Supporting Information

Novel *N*-Substituted Indol-3-ylglyoxylamides Probing the L_{Di} and L_1/L_2 Lipophilic Regions of the Benzodiazepine Receptor Site in Search for Subtype Selective Ligands

Giampaolo Primofiore, Sabrina Taliani, Federico Da Settimo, Anna Maria Marini, Concettina La Motta, Francesca Simorini, Maria Paola Patrizi, Valentina Sergianni, Ettore Novellino, Giovanni Greco, Barbara Cosimelli, Vincenzo Calderone, Marina Montali, François Besnard and Claudia Martini

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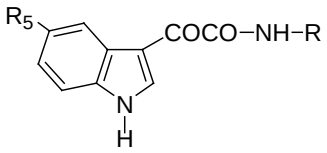
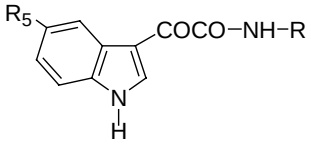
Table 1. Physical Properties of Indolylglyoxylamide derivatives **10-37**.



no	R_5	R	yield (%)	recryst. solvent	mp (°C)	formula[a]
10	H	$CH_2C_6H_4$-4'-CH_3	82	EtOH	184-186	$C_{18}H_{16}N_2O_2$
11	NO_2	$CH_2C_6H_4$-4'-CH_3	84	EtOH	>300	$C_{18}H_{15}N_3O_4$
12	H	$CH_2C_6H_4$-4'-CH_2CH_3	87	EtOH	>300	$C_{19}H_{18}N_2O_2$
13	NO_2	$CH_2C_6H_4$-4'-CH_2CH_3	80	EtOH	298-300	$C_{19}H_{17}N_3O_4$
14	H	$CH_2C_6H_4$-4'-Br	92	EtOH	208-210	$C_{17}H_{13}BrN_2O_2$
15	NO_2	$CH_2C_6H_4$-4'-Br	94	EtOH	>300	$C_{17}H_{12}BrN_3O_4$
16	H	$CH_2C_6H_4$-4'-C≡CSi$(CH_3)_3$	82	EtOH	220-222	$C_{22}H_{22}N_2O_2Si$
17	NO_2	$CH_2C_6H_4$-4'-C≡CSi$(CH_3)_3$	76	EtOH	176-178	$C_{22}H_{21}N_3O_4Si$
18	H	$CH_2C_6H_4$-4'-CH_2C≡CSi$(CH_3)_3$	82	EtOH	>300	$C_{23}H_{24}N_2O_2Si$
19	NO_2	$CH_2C_6H_4$-4'-CH_2C≡CSi$(CH_3)_3$	90	EtOH	273-275	$C_{23}H_{23}N_3O_4Si$
20	H	$CH_2C_6H_4$-4'-C≡CH	82	Toluene	192-194	$C_{19}H_{14}N_2O_2$
21	NO_2	$CH_2C_6H_4$-4'-C≡CH	88	EtOH	273-275	$C_{19}H_{13}N_3O_4$
22	H	$CH_2C_6H_4$-4'-C≡C-CH_3	85	Toluene	187-190	$C_{20}H_{16}N_2O_2$
23	NO_2	$CH_2C_6H_4$-4'-C≡C-CH_3	85	EtOH	240-242	$C_{20}H_{15}N_3O_4$
24	H	$(CH_2)_3CH_3$	88	toluene	165-167	$C_{14}H_{16}N_2O_2$
25	NO_2	$(CH_2)_3CH_3$	89	EtOH	274-277	$C_{14}H_{15}N_3O_4$
26	H	$(CH_2)_4CH_3$	86	EtOH	154-156	$C_{15}H_{18}N_2O_2$
27	NO_2	$(CH_2)_4CH_3$	79	EtOH	270-273	$C_{15}H_{17}N_3O_4$
28	H	$(CH_2)_5CH_3$	80	EtOH/H_2O	151-153	$C_{16}H_{20}N_2O_2$
29	NO_2	$(CH_2)_5CH_3$	81	EtOH	273-276	$C_{16}H_{19}N_3O_4$
30	H	$CH(CH_3)_2$	83	toluene	192-194	$C_{13}H_{14}N_2O_2$
31	NO_2	$CH(CH_3)_2$	96	EtOH	262-265	$C_{13}H_{13}N_3O_4$
32	H	$CH(CH_3)CH_2CH_3$	75	EtOH	171-173	$C_{14}H_{16}N_2O_2$
33	NO_2	$CH(CH_3)CH_2CH_3$	77	EtOH	237-240	$C_{14}H_{15}N_3O_4$
34	H	$C(CH_3)_3$	83	Toluene	158-160	$C_{14}H_{16}N_2O_2$
35	NO_2	$C(CH_3)_3$	89	EtOH	> 300	$C_{14}H_{15}N_3O_4$
36	H	$CH_2CH(CH_3)_2$	81	Toluene	174-176	$C_{14}H_{16}N_2O_2$
37	NO_2	$CH_2CH(CH_3)_2$	95	EtOH	280-283	$C_{14}H_{15}N_3O_4$

