

## Supplementary Material

### Versatile synthesis of novel tetrahydroquinolines as potentially active semicarbazide-sensitive amine oxidase (SSAO) inhibitors via *tert*-amino effect

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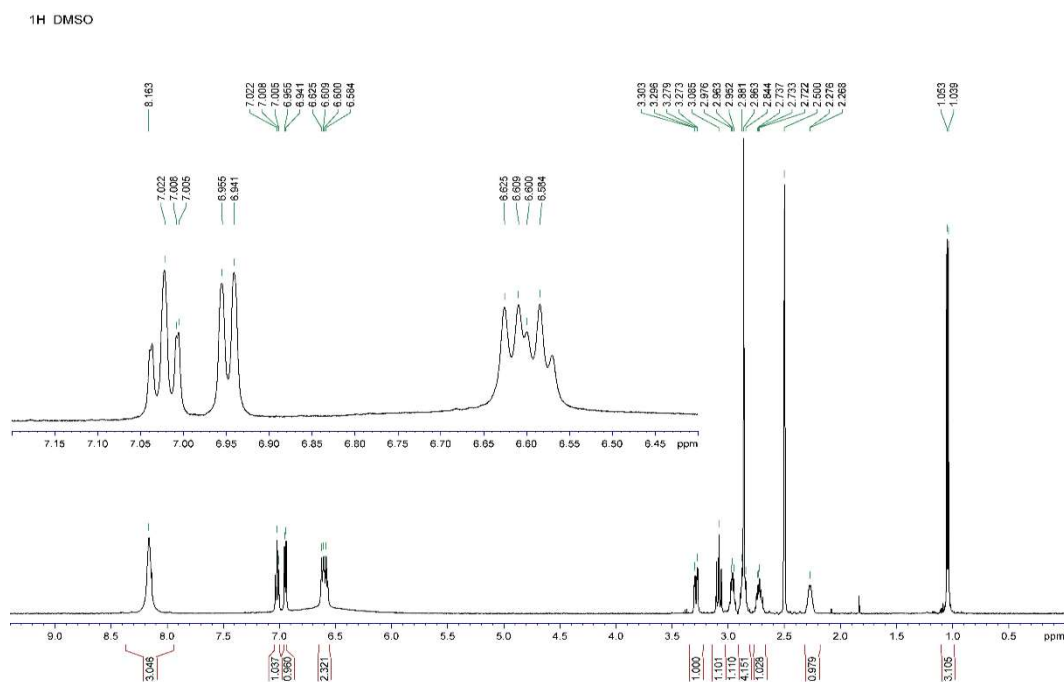
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Budapest, Hungary*

