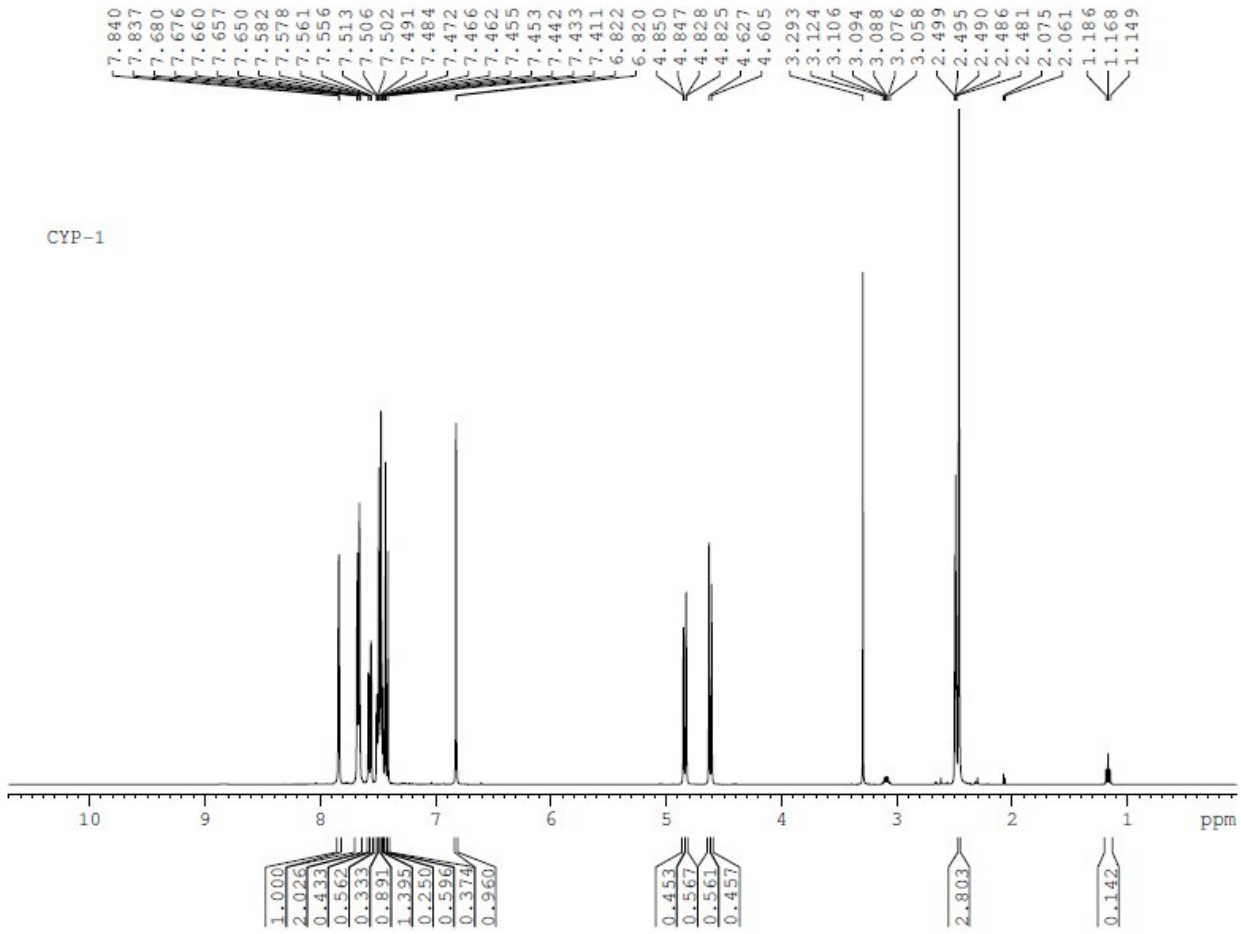
Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information Index



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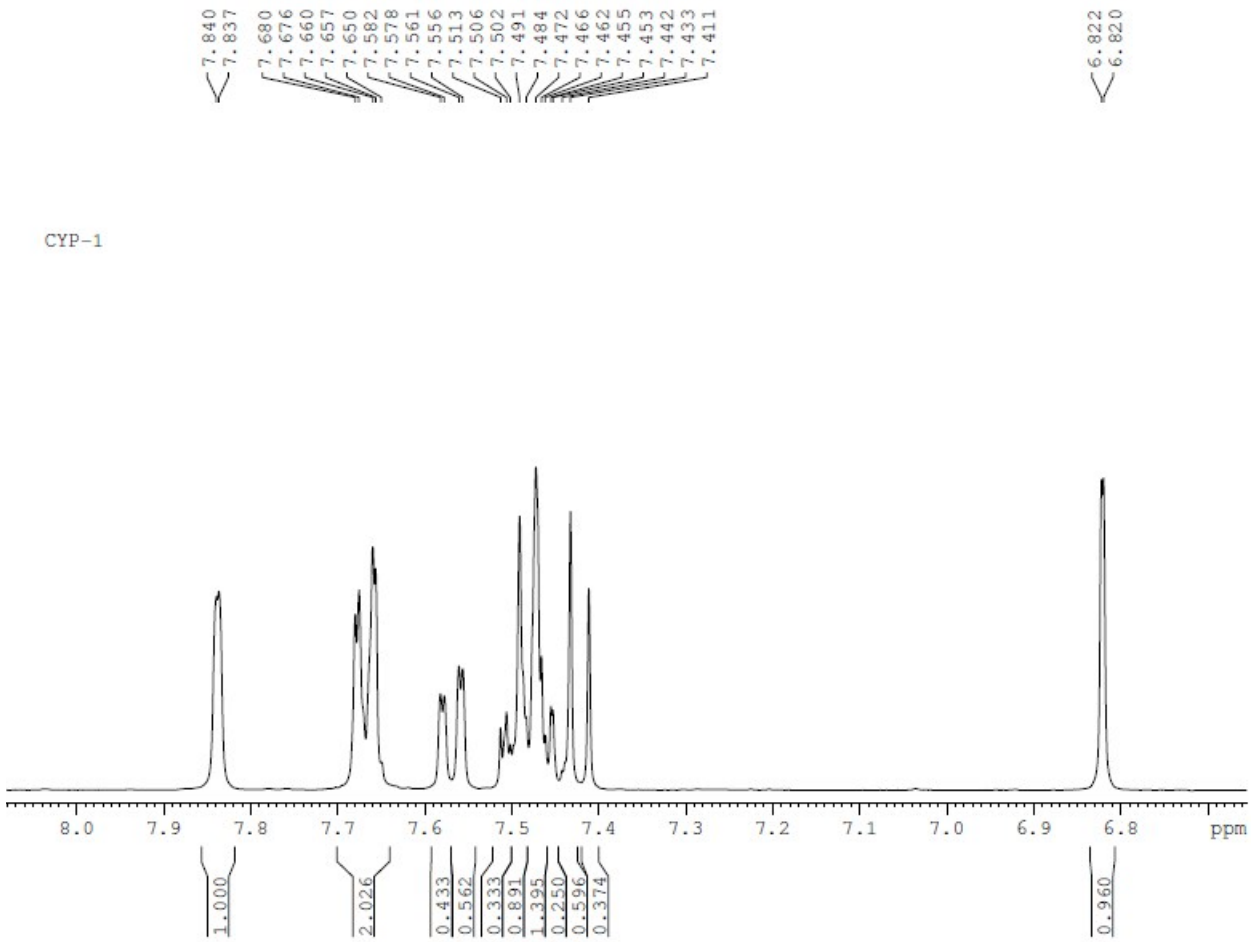

