Supporting Information

for

Investigation of the role of stereoelectronic effects in the conformation of piperidones by NMR spectroscopy and X-ray diffraction

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Additional schemes, figures, theoretical, spectra, and crystallographic data

Content:

Theoretical calculations summary
Compound **3**
Cartesian coordinates s3
Natural population analysis s4
Perturbation theory energy analysis of Fock matrix s5
Compound **1**
Cartesian Coordinates s6
Natural population analysis s8
Perturbation theory energy analysis of Fock matrix s9
Crystallography data
Compound **1** s10
Compound **6** s10
Compound **7** s10
NMR Data:
Table S1. ^{1}H NMR data: chemical shift (δ) and $^{n}J_{H,H}$ (Hz) for compound **1-8** in CDCl3 s11
Table S2. ^{13}C NMR data: chemical shift (δ) and $^{1}J_{C,H}$ (Hz) for compound **1-8** in CDCl3 s12
Schemes:
Scheme S1. (a) Stabilization of positive charges by the homohyperconjugation effect in organometallic molecules. (b) Stabilization of conformation by LPE (N, O and S) homohyperconjugation through W arrangement and Plough effect. s13
Scheme S2. Reaction mechanism proposed for the synthesis of piperidones **1** and **2** by double Mannich reaction s14

Supporting Information

Scheme S3. Reaction mechanism proposed for the synthesis of piperidones **3** to **8** by Mannich reaction s15

Scheme S4. A(1,3) allylic strain. s16

Scheme S5. (a) preferred conformation for the compound **1** and **2**. (b) dqf- COSY spectrum of compound **1** in $CDCl_3$. (c) t-ROESY spectrum of compound **1** in $CDCl_3$. s16

Scheme S6. NMR characterization of compound **4**. (a) ^1H spectrum in $CDCl_3$. (b) dqf-COSY spectrum. (c) HSQC spectrum$_3$. s17

Scheme S7. Determination of the conformation of piperidones by t-ROESY spectrum s18

Scheme S8. (a) ORTEP diagram of compounds **1**, thermal ellipsoids are drawn at 30% probability level for all atoms other than H. (b) crystal packing and C(15)···H(15)···π inter and intramolecular interaction of compound **1**. s19

Scheme S9. (a) ORTEP diagram of compounds **6** and **7**, thermal ellipsoids are drawn at 30% probability level for all atoms other than H. (b) Intermolecular hydrogen bonds of compound **6** and **7** s20

Scheme S10. $^1J_{C,H}$ coupling constant of compound **3**, **5**, **6** and **8** s21

Scheme S11. Schematic representation of $n_X \rightarrow \sigma^*_{C7\text{-}Heq}$ Hyperconjugation in the piperidones **3-8** s21

Scheme S12. Distance between N(3) and σ*C-H orbital of compound **3**, **5**, **6** and **7,** measured by X-ray s22

Select spectra

^1H NMR spectrum of **1** s23

^{13}C NMR spectrum of **1** s24

^1H NMR spectrum of **2** s25

^{13}C NMR spectrum of **2** s26

^1H spectrum of compound **3** s27

^{13}C spectrum of compound **3** s28

$^1H,^1H$ COSY spectrum of compound **3** s29

dqf spectrum of compound **3** s30

^1H NMR spectrum of compound **4** s31

^{13}C NMR spectrum of compound **4** s32

HSQC spectrum of compound **4** s33

t-ROESY spectrum of compound **4** s34

^1H spectrum of compound **5** s35

^{13}C spectrum of compound **5** s36

dqf spectrum of compound **5** s37

^1H spectrum of compound **6** s38

^{13}C spectrum of compound **6** s39

^1H NMR spectrum of compound **7** s40

^{13}C NMR spectrum of compound **7** s41

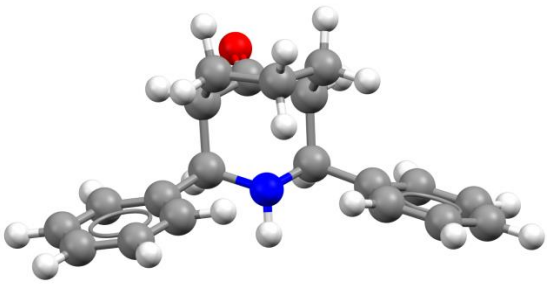
^1H-^1H COSY spectrum of compound **7** s42

HSQC spectrum of compound **7** s43

DQF spectrum of compound **7** s44

THEORETICAL CALCULATIONS SUMMARY

Compound 3:



Cartesian Coordinates

Atom	X	Y	Z
C1	1.248451	1.688571	0.067809
C2	1.227609	0.388289	-0.786319
C4	-1.22763	0.388297	-0.786296
C5	-1.248451	1.688559	0.067858
C6	-1.275225	1.482261	1.596693
C7	0.00005	0.844856	2.161153
C8	1.275296	1.482286	1.596647
C9	-0.000007	2.46291	-0.288211
H1eq	2.118875	2.273235	-0.238543
H2ax	1.289286	0.726162	-1.836822
H3	-0.000019	-1.203281	-1.109553
H4ax	-1.289326	0.726191	-1.836795
H5eq	-2.118891	2.27322	-0.238454
H6ax	-1.417508	2.470693	2.048846
H6eq	-2.151439	0.886662	1.868016
H7ax	0.000066	-0.221612	1.939009
H7eq	0.000069	0.947634	3.250751
H8ax	1.417576	2.470728	2.048789
H8eq	2.151529	0.886696	1.867929
N3	-0.000014	-0.359509	-0.547615
O9	-0.000025	3.551449	-0.81209
C10	2.450483	-0.461361	-0.514087
C11	3.646217	-0.163805	-1.167052
C12	4.801068	-0.886486	-0.899218
C13	4.773668	-1.925767	0.024532
C14	3.585269	-2.234243	0.674369
C15	2.431032	-1.505645	0.40814
C16	-2.450506	-0.461358	-0.514077
C17	-3.64628	-0.163699	-1.166921

C18	-4.801122	-0.886395	-0.899087
C19	-4.773672	-1.925797	0.024527
C20	-3.585229	-2.234378	0.674231
C21	-2.431	-1.505763	0.408008
H11	3.670975	0.642357	-1.894557
H12	5.722583	-0.642863	-1.416199
H13	5.673966	-2.492683	0.233242
H14	3.555276	-3.043893	1.395221
H15	1.504463	-1.742536	0.917638
H17	-3.671079	0.642557	-1.894315
H18	-5.722675	-0.64269	-1.415966
H19	-5.673962	-2.492724	0.233229
H20	-3.555192	-3.044123	1.394971
H21	-1.504392	-1.742751	0.917388

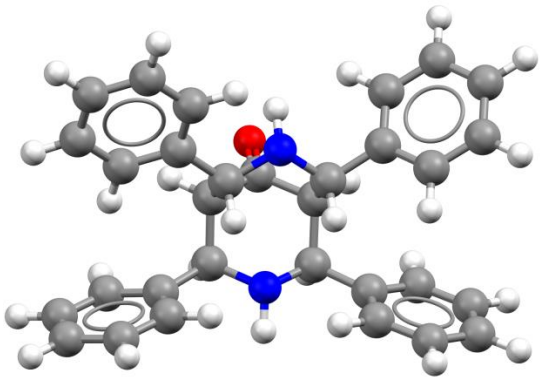
Natural population analysis in ωB97XD/6-311++G(d,p) level theory.

Atom	Mulliken atomic charges	Natural charge	core	Valence	Rydberg	Total
C1	0.218704	-0.30643	1.99906	4.28539	0.02197	6.30643
C2	-0.041174	-0.01803	1.99911	3.99161	0.02730	6.01803
C4	-0.041172	-0.01744	1.99911	3.99159	0.02674	6.01744
C5	0.218709	-0.30643	1.99906	4.28540	0.02197	6.30643
C6	-0.681972	-0.38763	1.99926	4.37394	0.01443	6.38763
C7	-0.128455	-0.39507	1.99927	4.38278	0.01302	6.39507
C8	-0.681931	-0.38763	1.99926	4.37393	0.01443	6.38763
H1eq	0.290847	0.23224	0.00000	0.76542	0.00234	0.76776
H2ax	0.255559	0.18168	0.00000	0.81565	0.00266	0.81832
H4ax	0.255564	0.18168	0.00000	0.81565	0.00267	0.81832
H5eq	0.290840	0.23224	0.00000	0.76542	0.00234	0.76776
H6ax	0.213837	0.20509	0.00000	0.79309	0.00182	0.79491
H6eq	0.171444	0.22001	0.00000	0.77819	0.00180	0.77999
H7ax	0.080061	0.20947	0.00000	0.78838	0.00215	0.79053
H7eq	0.220823	0.20328	0.00000	0.79479	0.00193	0.79672
H8ax	0.213841	0.20508	0.00000	0.79310	0.00182	0.79492
H8eq	0.171443	0.21999	0.00000	0.77819	0.00182	0.78001

Perturbation theory energy analysis of Fock Matrix

NBO interaction	E(2) [kcal/mol]	E(j)-E(i) [a.u.]	F(i,j) [a.u.]
$n_N \rightarrow \sigma^*_{C7Heq}$	0.55	0.89	0.02
$n_N \rightarrow \sigma^*_{C7Hax}$			
$\sigma_{C7Heq} \rightarrow \sigma^*_{C6C5}$	3.87	1.03	0.056
$\sigma_{C6C5} \rightarrow \pi^*_{CO}$	3.89	0.8	0.05
$\sigma_{C6C5} \rightarrow \pi^*_{CO}$	2.45	1.41	0.053
$\sigma_{C6Heq} \rightarrow \sigma^*_{C5C9}$	3.06	1.06	0.051
$\sigma_{C5C9} \rightarrow \sigma^*_{CO}$	0.93	1.44	0.033
$\sigma_{C6Hax} \rightarrow \sigma^*_{C5C4}$	4.71	1.01	0.062
$\sigma_{C7Hax} \rightarrow \sigma^*_{C6Hax}$	3.01	1.06	0.051
$\sigma_{C4C5} \rightarrow \pi^*_{CO}$	4.78	0.8	0.055
$\sigma_{C4C5} \rightarrow \sigma^*_{CO}$	2.14	1.4	0.049

Compound 1:



Cartesian Coordinates

Atom	X	Y	Z
C1	-1.243491	-0.113438	1.251766
C2	-1.136332	-1.636654	0.973133
C4	1.299463	-1.484838	1.053066
C5	1.240723	0.062772	1.240105
C6	1.140814	0.864805	-0.107886
C8	-1.285169	0.740091	-0.066921
C9	-0.022731	0.307571	2.030326
H1eq	-2.130018	0.067402	1.858983
H2ax	-1.187625	-2.138501	1.955315
H3	0.197201	-2.903095	0.09021
H4ax	1.30273	-1.91439	2.070501
H5eq	2.092893	0.382989	1.839914
H6ax	1.120411	0.126945	-0.915643
H7	-0.139347	2.3673	0.441115
H8ax	-1.266132	0.050218	-0.912243
N3	0.126492	-1.914697	0.304188
N7	-0.11546	1.599516	-0.223812
O9	-0.05136	0.762669	3.148714
C10	-2.323289	-2.101459	0.152445
C11	-3.57128	-2.204219	0.766862
C12	-4.697492	-2.5491	0.034268
C13	-4.59099	-2.807111	-1.328903
C14	-3.3512	-2.719839	-1.946861
C15	-2.223852	-2.366712	-1.211108
C16	2.580644	-1.920677	0.380644
C17	3.71843	-2.121612	1.162646
C18	4.937986	-2.429631	0.575837
C19	5.033826	-2.550572	-0.806658
C20	3.901522	-2.372727	-1.591077

C21	2.681025	-2.061933	-1.00169
C22	-2.565202	1.538207	-0.138267
C23	-3.534903	1.228721	-1.086931
C24	-4.732308	1.934867	-1.131341
C25	-4.971449	2.96035	-0.225753
C26	-4.01073	3.271053	0.731337
C27	-2.819587	2.559992	0.777522
C28	2.329298	1.77856	-0.368293
C29	3.631487	1.361577	-0.084463
C30	4.719886	2.173455	-0.374473
C31	4.529499	3.423422	-0.951675
C32	3.23979	3.845308	-1.244912
C33	2.150371	3.028509	-0.961482
H11	-3.663717	-2.001935	1.829885
H12	-5.660706	-2.617617	0.527029
H13	-5.470235	-3.077716	-1.902616
H14	-3.256464	-2.920815	-3.008354
H15	-1.261346	-2.279672	-1.701818
H17	3.647886	-2.019807	2.241659
H18	5.814187	-2.577186	1.197254
H19	5.985567	-2.786721	-1.268761
H20	3.968249	-2.470994	-2.668734
H21	1.800744	-1.920086	-1.617799
H23	-3.357356	0.41948	-1.788176
H24	-5.479296	1.679877	-1.874854
H25	-5.904633	3.511422	-0.259885
H26	-4.193806	4.063017	1.449038
H27	-2.091487	2.793511	1.549596
H29	3.811092	0.388219	0.355714
H30	5.721339	1.823614	-0.14876
H31	5.378938	4.059262	-1.17513
H32	3.075669	4.814407	-1.703406
H33	1.150357	3.353367	-1.219965

Natural population analysis in ωB97XD/6-311++G(d,p) level theory.

Atom	Mulliken atomic charges	Natural charge	core	Valence	Rydberg	Total
C1	-0.020307	-0.32407	1.99903	4.29887	0.02617	6.32407
C2	-0.282628	-0.01213	1.99911	3.98868	0.02435	6.01213
C4	-0.245294	-0.01732	1.9991	3.99145	0.02677	6.01732
C5	0.089815	-0.34843	1.99909	4.31377	0.03557	6.34843
C6	-0.346836	0.08808	1.99913	3.88578	0.02701	5.91192
C8	0.045344	-0.04055	1.99912	4.00347	0.03796	6.04055
C9	-0.615489	0.61974	1.99913	3.33092	0.05021	5.38026
H1eq	0.330551	0.24269	0	0.75538	0.00193	0.75731
H2ax	0.270595	0.18705	0	0.8103	0.00265	0.81295
H3	0.33721	0.37353	0	0.62336	0.00312	0.62647
H4ax	0.250479	0.18425	0	0.81301	0.00274	0.81575
H5eq	0.335355	0.24188	0	0.75534	0.00278	0.75812
H6ax	0.13706	0.21273	0	0.78296	0.00431	0.78727
H7	0.222254	0.35553	0	0.64042	0.00405	0.64447
H8ax	0.201887	0.2181	0	0.77855	0.00336	0.7819

Perturbation theory energy analysis of Fock Matrix

NBO interaction	E(2) [kcal/mol]	E(j)-E(i) [a.u.]	F(i,j) [a.u.]
$n_{N3}\rightarrow\sigma^*_{C1C2}$	1.41	0.83	0.031
$n_{N3}\rightarrow\sigma^*_{C5C4}$	2	0.82	0.037
$n_{N3}\rightarrow\sigma^*_{C4H4ax}$	10.53	0.72	0.079
$n_{N3}\rightarrow\sigma^*_{C4C16}$	0.86	0.88	0.025
$n_{N3}\rightarrow\sigma^*_{C2H2ax}$	9.89	0.87	0.084
$n_{N3}\rightarrow\sigma^*_{C2C10}$	1.07	0.89	0.028
$n_{N3}\rightarrow\sigma^*_{C25C24}$	0.81	0.3	0.014
$n_{N3}\rightarrow\sigma^*_{C27C26}$	1.42	0.2	0.015
$n_{N7}\rightarrow\sigma^*_{C1C8}$	11.54	0.82	0.088
$n_{N7}\rightarrow\sigma^*_{C5C6}$	0.91	0.48	0.019
$n_{N7}\rightarrow\sigma^*_{C6H6ax}$	1.99	0.93	0.039
$n_{N7}\rightarrow\sigma^*_{C8N7}$	2.97	0.78	0.044
$n_{N7}\rightarrow\sigma^*_{C8C22}$	0.86	0.92	0.025
$n_{N7}\rightarrow\sigma^*_{C4H4ax}$	7.57	0.73	0.067
$n_{N7}\rightarrow\sigma^*_{C4C16}$	0.51	0.89	0.019
$n_{N7}\rightarrow\sigma^*_{N3H3}$	0.6	0.89	0.021
$\sigma_{N3H3}\rightarrow\sigma^*_{C2C11}$	3.41	1.14	0.056
$\sigma_{N3H3}\rightarrow\sigma^*_{C3C9}$	3.42	1.13	0.056
$\sigma_{N3H3}\rightarrow\pi^*_{C5O8}$	1.3	0.21	0.015
$\sigma_{C4H4ax}\rightarrow\sigma^*_{C5C6}$	6.08	0.67	0.057
$\sigma_{C4H4ax}\rightarrow\pi^*_{C9O9}$	3.72	0.09	0.017
$\sigma_{C2H2ax}\rightarrow\sigma^*_{C1C8}$	3.94	1.01	0.057
$\sigma_{C2H2ax}\rightarrow\pi^*_{C9O9}$	7.54	0.09	0.024
$n_{O9}\rightarrow\sigma^*_{C1C9}$	2.54	1.26	0.051
$\pi_{O9}\rightarrow\sigma^*_{C1C9}$	24.43	0.83	0.129
$\pi_{O9}\rightarrow\sigma^*_{C5C6}$	1.38	0.43	0.022
$\sigma_{C5H5eq}\rightarrow\sigma^*_{C9O9}$	0.64	1.3	0.026
$\sigma_{C5H5eq}\rightarrow\pi^*_{C9O9}$	1.24	0.09	0.01
$\sigma_{C1H1eq}\rightarrow\sigma^*_{C9O9}$	0.68	1.3	0.027
$\sigma_{C8H8ax}\rightarrow\sigma^*_{N7H7}$	4.58	1.07	0.063
$\sigma_{C6H6ax}\rightarrow\sigma^*_{N7H7}$	4.85	1.05	0.064
$\sigma_{C6H6ax}\rightarrow\pi^*_{C9O9}$	57.12	0.06	0.052

Crystallography

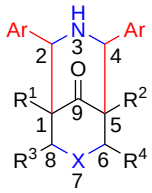
The crystallographic data for compounds **1, 6** and **7** have been deposited in the Cambridge Crystallographic Data Centre with the deposition numbers CCDC 928314 (**1**), 928315 (**6**), 933224 (**7**), respectively. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

Crystallographic data for 1 (2,4,6,8-tetraphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one): chemical formula: $C_{31}H_{28}N_2O$; formula weight (M): 444.55; temperature: 293(2) K; monoclinic; P21/n; a = 13.986(2) Å, b = 10.039(5) Å, c = 17.529(4) Å, α = 90.00°, β = 104.99(3)°, γ = 90.00°; V = 2377.4 $Å^3$; Z = 4; Density (calculated) = 1.320 Mg/m^3; number of reflections collected: 16 119; Final R indices [I>2sigma(I)] R1 = 0.0539, wR2 = 0.1350; Data / restraints / parameters = 5357 / 0 / 419, Goodness-of-fit on F^2 = 1.048.