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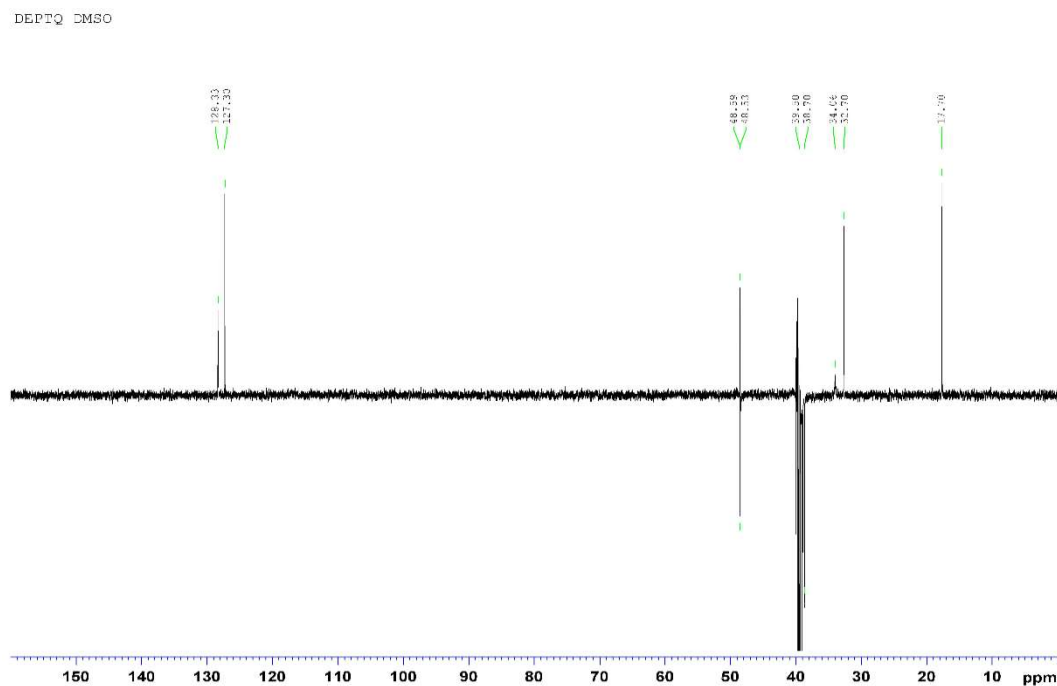
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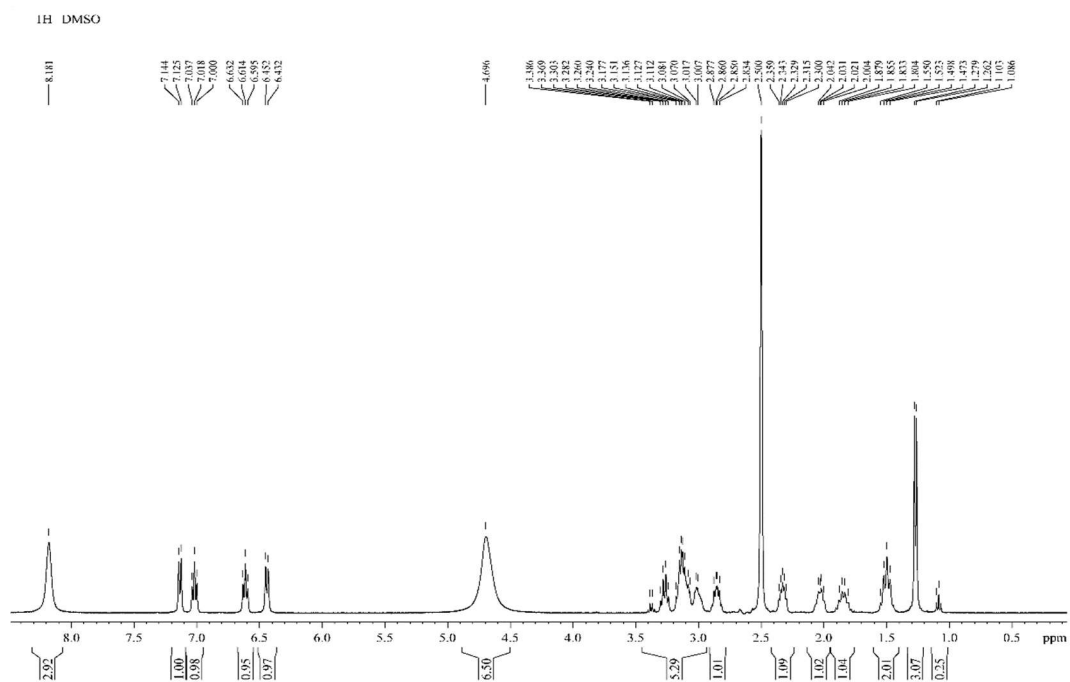
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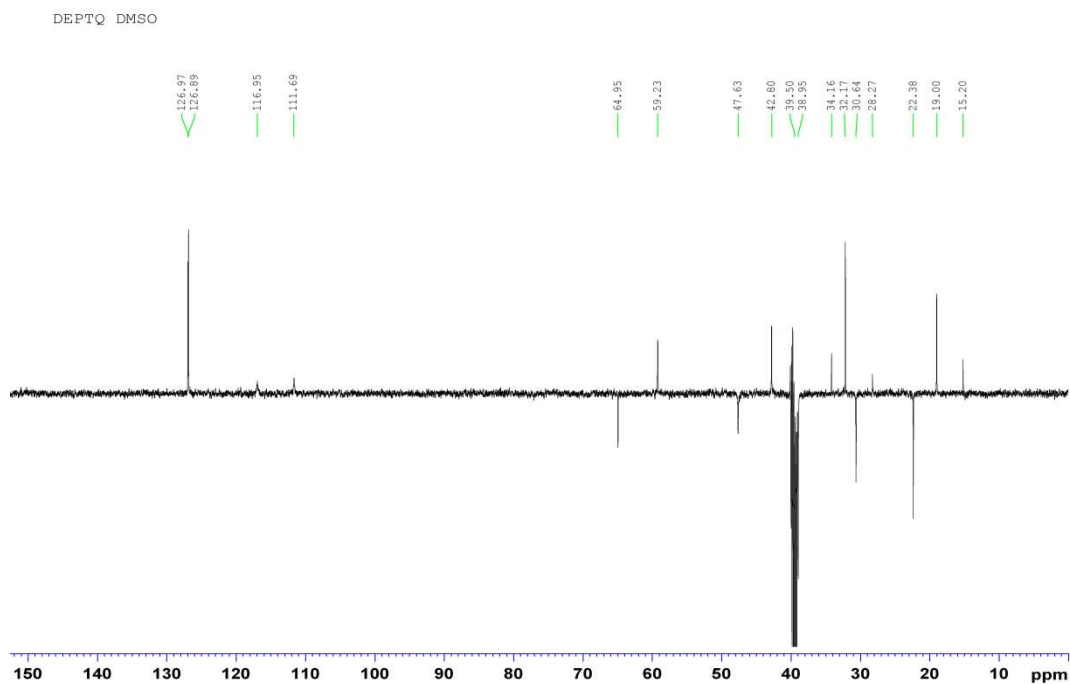
<sup>1</sup>H NMR spectrum of (*cis*-(±)-1,4-Dimethyl-1,2,3,4-tetrahydroquinolin-3-yl)methanamine dihydrochloride (**11a cis**); 500 MHz.



