crystals

Weak Interactions in the Structures of Newly Synthesized (–)-Cytisine Amino Acid Derivatives

Anna K. Przybył *, Anita M. Grześkiewicz and Maciej Kubicki *

N-[glycine-(*N*-phtaloyl)]cytisine (3A)

$C_{21}H_{19}N_3O_4$
MW 377 g/mol
creamy crystals
m.p. > 240 °C

Spectral analysis

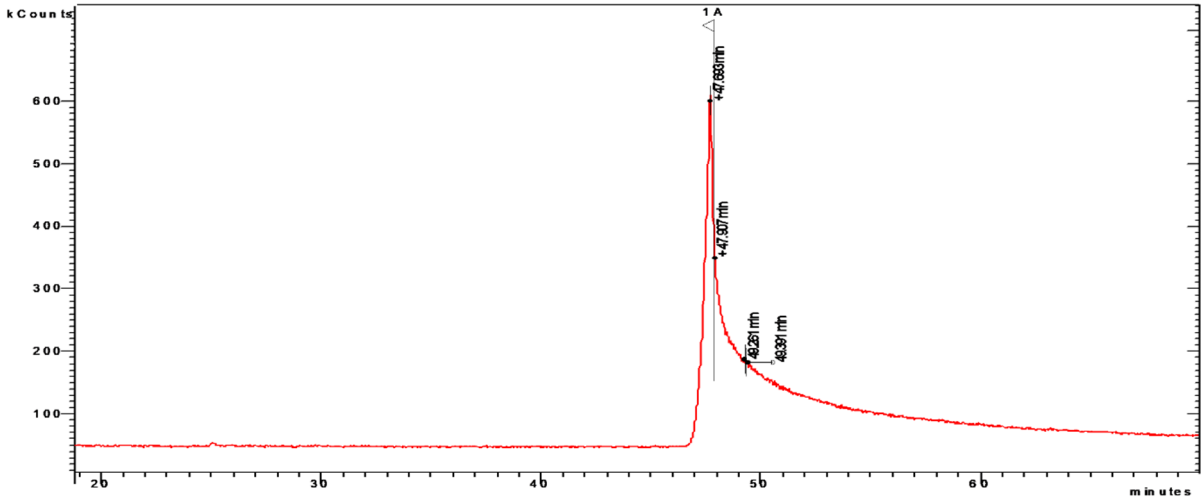


Figure S1. GC-MS spectrum of the probe with *N*-[glycine-(*N*-phtaloyl)]cytisine.

EI-MS: Rt 47.843; m/z 377 (M^+, 31%), 160 (100%), 146 (88%), 189 (40%), 147 (39%), 77 (30%), 133 (28%)

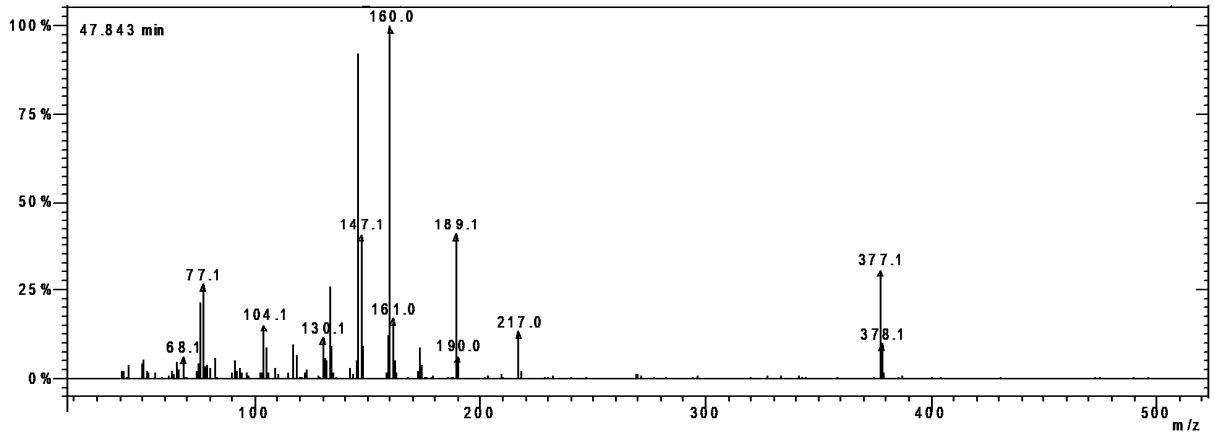


Figure S2. EI-MS spectrum of *N*-[glycine-(*N*-phtaloyl)]cytisine.

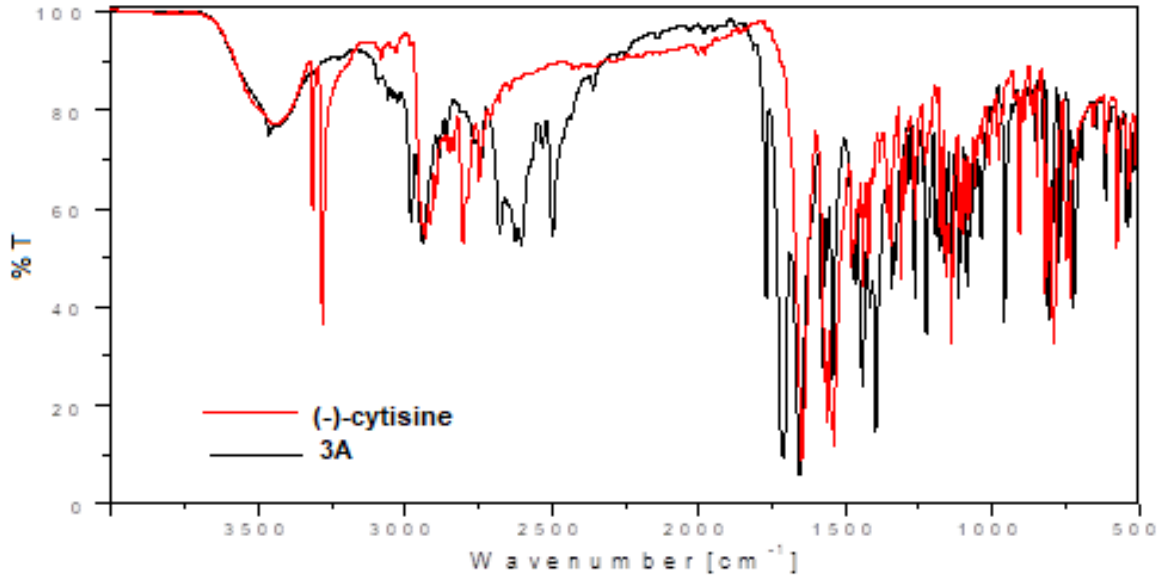


Figure S3. Comparison of the FTIR spectra of (-)-cytisine (**1**, red) and its *N*-[glycine-(*N*-phtaloyl)]cytisine (**3A**, black) (KBr).

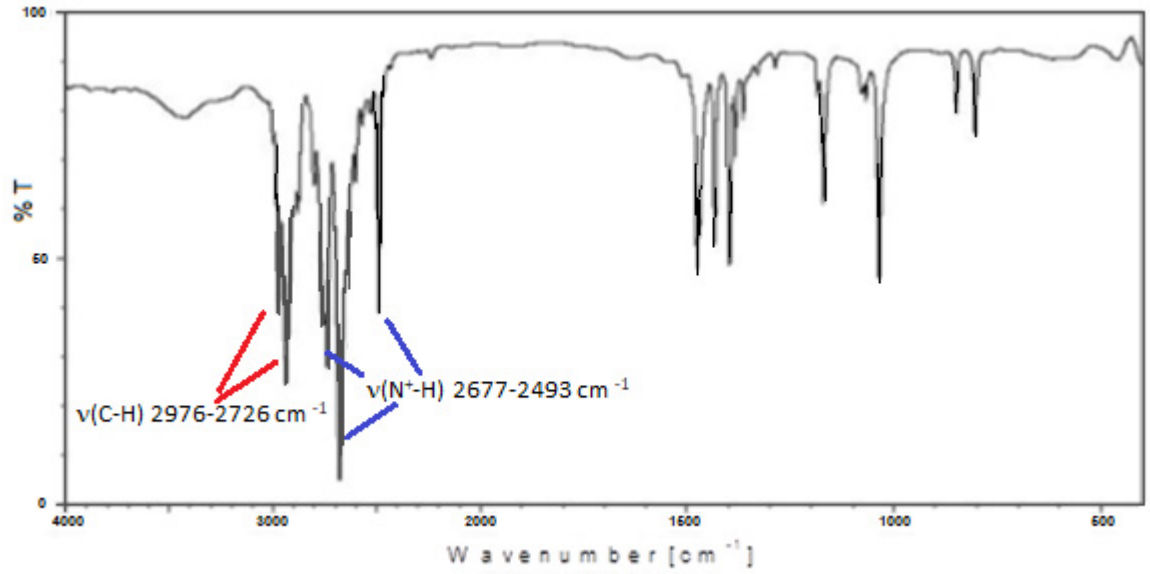


Figure S4. FTIR spectra of triethylamine x HCl (KBr).

FTIR spectra shows the intense bands in the area of 2677-2493 cm-1, are derived from the stretching vibrations ν (N + -H) of HCl x Et_3N salt impurities (Fig. 6). After subsequent purification on the Al_2O_3 column, these bands are no longer observed.

IR (KBr) [cm^{-1}**]:** 3462-3434, 3092-3023, 2977-2739, 1686,1655, 1769, 1711, 1579-1543

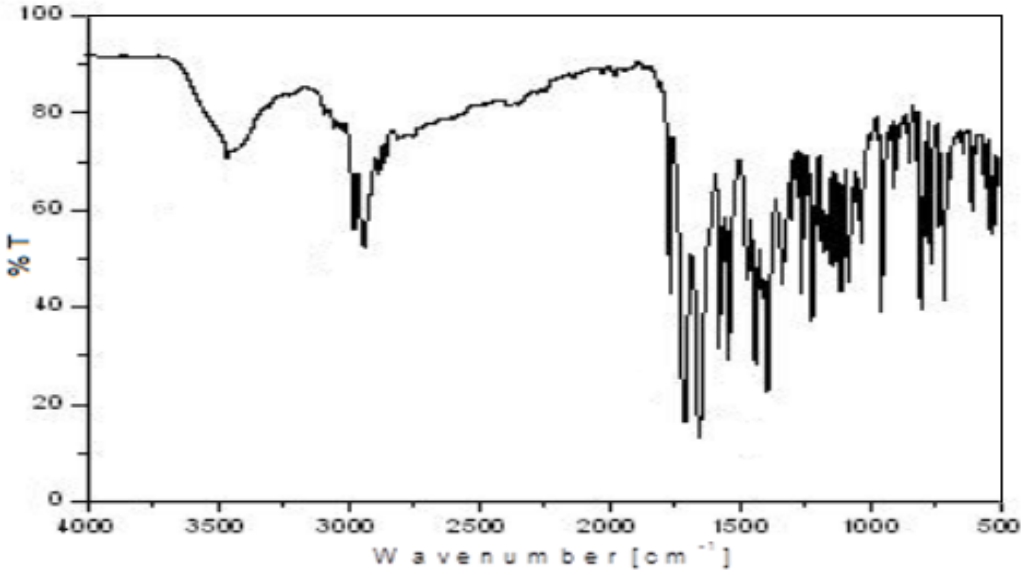


Figure S5. FTIR spectrum of *N*-[glycine-(*N*-phtaloyl)]cytisine (KBr).

^{13}C NMR ($CDCl_3$) ***(cis/ trans)*****:** 167.4; 165.1/164.6; 163.2; 147.7/147.7; 138.8/138.4; 133.9; 132.0; 123.3; 118.3/117.0; 105.6/104.7; 52.3/50.9; 49.4/48.3; 48.7/48.7; 45.7; 34.8/34.1; 27.3/27.3; 26.1/25.9 ppm.

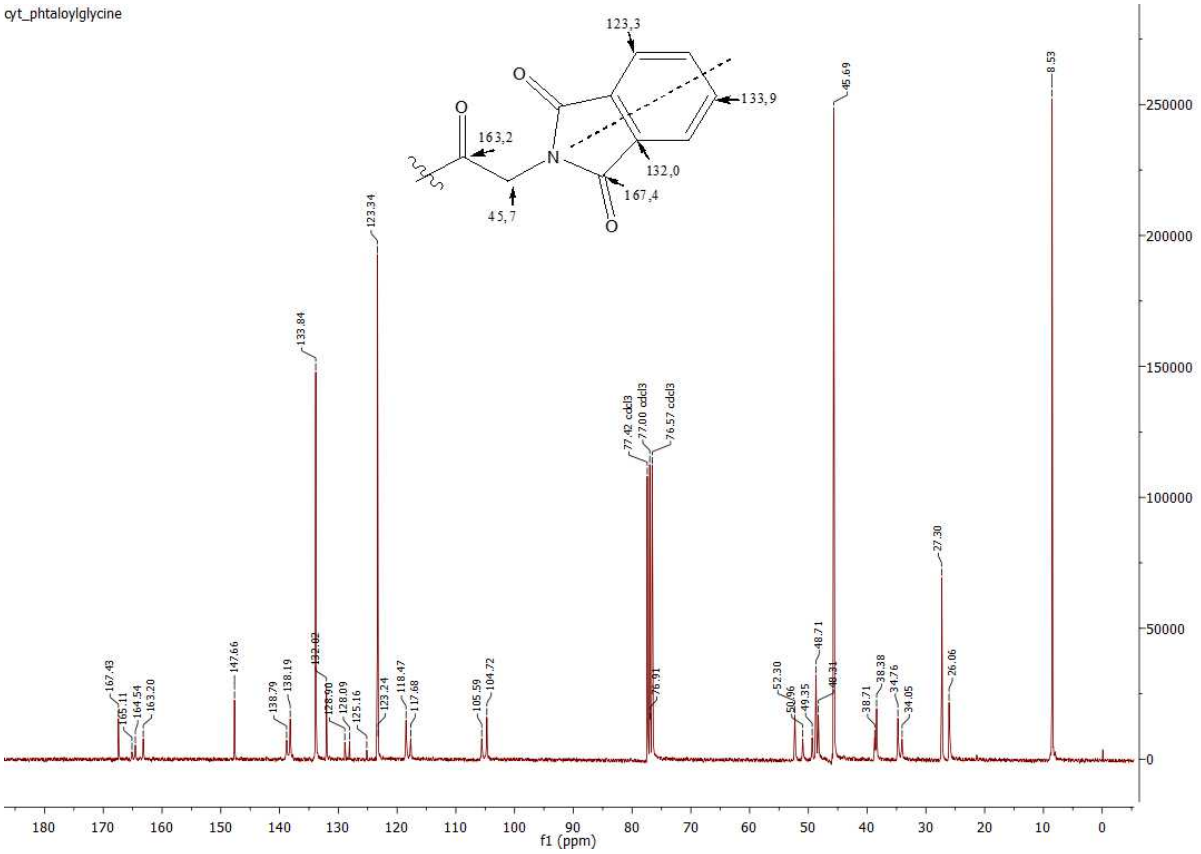


Figure S6 . ^{13}C NMR spectrum of *N*-[glycine-(*N*-phtaloyl)]cytisine ($CDCl_3$).

