ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO:

Spectroscopic FT-IR and NMR studies on 2-(2-Aminoethyl)-1,2,3,4,9-tetrahydrocarbazole supported by molecular modeling of their structure, selected spectroscopic and electronic parameters

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NLO (Non-Linear Optical) Analysis

The NLO tendency of the title compound have been predicted via the static dipole moment (μ), the mean polarizability (α0), the anisotropy of the polarizability (Δα), the frequency independent first-order hyperpolarizability (β) tensors, all equations to obtain the NLO tensors have been given as below [22- 23]:

$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2}$

$\alpha_0 = (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})/3$

$\Delta\alpha = 2^{-1/2}\left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xz}^2 + \alpha_{xy}^2 + \alpha_{yz}^2)\right]^{1/2}$

$\beta = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$

where,

$\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})$

$\beta_y = (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})$

$\beta_z = (\beta_{zzz} + \beta_{zyy} + \beta_{zxx})$

Global Reactivity Descriptors, FMO (Frontier Molecular Orbital) Analysis, MEP (Molecular Electrostatic Potential)

The chemical reactivity behavior of the title compound have been obtained by the ionization energy (*I*) and electron affinity (*A*) [24], electronic chemical potential (χ), global hardness (η), electrophilicity (ω) and the maximum charge transfer index (ΔNmax) [25-27]as follows

$I = -E_{HOMO}$ $A = -E_{LUMO}$

$\chi = -\frac{I+A}{2}$ $\eta = \frac{I-A}{2}$

$\omega = \frac{\mu^2}{2\eta}$ $\Delta N_{max} = \frac{I+A}{2(I-A)}$

FT-IR Spectral Analysis

Table S1. The selected observed and calculated vibrational frequencies (in cm^{-1}) of 2-(2-Aminoethyl)-1,2,3,4,9-tetrahydrocarbazole compound in the water phase