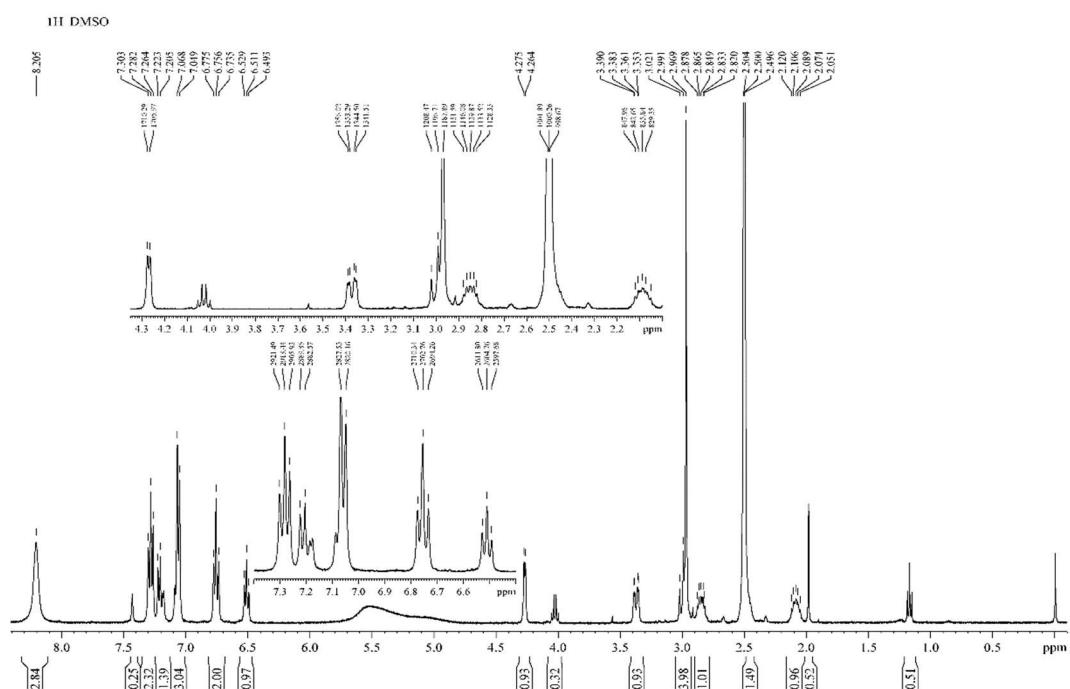
DEPTQ spectrum of (*cis*-(±)-1,4-Dimethyl-1,2,3,4-tetrahydroquinolin-3-yl)methanamine dihydrochloride (**11a cis**); 125 MHz.



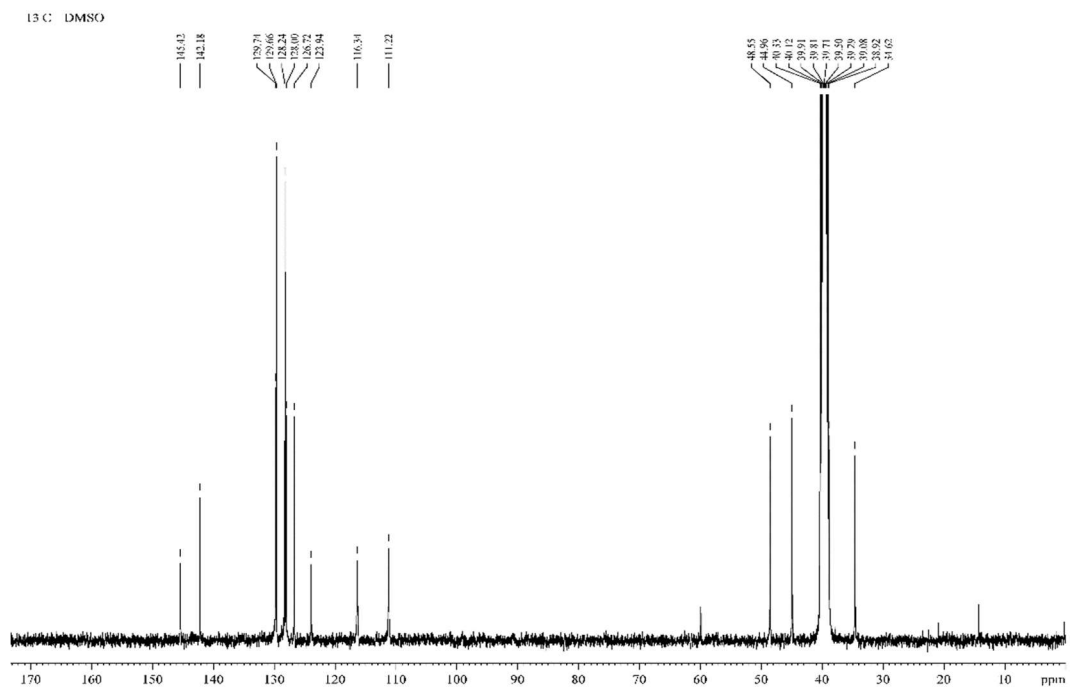
<sup>1</sup>H NMR spectrum of [cis-trans-(±)-5-Methyl-1,2,3,3a,4,5-hexahydropyrrolo[1,2-a]quinolin-4-yl]methanamine dihydrochloride (**11b cis-trans**); 400 MHz.



