Supporting Information

Inhibition of Nucleoside Transport Proteins by C8-alkylamine Substituted Purines.

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Table 1. Melting Points (**46**–**58**, **72**–**75**) and Mass Spectrometry Data (**20**, **21**, **46**–**58**, **72**–**75**).

Compd	**Melting Point (°C)**	**Mass** $[M + H]^+$ **(*m*/*z*)**	
		Found	**Calcd**
20		440.1	440.1
21		454.0	454.1
46	193 (decomp)	404.1408	404.1392
47	102–104	418.1510	418.1549
48	108	432.1746	432.1705
49	86	446.1818	446.1862
50	80–82	460.2022	460.2018
51	78	474.2135	474.2175
52	129	460.2013	460.2018
53	102	430.1497	430.1549
54	175–176	458.1851	458.1862
55	108–109	472.1994	472.2018
56	158 (decomp)	444.1678	444.1705
57	90–92	458.1834	458.1862
58	98–99	460.1625	460.1654
72	150–151	461.1736	461.1754
73	66–68	475.1955	475.1911
74	154	447.1594	447.1598
75	201	463.1583	463.1547

^{13}C NMR Data (7, 9–14, 16–58, 63–67, 69–75)

2',3',5'-Tri-*O*-acetyl-8-(methylamino)-inosine (7). ^{13}C NMR ($CDCl_3$) δ 19.9, 20.1, 20.3, 29.5, 62.6, 69.6, 70.4, 79.9, 84.4, 121.9, 142.5, 148.0, 151.8, 157.6, 169.1, 169.3, 169.8.

2',3',5'-Tri-*O*-acetyl-8-(*n*-propylamino)-inosine (9). ^{13}C NMR ($CDCl_3$) δ 10.9, 19.8, 20.1, 20.2, 22.2, 44.5, 62.6, 69.5, 70.5, 79.8, 84.5, 121.9, 142.1, 147.9, 151.1, 157.6, 169.1, 169.2, 169.8.

2',3',5'-Tri-*O*-acetyl-8-(*n*-butylamino)-inosine (10). ^{13}C NMR ($CDCl_3$) δ 13.4, 19.7, 19.9, 20.1, 20.3, 31.2, 42.6, 62.7, 69.6, 70.5, 79.9, 84.6, 122.0, 142.2, 148.0, 151.2, 157.7, 169.1, 169.3, 169.8.

2',3',5'-Tri-*O*-acetyl-8-(*n*-pentylamino)-inosine (11). ^{13}C NMR ($CDCl_3$) δ 13.5, 19.8, 20.0, 20.1, 21.9, 28.5, 28.7, 42.7, 62.6, 69.5, 70.5, 79.7, 84.5, 121.9, 142.0, 147.8, 151.1, 157.5, 169.0, 169.1, 169.7.

2',3',5'-Tri-*O*-acetyl-8-(*n*-hexylamino)-inosine (12). ^{13}C NMR ($CDCl_3$) δ 13.4, 19.7, 19.9, 20.0, 26.0, 28.8, 30.9, 42.7, 62.5, 69.4, 70.5, 79.6, 84.5, 121.9, 142.0, 147.7, 151.0, 157.4, 168.9, 169.1, 169.6.

2',3',5'-Tri-*O*-acetyl-8-[(2-methyl-butyl)-amino]-inosine (13). ^{13}C NMR ($CDCl_3$) δ 10.9, 16.7, 20.1, 20.2, 20.4, 26.6, 26.8, 34.1, 48.7, 62.8, 69.9, 70.7, 80.0, 84.7, 122.1, 142.1, 148.0, 151.4, 157.9, 169.2, 169.4, 169.9.

2',3',5'-Tri-*O*-acetyl-8-(cyclopropylamino)-inosine (14). ^{13}C NMR ($CDCl_3$) δ 7.1, 20.0, 20.2, 20.4, 24.8, 62.6, 69.5, 70.9, 79.7, 84.9, 122.0, 143.1, 148.1, 154.5, 157.7, 169.2, 169.3, 170.0.

