# N-Aminoimidazole Derivatives Inhibiting Retroviral Replication via a Yet **Unidentified Mode of Action**

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The synthesis of a series of N-aminoimidazoles (NAIMs) with an uncommon spectrum of antiretroviral activity is described. From a group of 60 closely related molecules, we were able to subdivide the molecules in different groups based on their anti-HIV and anti-SIV activity in vitro: (i) molecules acting on a new, immediate postintegration step, (ii) molecules acting on both postintegration and HIV-1 reverse transcriptase (RT) as NNRTI, and (iii) molecules that mainly act at the HIV-1 RT according to an NNRTI-type mode of action.

## Introduction

Replication of human immunodeficiency virus type 1 can be reduced in HIV-infected patients using a combination of antiviral drugs targeted at the reverse transcriptase (RT) and protease.1 Unfortunately, because of the high mutation rate of HIV, treatment, even combination therapy, is required for drug-resistant variants.<sup>2</sup>

Shortly after the discovery of the nonnucleoside reverse transcriptase inhibitors (NNRTIs), it became clear that resistance to this class of compounds emerges rapidly.<sup>3</sup> Moreover, cross-resistance is very important. If a patient's virus becomes resistant to NNRTIs, no other member of the group can be used effectively. Capravirine (S-1153), a 1,2,4,5-substituted imidazole derivative, is an NNRTI<sup>4</sup> that is able to inhibit HIV-1 strains that are resistant to other NNRTIs. This ability to cope with typical NNRTI-induced mutations is based, at least in part, on an extensive network of hydrogen bonds involving the main chain of residues 101, 103, and 236 of the p66 RT subunit. Side chain mutations are not likely to disrupt these interactions.<sup>5</sup>

We synthesized a series of N-aminoimidazoles via a one-pot synthesis. The similarity of this series of compounds to S-1153 is depicted in Chart 1.

The in vitro antiviral evaluation of a series of 60 N-aminoimidazole and N-aminoimidazole thiones yielded unexpected antiviral activity findings. Out of a series of 60 compounds, 7 compounds were equipotent against the replication of HIV-1 (strains III<sub>B</sub> and the molecular clone NL4.3), an NNRTI-resistant HIV-1 strain (with mutations K103N, Y181C in RT), HIV-2(ROD), and SIV(mac251). The most potent of these compounds were also active against MSV-induced transformation of C3H/ 3T3 embryo murine fibroblast in vitro.

Chart 1. Structure Analogy of S-1153 vs N-Aminoimidazole Derivatives 3 and 7



This very unusual antiviral activity pattern suggests that the antiretroviral activity of these compounds is not based on an inhibition of the reverse transcriptase activity as might have been expected from the structural similarity with capravirine.

Other members of the series had an activity profile that coincided with that of the NNRTIs (no activity against HIV-2(ROD) and reduced activity against an NNRTI-resistant strain), but some of these compounds inhibited the replication of SIV(mac251) to the same extent as wild-type HIV-1 strains, unlike the classical NNRTIs nevirapine, delavirdine, and efavirenz.

These results prompted us to study the structureactivity relationship and potential mode of action of these *N*-aminoimidazoles (NAIMs) more thoroughly.

#### Chemistry

Starting from cheap, easily available compounds such as hydrazines 1,  $\alpha$ -bromoketones 2, and potassium thiocyanate, N-substituted 1-amino-2,3-dihydro-1H-imidazole-2-thiones 3 were formed in good yield in a onepot reaction (Scheme 1).<sup>6</sup> By use of strategies of parallel synthesis and combination of starting materials 1 and 2, a broad range of differently substituted heterocycles 3 could be obtained.

This multistep reaction is considered to occur via the conversion of an  $\alpha$ -thiocyanatoketone (formed by nucleophilic substitution reaction) to the thiocyanato-

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**Scheme 1.** Synthesis of *N*-Aminoimidazoline-2-thiones **3** 



**Scheme 2.** Most Likely Pathway for the Formation of 2-Iminothiazoles **6** 



hydrazone **4**. Subsequent 1,4-elimination led to the corresponding azoalkene and thiocyanic acid. The thus formed two intermediates can undergo a [3 + 2] cycloaddition reaction, and following hydrogen shift, the 1-amino-2,3-dihydro-1*H*-imidazole-2-thiones **3** were obtained.

In the case of ortho-substituted ketones, it was found that the reaction did not follow the pathway outlined in Scheme 1. Instead of the cycloaddition, a 5-exo-dig cyclization reaction (Scheme 2) took place. Likewise, in this pathway the  $\alpha$ -thiocyanatohydrazone **4** is the key intermediate. In the case of substituents in the ortho position of the former ketone **2**, the 1,4-elimination giving rise to the formation of azoalkenes, which are planar, delocalized  $\pi$ -electron systems, is not favored. As shown in Scheme 2, a cyclization reaction yielding a 2-iminothiazole **6** took place instead. Attempts to convert the 2-iminothiazole **6** to the desired imidazoline-2-thione derivative **3** by way of a Dimroth rearrangement<sup>7</sup> failed.

The two isomers can be easily distinguished by NMR methods. The signal corresponding to the carbon 2 of the imidazoline-2-thione derivative **3** was found in the range  $\delta$  160–162 ppm, whereas the corresponding signal of the 2-iminothiazole **6** was found in the range  $\delta$  169–171 ppm.

In the case of isomer **3**, saturation of the 3-NH causes a 10% nuclear Overhauser enhancement (NOE) at the 4-substituent, whereas irradiation of the imino NH showed an NOE enhancement of 5% relative to the exocyclic NH. The results of structure elucidation are summarized in Chart 2.

Besides the restriction of having a substituent in the ortho position of ketone **2**, the method of generating *N*-aminoimidazoline-2-thiones **3** in a one-pot-reaction starting from hydrazines **1**, ketones **2**, and potassium thiocyanate is suitable for all substituents,  $R^1$ ,  $R^2$ , and  $R^3$  being either aryl or alkyl. The method is also suitable

**Chart 2.** Comparison between the NMR Data of 2-Iminothiazoles **6** and *N*-Aminoimidazoline-2-thiones **3** 



**Chart 3.** Structures of *N*-Aminoimidazoles **7** and *S*-Alkylaminoimidazoles **8** 



for the conversion of N,N-disubstituted hydrazines **1**, obtaining the corresponding imidazoline thione **3** with an N,N-disubstituted side chain. Further derivatization of heterocycle **3** could be achieved by desulfurization with hydrogen peroxide in acetic acid,<sup>8</sup> yielding the corresponding *N*-aminoimidazole derivatives **7**.

Alkylation of the imidazoline-2-thiones **3** quantitatively formed the *S*-alkyl product **8** (Chart 3), even under Mitsunobu<sup>9</sup> conditions. Substitution patterns, yields, melting points,  $R_f$  values and HRMS of the imidazole derivatives **3** and **7** are shown in Table 1.

### **Biological Results and Discussion**

**Inhibition of HIV and SIV Replication in Cell Culture by** *N*-**Aminoimidazoles 3 and 7.** We tested a series of *N*-arylaminoimidazoles **7** for their potential to inhibit the replication of HIV and SIV in a cell culture model for acute infection. The cytotoxicity of the compounds was determined in parallel. The antiviral activity and cytotoxicity data are presented in Table 2. From a series of 60 compounds, 26 compounds were active against the replication of at least one of the included virus strains. Seven compounds (**3.01**, **3.05**, **3.07**, **3.39**, **7.01**, **7.02**, and **7.03**) were equally potent inhibitors of the HIV-1, HIV-2, and SIV replication in MT-4 cells. Similar results were obtained in peripheral blood mononuclear cells (PBMCs) (data not shown).

Some molecules showed reduced activity against a clinically relevant NNRTI-resistant strain (mutations in RT K103N and Y181C), but unlike established NNRTIs as nevirapine, delavirdine, and efavirenz, they remained potent inhibitors of SIV(mac251) replication in vitro. Moreover, the most potent broad-spectrum *N*-aminoimidazole derivatives **3** and **7** inhibited MSV-induced transformation of C3H/3TC embryo murine fibroblasts in vitro (Table 3).

**Structure**–Activity Relationship (SAR) for *N*-Aminoimidazole Derivatives 3 and 7. All the antiretroviral-active *N*-aminoimidazoles 3 and 7 have in common the basic molecule depicted in Chart 4. No marked difference in antiviral activity and cytotoxicity was observed between the imidazoles 7 and their 2thiono homologue 3 series. However, alkylation (methylation or benzylation) of the sulfur led to complete

**Table 1.** Analytical Data of *N*-Aminoimidazole-2-thiones **3** (Written as Thiole Tautomer with  $R^4 = SH$ ) and *N*-Aminoimidazoles **7** ( $R^4 = H$ )<sup>*a*</sup>