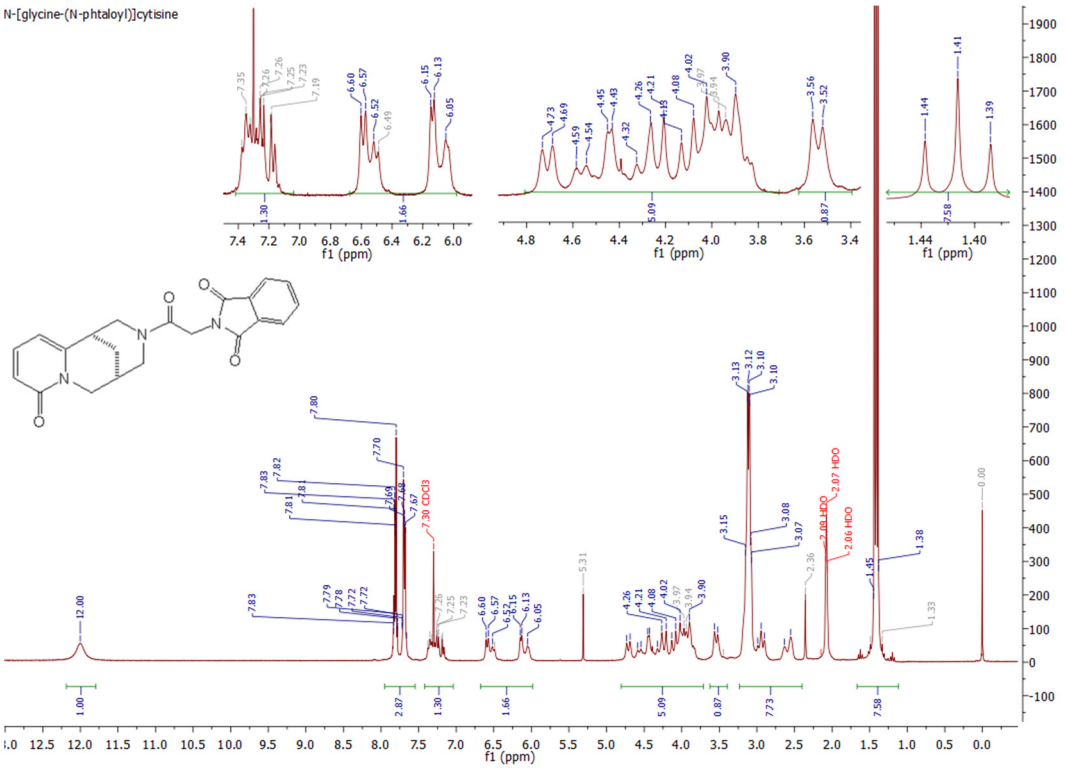


Figure S7. ^{1}H NMR spectrum of *N*-[glycine-(*N*-phtaloyl)]cytisine ($CDCl_3$).

***N*-[β-alanine-(*N*-phtaloyl)]cytisine (3B)**

$C_{22}H_{21}N_3O_4$

MW 391 g/mol

yellowish precipitate

yield 54%

m.p. 212-214 °C

Spectral analysis:

EI-MS Rt 69.855; m/z: 391 (M^+, 21%), 147 (100%), 146 (83%), 190 (49%), 189 (30%), 77 (30%), 76(27%).

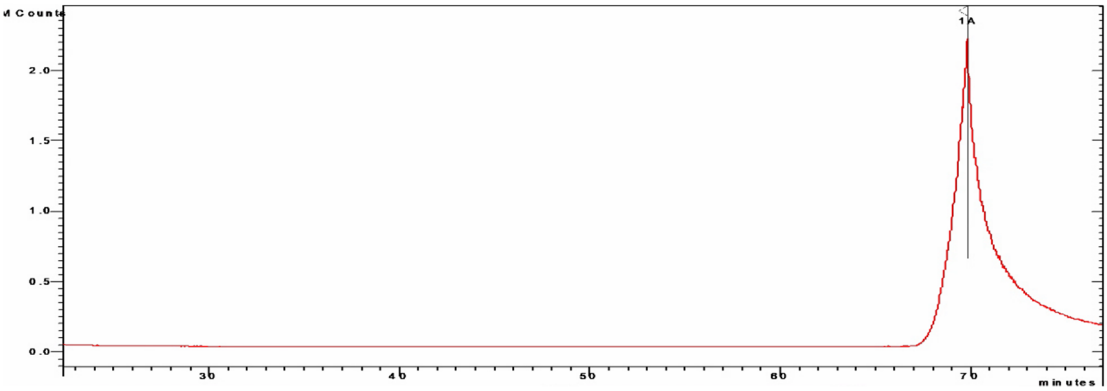


Figure S8. GC-MS spectrum of the probe with *N*-[β-alanine-(*N*-phtaloyl)]cytisine (**3B**).

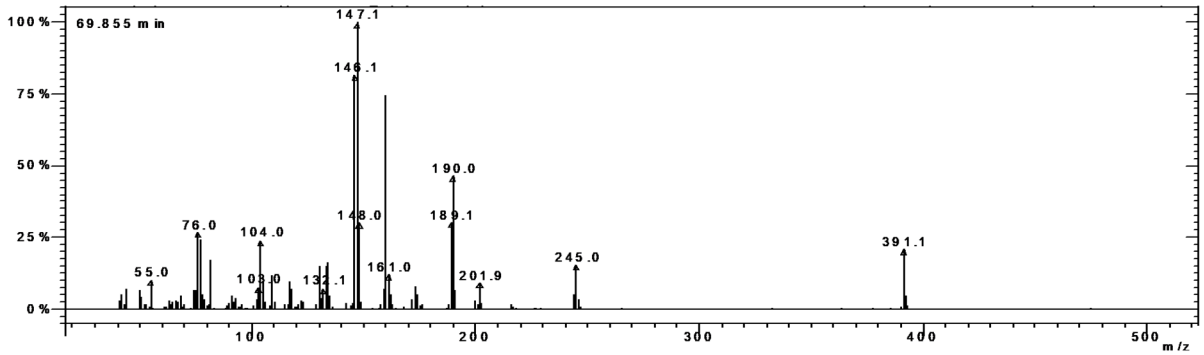


Figure S9. EI-MS spectrum of *N*-[β-alanine-(*N*-phtaloyl)]cytisine (**3B**).

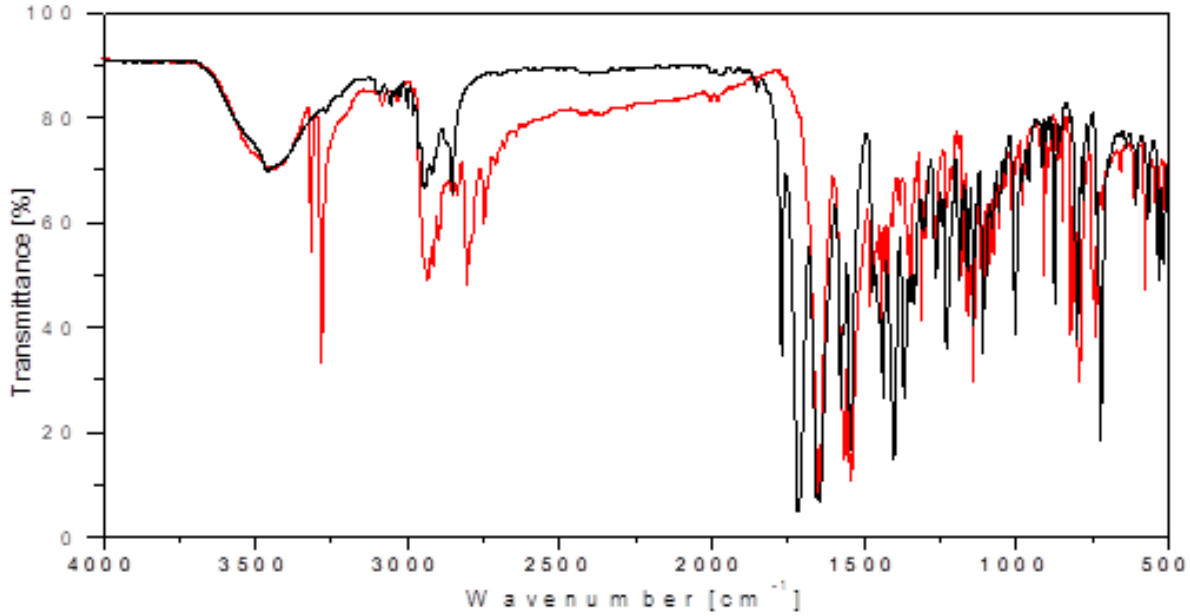


Figure S10. Comparison of the FTIR spectra of (-)-cytisine (**1,** red) and its *N*-[β-alanine (*N*-phtaloyl)]cytisine (**3B**, black) (KBr).

IR (KBr) 3459, 3096-3000, 2979-2852, 1654,1645, 1769, 1716, 1575-1543 [cm^{-1}].

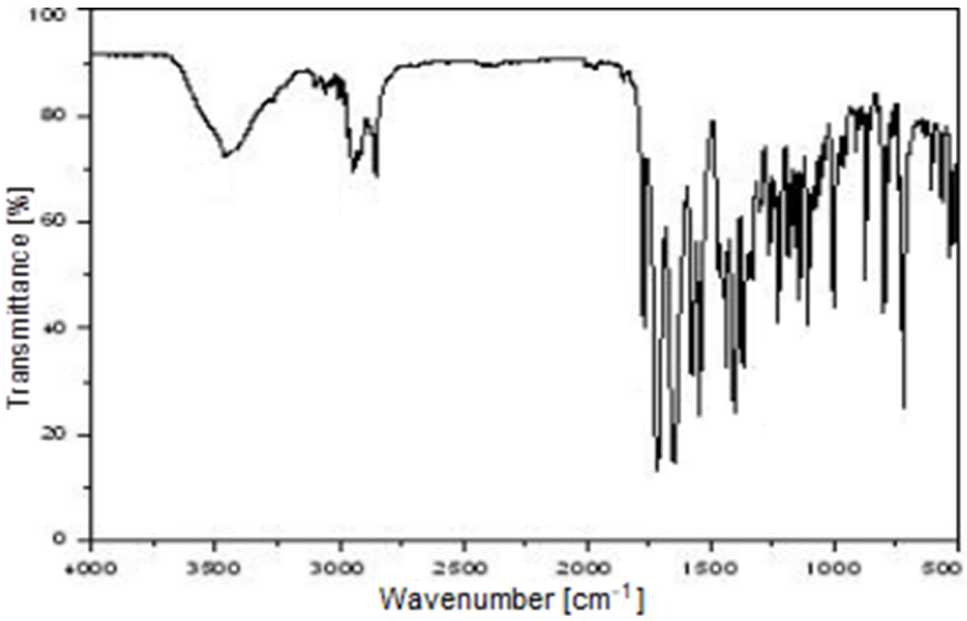


Figure S11 . FTIR spectrum of *N*-[β-alanine (*N*-phtaloyl)]cytisine **3B** (KBr).

^{13}C NMR ($CDCl_3$) *(cis/ trans)*: 169.7; 168.0; 163.6/163.5; 148.4/148.2; 139.5/139.1; 133.9; 131.7; 123.1; 117.4/116.9; 106.6/105.9; 52.78/51.4; 49.4/48.7; 48.4/47.5; 47.5; 34.7/34,0; 31.2; 27,2/27.0; 25.7/25.6 [ppm].

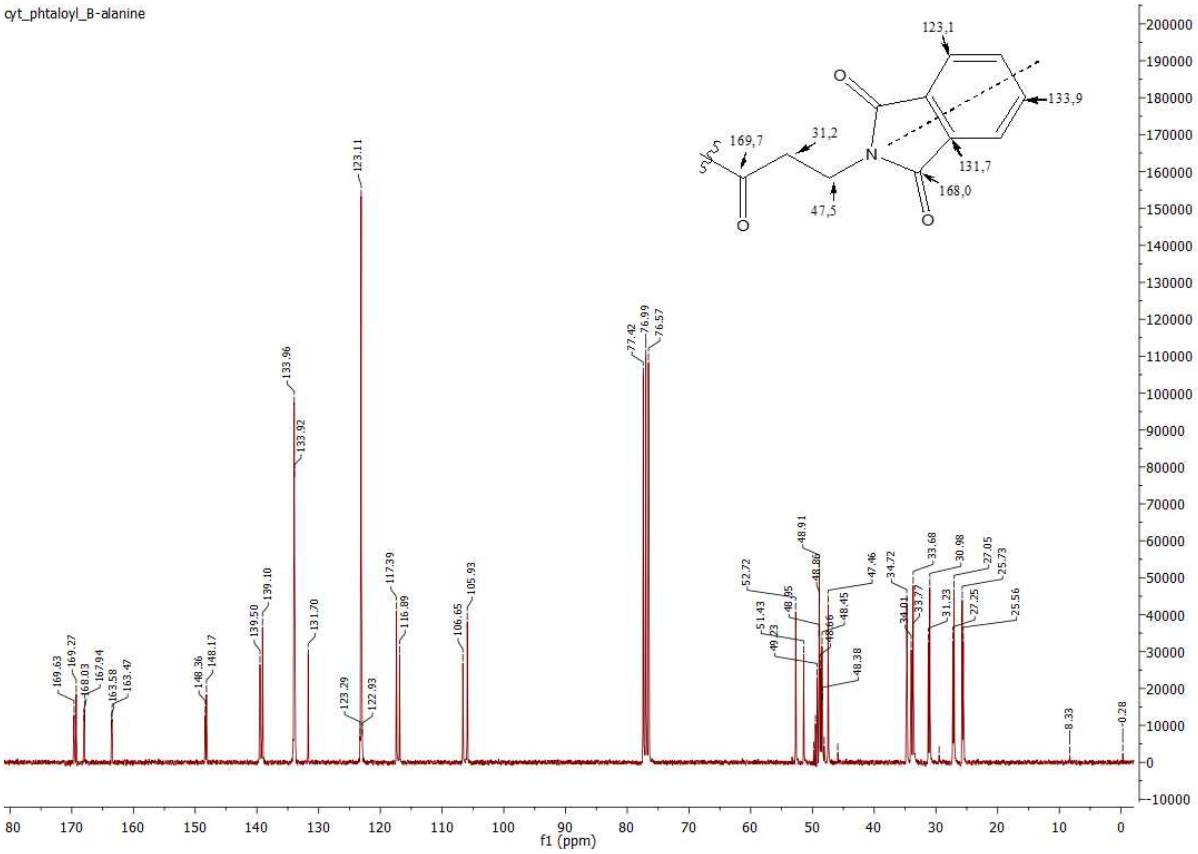


Figure S12. ^{13}C NMR spectrum of *N*-[β-alanine (*N*-phtaloyl)]cytisine ($CDCl_3$).