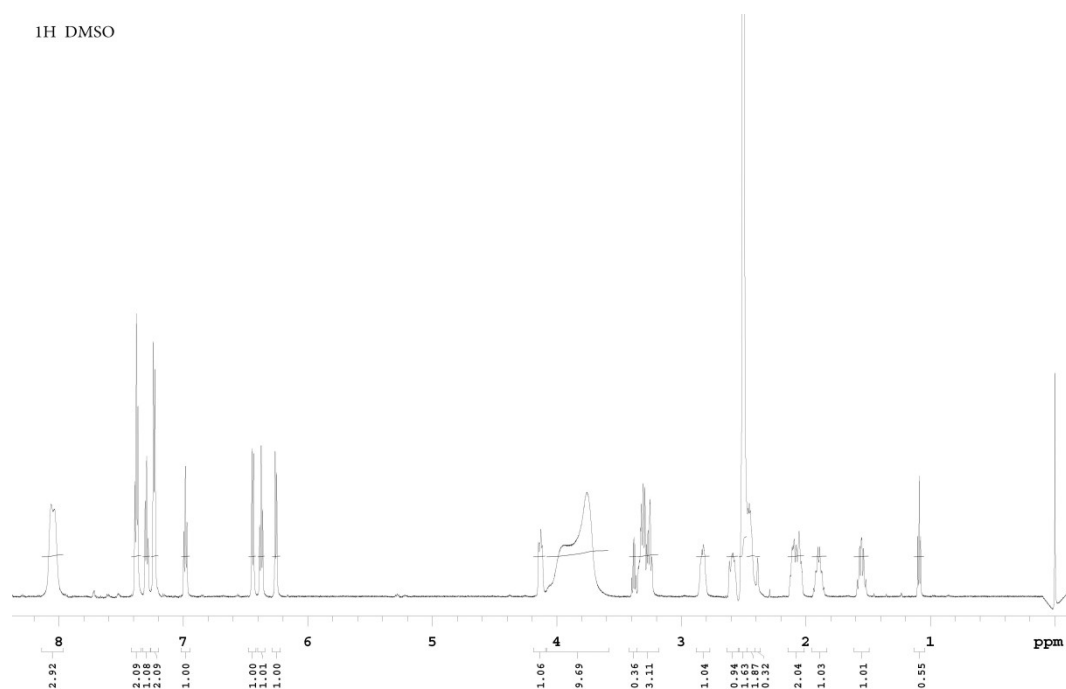
DEPTQ spectrum of [cis-trans-(±)-5-Methyl-1,2,3,3a,4,5-hexahydropyrrolo[1,2-a]quinolin-4-yl]methanamine dihydrochloride (**11b cis-trans**); 125 MHz.



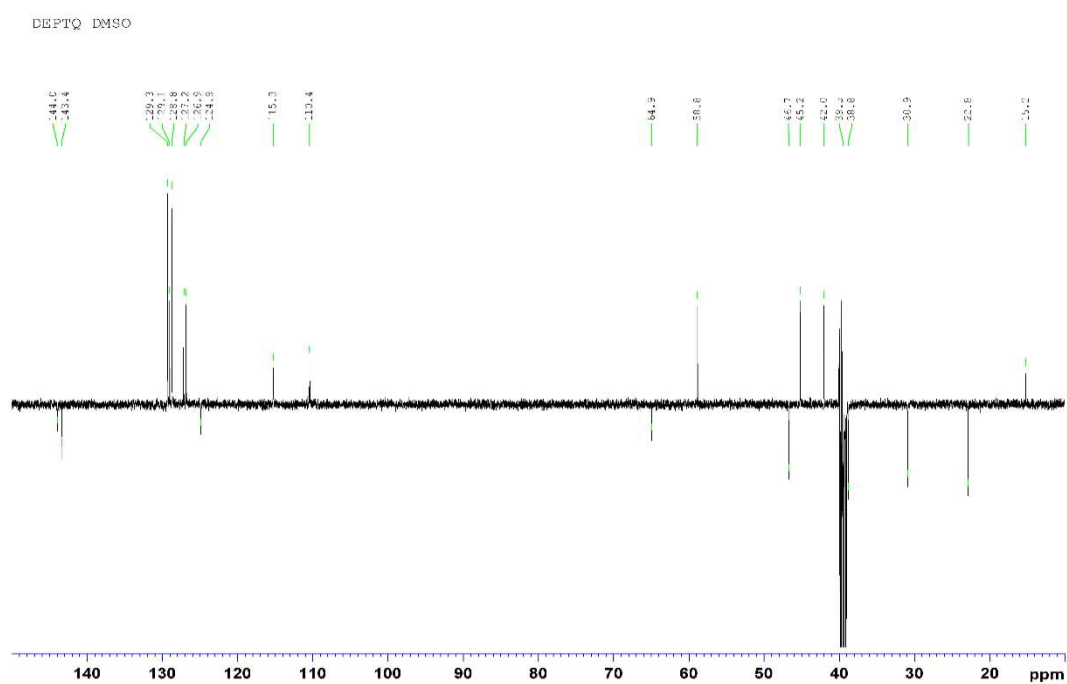
$^1\text{H}$  NMR spectrum of [*cis*-(±)-1-Methyl-4-phenyl-1,2,3,4-tetrahydroquinolin-3-yl]methanamine dihydrochloride (**12a cis**); 400 MHz.