[a]Elemental analyses for C, H, N, were within ±0.4% of the calculated values.

Table 2. Spectral Data of Indolylglyoxylamide derivatives **10-37**.



no.	R_5	R	IR (cm^{-1})	^{1}H-NMR (δ, ppm)
10	H	$CH_2C_6H_4$-4'-CH_3	3200, 1640, 1600, 1240, 720.	2.25 (s, 3H, CH_3); 4.36 (d, 2H, CH_2); 7.10-7.28 (m, 6H, Ar-H); 7.50-7.54 (m, 1H, 7-H); 8.19-8.24 (m, 1H, 4-H); 8.72 (s, 1H, 2-H); 9.22 (t, 1H, CONH, exch. with D_2O); 12.40 (bs 1H, 1-NH, exch. with D_2O).
11	NO_2	$CH_2C_6H_4$-4'-CH_3	3370, 3180, 1660, 1610, 1220, 740.	2.26 (s, 3H, CH_3); 4.37 (d, 2H, CH_2); 7.12 (d, 2H, 3'-H, 5'-H); 7.21 (d, 2H, 2'-H, 6'-H); 7.63 (d, 1H, 7-H); 8.16 (dd, 1H, 6-H); 8.97 (s, 1H, 2-H); 9.07 (d, 1H, 4-H); 9.36 (t, 1H, CONH, exch. with D_2O); 12.80 (bs, 1H, 1-NH, exch. with D_2O).
12	H	$CH_2C_6H_4$-4'-CH_2CH_3	3320, 3260, 1650, 1600, 1230, 740.	1.14 (t, 3H, CH_3); 2.56 (q, 2H, CH_2CH_3); 4.37 (d, 2H, NHCH_2); 7.10-7.26 (m, 6H, Ar-H); 7.50-7.54 (m, 1H, 7-H); 8.12-8.18 (m, 1H, 4-H); 8.72 (s, 1H, 2-H); 9.23 (t, 1H, CONH, exch. with D_2O); 12.22 (bs, 1H, 1-NH, exch. with D_2O).
13	NO_2	$CH_2C_6H_4$-4'-CH_2CH_3	3360, 3150, 1660, 1620, 1220, 740.	1.15 (t, 3H, CH_3); 2.57 (q, 2H, CH_2CH_3); 4.40 (d, 2H, NHCH_2); 7.16 (d, 2H, 3'-H, 5'-H); 7.25 (d, 2H, 2'-H, 6'-H); 7.75 (d, 1H, 7-H); 8.15 (dd, 1H, 6-H); 8.98 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 9.34 (t, 1H, CONH, exch. with D_2O); 12.70 (bs, 1H, 1-NH, exch. with D_2O).
14	H	$CH_2C_6H_4$-4'-Br	3270, 1640, 1600, 1220, 740.	4.39 (d, 2H, CH_2); 7.22-7.30 (m, 4H, Ar-H); 7.51-7.55 (m, 3H, Ar-H); 8.21-8.25 (m, 1H, 4-H); 8.74 (s, 1H, 2-H); 9.34 (t, 1H, CONH, exch. with D_2O); 12.20 (bs, 1H, 1-NH, exch. with D_2O).
15	NO_2	$CH_2C_6H_4$-4'-Br	3360, 3160, 1670, 1620, 1220, 790.	4.41 (d, 2H, CH_2); 7.30 (d, 2H, 2'-H, 6'-H); 7.54 (d, 2H, 3'-H, 5'-H); 7.74 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.98 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 9.45 (t, 1H, CONH, exch. with D_2O); 12.75 (bs, 1H, 1-NH, exch. with D_2O).
16	H	$CH_2C_6H_4$-4'-C≡CSi$(CH_3)_3$	3320, 3260, 2150, 1660, 1600, 1240, 740.	0.22 (s, 9H, $3CH_3$); 4.43 (d, 2H, CH_2); 7.24-7.56 (m, 7H, Ar-H); 8.21-8.26 (m, 1H, 4-H); 8.74 (s, 1H, 2-H); 9.33 (t, 1H, CONH, exch. with D_2O); 12.24 (bs, 1H, 1-NH, exch. with D_2O).
17	NO_2	$CH_2C_6H_4$-4'-C≡CSi$(CH_3)_3$	3340, 3160, 2160, 1670, 1620, 1230, 740.	0.22 (s, 9H, $3CH_3$); 4.45 (d, 2H, CH_2); 7.33 (d, 2H, 2'-H, 6'-H); 7.43 (d, 2H, 3'-H, 5'-H); 7.75 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 9.00 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 9.46 (t, 1H, CONH, exch. with D_2O); 12.80 (bs, 1H, 1-NH, exch. with D_2O).