Crystallographic data for 6 (2,4-bis(3-nitrophenyl)-3-azabicyclo[3.3.1]nonan-9-one): chemical formula:$C_{20}H_{19}N_3O_5$; formula weight (M): 381.38; temperature: 293(2) K; Triclinic; P-1; a = 7.226 (4), b = 8.2780(12), c = 16.0640(10) Å, α = 96.20(2) Å, β = 91.364(1) Å, γ = 99.900(1) Å; V = 940.2(5) $Å^3$; Z = 2; Density (calculated) = 1.347 Mg/m^3; number of reflections collected: 6 469; Final R indices [I>2sigma(I)] R1 = 0.0589, wR2 = 0.1366; Data / restraints / parameters = 4159 / 0 / 329, Goodness-of-fit on F^2 = 1.048.

Crystallographic data for 7 (1-methyl-2,4-bis(3-nitrophenyl)-3-azabicyclo[3.3.1]nonan-9-one): chemical formula:$C_{21}H_{21}N_3O_5$; formula weight (M): 395.4; temperature: 293(2) K; Orthorhombic; Pna21; a = 6.861 (4), b = 11.744(5), c = 23.713(2) Å, α = 90.0 Å, β = 90.0 Å, γ = 90.0 Å; V = 1910.7(14) $Å^3$; Z = 4; Density (calculated) = 1.375 Mg/m^3; number of reflections collected: 14 713; Final R indices [I>2sigma(I)] R1 = 0.0619, wR2 = 0.1607; Data / restraints / parameters = 3314 / 1 / 278, Goodness-of-fit on F^2 = 1.073.

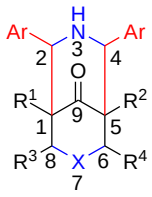
Table S1. ^{1}H NMR data: chemical shift (δ) and $^{n}J_{H,H}$ (Hz) for compounds **1–8** in $CDCl_3$.



Comp.	X	Ar	R^1	R^2	R^3	R^4
1	NH	C_6H_5	H	H	C_6H_5	C_6H_5
2	NH	C_6H_5	H	CH_3	C_6H_5	C_6H_5
3	CH_2	C_6H_5	H	H	H	H
4	CH_2	C_6H_5	H	CH_3	H	H
5	CH_2	C_6H_5	CH_3	CH_3	H	H
6	CH_2	$3NO_2$-C_6H_4	H	H	H	H
7	CH_2	$3NO_2$-C_6H_4	H	CH_3	H	H
8	CH_2	$3NO_2$-C_6H_4	CH_3	CH_3	H	H

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
$\delta_{H(1)eq}$	2.87	-	2.48	-	-	2.56	-	-
$\delta_{H(2)ax}$	4.37	5.3	4.41	3.95	3.93	4.58	4.12	3.96
$\delta_{H(4)ax}$	4.37	4.76	4.41	4.40	3.93	4.58	4.56	3.96
$\delta_{H(5)eq}$	2.87	3.00	2.48	2.57	-	2.56	2.63	NA
$\delta_{H(6)ax}$	4.72	4.37	1.70	1.71	1.50	1.78	1.76	1.56
$\delta_{H(6)eq}$	-	-	1.93	1.94	2.11	1.86	1.84	2.04
$\delta_{H(7)ax}$	-	-	2.9	3.19	3.49	2.82	3.11	3.49
$\delta_{H(7)eq}$	-	-	1.39	1.45	1.49	1.49	1.52	1.52
$\delta_{H(8)ax}$	4.72	3.86	1.70	1.46	1.5	1.78	1.54	1.56
$\delta_{H(8)eq}$	-	-	1.93	2.08	2.11	1.86	2.01	2.04
δ_{Me}	-	0.65	-	0.81	0.84	-	0.82	0.85
$^{3}J_{H(1)eq,H(2)ax}$	2.1	-	1.8	-	-	1.8	-	-
$^{3}J_{H(1)eq,H(8)}$	3.0	-	1.5	-	-	1.4	-	-
$^{3}J_{H(4)ax,H(5)eq}$	2.1	2.0	1.8	3.0	-	1.8	2.9	-
$^{3}J_{H(5)eq,H(6)}$	3.0	3.4	1.5	2.7	-	1.4	2.3	-
$^{2}J_{H(6)ax,H(6)eq}$	-	-	13.0	13.8	13.6	13.7	13.8	13.6
$^{2}J_{H(7)ax,H(7)eq}$	-	-	13.1	13.3	13.1	13.1	13.2	13.2
$^{2}J_{H(8)ax,H(8)eq}$	-	-	13.6	13.3	13.6	13.7	13.6	13.6
$^{3}J_{H(6)ax,H(7)ax}$	-	-	13.3	13.4	13.7	13.3	13.4	13.8
$^{3}J_{H(6)ax,H(7)eq}$	-	-	6.1	6.0	6.8	6.2	6.3	6.8
$^{3}J_{H(7)ax,H(8)ax}$	-	-	13.3	13.4	13.7	13.3	13.4	13.8
$^{3}J_{H(7)ax,H(8)eq}$	-	-	6.1	5.7	6.8	6.2	5.6	6.8

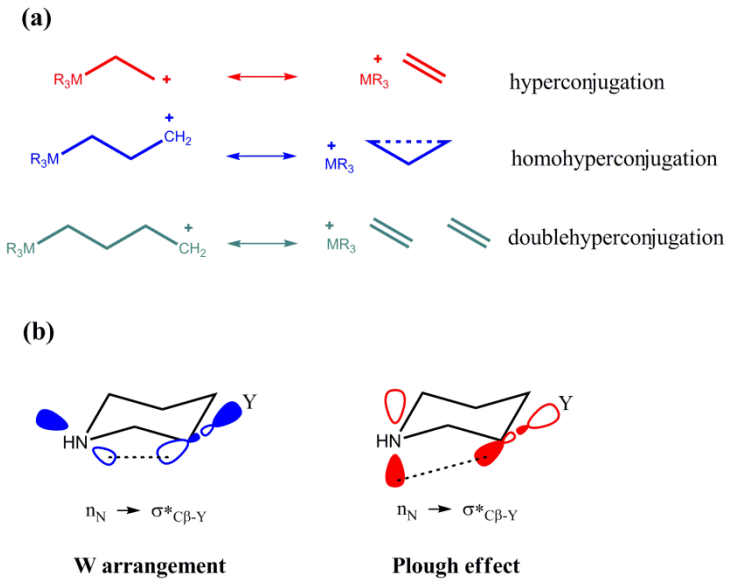
Table S2. ^{13}C NMR data: chemical shift (δ) and ^{1}JC,H (Hz) for compounds **1–8** in $CDCl_3$



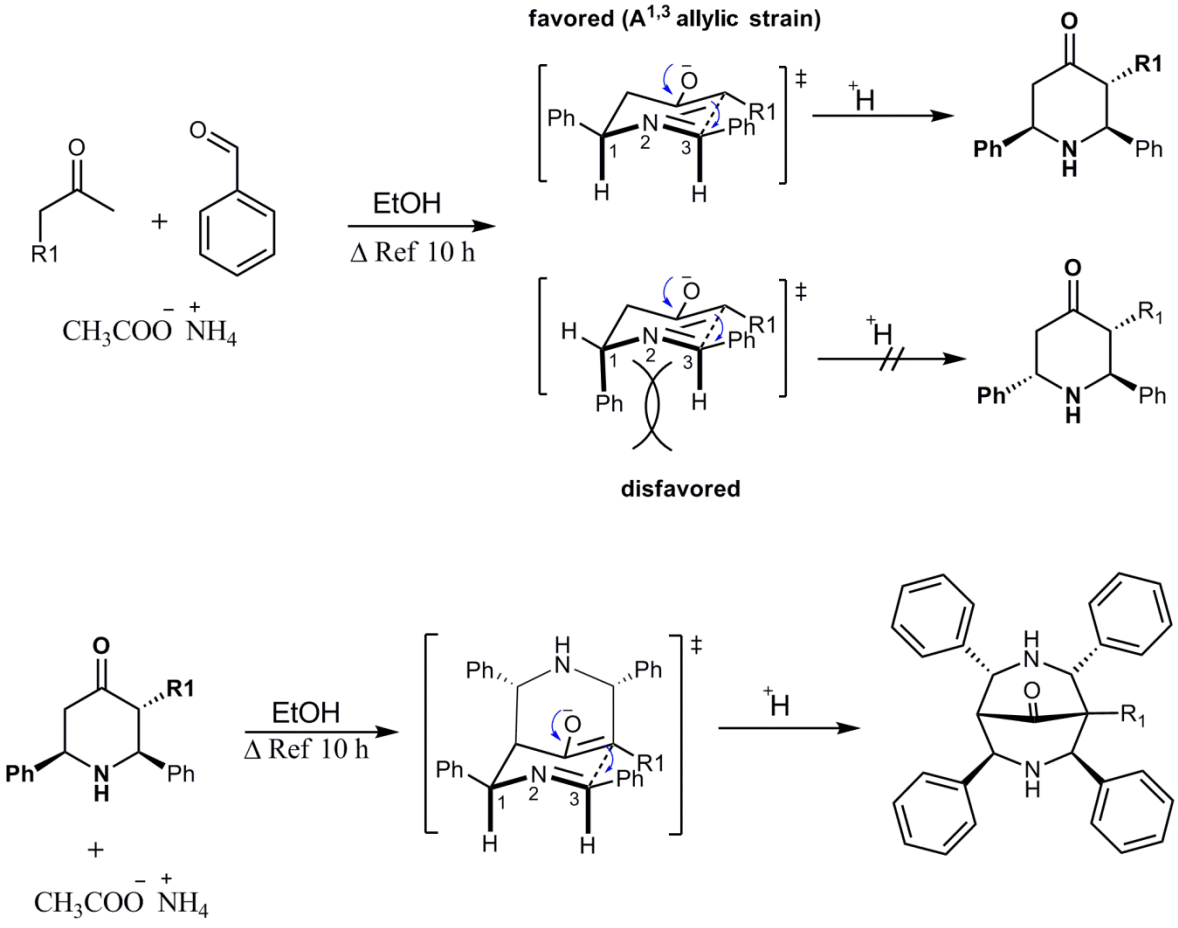
Comp.	X	Ar	R^1	R^2	R^3	R^4
1	NH	C_6H_5	H	H	C_6H_5	C_6H_5
2	NH	C_6H_5	H	CH_3	C_6H_5	C_6H_5
3	CH_2	C_6H_5	H	H	H	H
4	CH_2	C_6H_5	H	CH_3	H	H
5	CH_2	C_6H_5	CH_3	CH_3	H	H
6	CH_2	$3NO_2$-C_6H_4	H	H	H	H
7	CH_2	$3NO_2$-C_6H_4	H	CH_3	H	H
8	CH_2	$3NO_2$-C_6H_4	CH_3	CH_3	H	H

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
C(1)	63.41	54.84	54.1	50.94	51.11	53.29	50.55	51.06
C(2)	58.77	61.64	64.87	71.33	71.65	64.02	70.42	70.81
C(4)	58.77	58.64	64.87	65.06	71.65	64.02	64.21	71.20
C(5)	63.41	62.57	54.1	54.49	51.11	53.29	53.68	50.56
C(6)	61.80	63.31	29.17	29.23	37.02	28.92	29.01	36.98
C(7)	-	-	21.24	21.54	21.58	21.18	21.45	21.48
C(8)	61.80	70.30	29.17	36.96	37.02	28.92	36.74	36.94
C(9)	211.66	212.70	217.74	218.01	218.16	214.92	215.46	215.56
Me	-	18.41	-	20.43	20.93	-	20.25	20.73
$^{1}J_{C(1),Heq}$	138.7	-	136.3	-	-	136.3	-	-
$^{1}J_{C(2),Hax}$	140.5	138.4	134.4	133.9	134.0	137.4	135.9	136.0
$^{1}J_{C(4),Hax}$	140.5	138.7	134.4	135.0	134.0	137.4	135.9	135.9
$^{1}J_{C(5),Heq}$	138.7	138.0	136.3	136.3	-	136.3	136.2	-
$^{1}J_{C(6),Hax}$	140.6	136.4	125.9	128.1	125.3	133.4	127.6	132.2
$^{1}J_{C(6),Heq}$	-	-	130.4	131.8	130.5	133.5	130.2	131.4
$^{1}J_{C(7),Hax}$	-	-	131.5	131.7	130.9	130.2	130.0	130.5
$^{1}J_{C(7),Heq}$	-	-	125.9	125.9	125.2	125.5	126.4	125.4
$^{1}J_{C(8),Hax}$	140.6	136.4	125.9	124.4	125.3	125.4	126.8	125.5
$^{1}J_{C(8),Heq}$	-	-	130.4	130.2	130.5	133.5	131.7	133.3
Me	-	128.5	-	126.7	126.6	-	127.3	127.5

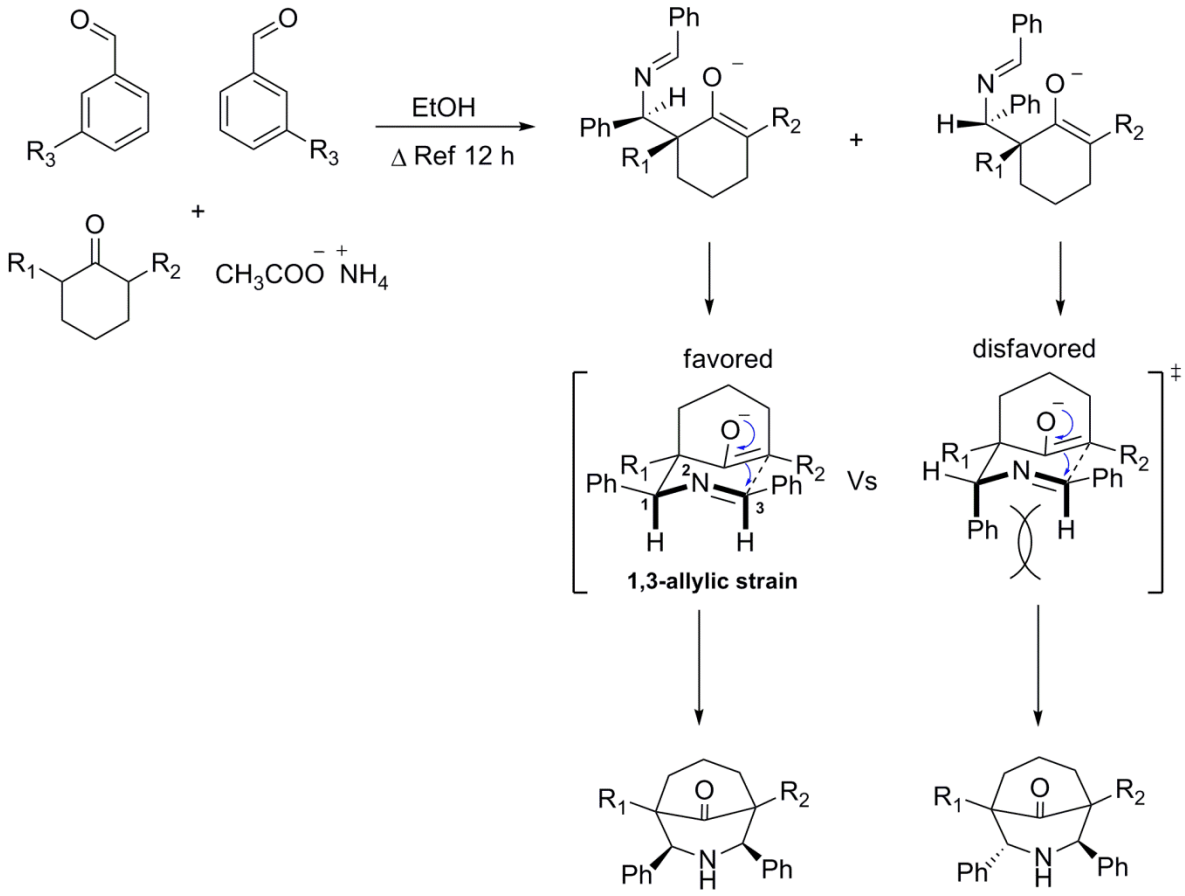
Schemes:



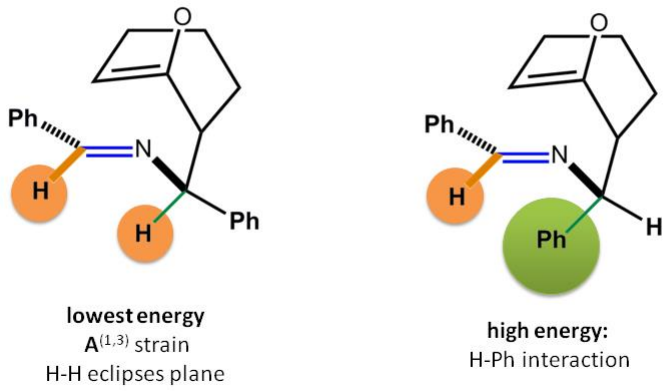
Scheme S1. (a) Stabilization of positive charges by the homohyperconjugation effect in organometallic molecules. (b) Stabilization of conformation by LPE (N, O and S) homohyperconjugation through W arrangement and Plough effect.