***N*-[*D,L*-valine-(*N*-phtaloyl)]cytisine (3C)**

$C_{24}H_{25}N_3O_4$

MW 419 g/mol

creamy foam

yield 61%

m.p. 130 °C (with decomposition)

Spectral analysis

GC-MS

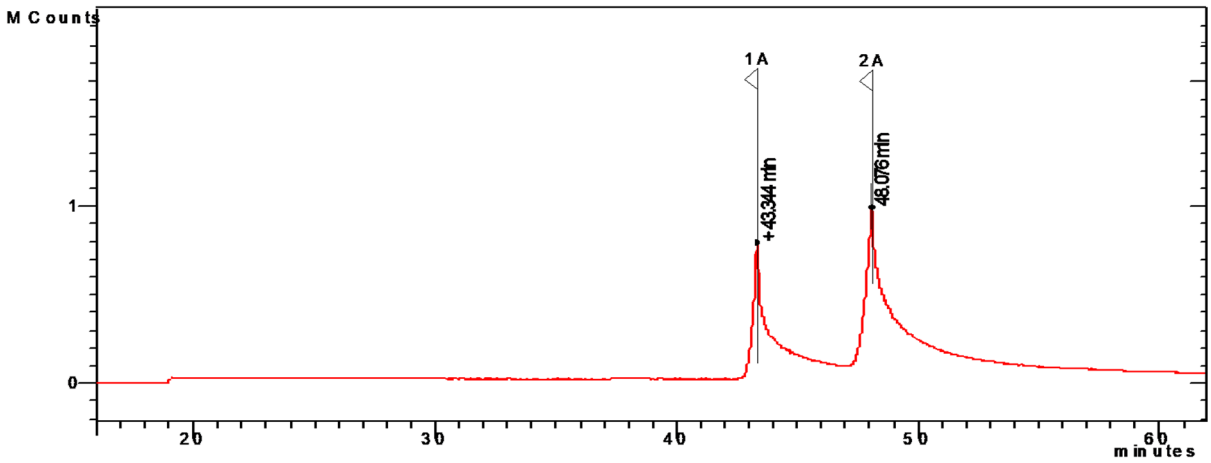
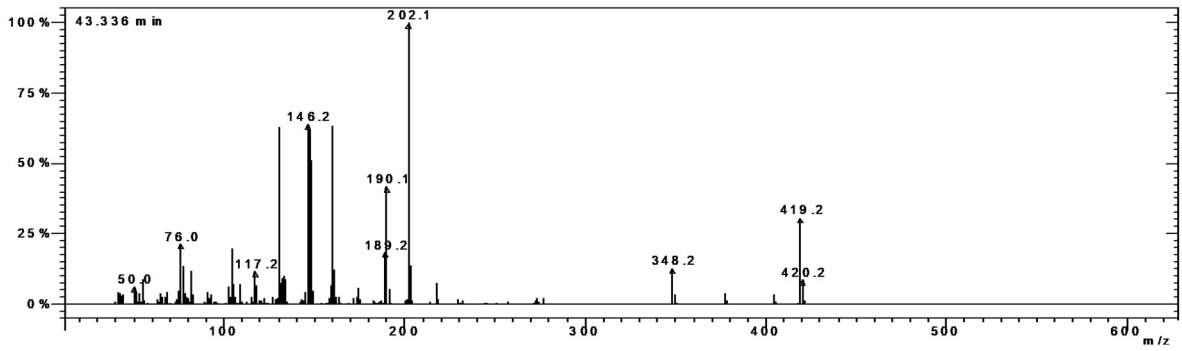


Figure S13. GC-MS spectrum of the probe with *N*-[*D,L*-valine-(*N*-phtaloyl)]cytisine (3C).

EI-MS

a) isomer *D*: Rt 43.336; m/z: 419 (M^+, 30%), 202 (100%), 146 (64%), 148 (51%), 190 (42%), 76 (22%), 189 (19%).



b) isomer *L*: Rt 48.161; m/z: 419 (M^+, 9%), 202 (100%), 147 (69%), 190 (68%), 146 (58%), 189(27%), 76 (24%).

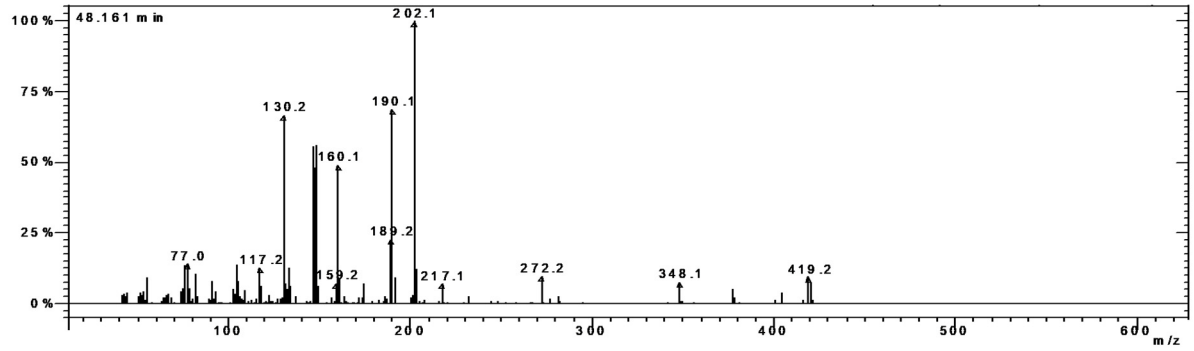


Figure S14. EI-MS spectra of a) *N*-[*D*-valine -(*N*-phtaloyl)]cytisine (**3C**) and b) *N*-[*D*-valine -(*N*-phtaloyl)]cytisine (**3D**).

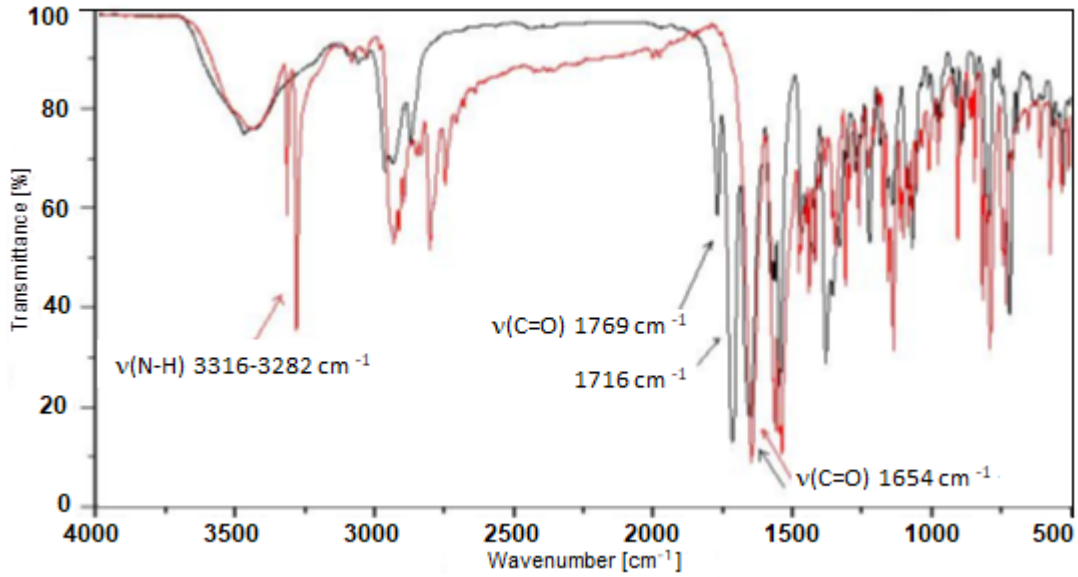


Figure S15. Comparison of the FTIR spectra of (-)-cytisine (**1**, red) and its *N*-[*D,L*-valine -(*N*-phtaloyl)]cytisine (**3C,** black) (KBr).

IR (KBr): 3468-3439, 3094-3031, 2961-2870, 1654, 1769, 1716, 1576-1545 [cm^{-1}].

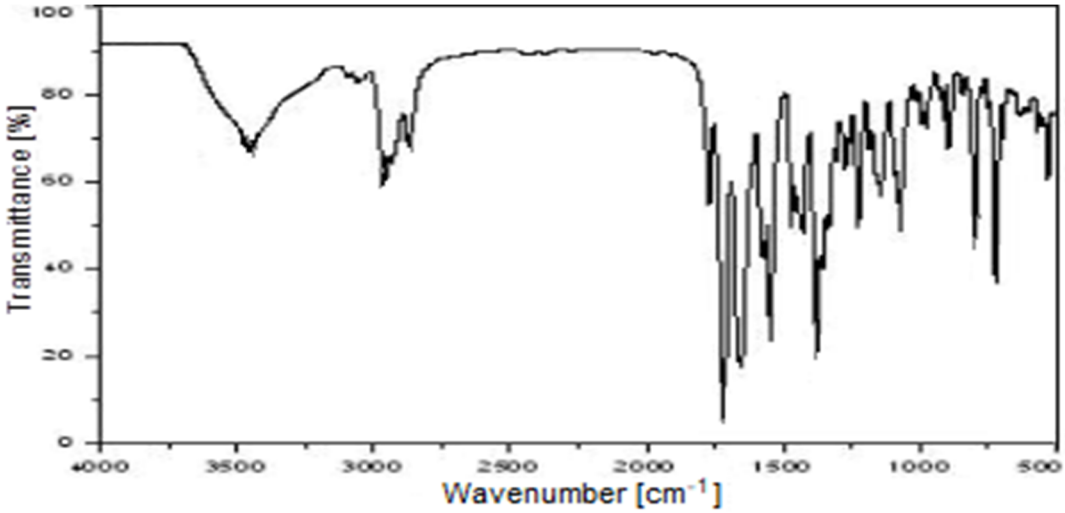


Figure S16. FTIR spectrum of *N*-[*D,L*-valine -(*N*-phtaloyl)]cytisine (**3C**). (KBr).

^{13}C NMR ($CDCl_3$) *(cis/ trans)*: 167.9; 167.0; 163.3/162.6; 139.0/136.8, 134.2; 134.2/131.4; 131.4; 123.6; 117.4/117.0, 105.8/104.0; 55.8/55.4; 51.4/51.0; 49.4/48.7; 48.7; 34.4; 27.2/27.0; 26.8/26.0; 20.8/19.7; 19.6; 18.5 [ppm].

***N*-[*L*-valine-(N-phtaloyl)]cytisine (3D)**

$C_{24}H_{25}N_3O_4$

MW 419 g/mol

white foam

yield 69%

m.p. 110 °C (with decomposition)

Spectral analysis

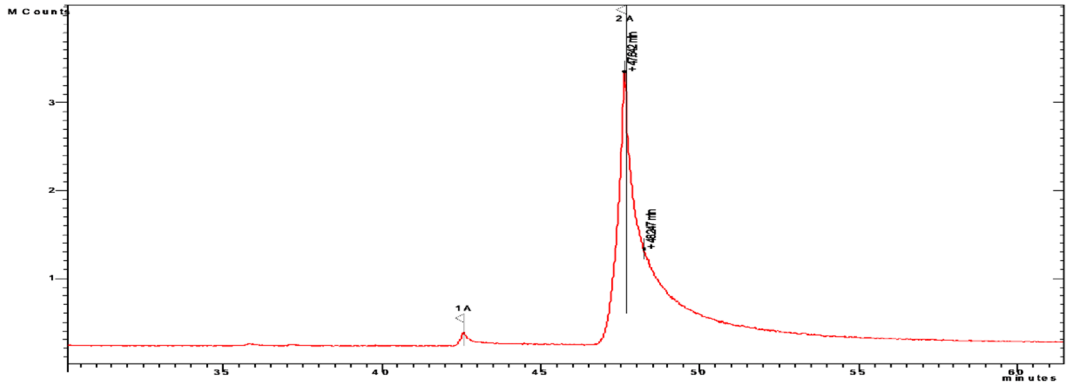


Figure S17. GC-MS spectrum of the probe with *N*-[*L*-valine -(*N*-phtaloyl)]cytisine (**3D,** 2A) with impurity of isomer *N*-[*D*-valine-(*N*-phtaloyl)]cytisine (**3C,** 1A**)**.

EI-MS: Rt 47.642; m/z 419 (M^+, 9%), 202 (100%), 147 (69%), 190 (68%), 146 (58%), 189 (27%), 76(24%).