	Conf1				Conf7			
Exp.	*Unscal.*	*Scal.*	I_{IR}	*PED %*[a]	*Unscal.*	*Scal.*	I_{IR}	*PED %*[a]
3402	3645	3524	134,5	$\nu N_{23}H$ (100)	3646	3525	131,0	$\nu N_{23}H$ (100)
	3554	3436	2,1	$\nu_{as}N_{32}H2$ (99)	3553	3435	2,1	$\nu_{as}N_{32}H2$ (99)
	3481	3365	0,2	$\nu N_{32}H2$ (99)	3480	3365	0,2	$\nu N_{32}H2$ (99)
	3185	3080	33,7	νCH R**A** (85)+ ν_{as}CH R**A** (12)	3185	3079	34,0	νCH R**A** (92)
	3175	3069	52,1	ν_{as}CH R**A** (83)	3174	3069	53,3	ν_{as}CH R**A** (88)
	3166	3061	5,8	ν_{as}CH R**A** (87)	3166	3061	5,6	ν_{as}CH R**A** (91)
3050	3158	3053	2,7	ν_{as}CH R**A** (89)	3157	3053	2,9	ν_{as}CH R**A** (88)
	3095	2992	32,9	$\nu_{as}C_{14}H$ (95)	3058	2956	84,4	$\nu(C_{14}H+C_{27}H)$ (90)
	3042	2941	144,1	$\nu_{as}(C_{26}H+ C_{27}H)$+ ν_{as}CH R**C** (90)	3054	2953	114,9	$\nu_{as}(C_{14}H+C_{27}H)$ (76)
	3033	2932	47,5	ν_{as}CH R**C** (81)	3050	2949	21,7	ν_{as}CH R**C** (88)
	3029	2928	43,5	$\nu(C_{26}H+ C_{27}H)$ (84)	3034	2934	43,9	$\nu C_{26}H$ (90)
	3028	2927	80,7	ν_{as}CH R**C** (83)	3030	2929	81,7	νCH R**C** (89)
2917	3006	2906	175,4	νCH R**C**+ $\nu(C_{26}H+ C_{27}H)$ (81)	3014	2914	70,7	νCH R**C** (87)
	2997	2897	13,6	νCH R**C**+ $\nu C_{26}H2$ (73)	3012	2912	67,9	νCH R**C** (86)
	2989	2890	5,1	νCH R**C** (84)	3002	2902	76,0	$\nu C_{26}H$ (88)
	2983	2884	87,0	νCH R**C** (88)	2984	2885	82,4	νCH R**C** (94)
	2982	2883	37,1	νCH R**C** (91)	2979	2880	33,2	νCH R**C** (87)
2849	2954	2856	136,3	$\nu C_{27}H$ (95)	2955	2856	130,4	$\nu C_{27}H$ (96)
1720	1654	1599	15,4	νCC R**A**+ ipb $HN_{23}C$ (50)	1653	1598	17,3	νCC R**A**+ ipb $HN_{23}C$ (44)
1619	1644	1589	51,3	$\sigma N_{32}H2$ (73)	1643	1589	50,9	$\sigma N_{32}H2$ (68)
	1613	1560	24,0	νCC R**AB**+ ipb $HN_{23}C$ (49)	1612	1558	27,9	νCC R**AB**+ ipb $HN_{23}C$+ $\nu N_{23}C$ (33)
	1595	1542	8,6	νCC R**AB** (51)	1594	1541	11,8	νCC R**AB** (54)
1486	1514	1463	7,9	νCC R**A** (14)+ ipb HCC R**A** (29)+ $\nu N_{23}C$ (10)	1513	1463	8,9	νCC R**A** (16)+ ipb HCC R**A** (23)+ $\nu N_{23}C$ (11)
1458	1506	1456	4,2	$\sigma C_{27}H2$ (85)	1512	1462	5,6	$\sigma C_{27}H2$ (86)
1444	1494	1445	14,7	σCH2 R**C** (82)	1491	1442	10,4	σCH2 R**C** (75)
	1485	1436	60,9	σCH2 R**C** (12)	1487	1438	45,7	σCH2 R**C** (18)
	1480	1431	10,7	σCH2 R**C** (74)	1482	1433	25,3	σCH2 R**C** (80)
	1478	1428	23,5	$\sigma C_{26}H2$+ σCH2 R**C** (59)	1479	1430	51,1	σCH2 R**C** (75)
	1474	1425	29,1	$\sigma C_{26}H2$+ σCH2 R**C** (71)	1473	1424	9,0	$\sigma C_{26}H2$ (86)
	1462	1413	28,3	ipb HCC R**A**+ σCH2 R**C** (43)+ α R**A** (14)	1464	1415	38,5	ipb HCC R**A**+ σCH2 R**C** (24)
1361	1423	1375	21,9	$\omega C_{27}H2$+ $\tau N_{32}H2$ (64)+ $\sigma C_{27}H2$ (22)	1427	1379	13,3	$\omega C_{27}H2$ (52)+ $\tau(C_{26}H2+ N_{32}H2)$ (10)
	1402	1355	5,9	ωCH2 R**C**+ $\omega C_{26}H2$ (12)	1405	1358	3,1	ωCH2 R**C**+ $\omega(C_{26}H2+ C_{27}H2)$ (33)
	1395	1349	0,5	ωCH2 R**C**+ $\omega C_{26}H2$	1396	1350	0,7	ωCH2 R**C**+ $\omega C_{26}H2$ (10)
	1392	1346	6,0	ωCH2 R**C**+ $\omega C_{26}H2$ (25)	1385	1339	14,1	ωCH2 R**C**+ $\omega C_{26}H2$ (19)
	1372	1326	16,5	χ HCCC R**C** (18)+ $\tau C_{26}H2$ (10)	1384	1338	4,3	χ HCCC R**C**+ $\tau C_{26}H2$ (54)
1314	1362	1316	10,5	χ HCCC R**C** (21)	1371	1326	14,7	νCC R**AB**+ $\nu N_{23}C$ (13)
1296	1341	1296	15,8	χ HCCC R**C** (44)	1345	1300	26,5	ipb HCC R**C** (12)
	1338	1293	5,9	$\tau(C_{26}H2+ C_{27}H2)$ (37)	1333	1289	4,4	(ω+ τ) CH2 R**C** (11)+ $\tau(C_{26}H2+ C_{27}H2)$ (29)
1275	1323	1279	111,9	ωCH2 R**C**+ $\tau C_{27}H2$ (19)	1322	1278	65,0	ωCH2 R**C**+ $\tau(C_{26}H2+ C_{27}H2)$ (30)
	1303	1259	23,7	ipb HCN_{32} (26)+ $\tau(C_{26}H2+ C_{27}H2)$ (12)	1310	1267	20,0	$\tau(C_{26}H2+ N_{32}H2)$ (42)
	1297	1254	1,3	ipb HCN_{32}+ $\tau(C_{26}H2+ C_{27}H2)$ (23)	1299	1256	37,0	ipb HCN_{32}+ $\tau(C_{26}H2+ C_{27}H2)$ (33)+ χ HCCC R**C** (12)
1240	1283	1240	17,0	ipb HCC R**C** (35)	1284	1241	12,5	χ $HCCN_{23}$ (16)
	1267	1225	4,3	ipb HCC R**C** (37)	1263	1221	7,5	ipb HCC R**C** (18)+ ωCH2 R**C**+ $\tau(C_{26}H2+ C_{27}H2)$ (10)
1216	1255	1213	23,8	ipb HCC R**C** (18)	1250	1209	23,9	ipb HCC R**C** (32)
	1239	1198	9,7	ipb HCC R**C** (40)	1234	1193	5,3	ipb HCC R**C** (35)
1168	1215	1174	13,1	ipb $HN_{23}C$ (32)	1214	1173	13,8	ipb $HN_{23}C$ (44)