$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								
	compd	$\mathbb{R}^1$	R <sup>2</sup>	R <sup>3</sup>	yield (%)	$R_{f}{}^{b}$	mp (MeOH, °C)	exact mass
3.01         3.02         3.02         2.10         2.11         Calce         3.06         9.07         1.11         Found         3.0           3.02         2.CCLH         CH4	0.011		C II	CU	00	0 55	017 017	
3.02         2.1.C.974,         C.P1,         C.P1,         State         C.P1,         State         C.P1,         State         C.P1,         P.P1,         Found 3 10,           3.05         4.C.C.H.         4.B.C.H.         C.H.         6.0         4.2         2.2.14         Calcd 308, 3973 M + H17,         Found 3 10,           3.06         3.C.C.H.         4.B.C.H.         C.H.         86         0.52         2.2.2.2         Calcd 308, 3973 M + H17,         Found 3 10,           3.07         3.C.C.H.         4.C.C.J.H.         C.C.J.H.         80         0.53         2.2.2.2.2         Calcd 30, 0355 M + H17,         Found 3 10,           3.08         3.C.C.J.H.         4.C.C.J.H.         C.L.G.H.         C.H.         S.0.3         2.2.2.2.2.2         Calcd 316, 0375 M + H17,         Found 3 31,           3.10         3.C.C.J.H.         4.C.C.J.H.         C.H.         C.A.B.         0.53         2.2.2.2.22         Calcd 310, 0370 M + H17,         Found 3 31,           3.11         3.D.C.C.H.         C.H.         C.H.         C.A.B.         0.3.2         2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.2.	3.01	$3-ClC_6H_4$	$C_6H_5$	CH <sub>3</sub>	82	0.55	215-217	Calcd: $316.0675 [M + H]^+$ . Found: $316.0660$
3.00         +FC_QFI         Capits         CH3         633         220-210         Calication         Calicati	3.0211	$2-CIC_6H_4$	$C_6H_5$	$CH_3$	80	0.54	220-221	Calcd: $316.0675 [M + H]^{+}$ . Found: $316.0703$
3.00         3.01         3.02         212–214         Calcet 380.970         M+17: Found: 39           3.00         3.CCGH4         4.BCGH4         CH5         84         0.52         220–222         Calcet 380.970         M+117: Found: 39           3.00         3.CCGH4         4.BCGH4         CH5         84         0.52         220–227         Calcet 380.985         M+117: Found: 39           3.00         3.CCGH4         4.CCGH4         CH5         84         0.53         226–220         Calcet 380.0855         M+117: Found: 39           3.10         3.CCGH4         4.CH3OCH4         CH5         84         0.53         228–240         Calcet 380.0875         M+117: Found: 39           3.11         3.CCGH4         CH5         CH4         CH4         CH20-77         79         52         148         151         Calcet 380.0170         M+117: Found: 39           3.13         3.CCGH4         CH4         CH3         20         52         0.52         190–193         Calcet 380.0282         M+117: Found: 39           3.14         3.BCGH4         CA14         CA15         CH4         CH3         20         522         120–192         Calcet 380.0282         M+117: Found: 39         321         33.14	3.03	4-FC <sub>6</sub> H <sub>4</sub>	$C_6H_5$	$CH_3$	68	0.53	228-231	Calcd: $300.0971 \text{ [M + H]}^+$ . Found: $300.0996$
<b>3.05</b> 3-C(C <sub>4</sub> H <sub>4</sub> 3-BrC <sub>4</sub> H <sub>4</sub> CH <sub>4</sub> 8H C <sub>4</sub> H <sub>4</sub> CH <sub>4</sub> 86 0.52 196-200 Calct 339.3970 [M + H] <sup>-</sup> , Found 39 <b>3.07</b> 3-C(C <sub>4</sub> H <sub>4</sub> 4-C(C <sub>4</sub> H <sub>4</sub> CH <sub>4</sub> (H <sub>5</sub> 85 0.52 204-227 Calct 330.0855 [M + H] <sup>-</sup> , Found 35 <b>3.09</b> 3-C(C <sub>4</sub> H <sub>4</sub> 4-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> 82 0.52 226-226 Calct 340.055 [M + H] <sup>-</sup> , Found 35 <b>3.09</b> 3-C(C <sub>4</sub> H <sub>4</sub> 4-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> 88 0.33 226-229 Calct 340.075 [M + H] <sup>-</sup> , Found 35 <b>3.10</b> 3-C(C <sub>4</sub> H <sub>4</sub> 4-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> 84 0.33 226-229 Calct 340.075 [M + H] <sup>-</sup> , Found 35 <b>3.11</b> 3-C(C <sub>4</sub> H <sub>4</sub> 4-C(H <sub>2</sub> ) <sub>C</sub> 79 0.52 148-151 Calct 280.0765 [M + H] <sup>-</sup> , Found 36 <b>3.13</b> 3-C(C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 80 0.32 228-220 Calct 310.075 [M + H] <sup>-</sup> , Found 37 <b>3.11</b> 3-C(C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 0.42 20 <b>3.12</b> 4-C(H <sub>2</sub> ) <sub>C</sub> 79 0.52 148-151 Calct 280.095 [M + H] <sup>-</sup> , Found 38 <b>3.13</b> 3-C(H <sub>4</sub> -4CH <sub>5</sub> -C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 0.52 228-220 Calct 310.075 [M + H] <sup>-</sup> , Found 38 <b>3.14</b> 3-C(H <sub>4</sub> -4CH <sub>5</sub> -C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 0.54 260-292 Calct 300.0952 [M + H] <sup>-</sup> , Found 38 <b>3.16</b> 2-(D-5-C(C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.53 226-229 Calct 300.0952 [M + H] <sup>+</sup> , Found 38 <b>3.16</b> 3-C(H <sub>4</sub> -CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.53 226-229 Calct 320.0958 [M + H] <sup>+</sup> , Found 38 <b>3.17 3.</b> NO <sub>5</sub> CH <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.53 226-227 Calct 320.0958 [M + H] <sup>+</sup> , Found 28 <b>3.20</b> 3-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.54 220-222 Calct 320.191 [M + H] <sup>+</sup> , Found 25 <b>3.22 3.</b> C(H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.54 220-222 Calct 320.191 [M + H] <sup>+</sup> , Found 25 <b>3.23</b> 3-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 17-219 Calct 320.0908 [M + H] <sup>+</sup> , Found 32 <b>3.24</b> 3-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.47 210-219 Calct 320.131 [M + H] <sup>+</sup> , Found 33 <b>3.26</b> 2-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 178-180 Calct 320.137 [M + H] <sup>+</sup> , Found 33 <b>3.26</b> 2-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 178-180 Calct 320.137 [M + H] <sup>+</sup> , Found 33 <b>3.26</b> 2-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 178-180 Calct 320.137 [M + H] <sup>+</sup> , Found 33 <b>3.26</b> 2-C(C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 178-180 Calct 320.137 [M + H] <sup>+</sup> , Found 33 <b>3.33</b> 3-C(C <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> 80 0.57 178-180 Calct 320.1	3.04°	$4-CIC_6H_4$	$C_6H_5$	CH <sub>3</sub>	85	0.54	212 - 214	Calcd: $316.0675 [M + H]^+$ . Found: $316.0662$
3.06       3-ClC <sub>4</sub> H <sub>4</sub> 4-BrC <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> 84       0.52       220-222       Calcle: 350.0855 [M + H]: Found: 35         3.07       3-ClC <sub>4</sub> H <sub>4</sub> 4-ClC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> 85       0.52       225-226       Calcle: 350.0855 [M + H]: Found: 35         3.08       3-ClC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> O <sub>4</sub> CH <sub>4</sub> CH <sub>5</sub> O <sub>4</sub> CH <sub>4</sub> CH <sub>6</sub> O <sub>4</sub> C	3.05	$3-ClC_6H_4$	$3-BrC_6H_4$	$CH_3$	86	0.52	196 - 200	Calcd: $393.9790 [M + H]^+$ . Found: $393.9839$
	3.06	$3-ClC_6H_4$	$4-BrC_6H_4$	$CH_3$	84	0.52	220 - 222	Calcd: 393.9790 [M + H] <sup>+</sup> . Found: 393.9779
3.00       3-Clc_6H <sub>4</sub> 4-Clc_QL <sub>4</sub> CH <sub>3</sub> 82       0.52       225-226       Cahch: 346.0781 M + H]: Found: 55         3.10       3-Clc_6H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> 0.53       228-229       Cahch: 346.0781 M + H]: Found: 35         3.11       3-Clc_6H <sub>4</sub> CH <sub>4</sub> CH <sub>3</sub> 9       0.40       224-226       Cahch: 340.0781 M + H]: Found: 31         3.13       3-CH <sub>2</sub> -4-CH <sub>3</sub> -C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>3</sub> 2       0.52       190-192       Cahch: 300.0825 M + H]: Found: 33         3.14       3-Clc_6H <sub>4</sub> CH <sub>5</sub> CH <sub>3</sub> 2       0.52       190-192       Cahch: 300.0826 M + H]: Found: 33         3.15       3-Cl-4-CH <sub>5</sub> -CH <sub>5</sub> CH <sub>5</sub> CH <sub>3</sub> 2       0.52       190-192       Cahch: 300.0826 M + H]: Found: 33         3.16       2-Cl-5-ClC <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>3</sub> 6       0.53       226-270       Cahch: 300.0826 M + H]: Found: 32         3.18       3-ClC <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>3</sub> 6       0.53       226-229       Cahch: 300.0821 M + H]: Found: 32         3.20       3-ClC <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>3</sub> 6       0.53       217-219       Cahch: 300.081 M + H]: Found: 32         3.21       CH <sub>4</sub> CH <sub></sub>	3.07	3-ClC <sub>6</sub> H <sub>4</sub>	3-ClC <sub>6</sub> H <sub>4</sub>	$CH_3$	85	0.52	204 - 207	Calcd: 350.0855 [M + H] <sup>+</sup> . Found: 350.0271
3.00         3.Clc_4H <sub>4</sub> 4.Cl <sub>4</sub> D <sub>0</sub> C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> Calc         3.228-228         Calc         3.60781 [M + H] <sup>+</sup> , Found: 33           3.11         3.Clc_6H <sub>4</sub> $-(CH_2)_{-}$ 79         0.52         148-151         Calcd: 316.0075 [M + H] <sup>+</sup> , Found: 28           3.128         CA <sub>4</sub> CA <sub>4</sub> CH <sub>5</sub> 224-226         Calcd: 328.1065 [M + H] <sup>+</sup> , Found: 38           3.13         3.5Cl <sub>7</sub> -4.Cl <sub>7</sub> C <sub>6</sub> H <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> 0.52         190-192         Calcd: 300.0275 [M + H] <sup>+</sup> , Found: 38           3.15         3.Cl-4.CH <sub>5</sub> C <sub>6</sub> H <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> 20.52         190-193         Calcd: 300.0821 [M + H] <sup>+</sup> , Found: 39           3.16         2.ClCH <sub>5</sub> C <sub>6</sub> H <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> 80.49         214-116         Calcd: 300.0821 [M + H] <sup>+</sup> , Found: 39           3.17         3.No <sub>5</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 8.053         226-220         Calcd: 300.081 [M + H] <sup>+</sup> , Found: 33           3.28         3.Clc_6H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 8.053         226-221         Calcd: 300.081 [M + H] <sup>+</sup> , Found: 33           3.223         3.Clc_6H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 8.053         226-221         Calcd: 300.081 [M + H] <sup>+</sup> , Found: 33           3.223	3.08	3-ClC <sub>6</sub> H <sub>4</sub>	4-ClC <sub>6</sub> H <sub>4</sub>	$CH_3$	82	0.52	225 - 226	Calcd: 350.0855 [M + H] <sup>+</sup> . Found: 350.0356
3.10       3-ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> C <sub>1</sub> H <sub>3</sub> 8       0.53       238-240       Calcd: 280.0675 [M + H]'. Found: 28         3.12 <sup>8</sup> C <sub>6</sub> H <sub>5</sub> C <sub>1</sub> H <sub>3</sub> CH <sub>3</sub> 9       0.49       224-226       Calcd: 280.0675 [M + H]'. Found: 28         3.13       3-CH <sub>3</sub> -4-CH <sub>3</sub> -C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 0.52       190-192       Calcd: 300.078 [M + H]'. Found: 33         3.14       3-BrC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 20       0.52       190-192       Calcd: 300.082 [M + H]'. Found: 33         3.16       2-CL-5-ClC <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 80       0.53       226-270       Calcd: 300.082 [M + H]'. Found: 32         3.17       3-NO <sub>5</sub> C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 86       0.53       226-229       Calcd: 300.082 [M + H]'. Found: 32         3.20       3-ClC <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 86       0.53       217-219       Calcd: 240.090 [M + H]'. Found: 32         3.20       3-ClC <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 78       0.54       230-222       Calcd: 300.81 [M + H]'. Found: 32         3.22       3-ClC <sub>6</sub> C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 78       0.53       230-2240       Calcd: 300.81 [M + H]'. Found: 32         3.23	3.09	3-ClC <sub>6</sub> H <sub>4</sub>	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub>	$CH_3$	88	0.53	226 - 229	Calcd: 346.0781 [M + H] <sup>+</sup> . Found: 350.0831
3.11         3-ClCqH <sub>2</sub> -(CH <sub>2</sub> ) <sub>-</sub> 79         0.52         148-151         Calcd: 282.065 [M + H]; Found: 28           3.12 <sup>6</sup> GH <sub>5</sub> CH <sub>5</sub> Q         0.49         224-226         Calcd: 282.065 [M + H]; Found: 28           3.13         3-BCrGH <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 0.52         190-192         Calcd: 300.075 [M + H]; Found: 30           3.15         3-Cl-4-CH <sub>5</sub> CqH <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 0.52         190-192         Calcd: 300.083 [M + H]; Found: 33           3.16         2-Cl-5-ClC <sub>3</sub> H <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> 80         0.53         226-220         Calcd: 300.083 [M + H]; Found: 33           3.17         3-NO <sub>5</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 60         0.53         226-227         Calcd: 300.081 [M + H]; Found: 23           3.20         3-ClC <sub>6</sub> C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> 78         0.53         217-212         Calcd: 230.081 [M + H]; Found: 23           3.21         C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 78         0.53         217-212         Calcd: 300.081 [M + H]; Found: 33           3.22         3-ClC <sub>6</sub> C <sub>4</sub> H <sub>4</sub> CH <sub>5</sub> 60         57         230-22         Calcd: 310.0137 [M + H]; Found: 33           3.23         3-Cl	3.10	3-ClC <sub>6</sub> H <sub>4</sub>	$CH_3$	$C_6H_5$	83	0.53	238 - 240	Calcd: 316.0675 [M + H] <sup>+</sup> . Found: 316.0684
3.12 <sup>a</sup> C <sub>H</sub> C <sub>H</sub> Q2       0.49       224-226       Calct: 282.1065 [M + H] <sup>+</sup> , Found: 31         3.13       3.5H       3.5H       4.4CH, G <sub>H</sub> C <sub>H</sub> 62       0.52       190-192       Calct: 310.1378 [M + H] <sup>+</sup> , Found: 33         3.14       3.5H       3.5H       4.4CH, C <sub>H</sub> C <sub>H</sub> 12       105-193       Calct: 330.0285 [M + H] <sup>+</sup> , Found: 33         3.16       3.2C-4.2H, C <sub>G</sub> H <sub>3</sub> C <sub>H</sub> C <sub>H</sub> 14       80       141-16       Calct: 330.0285 [M + H] <sup>+</sup> , Found: 32         3.17       3.NO <sub>C</sub> GH <sub>4</sub> C <sub>H</sub> C <sub>H</sub> 80       0.53       226-229       Calct: 300.0971 [M + H] <sup>+</sup> , Found: 32         3.19       3.CH <sub>C</sub> G <sub>H</sub> C <sub>H</sub> T       80       0.53       226-229       Calct: 324.0968 [M + H] <sup>+</sup> , Found: 32         3.20       3.20       3.21       C <sub>H</sub> C <sub>H</sub> C <sub>H</sub> 78       0.53       217-219       Calct: 324.0968 [M + H] <sup>+</sup> , Found: 32         3.22       3.CH <sub>C</sub> C <sub>H</sub> C <sub>H</sub> C <sub>H</sub> 78       0.54       230-232       Calct: 324.1056 [M + H] <sup>+</sup> , Found: 32         3.23       3.CH <sub>C</sub> C <sub>H</sub> C <sub>H</sub> C <sub>H</sub> 78       0.52       224       234       234       234       234       23	3.11	3-ClC <sub>6</sub> H <sub>4</sub>	$-(CH_2)$	4-	79	0.52	148 - 151	Calcd: 280.0675 [M + H] <sup>+</sup> . Found: 280.0733
3.13       3-Cf4,C,H-,-C,H,       C,H,       CH,       62       0.53       228-230       Calck : 310.1378 [M + H] <sup>+</sup> . Found: 38         3.14       3-BrC-H,       C,H,       CH,       52       190-193       Calck : 300.078 [M + H] <sup>+</sup> . Found: 33         3.15       3-C1-4-CH,CaH,       C,H,       CH,       60       0.54       280-270       Calck : 300.082 [M + H] <sup>+</sup> . Found: 33         3.17       3-NO,CaH,       C,H,       CH,       60       0.53       228-229       Calck : 300.082 [M + H] <sup>+</sup> . Found: 30         3.18       3-FCaH,       C,H,       CH,       64       0.64       220-220       Calck : 320.091 [M + H] <sup>+</sup> . Found: 32         3.20       3-CLCaH,       C,H,       CH,       78       0.53       221-219       Calck : 240.090 [M + H] <sup>+</sup> . Found: 32         3.22       3-CH,G,H,       C,H,       CH,       78       0.53       217-219       Calck : 341.051 [M + H] <sup>+</sup> . Found: 32         3.23       3-CH,G,G,H,       C,H,       CH,       78       0.53       217-219       Calck : 341.051 [M + H] <sup>+</sup> . Found: 32         3.23       3-CL,G,A,       C,H,       C,H,       CH,       78       0.53       220-220       Calck : 341.051 [M + H] <sup>+</sup> . Found: 33       320         3.23       3-CL,G,A,	3.12 <sup>6</sup>	C <sub>6</sub> H <sub>5</sub>	C <sub>6</sub> H <sub>5</sub>	CH <sub>3</sub>	92	0.49	224 - 226	Calcd: 282.1065 $[M + H]^+$ . Found: 282.1037
3.14       3-Br C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 52       0.52       190-192       Calcit.       380.0170       M+ H <sup>1</sup> Found. 33         3.16       3-CL4-CHLC <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 60       0.54       286-270       Calcit.       380.0385       M+ H <sup>1</sup> Found. 33         3.17       3-No <sub>7</sub> C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 48       0.53       226-229       Calcit.       280.0971       M+ H <sup>1</sup> Found. 32         3.18       3-FC <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> 88       0.53       226-229       Calcit.       280.019       M+ H <sup>1</sup> Found. 39         3.20       3-CLG <sub>2</sub> H <sub>4</sub> CH <sub>8</sub> CH <sub>3</sub> CH <sub>8</sub> 87       0.53       217-219       Calcit.       280.058       M+ H <sup>1</sup> Found. 39         3.21       3-CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>8</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> 230.23       Calcit.       280.058       M+ H <sup>1</sup> Found. 33         3.22       3-CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>8</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> 20.222       Calcit.       280.058       M+ H <sup>1</sup> Found. 33         3.23       3-CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>2</sub> CH <sub>4</sub> <th>3.13</th> <th><math>3-CH_3-4-CH_3-C_6H_3</math></th> <th>C<sub>6</sub>H<sub>5</sub></th> <th>CH<sub>3</sub></th> <th>62</th> <th>0.53</th> <th>228-230</th> <th>Calcd: 310.1378 [M + H]<sup>+</sup>. Found: 310.1373</th>	3.13	$3-CH_3-4-CH_3-C_6H_3$	C <sub>6</sub> H <sub>5</sub>	CH <sub>3</sub>	62	0.53	228-230	Calcd: 310.1378 [M + H] <sup>+</sup> . Found: 310.1373
3.16       2.0.1-4.CH, C.H., 3.16       2.0.1-2.2       190-193       Calk: 330.082 M + H1'. Found: 35         3.16       2.0.1-5-ClCaH <sub>3</sub> C.H., C.H., 3.17       3.N.O, C.H., 3.16       C.H., C.H., 3.17       3.N.O, C.H., 3.17       C.H., 3.18       3.FC, C.H., 3.14       C.H., 3.14       C.H., C.H., 3.15       3.FC, C.H., 3.16       C.H.C., 3.17       3.N.O, C.H., 3.16       C.H.C., 3.17       3.N.O, C.H., 3.16       C.H.C., 3.17       3.N.O, C.H., 3.16       C.H.C., 3.16       C.H.C., 3.16       2.0.12       M.H.I'. Found: 30         3.19       3.CH <sub>2</sub> C <sub>4</sub> H <sub>4</sub> C.H., C.H., 3.22       C.H.C., 3.24       S.C.C., 3.24       C.H.C., 3.24       S.C.C., 3.24       C.H.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       C.H.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       S.C.C., 3.24       C.H.C., 3.24       S.C.C., 3.24	3.14	3-BrCeH4	CeHs	CH <sub>2</sub>	52	0.52	190-192	Calcd: $360.0170 [M + H]^+$ Found: $360.0168$
16         2-Cl $-5-ClC_{H_2}$ CH <sub>2</sub> 60         0.54         286-270         Calc:         250.0285         M + H1 <sup>+</sup> , Found:         250.235           3.16         3-FC <sub>4</sub> H <sub>4</sub> C <sub>H</sub> <sub>3</sub> CH <sub>3</sub> 36         0.49         214-116         Calc:         250.0285         M + H1 <sup>+</sup> , Found:         250.320           3.18         3-FC <sub>4</sub> H <sub>4</sub> C <sub>H</sub> <sub>3</sub> CH <sub>3</sub> 78         0.53         226-229         Calc:         250.1621         M + H1 <sup>+</sup> , Found:         250.321           3.20         3-CH <sub>2</sub> C <sub>4</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> 87         8.053         227-222         Calc:         250.1065         M + H1 <sup>+</sup> , Found:         250.323           3.22         3-CH <sub>2</sub> C <sub>4</sub> H <sub>4</sub> C <sub>H</sub> <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> 80.52         116-118         Calc:         3105         M + H1 <sup>+</sup> , Found:         323.33         3-CH <sub>4</sub> C <sub>4</sub> C <sub>4</sub> H <sub>4</sub> C <sub>H</sub> <sub>4</sub> CH <sub>3</sub> CH <sub>4</sub> 68         0.52         116-118         Calc:         310.317         M + H1 <sup>+</sup> , Found:         323.32           3.21         3-ClC <sub>4</sub> H <sub>4</sub> C <sub>H</sub> <sub>4</sub> CH <sub>3</sub> CH <sub>4</sub> 68         0.52         116-118         Calc:         310.311.371         M + H1 <sup>+</sup> , Found:         333.33	3.15	3-Cl-4-CH <sub>2</sub> C <sub>6</sub> H <sub>2</sub>	CeHr	CH <sub>2</sub>	32	0.52	190-193	Calcd: 330 0832 $[M + H]^+$ Found: 330 0834