18	H	$CH_2C_6H_4$-4'-$CH_2C{\equiv}CSi(CH_3)_3$	3360,3140, 2130, 1650, 1610, 1180, 740.	0.12 (s, 9H, $3CH_3$); 1.74 (s, 2H, CH_2-Si); 4.39 (d, 2H, NH*CH_2*); 7.20-7.56 (m, 7H, Ar-H); 8.20-8.25 (m, 1H, 4-H); 8.73 (s, 1H, 2-H); 9.32 (t, 1H, CONH, exch. with D_2O); 12.30 (bs, 1H, 1-NH, exch. with D_2O).
19	NO_2	$CH_2C_6H_4$-4'-$CH_2C{\equiv}CSi(CH_3)_3$	3360, 3180, 2190, 1660, 1610, 1100, 740.	0.12 (s, 9H, $3CH_3$); 1.75 (s, 2H, CH_2-Si); 4.41 (d, 2H, NH*CH_2*); 7.24-7.33 (m, 4H, Ar-H); 7.74 (d, 1H, 7-H); 8.16 (dd, 1H, 6-H); 8.99 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 9.42 (t, 1H, CONH, exch. with D_2O); 12.80 (bs, 1H, 1-NH, exch. with D_2O).
20	H	$CH_2C_6H_4$-4'-C≡CH	3370, 3240, 2100, 1680, 1600, 1230, 750.	4.15 (s, 1H, CH); 4.43 (d, 2H, CH_2); 7.18-7.35 (m, 4H, Ar-H); 7.43-7.55 (m, 3H, Ar-H); 8.19-8.25 (m, 1H, 4-H); 8.74 (s, 1H, 2-H); 9.34 (t, 1H, CONH, exch. with D_2O); 12.24 (bs, 1H, 1-NH, exch. with D_2O).
21	NO_2	$CH_2C_6H_4$-4'-C≡CH	3370, 3160, 2100, 1670, 1615, 1240, 790.	4.15 (s, 1H, CH); 4.45 (d, 2H, CH_2); 7.34 (d, 2H, 2'-H, 6'-H); 7.45 (d, 2H, 3'-H, 5'-H); 7.74 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.99 (s, 1H, 2-H); 9.09 (d, 1H, 4-H); 9.44 (t, 1H, CONH, exch. with D_2O); 12.65 (bs, 1H, 1-NH, exch. with D_2O).
22	H	$CH_2C_6H_4$-4'-C≡C-CH_3	3250, 1930, 1650, 1600, 1130, 740.	2.02 (s, 3H, CH_3); 4.41 (d, 2H, CH_2); 7.23-7.37 (m, 6H, Ar-H); 7.51-7.55 (m, 1H, 7-H); 8.21-8.25 (m, 1H, 4-H); 8.75 (s, 1H, 2-H); 9.33 (t, 1H, CONH, exch. with D_2O); 12.25 (bs, 1H, 1-NH, exch. with D_2O).
23	NO_2	$CH_2C_6H_4$-4'-C≡C-CH_3	3360, 3150, 1670, 1610, 1220, 740.	2.02 (s, 3H, CH_3); 4.42 (d, 2H, CH_2); 7.23-7.37 (m, 4H, Ar-H); 7.74 (d, 1H, 7-H); 8.18 (dd, 1H, 6-H); 9.00 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 9.44 (t, 1H, CONH, exch. with D_2O); 12.78 (bs, 1H, 1-NH, exch. with D_2O).
24	H	$(CH_2)_3CH_3$	3320, 3230, 1660, 1600, 1230, 740.	0.89 (t, 3H, CH_3); 1.25-1.53 (m, 4H, $NHCH_2(CH_2)_2CH_3$); 3.15-3.25 (m, 2H, NH*CH_2*); 7.20-7.30 (m, 2H, 5-H, 6-H); 7.50-7.55 (m, 1H, 7-H); 8.20-8.24 (m, 1H, 4-H); 8.68-8.74 (m, 2H, 2-H, CONH, exch. with D_2O); 12.21 (bs, 1H, 1-NH, exch. with D_2O)
25	NO_2	$(CH_2)_3CH_3$	3340, 3180, 1670, 1620, 1260, 740.	0.89 (t, 3H, CH_3); 1.24-1.54 (m, 4H, $NHCH_2(CH_2)_2CH_3$); 3.17-3.27 (m, 2H, NH*CH_2*); 7.74 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.83 (t, 1H, CONH, exch. with D_2O); 8.98 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 12.75 (bs, 1H, 1-NH, exch. with D_2O)
26	H	$(CH_2)_4CH_3$	3340, 3230, 1660, 1600, 1240, 740.	0.87 (t, 3H, CH_3); 1.25-1.54 (m, 6H, $NHCH_2(CH_2)_3CH_3$); 3.17-3.27 (m, 2H, NH*CH_2*); 7.21-7.30 (m, 2H, 5-H, 6-H); 7.51-7.55 (m, 1H, 7-H); 8.20-8.24 (m, 1H, 4-H); 8.68-8.74 (m, 2H, 2-H, CONH, exch. with D_2O); 12.21 (bs, 1H, 1-NH, exch. with D_2O)
27	NO_2	$(CH_2)_4CH_3$	3350, 3150, 1670, 1620, 1220, 740.	0.87 (t, 3H, CH_3); 1.26-1.56 (m, 6H, $NHCH_2(CH_2)_3CH_3$); 3.17-3.27 (m, 2H, NH*CH_2*); 7.74 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.85 (t, 1H, CONH, exch. with D_2O); 8.98 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 12.78 (bs, 1H, 1-NH, exch. with D_2O)