1141	1172	1134	6,8	ipb HCC R**A** (36)	1181	1142	3,4	τ(C_{26}H2+ N_{32}H2) (29)
	1169	1131	6,9	τCH2 R**C** (39)	1172	1133	6,7	ipb HCC R**A** (45)+ α R**A** (15)
	1161	1122	12,9	ipb HCC R**A** (25)	1162	1123	12,0	ipb HCC R**A**+ τCH2 R**C** (44)
	1151	1113	6,4	ipb HCC R**C** (10)	1155	1117	20,7	ipb HCC R**AC** (49)
	1126	1089	1,5	α R**A** (21)+ ipb HCC R**A** (22)	1126	1088	4,2	α R**A** (29)+ νCC R**A** (10)
	1111	1074	23,7	ν(N_{32}C+ $C_{13}C_{26}$) (61)	1114	1077	8,4	ν(N_{32}C+ $C_{26}C_{27}$) (51)
	1106	1069	5,7	ν(N_{32}C+ $C_{26}C_{27}$)	1096	1060	15,4	ν(N_{32}C+ $C_{26}C_{27}$) (14)
1044	1076	1041	2,1	ipb HCC R**C**+ τN_{32}H2 (15)	1070	1035	1,3	τN_{32}H2+ α R**C** (17)
	1055	1020	13,1	ν(N_{32}C+ $C_{13}C_{26}$) (30)+ β R**C** (16)	1029	995	16,1	νCC R**A** (32)
1009	1029	994	22,3	α R**A** (33)	1027	992	12,9	ν(N_{32}C+ $C_{13}C_{26}$) (48)
981	1000	967	7,2	(ωCH2+ νCC) R**C** (32)	1010	977	19,0	ωC_{26}H2+ ρN_{32}H2 (17)
	985	952	7,0	χ HN_{32}CC (14)+ σN_{32}H2 (22)	998	965	2,1	τ(C_{26}H2+ C_{27}H2)
	975	942	3,3	νCC R**C** (12)	974	942	0,0	opb HCC R**A** (86)
	974	942	0,1	opb HCC R**A** (85)	962	930	10,0	νCC R**C** (32)+ τN_{32}H2 (15)
923	940	908	4,1	opb HCC R**A** (91)	939	908	4,6	opb HCC R**A** (89)
	925	894	46,2	χ HN_{32}CC (26)	929	898	5,8	χ $HCCN_{23}$ (10)
	915	884	11,2	ρ(CH2) R**C** (10)+ χ $HCCN_{23}$ (15)	919	889	16,6	ρ(CH2) R**C**
	893	863	3,2	ν(N_{32}C+ $C_{26}C_{27}$)+ νCC R**C** (23)+ χ HN_{32}CC (13)	892	862	21,4	ωN_{32}H2 (11)
841	886	856	31,6	ρ(CH2) R**C** (12)+ ipb CCN_{32} (11)	864	836	25,8	νCC R**AB**+ νN_{23}C (31)
	856	828	5,1	opb HCC R**A** (45)	856	827	2,1	opb HCC R**A** (77)
	854	826	9,3	opb HCC R**A** (27)	848	820	41,8	ν($C_{13}C_{26}$+ $C_{26}C_{27}$) (18)
788	824	796	97,5	ωN_{32}H2+ ρC_{27}H2 (45)	825	797	89,2	ωN_{32}H2+ ρ(C_{26}H2+ C_{27}H2) (29)+ σN_{32}H2 (28)
	806	779	8,6	ρ(CH2) R**C**+ ρC_{26}H2(15)+ ν(N_{32}C+ $C_{13}C_{26}$) (28)	791	765	3,1	ρ(CH2) R**C** (12)+ ν($C_{13}C_{26}$+ $C_{26}C_{27}$) (32)
	766	741	0,3	β R**A**+ χCN_{23}CC) (63)	765	739	0,5	β R**A** (46)+ χ(CCN_{23}C+ $CCCN_{23}$) (11)
733	746	722	130,4	opb HCC R**A** (89)	746	721	131,4	opb HCC R**A** (90)
	726	702	3,7	νCC R**C** (25)+ ipb CCN_{23} (23)	722	698	3,0	νCC R**C** (33)