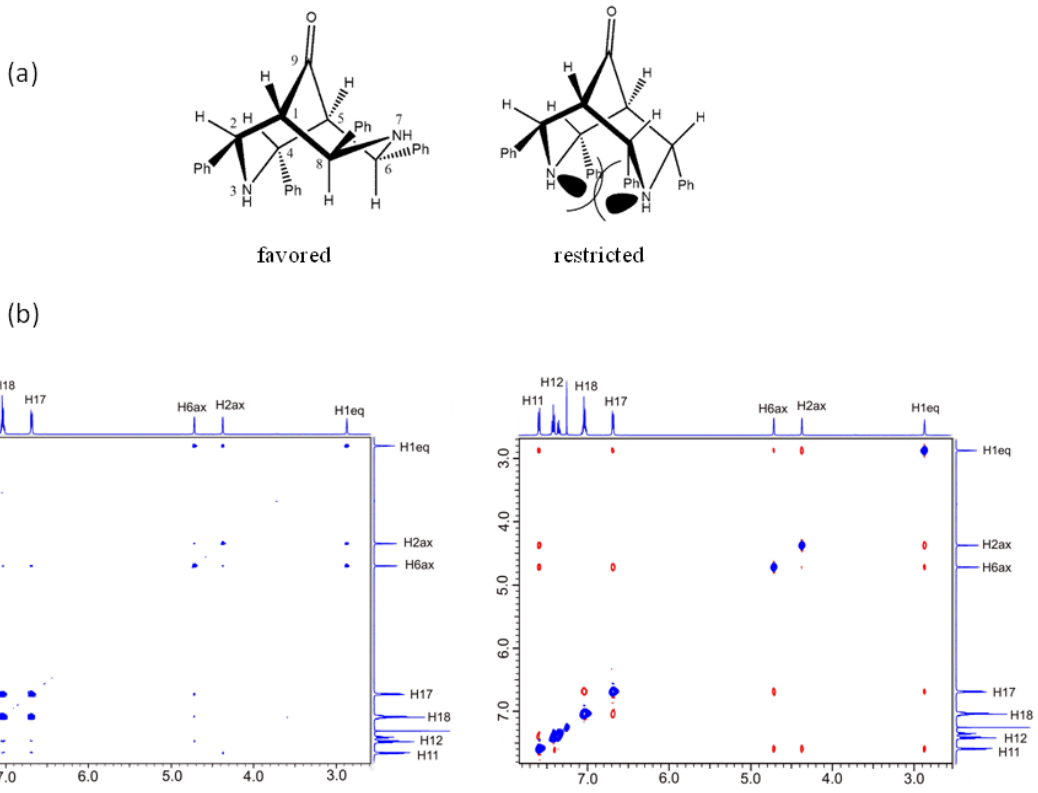
Scheme S2. Reaction mechanism proposed for the synthesis of piperidones **1** and **2** by double Mannich reaction.



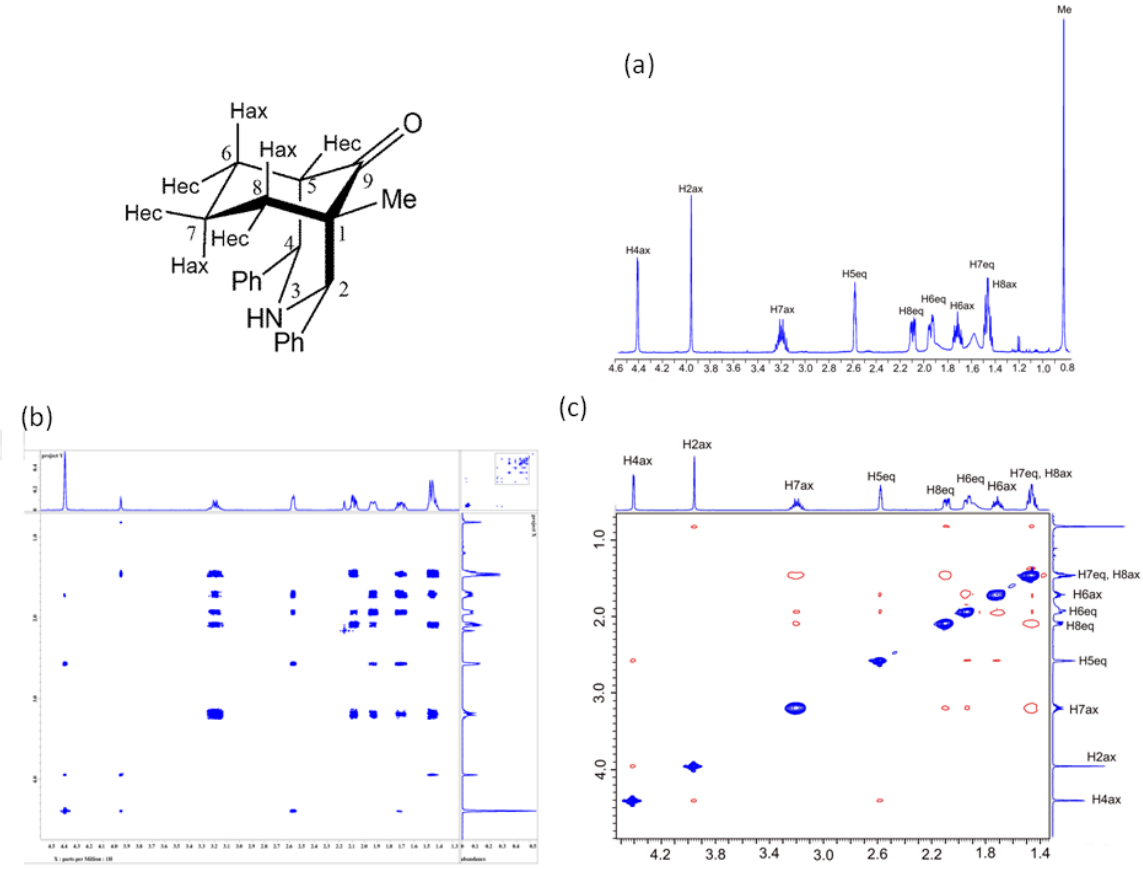
Scheme S3. Reaction mechanism proposed for the synthesis of piperidones **3** to **8** by Mannich reaction.



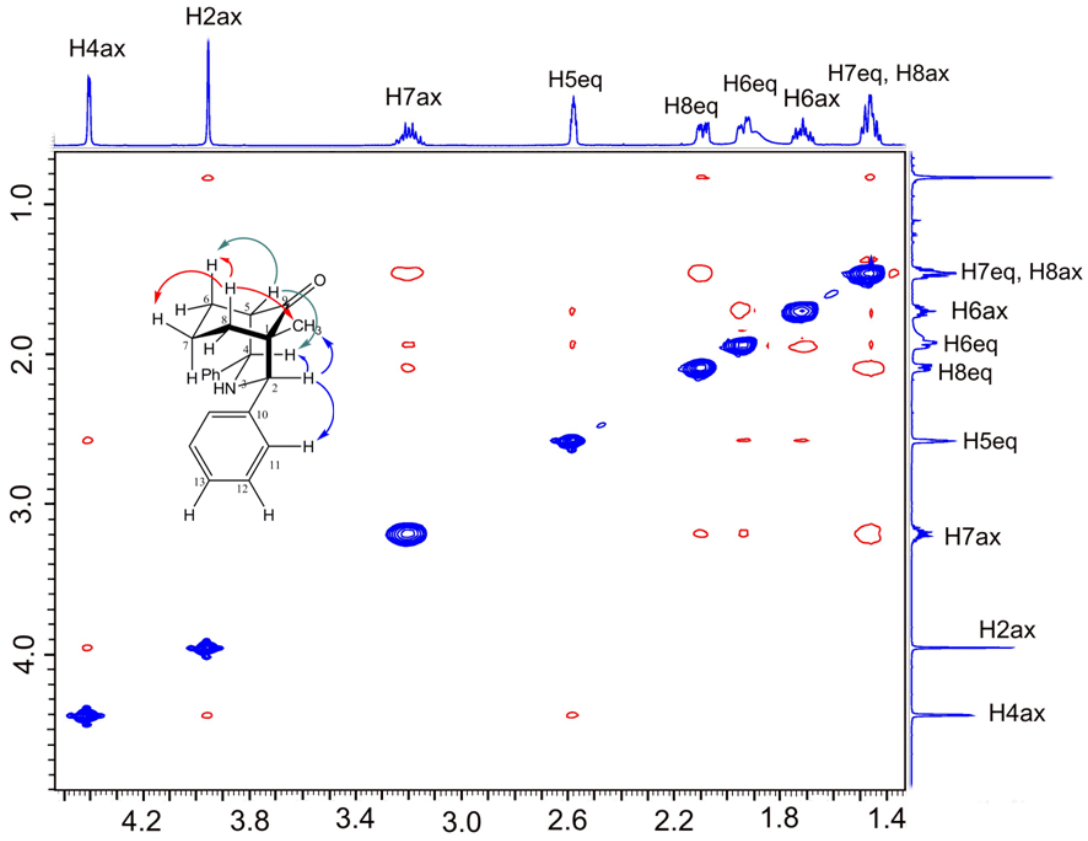
Scheme S4. A(1,3) allylic strain.



Scheme S5. (a) preferred conformation for the compound **1** and **2**. (b) dqf- COSY spectrum of compound **1** in $CDCl_3$. (c) t-ROESY spectrum of compound **1** in $CDCl_3$.



Scheme S6. NMR characterization of compound **4** in $CDCl_3$. (a) ^1H spectrum. (b) dqf-COSY spectrum. (c) HSQC spectrum.



Scheme S7. Determination of the conformation of piperidones by t-ROESY spectrum

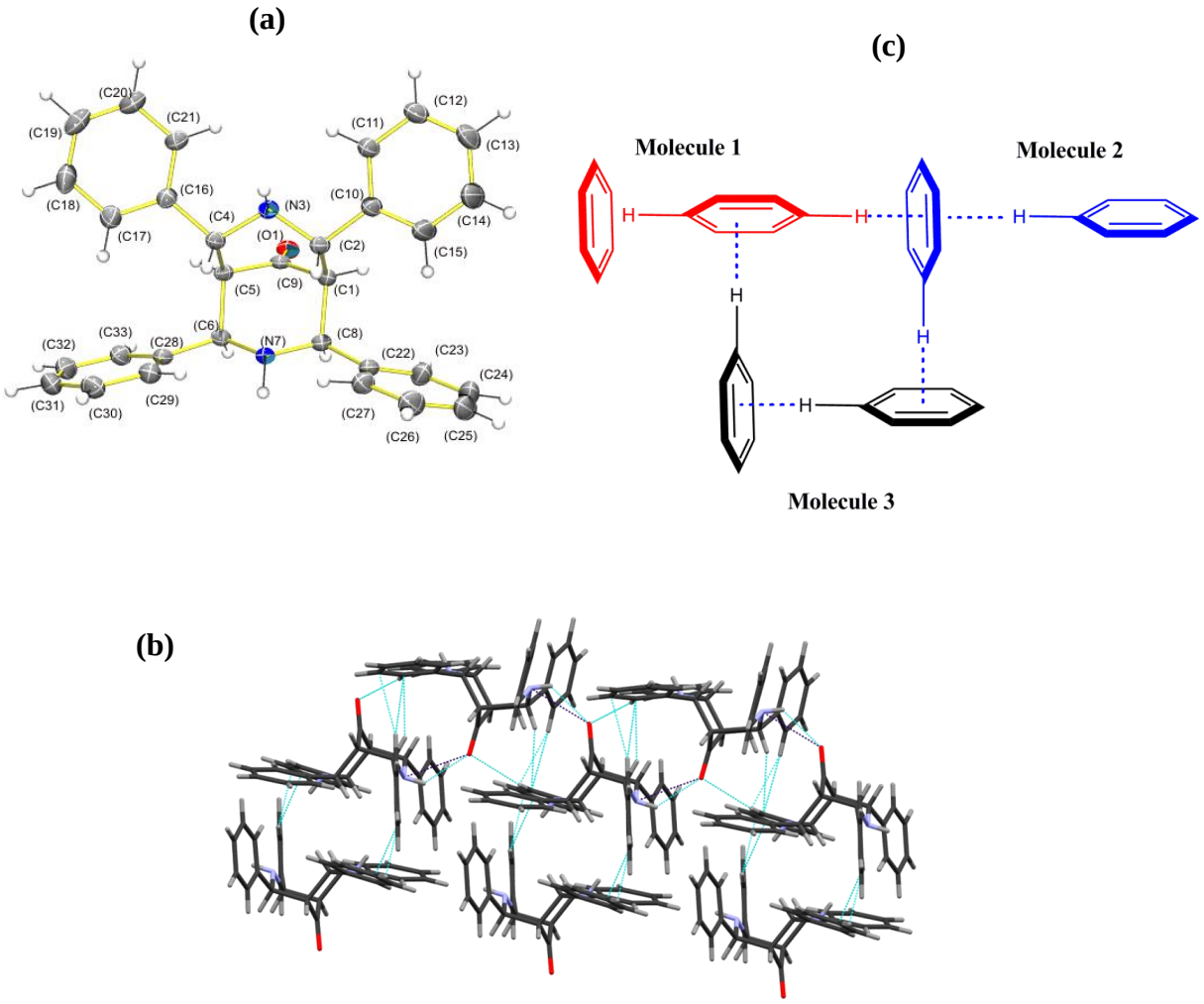
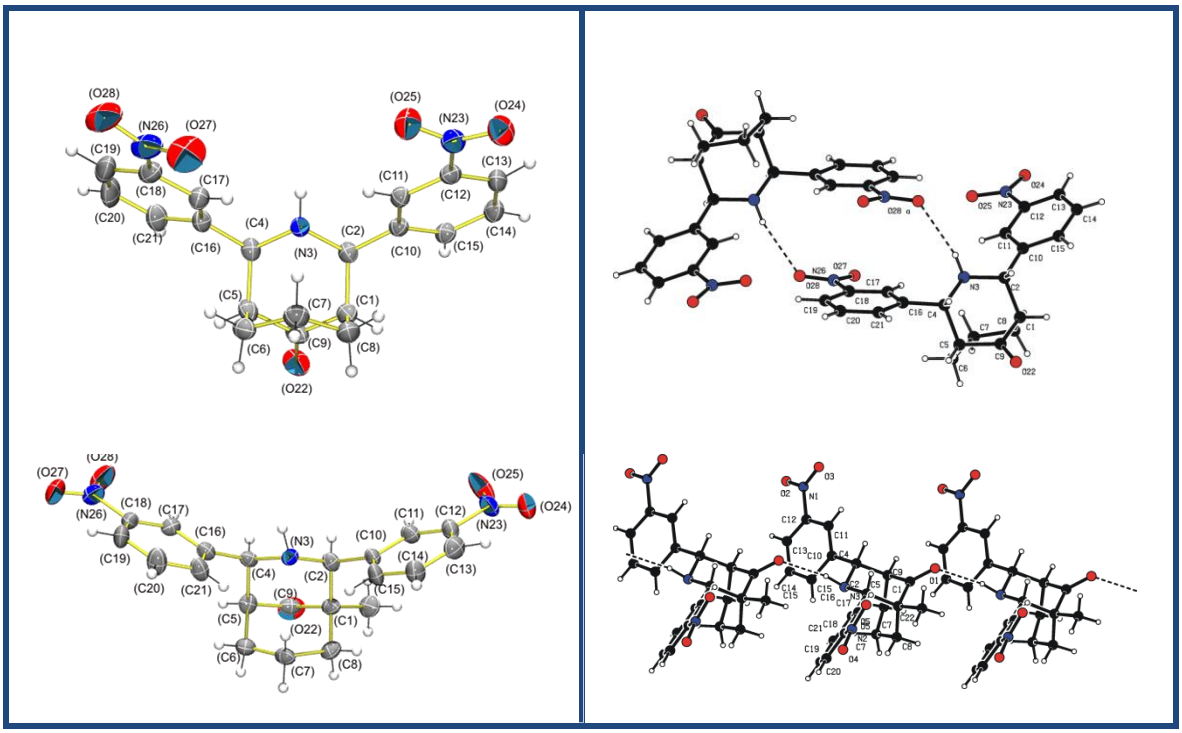
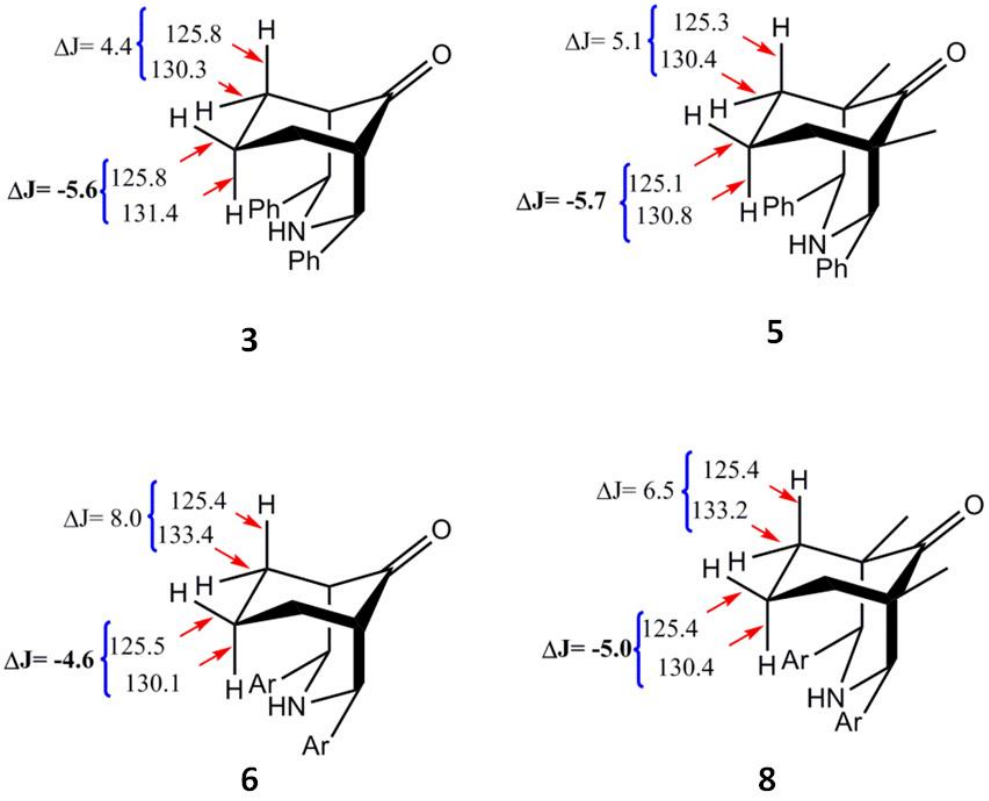


