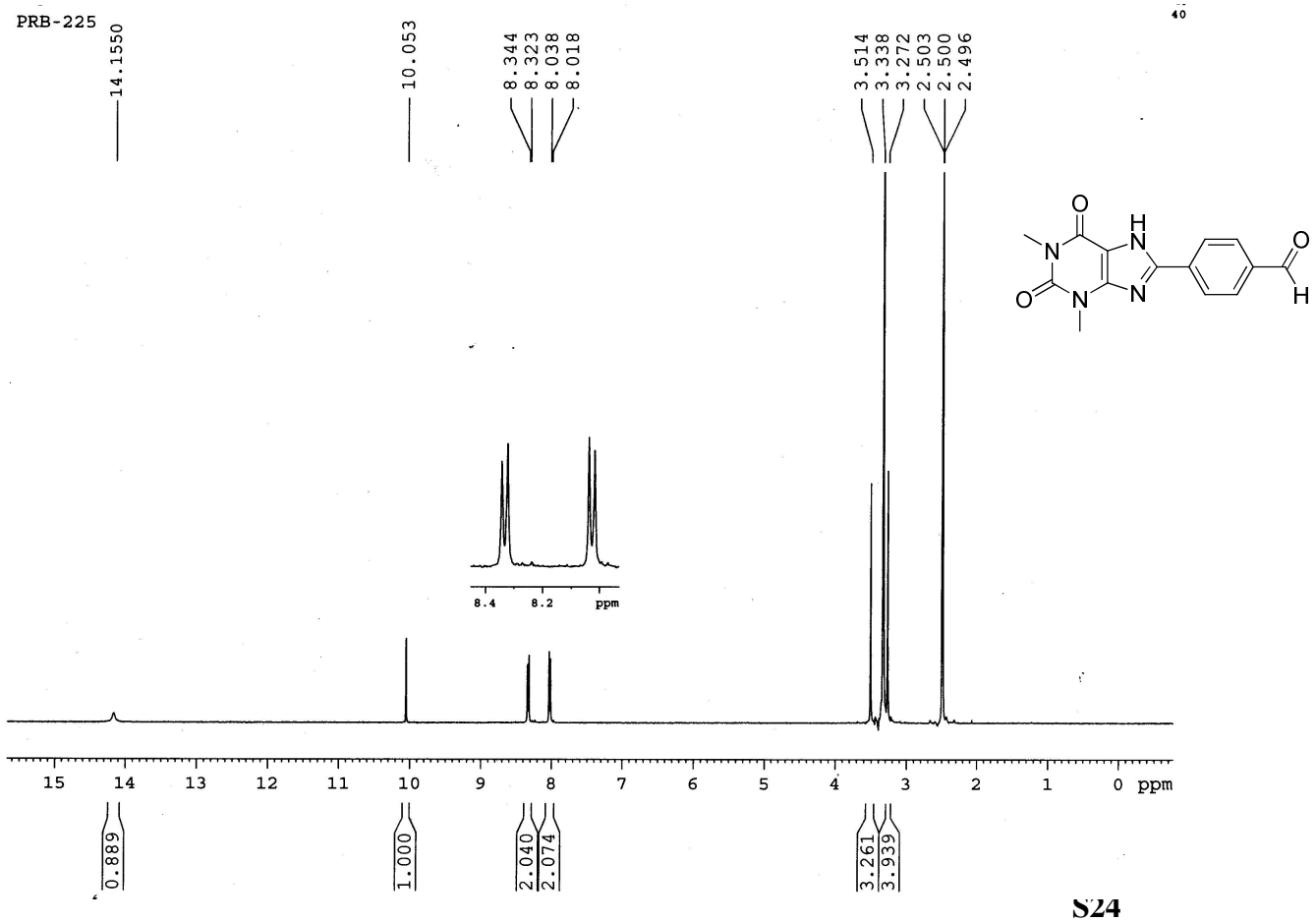
^{1}H-NMR spectrum of 8-(5-bromo-2-methoxyphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6j) (DMSO-d$_6$)



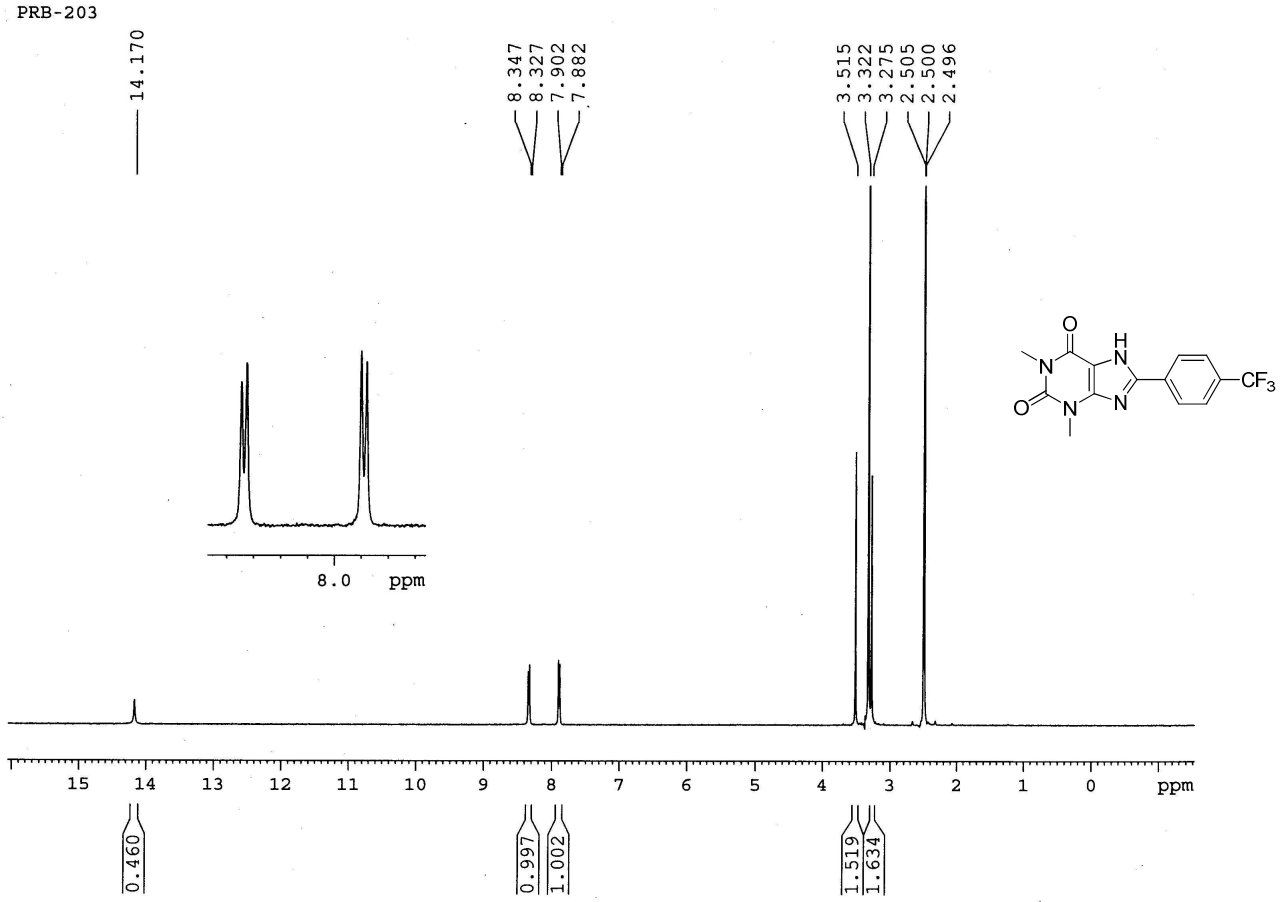