	707	684	2,0	νCC R**AC** (20)+ opb CN_{23}C (15)	708	684	0,9	νCC R**C**+ β R**A**
	653	631	15,7	χ (CCCC+CN_{23}CC)+ β R**A** (51)	654	632	13,5	χ (CCCC+CN_{23}CC)+ β R**A** (52)
	611	591	0,6	ipb CCN_{23}+ α R**A** (22)	605	585	2,4	ipb CCN_{23}+ α R**A** (36)
	589	569	7,3	opb HCC R**A**+ opb HN_{23}C (71)	589	569	4,3	opb HCC R**A**+ opb HN_{23}C (59)
	557	538	3,4	α R**A** (53)	579	560	7,6	opb ($C_{13}C_{26}C_{27}$+ CCN_{32}) (33)+ νCC R**C** (11)
	537	519	11,0	opb ($C_{13}C_{26}C_{27}$+ CCN_{23}) (23)	546	528	6,3	α R**A**+ ipb $C_{13}C_{26}C_{27}$+ opb CCN_{23} (32)+ νCC R**A** (16)
	498	482	4,8	ipb (HN_{23}C+$C_{13}C_{26}C_{27}$+ CN_{23}C) (40)	514	497	7,0	ipb CCN_{23} (55)
	469	453	2,3	β R**C**+ opb CCN_{23} (26)	449	434	2,8	ipb $C_{13}C_{26}C_{27}$+ opb CCN_{23} (12)
	438	423	4,0	β R**A** (77)	437	423	4,7	β R**A** (74)
	408	395	31,4	ipb CCN_{32} (29)	409	395	11,4	ωN_{32}H2 (12)+ χHCCH R**C** (10)
	399	386	110,3	opb HN_{23}C (79)	402	388	136,2	opb HN_{23}C (84)
	346	335	12,2	opb ($C_{13}C_{26}C_{27}$+ CCN_{32}) (30)+ νCC R**C** (15)	368	355	0,6	opb ($C_{14}C_{23}C_{26}$+ CCN_{32}) (37)
	318	308	0,7	ρ(CH2) R**C**+ χCCCC R**C** (46)	318	307	0,0	ρ(CH2) R**C**+ χ(CCCC+ CCN_{23}C) (59)
	305	295	4,1	ρ(C_{26}H2+ N_{32}H2) (44)	297	287	0,6	ρC_{26}H2+ χ(CCCC+ CCN_{23}C) (47)
	283	274	11,7	χCCCC R**C**+ ρN_{32}H2 (24)	283	274	11,7	χ($CCCN_{32}$+ CCN_{23}C) (16)+ β R**A** (11)
	248	240	34,8	ρN_{32}H2 (31)	254	245	19,7	ρN_{32}H2 (36)+ χ($CCCN_{32}$+ CCN_{23}C) (19)
	240	232	25,1	ρN_{32}H2+ χC_{26}CCC (16)	232	225	29,1	ρN_{32}H2 (41)
	202	195	14,6	χ(CCCC R**AC**+ $CCCN_{23}$) (39)	204	198	32,0	χ($CCCN_{32}$+ CCN_{23}C) (35)
	175	169	6,2	χCCCC R**AC**	175	169	1,6	ipb ($C_{13}C_{26}C_{27}$+ CCN_{32}) (12)
	145	140	0,3	χ ($CCCN_{23}$+ CCCC R**C**) (33)	150	145	3,4	ipb ($C_{13}C_{26}C_{27}$+ CCN_{32}) (17)
	134	130	0,5	χ(CCCC R**C**+ $CCCN_{23}$) (23)	129	125	0,6	χ(CCN_{23}C+ $CCCN_{23}$) (14)
	93	90	1,8	χ(CCCC R**C**+ $CCCN_{32}$) (43)	104	100	4,1	χ($CCCN_{32}$+ CCN_{23}C) (40)
	56	54	2,2	χ(CCCC R**C**+ $CCCN_{32}$) (39)	46	44	1,6	χ(CCCC R**C**+ $CCCN_{23}$) (44)
	38	36	0,3	χ(CCCC R**C**+ $CCCN_{32}$) (60)	39	38	1,0	χ(CCCC R**C**+ $CCCN_{32}$) (57)