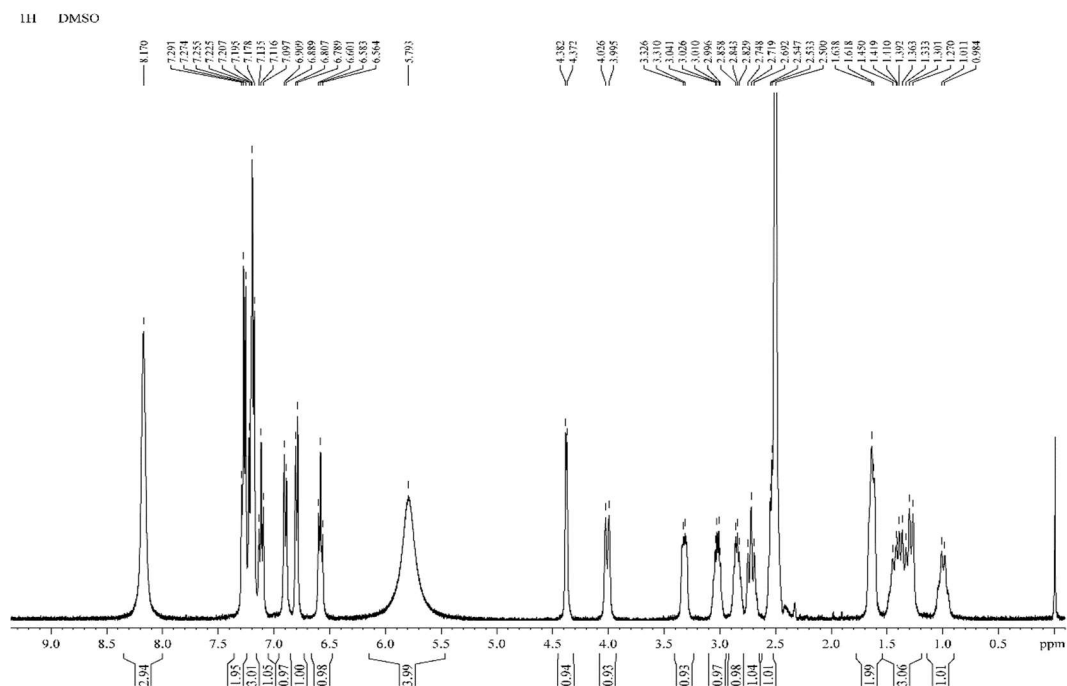
$^{13}\text{C}$  NMR spectrum of [*cis*-(±)-1-Methyl-4-phenyl-1,2,3,4-tetrahydroquinolin-3-yl]methanamine dihydrochloride (**12a cis**); 100 MHz.



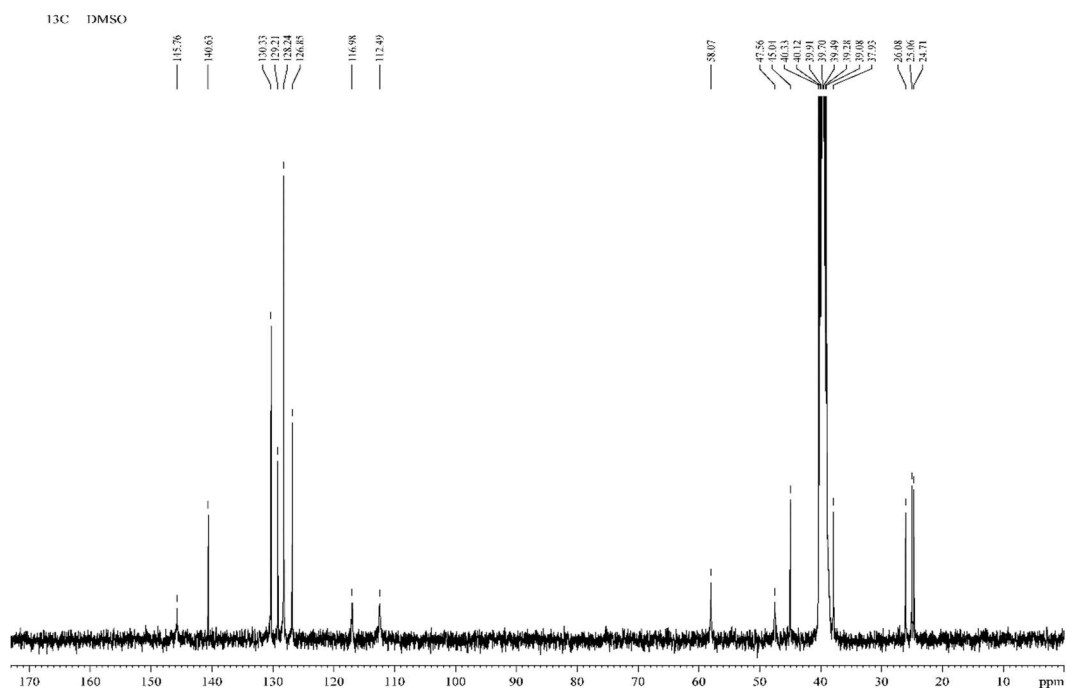
<sup>1</sup>H NMR spectrum of [*cis-trans*-(±)-5-Phenyl-1,2,3,3a,4,5-pyrrolo[1,2-*a*]quinolin-4-yl]methanamine dihydrochloride (**12b cis-trans**); 600 MHz.



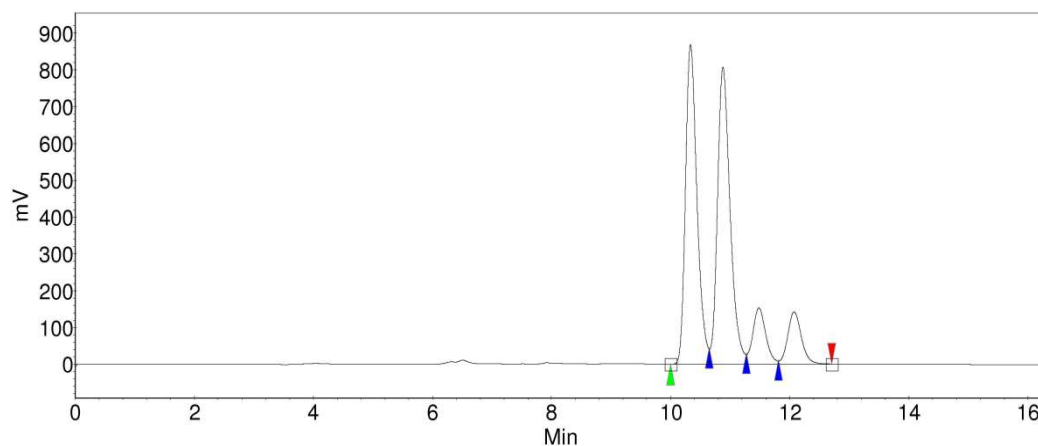
DEPTQ spectrum of [*cis-trans*-(±)-5-Phenyl-1,2,3,3a,4,5-pyrrolo[1,2-*a*]quinolin-4-yl]methanamine dihydrochloride (**12b cis-trans**); 125 MHz.