2',3',5'-Tri-*O*-acetyl-8-(cyclohexylamino)-inosine (16). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.2, 20.5, 24.7, 25.4, 33.0, 33.2, 51.3, 62.7, 69.7, 71.0, 79.8, 84.9, 122.2, 141.9, 147.9, 150.6, 157.9, 169.3, 170.0.

2',3',5'-Tri-*O*-acetyl-8-pyrrolidino-inosine (17). ^{13}C NMR ($CDCl_3$) δ 19.8, 19.9, 20.0, 25.0, 50.7, 62.4, 69.9, 71.1, 79.0, 86.2, 122.5, 142.4, 147.8, 153.8, 157.4, 168.6, 168.8, 169.8.

2',3',5'-Tri-*O*-acetyl-8-piperidino-inosine (18). ^{13}C NMR ($CDCl_3$) δ 19.9, 20.1, 23.4, 24.9, 51.9, 62.5, 69.9, 71.5, 79.0, 86.2, 122.2, 143.8, 147.9, 155.2, 157.7, 168.6, 168.9, 169.9.

2',3',5'-Tri-*O*-acetyl-8-*N*-morpholino-inosine (19). ^{13}C NMR ($CDCl_3$) δ 19.9, 20.0, 51.0, 62.4, 65.7, 69.9, 71.4, 79.1, 86.1, 122.1, 144.1, 147.9, 153.9, 157.5, 168.7, 168.9, 169.9.

2',3',5'-Tri-*O*-acetyl-8-methylamino-thioinosine (20). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.2, 20.4, 29.6, 62.7, 69.6, 70.7, 79.9, 84.9, 134.3, 142.6, 143.9, 153.7, 168.5, 169.4, 169.5, 170.1.

2',3',5'-Tri-*O*-acetyl-8-ethylamino-thioinosine (21). ^{13}C NMR ($CDCl_3/CD_3OD$ 1/1, v/v) δ 13.7, 19.3, 19.4, 19.6, 37.1, 62.4, 69.9, 70.8, 79.2, 84.8, 134.7, 141.3, 143.4, 152.8, 168.8, 169.3, 169.5, 170.4.

2',3',5'-Tri-*O*-acetyl-8-(*n*-propylamino)-thioinosine (22). ^{13}C NMR ($CDCl_3$) δ 10.8, 19.8, 20.1, 20.5, 22.1, 44.5, 62.5, 69.5, 70.5, 79.9, 84.6, 134.4, 142.0, 143.8, 152.8, 168.8, 169.0, 169.2, 169.8.

2',3',5'-Tri-*O*-acetyl-8-(*n*-butylamino)-thioinosine (23). ^{13}C NMR ($CDCl_3$) δ 13.5, 19.7, 20.0, 20.2, 20.4, 31.2, 42.8, 62.7, 69.6, 70.6, 80.2, 84.6, 134.5, 142.1, 144.0, 152.9, 168.8, 169.2, 169.4, 169.9.

2',3',5'-Tri-*O*-acetyl-8-(*n*-pentylamino)-thioinosine (24). ^{13}C NMR ($CDCl_3$) δ 13.4, 19.8, 20.1, 20.2, 21.8, 28.6, 28.8, 42.8, 62.5, 69.4, 70.5, 79.9, 84.5, 134.4, 142.0, 143.8, 152.7, 168.5, 169.1, 169.2, 169.8.

2',3',5'-Tri-*O*-acetyl-8-(*n*-hexylamino)-thioinosine (25). ^{13}C NMR ($CDCl_3$) δ 13.7, 20.1, 20.3, 20.4, 22.2, 26.2, 29.2, 31.2, 43.1, 62.7, 69.6, 70.6, 80.3, 84.7, 134.5, 142.0, 144.1, 152.9, 168.8, 169.2, 169.4, 169.9.