28	H	$(CH_2)_5CH_3$	3320, 3220, 1650, 1600, 1240, 740.	0.86 (t, 3H, CH_3); 1.21-1.54 (m, 8H, $NHCH_2(CH_2)_4CH_3$); 3.15-3.25 (m, 2H, $NHCH_2$); 7.23-7.28 (m, 2H, 5-H, 6-H); 7.50-7.55 (m, 1H, 7-H); 8.20-8.24 (m, 1H, 4-H); 8.69-8.73 (m, 2H, 2-H, CONH, exch. with D_2O); 12.22 (bs, 1H, 1-NH, exch. with D_2O)
29	NO_2	$(CH_2)_5CH_3$	3360, 3180, 1670, 1630, 1230, 740.	0.86 (t, 3H, CH_3); 1.23-1.55 (m, 8H, $NHCH_2(CH_2)_4CH_3$); 3.17-3.27 (m, 2H, $NHCH_2$); 7.75 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.84 (t, 1H, CONH, exch. with D_2O); 8.98 (s, 1H, 2-H); 9.07 (d, 1H, 4-H); 12.86 (bs, 1H, 1-NH, exch. with D_2O)
30	H	$CH(CH_3)_2$	3300, 3250, 1650, 1600, 1240, 740.	1.15 (d, 6H, $2CH_3$); 3.94-4.09 (m, 1H, CH); 7.22-7.29 (m, 2H, 5-H, 6-H); 7.50-7.55 (m, 1H, 7-H); 8.19-8.24 (m, 1H, 4-H); 8.53 (d, 1H, CONH, exch. with D_2O); 8.71 (s, 1H, 2-H); 12.22 (bs, 1H, 1-NH, exch. with D_2O)
31	NO_2	$CH(CH_3)_2$	3280, 3190, 1650, 1610, 1220, 730.	1.17 (d, 6H, $2CH_3$); 3.98-4.08 (m, 1H, CH); 7.67 (d, 1H, 7-H); 8.08 (dd, 1H, 6-H); 8.56 (d, 1H, CONH, exch. with D_2O); 8.90 (s, 1H, 2-H); 9.04 (d, 1H, 4-H); 12.80 (bs, 1H, 1-NH, exch. with D_2O)
32	H	$CH(CH_3)CH_2CH_3$	3270, 3150, 1650, 1600, 1240, 740.	0.85 (t, 3H, CH_2CH_3); 1.13 (d, 3H, $CHCH_3$); 1.43-1.55 (m, 2H, CH_2CH_3); 3.75-3.90 (m, 1H, CH); 7.23-7.28 (m, 2H, 5-H, 6-H); 7.51-7.55 (m, 1H, 7-H); 8.20-8.24 (m, 1H, 4-H); 8.47 (d, 1H, CONH, exch. with D_2O); 8.69 (s, 1H, 2-H); 12.21 (bs, 1H, 1-NH, exch. with D_2O)