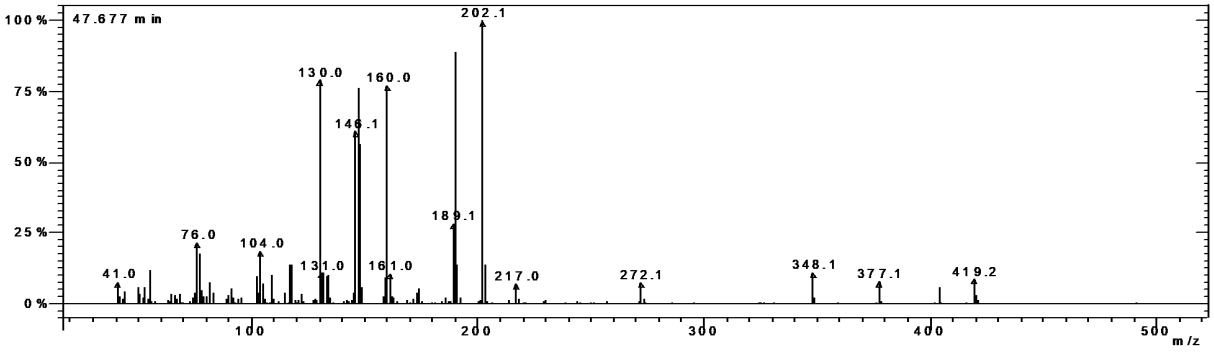


Figure S18. EI-MS spectra of *N*-[*D*-valine-(*N*-phtaloyl)]cytisine (**3D**).

IR (KBr): 3468-3439, 3094-3031, 2961-2870, 1654, 1769,1716, 1576-1545 [cm^{-1}].

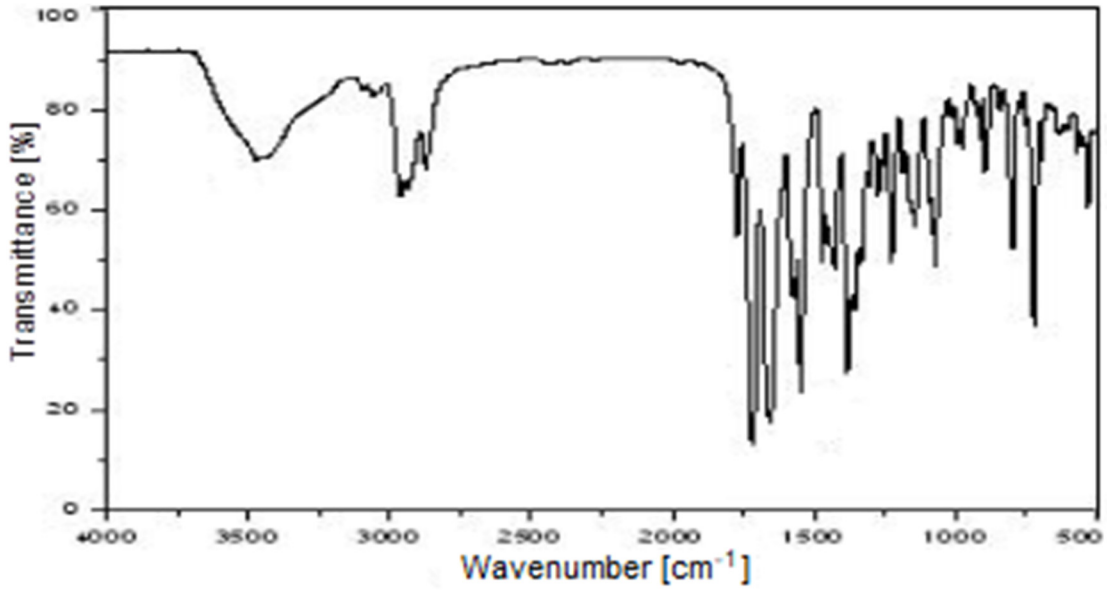


Figure S19. FTIR spectrum of *N*-[*L*-valine-(*N*-phtaloyl)]cytisine (**3D**) in KBr.

^{13}C NMR ($CDCl_3$) ***(cis/ trans)*****:** 167.9, 167.0, 163.3/162.6, 139.0/136.8, 134.2, 134.2/131.4, 131.4, 123.6, 117.4/117.0, 105.8/104.0, 55.8/55.4, 51.4/51.0, 49.4/48.7, 48.7, 34.4, 27.2/27.0, 26,8/26,0, 20.8/19.7, 19.6, 18.5 [ppm].

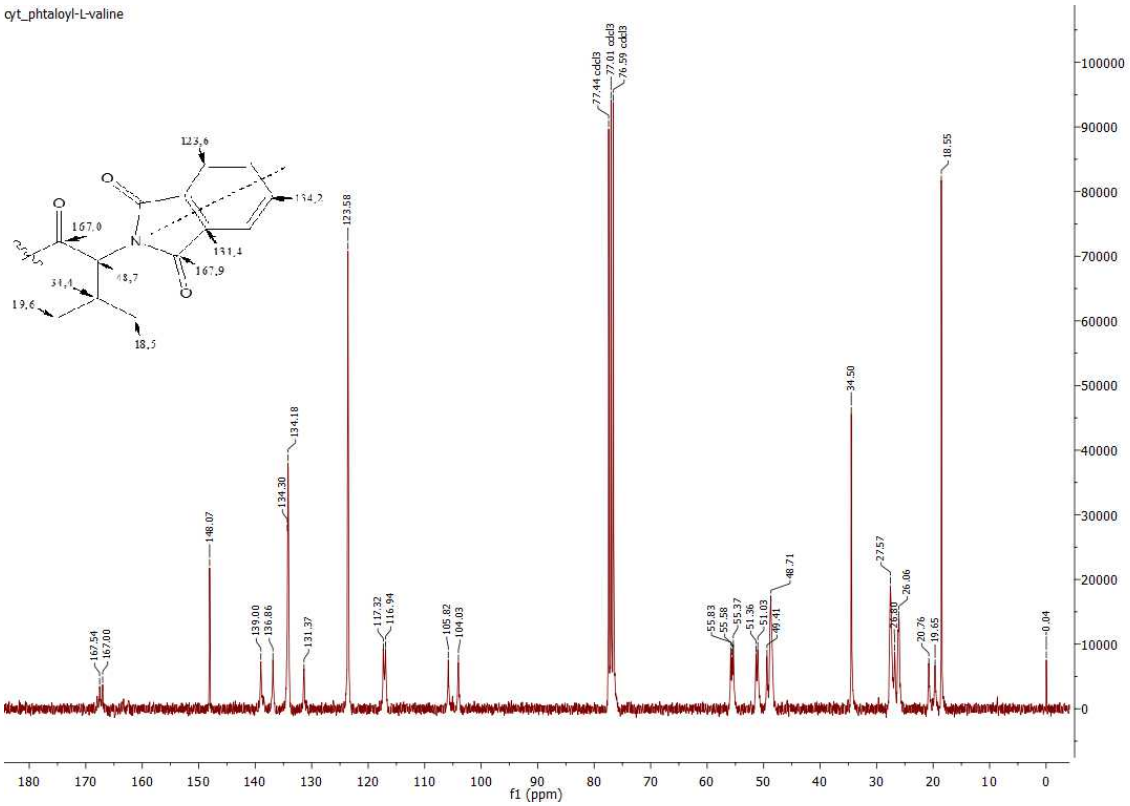


Figure S20. ^{13}C NMR spectrum of *N*-[*D*-valine-(*N*-phtaloyl)]cytisine (**3D**) in $CDCl_3$.

***N*-[*L*-isoleucine-(*N*-phtaloyl)]cytisine (3E)**

$C_{25}H_{27}N_3O_4$

MW 433 g/mol

Light yellow crystals

yield 58%

m.p. 80-84 °C (with decomposition)

Spectral analysis

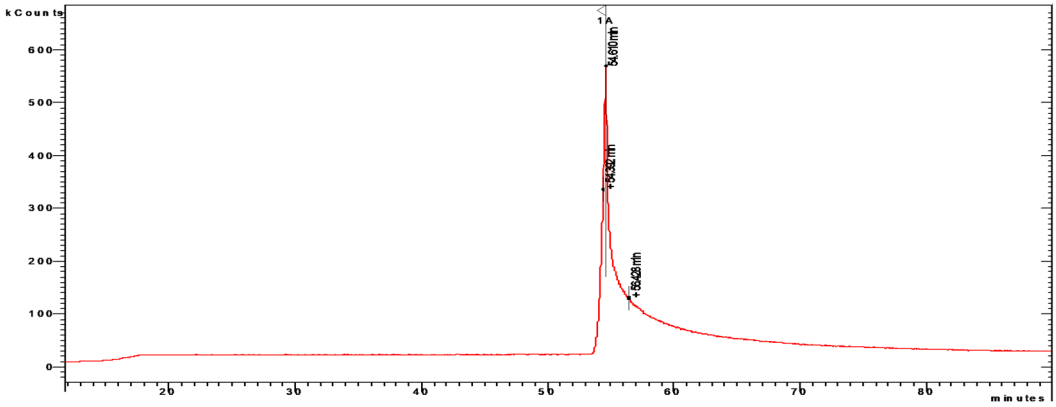


Figure S21. GC-MS spectrum of the probe with *N*-[*L-isoleucine*-(*N*-phtaloyl)]cytisine (**3E**).

EI-MS: Rt 54.604; m/z: 433 (M^+), 160 (100%), 377 (46%), 216 (41%), 147 (39%), 190 (28%).

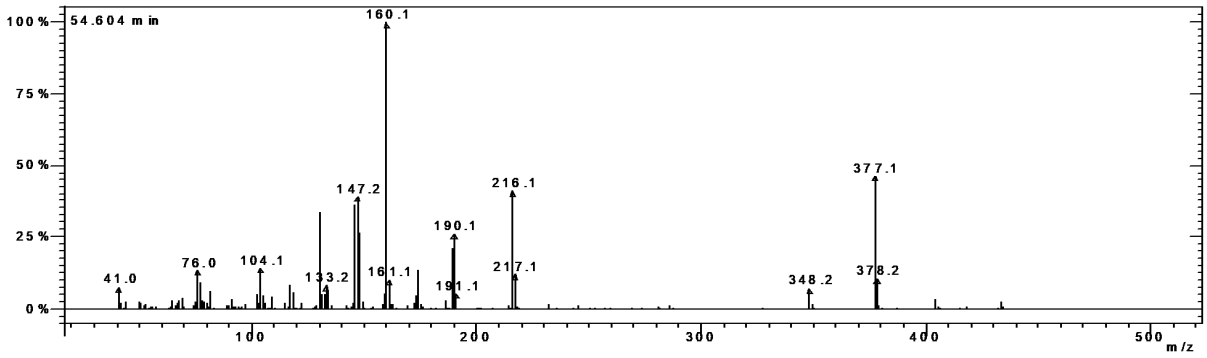


Figure S22. EI-MS spectra of *N*-[*L-isoleucine*-(*N*-phtaloyl)]cytisine (**3E**).

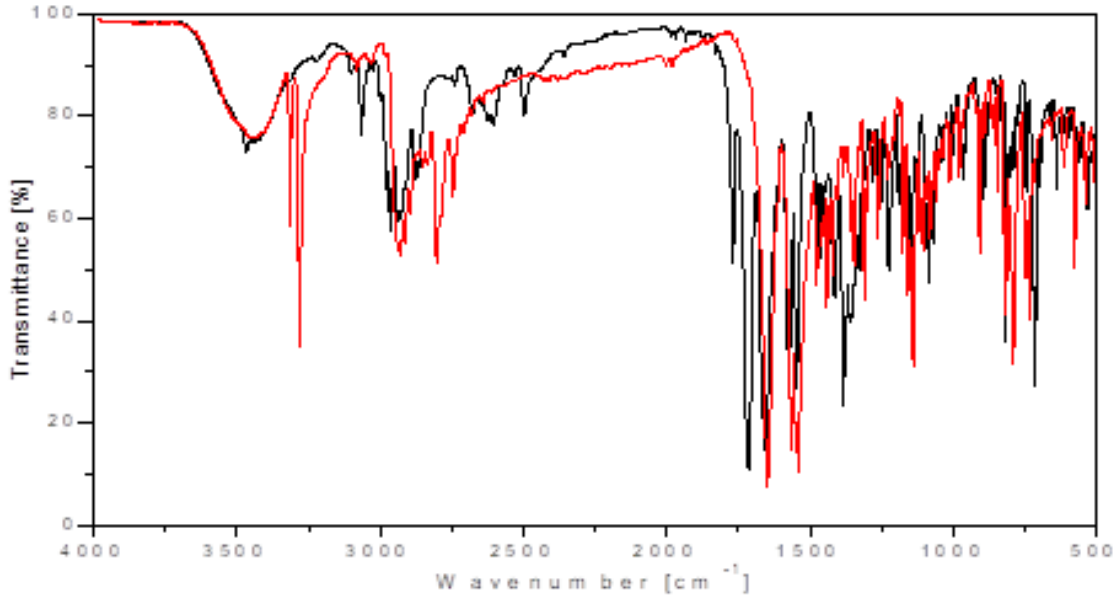


Figure S23. Comparison of the FTIR spectra of (-)-cytisine (**1**, red) and its *N*-[*L*-isoleucine-(*N*-phtaloyl)]cytisine (**3E**, black) (KBr).

IR (KBr): 3466-3436, 3100-3023, 2978-2860, 1664, 1653, 1768, 1713, 1576-1547 [cm^{-1}].

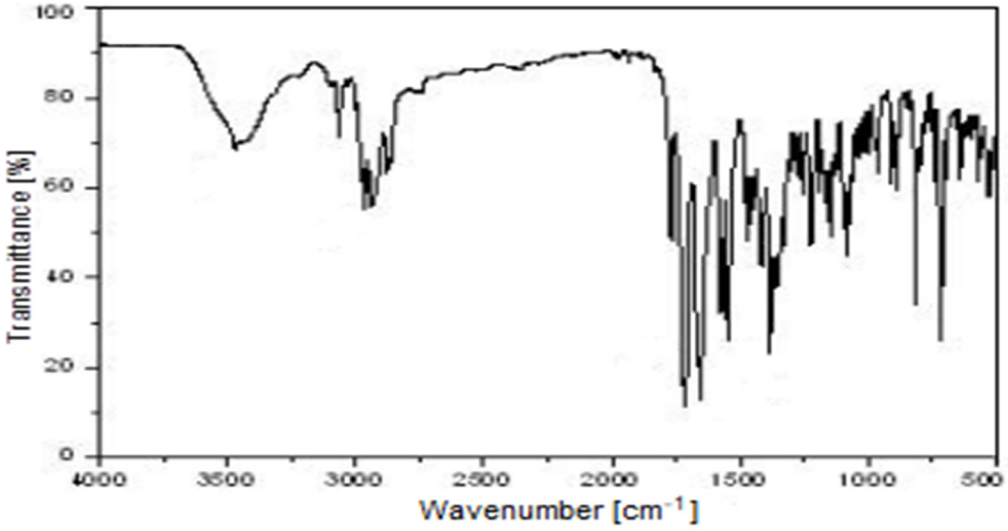


Figure S24. FTIR spectrum of *N*-[*L-isoleucine*-(*N*-phtaloyl)]cytisine (**3E**) in KBr.