^{1}H-NMR spectrum of 8-(3-(trifluoromethoxy)phenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6k) (DMSO-d_6)



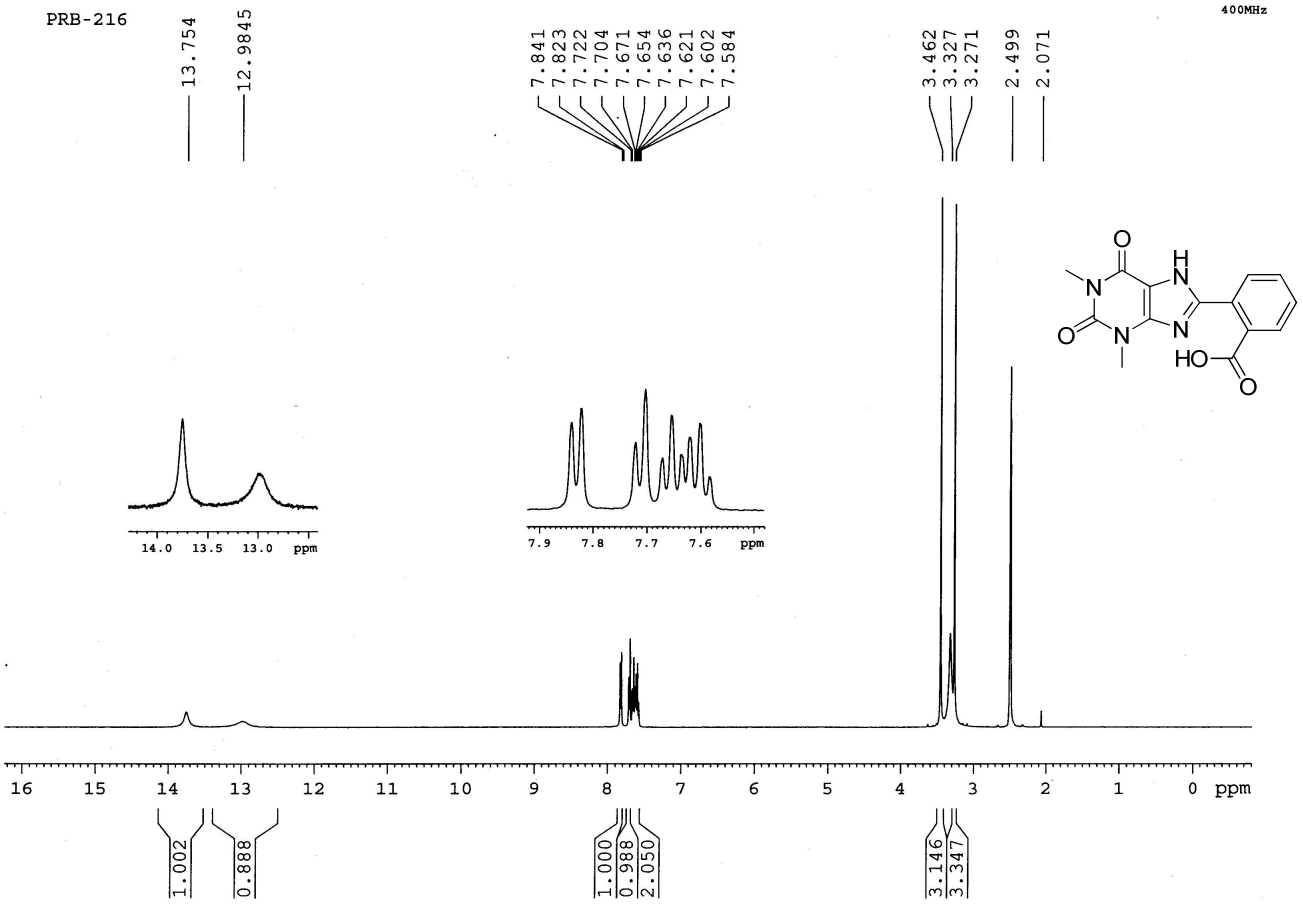
^{1}H-NMR spectrum of 