2',3',5'-Tri-*O*-acetyl-8-[(2-methyl-butyl)-amino]-thioinosine (26). ^{13}C NMR ($CDCl_3$) δ 10.9, 16.8, 20.1, 20.3, 20.5, 26.6, 26.8, 34.2, 48.8, 62.8, 69.7, 70.7, 80.3, 84.8, 134.6, 142.0, 144.2, 153.1, 168.8, 169.3, 169.5, 170.0.

2',3',5'-Tri-*O*-acetyl-8-(cyclopropylamino)-thioinosine (27). ^{13}C NMR ($CDCl_3$) δ 7.3, 20.1, 20.3, 20.5, 24.8, 62.6, 69.6, 70.8, 80.0, 84.9, 134.2, 143.1, 143.9, 153.4, 169.3, 169.5, 169.6, 170.1.

2',3',5'-Tri-*O*-acetyl-8-(cyclopentylamino)-thioinosine (28). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.3, 20.4, 23.3, 32.8, 32.9, 54.5, 62.7, 69.6, 71.0, 80.1, 85.0, 134.6, 142.0, 144.0, 152.7, 168.9, 169.4, 170.1.

2',3',5'-Tri-*O*-acetyl-8-(cyclohexylamino)-thioinosine (29). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.3, 20.6, 24.6, 25.3, 33.0, 33.3, 51.3, 62.7, 69.6, 70.9, 80.2, 84.9, 134.7, 141.9, 144.0, 152.3, 168.7, 169.3, 169.4, 170.1.

2',3',5'-Tri-*O*-acetyl-8-pyrrolidino-thioinosine (30). ^{13}C NMR ($CDCl_3$) δ 20.0, 20.1, 20.2, 25.3, 50.7, 62.5, 70.0, 70.9, 79.3, 86.3, 134.8, 141.9, 143.6, 155.3, 168.8, 169.0, 170.1, 170.7.

2',3',5'-Tri-*O*-acetyl-8-piperidino-thioinosine (31). ^{13}C NMR ($CDCl_3$) δ 19.9, 20.0, 20.2, 23.3, 24.9, 51.5, 62.4, 69.9, 71.1, 79.2, 86.4, 134.0, 143.3, 143.5, 157.0, 168.7, 169.0, 170.1, 170.6.

