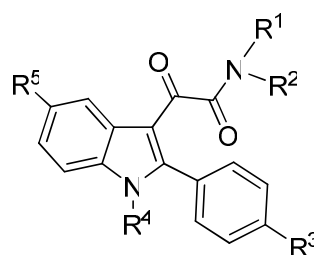


Supporting Information

Evaluation of Novel *N*¹-Methyl-2-phenylindol-3-ylglyoxylamides as a New Chemotype of 18 kDa Translocator Protein-Selective Ligand Suitable for the Development of Positron Emission Tomography Radioligands

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Table 1. Spectral Data of *N,N*-dialkylindolylglyoxylamide Derivatives **17-31**.**9–23**

Compd	R ¹	R ²	R ³	R ⁴	R ⁵	IR (ν, cm ⁻¹)	¹ H-NMR (δ, ppm)
17	Me	Bn	H	H	H	3330, 1610, 1078, 866, 743.	2.30, 2.73 (2s, 3H); 4.09, 4.30 (2s, 2H); 7.14-7.63 (m, 13H); 8.07-8.11 (m, 1H); 12.47 (bs; 1H, exch. with D ₂ O).
18	Me	Bn	F	H	H	3188, 1631, 1611, 1081, 869, 753.	2.35, 2.76 (2s, 3H); 4.17, 4.34 (2s, 2H); 7.17-7.54 (m, 10H); 7.65-7.71 (m, 2H); 8.06-7.15 (m, 1H); 12.59 (bs, 1H, exch. with D ₂ O).
19	ⁿ Pr	ⁿ Pr	H	Me	H	1641, 1610, 1077, 753, 706.	0.67-0.77 (m, 6H); 1.06-1.13 (m, 2H); 1.44-1.48 (m, 2H); 2.69, 2.94 (2t, <i>J</i> =7.8 Hz, <i>J</i> =7.4 Hz, 4H); 3.51 (s, 3H); 7.29-7.70 (m, 8H); 8.19-8.23 (m, 1H).
20	ⁿ Bu	ⁿ Bu	H	Me	H	1634, 1611, 1078, 869, 760	0.73-0.85 (m, 6H); 1.06-1.17 (m, 6H); 1.38-1.41 (m, 2H); 2.72, 2.97 (2t, <i>J</i> =7.6 Hz, 4H); 3.49 (s, 3H); 7.32-7.67 (m, 8H); 8.20-8.24 (m, 1H).
21	ⁿ Hex	ⁿ Hex	H	Me	H	1648, 1627, 1225, 1078, 753.	0.79, 0.87 (2t, <i>J</i> =6.5 Hz, <i>J</i> =6.6 Hz, 6H); 1.13-1.43 (m, 16H); 2.73, 2.79 (2t, <i>J</i> =7.2 Hz, <i>J</i> =7.0 Hz, 4H); 3.49 (s, 3H); 7.33-7.65 (m, 8H); 8.19-8.23 (m, 1H).
22	Et	ⁿ Bu	H	Me	H	1638, 1611, 1078, 852, 753	0.65-0.85 (m, 6H); 0.97-1.18 (m, 4H); 2.69-2.83 (m, 2H); 2.92-3.11 (m, 2H); 3.48 (s, 3H); 7.30-7.67 (m, 8H); 8.16-8.21 (m, 1H).
23	Et	Bn	H	Me	H	1638, 1607, 1074, 805, 757	0.44, 0.83 (2t, <i>J</i> =7.0 Hz, <i>J</i> =7.2 Hz, 3H); 2.70-3.14 (2q, <i>J</i> =6.8 Hz, <i>J</i> =6.7 Hz, 2H); 3.52 (s, 3H); 3.97, 4.23 (2s, 2H); 7.10-7.69 (m, 13H); 8.16-8.29 (m, 1H).
24	Me	ⁿ Bu	H	Me	H	1641, 1621, 1071, 866, 757	0.75-0.83 (m, 3H); 1.08-1.19 (m, 4H); 2.22, 2.69 (2s, 3H); 2.63, 2.93 (2t, <i>J</i> =7.0 Hz, <i>J</i> =7.2 Hz, 2H); 3.51 (s, 3H); 7.30-7.68 (m, 8H); 8.23-8.27 (m, 1H).