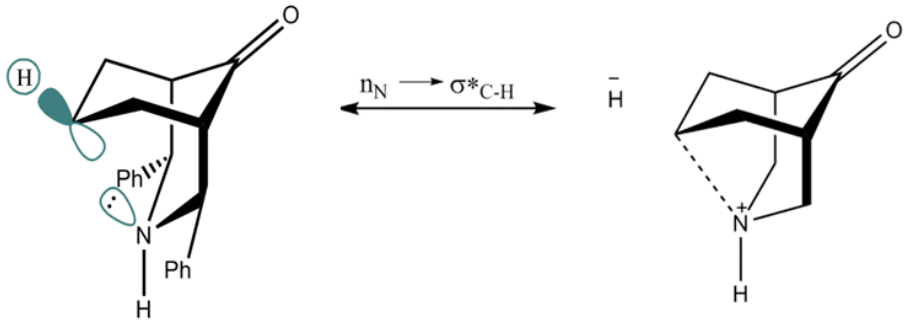
Figure S8. (a) ORTEP diagram of compounds **1**, thermal ellipsoids are drawn at 30% probability level for all atoms other than H. **(b)** crystal packing and C(15)···H(15)···π inter and intramolecular interaction of compound **1**.



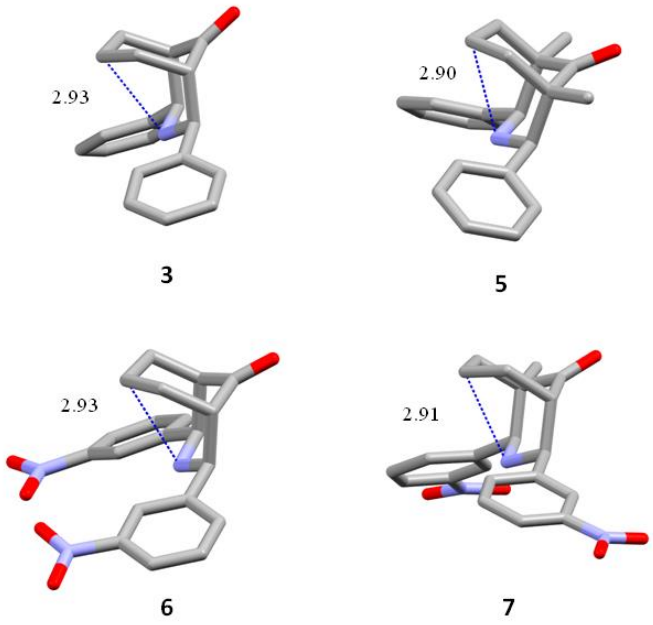
Scheme S9. (a) ORTEP diagram of compounds **6** and **7**, thermal ellipsoids are drawn at 30% probability level for all atoms other than H. **(b)** Intermolecular hydrogen bonds of compound **6** and **7.**



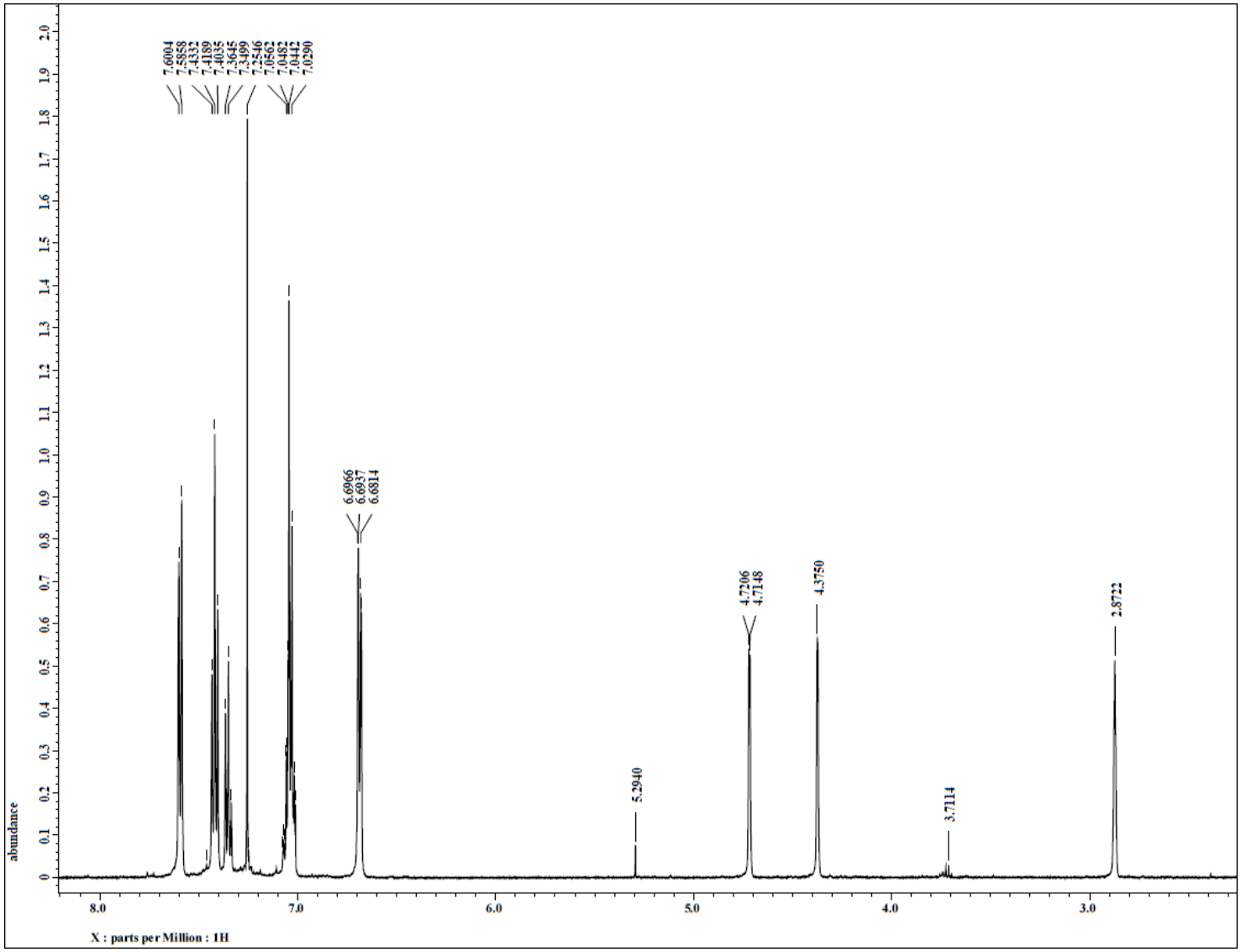
Scheme S10. $^{1}J_{C,H}$ coupling constant of compound **3**, **5**, **6** and **8**



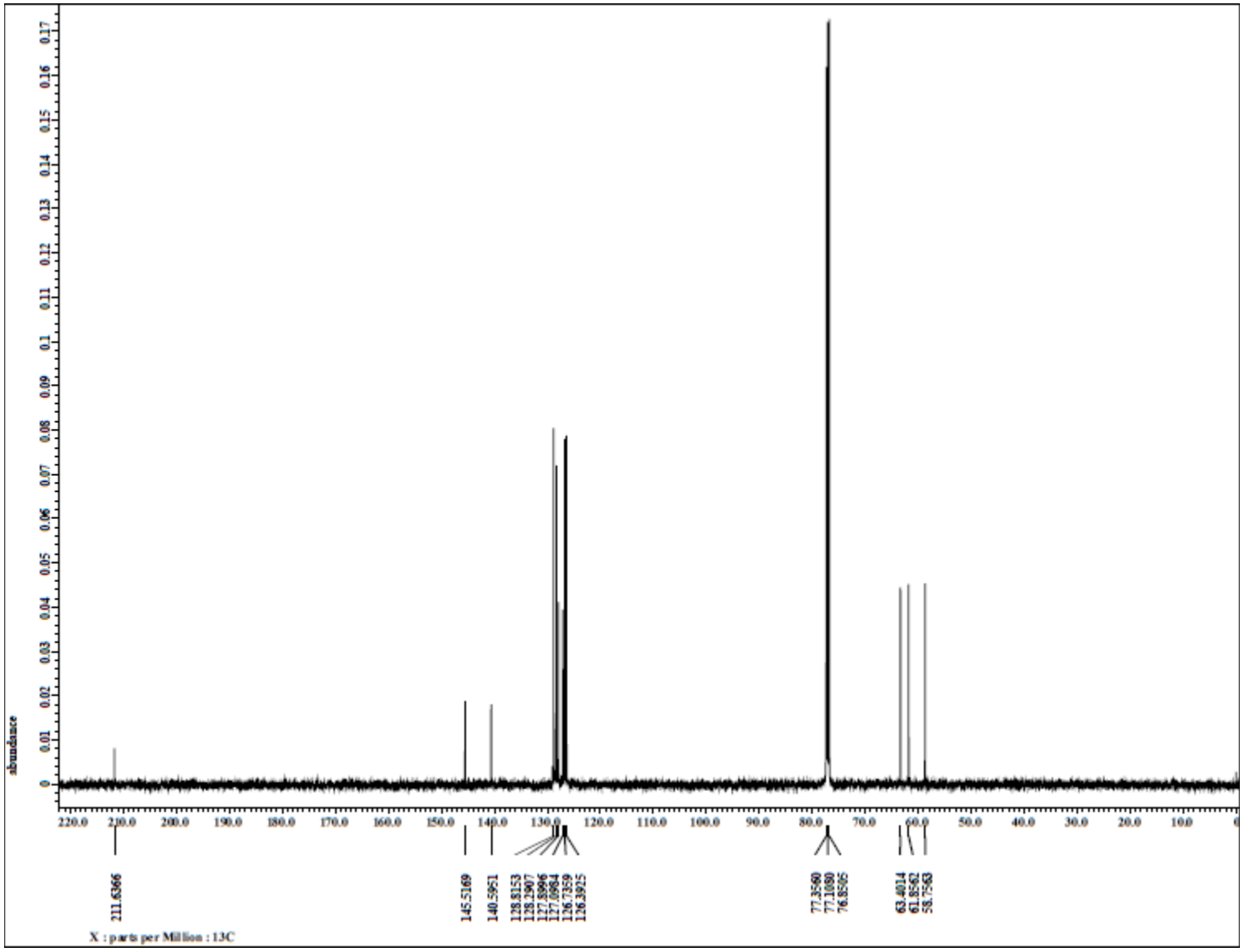
Scheme S11. Schematic representation of $n_X \rightarrow \sigma^*_{C7\text{-}Heq}$ Hyperconjugation in the piperidones **3**-**8**.



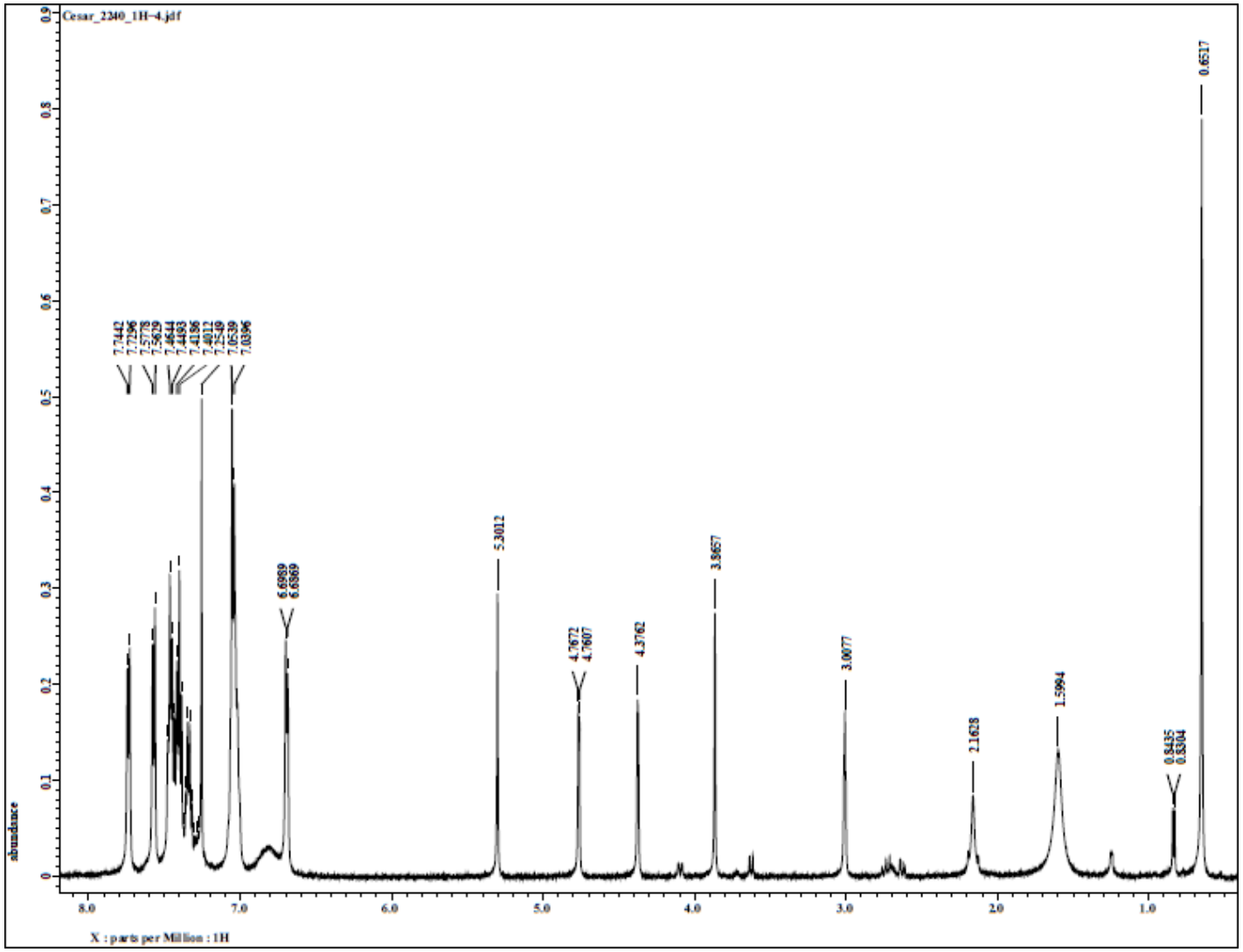
Scheme S12. Distance between N(3) and σ*C-H orbital of compounds **3**, **5**, **6** and **7,** measured by X-ray