33	NO_2	$CH(CH_3)CH_2CH_3$	3320, 3190, 1660, 1620, 1220, 740.	0.86 (t, 3H, CH_2CH_3); 1.25 (d, 3H, $CHCH_3$); 1.45-1.57 (m, 2H, CH_2CH_3); 3.77-3.92 (m, 1H, CH); 7.74 (d, 1H, 7-H); 8.17 (dd, 1H, 6-H); 8.60 (d, 1H, CONH, exch. with D_2O); 8.94 (s, 1H, 2-H); 9.08 (d, 1H, 4-H); 12.77 (bs, 1H, 1-NH, exch. with D_2O).
34	H	$C(CH_3)_3$	3340, 3170, 1660, 1630, 1240, 740.	1.39 (s, 9H, $3CH_3$); 7.21–7.30 (m, 2H, 5-H, 6-H); 7.51-7.56 (m, 1H, 7-H); 8.00 (bs, 1H, CONH, exch. with D_2O); 8.19-8.23 (m, 1H, 4-H); 8.66 (s, 1H, 2-H); 12.23 (bs, 1H, CONH, exch. with D_2O)
35	NO_2	$C(CH_3)_3$	3350, 3260, 1680, 1600, 1220, 740.	1.39 (s, 9H, $3CH_3$); 7.71 (d, 1H, 7-H); 8.08 (bs, 1H, CONH, exch. with D_2O); 8.13 (dd, 1H, 6-H); 8.86 (s, 1H, 2-H); 9.04 (dd, 1H, 4-H); 12.78 (bs, 1H, 1-NH, exch. with D_2O)
36	H	$CH_2CH(CH_3)_2$	3310, 3250, 1650, 1600, 1240, 740.	0.89 (d, 6H, $2CH_3$); 1.75-1.91 (m, 1H, CH); 3.01-3.07 (m, 2H, CH_2); 7.24-7.30 (m, 2H, 5-H, 6-H); 7.52-7.56 (m, 1H, 7-H); 8.21-8.25 (m, 1H, 4-H); 8.70-8.73 (m, 2H, 2-H, CONH, exch. with D_2O); 12.23 (bs, 1H, 1-NH, exch. with D_2O)
37	NO_2	$CH_2CH(CH_3)_2$	3360, 3120, 1670, 1630, 1240, 740.	0.88 (d, 6H, $2CH_3$); 1.81-1.88 (m, 1H, CH); 3.02-3.09 (m, 2H, CH_2); 7.74 (d, 1H, 7-H); 8.16 (dd, 1H, 6-H); 8.83 (t, 1H, CONH, exch. with D_2O); 8.95 (s, 1H, 2-H); 9.07 (d, 1H, 4-H); 12.80 (bs, 1H, 1-NH, exch. with D_2O)