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 16	2 - C = 5 - C = C + 3	C <sub>0</sub> H <sub>2</sub>	CH <sub>0</sub>	60	0.54	266-270	Calcd: $350.0285 [M + H]^+$ Found: $350.0248$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 17	3-NO <sub>2</sub> C <sub>2</sub> H	C <sub>0</sub> H <sub>2</sub>	CH <sub>2</sub>	/8	0.01	214-116	Calcd: $327.0916 [M + H]^+$ Found: $327.0928$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	218	3-FC-H.	C.H.	CH <sub>2</sub>	36	0.45	226-220	Calcd: $327.0010 [M + H]^{+}$ Found: $327.0020$
3.19       3-CLT3CH14       CH33       CH3       CH4       234-236       Calcdt       234.0151       H + H) <sup>+</sup> , Found       22         3.21       3-CH3CH4       CH3       CH3       CH3       CH4       6       0.50       220-222       Calcdt       224.1065       H + H) <sup>+</sup> , Found       32         3.223       3-CH3CH4       CaH3       CH4, CH3       CH4       6       0.50       220-222       Calcdt       320.0831       M + H) <sup>+</sup> , Found       33         3.23       3-CH4, CH4, CH4       CH4       CH4       CH4       CA       0.57       178-180       Calcdt       310.1377       M + H) <sup>+</sup> , Found       33         3.26       3-CICeH4       CH4, CH3       CH3       52       0.30       166-162       Calcdt       284.0261       M + H) <sup>+</sup> , Found       32         3.31       3-CH2, CH4       CH4       CH3       CH3       82       0.53       168-170       Calcdt       310.171       M + H) <sup>+</sup> , Found       33       3.33       3.33       3.33       3.33       3.33       3.33       3.33       3	J.10 9 10	2 CH C H			50	0.55	206 207	Calcd: $300.0371$ [M + H] <sup>+</sup> Found: $300.0335$
3.21       C.H.3       C.H.4       C.H.4       C.H.4       C.H.3       C.H.3       C.H.3       C.H.4       C.H.4       C.H.4       C.H.3       C.H.3       C.H.3       C.H.4       C.H.4       C.H.4       C.H.3       C.H.3       C.H.4       C.H.3       C.H.3       C.H.4       C.H.4       H.H.7       Found: 31       S.J.3       C.H.2       C.H.4       C.H.3       S.G.       C.H.4       C.H.3       S.G.       C.H.4       C.H.3       S.G.       C.H.4 <t< th=""><th>3.19 2 90</th><th><math>3-CH_{3}C_{6}H_{4}</math></th><th></th><th></th><th>07</th><th>0.55</th><th>200-207</th><th>Calcu. 290.1221 <math>[M + H]^+</math> Found: 290.1206</th></t<>	3.19 2 90	$3-CH_{3}C_{6}H_{4}$			07	0.55	200-207	Calcu. 290.1221 $[M + H]^+$ Found: 290.1206
3.2.2       3.2.4       3.2.4.4       CH3       CH3       CH3       CH3       CH3       CH4	3.2U 9.91	$5 - C I C_6 \Pi_4$		$CH_3$	01 70	0.54	234-230	Calcd: $234.0319$ [W $\pm$ H] <sup>+</sup> Found: $234.0321$
<b>3.22 3</b> -CH <sub>3</sub> C <sub>4</sub> F <sub>4</sub> , CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> <b>3 0</b> .34 230–232 Calc: 234.105 [M + H] <sup>+</sup> , Found: 32 <b>3.24 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> (H <sub>2</sub> H <sub>6</sub> <b>6</b> .50 220–222 Calc: 324.1534 [M + H] <sup>+</sup> , Found: 32 <b>3.25 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>5</sub> (CH <sub>2</sub> <b>7 0</b> .53 202–204 Calc: 310.1377 [M + H] <sup>+</sup> , Found: 31 <b>3.26 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>2</sub> (CH <sub>2</sub> <b>7 0</b> .57 178–180 Calc: 310.1377 [M + H] <sup>+</sup> , Found: 31 <b>3.27 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> (CO + H <sub>3</sub> <b>6</b> 8 0.49 194–196 Calc: 298.0417 [M + H] <sup>+</sup> , Found: 29 <b>3.28 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> <b>5 0</b> .05 160–162 Calc: 310.1377 [M + H] <sup>+</sup> , Found: 29 <b>3.28 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> CH <sub>5</sub> <b>2</b> 0.53 240–242 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.31 3</b> -CH <sub>5</sub> O <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub> CH <sub>5</sub> <b>2</b> 0.53 240–242 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.32 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>5</sub> <b>8 0</b> .053 184–186 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.33 3</b> -MC <sub>6</sub> C <sub>4</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.53 184–186 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.34 3</b> -CH <sub>5</sub> O <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.54 160–162 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.35 3</b> -CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.54 160–162 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.36 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.54 160–162 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 34 <b>3.38 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.54 160–168 Calc: 340.0120 [M + H] <sup>+</sup> , Found: 34 <b>3.38 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -H0COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>61</b> 0.33 166–168 Calc: 330.1147 [M + H] <sup>+</sup> , Found: 34 <b>3.39 3</b> -CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -H0COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>70</b> 0.34 170–172 Calc: 330.137 [M + H] <sup>+</sup> , Found: 34 <b>3.39 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -H0COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>71</b> 0.56 194–196 Calc: 330.1137 [M + H] <sup>+</sup> , Found: 34 <b>3.40</b> 4-CH <sub>5</sub> SC <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>73</b> 0.35 164–166 Calc: 330.1137 [M + H] <sup>+</sup> , Found: 33 <b>3.40</b> 4-CH <sub>5</sub> SC <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>58</b> 0.50 180–182 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.40</b> 4-CH <sub>5</sub> SC <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>58</b> 0.50 180–182 Calc: 310.1378 [M + H] <sup>+</sup> , Found: 32 <b>702 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -H0COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>50</b> 0	3.61	$C_6\Pi_5$			10	0.55	217-219	Calcu: $220.0906 [W + H]^+$ . Found: $220.0644$
$      3.2.3  3-CH_{3}C_{4}H_{4} \qquad C_{4}H_{5} \qquad (CH_{3}D_{2}CH)  46 \qquad 0.30 \qquad 220-222 \qquad CalcG: 324.134 \\ M + H1', Found: 33 \\ 3.2.5 \qquad 3-CH_{3}C_{4}H_{4} \qquad C_{4}H_{5} \qquad CH_{3}CH_{2}  CR \\ 3.2.5 \qquad 3-CC_{6}H_{4} \qquad C_{6}H_{5} \qquad CH_{5}C_{4}H_{2} \qquad 72 \qquad 0.53 \qquad 202-204 \qquad CalcG: 310.01377 \\ M + H1', Found: 31 \\ 3.2.6 \qquad 3-CC_{6}H_{4} \qquad C_{4}H_{5} \qquad C_{6}H_{5} \qquad 6.57 \qquad 178-180 \qquad CalcG: 320.081 \\ M + H1', Found: 32 \\ 3.2.8 \qquad 3-CC_{6}H_{4} \qquad COH \qquad CH_{3} \qquad 68 \qquad 0.49 \qquad 194-196 \qquad CalcG: 280.0417 \\ M + H1', Found: 29 \\ 3.2.9 \qquad 3-CC_{6}H_{4} \qquad COH \qquad CH_{3} \qquad 52 \qquad 0.30 \qquad 166-168 \qquad CalcG: 280.0417 \\ M + H1', Found: 29 \\ 3.30 \qquad 3-CH_{3}-5-CH_{3}C_{6}H_{4} \qquad C_{4}H_{5} \qquad CH_{3} \qquad 80 \qquad 0.53 \qquad 184-186 \qquad CalcG: 312.1171 \\ M + H1', Found: 29 \\ 3.30 \qquad 3-CH_{3}-5-CH_{3}C_{6}H_{4} \qquad C_{4}H_{5} \qquad CH_{3} \qquad 80 \qquad 0.53 \qquad 184-186 \qquad CalcG: 312.1171 \\ M + H1', Found: 31 \\ 3.32 \qquad 3-CC_{6}H_{4} \qquad 3-CNC_{6}H_{4} \qquad CH_{3} \qquad 80 \qquad 0.53 \qquad 184-186 \qquad Calcd: 312.1171 \\ M + H1', Found: 31 \\ 3.33 \qquad 3-MeC_{4}H_{4} \qquad 3-CNC_{6}H_{4} \qquad CH_{3} \qquad 80 \qquad 0.54 \qquad 170-172 \qquad Calcd: 310.1378 \\ M + H1', Found: 32 \\ 3.34 \qquad 3-CC_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 80 \qquad 0.52 \qquad 164-166 \qquad Calcd: 321.1174 \\ M + H1', Found: 35 \\ 3.36 \qquad 3-CC_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 80 \qquad 0.52 \qquad 164-166 \qquad Calcd: 350.1119 \\ M + H1', Found: 35 \\ 3.36 \qquad 3-CC_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 70 \qquad 0.34 \qquad 170-172 \qquad Calcd: 340.0573 \\ M + H1', Found: 35 \\ 3.39 \qquad c-naphthyl \qquad C_{4}H_{5} \qquad CH_{3} \qquad F0 \qquad 0.34 \qquad 170-172 \qquad Calcd: 340.01119 \\ M + H1', Found: 35 \\ 3.39 \qquad c-CL_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 70 \qquad 0.34 \qquad 170-172 \qquad Calcd: 310.1378 \\ M + H1', Found: 36 \\ 3.37 \qquad 3-CCL_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 70 \qquad 0.34 \qquad 170-172 \qquad Calcd: 340.0457 \\ M + H1', Found: 36 \\ 3.39 \qquad 3-CL_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 61 \qquad 0.33 \qquad 166-168 \qquad Calcd: 350.0573 \\ M + H1', Found: 36 \\ 3.39 \qquad c-CL_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 70 \qquad 0.34 \qquad 170-172 \qquad Calcd: 310.1378 \\ M + H1', Found: 37 \\ 3.36 \qquad -CL_{6}H_{4} \qquad 3-MeOCOC_{6}H_{4} \qquad CH_{3} \qquad 70 \qquad 0.34 \qquad 170-172 \qquad Cal$	3.22	$3-CH_3C_6H_4$		$(CH_3)$	80	0.54	230-232	Calcd: $234.1005$ [M + H] · Found: $234.1078$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3.23	$3-CH_3C_6H_4$	$C_6H_5$	$(CH_3)_2CH$	40	0.50	220-222	Calcd: $324.1534 [M + H]^+$ . Found: $324.1524$
<b>3.25 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>2</sub> 72 0.33 202–204 Calcd: <b>310</b> .1377 [M + H] <sup>-</sup> . Found: <b>31</b> <b>3.26 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> OC CH <sub>3</sub> <b>68</b> 0.49 194–196 Calcd: <b>328</b> .0382 [M + H] <sup>-</sup> . Found: <b>29</b> <b>3.28 3</b> -ClC <sub>6</sub> H <sub>4</sub> COOH CH <sub>3</sub> <b>52</b> 0.30 166–168 Calcd: <b>298</b> .0417 [M + H] <sup>-</sup> . Found: <b>29</b> <b>3.29 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> OC CH <sub>5</sub> CH <sub>3</sub> <b>82</b> 0.53 240–242 Calcd: <b>310</b> .1378 [M + H] <sup>-</sup> . Found: <b>31</b> <b>3.31 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> <b>80</b> 0.53 184–186 Calcd: <b>298</b> .0417 [M + H] <sup>-</sup> . Found: <b>31</b> <b>3.32 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> <b>80</b> 0.53 184–186 Calcd: <b>321</b> .1171 [M + H] <sup>+</sup> . Found: <b>31</b> <b>3.32 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> <b>4</b> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> CH <sub>3</sub> <b>80</b> 0.53 168–170 Calcd: <b>321</b> .0174 [M + H] <sup>-</sup> . Found: <b>32</b> <b>3.33 3</b> -MeC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>88</b> 0.53 160–162 Calcd: <b>321</b> .1174 [M + H] <sup>+</sup> . Found: <b>32</b> <b>3.34</b> 3-ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>80</b> 0.52 164–166 Calcd: <b>321</b> .1174 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.36 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -MOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>70</b> 0.34 170–172 Calcd: <b>334</b> .0730 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.37 3</b> -CH <sub>5</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -MOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>71</b> 0.33 166–166 Calcd: <b>332</b> .1176 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.39</b> a-cnaphthyl CaH <sub>5</sub> CH <sub>5</sub> CH <sub>3</sub> <b>58</b> 0.50 180–188 Calcd: <b>330</b> .1138 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.40</b> 4-CH <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> <b>3</b> -NH <sub>2</sub> COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>58</b> 0.50 180–182 Calcd: <b>330</b> .073 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.40</b> 4-CH <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> <b>3</b> -NH <sub>2</sub> COC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>58</b> 0.48 215–217 Calcd: <b>320</b> .0242 [M + H] <sup>+</sup> . Found: <b>35</b> <b>3.40</b> 4-CH <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>58</b> 0.48 215–217 Calcd: <b>328</b> .0242 [M + H] <sup>+</sup> . Found: <b>31</b> <b>3.40</b> 4-CH <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>58</b> 0.48 165–167 Calcd: <b>338</b> .0259 [M + H] <sup>+</sup> . Found: <b>36</b> <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BC <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>66</b> 0.83 188–170 Calcd: <b>380</b> .059 [M + H] <sup>+</sup> . Found: <b>26</b> <b>7.05</b> C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>5</sub> CH <sub>3</sub> <b>86</b> 0.84 165–167 Calcd: <b>326</b> .0298 [M + H] <sup>+</sup> . Found: <b>36</b> <b>7.06</b> C <sub>6</sub> H <sub>5</sub> CH <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>70 71</b> 46–148 Calcd: <b>320</b> .0298 [M + H] <sup>+</sup> . Found: <b>27</b> <b>7.16 3</b> -CH <sub>5</sub> CH <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub> CH <sub>3</sub> <b>79 0</b> ,76 178–180 Calcd: <b>38</b> .1867 [M +	3.24	$3-CIC_6H_4$	$C_6H_5$	CH <sub>3</sub> CH <sub>2</sub>	68	0.52	116-118	Calcd: $330.0831 \text{ [M + H]}^+$ . Found: $330.0833$
3.26 $3-Clc_{BH_4}$ $C_{BH_5}$ $C_{BH_5}$ $56$ $0.57$ $178-180$ Calcd: $284.0817$ $M+H^+$ Found: $37$ 3.28 $3-Clc_{BH_4}$ COOH $CH_3$ $52$ $0.30$ $166-168$ Calcd: $284.0261$ $M+H^+$ Found: $28$ 3.29 $3-Clc_{BH_4}$ CH_3       CH_3COO $75$ $0.45$ $160-162$ Calcd: $280.017$ $M+H^+$ Found: $28$ 3.31 $3-CH_3Ce_{BH_4}$ $C_{BH_5}$ CH_3 $80$ $0.53$ $168-170$ Calcd: $310.1378$ $M+H^+$ Found: $31$ 3.31 $3-CH_3Ce_{BH_4}$ $3-CNC_6H_4$ $CH_3$ $84$ $0.53$ $168-170$ Calcd: $312.1174$ $M+H^+$ Found: $31$ 3.33 $3-MC_2G_4H_4$ $3-CNC_6H_4$ $H=3$ $80$ $52$ $164-166$ Calcd: $321.1174$ $M+H^+$ Found: $35$ $3.34$ $3-Clc_2H_4$ $3-MeCOCc_4H_4$ $CH_3$ $70$ $0.34$ $170-172$ Calcd: $350.073$ $M+H^+$ Found: $35$ $3.36$ $3-Clc_2H_4$ $3-MeCOCc_4H_4$ $CH_3$ $70$ $3.5$	3.25	$3-CH_3C_6H_4$	$C_6H_5$	$CH_3CH_2$	72	0.53	202-204	Calcd: $310.1377 [M + H]^+$ . Found: $310.1375$
<b>3.27 3</b> -ClC <sub>4</sub> H <sub>4</sub> CH <sub>3</sub> OCO CH <sub>3</sub> 68 0.49 194-196 Calcd: 298.0417 [M + H] <sup>+</sup> , Found: 28 <b>3.29 3</b> -ClC <sub>4</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> OCO T5 0.45 160-162 Calcd: 298.0417 [M + H] <sup>+</sup> , Found: 28 <b>3.29 3</b> -ClC <sub>4</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> OCO 75 0.45 160-162 Calcd: 298.0417 [M + H] <sup>+</sup> , Found: 31 <b>3</b> -CH <sub>3</sub> O <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> 82 0.53 240-242 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3</b> -CH <sub>3</sub> O <sub>6</sub> C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> 80 0.53 184-186 Calcd: 284.0261 [M + H] <sup>+</sup> , Found: 31 <b>3</b> -CH <sub>3</sub> O <sub>6</sub> C <sub>4</sub> H <sub>4</sub> 3-CNC <sub>6</sub> H <sub>4</sub> CH <sub>5</sub> 84 0.53 168-170 Calcd: 341.0628 [M + H] <sup>+</sup> , Found: 31 <b>3</b> -CH <sub>3</sub> O <sub>6</sub> C <sub>4</sub> H <sub>4</sub> 3-CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 80 0.53 168-170 Calcd: 341.0628 [M + H] <sup>+</sup> , Found: 32 <b>3</b> -ClC <sub>4</sub> H <sub>4</sub> 3-CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 80 0.54 170-172 Calcd: 374.0730 [M + H] <sup>+</sup> , Found: 37 <b>3</b> -S5 3-ClC <sub>6</sub> C <sub>4</sub> H <sub>4</sub> 3-MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 70 0.54 170-172 Calcd: 370.0573 [M + H] <sup>+</sup> , Found: 36 <b>3</b> -37 3-CH <sub>3</sub> C <sub>4</sub> H <sub>4</sub> 3-MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 70 0.54 170-172 Calcd: 360.0573 [M + H] <sup>+</sup> , Found: 36 <b>3</b> -37 3-CH <sub>3</sub> C <sub>4</sub> H <sub>4</sub> 3-MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 70 0.55 164-166 Calcd: 0.571, [M + H] <sup>+</sup> , Found: 37 <b>3</b> -35 3-3 CH <sub>5</sub> C <sub>4</sub> H <sub>4</sub> 3-MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 71 0.56 194-196 Calcd: 332.1143 [M + H] <sup>+</sup> , Found: 33 <b>3</b> -60 CH <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> 58 0.50 180-182 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 33 <b>3</b> -0 CH <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> 58 0.50 180-182 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 32 <b>3</b> -245 Calcd, 340.1119 [M + H] <sup>+</sup> , Found: 32 <b>3</b> -245 Calcd, 44 - CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 58 0.61 22-225 Calcd: 296.1221 [M + H] <sup>+</sup> , Found: 32 <b>3</b> -245 Calcd, 44 - CH <sub>5</sub> CH <sub>4</sub> CH <sub>3</sub> 58 0.62 223-225 Calcd: 296.1221 [M + H] <sup>+</sup> , Found: 28 7.02 3 3-ClC <sub>6</sub> H <sub>4</sub> C <sub>4</sub> H <sub>5</sub> CH <sub>3</sub> 66 0.83 168-170 Calcd: 318.056 [M + H] <sup>+</sup> , Found: 28 7.02 3 3-ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 3-ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 67 0.76 176-178 Calcd: 284.0945 [M + H] <sup>+</sup> , Found: 28 7.05 CAH <sub>5</sub> CH <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub> Calcd: 220.7948 [M + H] <sup>+</sup> , Found: 27 7.0 3-ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>5</sub>	3.26	$3-CIC_6H_4$	$C_6H_5$	$C_6H_5$	56	0.57	178-180	Calcd: $378.0832 [M + H]^+$ . Found: $378.0863$
<b>3.28 3</b> -ClC <sub>6</sub> H <sub>4</sub> COOH CH <sub>3</sub> 52 0.30 166-168 Calct 284.0261 [M + H] <sup>+</sup> , Found: 28 (3) 3 CH <sub>3</sub> -5-CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 82 0.53 240-242 Calct 29.80417 [M + H] <sup>+</sup> , Found: 11 (3.1) 3.31 <b>3</b> -CH <sub>3</sub> O <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> (CH <sub>3</sub> 80 0.53 168-170 Calct 312.1171 [M + H] <sup>+</sup> , Found: 31 (3.33 <b>3</b> -MeC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> 84 0.53 168-170 Calct 312.1171 [M + H] <sup>+</sup> , Found: 31 (3.33 <b>3</b> -MeC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> 84 0.53 168-170 Calct 314.10628 [M + H] <sup>+</sup> , Found: 31 (3.35 <b>3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -MeCOC <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> 88 0.52 164-166 Calct 324.17730 [M + H] <sup>+</sup> , Found: 37 (3.35 <b>3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> <b>80 0.52 164-166 Calct 374.1776 [M + H]<sup>+</sup>, Found: 37 (3.35 <b>3</b>-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub> <b>3</b>-MeOCOC<sub>6</sub>H<sub>4</sub> (CH<sub>3</sub> 70 0.34 170-172 Calct 340.0119 [M + H]<sup>+</sup>, Found: 35 <b>3.36 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>3</b>-MeOCOC<sub>6</sub>H<sub>4</sub> (CH<sub>3</sub> 70 0.34 170-172 Calct 360.0573 [M + H]<sup>+</sup>, Found: 35 <b>3.39</b> c-naphthyl Co<sub>6</sub>H<sub>5</sub> CH<sub>3</sub> (CH<sub>3</sub> <b>47 0.56 194-166 Calct 354.1276 [M + H]<sup>+</sup>, Found: 35 <b>3.39</b> a-naphthyl C<sub>6</sub>H<sub>5</sub> CH<sub>3</sub> CH<sub>3</sub> <b>5 8</b> 0.50 180-182 Calct 310.1119 [M + H]<sup>+</sup>, Found: 31 <b>3.41</b> 4-CH<sub>5</sub>CC<sub>6</sub>H<sub>4</sub> C<sub>6</sub>H<sub>5</sub> CH<sub>3</sub> CH<sub>3</sub> <b>5</b> 0.62 223-216 Calct 320.11378 [M + H]<sup>+</sup>, Found: 31 <b>3.41</b> 4-CH<sub>5</sub>CC<sub>6</sub>H<sub>4</sub> C<sub>6</sub>H<sub>5</sub> CH<sub>3</sub> <b>5</b> 0.62 223-225 Calct 296.1221 [M + H]<sup>+</sup>, Found: 31 <b>3.41</b> 4-CH<sub>5</sub>C<sub>6</sub>H<sub>4</sub> C<sub>6</sub>H<sub>5</sub> CH<sub>3</sub> <b>6</b> 0.62 223-225 Calct 284.0945 [M + H]<sup>+</sup>, Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>3</b>-BrC<sub>6</sub>H<sub>4</sub> CH<sub>3</sub> <b>5</b> 0.76 <b>179-180</b> Calct 310.565 [M + H]<sup>+</sup>, Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>3</b>-BrC<sub>6</sub>H<sub>4</sub> CH<sub>3</sub> <b>6</b> 0.83 <b>168-170</b> Calct 284.0945 [M + H]<sup>+</sup>, Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>3</b>-BrC<sub>6</sub>H<sub>4</sub> CH<sub>3</sub> <b>6</b> 0.83 <b>168-167</b> Calct 284.0945 [M + H]<sup>+</sup>, Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>5</b>-CH<sub>5</sub> CH<sub>5</sub> CH<sub>3</sub> <b>8</b> 0.62 215-217 Calct 328.0942 [M + H]<sup>+</sup>, Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>5</b>-CH<sub>5</sub> CH<sub>5</sub> <b>6</b>-CH<sub>5</sub> <b>6</b>-CH<sub>5</sub> <b>6</b>-CH<sub>5</sub> <b>6</b>-CH<sub>5</sub> <b>7.04 1</b>+], Found: 31 <b>7.04 3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>7.05</b> CaH<sub>5</sub> <b>C</b>+H<sub>5</sub> <b>CH</b>-16 <b>1.06</b> Calct <b>2</b>-284.0945 [M + H]<sup>+</sup>, Found: 20 <b>7.05</b> CaH<sub>5</sub> <b>C</b>-144 <b>3</b>-ClC<sub>6</sub>H<sub>4</sub> <b>C</b>-147 <b>C</b>-147 <b>Calct 1.081.119 C</b>-147 <b>C</b></b></b>	3.27	$3-ClC_6H_4$	CH <sub>3</sub> OCO	$CH_3$	68	0.49	194-196	Calcd: 298.0417 $[M + H]^+$ . Found: 298.0421