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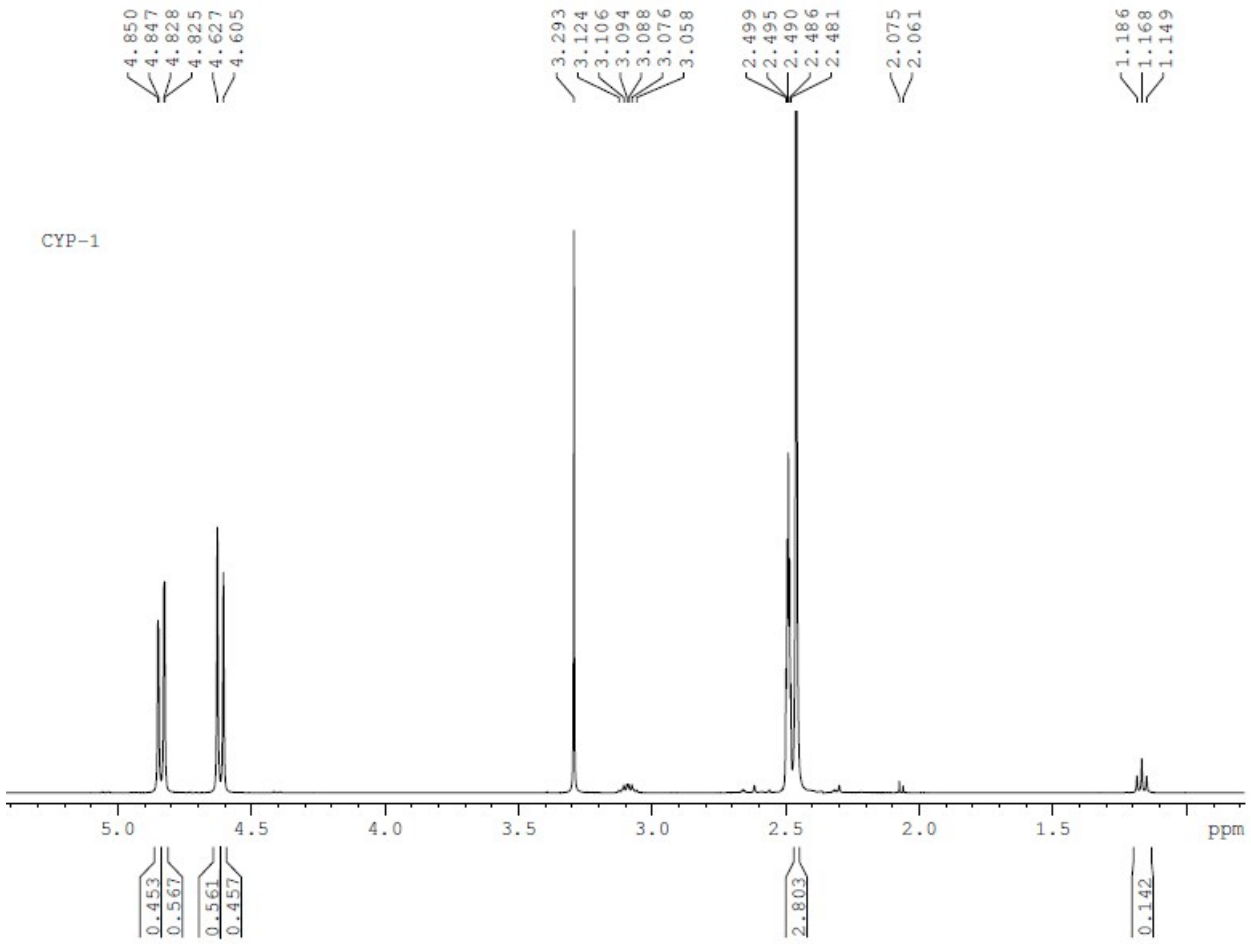

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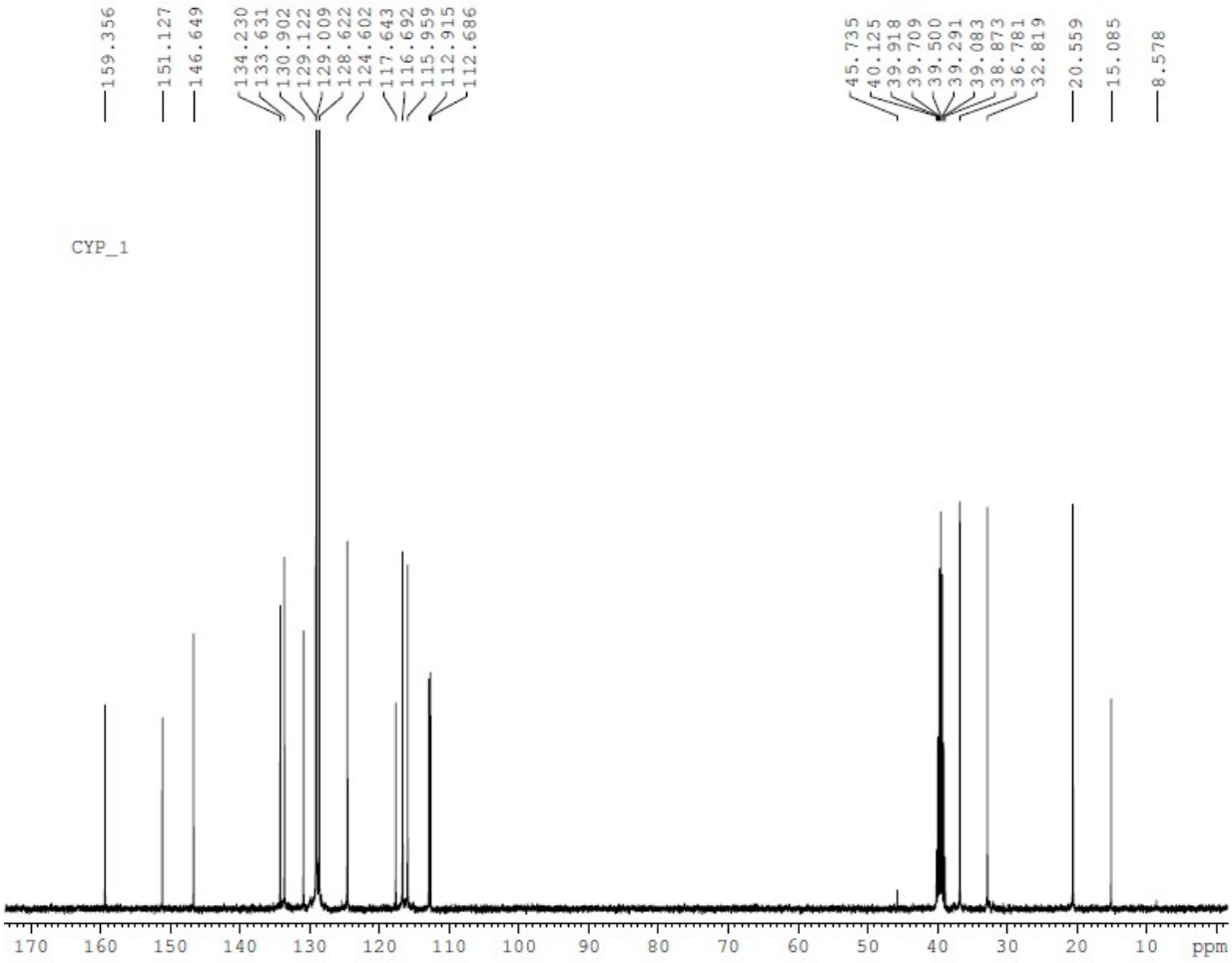