^{13}C NMR ($CDCl_3$) ***(cis/ trans)*****:** 168.0; 167.6; 163.3/162.4; 148.1/148.1; 139.0/136.9; 134.2; 131.7; 123.5; 117.3/116.8; 105.8/104.1; 54.7/54.3; 51;5/51.1; 49.4; 48.9/48.5; 34.4;33.3/32.9; 27.6/26.7; 26.1/25.9; 24.7; 16.8; 10.61 [ppm].

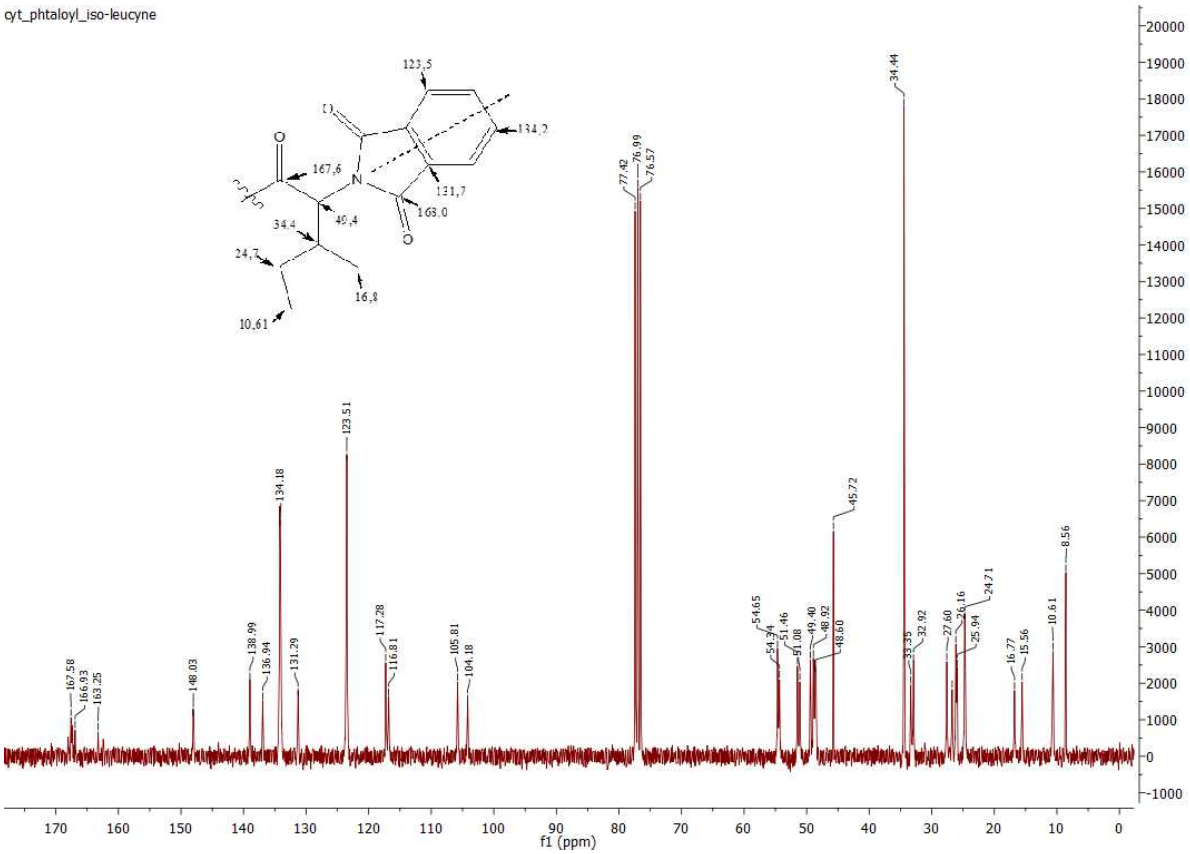


Figure S 25. ^{13}C NMR spectrum of *N*-[*L-isoleucine*-(*N*-phtaloyl)]cytisine (**3E**) in $CDCl_3$.

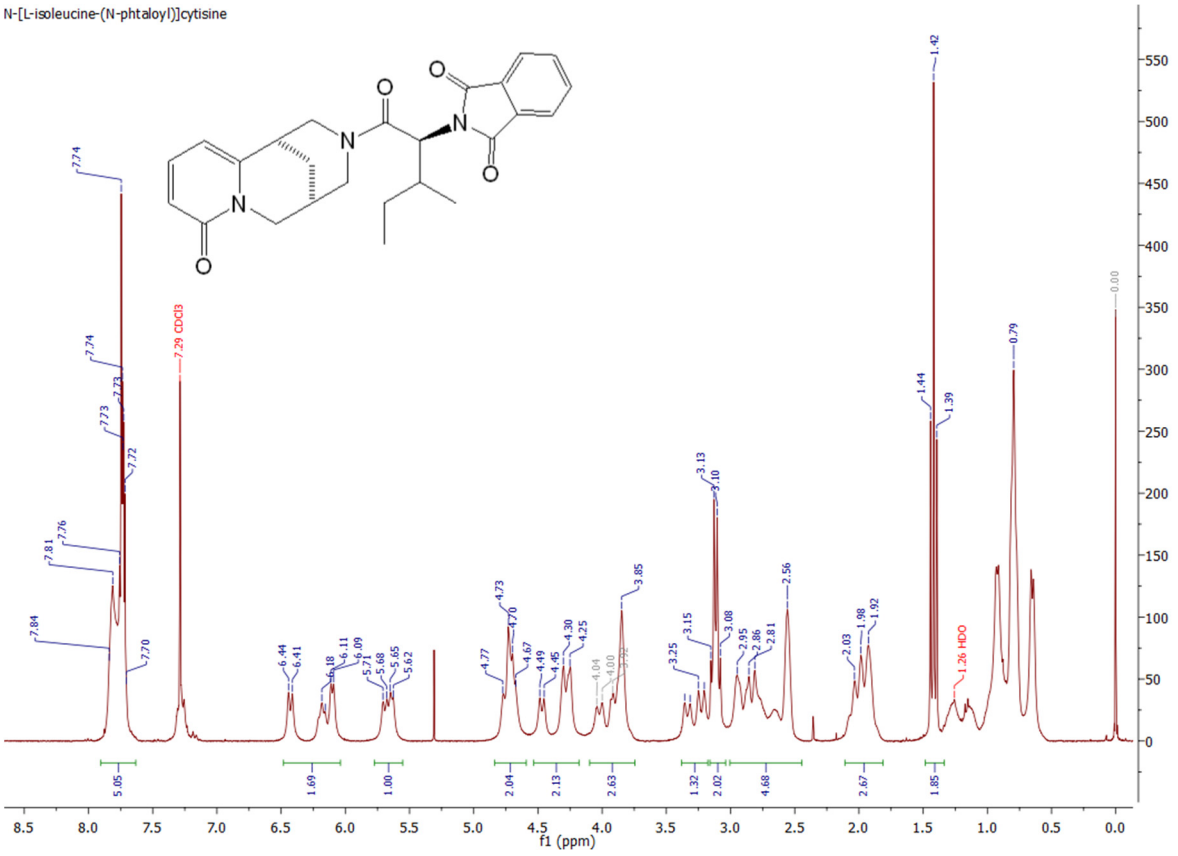


Figure S26. ^{1}H NMR spectrum of *N*-[*L-isoleucine*-(*N*-phtaloyl)]cytisine (**3E**) in $CDCl_3$.

N-[*L*-leucine-(*N*-phtaloyl)]cytisine (3F)

$C_{25}H_{27}N_3O_4$

MW 433 g/mol

creamy precipitate

yield 89%

m.p. 101-104 °C (with decomposition)

Spectral analysis

EI-MS: Rt 53.591; m/z: 433 (M^+, 1%), 160 (100%), 147 (78%), 377 (70%), 189 (38%), 130 (25%)

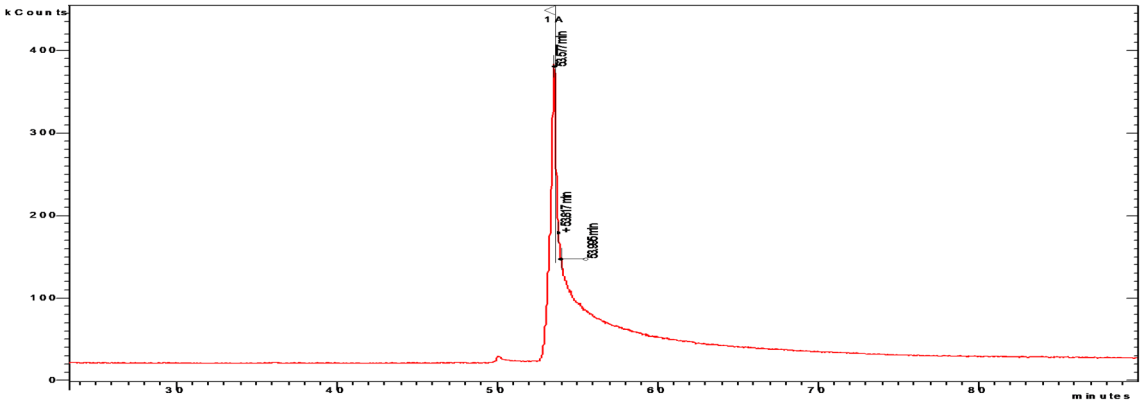


Figure S27. GC-MS spectrum of the probe with *N*-[*L-leucine*-(*N*-phtaloyl)]cytisine (**3F**).

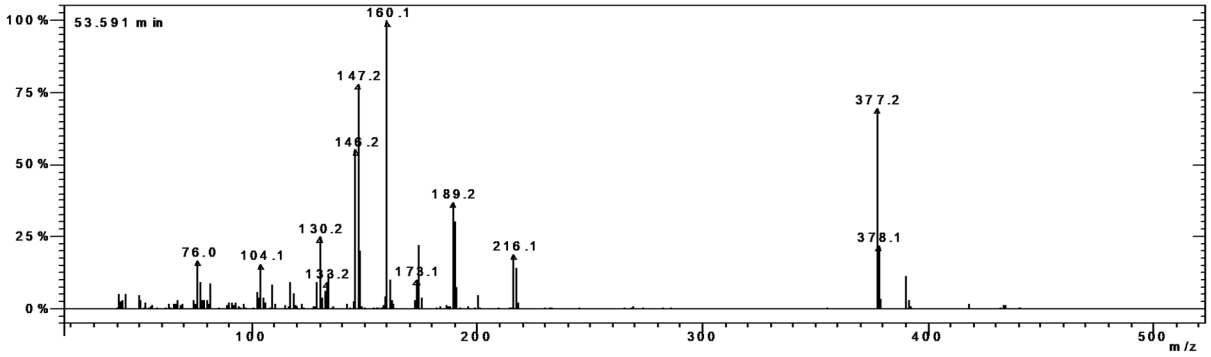


Figure S28. EI-MS spectra of *N*-[*L-leucine*-(*N*-phtaloyl)]cytisine (**3F**).

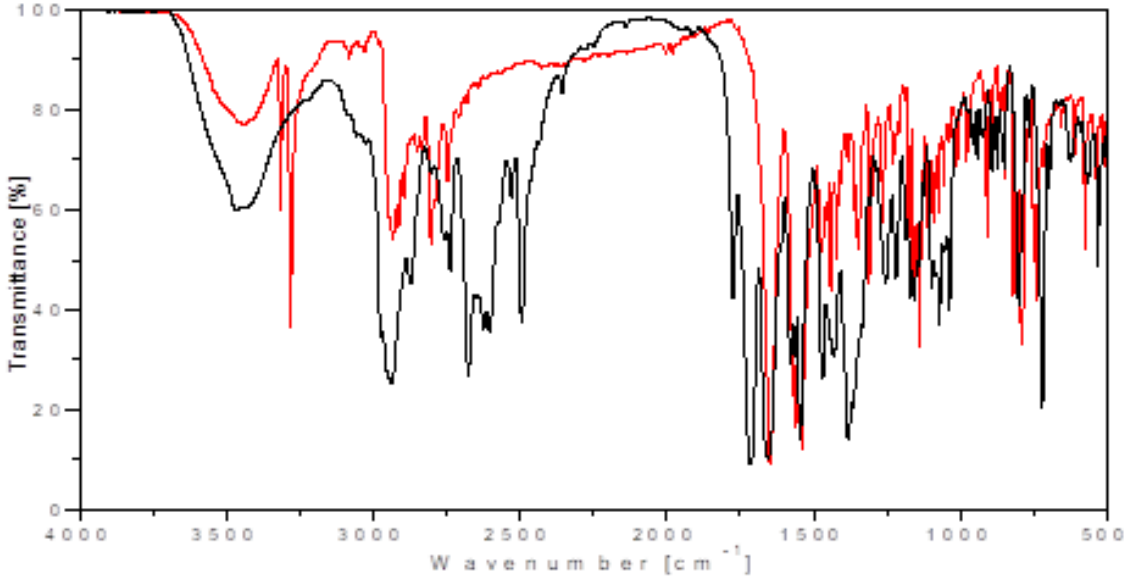


Figure S29. Comparison of the FTIR spectra of (-)-cytisine (**1**, red) and its *N*-[*L*-leucine-(*N*-phtaloyl)]cytisine (**3F** and Et3NxHCl impurities, black) (KBr).

IR (KBr): 3468-3447, 3085-3028, 2975-2738, 1654, 1774, 1714 cm^{-1}, 1577-1546 [cm^{-1}].