25	Me	ⁿ Pen	H	Me	H	1641, 1621, 1071, 866, 757	0.77-0.88 (m, 3H); 1.10-1.25 (m, 6H); 2.22, 2.69 (2s, 3H); 2.63, 2.94 (2t, <i>J</i> =6.8 Hz, <i>J</i> =6.9 Hz, 2H); 3.51 (s, 3H); 7.31-7.69 (m, 8H); 8.23-8.29 (m, 1H).
26	Me	Bn	H	Me	H	1641, 1614, 1068, 870, 750.	2.12, 2.68 (2s, 3H); 3.57 (s, 3H); 3.82, 4.21 (2s, 2H); 7.13-7.70 (m, 13H); 8.23-8.29 (m, 1H).
27	ⁿ Pr	ⁿ Pr	H	Me	F	1636, 1581, 1072, 869, 747	0.65-0.74 (m, 6H); 1.07-1.16 (m, 2H); 1.39-1.51 (m, 2H); 2.67, 2.94 (2t, <i>J</i> =7.6 Hz, <i>J</i> =7.4 Hz, 4H); 3.50 (s, 3H); 7.19-7.92 (m, 8H).
28	ⁿ Pr	ⁿ Pr	F	Me	H	1641, 1604, 1225, 1078, 753.	0.68-0.77 (m, 6H); 1.09-1.24 (m, 2H); 1.42-1.49 (m, 2H); 2.71-2.79 (m, 2H); 2.90-3.00 (m, 2H); 3.51 (s, 3H); 7.33-7.69 (m, 7H); 8.20-8.24 (m, 1H).
29	ⁿ Hex	ⁿ Hex	F	Me	H	1648, 1611, 1071, 870, 757.	0.75-0.90 (m, 6H); 1.13-1.44 (m, 16H); 2.79, 2.97 (2t, <i>J</i> =6.8 Hz, <i>J</i> =7.0 Hz, 4H); 3.49 (s, 3H); 7.32-7.68 (m, 7H); 8.20-8.24 (m, 1H).
30	Me	Bn	F	Me	H	1641, 1607, 1068, 866, 760.	2.19, 2.69 (2s, 3H); 3.56 (s, 3H); 3.93, 4.24 (2s, 2H); 7.14-7.72 (m, 12H); 8.23-8.27 (m, 1H).
31	ⁿ Pr	ⁿ Pr	NO ₂	Me	H	1635, 1577, 1078, 863, 747	0.66-0.75 (m, 6H); 1.14-1.24 (m, 2H); 1.46-1.49 (m, 2H); 2.79, 3.01 (2t, <i>J</i> =8.0 Hz, <i>J</i> =8.0 Hz, 4H); 3.54 (s, 3H); 7.35-7.42 (m, 2H); 7.69-7.81 (m, 3H); 8.15-8.40 (m, 3H).

ANALYTICAL DATA

Compd	formula	Calcd. %			Found %		
		C	H	N	C	H	N
17	C ₂₄ H ₂₀ N ₂ O ₂	78.24	5.47	7.60	78.08	5.73	7.45
18	C ₂₄ H ₁₉ FN ₂ O ₂	74.60	4.96	7.25	74.75	4.78	7.41
19	C ₂₃ H ₂₆ N ₂ O ₂	76.21	7.23	7.73	76.33	7.32	7.72
20	C ₂₅ H ₃₀ N ₂ O ₂	76.89	7.74	7.17	76.88	7.67	7.12
21	C ₂₉ H ₃₈ N ₂ O ₂	77.99	8.58	6.27	77.77	8.56	6.07
22	C ₂₃ H ₂₆ N ₂ O ₂	76.21	7.23	7.73	76.33	7.32	7.62
23	C ₂₆ H ₂₄ N ₂ O ₂	78.76	6.10	7.07	78.91	6.12	7.17
24	C ₂₂ H ₂₄ N ₂ O ₂	75.83	6.94	8.04	75.98	6.77	8.32
25	C ₂₃ H ₂₆ N ₂ O ₂	76.21	7.23	7.73	76.03	7.17	7.84
26	C ₂₅ H ₂₂ N ₂ O ₂	78.51	5.80	7.32	78.34	5.91	7.57
27	C ₂₃ H ₂₅ FN ₂ O ₂	72.61	6.62	7.36	72.56	6.46	7.51
28	C ₂₃ H ₂₅ FN ₂ O ₂	72.61	6.62	7.36	72.87	6.47	7.43
29	C ₂₉ H ₃₇ FN ₂ O ₂	74.97	8.03	6.03	74.85	7.99	6.20
30	C ₂₅ H ₂₁ FN ₂ O ₂	74.98	5.29	7.00	74.76	5.30	6.82
31	C ₂₃ H ₂₅ N ₃ O ₄	67.80	6.18	10.31	67.75	6.02	10.09