$^1\text{H}$  NMR spectrum of [*cis-cis*-(±)-6-Phenyl-1*H*-2,3,4,4*a*,5,6-hexahydropyrido[1,2-*a*]quinolin-5-yl]methanamine dihydrochloride (**12c cis-cis**); 400 MHz.

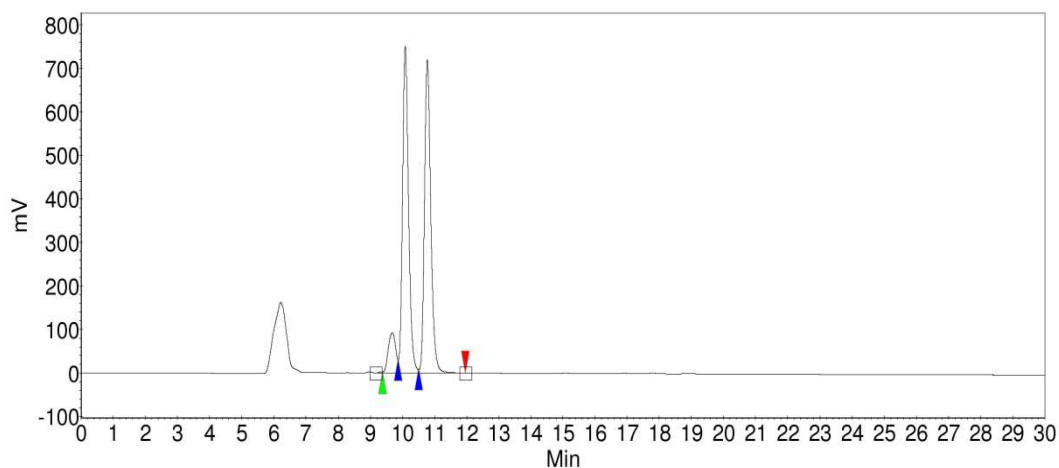


$^{13}\text{C}$  NMR spectrum of [*cis-cis*-(±)-6-Phenyl-1*H*-2,3,4,4*a*,5,6-hexahydropyrido[1,2-*a*]quinolin-5-yl]methanamine dihydrochloride (**12c cis-cis**); 100 MHz.



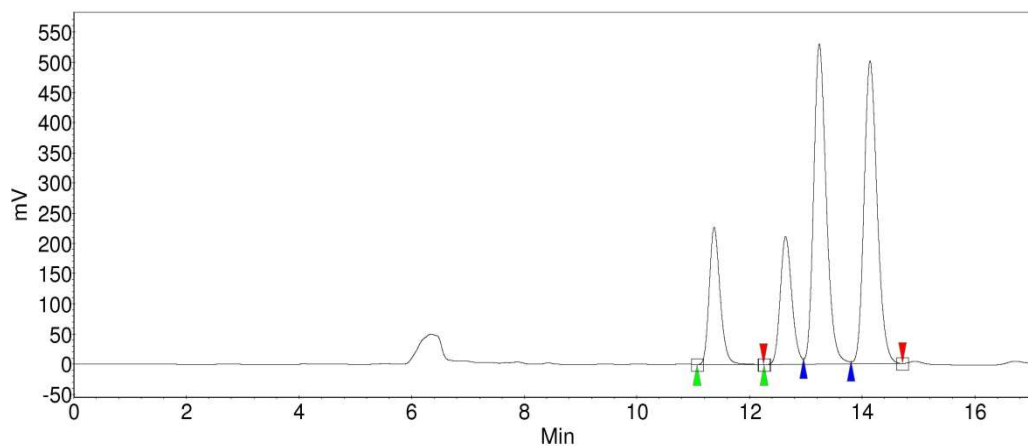
Index	Name	Time [Min]	Quantity [% Area]	Height [mV]	Area [mV.Min]	Area % [%]
1	UNKNOWN	10.337	41.38	867.9	193.5	41.378
2	UNKNOWN	10.882	42.35	806.9	198.1	42.352
3	UNKNOWN	11.485	8.24	152.7	38.5	8.238
4	UNKNOWN	12.075	8.03	141.9	37.6	8.032
Total			100.00	1969.4	467.7	100.000

HPLC chromatogram of *cis/trans*-(±)-5-Methyl-1,2,3,3a,4,5-hexahydropyrrolo[1,2-*a*]quinoline-4,4-dicarbonitrile (**5b cis/trans**) before the separation of the diastereomers; OJ-H, mobile phase ratio 10:90.



