

Supporting Information

Spirohexenolide A Targets Human Macrophage Migration Inhibitory Factor

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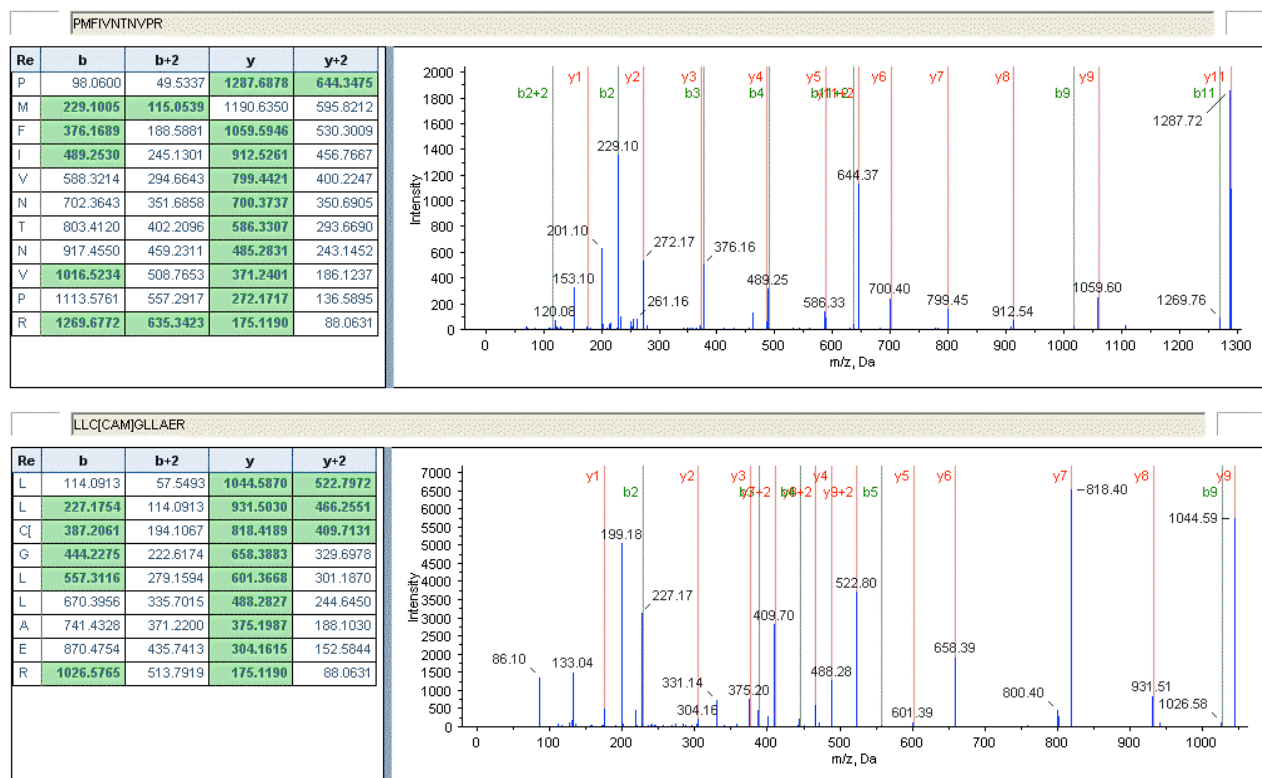
(a)

	Unused ProtScore	Total ProtScore	% Coverage	Accession #	Name	Peptides(95%)
1	27.35	27.35	44.1	gi 119395750	keratin 1 [Homo sapiens]	13
2	21.62	21.62	32	gi 40354192	keratin 10 [Homo sapiens]	10
3	12.37	12.37	25.8	gi 55956899	keratin 9 [Homo sapiens]	6
4	12	15.51	16.4	gi 47132620	keratin 2 [Homo sapiens]	7
5	8	8	27.5	gi 169217813	PREDICTED: hypothetical protein [Homo sapiens]	7
6	6	6	53.9	gi 4505185	macrophage migration inhibitory factor (glycosylation-inhibiting factor) [Homo sapiens]	8

(b)

Contribution	Confidence	Sequence	Δ Mass	Theoretical MW	Theoretical z	Score
2	99.00000095	AANVGWNNSTFA	0.01208865	1250.567993	2	16
2	99.00000095	LLCGLLAER	-0.043932918	1043.579712	2	12
2	99.00000095	PMFIVNTNVPR	0.020584069	1286.680542	2	13
0	99.00000095	AANVGWNNSTFA	0.01208865	1250.567993	2	15
0	0	AFGGSEPCALCSLHSIG KIGGAQNRSYSKLLCGL LAER	-0.02916191	4164.066895	4	7