2',3',5'-Tri-*O*-acetyl-8-*N*-morpholino-thioinosine (32). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.2, 20.5, 50.7, 62.5, 65.8, 69.9, 71.1, 79.3, 86.3, 133.9, 143.4, 144.5, 155.9, 168.8, 169.1, 170.1, 170.7.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-methylamino-thioinosine (33). ^{13}C NMR ($CDCl_3$) δ 18.8, 18.9, 19.0, 31.1, 34.8, 61.6, 68.9, 69.9, 78.3, 83.9, 125.7, 127.0, 127.7, 130.1, 137.0, 146.9, 148.3, 149.9, 153.1, 167.9, 168.1, 168.8.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-ethylamino-thioinosine (34). ^{13}C NMR ($CDCl_3$) δ 14.8, 20.2, 20.4, 20.5, 32.7, 37.9, 62.9, 70.0, 70.6, 80.5, 84.5, 126.9, 128.3, 129.0, 130.6, 137.7, 148.6, 149.2, 152.5, 152.9, 169.4, 169.5, 170.1.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(*n*-propylamino)-thioinosine (35). ^{13}C NMR ($CDCl_3$) δ 11.0, 19.9, 20.1, 20.2, 22.2, 32.5, 44.5, 62.7, 69.8, 70.6, 80.0, 84.4, 126.7, 128.0, 129.1, 130.5, 137.5, 148.3, 149.0, 152.0, 152.9, 169.1, 169.2, 169.8.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(*n*-butylamino)-thioinosine (36). ^{13}C NMR ($CDCl_3$) δ 13.6, 19.8, 20.1, 20.4, 31.4, 32.7, 42.8, 62.9, 69.9, 70.8, 80.3, 84.6, 126.9, 128.2, 128.9, 130.6, 137.7, 148.5, 149.2, 152.3, 153.0, 169.4, 169.5, 170.0.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(*n*-pentylamino)-thioinosine (37). ^{13}C NMR ($CDCl_3$) δ 13.5, 19.8, 20.0, 20.1, 21.9, 28.5, 28.6, 32.4, 42.7, 62.6, 69.7, 70.6, 79.9, 84.4, 126.6, 127.9, 128.6, 130.5, 137.5, 148.1, 149.0, 151.8, 152.8, 169.0, 169.1, 169.7.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(*n*-hexylamino)-thioinosine (38). ^{13}C NMR ($CDCl_3$) δ 13.9, 20.1, 20.3, 20.8, 22.3, 26.3, 29.2, 31.2, 32.7, 43.0, 62.9, 69.9, 70.8, 80.3, 84.6, 126.9, 128.2, 128.9, 130.6, 137.7, 148.5, 149.2, 152.3, 153.0, 169.3, 169.4, 170.0.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-[(2-methyl-butyl)-amino]-thioinosine (39). ^{13}C NMR ($CDCl_3$) δ 11.1, 17.0, 20.2, 20.5, 26.8, 26.9, 32.8, 34.5, 48.8, 63.0, 70.0, 71.0, 80.4, 84.7, 127.0, 128.3, 129.0, 130.7, 137.8, 148.6, 149.2, 152.5, 153.2, 169.4, 169.5, 170.0.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(cyclopropylamino)-thioinosine (40). ^{13}C NMR ($CDCl_3$) δ 7.0, 7.2, 20.1, 20.3, 20.4, 24.8, 32.7, 62.7, 69.8, 70.9, 80.1, 84.6, 126.9, 128.2, 128.9, 130.5, 137.6, 148.7, 149.0, 153.0, 153.3, 169.3, 169.4, 170.0.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(cyclopentylamino)-thioinosine (41). ^{13}C NMR ($CDCl_3$) δ 20.3, 20.4, 20.5, 23.5, 32.8, 33.0, 33.1, 54.6, 62.8, 70.0, 71.3, 80.2, 85.0, 126.9, 128.3, 129.0, 130.8, 137.7, 148.5, 149.0, 152.5, 152.7, 169.5, 169.6, 170.2.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-(cyclohexylamino)-thioinosine (42). ^{13}C NMR ($CDCl_3$) δ 20.3, 20.4, 20.6, 24.7, 25.5, 32.7, 32.9, 33.2, 51.5, 62.9, 70.0, 71.3, 80.2, 85.0, 126.9, 128.3, 129.0, 130.8, 137.7, 148.4, 149.0, 152.3, 169.5, 170.1.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-pyrrolidino-thioinosine (43). ^{13}C NMR ($CDCl_3$) δ 20.3, 20.4, 20.5, 25.6, 32.6, 50.8, 62.8, 70.5, 71.3, 79.6, 86.8, 126.9, 128.2, 129.0, 131.0, 137.7, 148.7, 149.4, 152.9, 155.7, 169.1, 169.3, 170.4.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-piperidino-thioinosine (44). ^{13}C NMR ($CDCl_3$) δ 20.3, 20.4, 20.5, 23.8, 25.2, 32.5, 51.8, 62.8, 70.4, 71.4, 79.5, 86.9, 126.9, 128.2, 128.9, 131.1, 137.5, 149.0, 149.9, 155.5, 157.4, 168.9, 169.2, 170.3.

2',3',5'-Tri-*O*-acetyl-6-benzyl-8-morpholino-thioinosine (45). ^{13}C NMR ($CDCl_3$) δ 20.1, 20.3, 20.4, 32.5, 50.9, 62.6, 65.8, 70.3, 71.3, 79.6, 86.6, 126.9, 128.2, 128.8, 129.7, 137.3, 148.8, 150.1, 156.3, 168.9, 169.2, 170.2.

6-Benzyl-8-methylamino-thioinosine (46). ^{13}C NMR ($CDCl_3$/MeOD 1/2) δ 29.2, 33.6, 62.6, 72.3, 72.6, 87.1, 88.3, 127.8, 129.1, 129.7, 131.7, 138.7, 148.7, 150.5, 152.1, 155.4.