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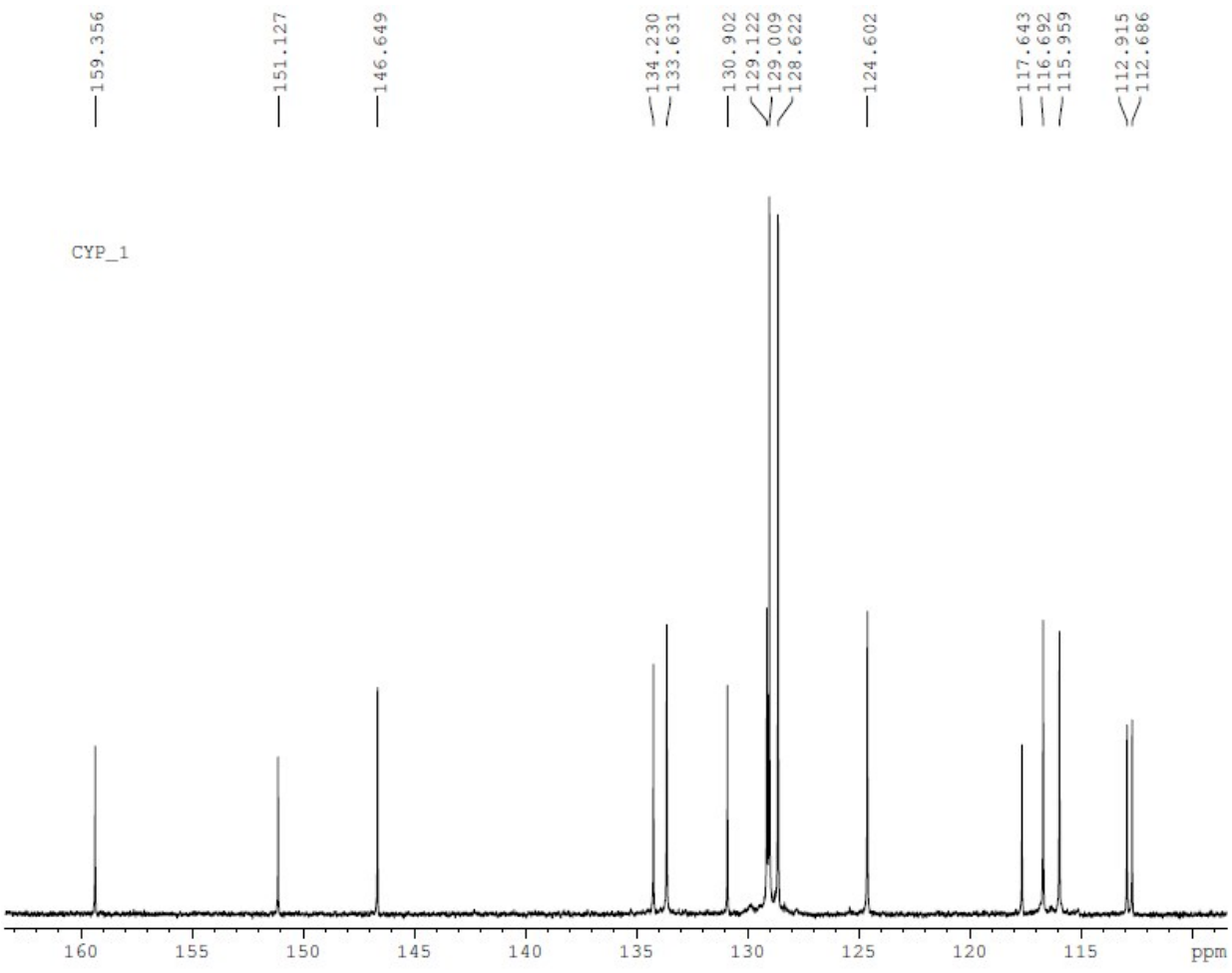

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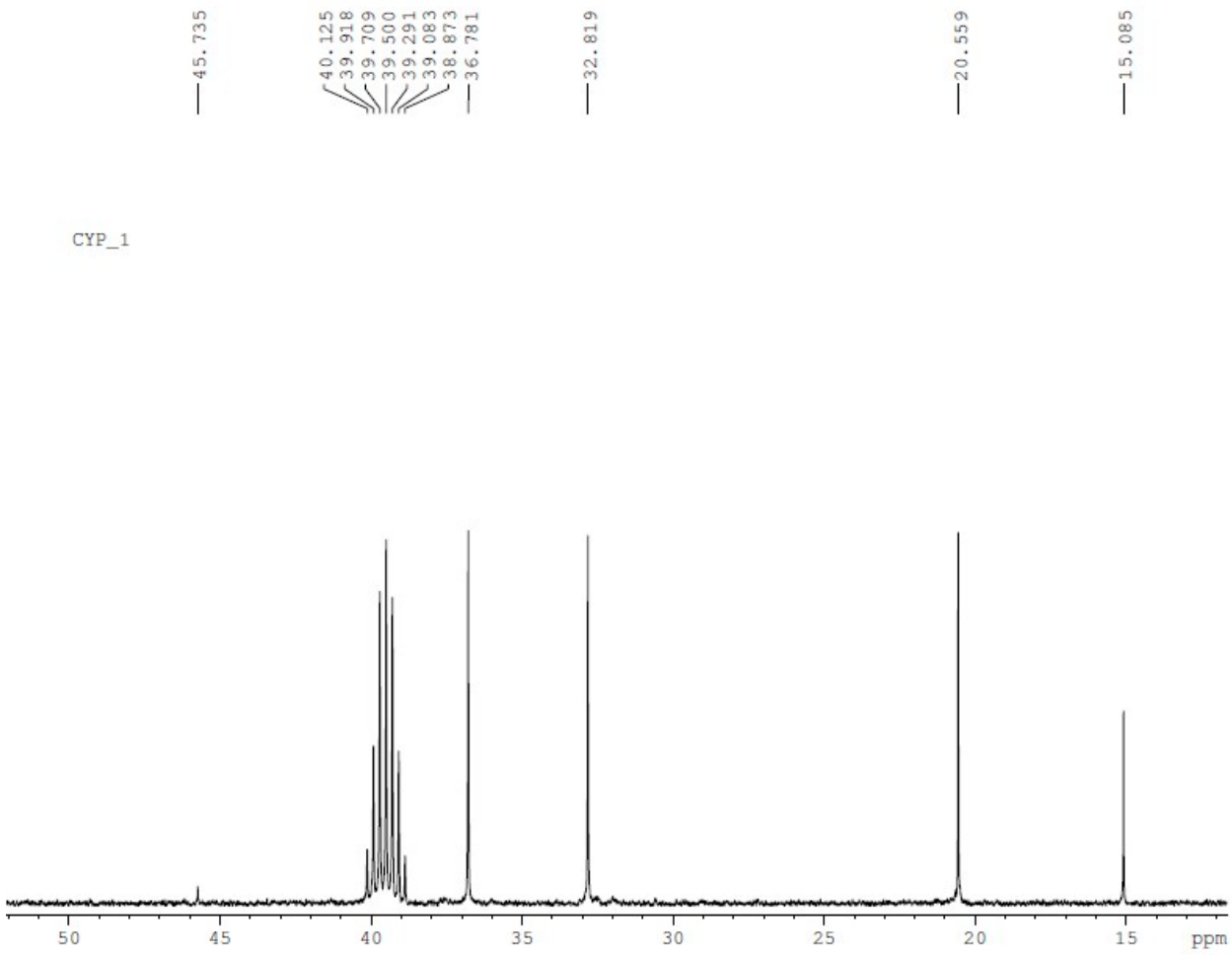

^{13}C-NMR of Compound 4a

KARNATAK UNIVERSITY
UNIVERSITY SCIENCE INSTRUMENTS CENTRE
DHARWAD

Sample Information

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Sample Type	: Unknown
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Sample Name	: CYP-1
Sample ID	:
IS Amount	: [1]=1

Spectrum

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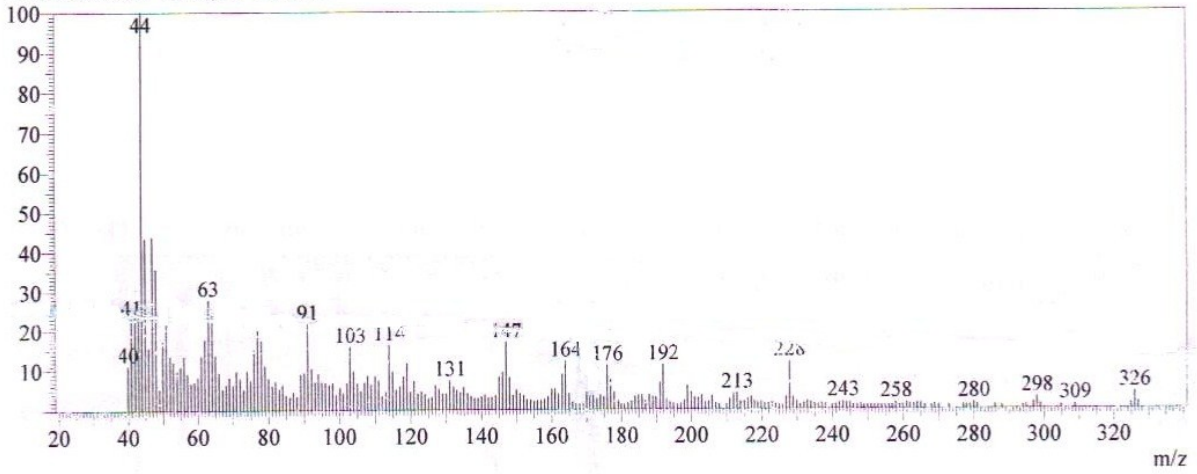