a. The abbreviation are $I_{IR,}$ IR intensity; ν, symmetric stretching; $\nu_{as,}$ asymmetric stretching; ω, wagging; τ, twisting; ρ, rocking; σ, scissoring; α, in-plan ring deformation; β, non-planar ring deformation; ipb, in-plane bending; opb, out-plane bending; sb, symmetric bending; χ, torsion; R, ring.

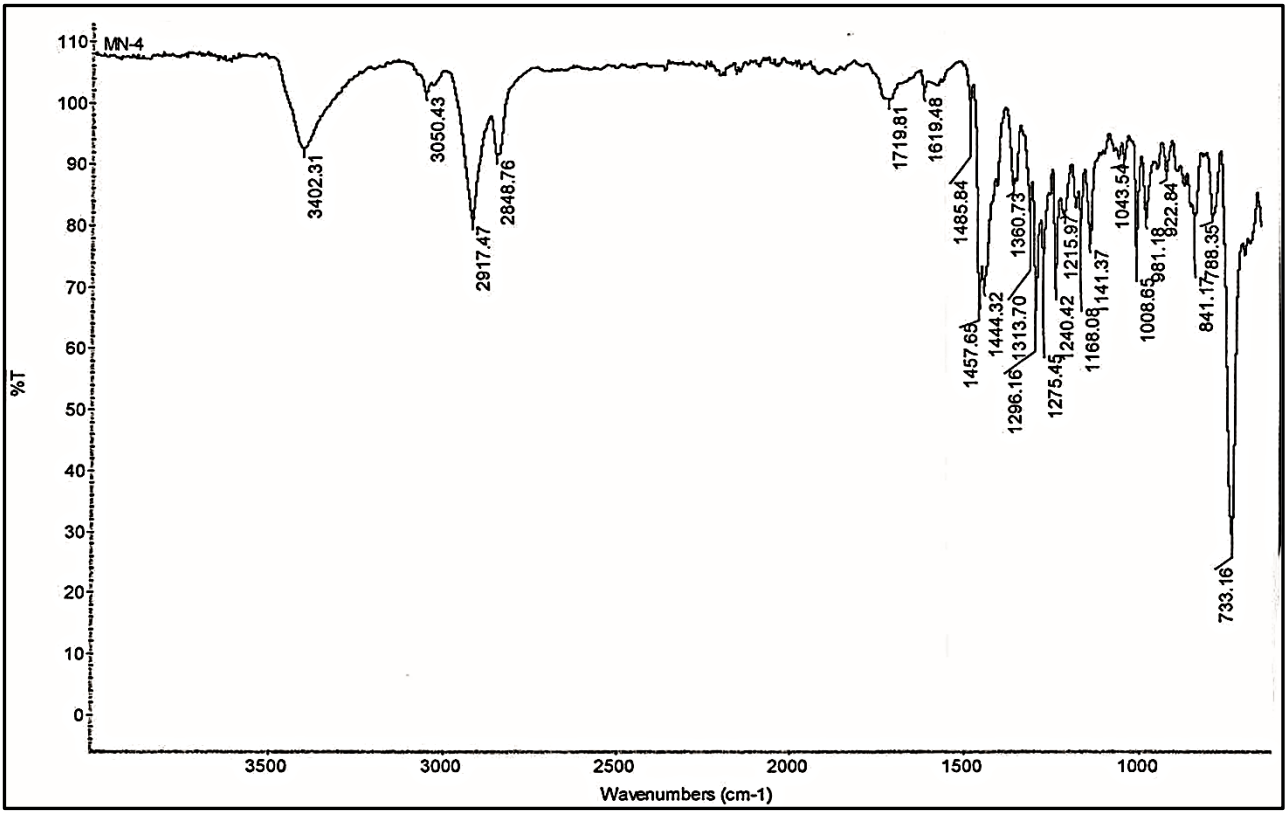

Figure S1. The recorded *FT-IR* spectra of the stable conformers for the 2-(2aminoethyl)1,2,3,4,9-tetrahydrocarbazole

^{13}C and ^{1}H NMR spectral analysis

Table S2. The observed and calculated ^{1}H and ^{13}C NMR chemical shifts (with respect to TMS, all values in ppm) for the Conf1 of the 2-(2-Aminoethyl)-1,2,3,4,9-tetrahydrocarbazole at B3LYP/6-311++G(d,p) in the gas phase

^{13}C	*Exp.*	Conf1	Conf2	Conf3	Conf4	Conf5	Conf6	Conf7
1C	119.2	125.2	125.4	125.3	125.3	125.3	125.2	125.1
2C	121.4	126.9	127.3	127.1	127.1	127.1	126.9	126.5
3C	108.9	114.0	114.2	114.1	114.2	114.2	114.1	114.0
4C	138.1	142.9	142.9	142.9	143.1	143.0	143.2	143.0
5C	128.7	135.2	134.9	135.1	135.0	135.0	135.2	135.2
6C	117.9	123.3	123.1	123.1	123.0	123.1	123.0	122.8
11C	135.2	139.6	139.6	139.9	139.9	139.7	140.0	142.0
12C	30.8	36.3	36.5	36.9	36.1	35.8	31.6	34.4
13C	32.9	45.0	42.2	42.9	35.9	39.8	35.2	41.6
14C	31.1	36.3	38.4	36.6	31.6	33.7	36.8	32.6
15C	22.1	26.0	26.2	26.3	26.2	26.2	26.1	26.7
16C	111.3	118.2	117.3	117.7	117.4	117.6	117.6	116.2
26C	41.2	43.6	47.0	43.4	44.0	45.3	44.3	41.7
27C	41.9	50.7	51.7	50.0	43.0	47.4	43.5	44.3

^{1}H	*Exp.*	Conf1	Conf2	Conf3	Conf4	Conf5	Conf6	Conf7
7H	6.95	7.22	7.24	7.23	7.23	7.23	7.22	7.21
8H	6.95	7.24	7.27	7.25	7.26	7.25	7.24	7.22
9H	7.26	7.25	7.27	7.27	7.27	7.27	7.26	7.25
10H	7.34	7.62	7.61	7.61	7.61	7.60	7.61	7.59
17H	2.00	2.51	2.54	2.57	2.50	2.58	2.22	4.35
18H	2.77	3.61	2.32	2.54	2.20	2.09	1.79	1.72
19H	2.77	2.87	2.89	2.90	2.97	2.93	2.91	2.98