4-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzaldehyde (6l) (DMSO-d_6)



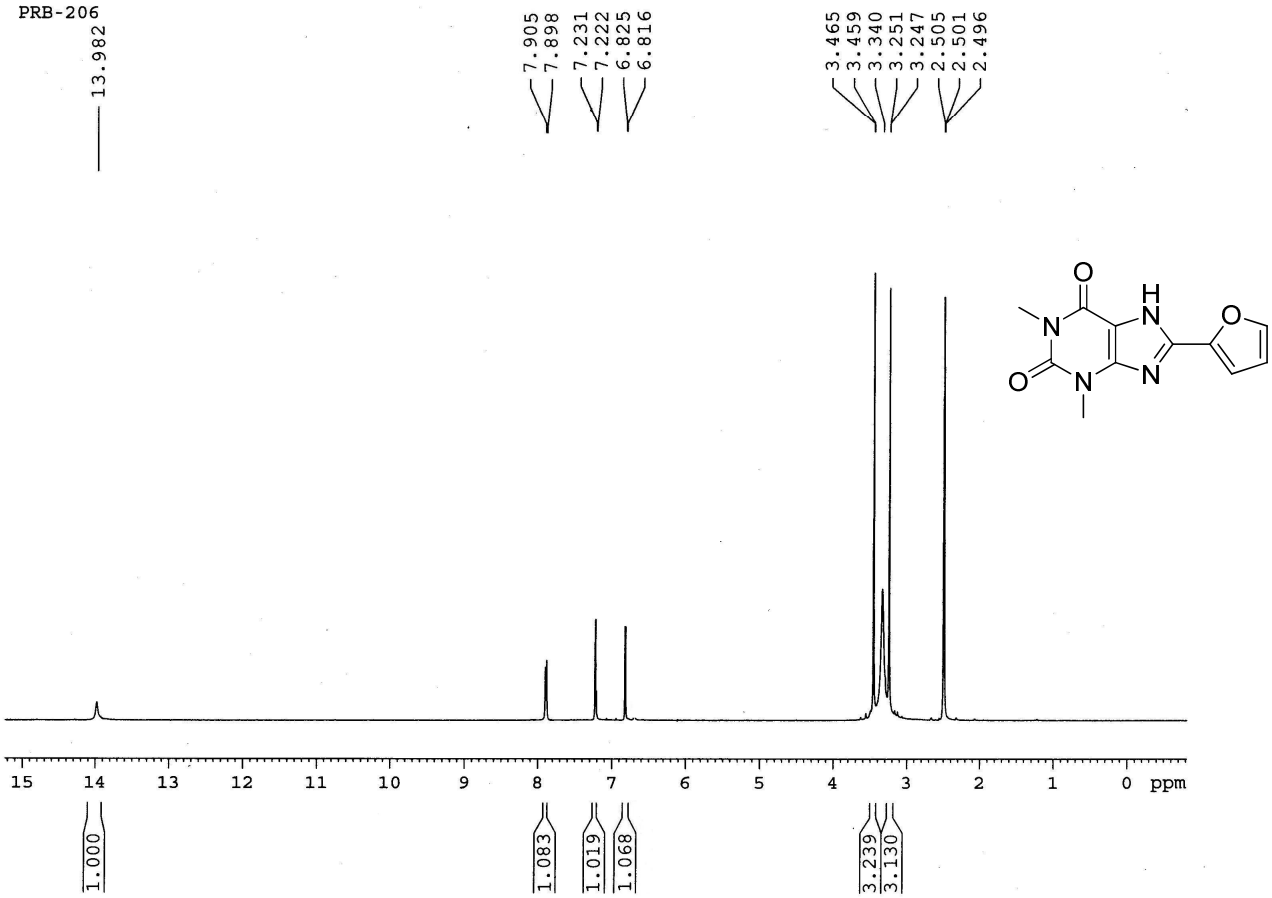
^{1}H-NMR spectrum of 8-(4-(trifluoromethylphenyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