<b>3.29</b> $3-ClC_{8}H_4$ CH <sub>3</sub> CH <sub>3</sub> OCO 75 0.45 160-162 Calcd: 298.0417 [M + H] <sup>+</sup> , Found: 29. <b>3.30</b> $3-ClC_{9}H_5$ CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>8</sub> H <sub>5</sub> CH <sub>3</sub> 82 0.53 240-242 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 31. <b>3.31</b> $3-CH_3OC_{6}H_4$ C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 84 0.53 168-170 Calcd: 31.1174 [M + H] <sup>+</sup> , Found: 31. <b>3.32</b> $3-ClC_{8}H_4$ $3-CNC_{8}H_4$ CH <sub>3</sub> 84 0.53 168-170 Calcd: 31.1174 [M + H] <sup>+</sup> , Found: 31. <b>3.33</b> $3-MeC_{6}H_4$ $3-CNC_{6}H_4$ CH <sub>3</sub> 84 0.53 160-162 Calcd: 32.1174 [M + H] <sup>+</sup> , Found: 32. <b>3.34</b> $3-ClC_{6}H_4$ $3-MeOCOC_{6}H_4$ CH <sub>3</sub> 90 0.54 170-172 Calcd: 374.0730 [M + H] <sup>+</sup> , Found: 35. <b>3.35</b> $3-ClC_{8}H_4$ $3-MeOCOC_{6}H_4$ CH <sub>3</sub> 70 0.34 170-172 Calcd: 340.1276 [M + H] <sup>+</sup> , Found: 35. <b>3.36</b> $3-ClC_{8}H_4$ $3-HOCOC_{6}H_4$ CH <sub>3</sub> 70 0.34 170-172 Calcd: 340.1119 [M + H] <sup>+</sup> , Found: 35. <b>3.36</b> $3-ClC_{6}H_4$ $3-HOCOC_{6}H_4$ CH <sub>3</sub> 71 0.35 164-166 Calcd: 330.0733 [M + H] <sup>+</sup> , Found: 35. <b>3.39</b> $\alpha$ -naphthyl CoH <sub>4</sub> CH <sub>3</sub> 77 0.56 194-196 Calcd: 330.1378 [M + H] <sup>+</sup> , Found: 35. <b>3.40</b> $4-CH_3CH_2C_{6}H_4$ C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 78 0.50 180-182 Calcd: 330.1378 [M + H] <sup>+</sup> , Found: 31. <b>3.41</b> $4-CH_3SC_{6}H_4$ C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 59 0.48 215-217 Calcd: 328.0942 [M + H] <sup>+</sup> , Found: 32. <b>3.42</b> Calch, CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 59 0.48 215-217 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 32. <b>3.42</b> Calch, CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> 50 0.62 223-225 Calcd: 296.1221 [M + H] <sup>+</sup> , Found: 32. <b>3.42</b> Calch, CH <sub>3</sub> CalcH <sub>4</sub> CalH <sub>4</sub> CH <sub>3</sub> 61 0.83 164-166 Calcd: 318.0959 [M + H] <sup>+</sup> , Found: 32. <b>7.02</b> $3-ClC_{6}H_4$ CalH <sub>4</sub> CalH <sub>4</sub> CH <sub>3</sub> 67 0.76 179-180 Calcd: 318.0565 [M + H] <sup>+</sup> , Found: 24. <b>7.05</b> CalH <sub>4</sub> CalH <sub>4</sub> Ch <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> 67 0.76 176-176 Calcd: 20.1344 [M + H] <sup>+</sup> , Found: 24. <b>7.06</b> Calds 314.0654 [M + H] <sup>+</sup> , Found: 31. <b>7.07</b> $3-ClC_{6}H_4$ CH <sub>3</sub> CH <sub>3</sub> 67 0.76 176-178 Calcd: 220.798 [M + H] <sup>+</sup> , Found: 27. <b>7.18</b> $3-CH_{6}C_{4}H_{4}$ CH <sub>3</sub> CH <sub>3</sub> 67 0.76 176-178 Calcd: 220.1344 [M + H] <sup>+</sup> , Found: 27. <b>7.18</b> $3-CH_{6}C_{4}H_{4}$ CH <sub>3</sub> CH <sub>3</sub> 67 0.76 176-178 Calcd: 278.1657 [M + H] <sup>+</sup> , Found: 27. <b>7.19</b> $3-ClC_{6}H_4$ CH <sub>3</sub> CH <sub>3</sub> 67 0.76	3.28	$3-CIC_6H_4$	СООН	CH <sub>3</sub>	52	0.30	166 - 168	Calcd: $284.0261 [M + H]^+$ . Found: $284.0261$
<b>3.30 3</b> -CH <sub>3</sub> <b>5</b> -CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>82</b> 0.53 240–242 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.31 3</b> -CH <sub>3</sub> <b>5</b> -CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>84</b> 0.53 184–186 Calcd: 312.1171 [M + H] <sup>+</sup> , Found: 31 <b>3.32 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>88</b> 0.53 168–170 Calcd: 312.1171 [M + H] <sup>+</sup> , Found: 31 <b>3.33 3</b> -MeC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>88</b> 0.53 168–170 Calcd: 312.1171 [M + H] <sup>+</sup> , Found: 32 <b>3.34 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>90</b> 0.54 170–172 Calcd: 374.0730 [M + H] <sup>+</sup> , Found: 37 <b>3.35 3</b> -CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>90</b> 0.54 170–172 Calcd: 340.1179 [M + H] <sup>+</sup> , Found: 37 <b>3.36 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>70</b> 0.34 170–172 Calcd: 340.1179 [M + H] <sup>+</sup> , Found: 34 <b>3.38 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -MOCOC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>71</b> 0.33 166–168 Calcd: 359.0733 [M + H] <sup>+</sup> , Found: 33 <b>3.40 4</b> -CH <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>77</b> 0.56 194–196 Calcd: 359.0733 [M + H] <sup>+</sup> , Found: 31 <b>3.41 4</b> -CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>58</b> 0.50 180–182 Calcd: 310.11378 [M + H] <sup>+</sup> , Found: 31 <b>3.41 4</b> -CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>58</b> 0.50 180–182 Calcd: 310.1378 [M + H] <sup>+</sup> , Found: 31 <b>3.41 4</b> -CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>58</b> 0.50 180–182 Calcd: 310.01378 [M + H] <sup>+</sup> , Found: 31 <b>3.42 4</b> -CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>58</b> 0.62 223–227 Calcd: 328.0494 [M + H] <sup>+</sup> , Found: 29 <b>7.01 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>66</b> 0.83 168–170 Calcd: 348.0454 [M + H] <sup>+</sup> , Found: 31 <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> <b>C</b> H <sub>3</sub> <b>52</b> 0.85 168–166 Calcd: 362.0059 [M + H] <sup>+</sup> , Found: 31 <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>6</b> -H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>66</b> 0.84 165–167 Calcd: 248.0954 [M + H] <sup>+</sup> , Found: 31 <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>67</b> 0.76 176–178 Calcd: 248.0954 [M + H] <sup>+</sup> , Found: 28 <b>7.05 C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>67</b> 0.76 176–178 Calcd: 248.0594 [M + H] <sup>+</sup> , Found: 27 <b>7.16 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>67</b> 0.76 176–178 Calcd: 248.0594 [M + H] <sup>+</sup> , Found: 27 <b>7.16 7.16 7.16 1.6</b> +H <sub>4</sub> <b>1.6</b> +H <sub>5</sub> <b>C</b> H <sub>3</sub> <b>67</b> 0.76 176–178 Calcd: 248.150 [M +	3.29	3-CIC <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub>	CH <sub>3</sub> OCO	75	0.45	160 - 162	Calcd: 298.0417 $[M + H]^+$ . Found: 298.0410
<b>3.31 3</b> -CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>80</b> 0.53 <b>184</b> -186 Calcd: <b>312</b> .1171 [M + H] <sup>+</sup> , Found: <b>34</b> <b>3.32 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>84</b> 0.53 <b>168</b> -170 Calcd: <b>311</b> .0128 [M + H] <sup>+</sup> , Found: <b>34</b> <b>3.33 3</b> -MeC <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>90</b> 0.54 <b>170</b> -172 Calcd: <b>374</b> .0730 [M + H] <sup>+</sup> , Found: <b>37</b> <b>3.34 3</b> -ClC <sub>8</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>90</b> 0.52 <b>164</b> -166 Calcd: <b>354</b> .1276 [M + H] <sup>+</sup> , Found: <b>37</b> <b>3.35 3</b> -ClC <sub>8</sub> H <sub>4</sub> <b>3</b> -MeOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>70</b> 0.34 <b>170</b> -172 Calcd: <b>374</b> .0730 [M + H] <sup>+</sup> , Found: <b>35</b> <b>3.36 3</b> -ClC <sub>8</sub> H <sub>4</sub> <b>3</b> -HOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>70</b> 0.34 <b>170</b> -172 Calcd: <b>360</b> .0573 [M + H] <sup>+</sup> , Found: <b>36</b> <b>3.37 3</b> -CH <sub>2</sub> C <sub>8</sub> H <sub>4</sub> <b>3</b> -HOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>71</b> 0.56 <b>194</b> -196 Calcd: <b>330</b> .1119 [M + H] <sup>+</sup> , Found: <b>38</b> <b>3.40</b> 4-CH <sub>3</sub> ClC <sub>8</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>47</b> 0.56 <b>194</b> -196 Calcd: <b>332</b> .1143 [M + H] <sup>+</sup> , Found: <b>33</b> <b>3.40</b> 4-CH <sub>3</sub> ClC <sub>6</sub> CH <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>58</b> 0.50 <b>180</b> -182 Calcd: <b>310</b> .1378 [M + H] <sup>+</sup> , Found: <b>33</b> <b>3.40</b> 4-CH <sub>3</sub> ClC <sub>6</sub> CH <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>58</b> 0.62 <b>233</b> -225 Calcd: <b>296</b> .1221 [M + H] <sup>+</sup> , Found: <b>32</b> <b>3.428</b> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>5</sub> CH <sub>3</sub> <b>88</b> 0.82 216-218 Calcd: <b>284</b> .0945 [M + H] <sup>+</sup> , Found: <b>29</b> <b>7.01 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 52 0.85 <b>164</b> -166 Calcd: <b>318</b> .0565 [M + H] <sup>+</sup> , Found: <b>29</b> <b>7.02 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 66 0.83 <b>168</b> -170 Calcd: <b>284</b> .0945 [M + H] <sup>+</sup> , Found: <b>29</b> <b>7.03 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86</b> 0.84 <b>165</b> -167 Calcd: <b>284</b> .0945 [M + H] <sup>+</sup> , Found: <b>20</b> <b>7.06</b> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>86</b> 0.48 <b>165</b> -167 Calcd: <b>281</b> .0504 [M + H] <sup>+</sup> , Found: <b>22</b> <b>7.06 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86</b> 0.78 <b>144</b> -146 Calcd: <b>222</b> .0798 [M + H] <sup>+</sup> , Found: <b>22</b> <b>7.08 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86</b> 0.78 <b>144</b> -146 Calcd: <b>222</b> .0798 [M + H] <sup>+</sup> , Found: <b>22</b> <b>7.13 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>76 77 76 77 166</b> -178 Calcd: <b>281</b> .1557 [M + H] <sup>+</sup> , Found: <b>22</b> <b>7.14 3</b> -ClC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>76 7 77 166</b> -178 Calcd: <b>281</b> .1557 [M + H] <sup>+</sup> , Found: <b>27</b> <b>7.15 3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86</b> 0.78 <b>144</b> -146 Calcd: <b>222</b> .0798 [M + H] <sup>+</sup> , Found:	3.30	$3-CH_3-5-CH_3C_6H_3$	$C_6H_5$	$CH_3$	82	0.53	240 - 242	Calcd: $310.1378 [M + H]^+$ . Found: $310.1394$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3.31	$3-CH_3OC_6H_4$	$C_6H_5$	$CH_3$	80	0.53	184 - 186	Calcd: $312.1171 [M + H]^+$ . Found: $312.1188$
<b>3.33</b> $3 - MeC_{6}H_{4}$ $3 - CNC_{6}H_{4}$ $CH_{3}$ <b>88</b> $0.53$ $160 - 162$ Calcd: $321.1174$ $[M + H]^+$ , Found: $37$ <b>3.34</b> $3 - CIC_{6}H_{4}$ $3 - MeCOCO_{6}H_{4}$ $CH_{3}$ <b>90</b> $0.54$ $170 - 172$ Calcd: $374.0730$ $[M + H]^+$ , Found: $37$ <b>3.35</b> $3 - CH_{3}C_{6}H_{4}$ $3 - MeCOCO_{6}H_{4}$ $CH_{3}$ <b>90</b> $0.52$ $164 - 166$ Calcd: $354.1276$ $[M + H]^+$ , Found: $36$ <b>3.36</b> $3 - CH_{2}C_{6}H_{4}$ $3 - MeCOCO_{6}H_{4}$ $CH_{3}$ <b>70</b> $0.34$ $170 - 172$ Calcd: $360.0573$ $[M + H]^+$ , Found: $36$ <b>3.37</b> $3 - CH_{2}C_{6}H_{4}$ $3 - NH_{2}COC_{6}H_{4}$ $CH_{3}$ <b>71</b> $0.35$ $164 - 166$ Calcd: $359.0733$ $[M + H]^+$ , Found: $31$ <b>3.39</b> $0 - naphthyl$ $C_{6}H_{5}$ $CH_{3}$ <b>47</b> $0.56$ $194 - 196$ Calcd: $352.0733$ $[M + H]^+$ , Found: $31$ <b>3.40</b> $4 - CH_{3}CH_{2}C_{6}H_{4}$ $C_{6}H_{5}$ $CH_{3}$ <b>58</b> $0.50$ $180 - 182$ Calcd: $310.178$ $[M + H]^+$ , Found: $31$ <b>3.40</b> $4 - CH_{3}CH_{2}C_{6}H_{4}$ $C_{6}H_{5}$ $CH_{3}$ <b>58</b> $0.48$ $215 - 217$ Calcd: $328.0942$ $[M + H]^+$ , Found: $31$ <b>3.42</b> $4 - CH_{3}CH_{2}C_{6}H_{4}$ $C_{6}H_{5}$ $CH_{3}$ <b>56</b> $0.62$ $223 - 225$ Calcd: $296.1221$ $[M + H]^+$ , Found: $32$ <b>3.42</b> $3 - CIC_{6}H_{4}$ $C_{6}H_{5}$ $CH_{3}$ <b>56</b> $0.68$ $216 - 218$ Calcd: $318.0945$ $[M + H]^+$ , Found: $28$ <b>7.02</b> $3 - CIC_{6}H_{4}$ $3 - BrC_{6}H_{4}$ $CH_{3}$ <b>52</b> $0.85$ $164 - 166$ Calcd: $362.0059$ $[M + H]^+$ , Found: $28$ <b>7.03</b> $3 - CIC_{6}H_{4}$ $3 - BrC_{6}H_{4}$ $CH_{3}$ <b>52</b> $0.85$ $164 - 166$ Calcd: $280.1954$ $[M + H]^+$ , Found: $24$ <b>7.04</b> $3 - CIC_{6}H_{4}$ $-(CH_{2})_{4} - 76$ $0.76$ $179 - 180$ Calcd: $248.0954$ $[M + H]^+$ , Found: $24$ <b>7.05</b> $C_{6}H_{5}$ $CH_{3}$ $CH_{3}$ <b>86</b> $0.78$ $144 - 146$ Calcd: $220.1344$ $[M + H]^+$ , Found: $27$ <b>7.06</b> $3 - CIC_{6}H_{4}$ $CH_{3}$ $CH_{3}$ <b>86</b> $0.78$ $144 - 146$ Calcd: $220.1344$ $[M + H]^+$ , Found: $27$ <b>7.06</b> $3 - CIC_{6}H_{4}$ $CH_{3}$ $CH_{3}$ <b>86</b> $0.78$ $144 - 146$ Calcd: $220.1344$ $[M + H]^+$ , Found: $27$ <b>7.16</b> $3 - CIC_{6}H_{4}$ $CH_{3}$ $CH_{3}$ <b>77</b> $0.68$ $138 - 138 - 140$ Calcd: $278.1657$ $[M + H]^+$ , Found: $27$ <b>7.13</b> $3 - CIC_{6$	3.32	$3-ClC_6H_4$	$3-CNC_6H_4$	$CH_3$	84	0.53	168 - 170	Calcd: $341.0628 [M + H]^+$ . Found: $341.0675$
<b>3.34</b> $3-\text{ClC}_{6}\text{H}_4$ $3-\text{Me}\text{COC}_{6}\text{H}_4$ $\text{CH}_3$ <b>90 0.54 170-172 Calcd: 374.0730</b> [M + H] <sup>+</sup> , Found: <b>37 3.35 3</b> -CH}_3C_6H_4 <b>3</b> -Me $\text{COC}_6H_4$ CH}_3 <b>70 0.34 170-172 Calcd: 354.1276</b> [M + H] <sup>+</sup> , Found: <b>36 3.37 3</b> -CH}_3C_6H_4 <b>3</b> -HOCCC}_6H_4 CH}_3 <b>70 0.34 170-172 Calcd: 360.0573</b> [M + H] <sup>+</sup> , Found: <b>36 3.37 3</b> -CH}_6C_H_4 <b>3</b> -HOCCC}_6H_4 CH}_3 <b>71 0.35 164-166 Calcd: 350.0733</b> [M + H] <sup>+</sup> , Found: <b>37 3.340 4</b> -CH}_3C_6H_4 <b>C</b> _6H_5 CH}_3 <b>47 0.56 194-196 Calcd: 350.0733</b> [M + H] <sup>+</sup> , Found: <b>33 3.40 4</b> -CH}_3C_6H_4 C_6H_5 CH}_3 <b>59 0.48 215-217 Calcd: 320.01378</b> [M + H] <sup>+</sup> , Found: <b>31 3.40 4</b> -CH}_3C_6H_4 C_6H_5 CH}_3 <b>59 0.48 215-217 Calcd: 328.0942</b> [M + H] <sup>+</sup> , Found: <b>31 3.42 6</b> -Ch}_3C_6H_4 C_6H_5 CH}_3 <b>56 0.62 223-225 Calcd: 296.1221</b> [M + H] <sup>+</sup> , Found: <b>29 7.01 3</b> -CIC}_6H_4 C_6H_5 CH}_3 <b>56 0.62 223-225 Calcd: 296.1221</b> [M + H] <sup>+</sup> , Found: <b>29 7.01 3</b> -CIC}_6H_4 <b>C</b> _6H_5 CH}_3 <b>60 0.83 164-166</b> Calcd: <b>322.095</b> [M + H] <sup>+</sup> , Found: <b>29 7.01 3</b> -CIC}_6H_4 <b>3</b> -CIC}_6H_4 CH}_3 <b>66 0.83 168-170</b> Calcd: <b>310.1378</b> [M + H] <sup>+</sup> , Found: <b>31 7.04 3</b> -CIC}_6H_4 <b>3</b> -CIC}_6H_4 CH}_3 <b>66 0.83 164-166</b> Calcd: <b>322.0059</b> [M + H] <sup>+</sup> , Found: <b>24 7.05</b> C6H_5 CH}_4 <b>CH</b> _3 <b>CH</b> _3 <b>67 0.76 179-180</b> Calcd: <b>284.0945</b> [M + H] <sup>+</sup> , Found: <b>21 7.06 C</b> _6H_5 CH}_3 <b>CH</b> _3 <b>CH</b> _3 <b>CH</b> _3 <b>CH</b> _4 <b>CH</b> _4 <b>CH</b> _3 <b>CH</b> _3 <b>86 0.77 146-148</b> Calcd: <b>220.1344</b> [M + H] <sup>+</sup> , Found: <b>22 7.06 C</b> _6H_4 CH}_3 <b>CH</b> _3 <b>86 0.77 146-148</b> Calcd: <b>220.1344</b> [M + H] <sup>+</sup> , Found: <b>22 7.06 C</b> _6H_4 <b>C</b> _6H_5 <b>CH</b> _3 <b>79 0.76 179-180</b> Calcd: <b>220.1344</b> [M + H] <sup>+</sup> , Found: <b>22 7.08 3</b> -CH}_3C_6H_4 <b>CH</b> _3 <b>CH</b> _3 <b>79 0.76 179-180</b> Calcd: <b>220.1344</b> [M + H] <sup>+</sup> , Found: <b>22 7.06 C</b> _6H_4 <b>C</b> _6H_5 <b>CH</b> _3 <b>79 0.76 179-180</b> Calcd: <b>220.1344</b> [M + H] <sup>+</sup> , Found: <b>22 7.06 C</b> _6H_4 <b>C</b> _6H_5 <b>CH</b> _3 <b>79 0.76 179-180</b> Calcd: <b>228.1657</b> [M + H] <sup>+</sup> , Found: <b>27 7.16 3</b> -CH}_3C_6H_4 <b>C</b> _6H_5 <b>CH</b> _3 <b></b>	3.33	$3-MeC_6H_4$	$3-CNC_6H_4$	$CH_3$	88	0.53	160 - 162	Calcd: $321.1174 [M + H]^+$ . Found: $321.1152$
<b>3.35</b> $3-CH_3C_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ $R_1$ $CH_3$ $R_1$ $R_2$ $R_1$	3.34	$3-ClC_6H_4$	3-MeOCOC <sub>6</sub> H <sub>4</sub>	$CH_3$	90	0.54	170 - 172	Calcd: 374.0730 [M + H] <sup>+</sup> . Found: 374.0757
<b>3.36</b> $3-\text{Cl}_{G}\text{H}_4$ <b>3</b> -HOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>70 0</b> .34 <b>170-172</b> Calcd: 360.0573 [M + H] <sup>+</sup> . Found: 36 <b>3.37 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -HOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>61 0</b> .33 <b>166-168</b> Calcd: 340.1119 [M + H] <sup>+</sup> . Found: 35 <b>3.39 c</b> -naphthyl C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>71 0</b> .56 <b>194-196</b> Calcd: 350.0733 [M + H] <sup>+</sup> . Found: 33 <b>3.40 4</b> -CH <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>58 0</b> .50 <b>180-182</b> Calcd: 332.1143 [M + H] <sup>+</sup> . Found: 31 <b>3.41 4</b> -CH <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>59 0</b> .48 <b>215-217</b> Calcd: 328.0942 [M + H] <sup>+</sup> . Found: 32 <b>3.42</b> <sup>8</sup> C <sub>6</sub> H <sub>5</sub> , CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>56 0</b> .62 <b>223-225</b> Calcd: 296.1221 [M + H] <sup>+</sup> . Found: 29 <b>7.01 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>C</b> <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>56 0</b> .62 <b>223-225</b> Calcd: 280.092 [M + H] <sup>+</sup> . Found: 32 <b>3.42</b> <sup>8</sup> C <sub>6</sub> H <sub>5</sub> , CH <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>52 0</b> .85 <b>164-166</b> Calcd: 320.059 [M + H] <sup>+</sup> . Found: 31 <b>7.02 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>52 0</b> .85 <b>164-166</b> Calcd: 320.059 [M + H] <sup>+</sup> . Found: 31 <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -BrC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>52 0</b> .85 <b>164-166</b> Calcd: 340.045 [M + H] <sup>+</sup> . Found: 31 <b>7.04 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>66 0</b> .83 <b>168-170</b> Calcd: <b>248.0954</b> [M + H] <sup>+</sup> . Found: 25 <b>7.06</b> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86 0</b> .76 <b>179-180</b> Calcd: <b>248.0954</b> [M + H] <sup>+</sup> . Found: 22 <b>7.06</b> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86 0</b> .78 <b>144-146</b> Calcd: 320.1344 [M + H] <sup>+</sup> . Found: 22 <b>7.08 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> <b>86 0</b> .78 <b>144-146</b> Calcd: 220.1344 [M + H] <sup>+</sup> . Found: 20 <b>7.09 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-155</b> Calcd: 220.1344 [M + H] <sup>+</sup> . Found: 20 <b>7.10 4</b> -FC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-155</b> Calcd: 268.1250 [M + H] <sup>+</sup> . Found: 26 <b>7.11 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-155</b> Calcd: 268.1250 [M + H] <sup>+</sup> . Found: 27 <b>7.12 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b> -ClC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-155</b> Calcd: 280.1450 [M + H] <sup>+</sup> . Found: 27 <b>7.13 3</b> -CH <sub>3</sub> -G <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-156</b> Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 27 <b>7.14 3</b> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> <b>3</b> -CNC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> <b>79 0</b> .76 <b>153-156</b> Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 28 <b>7.15 3</b> -ClC <sub>6</sub> H <sub>4</sub> <b>3</b>	3.35	$3-CH_3C_6H_4$	$3-MeOCOC_6H_4$	$CH_3$	80	0.52	164 - 166	Calcd: $354.1276 [M + H]^+$ . Found: $354.1305$
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	3.36	$3-CIC_6H_4$	$3-HOCOC_6H_4$	$CH_3$	70	0.34	170 - 172	Calcd: $360.0573 [M + H]^+$ . Found: $360.0608$
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	3.37	$3-CH_3C_6H_4$	$3-HOCOC_6H_4$	$CH_3$	61	0.33	166 - 168	Calcd: 340.1119 [M + H] <sup>+</sup> . Found: 340.1147
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	3.38	$3-CIC_6H_4$	$3-NH_2COC_6H_4$	$CH_3$	73	0.35	164 - 166	Calcd: $359.0733 [M + H]^+$ . Found: $359.0702$
$      \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	3.39	α-naphthyl	$C_6H_5$	$CH_3$	47	0.56	194 - 196	Calcd: $332.1143 [M + H]^+$ . Found: $332.1224$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3.40	$4-CH_3CH_2C_6H_4$	$C_6H_5$	$CH_3$	58	0.50	180 - 182	Calcd: $310.1378 [M + H]^+$ . Found: $310.1361$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3.41	$4-CH_3SC_6H_4$	$C_6H_5$	$CH_3$	59	0.48	215 - 217	Calcd: $328.0942 [M + H]^+$ . Found: $328.0928$