20H	2.77	2.83	2.86	2.79	2.77	2.75	2.87	2.83
21H	2.39	2.58	2.60	2.59	2.65	2.61	3.01	2.49
22H	1.46	1.33	1.56	1.53	1.25	1.42	1.59	1.97
24H		6.92	6.95	6.94	6.97	6.95	6.97	6.96
25H	2.00	1.95	1.82	1.78	1.99	1.84	2.71	2.16
28H	1.46	1.42	1.37	1.81	1.36	1.72	1.71	1.75
29H	2.00	1.52	1.41	1.37	1.92	1.45	1.42	1.79
30H	2.77	3.62	3.11	2.86	3.48	3.10	3.30	3.31
31H	2.60	2.80	2.85	3.38	2.64	2.97	2.84	3.06
33H	1.46	0.82	0.13	0.65	0.78	0.88	0.68	0.73
34H	1.46	0.18	0.99	0.86	0.61	0.28	0.03	0.15

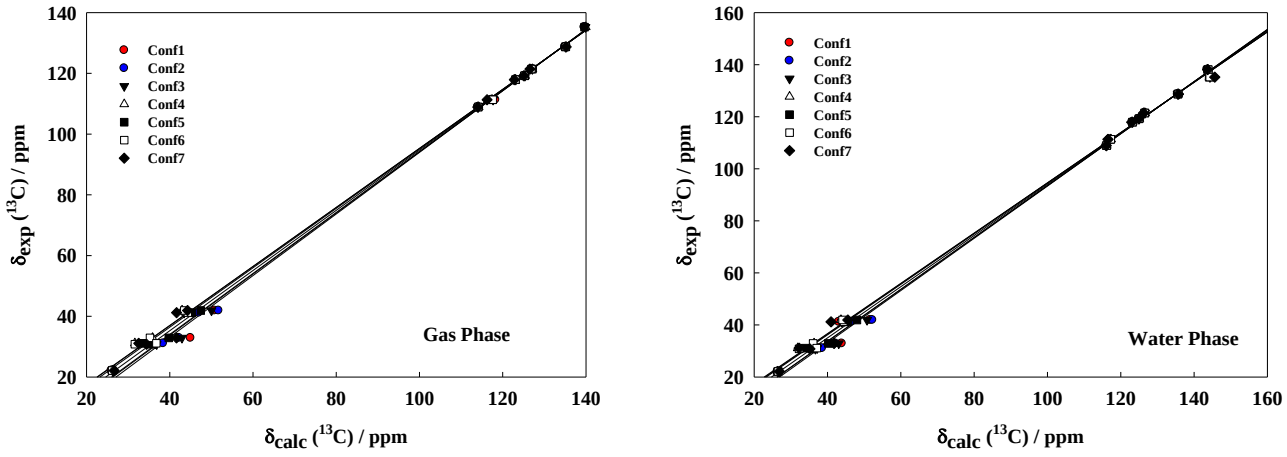

Figure S2a. The comparison of the experimental and calculated *13C* NMR isotropic chemical shifts (with respect to TMS) for the most stable conformers of 2-(2aminoethyl)1,2,3,4,9-tetrahydrocarbazole

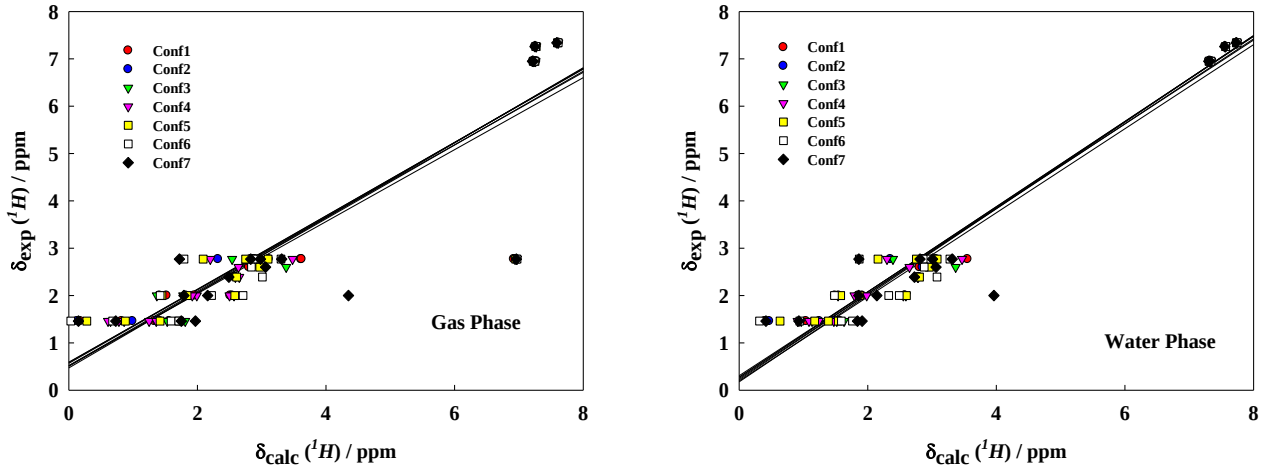

Figure S2b. The comparison of the experimental and calculated ^{1}H isotropic chemical shifts (with respect to TMS) for the most stable conformers of 2-(2aminoethyl)1,2,3,4,9-tetrahydrocarbazole