6m) (DMSO-d_6)



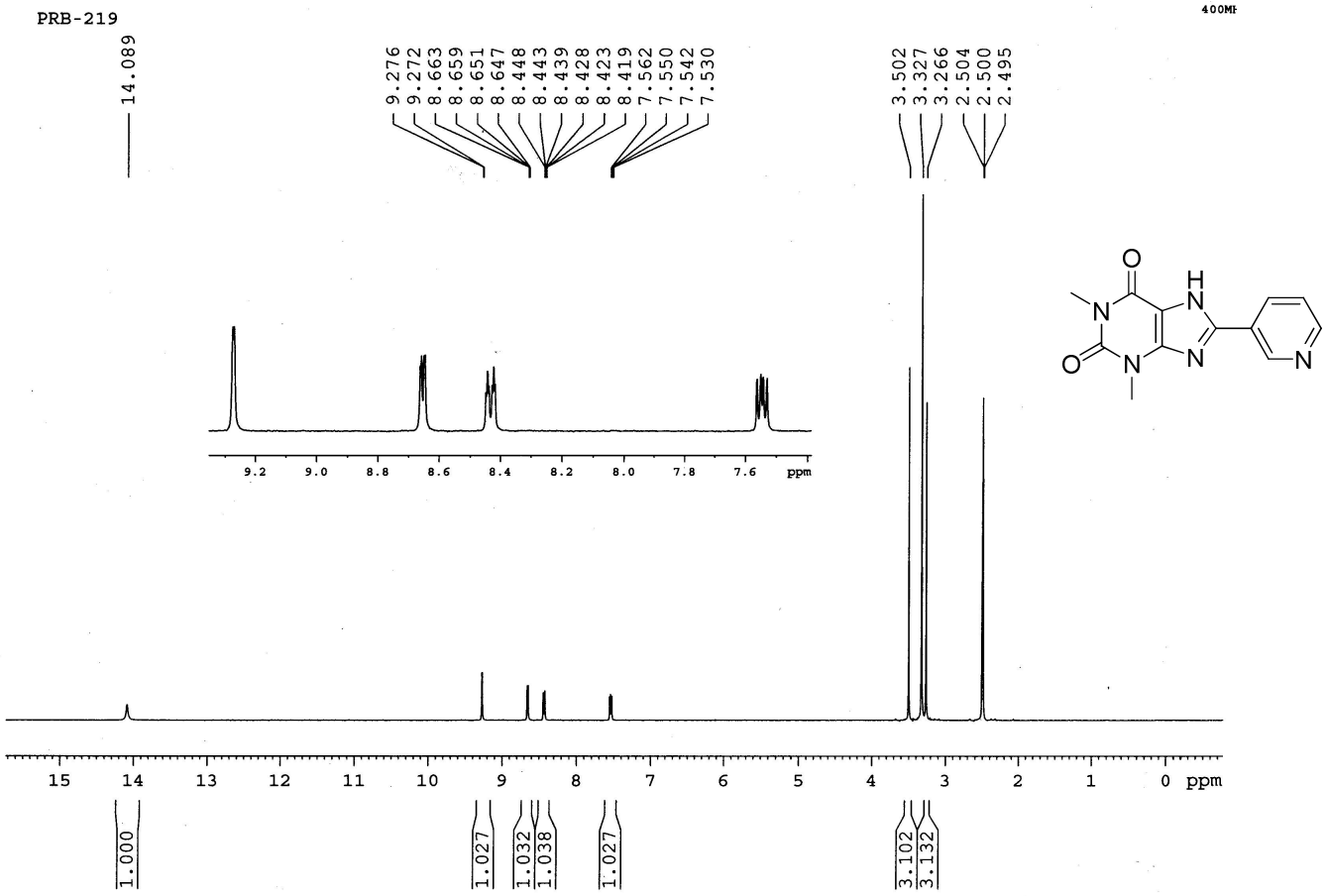
^{1}H-NMR spectrum of 2-(1,3-dimethyl-2,6-dioxo-1*H*-purin-8-yl)benzoic acid (6n) (DMSO-d_6)



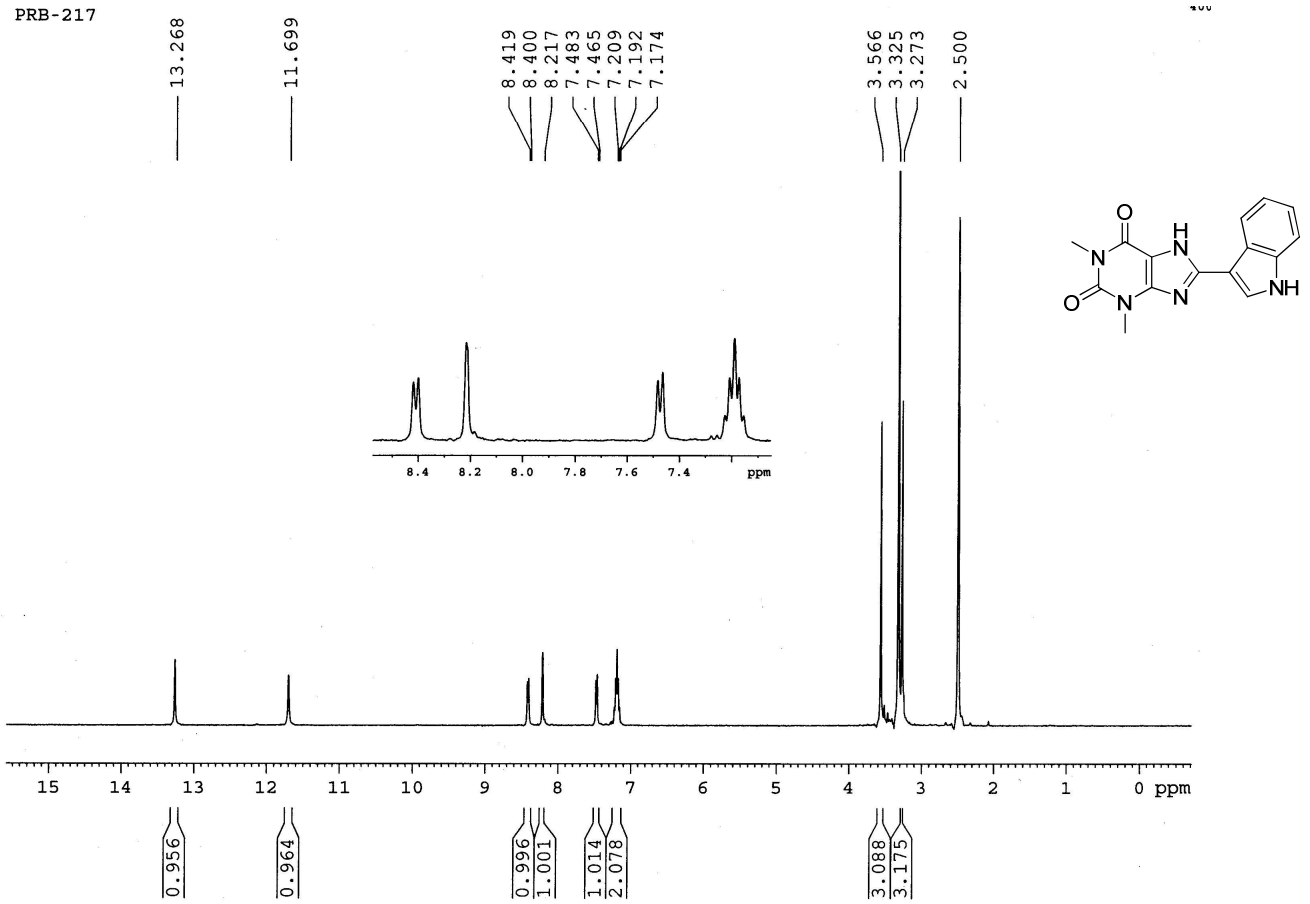