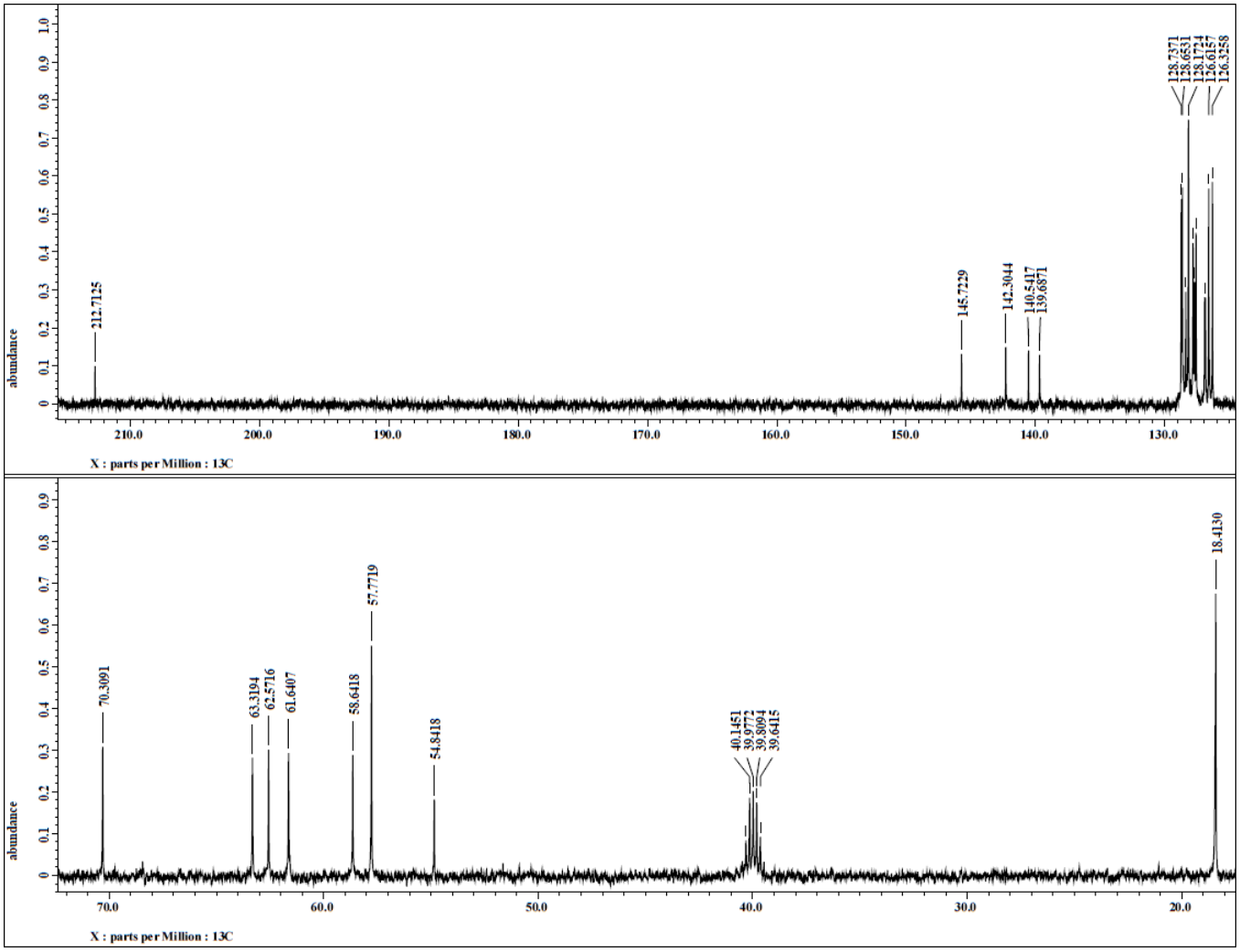
^{1}H NMR spectrum of **1**



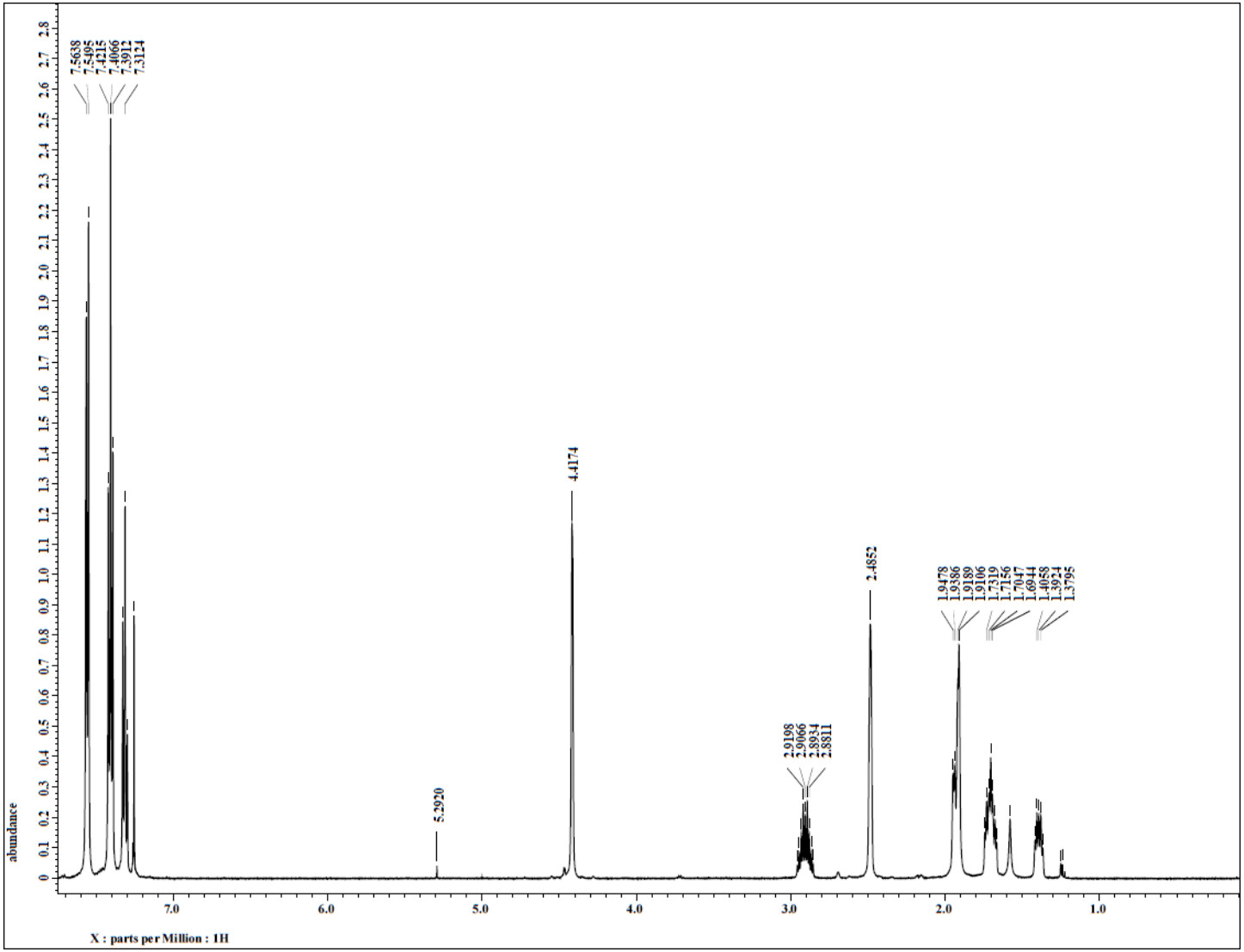
^{13}C NMR spectrum of **1**



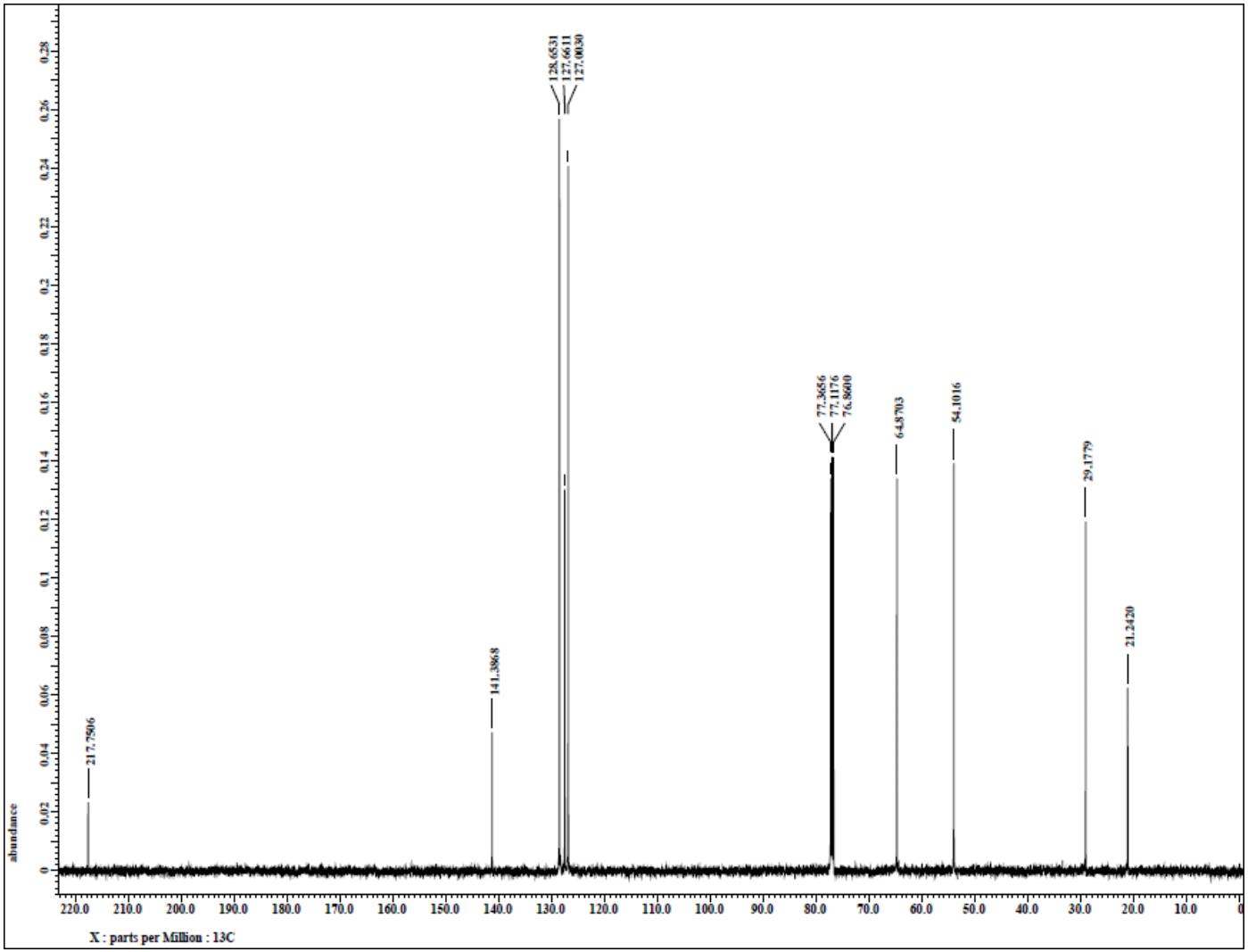
^{1}H NMR spectrum of **2**



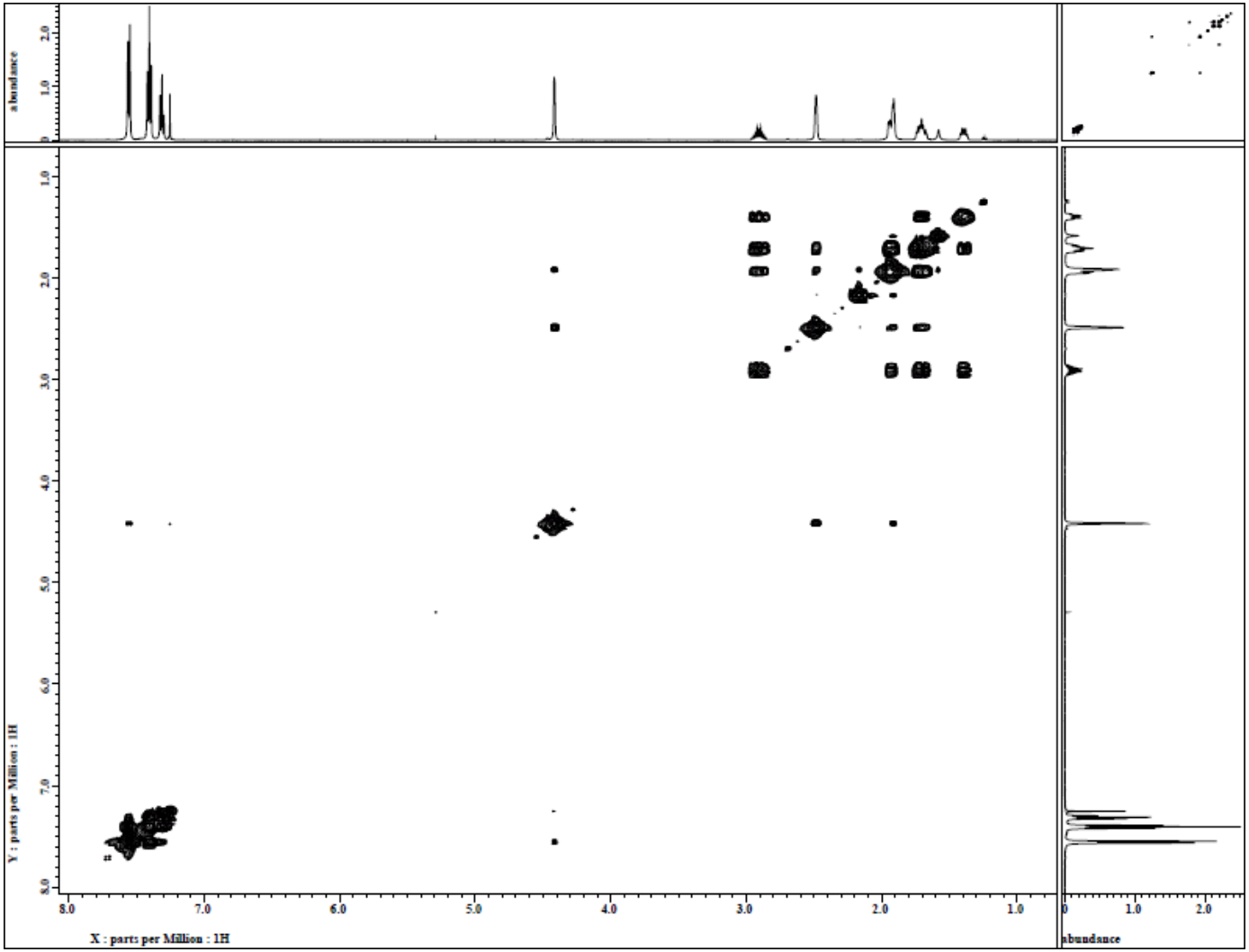
^{13}C NMR spectrum of **2**



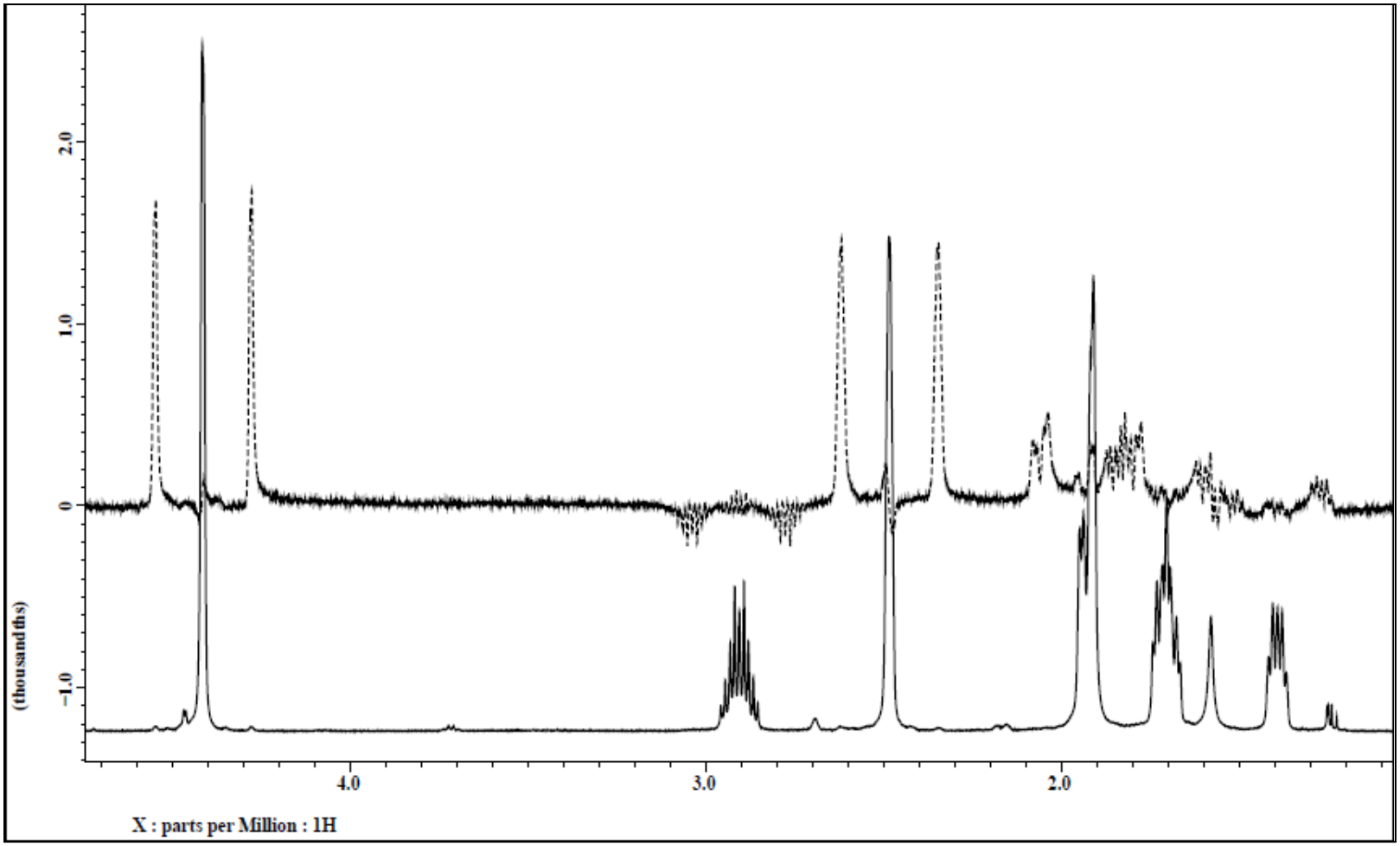
^{1}H spectrum of compound **3**



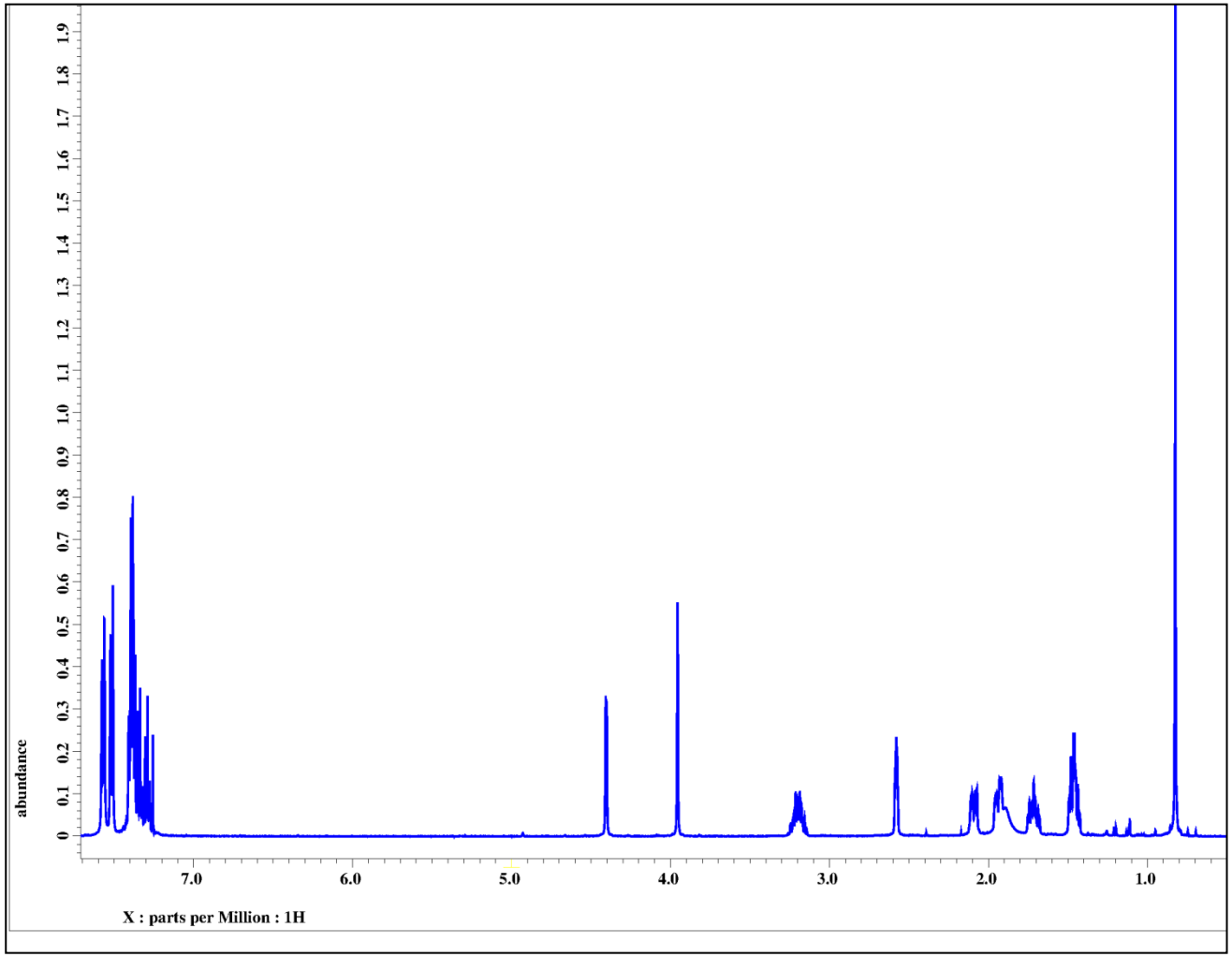
^{13}C spectrum of compound **3**



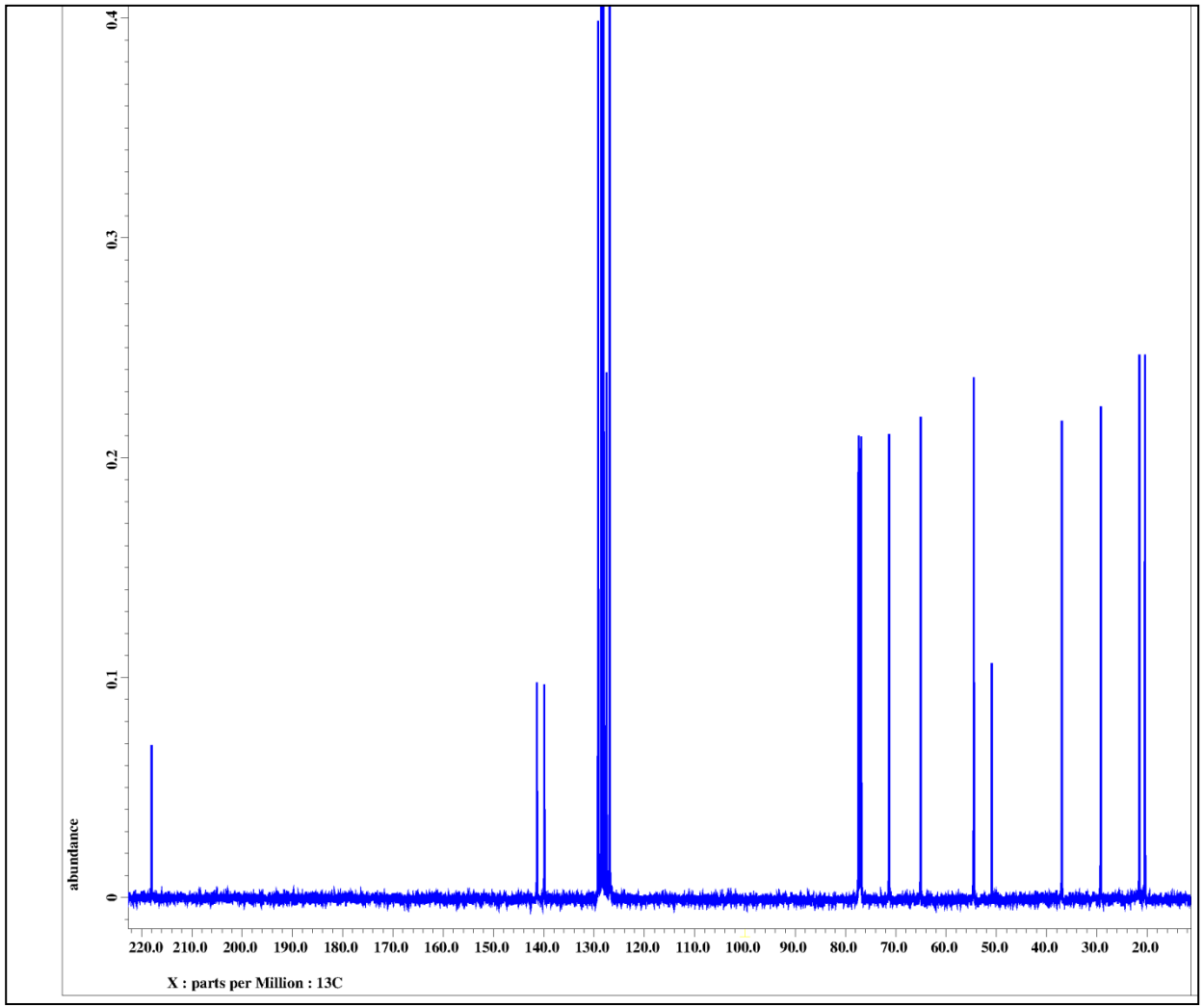
^{1}H-^{1}H COSY spectrum of compound **3**