7.01 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ 88 $0.82$ $216-218$ $Calcd: 284.0945$ $[M + H]^+$ . Found: 287.02 $3-ClC_6H_4$ $3-BrC_6H_4$ $CH_3$ $52$ $0.85$ $164-166$ $Calcd: 362.0059$ $[M + H]^+$ . Found: 317.03 $3-ClC_6H_4$ $3-ClC_6H_4$ $CH_3$ $66$ $0.83$ $168-170$ $Calcd: 248.0954$ $[M + H]^+$ . Found: 31:7.04 $3-ClC_6H_4$ $-(CH_2)_4 76$ $0.76$ $179-180$ $Calcd: 248.0954$ $[M + H]^+$ . Found: 247.05 $C_6H_5$ $C_6H_5$ $CH_3$ $86$ $0.84$ $165-167$ $Calcd: 210.1344$ $[M + H]^+$ . Found: 257.06 $C_6H_5$ $CH_3$ $CH_3$ $82$ $0.77$ $146-148$ $Calcd: 222.0798$ $[M + H]^+$ . Found: 267.08 $3-ClC_6H_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ $Calcd: 202.1344$ $[M + H]^+$ . Found: 267.10 $4-FC_6H_4$ $CH_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calcd: 264.1500$ $[M + H]^+$ . Found: 267.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.11 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.12 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.13 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ <	3.42 <sup>8</sup>	$C_6H_{5,}CH_3$	$C_6H_5$	$CH_3$	56	0.62	223 - 225	Calcd: 296.1221 [M + H] <sup>+</sup> . Found: 296.1205
7.02 $3-\text{ClC}_6\text{H}_4$ $3-\text{BrC}_6\text{H}_4$ $C\text{H}_3$ $52$ $0.85$ $164-166$ Calcd: $362.0059$ $[M + H]^+$ . Found: $36$ 7.03 $3-\text{ClC}_6\text{H}_4$ $3-\text{ClC}_6\text{H}_4$ $C\text{H}_3$ $66$ $0.83$ $168-170$ Calcd: $318.0565$ $[M + H]^+$ . Found: $31.70$ 7.04 $3-\text{ClC}_6\text{H}_4$ $-(\text{CH}_2)_4 76$ $0.76$ $179-180$ Calcd: $248.0954$ $[M + H]^+$ . Found: $24.75$ 7.05 $C_6\text{H}_5$ $C\text{H}_3$ $C\text{H}_3$ $67$ $0.76$ $176-178$ Calcd: $250.1344$ $[M + H]^+$ . Found: $25.76$ 7.06 $C_6\text{H}_5$ $C\text{H}_3$ $C\text{H}_3$ $67$ $0.76$ $176-178$ Calcd: $222.0798$ $[M + H]^+$ . Found: $22.708$ $7.07$ $3-\text{ClC}_6\text{H}_4$ $C\text{H}_3$ $C\text{H}_3$ $82$ $0.77$ $146-148$ Calcd: $222.0798$ $[M + H]^+$ . Found: $22.708$ $7.09$ $3-\text{CH}_3\text{C}_6\text{H}_4$ $C\text{H}_3$ $C\text{H}_3$ $86$ $0.78$ $144-146$ Calcd: $202.1344$ $[M + H]^+$ . Found: $20.77$ $7.09$ $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $79$ $0.76$ $153-155$ Calcd: $264.1500$ $[M + H]^+$ . Found: $26.77$ $7.10$ $4-\text{F}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $79$ $0.76$ $153-155$ Calcd: $278.1657$ $[M + H]^+$ . Found: $27.71$ $7.12$ $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $81$ $0.85$ $138-140$ Calcd:	7.01	$3-ClC_6H_4$	$C_6H_5$	$CH_3$	88	0.82	216 - 218	Calcd: 284.0945 [M + H] <sup>+</sup> . Found: 284.0955
7.03 $3-\text{ClC}_6\text{H}_4$ $3-\text{ClC}_6\text{H}_4$ $C\text{H}_3$ $66$ $0.83$ $168-170$ $Calcd:$ $318.0565$ $[M + H]^+$ . Found: $31.704$ 7.04 $3-\text{ClC}_6\text{H}_4$ $-(\text{CH}_2)_4-$ 76 $0.76$ $179-180$ $Calcd:$ $248.0954$ $[M + H]^+$ . Found: $24.704$ 7.05 $C_6\text{H}_5$ $C_6\text{H}_5$ $CH_3$ $86$ $0.84$ $165-167$ $Calcd:$ $250.1344$ $[M + H]^+$ . Found: $24.704$ 7.06 $C_6\text{H}_5$ $CH_3$ $CH_3$ $67$ $0.76$ $176-178$ $Calcd:$ $250.1344$ $[M + H]^+$ . Found: $25.704$ 7.07 $3-\text{Cl}_6\text{H}_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-148$ $Calcd:$ $220.798$ $[M + H]^+$ . Found: $20.709$ 7.08 $3-\text{CH}_3\text{C}_6\text{H}_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ $Calcd:$ $220.798$ $[M + H]^+$ . Found: $20.709$ 7.09 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calcd:$ $20.1344$ $[M + H]^+$ . Found: $20.709$ 7.10 $4-\text{FC}_6\text{H}_4$ $C_6\text{H}_5$ $CH_3$ $79$ $0.76$ $153-155$ $Calcd:$ $268.1250$ $[M + H]^+$ . Found: $27.714$ 7.12 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $27.714$ 7.13 $3-\text{CH}_3-6\text{H}_4$ $C_6\text{H}_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $27.714$ 7.14 $3-CH$	7.02	$3-ClC_6H_4$	3-BrC <sub>6</sub> H <sub>4</sub>	$CH_3$	52	0.85	164 - 166	Calcd: 362.0059 [M + H] <sup>+</sup> . Found: 362.0062
7.04 $3-\text{ClC}_6\text{H}_4$ $-(\text{CH}_2)_4-$ 76 $0.76$ $179-180$ Calcd: $248.0954$ $[\text{M} + \text{H}]^+$ , Found: $24$ 7.05 $C_6\text{H}_5$ $C_6\text{H}_5$ $C\text{H}_3$ $C\text{H}_3$ 86 $0.84$ $165-167$ Calcd: $250.1344$ $[\text{M} + \text{H}]^+$ . Found: $25$ 7.06 $C_6\text{H}_5$ $C\text{H}_3$ $C\text{H}_3$ $67$ $0.76$ $176-178$ Calcd: $250.1344$ $[\text{M} + \text{H}]^+$ . Found: $25$ 7.07 $3-\text{Cl}_6\text{H}_4$ $C\text{H}_3$ $C\text{H}_3$ $82$ $0.77$ $146-148$ Calcd: $222.0798$ $[\text{M} + \text{H}]^+$ . Found: $22$ 7.08 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C\text{H}_3$ $C\text{H}_3$ $86$ $0.78$ $144-146$ Calcd: $202.1344$ $[\text{M} + \text{H}]^+$ . Found: $26$ 7.09 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $75$ $0.84$ $159-160$ Calcd: $264.1500$ $[\text{M} + \text{H}]^+$ . Found: $26$ 7.10 $4-\text{FC}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $79$ $0.76$ $153-155$ Calcd: $268.1250$ $[\text{M} + \text{H}]^+$ . Found: $27$ 7.13 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $81$ $0.85$ $138-140$ Calcd: $278.1657$ $[\text{M} + \text{H}]^+$ . Found: $27$ 7.13 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $66$ $0.86$ $154-156$ Calcd: $280.1450$ $[\text{M} + \text{H}]^+$ . Found: $27$ 7.13 $3-\text{CH}_3\text{C}_6\text{H}_4$ $C_6\text{H}_5$ $C\text{H}_3$ $66$ $0.84$ $156-158$ Calcd: $280.1450$ $[\text{M} + \text{H}]^+$ . Found: $27$ 7.14 $3-\text{CH}_3\text{C}_6\text{H}_4$	7.03	$3-ClC_6H_4$	3-ClC <sub>6</sub> H <sub>4</sub>	$CH_3$	66	0.83	168 - 170	Calcd: 318.0565 $[M + H]^+$ . Found: 318.0616
7.05 $C_6H_5$ $C_6H_5$ $CH_3$ 86 $0.84$ $165-167$ $Calct:$ $250.1344$ $[M + H]^+$ . Found: $250.1344$ 7.06 $C_6H_5$ $CH_3$ $CH_3$ $CH_3$ $67$ $0.76$ $176-178$ $Calct:$ $188.1188$ $[M + H]^+$ . Found: $18$ 7.07 $3-ClC_6H_4$ $CH_3$ $CH_3$ $82$ $0.77$ $146-148$ $Calct:$ $222.0798$ $[M + H]^+$ . Found: $22$ 7.08 $3-CH_3C_6H_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ $Calct:$ $202.1344$ $[M + H]^+$ . Found: $20$ 7.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calct:$ $264.1500$ $[M + H]^+$ . Found: $26$ 7.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ $Calct:$ $268.1250$ $[M + H]^+$ . Found: $27$ 7.11 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calct:$ $278.1657$ $[M + H]^+$ . Found: $27$ 7.12 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $81$ $0.85$ $138-140$ $Calct:$ $278.1657$ $[M + H]^+$ . Found: $27$ 7.13 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calct:$ $278.1657$ $[M + H]^+$ . Found: $27$ 7.14 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calct:$ $280.1450$ $[M + H]^+$ . Found: $28$ 7.15 $3-ClC_6H_4$ <	7.04	$3-ClC_6H_4$	$-(CH_2)$	4	76	0.76	179 - 180	Calcd: 248.0954 $[M + H]^+$ . Found: 248.0953
7.06 $C_6H_5$ $CH_3$ $CH_3$ $CH_3$ $67$ $0.76$ $176-178$ Calcd: 188.1188 [M + H] <sup>+</sup> . Found: 187.07 $3-ClC_6H_4$ $CH_3$ $CH_3$ $82$ $0.77$ $146-148$ Calcd: 222.0798 [M + H] <sup>+</sup> . Found: 227.08 $3-CH_3C_6H_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ Calcd: 202.1344 [M + H] <sup>+</sup> . Found: 207.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $75$ $0.84$ $159-160$ Calcd: 264.1500 [M + H] <sup>+</sup> . Found: 267.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ Calcd: 268.1250 [M + H] <sup>+</sup> . Found: 267.11 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 277.12 $3-ClC_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 277.13 $3-CH_3C_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 277.14 $3-CH_3OC_6H_4$ $CH_3$ $CH_3$ $68$ $0.84$ $156-158$ Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 277.14 $3-CH_3OC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 277.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ Calcd: 280.1450 [M + H] <sup>+</sup> . Found: 287.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ Calcd: 280.1450 [M + H] <sup>+</sup> . Found: 32	7.05	$C_6H_5$	$C_6H_5$	$CH_3$	86	0.84	165 - 167	Calcd: 250.1344 $[M + H]^+$ . Found: 250.1322
7.07 $3-ClC_6H_4$ $CH_3$ $CH_3$ $82$ $0.77$ $146-148$ $Calcd:$ $222.0798$ $[M + H]^+$ . Found: $22$ 7.08 $3-CH_3C_6H_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ $Calcd:$ $202.1344$ $[M + H]^+$ . Found: $20$ 7.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calcd:$ $202.1344$ $[M + H]^+$ . Found: $20$ 7.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calcd:$ $202.1344$ $[M + H]^+$ . Found: $26$ 7.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ $Calcd:$ $268.1250$ $[M + H]^+$ . Found: $26$ 7.11 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $27.7$ 7.12 $3-ClC_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $27.7$ 7.13 $3-CH_3-C_6H_3$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $27.7$ 7.15 $3-ClC_6H_4$ $G_6H_5$ $CH_3$ $68$ $0.84$ $140-142$ $Calcd:$ $280.1450$ $[M + H]^+$ . Found: $28.7$ 7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd:$ $289.1453$ $[M + H]^+$ . Found: $28.7$ 7.16 $3-MeC_6H_4$	7.06	$C_6H_5$	$CH_3$	$CH_3$	67	0.76	176 - 178	Calcd: 188.1188 [M + H] <sup>+</sup> . Found: 188.1153
7.08 $3-CH_3C_6H_4$ $CH_3$ $CH_3$ $86$ $0.78$ $144-146$ $Calcd: 202.1344$ $[M + H]^+$ . Found: 207.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $75$ $0.84$ $159-160$ $Calcd: 264.1500$ $[M + H]^+$ . Found: 267.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ $79$ $0.76$ $153-155$ $Calcd: 268.1250$ $[M + H]^+$ . Found: 267.11 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.12 $3-ClC_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.13 $3-CH_3-G_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.13 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 277.14 $3-ClC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd: 280.1450$ $[M + H]^+$ . Found: 287.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ $Calcd: 280.1450$ $[M + H]^+$ . Found: 287.17 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 289.1453$ $[M + H]^+$ . Found: 287.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd: 327.1013$ $[M + H]^+$ . Found: 327.18 $3-MeC_6H_4$ $3-MeCCC_6$	7.07	$3-ClC_6H_4$	$CH_3$	$CH_3$	82	0.77	146 - 148	Calcd: 222.0798 [M + H] <sup>+</sup> . Found: 222.0793.
7.09 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ 75 $0.84$ $159-160$ $Calcd:$ $264.1500$ $[M + H]^+$ . Found: $266.7.10$ 7.10 $4-FC_6H_4$ $C_6H_5$ $CH_3$ 79 $0.76$ $153-155$ $Calcd:$ $268.1250$ $[M + H]^+$ . Found: $266.7.11$ $3-CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $276.7.13$ $3-CH_3C_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $276.7.13$ $3-CH_3-5-CH_3C_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $276.7.14$ $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd:$ $278.1657$ $[M + H]^+$ . Found: $276.7.14$ $3-CH_3C_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd:$ $280.1450$ $[M + H]^+$ . Found: $287.7.15$ $7.16$ $3-CN_6H_4$ $3-CN_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ $Calcd:$ $280.1450$ $[M + H]^+$ . Found: $287.7.16$ $7.17$ $3-ClC_6H_4$ $3-CN_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd:$ $280.1453$ $[M + H]^+$ . Found: $287.7.1013$ $7.18$ $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd:$ $327.1013$ $[M + H]^+$ . Found: $347.7.1013$ $[M + H]^+$ . Found: </th <th>7.08</th> <th><math>3-CH_3C_6H_4</math></th> <th><math>CH_3</math></th> <th><math>CH_3</math></th> <th>86</th> <th>0.78</th> <th>144 - 146</th> <th>Calcd: 202.1344 [M + H]<sup>+</sup>. Found: 202.1356.</th>	7.08	$3-CH_3C_6H_4$	$CH_3$	$CH_3$	86	0.78	144 - 146	Calcd: 202.1344 [M + H] <sup>+</sup> . Found: 202.1356.
7.10 $4 \cdot FC_6H_4$ $C_6H_5$ $CH_3$ 79 $0.76$ $153-155$ $Calcd: 268.1250 [M + H]^+$ . Found: 267.11 $3 \cdot CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calcd: 278.1657 [M + H]^+$ . Found: 277.12 $3 \cdot CL_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd: 278.1657 [M + H]^+$ . Found: 277.13 $3 \cdot CH_3 - 5 \cdot CH_3C_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd: 278.1657 [M + H]^+$ . Found: 277.14 $3 \cdot CH_3OC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd: 278.1657 [M + H]^+$ . Found: 277.14 $3 \cdot CH_3OC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd: 280.1450 [M + H]^+$ . Found: 287.15 $3 \cdot ClC_6H_4$ $3 \cdot CNC_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ $Calcd: 280.1450 [M + H]^+$ . Found: 287.16 $3 \cdot MeC_6H_4$ $3 - CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 280.1453 [M + H]^+$ . Found: 287.17 $3 \cdot ClC_6H_4$ $3 - NH_2COC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 327.1013 [M + H]^+$ . Found: 327.18 $3 \cdot MeC_6H_4$ $3 - MeCOCO_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd: 342.1009 [M + H]^+$ . Found: 347.20 $3 - ClC_6H_4$ $3 - MeOCOC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd: 328.0853 [M + H]^+$ . Found: 32	7.09	$3-CH_3C_6H_4$	$C_6H_5$	$CH_3$	75	0.84	159 - 160	Calcd: 264.1500 [M + H] <sup>+</sup> . Found: 264.1536.
7.11 $3-CH_3C_6H_4$ $C_6H_5$ $CH_3CH_2$ $81$ $0.85$ $158-160$ $Calcd: 278.1657 [M + H]^+$ . Found: 27.7.12 $3-ClC_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd: 278.1657 [M + H]^+$ . Found: 27.7.13 $3-CH_3-5-CH_3C_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd: 278.1657 [M + H]^+$ . Found: 27.7.14 $3-CH_3OC_6H_4$ $C_6H_5$ $CH_3$ $66$ $0.84$ $156-158$ $Calcd: 280.1450 [M + H]^+$ . Found: 28.7.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ $Calcd: 280.1450 [M + H]^+$ . Found: 30.7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 289.1453 [M + H]^+$ . Found: 32.7.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 289.1453 [M + H]^+$ . Found: 32.7.18 $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd: 307.1556 [M + H]^+$ . Found: 34.7.19 $3-ClC_6H_4$ $3-MeCOCC_6H_4$ $CH_3$ $77$ $0.63$ $172-174$ $Calcd: 328.0853 [M + H]^+$ . Found: 34.7.20 $3-ClC_6H_4$ $3-HOCOCC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd: 328.0853 [M + H]^+$ . Found: 32.7.14 $3-ClC_6H_4$ $3-HOCOCC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd: 328.0853 [M + H]^+$ . Found: 32.	7.10	$4-FC_6H_4$	C <sub>6</sub> H <sub>5</sub>	$CH_3$	79	0.76	153 - 155	Calcd: 268.1250 [M + H] <sup>+</sup> . Found: 268.1237
7.12 $3-ClC_6H_4$ $CH_3OCO$ $CH_3$ $81$ $0.85$ $138-140$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 27.7.13 $3-CH_3-5-CH_3C_6H_3$ $C_6H_5$ $CH_3$ $66$ $0.86$ $154-156$ $Calcd: 278.1657$ $[M + H]^+$ . Found: 27.7.14 $3-CH_3OC_6H_4$ $C_6H_5$ $CH_3$ $68$ $0.84$ $156-158$ $Calcd: 280.1450$ $[M + H]^+$ . Found: 28.7.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ $Calcd: 280.1450$ $[M + H]^+$ . Found: 28.7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ $Calcd: 289.1453$ $[M + H]^+$ . Found: 28.7.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd: 327.1013$ $[M + H]^+$ . Found: 32.7.18 $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ $Calcd: 342.1009$ $[M + H]^+$ . Found: 34.7.20 $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd: 328.0853$ $[M + H]^+$ . Found: 32.	7.11	$3-CH_3C_6H_4$	C <sub>6</sub> H <sub>5</sub>	CH <sub>3</sub> CH <sub>2</sub>	81	0.85	158 - 160	Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 278.1641
7.13 $3-CH_3-5-CH_3C_6H_3$ $C_6H_5$ $CH_3$ 66 $0.86$ $154-156$ Calcd: $278.1657$ $(M + H)^+$ . Found: $274.1657$ 7.14 $3-CH_3OC_6H_4$ $C_6H_5$ $CH_3$ 68 $0.84$ $156-158$ Calcd: $280.1450$ $(M + H)^+$ . Found: $284.1450$ 7.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ 75 $0.84$ $140-142$ Calcd: $280.1450$ $(M + H)^+$ . Found: $284.1450$ 7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ 70 $0.84$ $138-140$ Calcd: $289.1453$ $(M + H)^+$ . Found: $284.1450$ 7.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ 84 $0.67$ $228-230$ Calcd: $327.1013$ $(M + H)^+$ . Found: $324.1450$ 7.18 $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ 70 $0.66$ $220-222$ Calcd: $342.1009$ $(M + H)^+$ . Found: $34.1450$ 7.19 $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ 77 $0.63$ $176-178$ Calcd: $328.0853$ $(M + H)^+$ . Found: $32.1450$ 7.20 $3-ClC_6H_4$ $3-HOOCC_6H_4$ $CH_3$ 77 $0.63$ $176-178$ Calcd: $328.0853$ $(M + H)^+$ . Found: $32.1450$	7.12	3-ClC <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub> OCO	$CH_3$	81	0.85	138 - 140	Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 278.1641
7.14 $3-CH_3OC_6H_4$ $C_6H_5$ $CH_3$ 68 $0.84$ $156-158$ Calcd: $280.1450$ $(M + H)^+$ . Found: $280.1450$ 7.15 $3-ClC_6H_4$ $3-CNC_6H_4$ $CH_3$ $75$ $0.84$ $140-142$ Calcd: $309.0907$ $(M + H)^+$ . Found: $300.0907$ 7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ $70$ $0.84$ $138-140$ Calcd: $289.1453$ $(M + H)^+$ . Found: $280.1450$ 7.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $84$ $0.67$ $228-230$ Calcd: $327.1013$ $(M + H)^+$ . Found: $320.0907$ 7.18 $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ $70$ $0.66$ $220-222$ Calcd: $307.1556$ $(M + H)^+$ . Found: $300.0907$ 7.19 $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ $65$ $0.800$ $172-174$ Calcd: $342.1009$ $(M + H)^+$ . Found: $340.090$ 7.20 $3-ClC_6H_4$ $3-HOCOC_6H_4$ $CH_3$ $77$ $0.630.090$ $176-178$ Calcd: $328.0853$ $(M + H)^+$ . Found: $320.090$	7.13	3-CH3-5-CH3C6H3	C <sub>6</sub> H <sub>5</sub>	$CH_3$	66	0.86	154 - 156	Calcd: 278.1657 [M + H] <sup>+</sup> . Found: 278.1636.
7.15 $3-CNC_6H_4$ $CH_3$ 75 $0.84$ $140-142$ $Calcd:$ $30.0907$ $[M + H]^+$ . Found: $30.0907$ 7.16 $3-MeC_6H_4$ $3-CNC_6H_4$ $CH_3$ 70 $0.84$ $138-140$ $Calcd:$ $289.1453$ $[M + H]^+$ . Found: $288.0466666666666666666666666666666666666$	7.14	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub>	$C_6H_5$	$CH_3$	68	0.84	156 - 158	Calcd: 280.1450 [M + H] <sup>+</sup> . Found: 280.1449.
7.16 $3-\text{CNC}_6\text{H}_4$ $C\text{H}_3$ 70 $0.84$ $138-140$ Calcd: $289.1453$ $[\text{M} + \text{H}]^+$ . Found: $28$ 7.17 $3-\text{CIC}_6\text{H}_4$ $3-\text{NH}_2\text{COC}_6\text{H}_4$ $C\text{H}_3$ 84 $0.67$ $228-230$ Calcd: $289.1453$ $[\text{M} + \text{H}]^+$ . Found: $28$ 7.18 $3-\text{MeC}_6\text{H}_4$ $3-\text{NH}_2\text{COC}_6\text{H}_4$ $C\text{H}_3$ 70 $0.66$ $220-222$ Calcd: $307.1556$ $[\text{M} + \text{H}]^+$ . Found: $30$ 7.19 $3-\text{CIC}_6\text{H}_4$ $3-\text{MeOCOC}_6\text{H}_4$ $C\text{H}_3$ 65 $0.80$ $172-174$ Calcd: $342.1009$ $[\text{M} + \text{H}]^+$ . Found: $34$ 7.20 $3-\text{CIC}_6\text{H}_4$ $3-\text{MOCOC}_6\text{H}_4$ $C\text{H}_3$ 77 $0.63$ $176-178$ Calcd: $328.0853$ $[\text{M} + \text{H}]^+$ . Found: $32$	7.15	3-ClC <sub>6</sub> H <sub>4</sub>	3-CNC <sub>6</sub> H₄	CH <sub>3</sub>	75	0.84	140-142	Calcd: 309.0907 [M + H] <sup>+</sup> . Found: 309.0911
7.17 $3-ClC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ 84 $0.67$ $228-230$ Calcd: $327.1013$ $[M + H]^+$ . Found: $32$ 7.18 $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ 70 $0.66$ $220-222$ Calcd: $307.1556$ $[M + H]^+$ . Found: $30$ 7.19 $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ 65 $0.80$ $172-174$ Calcd: $342.1009$ $[M + H]^+$ . Found: $34$ 7.20 $3-ClC_6H_4$ $3-HOCOC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ Calcd: $328.0853$ $[M + H]^+$ . Found: $32$	7.16	3-MeC <sub>6</sub> H <sub>4</sub>	3-CNC <sub>6</sub> H₄	CH <sub>3</sub>	70	0.84	138-140	Calcd: 289.1453 [M + H] <sup>+</sup> . Found: 289.1456
<b>7.18</b> $3-MeC_6H_4$ $3-NH_2COC_6H_4$ $CH_3$ 70 $0.66$ $220-222$ Calcd: $307.1556$ $(M + H)^+$ . Found: $30$ <b>7.19</b> $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ 65 $0.80$ $172-174$ Calcd: $342.1009$ $(M + H)^+$ . Found: $34$ <b>7.20</b> $3-ClC_6H_4$ $3-HOCOC_6H_4$ $CH_3$ 77 $0.63$ $176-178$ Calcd: $328.0853$ $(M + H)^+$ . Found: $32$	7.17	3-ClC <sub>6</sub> H <sub>4</sub>	3-NH2COC6H4	CH <sub>3</sub>	84	0.67	228-230	Calcd: 327.1013 [M + H] <sup>+</sup> . Found: 327.1017
7.19 $3-ClC_6H_4$ $3-MeOCOC_6H_4$ $CH_3$ $65$ $0.80$ $172-174$ $Calcd:$ $342.1009$ $(M + H)^+$ . Found: $34$ 7.20 $3-ClC_6H_4$ $3-HeOCOC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd:$ $342.1009$ $(M + H)^+$ . Found: $34$ 7.20 $3-ClC_6H_4$ $3-HeOCOC_6H_4$ $CH_3$ $77$ $0.63$ $176-178$ $Calcd:$ $328.0853$ $(M + H)^+$ . Found: $32$	7.18	3-MeC <sub>6</sub> H <sub>4</sub>	3-NH <sub>2</sub> COC <sub>6</sub> H <sub>4</sub>	$CH_3$	70	0.66	220-222	Calcd: 307.1556 [M + H] <sup>+</sup> . Found: 307.1544
<b>7.20</b> 3-ClC <sub>6</sub> H <sub>4</sub> 3-HOCOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> 77 0.63 176-178 Calcd: 328.0853 [M + H] <sup>+</sup> . Found: 32.	7.19	3-ClC <sub>6</sub> H <sub>4</sub>	3-MeOCOC <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub>	65	0.80	172 - 174	Calcd: 342.1009 [M + H] <sup>+</sup> . Found: 342.1015
	7.20	3-ClC <sub>6</sub> H <sub>4</sub>	3-HOCOC <sub>6</sub> H₄	$CH_3$	77	0.63	176-178	Calcd: 328.0853 [M + H] <sup>+</sup> . Found: 328.0854
<b>7.21°</b> $C_6H_5$ , $CH_3$ $C_6H_5$ $CH_3$ <b>54 0.82</b> 110-112 Calcd: 264.1501 [M + H] <sup>+</sup> . Found: 26	7.21 <sup>8</sup>	C <sub>6</sub> H <sub>5</sub> , CH <sub>3</sub>	C <sub>6</sub> H <sub>5</sub>	$CH_3$	54	0.82	110-112	Calcd: 264.1501 [M + H] <sup>+</sup> . Found: 264.1517