^{1}H-NMR spectrum of 8-(furan-2-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6o) (DMSO-d_6)



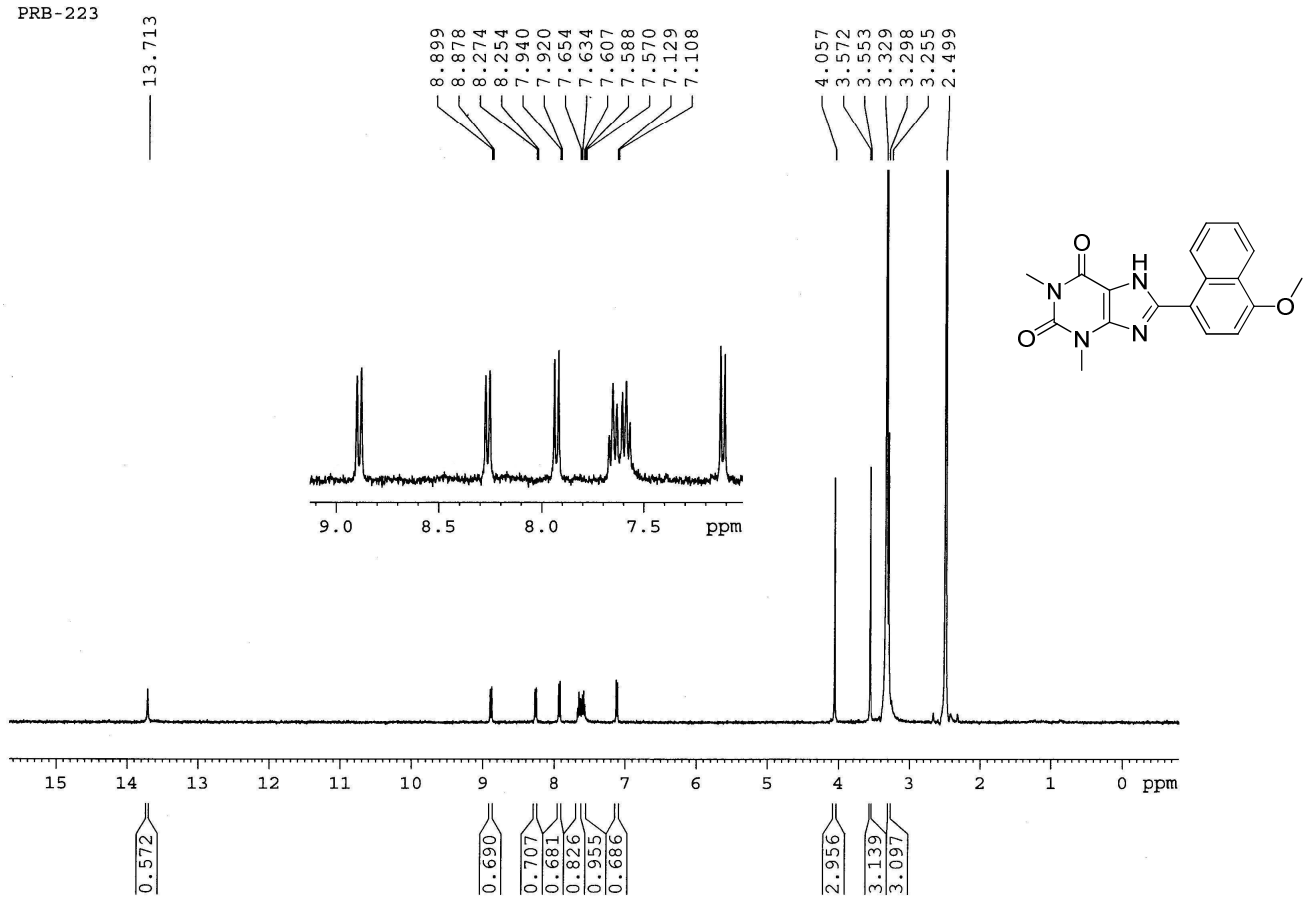
^{1}H-NMR spectrum of 8-(pyridin-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6p) (DMSO-d_6)



^{1}H-NMR spectrum of 8-(1*H*-indol-3-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6q) (DMSO-d_6)



^{1}H-NMR spectrum of 8-(4-methoxynaphthalen-1-yl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6r) (DMSO-d_6)



^{1}H-NMR spectrum of 8-styryl-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione (6s) (DMSO-d_6)