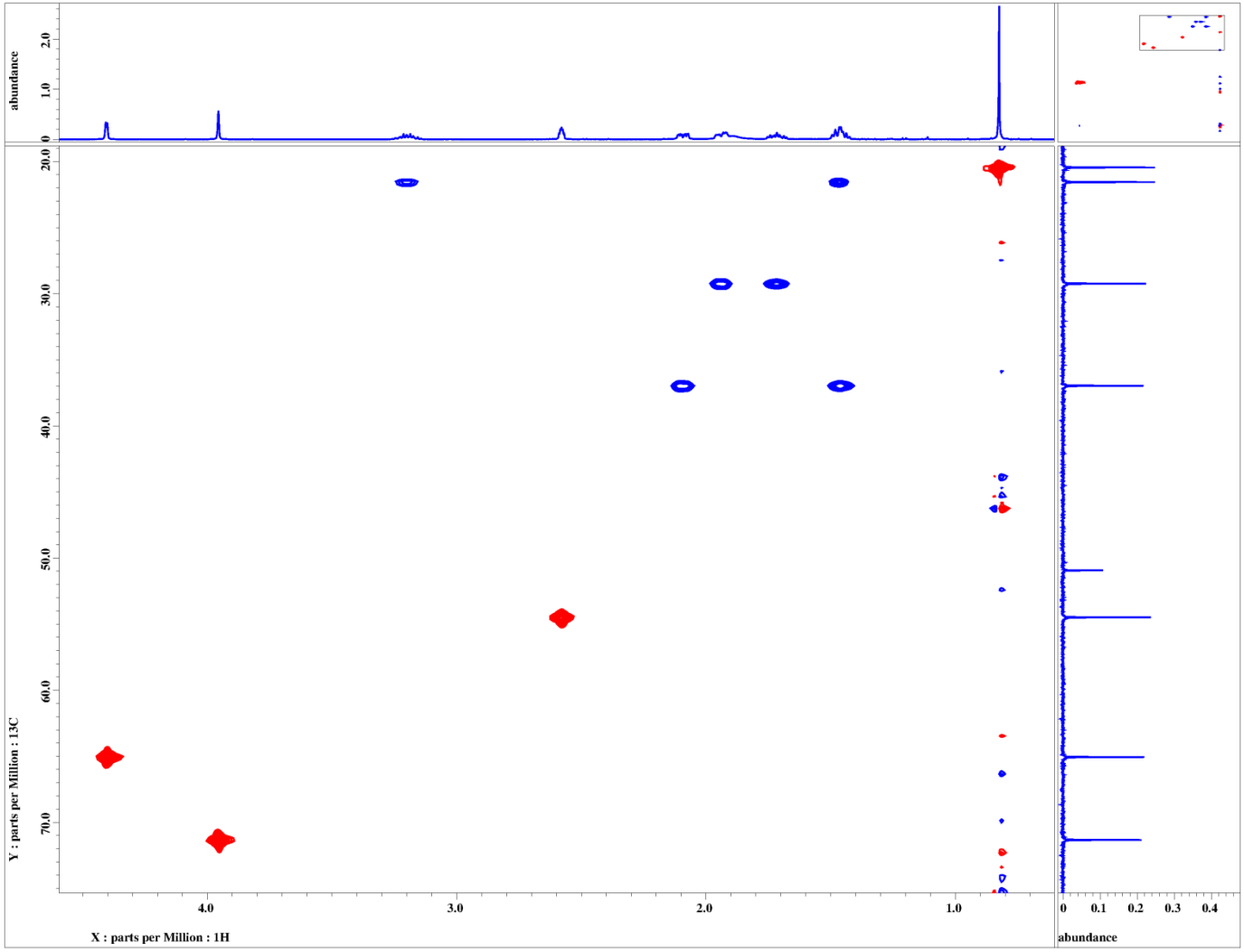
DQF spectrum of compound **3**



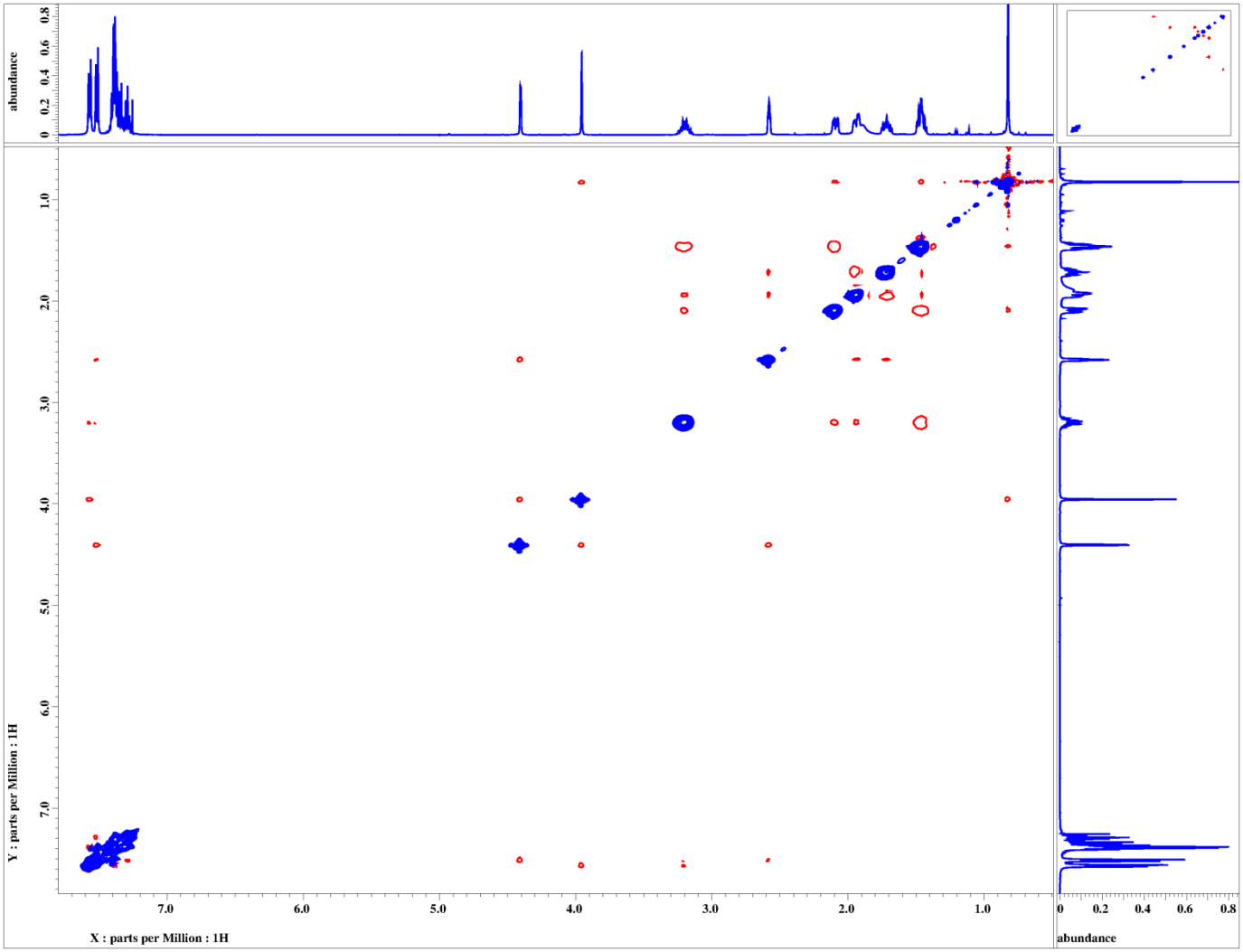
^{1}H NMR spectrum of compound **4**



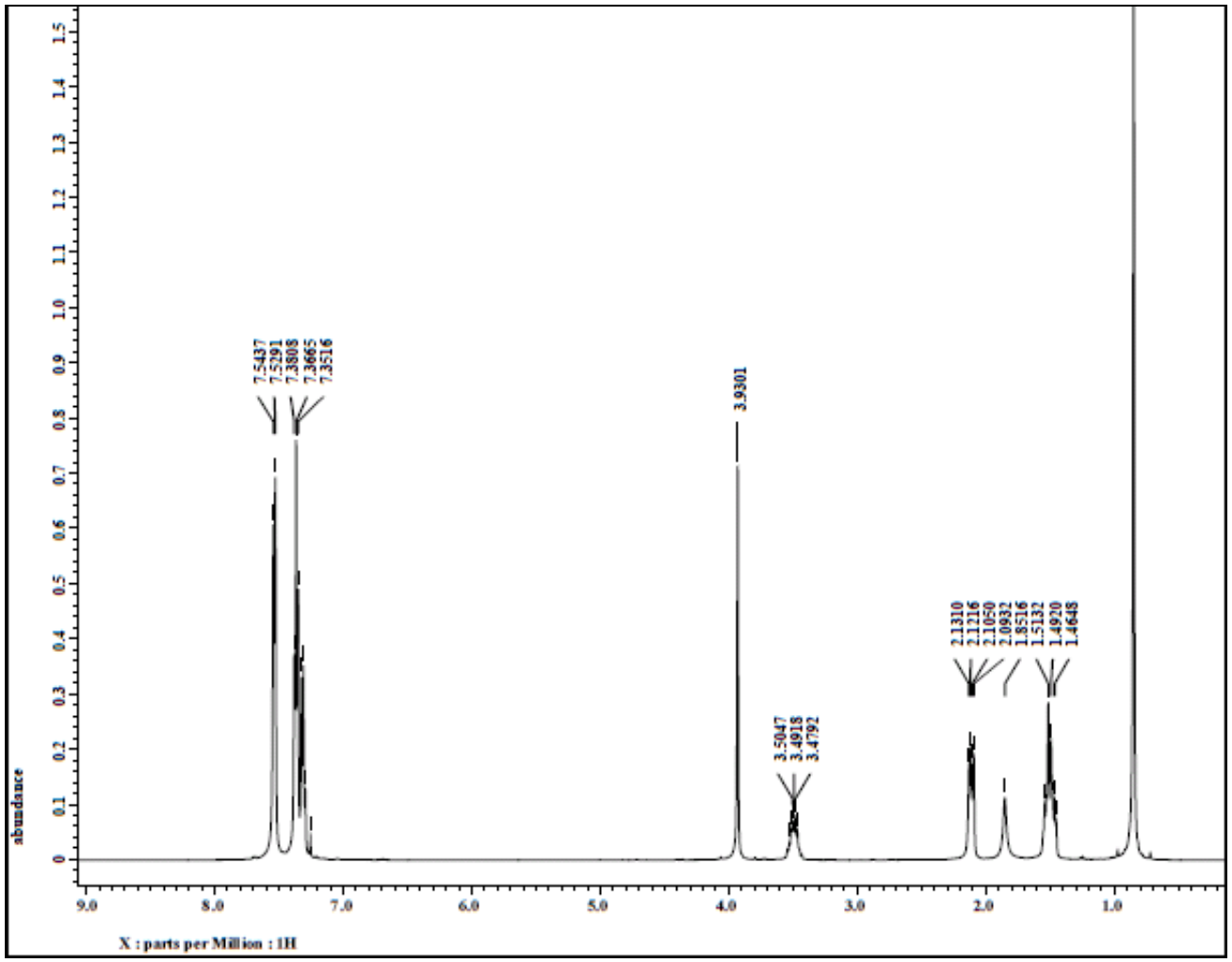
^{13}C NMR spectrum of compound **4**



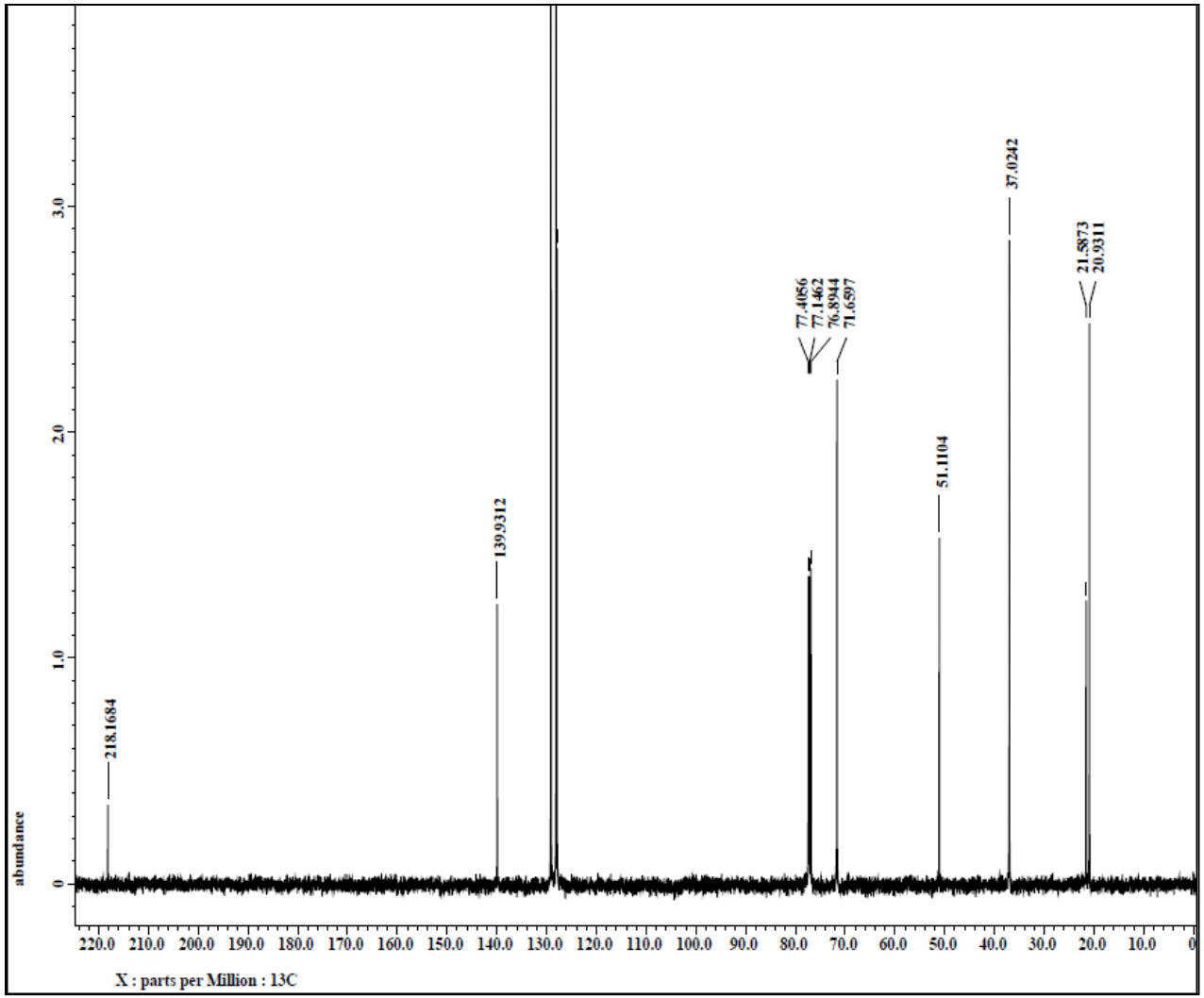
HSQC spectrum of compound **4**



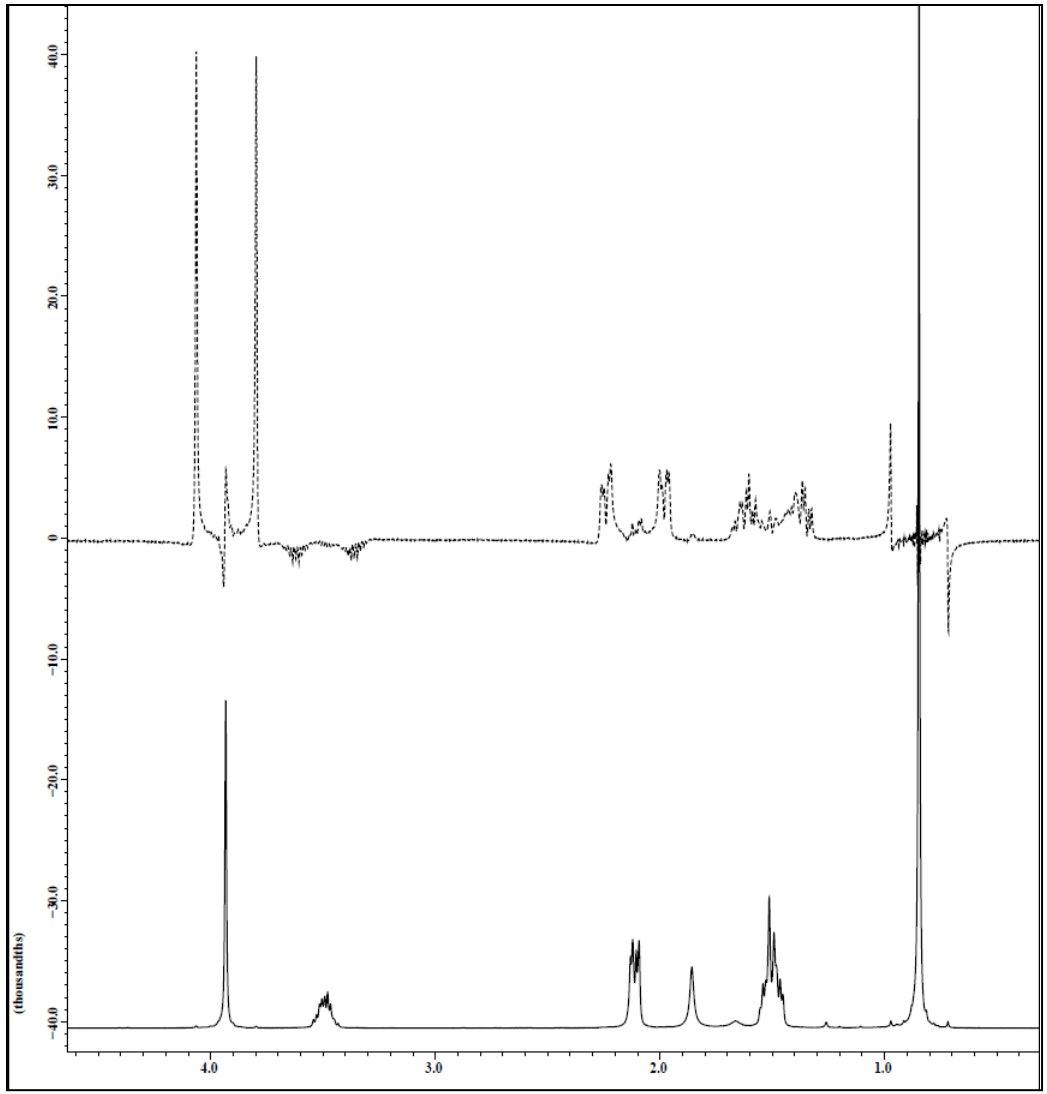