6-Benzyl-8-ethylamino-thioinosine (47). ^{13}C NMR ($CDCl_3$/MeOD 1/1, v/v) δ 14.6, 33.5, 38.1, 62.4, 72.0, 72.3, 86.8, 87.9, 127.6, 128.9, 129.5, 131.7, 138.4, 148.3, 150.1, 151.9, 154.3.

6-Benzyl-8-(*n*-propylamino)-thioinosine (48). ^{13}C NMR (MeOD) δ 11.8, 23.4, 33.8, 45.4, 62.9, 72.6, 72.8, 87.5, 88.4, 128.1, 129.4, 130.0, 132.0, 139.4, 149.1, 151.1, 152.1, 155.1.

6-Benzyl-8-(*n*-butylamino)-thioinosine (49). ^{13}C NMR (MeOD) δ 14.2, 21.1, 32.2, 33.8, 43.4, 62.9, 72.6, 72.7, 87.5, 88.3, 128.0, 129.4, 130.0, 132.0, 139.3, 149.0, 151.0, 152.0, 155.0.

6-Benzyl-8-(*n*-pentylamino)-thioinosine (50). ^{13}C NMR (MeOD) δ 14.4, 23.3, 29.7, 30.1, 33.8, 43.7, 62.8, 72.7, 87.4, 91.1, 128.0, 129.3, 129.9, 131.9, 139.1, 148.9, 150.8, 152.0, 154.9.

6-Benzyl-8-(*n*-hexylamino)-thioinosine (51). ^{13}C NMR (MeOD) δ 14.4, 23.6, 27.7, 30.1, 32.6, 33.8, 43.7, 62.9, 72.6, 72.7, 87.5, 88.4, 128.0, 129.4, 130.0, 132.0, 139.4, 149.0, 151.0, 152.1, 155.0.

6-Benzyl-8-[(2-methyl-butyl)-amino]-thioinosine (52). ^{13}C NMR (MeOD) δ 11.5, 17.4, 27.9, 28.0, 33.9, 35.4, 62.9, 72.7, 72.8, 87.6, 88.3, 128.1, 129.4, 130.0, 132.1, 139.4, 149.0, 151.2, 152.0, 155.2.

6-Benzyl-8-(cyclopropylamino)-thioinosine (53). ^{13}C NMR (MeOD) δ 7.0, 7.6, 25.5, 33.8, 62.9, 72.5, 72.7, 87.5, 88.4, 128.1, 129.4, 130.0, 131.7, 139.4, 149.3, 150.9, 152.8, 155.6.

6-Benzyl-8-(cyclopentylamino)-thioinosine (54). ^{13}C NMR ($CDCl_3$/MeOD 1/1) δ 24.6, 33.0, 33.1, 33.6, 55.1, 62.4, 72.0, 72.3, 86.9, 87.7, 127.7, 128.9, 130.0, 131.8, 138.4, 148.2, 150.2, 151.8, 154.1.

6-Benzyl-8-(cyclohexylamino)-thioinosine (55). ^{13}C NMR ($CDCl_3$/MeOD 1/5, v/v) δ 26.3, 26.4, 26.5, 33.8, 33.9, 34.2, 53.2, 62.8, 72.5, 72.6, 87.4, 88.3, 128.0, 129.4, 130.0, 132.1, 139.3, 148.9, 151.0, 151.9, 154.4.

6-Benzyl-8-pyrrolidino-thioinosine (56). ^{13}C NMR ($CDCl_3$/MeOD 2/1, v/v) δ 26.1, 33.3, 51.6, 63.6, 72.1, 72.2, 87.2, 89.5, 127.5, 128.8, 129.4, 132.0, 138.0, 147.9, 149.3, 153.8, 156.3.

6-Benzyl-8-piperidino-thioinosine (57). ^{13}C NMR ($CDCl_3$) δ 23.8, 25.1, 32.9, 52.1, 63.3, 72.1, 86.5, 89.0, 127.1, 128.3, 129.0, 130.2, 137.0, 147.9, 148.4, 156.4, 158.3.