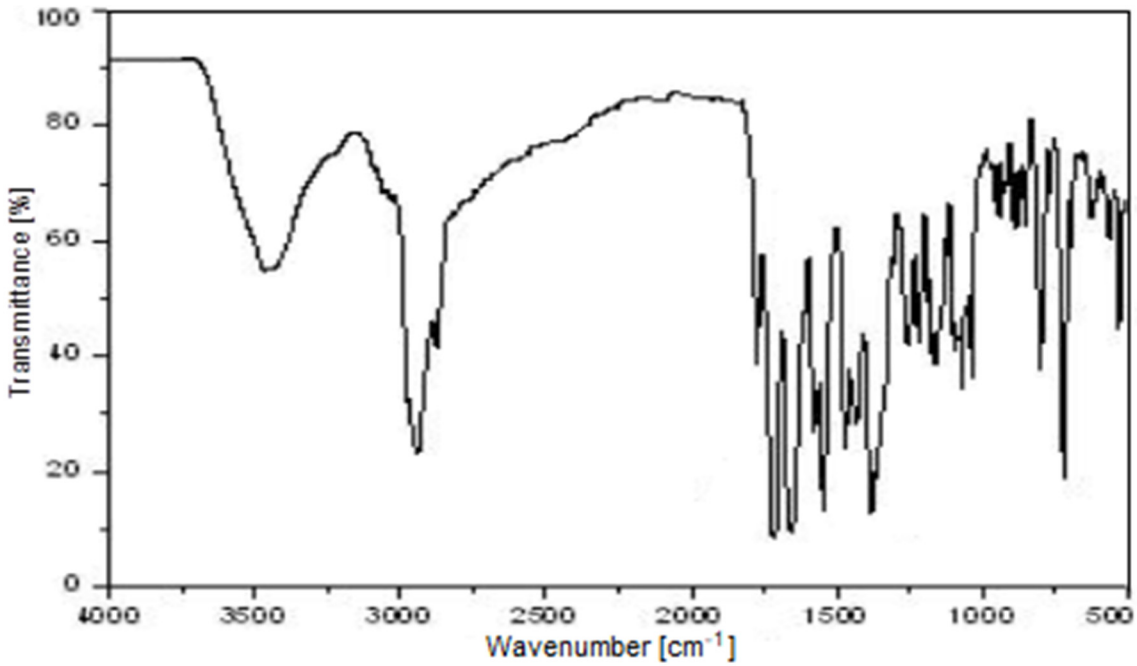


Figure S30. FTIR spectrum of *N*-[*L-leucine*-(*N*-phtaloyl)]cytisine (**3F**) in KBr.

^{13}C NMR ($CDCl_3$): 169.1; 167.6; 162.9/162.9; 147.9/147.9, 138.6/137.4; 134.1; 131.6; 123.5; 117.9/117.3; 51.6/51.6; 50.6/50.2; 49.2/48.7; 37.6; 30.0/29.6; 27.2/27.0; 26.0; 24.9/24.8; 22.9; 21.5 [ppm].

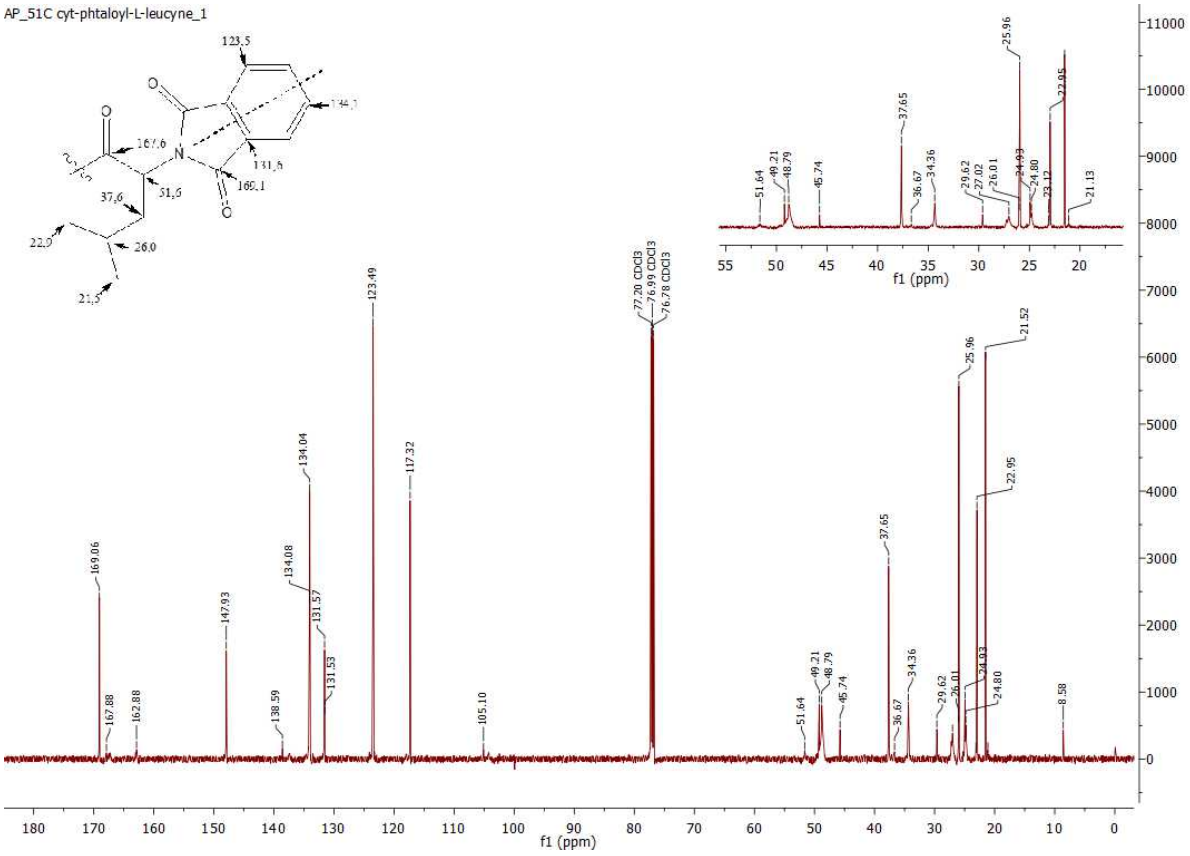


Figure S31 . ^{13}C NMR spectrum of *N*-[*L-leucine*-(*N*-phtaloyl)]cytisine (**3F**) in $CDCl_3$.

***N*-[*D*-leucine-(*N*-phtaloyl)]cytisine (3G)**

$C_{25}H_{27}N_3O_4$

MW 433 g/mol

orange precipitate

yield 61%

m.p. 101-105 °C (with decomposition)

Spectral analysis

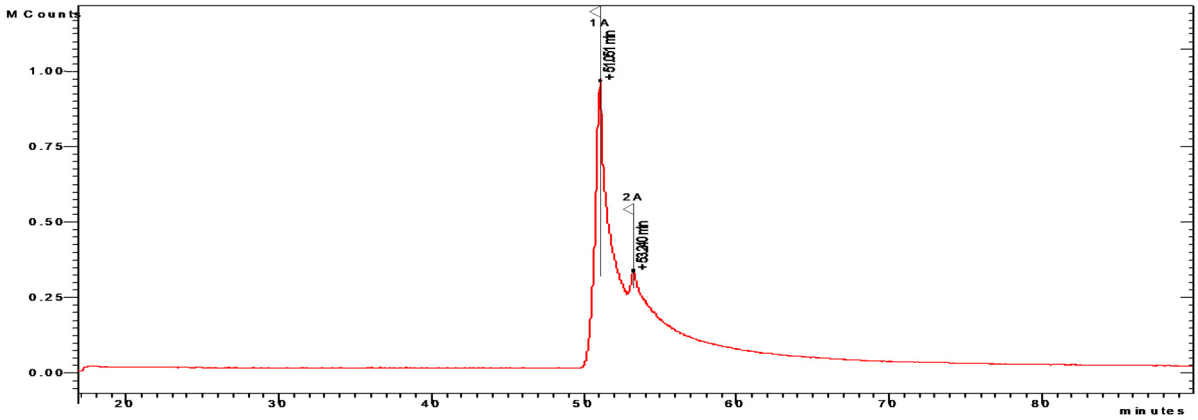
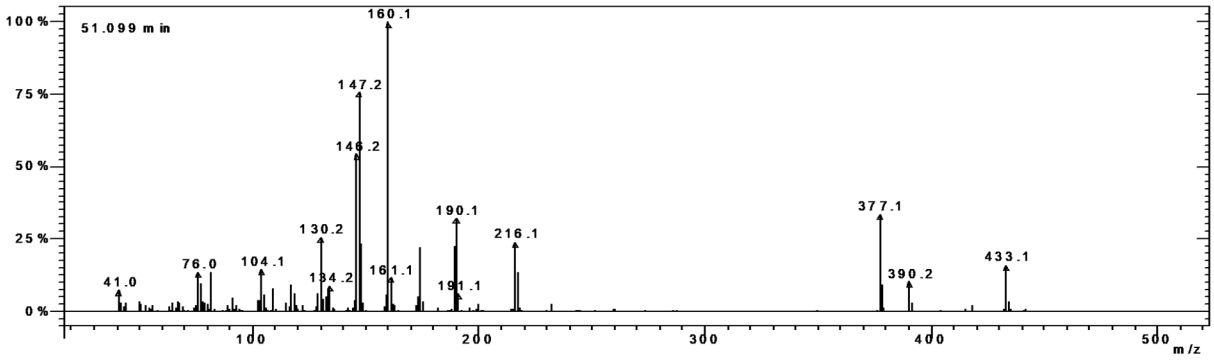


Figure S32. GC-MS spectrum of the probe with *N*-[*D-leucine*-(*N*-phtaloyl)]cytisine (**3G**).

EI-MS

N-[*D*-leucine-(*N*-phtaloyl)]cytisine (**3G**):

Rt 51.099; m/z 433 (M^+, 16%), 160 (100%), 147 (75%), 377 (33%), 190 (32%), 130 (25%),



and impurity of *N*-[*L*-leucine-(*N*-phtaloyl)]cytisine Rt 53.225, m/z 433 (M^+, 10%), 160 (100%), 147 (61%), 377 (50%), 190 (41%), 130 (22%).

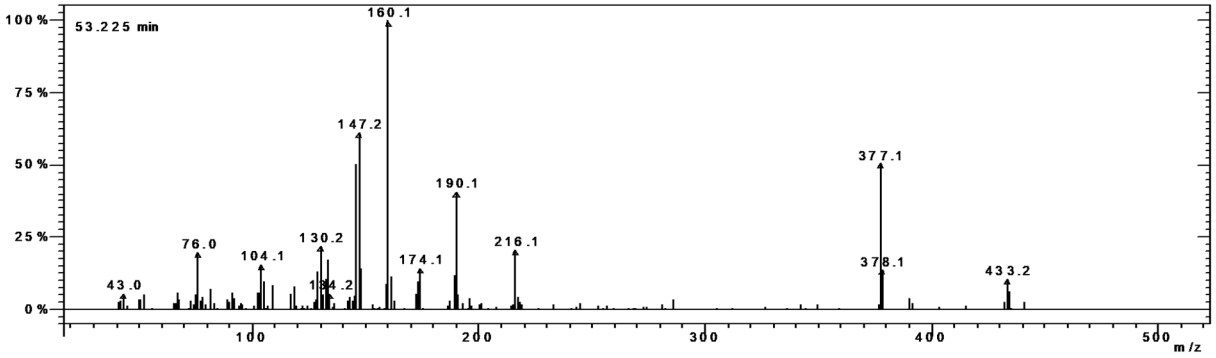


Figure S33. EI-MS spectra of a) *N*-[*D-leucine*-(*N*-phtaloyl)]cytisine (**3F**) and b) *N*-[*L-leucine* -(*N*-phtaloyl)]cytisine (**3G**)

IR (KBr): 3468-3447, 3085-3028, 2975-2738, 1654, 1774, 1714, 1577-1546 [cm^{-1}].

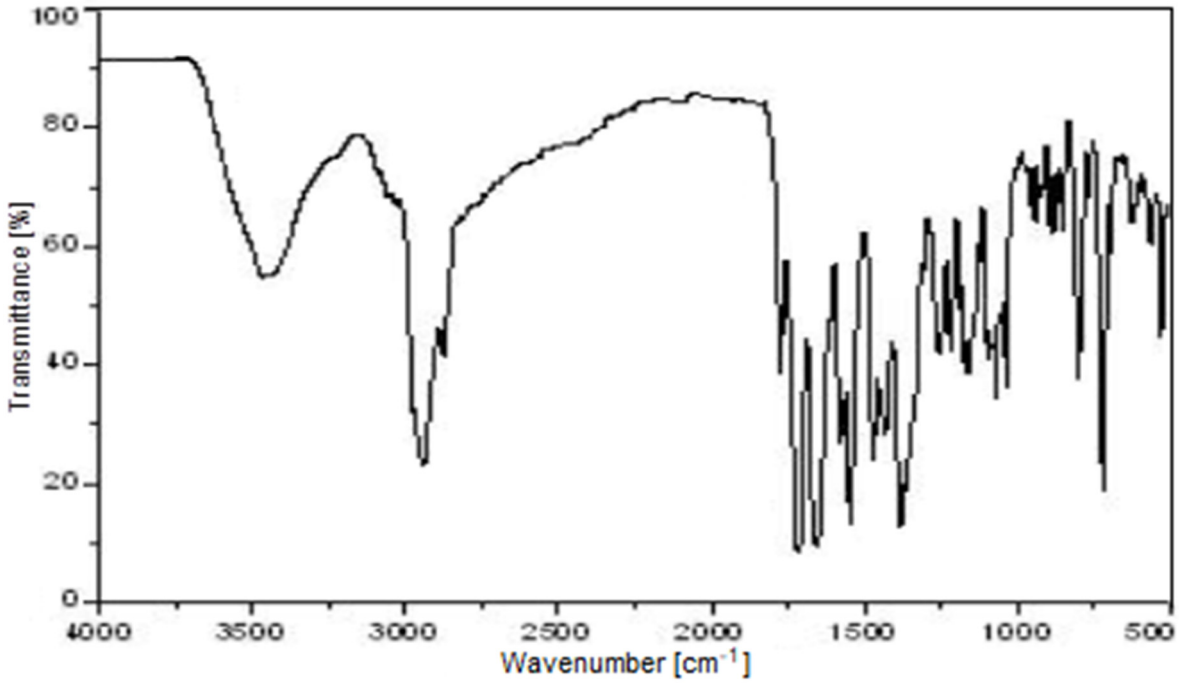


Figure S34. FTIR spectrum of *N*-[*D*-leucine-(*N*-phtaloyl)]cytisine (**3G**) in KBr.