t-ROESY spectrum of compound **4**



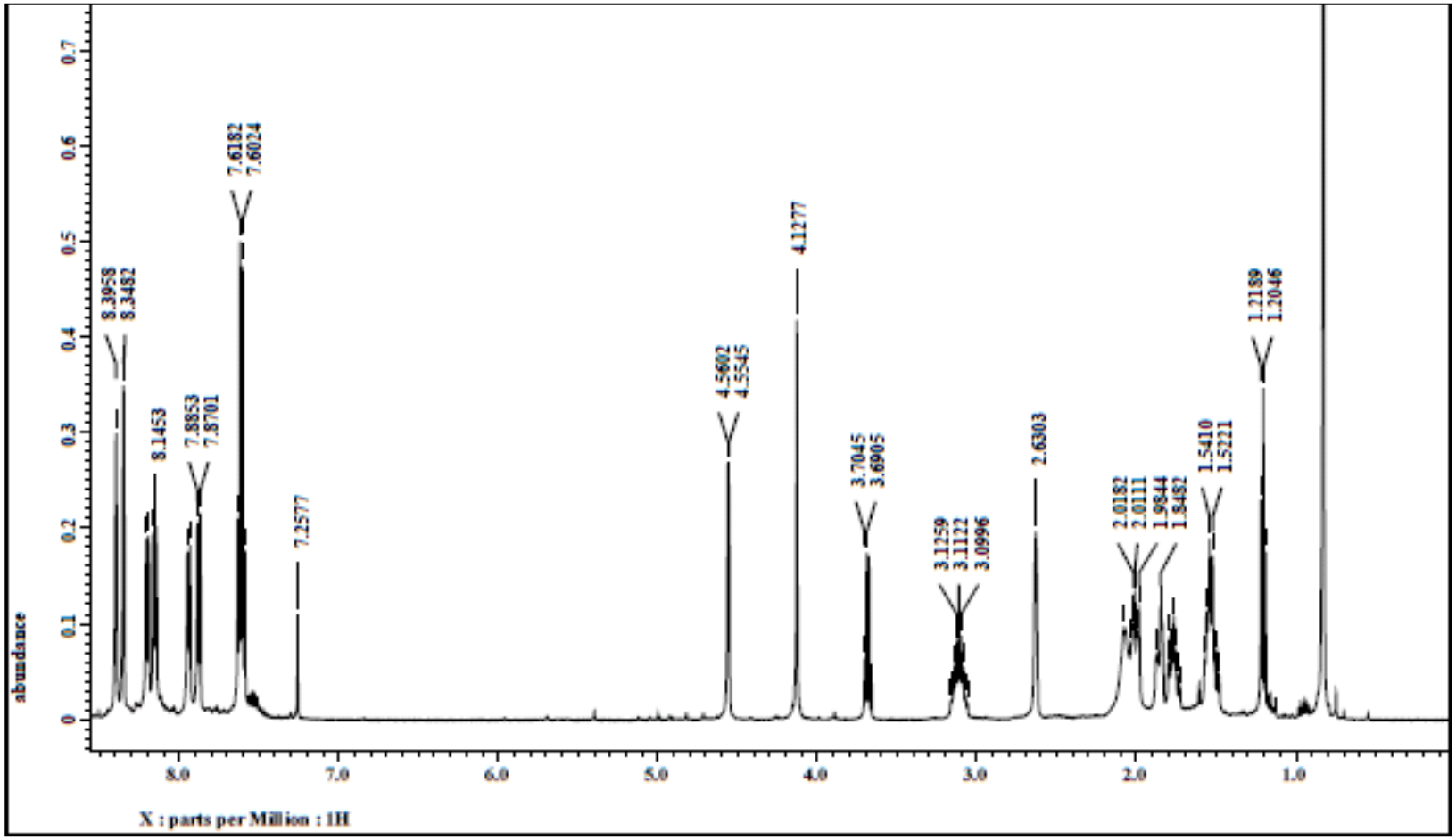
^{1}H spectrum of compound **5**



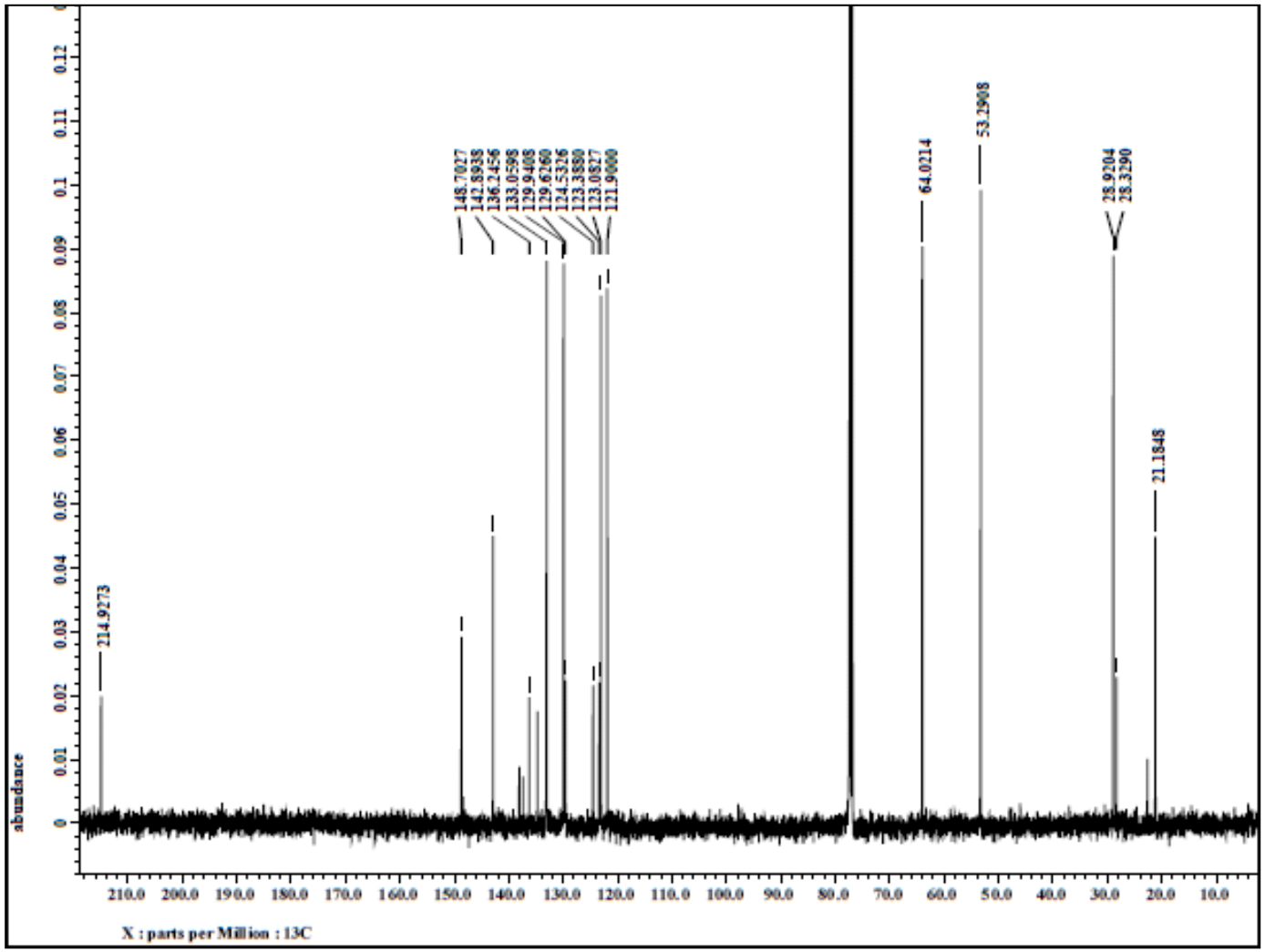
^{13}C spectrum of compound **5**



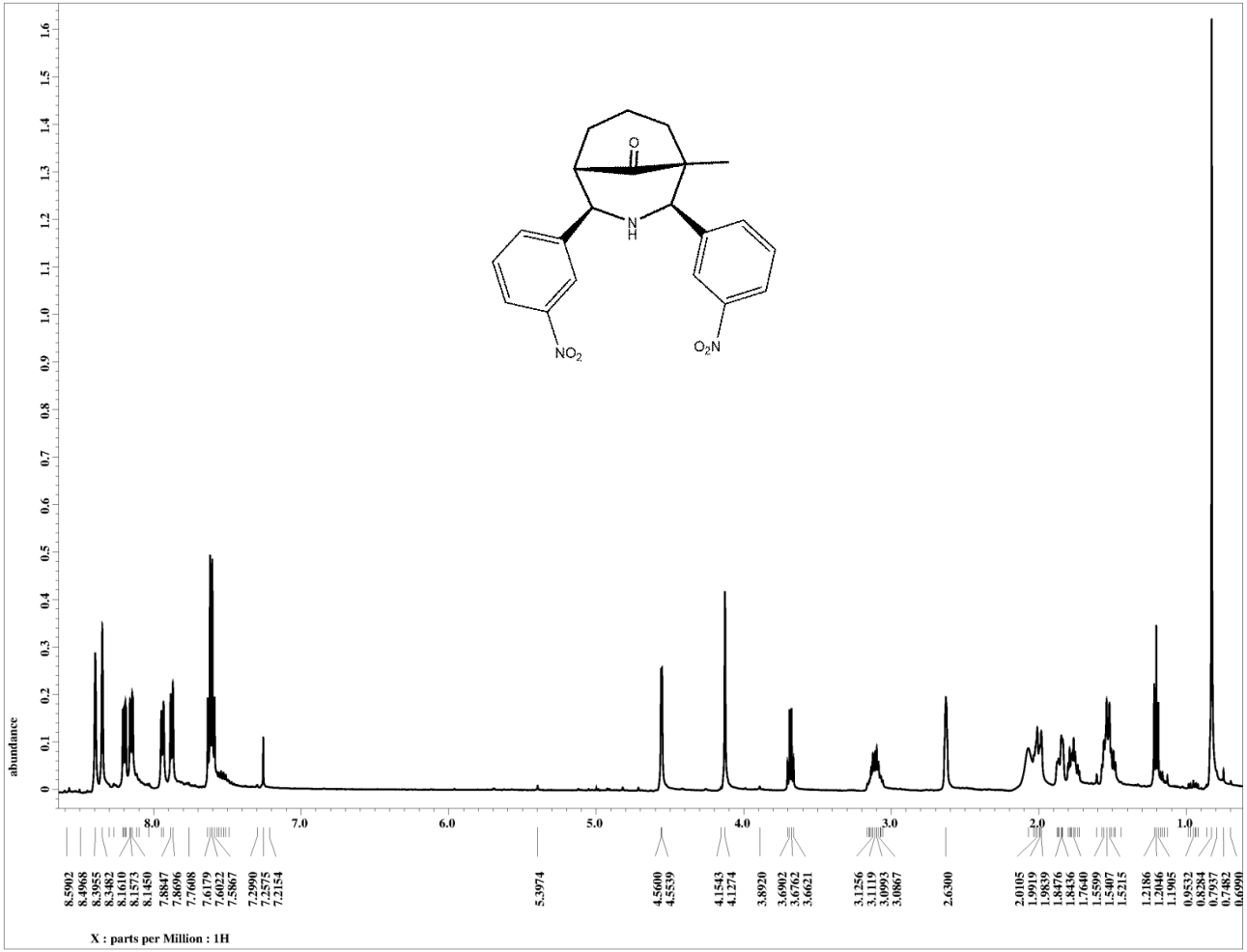
dqf spectrum of compound **5**



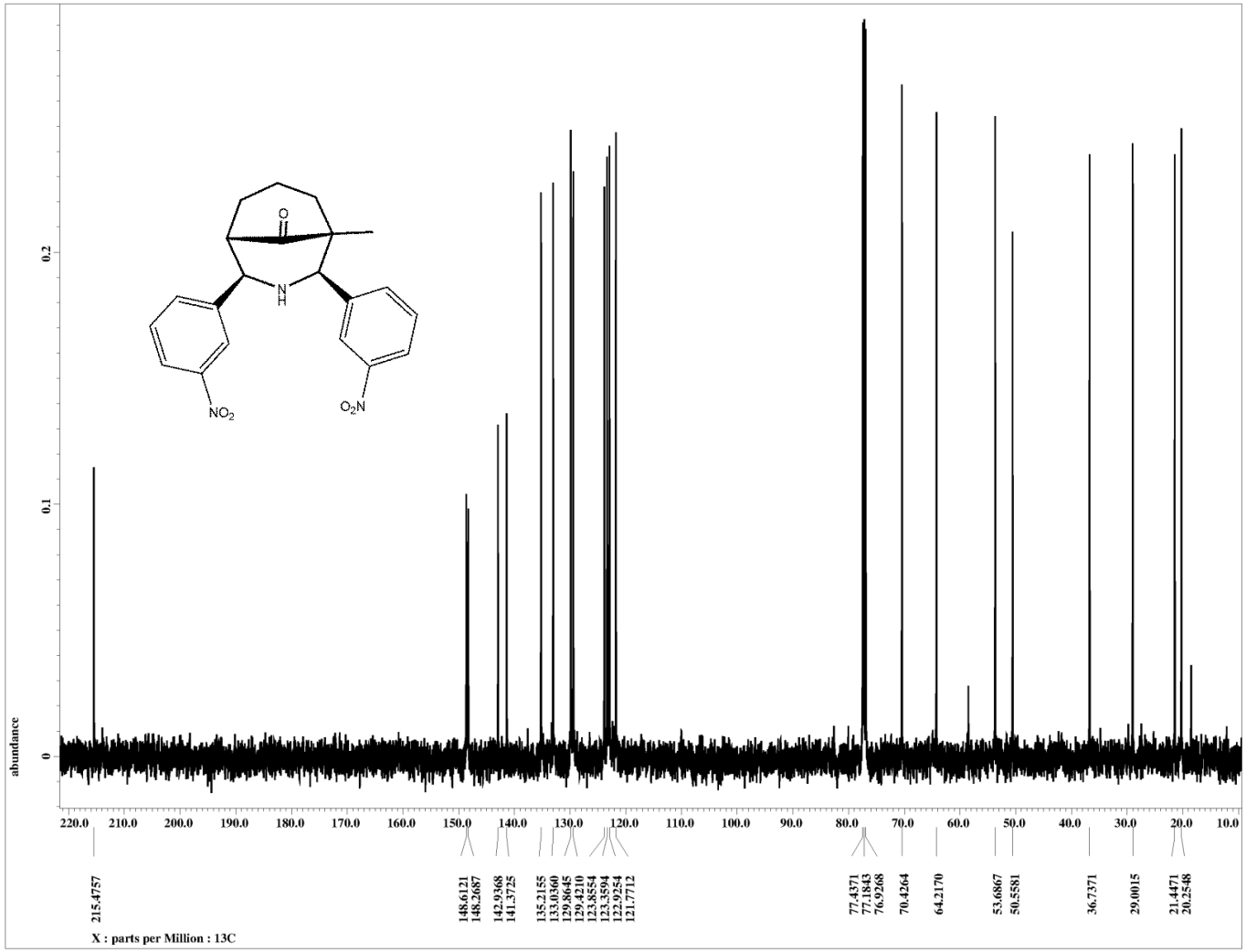
^{1}H spectrum of compound **6**