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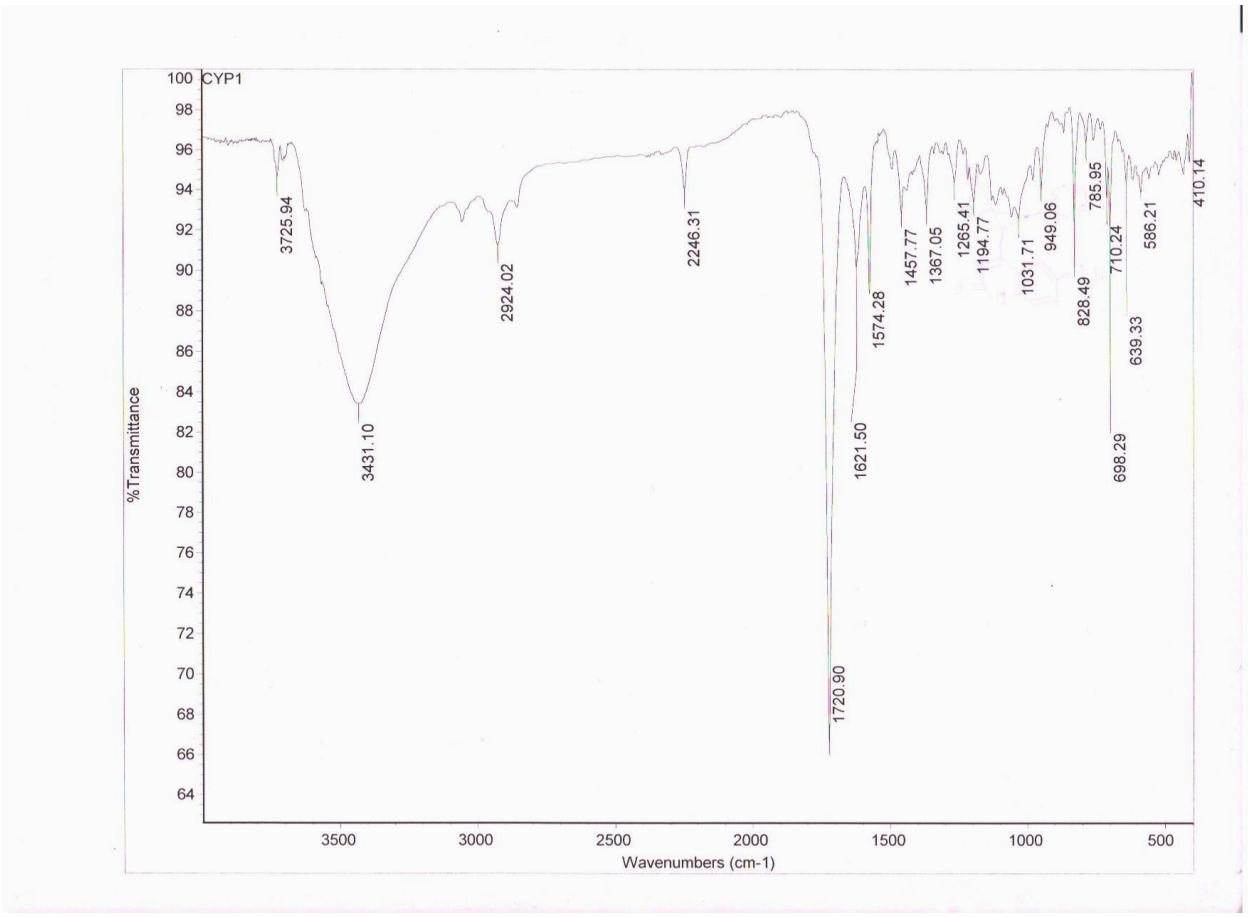
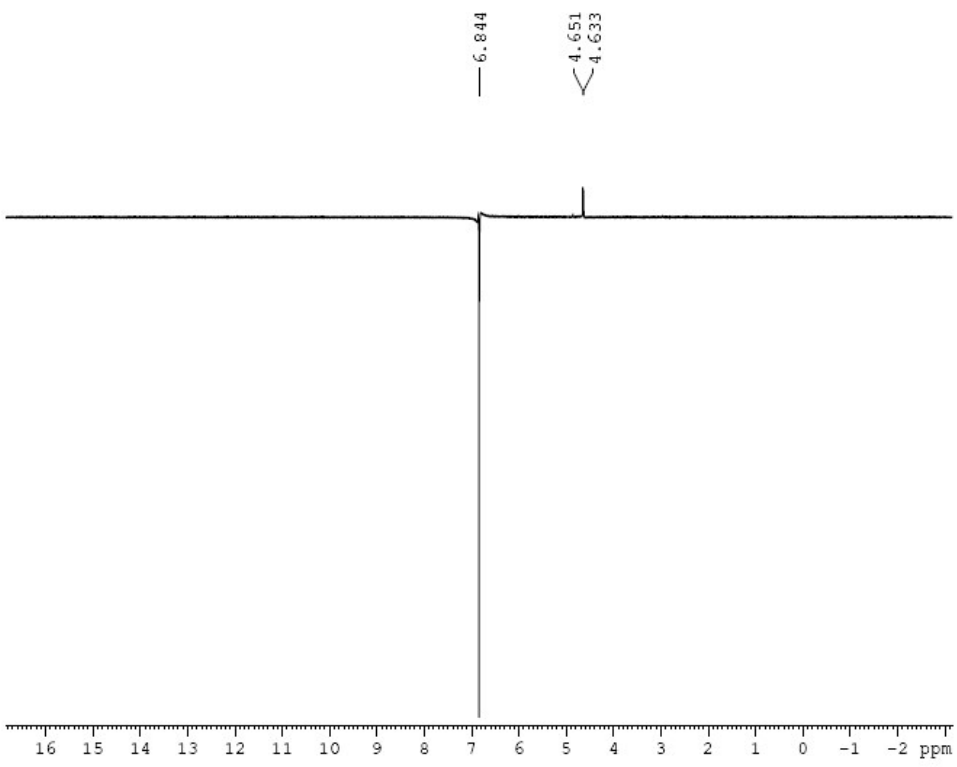


IR Spectra of Compound 4a

NOE Studies

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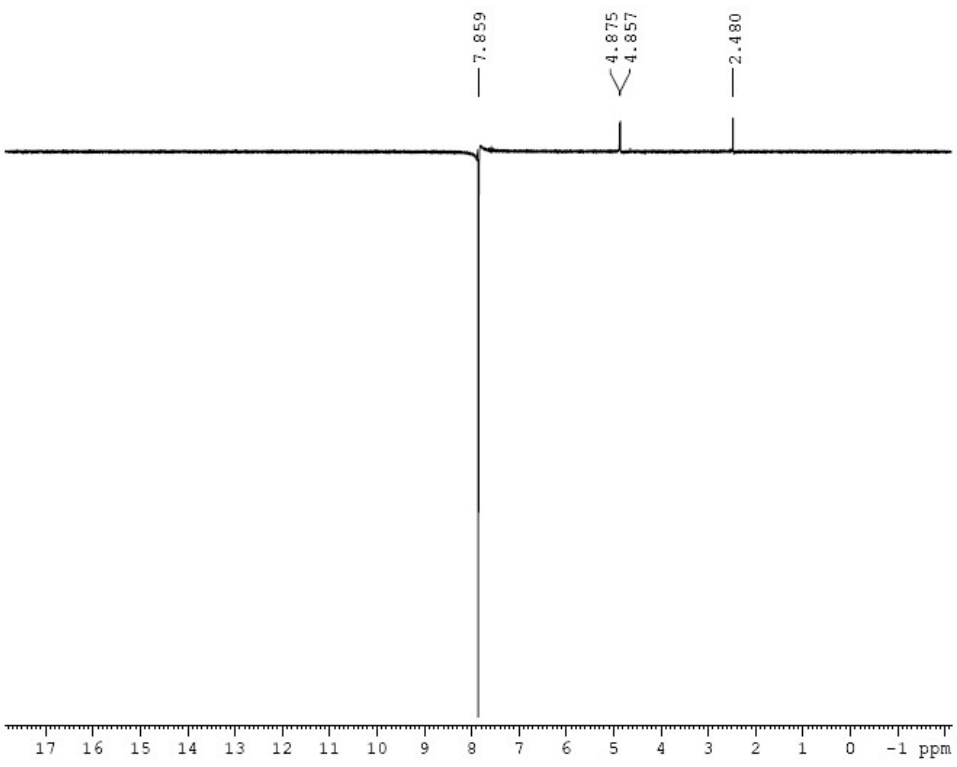
Irradiation at 6.84 ppm of Compound 4a