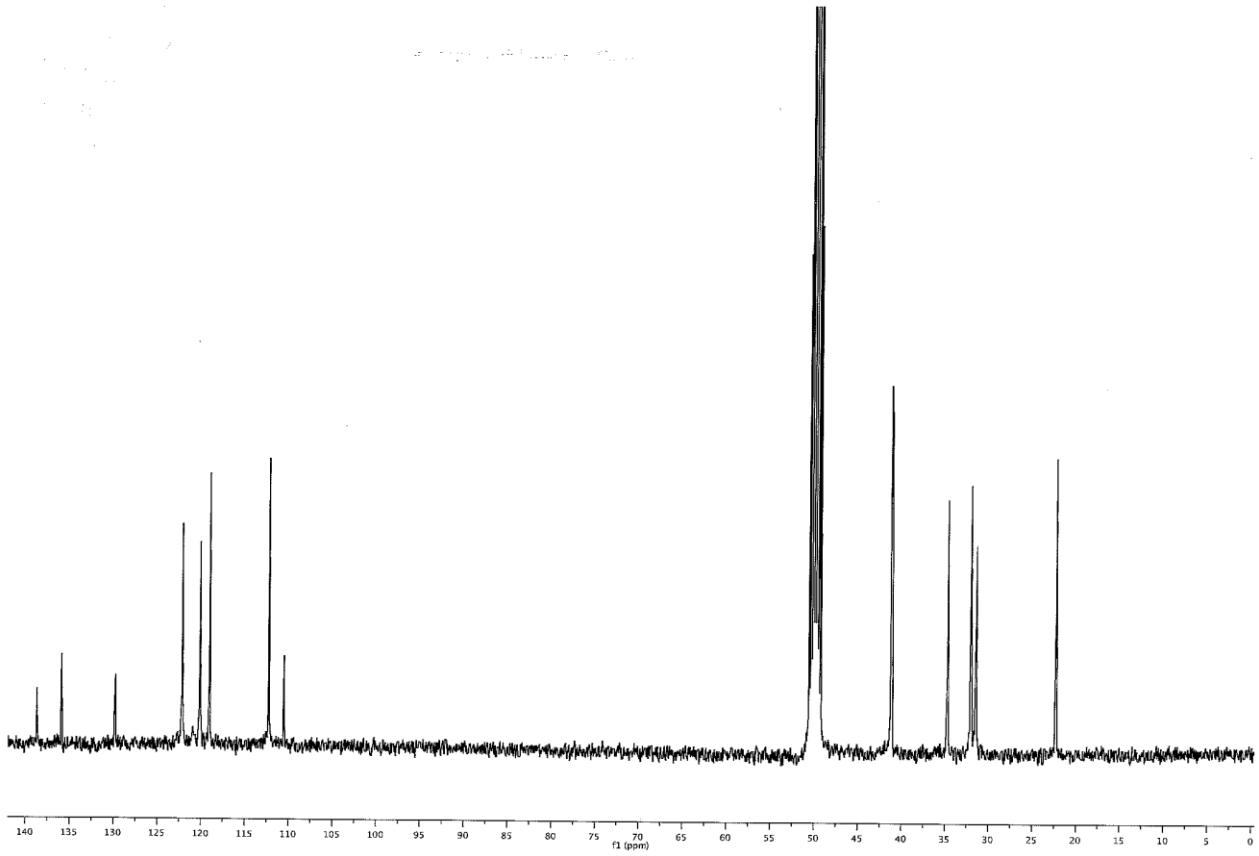

Figure S3a. The recorded *^{13}C NMR* spectrum of 2-(2aminoethyl)1,2,3,4,9-tetrahydrocarbazole