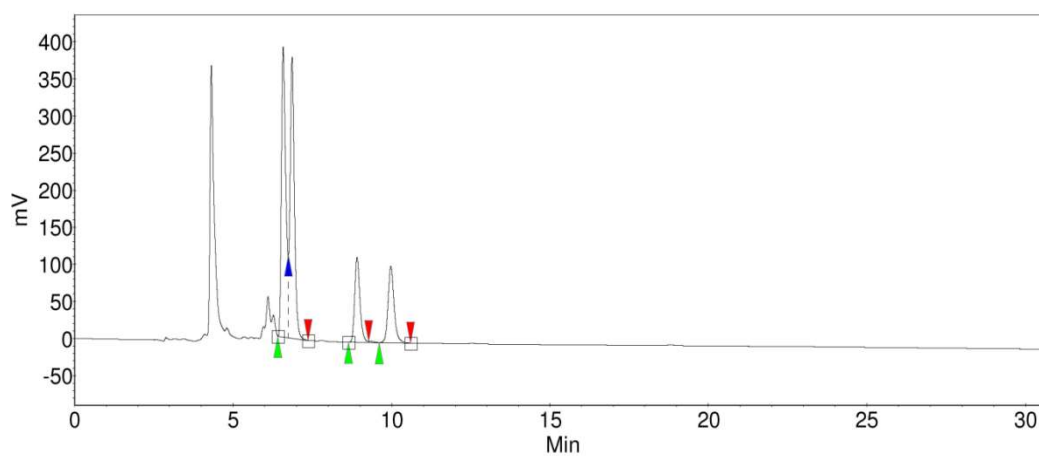
Index	Name	Time [Min]	Quantity [% Area]	Height [mV]	Area [mV.Min]	Area % [%]
1	UNKNOWN	9.683	7.05	92.6	24.8	7.054
2	UNKNOWN	10.087	46.29	750.3	162.7	46.291
3	UNKNOWN	10.772	46.65	720.0	163.9	46.655
Total			100.00	1562.8	351.4	100.000

HPLC chromatogram of *cis/trans*-(±)-6-Methyl-1*H*-2,3,4,4a,5,6-hexahydropyrido[1,2-*a*]quinoline-5,5-dicarbonitrile (**5c cis/trans**) before the separation of the diastereomers; AD-H, mobile phase ratio 75:25.



Index	Name	Time [Min]	Quantity [% Area]	Height [mV]	Area [mV.Min]	Area % [%]
1	UNKNOWN	11.373	13.58	227.1	50.8	13.584
2	UNKNOWN	12.643	13.51	211.7	50.6	13.512
3	UNKNOWN	13.240	36.69	530.4	137.3	36.694
4	UNKNOWN	14.142	36.21	502.1	135.5	36.210
Total			100.00	1471.3	374.2	100.000

HPLC chromatogram of *cis/trans*-(±)-1,4-Dimethyl-1,2,3,4-tetrahydroquinoline-3-carbonitrile (**7a cis/trans**) before the separation of the diastereomers; OJ-H, mobile phase ratio 50:50.

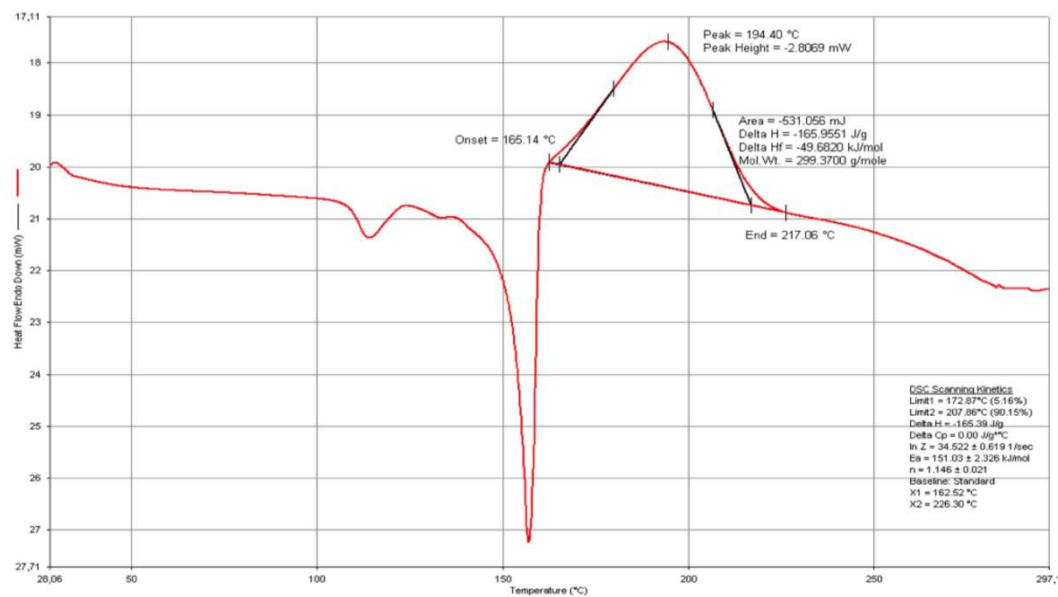


Index	Name	Time [Min]	Quantity [% Area]	Height [mV]	Area [mV.Min]	Area % [%]
1	UNKNOWN	6.580	36.97	391.1	61.7	36.974
2	UNKNOWN	6.862	36.40	379.2	60.8	36.401
3	UNKNOWN	8.910	13.07	114.8	21.8	13.070
4	UNKNOWN	9.975	13.56	103.5	22.6	13.555
Total			100.00	988.6	166.9	100.000

HPLC chromatogram of *cis-cis/cis-trans*-(±)-6-Phenyl-1H-2,3,4,4a,5,6-hexahydropyrido[1,2-a]quinoline-5-carbonitrile (**8c cis-cis/cis-trans**) before the separation of the diastereomers; AD-H, mobile phase ratio 50:50.