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RG                         71.8
DW                       50.000 usec
DE                        6.50 usec
TE                       298.0 K
D1                  2.00000000 sec
D8                  0.50000000 sec
D16                 0.00020000 sec
D20                 0.24879999 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
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P2                       14.18 usec
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PL1                       1.50 dB
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PL1W               17.96062279 W
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SP2                      68.10 dB
SPNAM[2] Gaus1_180r.1000
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SPOFFS2  0 Hz

====== GRADIENT CHANNEL =====
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GPZ1                     15.00 %
GPZ2                     40.00 %
P16                    1000.00 usec

F2 - Processing parameters
SI                        65536
SF                 500.1300000 MHz
WDW                          EM
SSB        0
LB                        0.10 Hz
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Irradiation at 7.85 ppm of Compound 4a

Experimental

Instrumentation: Melting points were determined by open capillary method and are uncorrected. IR spectra (KBr disc) were recorded on a Nicolet-5700 FT-IR spectrophotometer. ^{1}H-NMR spectra were recorded on a Bruker 400 MHz spectrometer using DMSO-d_6 as solvent and TMS as an internal standard. Chemical shifts are expressed in δ ppm. Mass spectra were recorded using Agilent-single Quartz GC-MS. Elemental analysis was carried out using Heraus CHN rapid analyzer. Purity of the compound was checked by T.L.C. All the chemicals purchased were of analytical grade and were used without further purification unless otherwise stated.

General procedure for the synthesis of 4-(bromomethyl)-2H-chromen-2-ones.

Required 4-(bromomethyl)-2*H*-chromen-2-ones [31] have been synthesized by the Pechmann cyclization of substituted phenols with ethyl 4-bromoacetoacetate.

General procedure for the synthesis of 4-(bromomethyl) quinolin-2(1H)-ones.

Initially, substituted acetoacetanilides were brominated in the presence of $CHCl_3$ to get the corresponding ω-bromoacetoacetanilides. Further 8g of ω-bromoacetoacetanilides in 32 mL of concentrated sulphuric acid was warmed on a water bath for 4hrs. The reaction mixture was then quenched in ice-water and the separated solid was filtered and washed thoroughly with water, dried and recrystallised using acetic acid.

General procedure for the synthesis of coumarinyl/ 1-azacoumarinyl pyridinium ylide (5)

Pyridinium ylides **5** were synthesized by refluxing **1** (0.001M) and pyridine (0.0012M) in acetonitrile for 3 h. The separated pyridinium salt was filtered and washed with absolute alcohol and dried.

Spectral Characterization

All the synthesized compounds were characterized using IR, ^{1}H-NMR, ^{13}C-NMR and EI-MS. For a typical compound **4a,** (R= -H, R'= 6-CH_3, R"= -CN, X=O) IR spectrum showed band at 2246 cm^{-1} (cyanide) and 1720 cm^{-1} (lactone). Further, the formation of cyclopropane ring was confirmed by the ^{1}H-NMR wherein the C_5-H of coumarin ring resonated at 7.83 ppm as a doublet with $^{5}J_{C5\text{-}H}$ = 1.2 Hz showing a 5-bond coupling with the C_4-CH of coumarin ring. C_4-CH of coumarin ring appeared at 4.83 ppm as doublet of doublets with $J_{vic(CH)}$ = 8.8 Hz, Cou-CH $^{5}J_{C5\text{-}H}$ = 1.2 Hz. CH attached to aryl group resonated at 4.61 ppm as a doublet with $J_{vic(CH)}$ = 8.8 Hz. C_6-CH_3 protons appeared at 2.45 as a singlet. C_3-H was observed as a singlet at 6.82 ppm. Other aromatic protons resonated between 7.68-7.41 ppm.

In ^{13}C-NMR, the carbon attached to two cyano group resonated at 15.08 ppm, the methyl carbon appeared at 20.55 ppm. Cyclopropane ring carbon attached to aryl group resonated at 32.81 ppm whereas the one attached to coumarin appeared at 36.78 ppm. Carbon of two cyano group resonated at 112.68 and 112.91 ppm. The lactone carbon of the coumarin ring appeared at 159.35 ppm. Aromatic carbons resonated in the range of 112-159 ppm. Formation of the product was further confirmed by EI-MS where the molecular ion peak was observed at 326 *m/z*.

2-(6-Methyl-2-oxo-2H-chromen-4-yl)-3-phenyl-cyclopropane-1,1-dicarbonitrile (4a)

White; Yield 85%; m.p: 268-270°C; IR (KBr) cm^{-1} 1720 (C=O lactone), 2246 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.83(d, 1H, $^{5}J_{C5\text{-}H}$ = 1.2 Hz, C_5-H), 7.68-7.41(m, 7H, Ar-H), 6.82(s, 1H, C_3-H), 4.83(dd, 1H, $J_{vic(CH)}$ = 8.8Hz, Cou-CH, $^{5}J_{C5\text{-}H}$ = 1.2 Hz), 4.61(d, 1H, $J_{vic(CH)}$ = 8.8Hz, Ar-CH), 2.45(s, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ (ppm): 8.57, 15.08, 20.55, 32.81, 36.78, 45.73, 112.68, 112.91, 115.95, 116.69, 117.64, 124.60, 128.62, 129.00,

129.12, 130.90, 133.63, 134.23, 146.64, 151.12, 159.35; MS *m/z* 326(100%); Anal Calcd. for $C_{21}H_{14}N_2O_2$ (%), Calcd: C, 77.29; H, 4.32; N, 8.58; found: C, 77.26; H, 4.29; N, 8.55

2-(7-methyl-2-oxo-2H-chromen-4-yl)-3-phenylcyclopropane-1,1-dicarbonitrile (4b)

White; Yield 61%; m.p: 214-216°C; IR (KBr) cm^{-1} 1719 (C=O lactone), 2248 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 8.19-7.11(m, 8H, Ar-H), 6.76(s, 1H, C_3-H), 4.84(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Cou-CH), 4.57(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Ar-CH), 2.46(s, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ (ppm): 7.96, 14.85, 20.95, 21.07, 32.94, 35.29, 36.85, 112.70, 112.91, 114.99, 115.51, 116.96, 124.49, 125.19, 125.87, 129.78, 143.65, 143.90, 146.80, 153.04, 159.40; Anal Calcd. for $C_{21}H_{14}N_2O_2$ (%), Calcd: C, 77.29; H, 4.32; N, 8.58; found: C, 77.25; H, 4.28; N, 8.54

2-(5,7-dimethyl-2-oxo-2H-chromen-4-yl)-3-phenylcyclopropane-1,1-dicarbonitrile (4c)

White; Yield 82%; m.p: 295-297°C; IR (KBr) cm^{-1} 1717 (C=O lactone), 2246 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.65-7.04(m, 7H, Ar-H), 6.71(s, 1H, C_3-H), 4.78(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Cou-CH), 4.63(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Ar-CH), 2.87(s, 3H, -CH_3), 2.50(s, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ (ppm): 16.63, 20.60, 22.97, 37.16, 38.51, 38.87, 40.12, 113.03, 113.06, 114.83, 115.82, 117.34, 128.60, 129.00, 129.07, 129.97, 131.14, 135.63, 142.81, 147.36, 154.56, 158.88; Anal Calcd. for $C_{22}H_{16}N_2O_2$ (%), Calcd: C, 77.63; H, 4.74; N, 8.23; found: C, 77.63; H, 4.70; N, 8.20