(c)



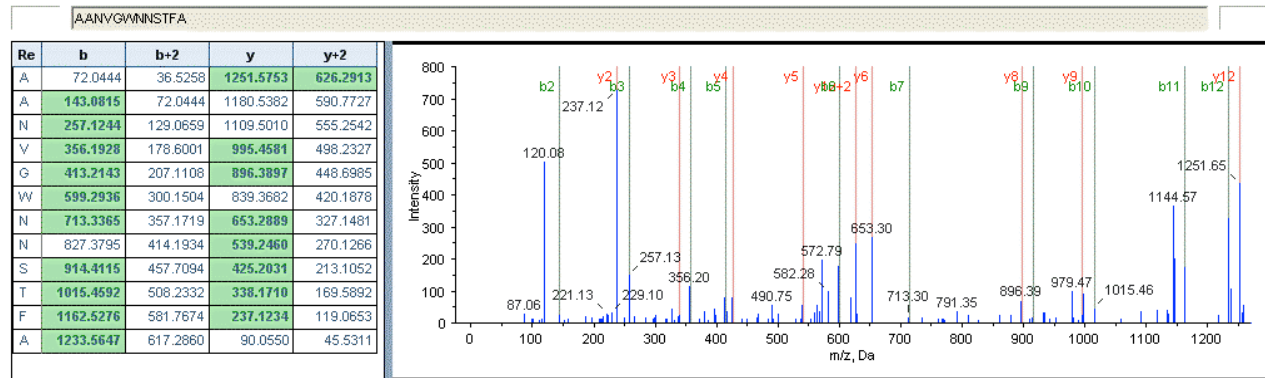


Figure S1. Protein ID data. (a) Protein ID of the 12 kDa band excised from SDS-PAGE. (b) List of peptides detected in the hMIF Protein ID group. (c) MS/MS fragmentation spectra of the first three hMIF peptides.

	Exp.1 (p-ratio / adjusted p-ratio)	Exp.2 (p-ratio / adjusted p-ratio)	Exp.3 (p-ratio / adjusted p-ratio)	Average	Standard deviation
L7	0.227 / 1	0.269 / 1	0.158 / 1	1	-
L8	0.451 / 2.019	0.558 / 2.073	0.319 / 2.019	2.04	0.03
L9	0.317 / 1.418	0.304 / 1.129	0.233 / 1.475	1.34	0.19
L10	0.458 / 2.052	0.596 / 2.215	0.344 / 2.177	2.15	0.09
L11	0.239 / 1.069	0.381 / 1.415	0.154 / 0.973	1.15	0.23

Table S1. p-Ratio data from the pAkt phosphorylation assay.

Figure S2. Spectral data for azide **5a**. ^1H -NMR (400 MHz) in CDCl_3 .