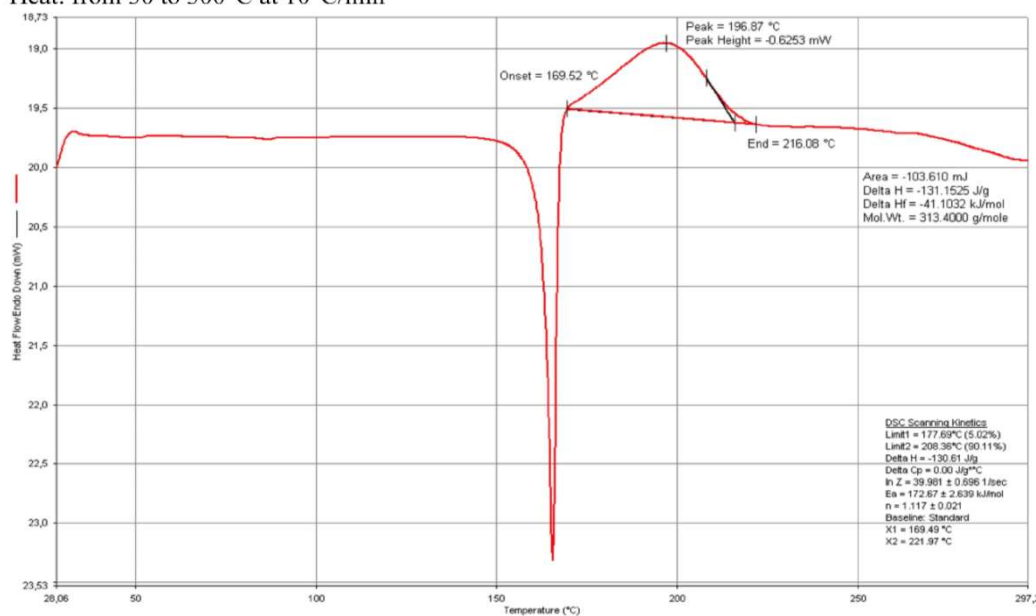


wt: 3.20 mg  
Heat: from 30 to 300°C at 10°C/min

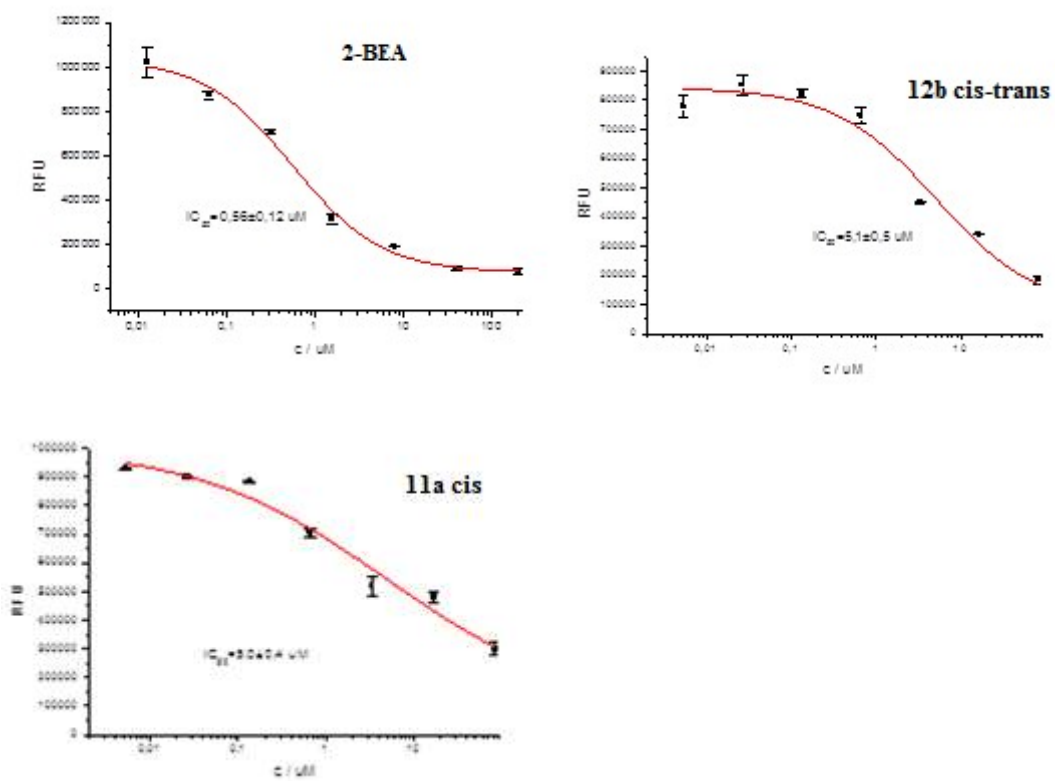


DSC curve of 2-{Phenyl[2''-(pyrrolidin-1''-yl)phenyl]methylidene}propanedinitrile (**4b**)

wt: 0.79 mg  
Heat: from 30 to 300°C at 10°C/min



DSC curve of 2-{Phenyl[2''-(piperidin-1''-yl)phenyl]methylidene}propanedinitrile (**4c**)



Dose response curves of 2-BEA, compound **11a cis** and **12b cis-trans**