^{13}C NMR ($CDCl_3$): 169.1; 167.6; 162.9/162.9; 147.9/147.9; 138.6/137.4; 134.1; 131.6; 123.5; 117.9/117.3; 51.6/51.6; 50.6/50.2; 49.2/48.7; 37.6; 30.0/29.6; 27.2/27.0; 26.0; 24.9/24.8; 22.9; 21.5 [ppm].

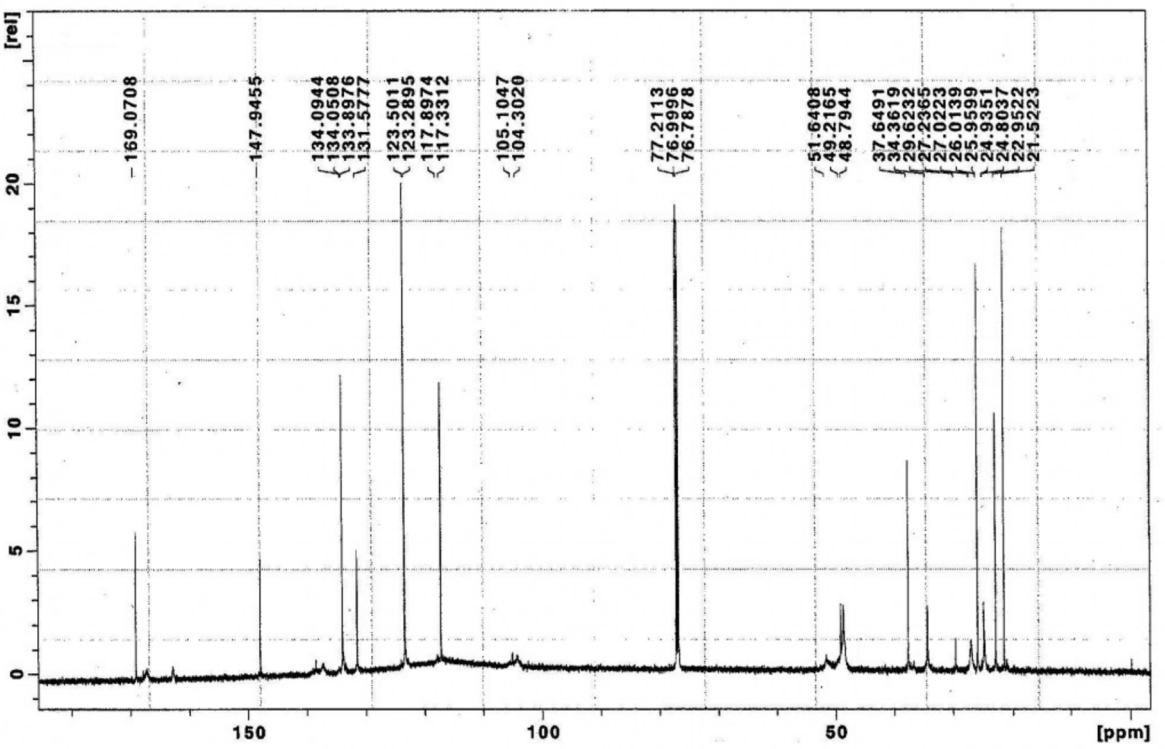


Figure S35. ^{13}C NMR spectrum of *N*-[*D-leucine*-(*N*-phtaloyl)]cytisine (**3G**) in $CDCl_3$.

***N*-[*D,L*-phenylalanine-(*N*-phtaloyl)]cytisine (3H)**

$C_{28}H_{25}N_3O_4$

MW 467 g/mol

in the form of cream "plates".

yield 47%

m.p. 143-150 °C (with decomposition)

Spectral analysis

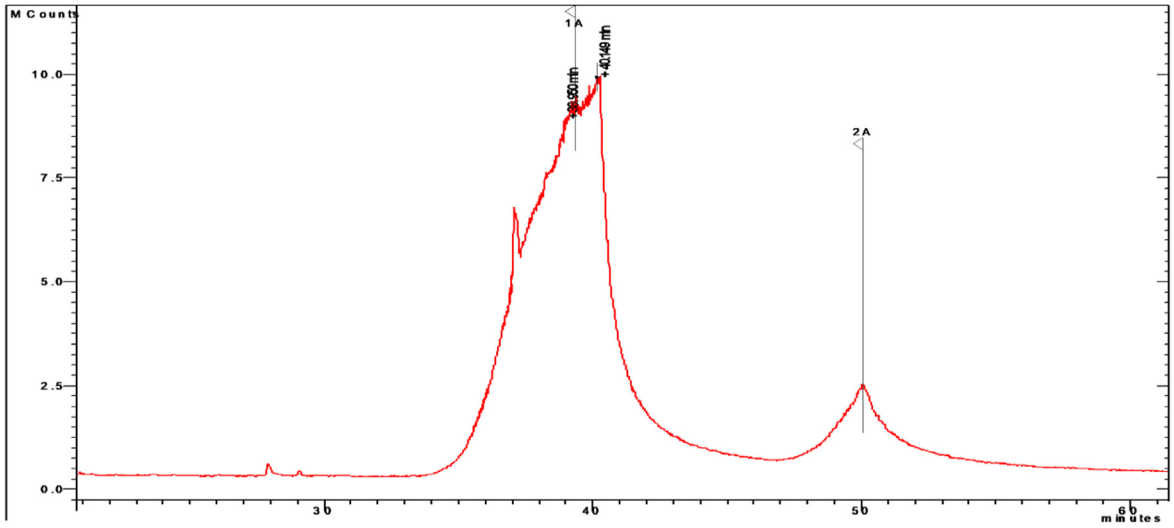
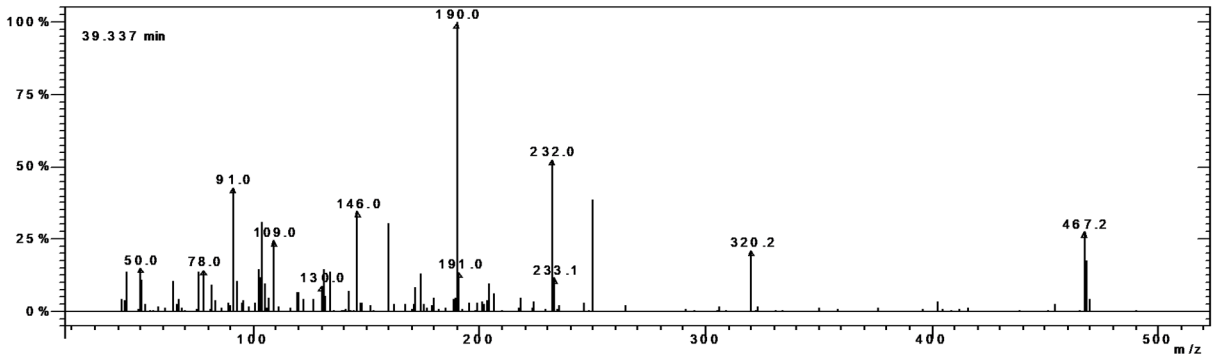


Figure S36. GC-MS spectrum of the probe with *N*-[*D,L-phenylalanine*-(*N*-phtaloyl)]cytisine (**3H**).

EI-MS

isomer *D* m/z: 467 (M^+), 190 (100%), 232 (53%), 91 (43%), 146 (35%), 320 (20%).



isomer *L* m/z: 467 (M^+), 190 (100%), 147 (74%), 232 (42%), 146 (38%), 77 (26%).

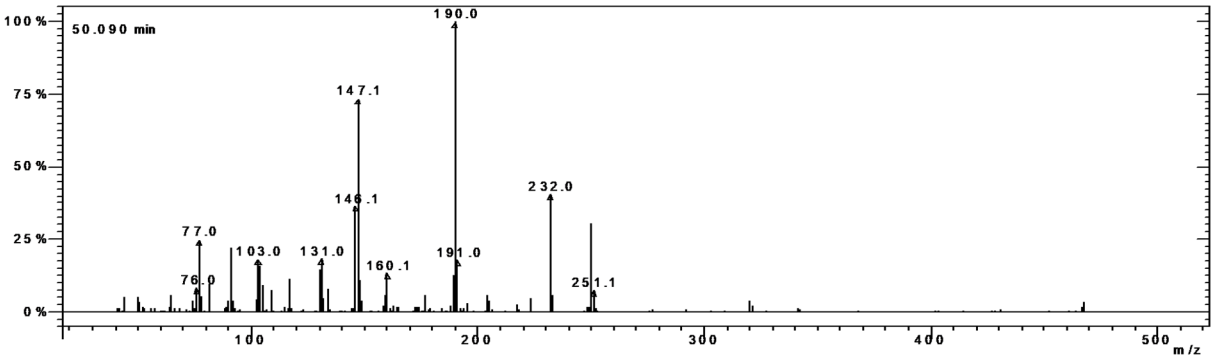


Figure S37. EI-MS spectra of a) *N*-[*D-phenylalanine*-(*N*-phtaloyl)]cytisine (**3H**) and b) *N*-[*L-phenylalanine*-(*N*-phtaloyl)]cytisine (**3H**).

IR (KBr): 3471-3413, 3084-3002, 2926-2864, 1653, 1776, 1713, 1576-1544, 1496-1426 [cm^{-1}].

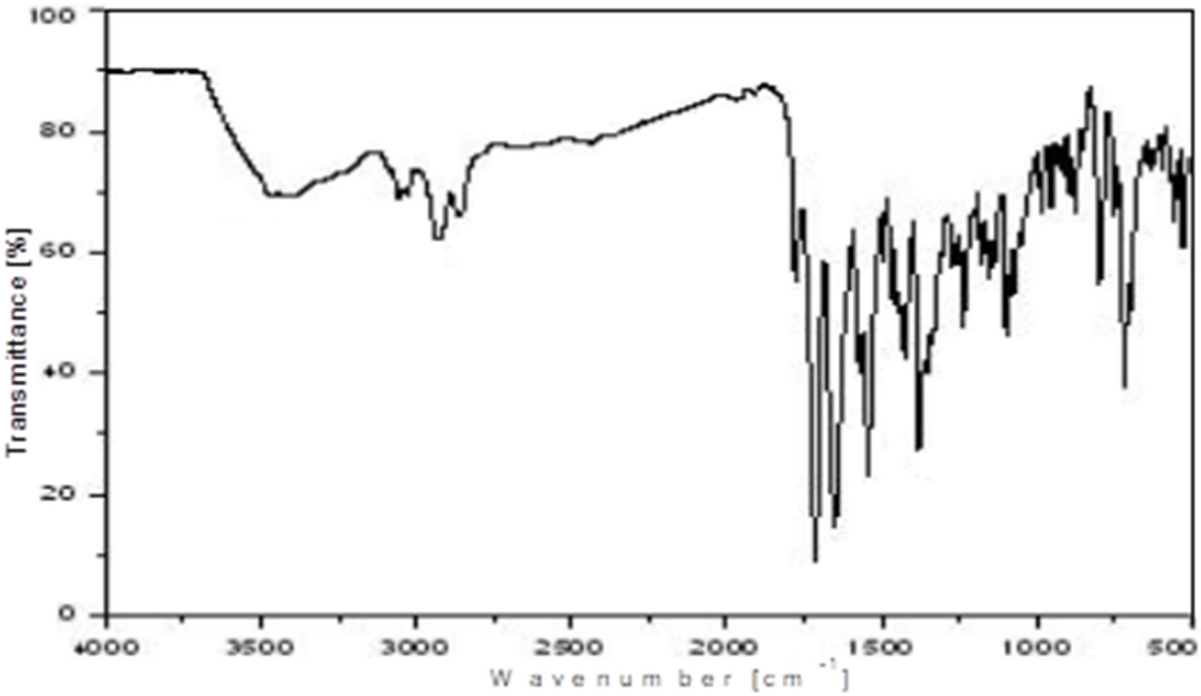


Figure S38. FTIR spectrum of N-[D,L-phenylalanine-(N-phtaloyl)]cytisine (**3H**) in KBr.

^{13}C NMR ($CDCl_3$) *(cis/ trans)*: 167.3; 166.6; 162.9/162.9; 137.0/136.8; 136.8; 134.1; 134.1/133.9; 131.4; 131.3;129.1; 128.4; 123.5; 118.1/117.2; 105.9/105.1; 52.4; 52.4/51.7; 51.7/51.3; 51.3/48.7; 35.2/34.3; 34.3; 27.4/26.8; 26.1/25.9 [ppm].

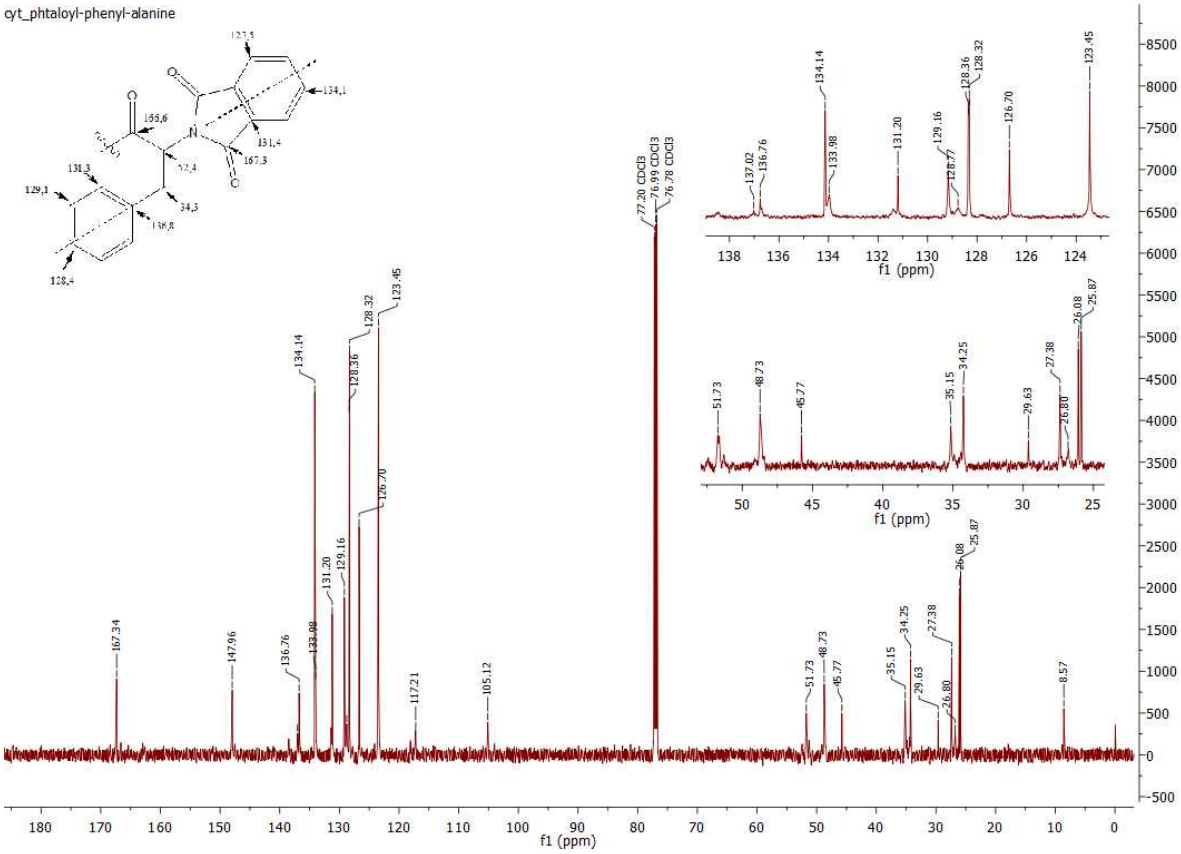


Figure S39. ^{13}C NMR spectrum of *N*-[*D,L*-phenylalanine-(*N*-phtaloyl)]cytisine (**3H**) in $CDCl_3$.