<sup>*a*</sup> The results of elemental analyses (C, H, N) of all active compounds were within  $\pm 0.4\%$  of the theoretical values. <sup>*b*</sup> Solvent system for *N*-aminoimidazoline-2-thiones **3**: CH<sub>2</sub>Cl<sub>2</sub>/MeOH, 99:1. Solvent system for *N*-aminoimidazoles **7**: CH<sub>2</sub>Cl<sub>2</sub>/MeOH, 9:1.

Table 2. Inhibition of Viral Replication in MT-4 Cells by *N*-Aminoimidazole Derivatives 3 and 7

			IC <sub>50</sub> <sup>a</sup> (µM)			
		HIV-1				
compd	III <sub>B</sub>	NL4.3	NNRTI(res) <sup>b</sup>	HIV-2 ROD	SIV mac251	СС <sub>50</sub> (µМ) <sup>с</sup>
3.01	$6.39 \pm 0.94$	$8.99 \pm 6.14$	$9.72 \pm 4.99$	$8.11\pm0.38$	$8.20 \pm 4.62$	$66.65 \pm 19.00$
3.05	$\textbf{8.54} \pm \textbf{1.06}$	$5.60 \pm 4.81$	$3.00 \pm 1.20$	$10.46\pm6.71$	$1.75\pm0.20$	$43.98 \pm 20.60$
3.07	$5.00 \pm 1.17$	$2.48 \pm 0.91$	$1.86 \pm 1.20$	$3.91\pm0.65$	$1.22\pm0.77$	$30.95 \pm 11.93$
3.39	$5.55 \pm 2.14$	$6.58 \pm 4.80$	$11.89 \pm 5.31$	$5.10 \pm 3.77$	$4.68\pm0.30$	$32.05 \pm 9.17$
7.01	$1.59 \pm 0.32$	$1.90 \pm 0.60$	$1.73 \pm 0.74$	$1.65 \pm 1.55$	$2.15 \pm 0.42$	$17.48 \pm 7.58$
7.02	$0.38 \pm 0.08$ 0.72 ± 0.50	$1.30 \pm 0.77$ 0.62 $\pm$ 0.02	$0.97 \pm 0.14$ 0.28 $\pm$ 0.28	$0.91 \pm 0.19$ 0.72 $\pm$ 0.02	$0.00 \pm 0.23$ 0.21 $\pm$ 0.12	$10.41 \pm 7.94$ 11.04 $\pm$ 0.02
7.03	$0.72 \pm 0.39$ $0.30 \pm 0.55$	$0.03 \pm 0.03$ 3 54 $\pm$ 0.81	$0.30 \pm 0.20$	$0.72 \pm 0.03$	$0.31 \pm 0.13$ 10.31 $\pm$ 3.50	$11.34 \pm 3.33$ 55.58 $\pm$ 18.68
3.13	$9.30 \pm 0.33$ $9.96 \pm 1.61$	$452 \pm 380$	$577 \pm 0.28$	> 44 94	$272 \pm 0.17$	$33.38 \pm 10.08$ $44.94 \pm 14.15$
3.17	$7.29 \pm 1.53$	$11.25 \pm 4.57$	$42.18 \pm 2.39$	>48.26	$7.54 \pm 1.59$	$48.26 \pm 22.49$
3.19	$1.56\pm0.61$	$2.17\pm0.88$	$26.10\pm3.96$	>35.71	$6.50\pm4.60$	$88.25\pm35.71$
3.25	$17.64 \pm 13.02$	$12.80\pm3.39$	$\geq \! 53.55$	> 53.55	> 53.55	$53.55 \pm 28.73$
3.30	$1.03\pm0.58$	$0.87 \pm 0.52$	>194.21	>194.21	>194.21	$194.21 \pm 132.79^{d}$
3.31	$4.78 \pm 1.38$	$9.79 \pm 0.22$	>38.02	>38.02	>38.02	$38.02\pm5.34$
7.05	≥11.67	$20.98 \pm 2.64$	>52.18	>52.18	>52.18	$52.18 \pm 11.52$
7.09	$3.26 \pm 0.91$	$5.20 \pm 0.04$	$3.99 \pm 0.04$	>27.04	$3.08 \pm 0.41$	$27.04 \pm 11.81$
7.15	$6.96 \pm 2.00$	$8.91 \pm 3.01$	$22.57 \pm 5.05$	>36.79	$7.22 \pm 0.027$	$36.79 \pm 5.15$
3.U2 3.02	>101.81	$23.27 \pm 8.49$	>101.81	>101.81	$^{-101.01}$ 7 71 $\pm$ 3 88	$101.81 \pm 32.84$ $40.80 \pm 13.00$
3.08	> 38 69	> 38 69	>38.69	>38.69	$10.12 \pm 3.66$	$40.80 \pm 13.90$ 38.69 + 13.01
3.13	>44.29	$10.85 \pm 0.82$	>44.29	>44.29	$10.12 \pm 11.00$ $10.88 \pm 8.45$	$44.29 \pm 14.34$
3.18	>108.23	$18.44 \pm 9.39$	$\geq 43.42$	>108.23	$33.80 \pm 20.36$	$108.23 \pm 71.38$
3.23	>42.63	$\geq 42.63$	>42.63	>42.63	>42.63	$42.63 \pm 16.79$
3.24	$9.06 \pm 1.55$	>38.96	>38.96	>38.96	$3.88 \pm 3.27$	$38.96 \pm 15.86$
3.32	$\geq \! 99.40$	$41.96 \pm 2.08$	>99.40	>99.40	>99.40	$99.40 \pm 42.13$
7.13	>20.44	$10.99 \pm 2.85$	>20.44	>20.44	>20.44	$20.44 \pm 9.55$
3.03	>220.13	>220.13	ND	>220.13	>220.13	$220.13 \pm 60.29$
3.04	>134.41	>134.41	ND ND	>134.41	>134.41	$134.41 \pm 33.82$
3.00 3.10	>33.24 >40.06	~ 33.24 >40.06	ND	> 10.06	>33.24 >40.06	$33.24 \pm 14.31$ $40.06 \pm 27.07$
3.10	> 126 42	> 126 42	ND	> 126 42	> 126 42	$43.30 \pm 27.07$ 126 42 + 40 14
3.12	>191.27	>191.27	ND	>191.27	>191.27	$191.27 \pm 72.25$
3.16	>147.12	>147.12	ND	>147.12	>147.12	$147.12 \pm 78.80$
3.20	>259.42	>259.42	ND	>259.42	>259.42	$259.42\pm25.69$
3.21	>180.79	>180.79	ND	>180.79	>180.79	$180.79\pm29.78$
3.22	>359.86	>359.86	ND	>359.86	>359.86	$359.86 \pm 77.44$
3.26	> 36.31	>36.31	>36.31	> 36.31	>36.31	$36.31 \pm 14.87$
3.27	> 190.31	> 190.31	ND	> 190.31	> 190.31	$190.31 \pm 41.98$
3.28 2.90	~203.30	~ 203.30	ND	~203.30	~203.30	$203.30 \pm 41.94$
3.23	>45.63	>45.60	ND	>45.63	>45.63	$46.60 \pm 26.14$ 45.63 + 36.45
3.34	>67.36	>67.36	ND	>67.36	>67.36	$67.36 \pm 59.70$
3.36	>120.03	>120.03	ND	>120.03	>120.03	$120.03 \pm 40.10$
3.37	>187.13	>187.13	ND	>187.13	>187.13	$187.13\pm45.74$
3.38	>42.16	>42.16	ND	>42.16	>42.16	$42.16\pm12.49$
3.40	>34.45	>34.45	ND	>34.45	>34.45	$34.45 \pm 2.37$
3.41	> 53.04	>53.04	ND	> 53.04	>53.04	$53.04 \pm 14.87$
7.04	>67.29	>67.29	>67.29	>67.29	>67.29	$67.29 \pm 16.95$
7.00	>913.68	>213 68	ND	>913.68	>913 68	$331.42 \pm 33.09$ 213.68 + 55.17
7.08	>312 12	>312.12	ND	>312 12	> 312 12	312 12 + 29 36
7.10	> 30.82	> 30.82	ND	> 30.82	> 30.82	$30.82 \pm 9.39$
7.11	>27.87	>27.87	ND	>27.87	>27.87	$27.87 \pm 13.45$
7.12	>106.70	>106.70	ND	>106.70	>106.70	$106.70\pm70.83$
7.14	>34.44	>34.44	ND	>34.44	>34.44	$34.44 \pm 10.81$
7.16	>44.70	>44.70	ND	>44.70	>44.70	$44.70\pm9.68$
7.17	>260.50	>260.50	ND	>260.50	>260.50	$260.50\pm62.76$
7.18	>162.31	>162.31	ND ND	>162.31	>162.31	$162.31 \pm 56.76$
7.19 7.90	≥33.13 >160.57	> 33.15 > 160 57	ND ND	>33.15 >160.57	> 33.15 > 160 57	$33.13 \pm 3.83$ 160 57 $\pm$ 91 14
8.01	> 42.11	>42.11	ND	>42.11	> 42 11	42.11 + 17.19
8.02	> 39.66	>39.66	ND	>39.66	>39.66	$39.66 \pm 17.29$
R89439 (α-APA)	0.014	0.006	>10	>10	>10	>10