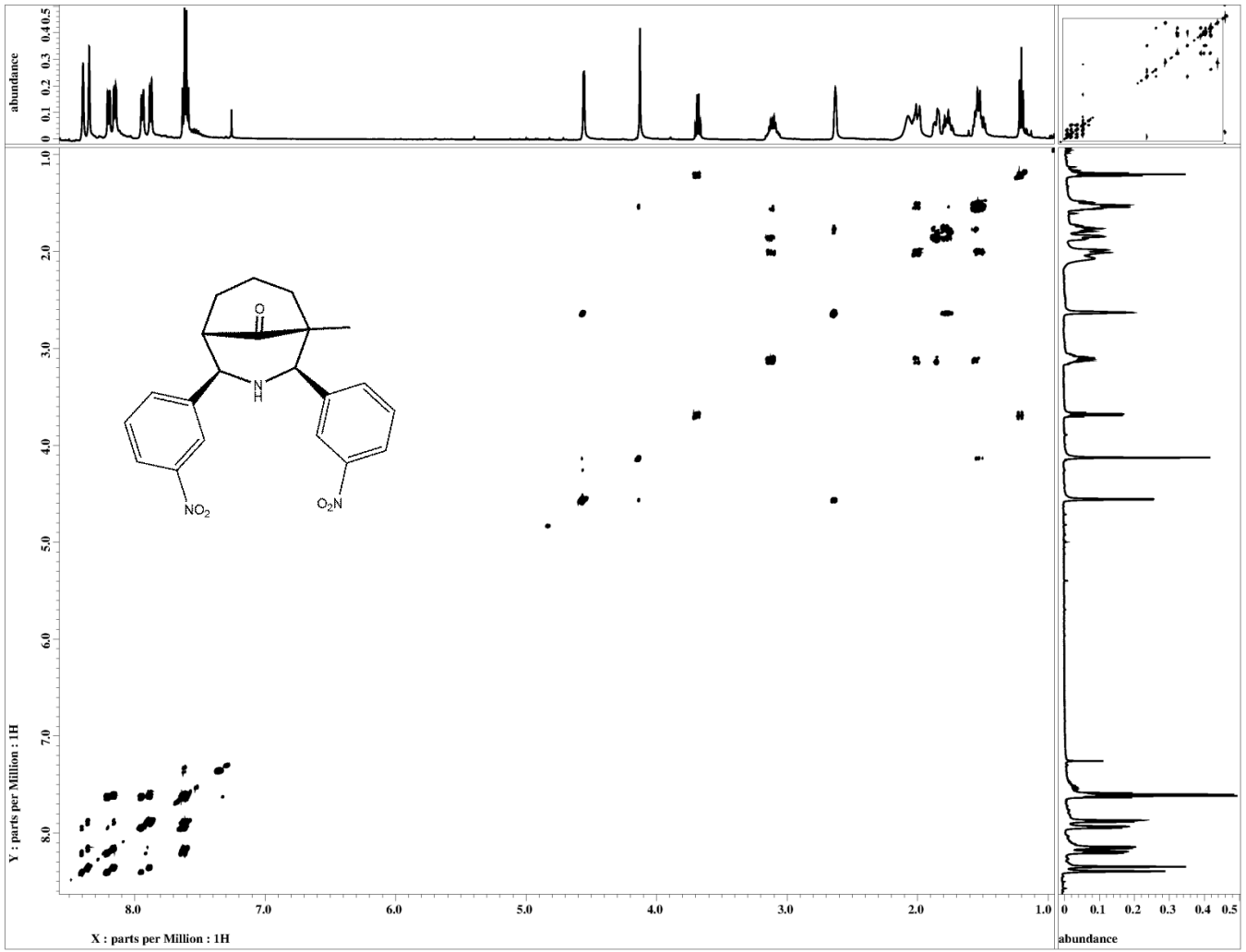
^{13}C spectrum of compound **6**



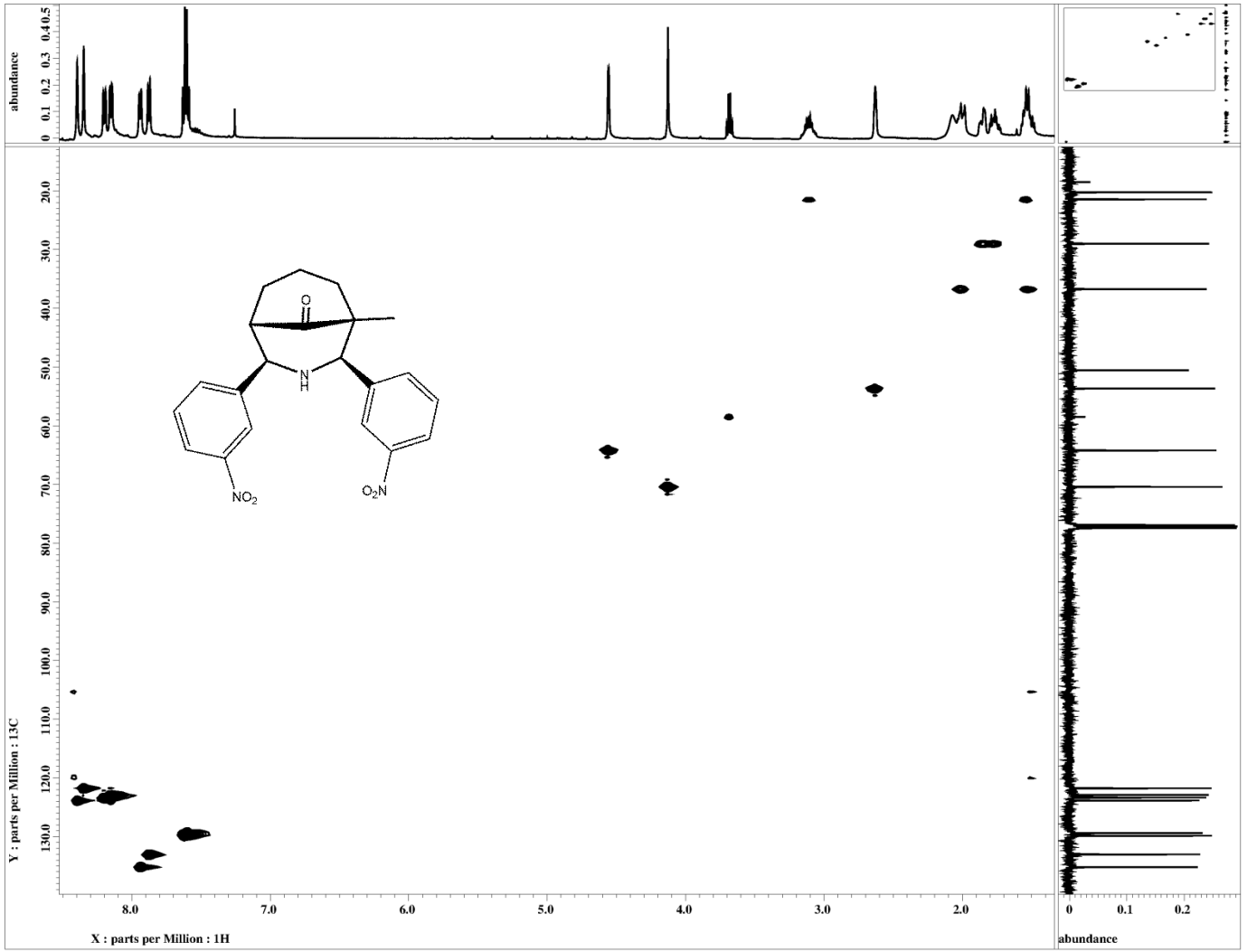
^{1}H NMR spectrum of compound **7**



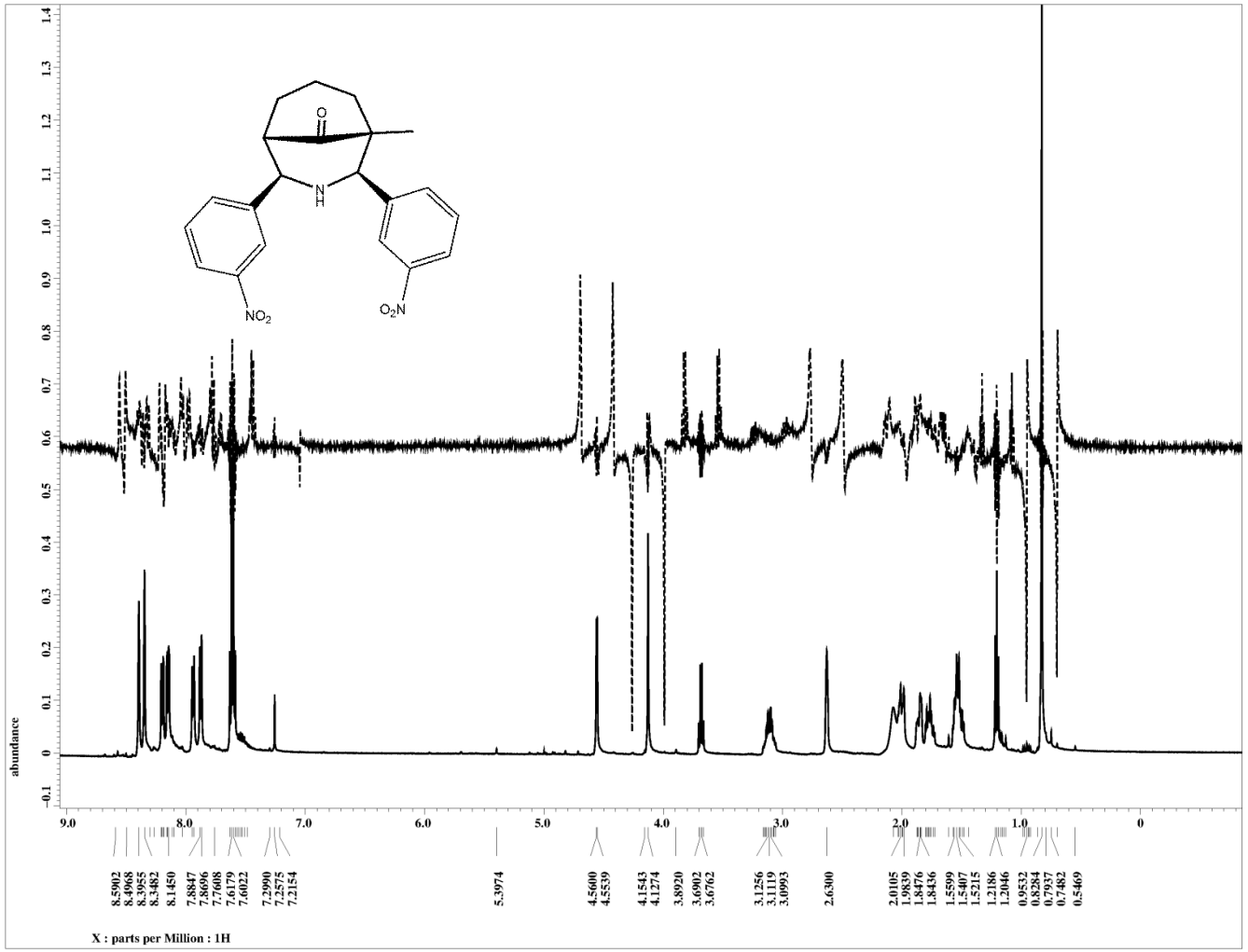
^{13}C NMR spectrum of compound **7**



^{1}H-^{1}H COSY spectrum of compound **7**



HSQC spectrum of compound **7**



DQF spectrum of compound **7**