6-Benzyl-8-morpholino-thioinosine (58). ^{13}C NMR ($CDCl_3$) δ 33.0, 51.3, 63.3, 66.0, 72.2, 72.5, 86.6, 88.7, 127.2, 128.4, 129.0, 130.2, 136.9, 147.9, 148.6, 157.2, 157.6.

9-Benzyl-8-bromo-hypoxanthine (63). ^{13}C NMR (DMSO-d_6) δ 42.7, 124.3, 125.5, 127.2, 128.9, 135.6, 146.7, 150.0, 155.4.

9-Benzyl-8-(cyclopentylamine)-hypoxanthine (64). ^{13}C NMR ($CDCl_3$) δ 23.1, 33.0, 44.6, 54.3, 121.6, 126.8, 128.1, 128.9, 134.8, 142.3, 149.0, 151.3, 158.0.

9-Benzyl-8-(cyclohexylamine)-hypoxanthine (65). ^{13}C NMR ($CDCl_3$) δ 24.1, 24.8, 32.1, 43.4, 50.7, 120.8, 126.2, 127.1, 128.0, 134.8, 141.4, 148.0, 150.9, 155.8.

9-Benzyl-8-pyrrolidino-hypoxanthine (66). ^{13}C NMR ($CDCl_3$/MeOD 1/1, v/v) δ 24.7, 45.7, 49.0, 121.1, 125.1, 127.0, 128.2, 136.0, 141.9, 149.1, 152.8, 156.1.

9-Benzyl-8-morpholino-hypoxanthine (67). ^{13}C NMR ($CDCl_3$/MeOD 4/1, v/v) δ 46.3, 50.3, 66.1, 121.4, 126.3, 127.8, 128.7, 135.4, 143.9, 149.4, 154.2, 157.4.

9-Benzyl-8-(cyclohexylamine)-6-mercaptopurine (69). ^{13}C NMR ($CDCl_3$/MeOD 1/1, v/v) δ 24.1, 24.7, 32.2, 43.5, 50.6, 126.2, 127.3, 128.1, 134.0, 134.3, 141.5, 144.4, 152.6, 167.0.

9-Benzyl-8-pyrrolidino-6-mercaptopurine (70). ^{13}C NMR ($CDCl_3$/MeOD 5/1, v/v) δ 25.1, 46.2, 49.6, 125.2, 127.5, 128.6, 134.2, 135.7, 141.7, 145.5, 154.3, 168.4.

9-Benzyl-8-morpholino-6-mercaptopurine (71). ^{13}C NMR (DMSO-d_6) δ 46.0, 49.7, 65.5, 126.6, 127.6, 128.7, 133.0, 136.0, 144.2, 145.4, 155.3, 172.1.

9-Benzyl-8-(cyclopentylamine)-6-(4-nitrobenzyl)-6-mercaptopurine (72). ^{13}C NMR ($CDCl_3$) δ 23.2, 31.9, 33.2, 44.5, 54.4, 123.5, 127.0, 128.6, 129.3, 129.9, 131.0, 134.3, 146.6, 146.8, 148.7, 149.9, 150.3, 153.3.

9-Benzyl-8-(cyclohexylamine)-6-(4-nitrobenzyl)-6-mercaptopurine (73). ^{13}C NMR ($CDCl_3$) δ 24.2, 25.3, 31.8, 32.9, 44.5, 50.9, 123.5, 126.9, 128.5, 129.2, 129.9, 134.3, 146.6, 146.8, 148.6, 149.7, 150.2, 153.0.

9-Benzyl-6-(4-nitrobenzyl)-8-pyrrolidino-6-mercaptopurine (74). ^{13}C NMR ($CDCl_3$) δ 25.1, 31.6, 46.1, 49.2, 123.2, 125.2, 127.5, 128.6, 129.7, 130.5, 135.9, 146.3, 146.5, 148.2, 149.6, 151.1, 154.6.