 $^a$  50% inhibitory concentration, or concentration required to inhibit the viral cytopathic effect by 50% in MT-4 cells. Data represent average values  $\pm$  SD for at least two independent experiments.  $^b$  S0561945.  $^c$  50% cytotoxic concentration, or concentration that reduced the MT-4 cell viability by 50%.  $^d$  Crystals observed at 16.15  $\mu$ M.

abolishment of the antiviral activity (8.01, 8.02 vs 3.01, 3.19). Comparison of the antiviral activity of a series of compounds bearing methyl, ethyl, propyl, or phenyl at position 4 of the imidazole moiety revealed that the

smaller the substituent, the more pronounced was the antiviral activity. The nature of the different substituents at position 5 of the imidazole ring suggested the need of an aromatic group with certain limitations to

**Table 3.** Inhibitory effects of *N*-Aminoimidazoles **3** and **7** on MSV-Induced Transformation of C3H/3T3 Embryo Murine Fibroblast in Vitro

compd	IC <sub>50</sub> <sup>a</sup> (µM)	MIC <sup>b</sup> (µM)
3.01	$38.0\pm14.2$	>63.3 (316.6)
3.02	>12.7	≥12.7
3.05	>10.1	>10.1 (50.7)
3.07	>11.4	>11.4 (57.1)
3.13	>64.6	>64.6 (323.2)
3.19	>67.7	>67.7 (338.5)
3.24	>12.13	>12.13 (60.63)
3.39	>12.07	>12.07 (60.35)
7.01	$6.9\pm3.8$	>14.1 (70.5)
7.02	$6.89 \pm 1.10$	>11.03 (55.15)
7.03	$5.37 \pm 1.04$	≥12.6
7.09	$13.37\pm2.05$	>15.2 (75.95)

<sup>a</sup> 50% effective dose. <sup>b</sup> Minimal inhibitory concentration.

**Chart 4.** General Structural Requirements of the *N*-Aminoimidazole Derivatives **3** and **7** 



its substitution pattern. Chloro or bromo being well accepted in the meta position, the same halogens introduced at the para position reduced the antiviral properties of the molecules.

The nature of the substitutions on the anilino substitutent at position 1 of the imidazole has serious repercussions on the antiviral activity of the N-aminoimidazoles and 2-thiones (NAIMs) 3 and 7. Not only do these substitutions influence the potency, more importantly they do influence the activity spectrum of the molecules. The most active molecules were found among meta-substituted anilino derivatives. The active molecules bearing a chlorine at position 3 of the anilino phenyl ring had a broader activity spectrum [HIV-1 (strains III<sub>B</sub> and NL4.3), HIV-1 (NNRTI-resistant strain with mutations K103N, Y181C in the RT), HIV-2(ROD), SIV(mac251), and MSV(Moloney)]. The activity of these molecules is mainly due to a yet unidentified mode of action taking place immediately after the integration is finished. Replacement of the *m*-chloro on the aniline moiety by a methyl increases the NNRTI action of the molecules (see 3.01 vs 3.19).

