Discovery of Benzo[d]imidazole-6-sulfonamides as Bromodomain and Extra-Terminal Domain (BET) Inhibitors with Selectivity for the First Bromodomain

Alessandra Cipriano+, Ciro Milite+, Alessandra Feoli, Monica Viviano, Giacomo Pepe, Pietro Campiglia, Giuliana Sarno, Sarah Picaud, Satomi Imaide, Nikolai Makukhin, Panagis Filippakopoulos, Alessio Ciulli, Sabrina Castellano,* and Gianluca Sbardella
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\(^{1}\)H-NMR and \(^{13}\)C-NMR spectra of compounds 9a–p  
HRMS spectra of compounds 9a–p  
HPLC traces of compounds 9a–p
$m/z \,[M+H]^+$ calcd. for  
$C_{20}H_{18}N_4O_5S + H^+: 396.1172$
$m/z\ [M + H]^+$ calcd. for $C_{16}H_{16}N_3O_3S + H^+\ :\ 318.0907$
$m/z \ [M + H]^+ \text{ calcd. for}$

$C_{18}H_{17}N_2O_2S + H^+ \text{ 332.1063}$
$m/z \ [M + H]^+$ calcd. for $C_2H_{20}N_4O_3S + H^+: 409.1329$
$m/z$ [M + H]$^+$ calcd. for $C_{21}H_{20}N_4O_3S + H^+: 409.1329$
$m/z$ [M + H]$^+$ calcd. for $C_{19}H_{19}N_2O_3S + H^+ 358.1220$
$m/z$ [M + H]$^+$ calcd. for $C_{20}H_{23}N_2O_3S + H^+ : 385.1533$
m/z [M + H]^+ calcd. for C_{21}H_{28}N_3O_3S + H^+ : 400.1689
$m/z$ [M + H]$^+$ calcd. for
$C_{15}H_{18}N_4O_3S + H^+ \cdot 381.1016$
$m/z \ [M + H]^+ \text{ calcd. for}$

$C_{22}H_{16}N_4O_3S + H^+ : 395.1172$
$m/z \ [M+H]^+$ calculated for C$_{15}$H$_{14}$N$_4$O$_3$S + H$^+$. 367.0859
9m

$\text{m/z \ [M + H]^+ \text{ calcd. for}}$

$\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3\text{S} + \text{H}^+ ; 367.0859$
$m/z \text{ [M + H]}^+ \text{ calcd. for}$

$C_{13}H_{13}CN_4O_2S + H^+: 385.0521$
**Compounds in this group**

- **9o**

  - *m/z [M + H]+ calc. for C_{10}H_{13}N_{4}O_{4}S + H:\ 383.0809*
$m/z$ (M + H)$^+$ calc. for $C_{12}H_{14}N_4O_4S + H^+$. 383.0809
HPLC traces of 9a
HPLC traces of 9b
HPLC traces of 9c
HPLC traces of 9d

SHIMADZU HPLC ANALYSIS REPORT
Data File Name: 9d.led

Chromatogram 220 nm

| Peak# | Ret. Time | Height | Area  | Area% |
|-------|-----------|--------|-------|-------|
| 1     | 4.408     | 41405  | 143761| 0.591 |
| 2     | 4.595     | 3268500| 23753726 | 97.662|
| 3     | 5.289     | 24918  | 104063 | 0.428 |
| 4     | 5.696     | 63523  | 320720 | 1.319 |
| Total |           |        | 3398347| 100.000|

Chromatogram 254 nm

| Peak# | Ret. Time | Height | Area  | Area% |
|-------|-----------|--------|-------|-------|
| 1     | 4.589     | 1154286| 6490078 | 99.125|
| 2     | 5.287     | 13246  | 57271 | 0.875 |
| Total |           |        | 1167532| 100.000|

S53
HPLC traces of 9e
HPLC traces of 9f
HPLC traces of 9g
HPLC traces of 9h
HPLC traces of 9i
HPLC traces of 9j
HPLC traces of 9k
HPLC traces of 91
HPLC traces of 9m
HPLC traces of 9n
HPLC traces of 9o
HPLC traces of 9p