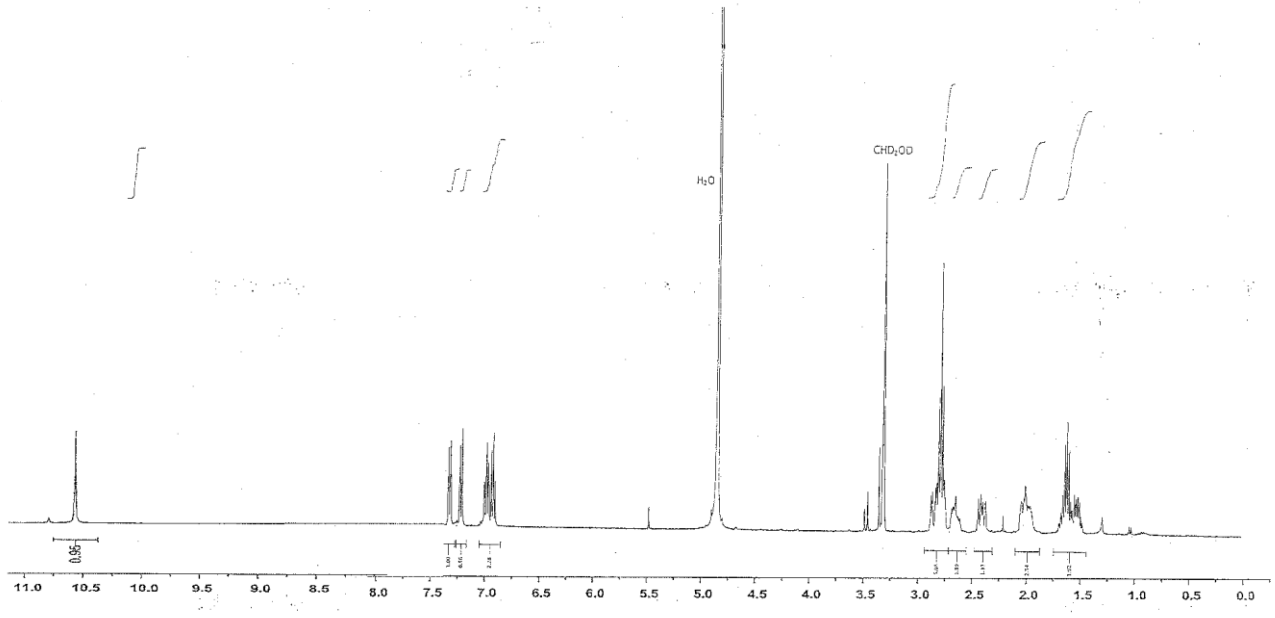

Figure S3b. The recorded *^{1}H NMR* spectrum of 2-(2aminoethyl)1,2,3,4,9-tetrahydrocarbazole

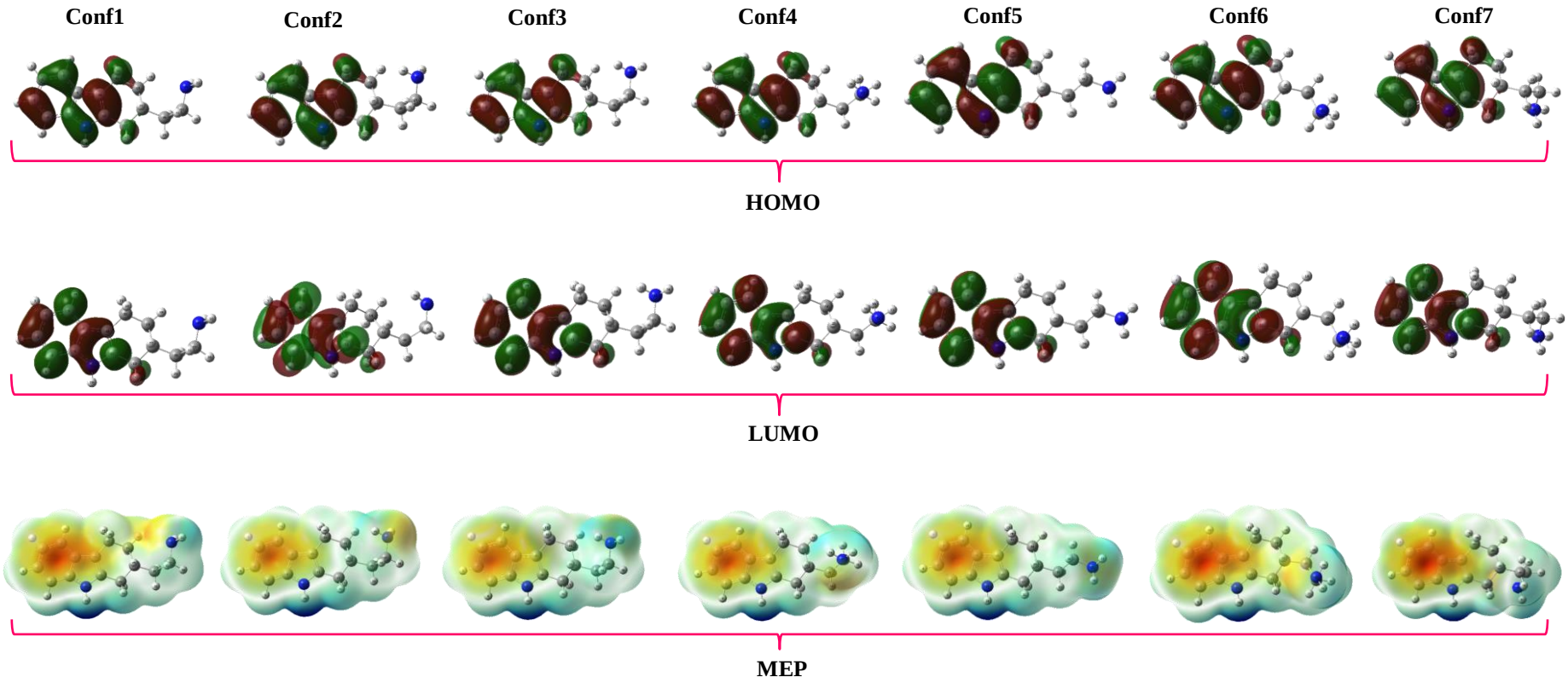

Fig. S4. HOMO and LUMO amplitudes (isoval:0.02) and MEP diagrams (isoval:0.0004) of the seven stable conformers for the title compound at B3LYP/6-311++G(d,p) basis set in the water phase