9-Benzyl-8-morpholino-6-(4-nitrobenzyl)-6-mercaptopurine (75). ^{13}C NMR (Bruker DMX 600 MHz, DMSO-d_6, 60°C) δ 30.7, 46.1, 49.0, 65.2, 123.1, 126.4, 127.3, 128.4, 129.2, 129.8, 135.7, 146.3, 146.5, 149.5, 150.8, 152.0, 156.2.

Elemental Analyses

Compd	Theoretical in %				Experimental in %				Deviation in %				Molecular Formula
	C	H	N	S	C	H	N	S	C	H	N	S	
46	52.38	5.16	16.83	7.70	52.11	5.25	16.79	7.74	-0.27	0.09	-0.04	0.04	$C_{18}H_{21}N_5O_4S$•$0.15CH_2Cl_2$
47	54.25	5.52	16.61	7.60	53.93	5.64	16.63	7.55	-0.32	0.12	0.02	-0.05	$C_{19}H_{23}N_5O_4S$•$0.05CH_2Cl_2$
48	55.67	5.84	16.23	7.43	55.48	5.73	16.21	7.43	-0.19	0.11	-0.02	0.00	$C_{20}H_{25}N_5O_4S$
49	56.61	6.11	15.72	7.20	56.34	6.06	15.73	7.14	-0.27	-0.05	0.01	-0.06	$C_{21}H_{27}N_5O_4S$
50	56.71	6.29	14.96	6.85	56.69	6.48	15.14	6.81	-0.03	0.19	0.17	-0.05	$C_{22}H_{29}N_5O_4S$•$0.1CH_2Cl_2$
51	56.43	6.42	14.15	6.48	56.24	6.65	14.02	6.30	-0.19	0.23	-0.13	-0.18	$C_{23}H_{31}N_5O_4S$•$0.25CH_2Cl_2$
52	57.10	6.32	15.10	6.91	56.95	6.29	15.11	6.88	-0.15	-0.03	0.01	-0.03	$C_{22}H_{29}N_5O_4S$•$0.05CH_2Cl_2$
53	54.34	5.28	15.69	7.18	54.18	5.39	15.85	7.12	-0.16	0.11	0.16	-0.07	$C_{20}H_{23}N_5O_4S$•$0.2CH_2Cl_2$
54	57.35	5.91	15.17	6.94	57.13	5.99	15.27	6.93	-0.22	0.07	0.10	-0.02	$C_{22}H_{27}N_5O_4S$•$0.05CH_2Cl_2$
55	56.67	6.03	14.21	6.51	56.35	6.00	14.34	6.33	-0.32	-0.03	0.13	-0.18	$C_{23}H_{29}N_5O_4S$•$0.25CH_2Cl_2$
56	58.58	6.20	14.85	6.80	56.83	5.62	16.00	7.13	0.04	0.07	-0.20	0.10	$C_{21}H_{25}N_5O_4S$
57	56.19	5.82	14.76	6.76	56.36	6.06	14.36	6.54	0.17	0.24	-0.40	-0.22	$C_{22}H_{27}N_5O_4S$•$0.2CH_2Cl_2$
58	53.44	5.37	14.70	6.73	53.05	5.66	15.01	6.71	-0.39	0.28	0.31	-0.02	$C_{21}H_{25}N_5O_5S$•$0.2CH_2Cl_2$
73	60.77	5.36	16.81	6.41	60.38	5.49	16.87	6.35	-0.39	0.12	0.06	-0.07	$C_{25}H_{26}N_6O_2S$•$0.3CH_2Cl_2$
74	60.12	4.87	18.13	6.92	60.34	4.80	17.98	6.69	0.22	-0.07	-0.15	-0.23	$C_{23}H_{22}N_6O_2S$•$0.2CH_2Cl_2$
75	58.90	4.75	17.84	6.81	58.60	4.51	17.83	6.48	-0.30	-0.25	-0.01	-0.33	$C_{23}H_{22}N_6O_3S$•$0.1CH_2Cl_2$