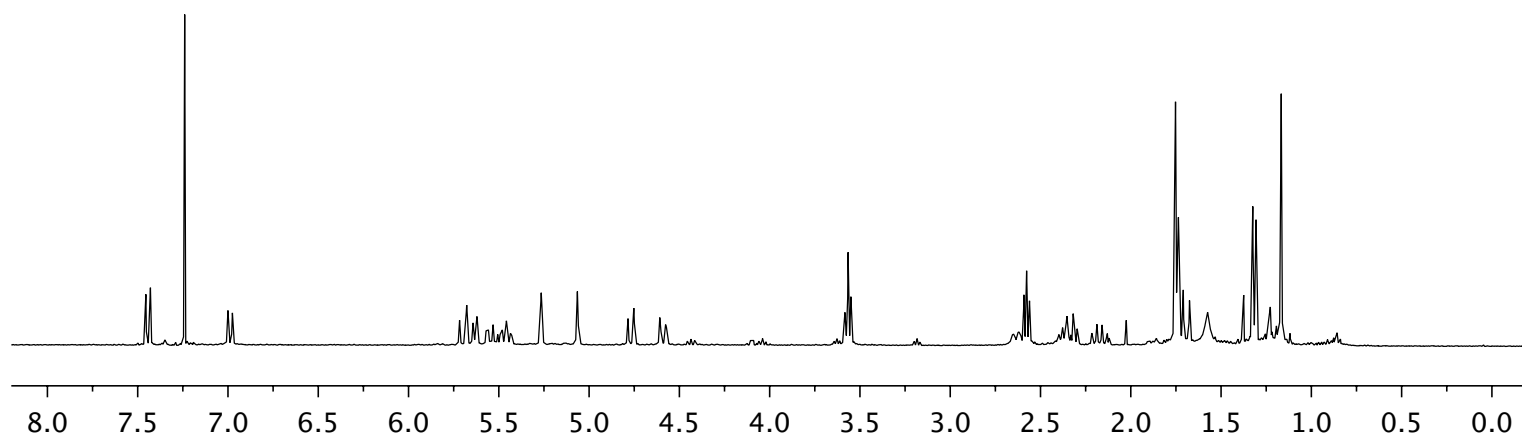


Figure S3. Spectral data for probe **2**. ^1H -NMR (400 MHz) and ^{13}C -NMR (125 MHz) spectra in CD_3OD .

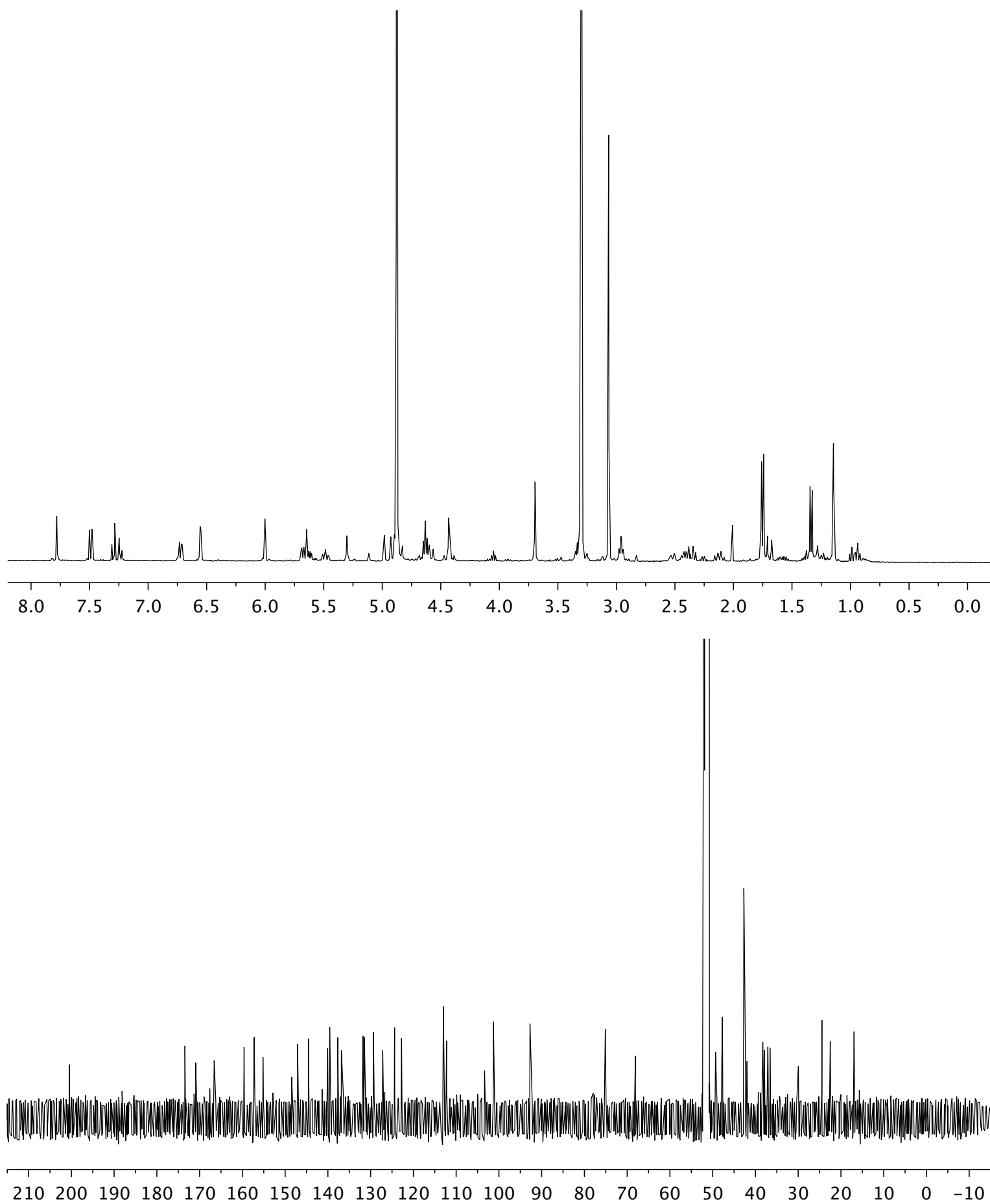


Figure S4. Spectral data for acid **5b**. ^1H -NMR (500 MHz) and ^{13}C -NMR (125 MHz) spectra in CDCl_3 .

