Supplementary Materials
for

Structural characterization of 4-(4-nitrophenyl)thiomorpholine, a precursor in medicinal chemistry

Paul R. Palme, Richard Goddard, Peter Imming and Rüdiger W. Seidel

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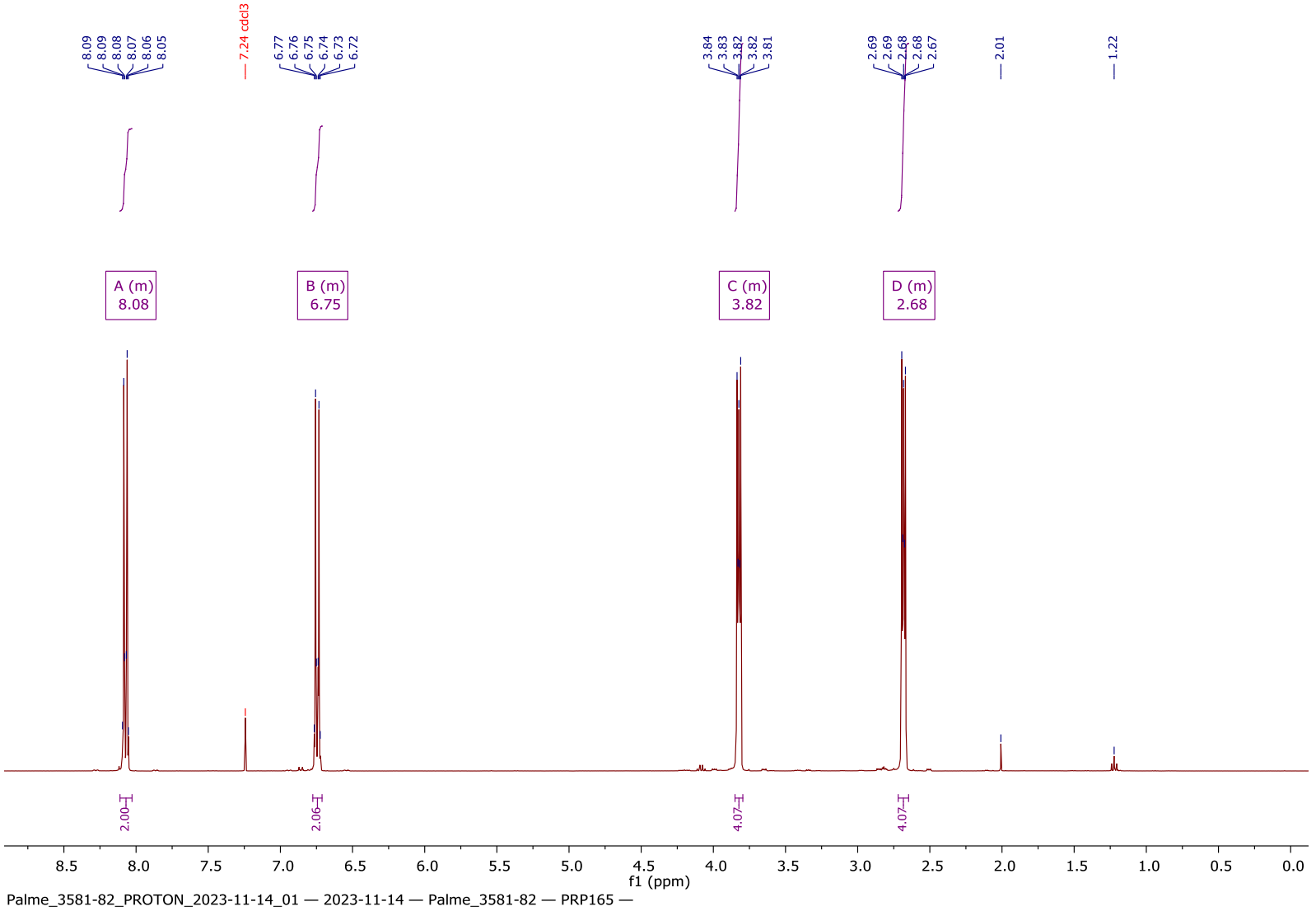


Figure S1 ^{1}H NMR spectrum of **1** in chloroform-*d*.