2-(7-methoxy-2-oxo-2H-chromen-4-yl)-3-phenylcyclopropane-1,1-dicarbonitrile (4d)

Off White; Yield 60%; m.p: 314-316°C; IR (KBr) cm^{-1} 1712 (C=O lactone), 2240 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 8.13-7.00(m, 8H, Ar-H), 6.64(s, 1H, C_3-H), 4.83(d, 1H, $J_{vic(CH)}$ = 9.2 Hz, Cou-CH), 4.55(d, 1H, $J_{vic(CH)}$ = 9.2 Hz, Ar-CH), 3.89(s, 3H, -OCH_3); ^{13}C-

NMR (100 MHz, DMSO-d_6) δ (ppm): 14.85, 33.01, 35.48, 55.99, 101.07, 111.82, 111.96. 114.51, 114.62, 125.92, 127.32, 128.63, 128.90, 129.45, 148.10, 155.30, 159.43, 162.86; MS *m/z* 342; Anal Calcd. for $C_{21}H_{14}N_2O_3$ (%), Calcd: C, 73.68; H, 4.12; N, 8.18; found: C, 73.64; H, 4.09; N, 8.14

2-(7-chloro-2-oxo-2H-chromen-4-yl)-3-phenylcyclopropane-1,1-dicarbonitrile (4e)

White; Yield 65%; m.p: 340-342°C; IR (KBr) cm^{-1} 1731 (C=O lactone), 2247 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 8.03-7.43(m, 8H, Ar-H), 6.89(s, 1H, C_3-H), 4.87(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Cou-CH), 4.59(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Ar-CH); ^{13}C-NMR (100 MHz, DMSO-d_6) δ (ppm): 15.00, 32.70, 36.81, 112.57, 112.85, 116.35, 116.95, 117.09, 125.30, 126.39, 128.63, 129.00, 129.14, 130.81, 137.15, 146.27, 153.38, 158.70; MS *m/z* 346(M^+), 348(M+2); Anal Calcd. for $C_{20}H_{11}ClN_2O_2$ (%), Calcd: C, 69.27; H, 3.20; N, 8.08; found: C, 69.24; H, 3.15; N, 8.04

2-(2-oxo-2H-benzo[h]chromen-4-yl)-3-phenylcyclopropane-1,1-dicarbonitrile (4f)

Dark Brown; Yield 81%; m.p: 352-354°C; IR (KBr) cm^{-1} 1720 (C=O lactone), 2235 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 8.45-6.96(m, 11H, Ar-H), 6.66(s, 1H, C_3-H), 4.99(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Cou-CH), 4.64(d, 1H, $J_{vic(CH)}$ = 8.8 Hz, Ar-CH); ^{13}C-NMR (100 MHz, DMSO-d_6) δ (ppm): 8.00, 14.98, 33.41, 37.16, 45.73, 53.76, 112.71, 112.95, 115.64, 120.27, 121.69, 122.15, 124.80, 127.84, 128.09, 128.66, 129.04, 129.15, 129.27, 130.93, 134.57, 147.69, 159.14; MS *m/z* 362; Anal Calcd. for $C_{24}H_{14}N_2O_2$ (%), Calcd: C, 79.55; H, 3.89; N, 7.73; found: C, 79.51; H, 3.84; N, 7.70

ethyl 1-cyano-2-(6-methyl-2-oxo-2H-chromen-4-yl)-3-phenylcyclopropanecarboxylate (4g)

White; Yield 85%; m.p: 128-130°C; IR (KBr) cm^{-1} 1733 (C=O lactone), 2243 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.58-7.34(m, 8H, Ar-H), 6.71(s, 1H, C_3-H), 4.50(d, 1H,

Cou-CH, $^{3}J_{vic}$ = 8.8 Hz), 4.02(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Ar-CH), 3.91(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz), 2.42(s, 3H, -CH_3), 0.77(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{23}H_{19}NO_4$ (%), Calcd: C, 73.98; H, 5.13; N, 3.75; found: C, 73.95; H, 5.10; N, 3.71

ethyl 1-cyano-2-(4-methoxyphenyl)-3-(6-methyl-2-oxo-2H-chromen-4-yl)cyclopropanecarboxylate (4h)

White; Yield 85%; m.p: 144-146°C; IR (KBr) cm^{-1} 1731 (C=O lactone), 2243 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.52(s, 1H, C_5-H), 7.51-6.97(m, 6H, Ar-H), 6.67(d, 1H, C_3-H, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 4.44(dd, 1H, Cou-CH, $^{3}J_{vic}$ = 8.8 Hz, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 3.95(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Ar-CH), 3.91(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz) 3.78(s, 3H, -OCH_3), 2.42(s, 3H, -CH_3), 0.77(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{24}H_{21}NO_5$ (%), Calcd: C, 71.45; H, 5.25; N, 3.47; found: C, 71.42; H, 5.22; N, 3.45

ethyl 1-cyano-2-(furan-2-yl)-3-(6-methyl-2-oxo-2H-chromen-4-yl) cyclopropanecarboxylate (4i)

Off White; Yield 56%; m.p: 114-116°C; IR (KBr) cm^{-1} 1721 (C=O lactone), 2249 (CN^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.76-6.53(m, 6H, Ar-H), 6.72(d, 1H, C_3-H, $^{4}J_{\text{allylic}}$ = 1.6 Hz), 4.42(dd, 1H, Cou-CH, $^{3}J_{vic}$ = 8.8 Hz, $^{4}J_{\text{allylic}}$ = 1.6 Hz), 4.06(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Furan-CH), 3.92(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz), 2.41(s, 3H, -CH_3), 0.77(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{21}H_{17}NO_5$ (%), Calcd: C, 69.41; H, 4.72; N, 3.85; found: C, 69.38; H, 4.70; N, 3.81

ethyl 1-cyano-2-(7,8-dimethyl-2-oxo-2H-chromen-4-yl)-3-p-tolylcyclopropanecarboxylate (4j)

White; Yield 82%; m.p: 132-134°C; IR (KBr) cm^{-1} 1724 (C=O lactone), 2244 (CN^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.48-7.23(m, 6H, Ar-H), 6.61(d, 1H, C_3-H, $^{4}J_{\text{allylic}}$ = 1.2 Hz),

4.42(dd, 1H, Cou-CH, $^{3}J_{vic}$ = 8.8Hz, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 3.95(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Ar-CH), 3.89(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz), 2.37(s, 3H, Ar-CH_3), 2.33(s, 3H, C_8-CH_3), 2.29(s, 3H, C_7-CH_3), 0.81(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{21}H_{17}NO_5$ (%), Calcd: C, 74.79; H, 5.77; N, 3.49; found: C, C, 74.75; H, 5.74; N, 3.45

ethyl 1-cyano-2-(7,8-dimethyl-2-oxo-2H-chromen-4-yl)-3-(4-nitrophenyl) cyclopropanecarboxylate (4k)

Dark Brown; Yield 65%; m.p: 115-117°C; IR (KBr) cm^{-1} 1732 (C=O lactone), 2247 (CN), 1348 and 1523 (NO_2); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 8.31-7.32(m, 6H, Ar-H), 6.72(d, 1H, C_3-H, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 4.65(dd, 1H, Cou-CH, $^{3}J_{vic}$ = 8.8 Hz, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 4.19(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Ar-CH), 3.90(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz), 2.38(s, 3H, C_8-CH_3), 2.29(s, 3H, C_7-CH_3), 0.81(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{24}H_{20}N_2O_6$ (%), Calcd: C, 66.66; H, 4.66; N, 6.48; found: C, 66.63; H, 4.62; N, 6.45

ethyl 2-(2-chlorophenyl)-1-cyano-3-(6-methoxy-2-oxo-2H-chromen-4-yl)cyclopropanecarboxylate (4l)