Table S1. Intermolecular interaction details for **3A**. symmetry coe, interaction energy, geometrical data and AIM topological analysis data

[ii] 1/2+x. 3/2-y. -z: 4 contacts with critical points.

E_{int}: -43.0 kJ/mol (CrystalExplorer); -40.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H15A	O24	17.28	-13.57	2.4147	0.9905	1.425	0.065	0.771
O2	C23	13.93	-10.09	3.1121	1.5056	1.6102	0.049	0.652
O24	H22	12.62	-8.4	2.598	1.5093	1.0887	0.039	0.618
H10B	O24	8.63	-6.37	2.7445	1.1418	1.6238	0.039	0.4

D	H	A	D-H	H···A	D···A	D-H···A
C15	H15A	O24[ii]	1.09	2.42	3.489	168
O2	C23[ii]				3.112	
C22[ii]	H22[ii]	O24	1.09	2.59	3.440	134
C10	H10B	O24[ii]	1.09	2.75	3.804	164

[iii] 1-x. ½+y. 1/2-z: 4 contacts with critical points.

E_{int}: -37.1 kJ/mol (CrystalExplorer); -33.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H8A	C4	11.47	-9.06	2.6709	1.0813	1.5933	0.051	0.509
H11B	C5	8.7	-6.43	2.8138	1.1316	1.701	0.039	0.403
O17	C8	12.88	-8.34	3.1831	1.5128	1.6897	0.037	0.64
H13A	C3	6.67	-4.98	3.0159	1.2093	1.8701	0.034	0.307
O14	H8B	3.12	-1.9	3.214	1.8013	1.4131	0.013	0.16

D	H	A	D-H	H···A	D···A	D-H···A
C8	H8A	C4^{iii}	1.09	2.67	3.721	161
C11	H11B	C5^{iii}	1.09	2.82	3.798	150
O17	C8^{iii}				3.183	
C13	H13A	C3^{ii}	1.09	3.02	4.018	153
C8^{iii}	H8B^{iii}	O14	1.09	3.22	4.236	156

^{iv} 2-x. -½+y. 1/2-z: 5 contacts with critical points.

E_{int}: -20.4 kJ/mol (CrystalExplorer); -20.4 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H4	O14	16.83	-11.19	2.5425	1.083	1.4687	0.046	0.825
H5	O14	12.11	-7.67	2.7014	1.1974	1.5334	0.033	0.608
H4	H13B	6.55	-4.27	2.4583	1.2308	1.2397	0.025	0.324
H5	O17	4.09	-2.73	3.0948	1.3163	1.8252	0.020	0.2
H7	C19	2.85	-1.82	3.3212	1.4111	1.9239	0.014	0.143

D	H	A	D-H	H···A	D···A	D-H···A
C4	H4	O14^{iv}	1.09	2.54	3.218	119
C5	H5	O14^{iv}	1.09	2.70	3.294	114
H4	H13B^{iv}				2.454	
C5	H5	O17^{iv}	1.09	3.09	4.146	164
C7	H7	C19^{iv}	1.09	3.33	4.283	147

^{v} 1+x. 1+y. z: 2 contacts with critical points.

E_{int}: -18.2 kJ/mol (CrystalExplorer); -8.2 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H20	O2	18.52	-12.65	2.4842	1.028	1.4572	0.052	0.896
H19	O2	10.82	-6.74	2.7483	1.2056	1.5655	0.030	0.547

D	H	A	D-H	H···A	D···A	D-H···A
C20	H20	O2[v]	1.09	2.48	3.243	126
C19	H19	O2[v]	1.09	2.75	3.350	115

[vi] 3/2+x. 3/2-y. -z: 2 contacts with critical points.

E_{int}: --17.8 kJ/mol (CrystalExplorer); -8.0 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H21	O2	15.83	-12.1	2.4429	1.0016	1.4424	0.059	0.718
H22	H9	1.32	-0.74	3.1857	1.6224	1.5878	0.0056	0.07

D	H	A	D-H	H···A	D···A	D-H···A
C21	H21	O2[vi]	1.09	2.44	3.502	166
H22	H9[vi]				3.025	

[vii] x. -1+y. -z: 1 contact with critical points.

E_{int}: --6.6 kJ/mol (CrystalExplorer); -7.7 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H3	O17	10.52	-6.8	2.6848	1.1319	1.5529	0.032	0.523

C3	H3	O17[vii]	1.09	2.68	3.499	131

[viii] ½+x. 5/2-y. -z: 1 contact with critical points.

E_{int}: --5.4 kJ/mol (CrystalExplorer); -8.4 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H20	C19	5.13	-3.39	3.0473	1.2526	1.8153	0.022	0.253

D	H	A	D-H	H···A	D···A	D-H···A
C20	H20	C19[viii]	1.09	3.04	3.880	134

Table S2. Intermolecular interaction details for **3E**. symmetry coe, interaction energy, geometrical data and AIM topological analysis data

[i] 1+x. y. z: 10 contacts with critical points.

E_{int}: --44.2 kJ/mol (CrystalExplorer); -43.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H5	O14	27.12	-22.4	2.2334	0.8943	1.3399	0.092	1.169
H7	O14	11.61	-7.79	2.6429	1.1201	1.5251	0.038	0.566
O17	H25	10.21	-6.68	2.7114	1.5597	1.153	0.033	0.505
H7	H11A	5.72	-4.09	2.4475	1.2347	1.2151	0.028	0.27
H4	O24	7.83	-4.76	2.8178	1.2065	1.6115	0.023	0.4
H5	O24	7.32	-4.43	2.8605	1.2263	1.636	0.021	0.375
C19	O24	5.83	-3.56	3.5262	1.8699	1.6669	0.019	0.297
H19	H25	5.44	-3.36	2.5544	1.2681	1.2919	0.019	0.276
H19	H28B	4.47	-2.71	2.6173	1.3034	1.3178	0.016	0.229
O17	H28B	4.34	-2.65	3.0464	1.7272	1.3338	0.016	0.222

D	H	A	D-H	H···A	D···A	D-H···A
C5	H5	O14[i]	1.09	2.23	3.257	157
C7	H7	O14[i]	1.09	2.65	3.798	136
C25[i]	H25[i]	O17	1.09	2.72	3.537	132
H7	H11A[i]				2.459	
C4	H4	O24[i]	1.09	2.81	3.551	125
C5	H5	O24[i]	1.09	2.86	3.566	123
C19	O24[i]				3.526	
H19	H25				2.558	
H19	H28B				2.605	
C28[i]	H28B[i]	O17	1.09	3.04	3.913	138

[ii] x. -1+yy. z: 8 contacts with critical points.

E_{int}: --41.7 kJ/mol (CrystalExplorer); -33.2 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H13A	O2	14.89	-9.87	2.5736	1.079	1.4956	0.042	0.731
H26C	H22	8.44	-5.79	2.2999	1.1582	1.1418	0.033	0.407
H27A	H22	9.48	-6.22	2.296	1.1609	1.1359	0.032	0.467
O17	H3	6.96	-4.79	2.7889	1.5966	1.1931	0.029	0.336
H15	O2	8.21	-5.13	2.8088	1.1909	1.6206	0.025	0.414
H15	H3	5.73	-3.84	2.4914	1.2655	1.2283	0.024	0.28
C26	O2	5.32	-3.14	3.6451	1.9549	1.7072	0.016	0.276
H26C	O24	3.2	-1.87	3.195	1.4087	1.8022	0.011	0.166

C13	H13A	O2[ii]	1.09	2.58	3.331	126
H26C	H22[i]				2.286	
H27A	H22[i]				2.294	
C3[ii]	H3[ii]	O17	1.09	2.78	3.870	176
C15	H15	O2[ii]	1.09	2.82	3.610	130
H15	H3[ii]				2.498	
C26	O2[ii]				3.645	
C26	H26C	O24[ii]	1.09	3.19	4.012	133

[ii] x. -1+y. z: 3 contacts with critical points.

E_{int}: --26.8 kJ/mol (CrystalExplorer); -8.9 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H3A2	O2	20.66	-16.56	2.3307	0.9435	1.3874	0.075	0.909
C2A	H10B	5.81	-3.53	3.1139	1.8349	1.2972	0.019	0.297
N1A	H11A	1.19	-0.65	3.692	2.1148	1.621	0.005	0.063

D	H	A	D-H	H···A	D···A	D-H···A
C3A	H3A2	O2^{ii}	1.09	2.32	3.401	172
C10^{ii}	H10B^{ii}	C2	1.09	3.12	3.795	121
C11^{ii}	H11A^{ii}	N1A	1.09	3.69	4.468	130

^{iv} 1+x. 1+y. z: 3 contacts with critical points.

E_{int}: --23.0 kJ/mol (CrystalExplorer); -16.6 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H8A	N1A	13.04	-9.69	2.5933	1.0654	1.5289	0.050	0.602
C3	H3A3	7.69	-5.24	2.855	1.7012	1.1554	0.030-	0.372
C6	N1A	5.59	-3.61	3.6104	1.839	1.8081	0.022-	0.278

D	H	A	D-H	H···A	D···A	D-H···A
C8	H8A	N1A^{iv}	1.09	2.60	3.590	151
C3A^{iv}	H3A3^{iv}	C3	1.09	2.85	3.721	137
C6	N1A^{iv}				3.610	

^{v} 1/2+x. 3/2-y. 1-z: 2 contacts with critical points.

E_{int}: --13.8 kJ/mol (CrystalExplorer); -17.2 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H20	C22	7.51	-4.88	3.061	1.2642	1.2642	0.027	0.372
H21	H28C	7.31	-4.95	2.4299	1.1851	1.1851	0.029	0.355

D	H	A	D-H	H···A	D···A	D-H···A
C20	H20	C22^{v}	1.09	3.06	3.650	115
H21	H28C^{v}				2.419	

x. y. z: 2 contacts with critical points.

E_{int}: --12.3 kJ/mol (CrystalExplorer); -8.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H26A	C3A	7.04	-4.96	3.0706	1.1974	1.8747	0.031	0.335
H11B	H3A1	8.77	-5.44	2.4111	1.1993	1.2141	0.026	0.444

D	H	A	D-H	H···A	D···A	D-H···A
C26	H26A	C3A	1.09	3.06	4.117	115
H11B	H3A1				2.405	164

[vi] -1/2+x. 1/2-y. 1-z: 3 contacts with critical points.

E_{int}: --12.1 kJ/mol (CrystalExplorer); -13.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H28C	O17	6.6	-4.44	2.8783	1.2256	1.6539	0.027	0.322
H28B	H28C	6.58	-4.32	2.4324	1.2202	1.2161	0.025	0.325
C28	H27A	6.55	-3.86	3.2387	1.8703	1.3766	0.018	0.339

D	H	A	D-H	H···A	D···A	D-H···A
C28	H28C	O17[vi]	1.09	2.87	3.902	159
H28B	H28C[vi]				2.415	
C27[vi]	H27A[vi]	C28	1.09	3.24	3.690	106

[vii] -x. ½+y. 1/2-z: 1 contacts with critical points.

E_{int}: --12.1 kJ/mol (CrystalExplorer); -13.3 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
N1A	H3A1	13.75	-10.48	2.527	1.5061	1.0235	0.054	0.625

D	H	A	D-H	H···A	D···A	D-H···A
C3A	H3A1	N1A[vii]	1.09	2.52	3.542	157

[viii] -1+x. 1+y. z: 2 contacts with critical points.

E_{int}: --10.7 kJ/mol (CrystalExplorer); -10.1 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H20	H28A	6.62	-4.33	2.4484	1.2295	1.229	0.025	0.327
C21	H26B	2.94	-1.89	3.3626	1.9553	1.4131	0.015	0.146

D	H	A	D-H	H···A	D···A	D-H···A
H20	H28A[viii]				2.435	
C26[viii]	H26B[viii]	C21	1.09	3.35	4.419	167

[ix] -x. 1/2+y. ½-z: 2 contacts with critical points.

E_{int}: --7.0 kJ/mol (CrystalExplorer); -7.1 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
N1A	H11B	8.41	-5.21	2.8991	1.6746	1.242	0.025	0.426
N1A	H9	2.87	-1.68	3.4921	2.1154	1.4318	0.011	0.149

D	H	A	D-H	H···A	D···A	D-H···A
C11	H11B	N1A[ix]	1.09	2.90	3.546	118
C26[viii]	H26B[viii]	C21	1.09	3.50	4.098	116

[x] 1-x. -1/2+y. ½-z: 2 contacts with critical points.

E_{int}: --10.4 kJ/mol (CrystalExplorer); -9.7 kJ/mol (PIXEL)

Atom 1	Atom 2	Gcp	Vcp	D12	Dcp1	Dcp2	Den	Lap
H10A	H8B	11.38	-8.27	2.1653	1.0755	1.0906	0.04414	0.532

D	H	A	D-H	H···A	D···A	D-H···A
H8B	H10A[x]				2.170	