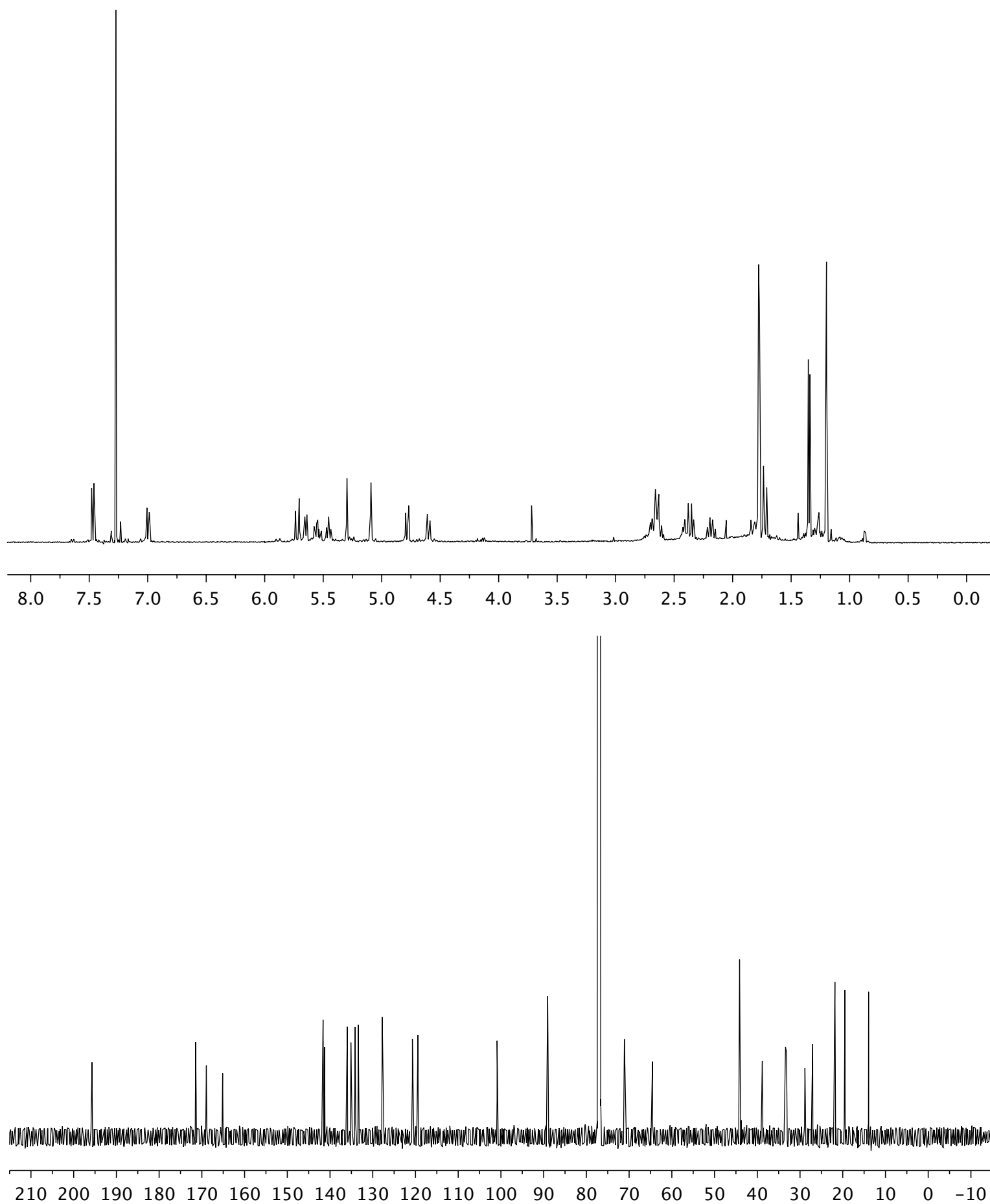


Figure S5. Spectral data for probe **3**. ^1H -NMR (500 MHz) in CDCl_3 and ^{13}C -NMR (125 MHz) spectra in CD_3OD .