White; Yield 87%; m.p: 164-166°C; IR (KBr) cm^{-1} 1725 (C=O lactone), 2250 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.63-7.20(m, 7H, Ar-H), 6.85(d, 1H, C_3-H, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 4.60(dd, 1H, Cou-CH, $^{3}J_{vic}$ = 8.8 Hz, $^{4}J_{\text{allylic}}$ = 1.2 Hz), 4.03(d, 1H, $^{3}J_{vic}$ = 8.8 Hz, Ar-CH), 3.97(q, 2H, -CH_2, $^{3}J_{vic}$ = 7.2 Hz), 3.84(s, 3H, -OCH_3), 0.78(t, 3H, -CH_3, $^{3}J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{23}H_{18}ClNO_5$ (%), Calcd: C, 65.18; H, 4.28; N, 3.30; found: C, 65.15; H, 4.25; N, 3.27

ethyl 2-(3-bromophenyl)-1-cyano-3-(5,7-dimethyl-2-oxo-2H-chromen-4-yl)cyclopropanecarboxylate (4m)

Purple; Yield 59%; m.p: 198-200°C; IR (KBr) cm^{-1} 1727 (C=O lactone), 2243 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.85(s, 1H, C_8-H), 7.59-7.06(m, 5H, Ar-H), 6.62(s, 1H, C_3-H), 4.59(d, 1H, Cou-CH, $^3J_{vic}$ = 8.8 Hz), 4.07(d, 1H, $^3J_{vic}$ = 8.8 Hz, Ar-CH), 3.95(q, 2H, -CH_2, $^3J_{vic}$ = 7.2 Hz), 2.84(s, 3H, C_5-CH_3), 2.34(s, 3H, C_7-CH_3), 0.83(t, 3H, -CH_3, $^3J_{vic}$ = 7.2 Hz). Anal Calcd. for $C_{24}H_{20}BrNO_4$ (%), Calcd: C, 61.81; H, 4.32; N, 3.00; found: C, 61.78; H, 4.28; N, 2.97

2-(furan-2-yl)-3-(6-methoxy-2-oxo-2H-chromen-4-yl)cyclopropane-1,1-dicarbonitrile (4n)

Black; Yield 75%; m.p: 190-192°C; IR (KBr) cm^{-1} 1718 (C=O lactone), 2219 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.83-7.05(m, 6H, Ar-H), 6.84(s, 1H, C_3-H), 4.78(d, 1H, Cou-CH, $^3J_{vic}$ = 8.8 Hz), 4.69(d, 1H, $^3J_{vic}$ = 8.8 Hz, Ar-CH), 3.87(s, 3H, -OCH_3). Anal Calcd. for $C_{19}H_{12}N_2O_4$ (%), Calcd: C, 68.67; H, 3.64; N, 8.43; found: C, 68.65; H, 3.62; N, 8.40

2-(5,7-dimethyl-2-oxo-2H-chromen-4-yl)-3-(4-methoxyphenyl)cyclopropane-1,1-dicarbonitrile (4o)

White; Yield 87%; m.p: 184-186°C; IR (KBr) cm^{-1} 1728 (C=O lactone), 2246 (CN); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 7.56(d, 1H, Ar-CH *meta* to -OCH_3, $^3J_{vic}$ = 8.8 Hz), 7.18(s, 1H, C_8-H), 7.15(s, 1H, C_6-H), 7.01(d, 1H, Ar-CH *ortho* to -OCH_3, $^3J_{vic}$ = 8.8 Hz), 6.68(s, 1H, C_3-H), 4.72(d, 1H, Cou-CH, $^3J_{vic}$ = 8.8 Hz), 4.55(d, 1H, $^3J_{vic}$ = 8.8 Hz, Ar-CH), 3.79(s, 3H, -OCH_3) 2.87(s, 3H, C_5-CH_3), 2.38(s, 3H, C_7-CH_3). Anal Calcd. for $C_{23}H_{18}N_2O_3$ (%), Calcd: C, 74.58; H, 4.90; N, 7.56; found: C, 74.55; H, 4.87; N, 7.52

2-(4-methoxyphenyl)-3-(2-oxo-1,2-dihydroquinolin-4-yl)cyclopropane-1,1-dicarbonitrile (4p)

White; Yield 58%; m.p: 282-284°C; IR (KBr) cm^{-1} 1664 (C=O lactam), 2247 (CN), 3435 (NH); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 11.93(s, 1H, NH), 7.90-7.01(m, 8H, Ar-H),

6.75(s, 1H, C_3-H), 4.73(d, 1H, C_4-CH, $^3J_{vic}$ = 9.2 Hz), 4.47(d, 1H, $^3J_{vic}$ = 9.2 Hz, Ar-CH), 3.79(s, 3H, -OCH_3). Anal Calcd. for $C_{21}H_{15}N_3O_2$ (%), Calcd: C, 73.89; H, 4.43; N, 12.31; found: C, 73.85; H, 4.40; N, 12.27

2-(2-chlorophenyl)-3-(8-methyl-2-oxo-1,2-dihydroquinolin-4-yl)cyclopropane-1,1-dicarbonitrile (4q)

White; Yield 75%; m.p: 250-252°C; IR (KBr) cm^{-1} 1662 (C=O lactam), 2249 (CN), 3435 (NH); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 11.05(s, 1H, NH), 7.72-7.26(m, 7H, Ar-H), 6.91(s, 1H, C_3-H), 4.79(dd, 1H, C_4-CH, $^3J_{vic}$ = 9.2 Hz, $^5J_{C5\text{-}H}$ = 1.2 Hz), 4.47(d, 1H, $^3J_{vic}$ = 9.2 Hz, Ar-CH), 2.07(s, 1H, C_8-CH_3) Anal Calcd. for $C_{21}H_{14}ClN_3O$ (%), Calcd: C, 70.10; H, 3.92; N, 11.68; found: C, 70.07; H, 3.90; N, 11.64

2-(7-chloro-2-oxo-1,2-dihydroquinolin-4-yl)-3-(4-methoxyphenyl)cyclopropane-1,1-dicarbonitrile (4r)

Off White; Yield 76%; m.p: 95-97°C; IR (KBr) cm^{-1} 1666 (C=O lactam), 2224 (CN), 3435 (NH); ^{1}H-NMR (400 MHz, DMSO-d_6, TMS) δ (ppm): 11.99(s, 1H, NH), 8.38-7.01(m, 7H, Ar-H), 6.79(s, 1H, C_3-H), 4.75(d, 1H, C_4-CH, $^3J_{vic}$ = 9.2 Hz), 4.45(d, 1H, $^3J_{vic}$ = 9.2 Hz, Ar-CH), 3.87(s, 3H, -OCH_3). Anal Calcd. for $C_{21}H_{14}ClN_3O_2$ (%), Calcd: C, 67.12; H, 3.75; N, 11.18; found: C, 67.09; H, 3.72; N, 11.14

Computational methods

Ab initio calculations were carried out using Gaussian W09 package. All the calculations were run on a HPz 200 workstation at RHF/STO-3G level.

Structure-I			**Structure-II**		
File name	C2C1C6C-13-180		File name	C2C1C6C13-0	
File type	.log		File type	.log	
Calculation type	FREQ		Calculation type	FREQ	
Calculation method	RHF		Calculation method	RHF	
Basis Set	STO-3G		Basis Set	STO-3G	
Charge	0		Charge	0	
Spin	Singlet		Spin	Singlet	
E(RHF)	-1048.75084476	a.u.	E(RHF)	-1048.74850478	a.u.
RMS Gradient Norm	0.00000550	a.u.	RMS Gradient Norm	0.00001081	a.u.
Imaginary Freq	0		Imaginary Freq	0	
Dipole Moment	3.5920	Debye		6.8583	Debye
Point Group	C1		Point Group	C1	

Energy Difference= 0.00233998 H = 1.4683608498 kcal/mol.