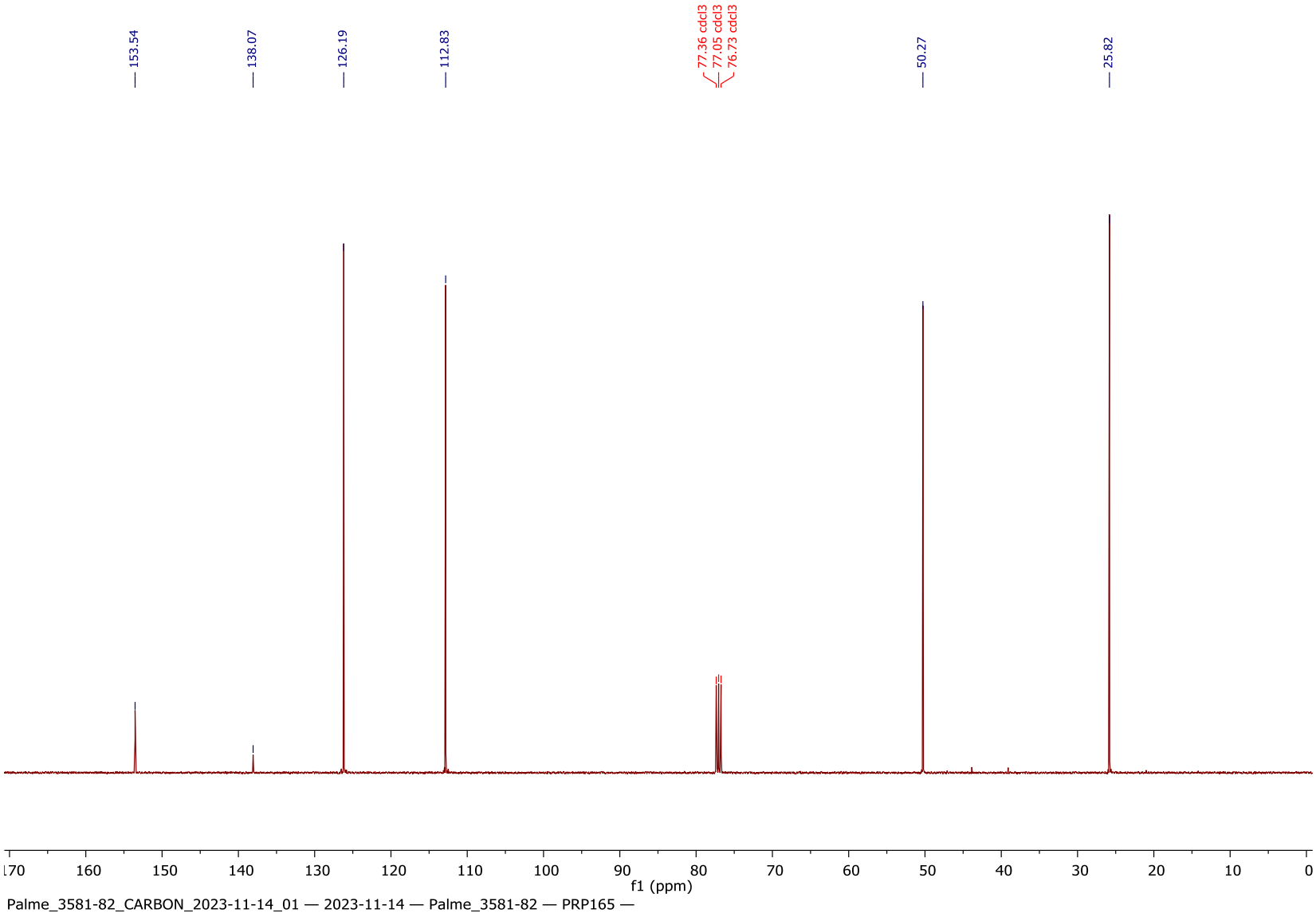


Figure S2 $^{13}C\{H\}$ NMR spectrum of **1** in chloroform-*d*.

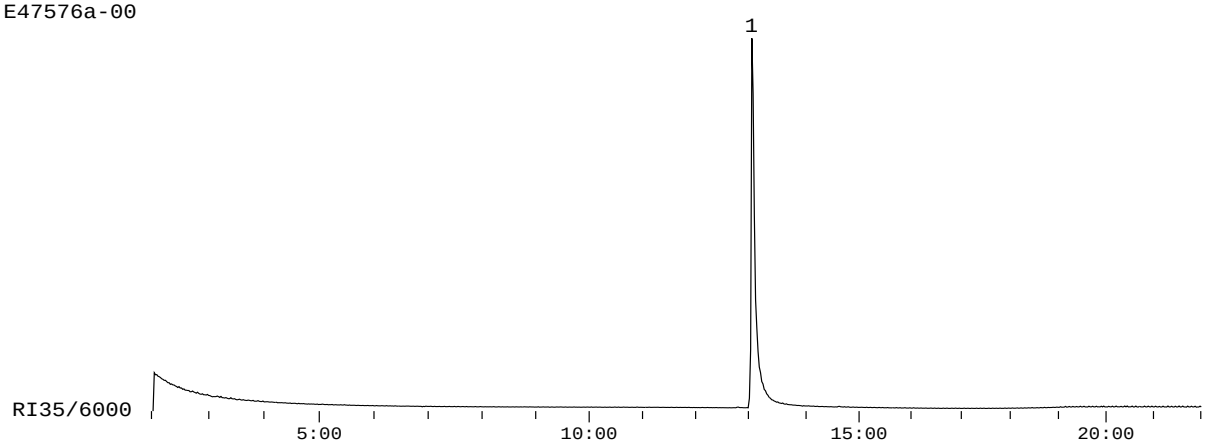
No.	MW.	Comment
1	224	Your proposed structure is possible Ref.-Spektr. Nr. OU6787:

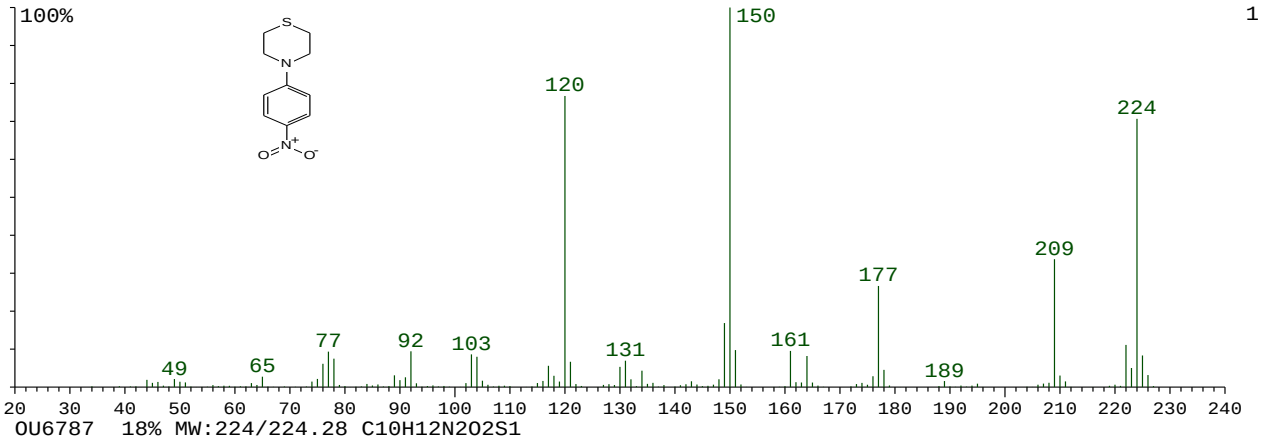
9.02.2024
File: E47576a-00.raw

Analyse: GOD-GB-170-01
LMN: Goddard,Richard

Messung:	GC-MS
Ionisierung:	GC-EI
Spektrometer:	QExactiveGC
Säule:	G211 XTI-5
Länge:	30
Temp.:	35-15-285-5
GC-Nr.:	-
MS-Nr.:	
Auswerter:	Kohler (2243)

E47576a-00





OU6787 18% MW:224/224.28 C10H12N2O2S1

34	0.19	62	0.20	87	0.16	109	0.37	136	1.12	162	1.29	195	0.90
39	0.22	63	1.05	88	0.27	110	0.28	137	0.12	163	1.21	196	0.05
41	0.16	64	0.56	89	3.10	114	0.17	138	0.53	164	8.19	204	0.10
42	0.19	65	2.74	90	1.83	115	1.07	140	0.16	165	1.20	206	0.63
44	1.91	66	0.14	91	2.58	116	1.62	141	0.48	166	0.39	207	0.92
45	1.12	67	0.07	92	9.43	117	5.61	142	0.75	167	0.08	208	1.14
46	1.36	69	0.16	93	1.00	118	2.98	143	1.53	172	0.19	209	33.69
47	0.38	71	0.08	94	0.12	119	1.46	144	0.68	173	0.80	210	3.04
48	0.18	73	0.15	95	0.28	120	76.70	145	0.26	174	1.11	211	1.50
49	2.12	74	1.45	96	0.44	121	6.67	146	0.34	175	0.62	212	0.07
50	1.41	75	2.15	97	0.16	122	0.80	147	0.64	176	2.86	219	0.34
51	1.23	76	6.14	98	0.30	123	0.30	148	2.06	177	26.64	220	0.63
52	0.13	77	9.34	99	0.10	127	0.58	149	16.87	178	4.54	221	0.32
54	0.05	78	7.49	101	0.05	128	0.77	150	100.00	179	0.42	222	11.11
55	0.10	79	0.56	102	1.05	129	0.54	151	9.75	188	0.26	223	5.03
56	0.52	80	0.27	103	8.62	130	5.33	152	0.69	189	1.59	224	70.68
57	0.24	82	0.11	104	7.99	131	6.95	153	0.05	190	0.19	225	8.33
58	0.37	83	0.16	105	1.68	132	2.05	158	0.05	191	0.07	226	3.17
59	0.34	84	0.83	106	0.61	133	0.25	159	0.08	192	0.40	227	0.27
60	0.11	85	0.42	107	0.15	134	4.32	160	0.24	193	0.12		
61	0.21	86	0.69	108	0.35	135	0.85	161	9.53	194	0.39		

OU6787 18% MW:224/224.28 C10H12N2O2S1 lim: 0.05%

Mass to be matched (m/z): 224.061650 Charge: 1

Mass Tolerance: ±0.005000
Restriction of atom numbers:

C	H	N	O	S
1-130	1-100	1-3	1-3	1-1

Number of calculated Formulas: 1

Formula	Diff.(ppm)	theor. m/z
C10 H12 N2 O2 S1	-1.12	224.061400

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MS-Nr.:	
Auswerter:	Kohler (2243)