Appendix

ANALYTICAL DATA

no.	formula	Calcd. %			Found %		
		C	H	N	C	H	N
2	$C_{17}H_{25}NO_2Si$	67.28	8.30	4.62	67.38	8.39	4.52
3	$C_{18}H_{27}NO_2Si$	68.09	8.57	4.41	67.95	8.61	4.49
4·HCl	$C_{12}H_{18}ClNSi$	60.10	7.57	5.84	59.98	7.55	5.77
5·HCl	$C_{13}H_{20}ClNSi$	61.51	7.94	5.52	61.32	8.03	5.47
6·HCl	$C_9H_{10}ClN$	64.48	6.01	8.36	64.62	5.95	8.19
7·HCl	$C_{10}H_{12}ClN$	66.12	6.66	7.71	66.07	6.71	7.58
10	$C_{18}H_{16}N_2O_2$	73.95	5.52	9.58	74.07	5.67	9.41
11	$C_{18}H_{15}N_3O_4$	64.09	4.48	12.46	63.93	4.37	12.51
12	$C_{19}H_{18}N_2O_2$	74.49	5.92	9.14	74.32	6.06	9.02
13	$C_{19}H_{17}N_3O_4$	64.95	4.88	11.96	64.77	4.82	11.92
14	$C_{17}H_{13}BrN_2O_2$	57.16	3.67	7.84	57.07	3.68	7.75
15	$C_{17}H_{12}BrN_3O_4$	50.77	3.01	10.45	50.81	3.20	10.31
16	$C_{22}H_{22}N_2O_2Si$	70.56	5.92	7.48	70.80	5.83	7.37
17	$C_{22}H_{21}N_3O_4Si$	62.99	5.05	10.02	62.81	5.00	10.18
18	$C_{23}H_{24}N_2O_2Si$	71.10	6.23	7.21	71.29	6.18	7.28
19	$C_{23}H_{23}N_3O_4Si$	63.72	5.35	9.69	63.78	5.42	9.78
20	$C_{19}H_{14}N_2O_2$	75.48	4.67	9.27	75.30	4.74	9.09
21	$C_{19}H_{13}N_3O_4$	65.70	3.77	12.10	65.89	3.71	11.99
22	$C_{20}H_{16}N_2O_2$	75.93	5.10	8.86	75.85	5.13	8.69
23	$C_{20}H_{15}N_3O_4$	66.48	4.18	11.63	66.36	4.24	11.57
24	$C_{14}H_{16}N_2O_2$	68.83	6.60	11.47	68.69	6.53	11.59
25	$C_{14}H_{15}N_3O_4$	58.13	5.23	14.53	58.27	5.19	14.71
26	$C_{15}H_{18}N_2O_2$	69.74	7.02	10.84	69.87	6.95	10.72
27	$C_{15}H_{17}N_3O_4$	59.40	5.65	13.85	59.31	5.57	13.97
28	$C_{16}H_{20}N_2O_2$	70.56	7.40	10.29	7.39	7.51	10.37
29	$C_{16}H_{19}N_3O_4$	60.56	6.03	13.24	60.47	5.95	13.13

30	$C_{13}H_{14}N_2O_2$	67.81	6.13	12.17	67.92	6.15	12.31
31	$C_{13}H_{13}N_3O_4$	56.72	4.76	15.27	56.60	4.63	15.13
32	$C_{14}H_{16}N_2O_2$	68.83	6.60	11.47	68.65	6.52	11.33
33	$C_{14}H_{15}N_3O_4$	58.13	5.23	14.53	58.34	5.17	14.62
34	$C_{14}H_{16}N_2O_2$	68.83	6.60	11.47	68.66	6.75	11.63
35	$C_{14}H_{15}N_3O_4$	58.13	5.23	14.53	58.06	5.31	14.71
36	$C_{14}H_{16}N_2O_2$	68.83	6.60	11.47	68.72	6.67	11.36
37	$C_{14}H_{15}N_3O_4$	58.13	5.23	14.53	58.02	5.33	14.65