Time of Intervention. A time of addition (TOA) experiment was carried out to investigate which step of the replicative cycle was inhibited by different Naminoimidazoles 3 and 7. Briefly, this experiment determines how long the addition of an anti-HIV compound can be postponed before losing its antiviral activity in the viral replication cycle. Virus was added at a high multiplicity of infection (moi = 0.5) to synchronize all steps of the viral replication. Reference compounds with a known mode of action were included. Dextran sulfate, a polyanion, is known to interfere with the binding of the virus to the cell. The nucleoside analogue AZT inhibits the reverse transcription process. L-708,906 is an established inhibitor of the strand transfer step of the integration process.<sup>10</sup> Ritonavir is an inhibitor of the proteolytic cleavage.



**Figure 1.** Time of addition experiment. MT-4 cells were infected with HIV-1(IIIB) at a multiplicity of infection of 0.5, and the test compounds were added at different times post-infection. Viral p24 Ag production was determined at 31 h postinfection and is expressed as the log 10 of the p24 Ag content in pg/mL. Symbols: ( $\diamond$ ) control; ( $\blacksquare$ ) dextran sulfate; ( $\blacktriangle$ ) AZT; ( $\blacklozenge$ ) L-708,906; (\*), 7.03; ( $\square$ ) ritonavir.

Addition of these compounds can be delayed for 0, 4, 7, and 18–19 h (Figure 1). Addition of **3.19** or **7.03** can be postponed for up to 7 h postinfection, suggesting a possible interaction at the moment of integration. These results should be interpreted with care, not excluding the possibility of an interaction with earlier processes in the HIV replication cycle because TOA experiments only reveal the last step targeted by the inhibitor.

**Reverse Transcriptase.** Several compounds from the **3** and **7** series have been evaluated against recombinant HIV-1 reverse transcriptase). **3.19** was inhibiting at 125  $\mu$ M using polyrA.oligodT as the template primer and at 105  $\mu$ M when using polyrC.oligodG. This compound was, however, inactive against Maloney murine leukaemia virus RT using endogenous RNA as the template at 1000  $\mu$ M.

Because the in vitro inhibition of the HIV-1 RT activity was observed for **3.19** and typical NNRTIresistance mutations were observed when genotypically analyzing the HIV-1(III<sub>B</sub>) strain selected in the presence of increasing concentrations of **3.19**, it is clear that **3.19** acts as an NNRTI in addition to its action at a later process in the viral replication cycle.

**Inhibition of HIV-1 Production from Chronically Infected Cells.** When **7.03** was evaluated for its influence on the production of virus from chronically HIV-1(NL4.3)-infected HUT-78 cells, we noticed an inhibitory effect. From TOA experiments, in vitro RT assays suggested the possibility of an action at the reverse transcription, integration, or later step in the replicative cycle of HIV. AZT, ritonavir, and L-708,906 were also included in the experiment. For molecules acting before the termination of the integration process, AZT and L-708,906, no inhibitory effect on release of virus could be observed (Figure 2).

As expected, for ritonavir an inhibition of the virus production was observed. **7.03** inhibited virus production up to the level of ritonavir. This fact reveals that although the unknown target of molecule **7.03** is situated around the moment of integration, it must coincide with a process taking place immediately after integration.



**Figure 2.** Percentage of virus (HIV-1 NL4.3) produced from chronically infected HUT78 cells in the presence of varying concentrations of compounds. After incubation for 44 h, virus p24 Ag production was determined. Symbols: ( $\blacktriangle$ ) AZT; ( $\blacklozenge$ ) L-708,906; (+) **3.19**; (\*) **7.03**; ( $\square$ ) ritonavir.

#### Conclusion

From a study to discover new NNRTIs with anti-HIV activity against clinically relevant mutants, a group of molecules with a new antiretroviral mode of action was identified. Although the exact molecular target remains to be resolved, the experiments clearly show that some of the *N*-aminoimidazole derivatives interfere with an (immediate) postintegrational event occurring after integration of the viral DNA into the host cell genome.

On the basis of a limited structure–activity relationship, it was possible to identify some structural requirements that confer antiretroviral activity via a new mode of action to these molecules.

#### **Experimental Section**

**Materials and General Chemical Methods.** NMR spectra were recorded on a Varian, Gemini 200 spectrometer (for <sup>1</sup>H (200 MHz) and <sup>13</sup>C). <sup>13</sup>C and <sup>1</sup>H are referenced to TMS. All NH and OH protons were assigned by exchange with D<sub>2</sub>O. Exact mass measurements were performed on a quadrupole time-of-flight mass spectrometer (Q-Tof-2, Micromass, Manchester, U.K.) equipped with a standard electrospray ionization (ESI) interface. Samples were infused in a 2-propanol/water (1:1) mixture at 3  $\mu$ L/min. TLC was performed with TLC aluminum sheets (Merck, silica gel 60 F254), and silica (200–425 mesh) was used for column chromatography. Melting points (mp [°C]) were determined with a Büchi-SMP-20 capillary melting apparatus. For all reactions, analytical grade solvents were used.

Syntheses of 1-Amino-2,3-dihydro-1H-imidazole-2thiones 3. General Procedure. To a stirred solution of the  $\alpha$ -haloketone **2** (2.5 mmol) in acetic acid (10 mL), potassium thiocyanate (0.37 g, 3.8 mmol) was added at ambient temperature. After 30 min the hydrazine 1 (2.5 mmol) or hydrazine hydrochloride was added. Following stirring for 4 h at 30 °C, the reaction mixture was evaluated by TLC ( $CH_2Cl_2/MeOH =$ 99 :1). In case no product formation could be observed, the mixture was warmed to 80 °C for 2 h. After addition of water (30 mL), the precipitate was filtered off and washed with water. In general, recrystallization from methanol afforded pure products. Only in some cases, further purification by column chromatography (silica,  $CH_2Cl_2/MeOH = 99$  :1) was necessary. When  $N, \hat{N}$ -methylphenylhydrazine was used as a starting material, 2,3-dihydro-4-methyl-1-(N-methyl-N-phenylamino)-5-phenyl-1H-imidazole-2-thione 3.42 could be obtained in an analogous way.

Synthesis of 1-(3-Chlorophenylamino)-2,3-dihydro-4,5diphenyl-1*H*-imidazole-2-thione (3.26). A mixture of benzoine (1.0 g, 7.1 mmol), KSCN (0.68 g, 7.1 mmol), and 3-chlorophenylhydrazine-HCl (1.26 g, 7.1 mmol) was stirred in acetic acid (10 mL) for 2 days. The white precipitate formed was filtered off (0.4 g). Water (50 mL) was added, and the additional precipitate formed was likewise filtered off. Recrystallization from MeOH/water (1:1) yielded 1.5 g (56%) of **3.26**.

**Conversion of Methoxycarbonyl Groups into the Free Acids. General Procedure.** The corresponding methoxycarbonyl-substituted imidazoline-2-thione derivative (1.33 mmol) (**3.27**, **3.34**, **3.35**) was stirred in a 10% solution of NaOH (25 mL) for 6 h. After washing with CH<sub>2</sub>Cl<sub>2</sub>, the aqueous layer was acidified. The precipitate formed was filtered off and dried.

Synthesis of 5-(3-Carboxamidophenyl)-1-(3-chlorophenylamino)-2,3-dihydro-4-methyl-1*H*-imidazole-2thione (3.38). A mixture of the corresponding methoxycarbonyl-substituted imidazoline-2-thione 3.34 (1.33 mmol) was stirred in NH<sub>3</sub>/MeOH fore 2 days. After removal of the solvent, the residue was recrystallized from MeOH/water (1:3) to yield 3.38 in 73% yield.

**Preparation of 1-(3-Chlorophenylamino)-4-methyl-2methylsulfanyl-5-phenyl-1***H***-imidazole (8.01). A mixture of 1-(3-chlorophenylamino)-2,3-dihydro-4-methyl-5-phenyl-1***H***imidazoline-2-thione (3.01) (0.1 g, 0.37 mmol) and methyl iodide (1.19 g, 8.40 mmol) in dichloromethane (5 mL) was heated under reflux for 1 h. Excess of methyl iodide and solvent were removed in vacuo. Further purification was achieved by recrystallization from CH\_2Cl\_2/n-hexane, 1:1.** 

**Preparation of 2-Benzylsulfanyl-1-(3-chlorophenylamino)-4-methyl-5-phenyl-1***H***-imidazole (8.02).** A mixture of 1-(3-chlorophenylamino)-2,3-dihydro-4-methyl-5-phenyl-1*H*imidazoline-2-thione (**3.01**) (0.20 g, 0.62 mmol) and benzyl chloride (0.08 g, 0.62 mmol) in pyridine (5 mL) was heated under reflux for 3 h. After removal of the solvent, the crude product was purified by column chromatography (silica gel, ethyl acetate/hexane = 2:1.

**Synthesis of 1-Arylamino-1***H***-imidazoles 7. General Procedure.** A suspension of the respective 1-amino-2,3dihydro-1*H*-imidazole-2-thione (**3**) (2 mmol) in glacial acetic acid (10 mL) was stirred in an ice bath. Upon dropwise addition of 30% hydrogen peroxide (1 mL, 9.76 mmol), the reaction mixture cleared up, resulting in a clear-brown solution. After stirring for another 15 min, the reaction mixture was made alkaline (pH 8–9) with 10% NaOH. The resulting precipitate was filtered off, washed with cold water, and recrystallized from water.

Experimental data concerning the syntheses of the starting hydrazines 1 and  $\alpha$ -bromo compounds 2, the NMR data of all NAIMs (*N*-aminoimidazole-2-thiones 3, *N*-aminoimidazoles 7, and imidazole derivatives **8**–10), and elemental analyses are available as Supporting Information.

**Reference Compounds.** Dextran sulfate with an average molecular weight of 5000 was purchased from Sigma. AZT was synthesized as previously described.<sup>11</sup> Loviride ( $\alpha$ -APA, R89439) was obtained from Janssen Research Foundation (Beerse, Belgium). The diketo acid L-708,906<sup>13a</sup> was kindly provided by Drs. N. Neamati and T. R. Burke (NIH, Bethesda, MD). Ritonavir (ABT538) was kindly provided by J. M. Leonard, Abbott Laboratories (Abbott Park, IL).

Viruses and Cells. The origin of HIV-1(III<sub>B</sub>) virus stock has been described.<sup>12</sup> The HIV-1(NL4.3) strain<sup>13</sup> is a molecular clone obtained from the National Institutes of Health (Bethesda, MD). HIV-1 and HIV-2(ROD)<sup>14</sup> stocks were obtained from the culture supernatant of HIV-1- or HIV-2infected MT-4 cells, respectively. Simian immunodeficiency virus, SIV(mac251), was originally isolated by Daniel et al.<sup>15</sup> and was obtained from C. Bruck (Smith Kline-RIT, Rixensart, Belgium). SIV(mac251) stocks were prepared from the supernatant of SIV-infected MT-4 cells. ^16 S0561945 is an HIV-1( $\dot{I}II_B)$ strain possessing the K103N and Y181C mutations in its reverse transcriptase gene, resulting in resistance toward nonnucleoside reverse transcriptase inhibitors. MSV was prepared from tumors induced following intramuscular inoculation of 3-day-old NMRI mice with MSV, as described previously.17

Antiviral Activity and Cytotoxicity Assays. The inhibitory effects of the *N*-aminoimidazole derivatives on HIV-1, HIV-2, and SIV replication were monitored by measuring the viability of MT-4 cells 5 days after infection.<sup>18</sup> Cytotoxicity of the compounds was determined in parallel by measuring the viability of mock-infected cells on day 5. The number of viable cells was quantified semiautomatically by a tetrazolium-based colorimetric method using 3-(4,5-dimethylthiazolyl-2-yl)-2,5-diphenyltetrazolium (MTT), as described by Pauwels et al.<sup>20</sup>

Peripheral blood mononuclear cells (PBMCs) from healthy donors were isolated by density centrifugation (Lymphoprep, Nycomed Pharma AS, Diagnostics, Oslo, Norway) and stimulated with phytohemagglutinin (PHA, 2  $\mu$ g/mL final concentration) (Sigma Chemical Co., Bornem, Belgium) for 3 days. The activated cells (PHA-stimulated blasts) were washed three times with PBS, and viral infections were done as described by the ACTG protocols.<sup>19</sup> HIV-infected or mock-infected PHAstimulated blasts were cultured in the presence of 25 U/mL of IL-2 and varying concentrations of drugs. The supernatant was collected at day 7, and HIV-1 core antigen (p24 Ag) in the supernatant was analyzed by enzyme linked immunosorbent assay (ELISA) (NEN, Brussels, Belgium).

C3H/3T3 cells were seeded at 20 000 cells per milliliter into wells of tissue culture cluster plates (48 wells per plate). Following a 24 h incubation period, cell cultures were infected with 80 focus-forming units of MSV for 120 min, whereafter the culture medium was replaced by 1 mL of fresh medium containing appropriate concentrations of the test compound. After 6 days, transformation of the cells was examined microscopically.<sup>20</sup>

**Time-of-Addition Experiment.** MT-4 cells were infected with HIV-1(III<sub>B</sub>) at a multiplicity of infection (moi) of 0.5. The test compounds were added at different times after infection.<sup>21</sup> Viral p24 Ag production was determined at 31 h postinfection by ELISA (NEN, Brussels, Belgium). The reference compounds were added at 100 times their 50% inhibitory concentration (IC<sub>50</sub>) obtained in the MT-4/MTT assay.

**Inhibition of HIV-1 Production from Chronically Infected Cells.** Persistently infected (NL4.3) HUT-78 cells were washed three times in order to remove cell-free virus. The test compounds at the required concentrations were transferred into the cups of a 48-well plate. To each cup 200 000 cells were added (final volume of 1 mL). The cultures were allowed to grow for 44 h. The supernatant was collected, and viral p24 Ag production was determined by ELISA (NEN, Brussels, Belgium).

**HIV-1 RT Assay.** Poly(rC).oligo(dG) and [<sup>3</sup>H]dGTP and poly(rA).oligo(dT) and [<sup>3</sup>H]dTTP were used as a template primer and radiolabeled substrate, respectively. The final [<sup>3</sup>H]dGTP and [<sup>3</sup>H]dTTP concentrations in the reaction mixture were both 2.5  $\mu$ M.

Selection of 3.19- and 7.03-Resistant Virus Strains. HIV-1(III<sub>B</sub>) was subjected to passages in MT-4 cells ( $4 \times 10^5$  cells/2 mL) in the presence of increasing concentrations of the compounds. Passages were performed every 3–4 days.

**Determination of the Amino Acid Sequence of the 3.19- and 7.03-Resistant HIV-1 Strains RT.** The procedures for the MT-4 cells infection with resistant HIV-1, preparation of the samples for the PCR assays, amplification of the proviral DNA, and sequencing of the 727-bp fragment covering amino acid residues 50–270 have been reported elsewhere.<sup>22</sup>

**HIV Integrase Assays.** Wild type His-tagged recombinant HIV-1 integrase and the substrate and target DNA were as previously described.<sup>23</sup> The following high-performance-liquid-chromatography-purified deoxynucleotides were purchased from Amersham-Pharmacia Biotech: INT1, 5'-TGTG-GAAAATCTCTAGCAGT; INT2, 5'-ACTGCTAGAGATTTTCCACAC; T35, 5'-ACTATACCAGACAATAATTGTCTGGCTG-TACCGT; SK70, 5'-ACGGTACAGGCCAGACAATTATTGTCTGGGTATAGT. The oligodeoxynucleotides INT1 and INT2 correspond to the U5 end of the HIV-1 LTR. The 3'-processing, overall integration, and strand-transfer assay were slightly modified from published procedures. The final reaction mixture of the 3'-processing assays contained 20 mM HEPES, pH 7.5, 5 mM dithiothreitol, 10 mM MgCl<sub>2</sub>, 75 mM NaCl, 5% (v/v) poly-(ethylene glycol) 8000, 15% dimethyl sulfoxide, 30 nM oligo-

deoxynucleotide substrate (INT1/INT2), and 230 nM His-tag IN in a volume of 10  $\mu$ L. Inhibitors were incubated briefly with the reaction components before the addition of IN. Reactions were started by addition of the enzyme. All the reactions were stopped by addition of formamide loading dye, and the products were separated in a 15% denaturating polyacryl-amide/urea gel. Autoradiography was performed by exposing the wet gel to X-ray film (CURIX RP1, Agfa). Quantification of the results was performed using the Cyclone (Canberra Packard, Zellik, Belgium).

To evaluate inhibition of 3'-processing, the reaction was allowed to proceed at 37 °C for 7 min. Inhibition of formation of the -2 band was determined. In the overall integration assay, the reaction was allowed to proceed for 60 min. Both inhibition of formation of the -2 band and DNA strand transfer products were scored. The DNA strand transfer was assayed in the following way. DNA substrate (INT1/INT2, 30 nM) was preincubated with 230 nM IN at 37 °C for 5 min to allow the cleavage reaction to occur. The composition of the reaction mixture was identical to that in the processing assay. After 5 min, 1  $\mu$ L of excess target DNA (SK70/T35, at a final concentration of 250 nM) was added with or without inhibitor and the samples were incubated at 37 °C for 1 h. The excess of unspecific target DNA competitively blocked further binding of IN to the viral substrate so that inhibition of DNA strand transfer in the preformed complexes can be monitored independently of DNA binding and 3'-processing.

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**Supporting Information Available:** Syntheses and NMR data of NAIM derivatives. This material is available free of charge via the Internet at http://pubs.acs.org.

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