Geometrical Parameters for Structure -I

! Geometrical Parameters of Structure I ! ! (Angstroms and Degrees) !		
! Name	Definition	Value
! R1	R(1,2)	1.5335
! R2	R(1,3)	1.5031
! R3	R(1,6)	1.5182
! R4	R(1,7)	1.0845
! R5	R(2,3)	1.5401
! R6	R(2,4)	1.475
! R7	R(2,5)	1.4743
! R8	R(3,8)	1.5149
! R9	R(3,9)	1.0837
! R10	R(4,10)	1.1559
! R11	R(5,11)	1.1559
! R12	R(6,12)	1.4849
! R13	R(6,13)	1.3242
! R14	R(8,14)	1.393
! R15	R(8,15)	1.3923
! R16	R(12,16)	1.3942
! R17	R(12,17)	1.402
! R18	R(13,18)	1.5022
! R19	R(13,19)	1.081
! R20	R(14,20)	1.3851
! R21	R(14,21)	1.0826
! R22	R(15,22)	1.3854
! R23	R(15,23)	1.0813
! R24	R(16,24)	1.4022
! R25	R(16,25)	1.3906
! R26	R(17,26)	1.3785
! R27	R(17,27)	1.0812
! R28	R(18,25)	1.4031
! R29	R(18,28)	1.219
! R30	R(20,29)	1.3865
! R31	R(20,30)	1.0827
! R32	R(22,29)	1.3866
! R33	R(22,31)	1.0827
! R34	R(24,32)	1.373
! R35	R(24,33)	1.0819
! R36	R(26,32)	1.4037
! R37	R(26,34)	1.5261
! R38	R(29,35)	1.0827
! R39	R(32,36)	1.0833
! R40	R(34,37)	1.085
! R41	R(34,38)	1.0876
! R42	R(34,39)	1.0876
! A1	A(2,1,6)	120.6753
! A2	A(2,1,7)	113.4883
! A3	A(3,1,6)	122.3029
! A4	A(3,1,7)	116.0656
! A5	A(6,1,7)	113.4892

! A6	A(1,2,4)	118.6874
! A7	A(1,2,5)	118.3195
! A8	A(3,2,4)	117.3598
! A9	A(3,2,5)	119.9556
! A10	A(4,2,5)	113.4822
! A11	A(1,3,8)	124.2342
! A12	A(1,3,9)	114.9006
! A13	A(2,3,8)	122.468
! A14	A(2,3,9)	111.9352
! A15	A(8,3,9)	112.9373
! A16	A(1,6,12)	118.9919
! A17	A(1,6,13)	122.1064
! A18	A(12,6,13)	118.8807
! A19	A(3,8,14)	118.1724
! A20	A(3,8,15)	122.9624
! A21	A(14,8,15)	118.8652
! A22	A(6,12,16)	117.817
! A23	A(6,12,17)	123.6564
! A24	A(16,12,17)	118.5266
! A25	A(6,13,18)	122.4585
! A26	A(6,13,19)	122.8646
! A27	A(18,13,19)	114.6751
! A28	A(8,14,20)	120.6914
! A29	A(8,14,21)	119.5723
! A30	A(20,14,21)	119.7363
! A31	A(8,15,22)	120.4223
! A32	A(8,15,23)	120.5591
! A33	A(22,15,23)	119.0186
! A34	A(12,16,24)	120.2011
! A35	A(12,16,25)	124.2425
! A36	A(24,16,25)	115.5564
! A37	A(12,17,26)	121.8534
! A38	A(12,17,27)	119.041
! A39	A(26,17,27)	119.1056
! A40	A(13,18,25)	118.0026
! A41	A(13,18,28)	124.5142
! A42	A(25,18,28)	117.483
! A43	A(14,20,29)	120.0359
! A44	A(14,20,30)	119.7876
! A45	A(29,20,30)	120.1764
! A46	A(15,22,29)	120.3029
! A47	A(15,22,31)	119.605
! A48	A(29,22,31)	120.0921
! A49	A(16,24,32)	119.9036
! A50	A(16,24,33)	118.6369
! A51	A(32,24,33)	121.4595
! A52	A(16,25,18)	118.5975
! A53	A(17,26,32)	118.4804
! A54	A(17,26,34)	121.3876
! A55	A(32,26,34)	120.132
! A56	A(20,29,22)	119.6823
! A57	A(20,29,35)	120.1857
! A58	A(22,29,35)	120.132
! A59	A(24,32,26)	121.0349

! A60	A(24,32,36)	119.5738
! A61	A(26,32,36)	119.3912
! A62	A(26,34,37)	110.8577
! A63	A(26,34,38)	110.73
! A64	A(26,34,39)	110.6816
! A65	A(37,34,38)	108.3889
! A66	A(37,34,39)	108.3347
! A67	A(38,34,39)	107.7425
! A68	L(2,4,10,12,-1)	179.955
! A69	L(2,5,11,22,-1)	180.2626
! A70	L(2,4,10,12,-2)	179.3766
! A71	L(2,5,11,22,-2)	179.4344
! D1	D(6,1,2,4)	6.1812
! D2	D(6,1,2,5)	-137.9979
! D3	D(7,1,2,4)	145.9164
! D4	D(7,1,2,5)	1.7373
! D5	D(6,1,3,8)	139.0048
! D6	D(6,1,3,9)	-7.6717
! D7	D(7,1,3,8)	-7.5291
! D8	D(7,1,3,9)	-154.2056
! D9	D(2,1,6,12)	79.5658
! D10	D(2,1,6,13)	-102.1225
! D11	D(3,1,6,12)	152.5223
! D12	D(3,1,6,13)	-29.1659
! D13	D(7,1,6,12)	-60.1691
! D14	D(7,1,6,13)	118.1427
! D15	D(4,2,3,8)	-137.5477
! D16	D(4,2,3,9)	1.4093
! D17	D(5,2,3,8)	7.1435
! D18	D(5,2,3,9)	146.1005
! D19	D(1,3,8,14)	-161.1647
! D20	D(1,3,8,15)	18.8853
! D21	D(2,3,8,14)	124.6726
! D22	D(2,3,8,15)	-55.2774
! D23	D(9,3,8,14)	-13.9217
! D24	D(9,3,8,15)	166.1282
! D25	D(1,6,12,16)	178.7404
! D26	D(1,6,12,17)	-1.2929
! D27	D(13,6,12,16)	0.3735
! D28	D(13,6,12,17)	-179.6597
! D29	D(1,6,13,18)	-178.7194
! D30	D(1,6,13,19)	0.7645
! D31	D(12,6,13,18)	-0.4059
! D32	D(12,6,13,19)	179.0781
! D33	D(3,8,14,20)	-179.8905
! D34	D(3,8,14,21)	0.1928
! D35	D(15,8,14,20)	0.0616
! D36	D(15,8,14,21)	-179.855
! D37	D(3,8,15,22)	179.8505
! D38	D(3,8,15,23)	-0.1589
! D39	D(14,8,15,22)	-0.0992
! D40	D(14,8,15,23)	179.8914
! D41	D(6,12,16,24)	179.9661
! D42	D(6,12,16,25)	-0.1127

! D43	D(17,12,16,24)	-0.0024
! D44	D(17,12,16,25)	179.9188
! D45	D(6,12,17,26)	-179.9623
! D46	D(6,12,17,27)	-0.0407
! D47	D(16,12,17,26)	0.0042
! D48	D(16,12,17,27)	179.9259
! D49	D(6,13,18,25)	0.1776
! D50	D(6,13,18,28)	-179.9866
! D51	D(19,13,18,25)	-179.3454
! D52	D(19,13,18,28)	0.4904
! D53	D(8,14,20,29)	0.0231
! D54	D(8,14,20,30)	-179.9707
! D55	D(21,14,20,29)	179.9397
! D56	D(21,14,20,30)	-0.0542
! D57	D(8,15,22,29)	0.0525
! D58	D(8,15,22,31)	-179.9697
! D59	D(23,15,22,29)	-179.9383
! D60	D(23,15,22,31)	0.0395
! D61	D(12,16,24,32)	-0.0098
! D62	D(12,16,24,33)	-179.9683
! D63	D(25,16,24,32)	-179.9376
! D64	D(25,16,24,33)	0.1039
! D65	D(12,16,25,18)	-0.1142
! D66	D(24,16,25,18)	179.8103
! D67	D(12,17,26,32)	0.006
! D68	D(12,17,26,34)	179.9016
! D69	D(27,17,26,32)	-179.9156
! D70	D(27,17,26,34)	-0.0199
! D71	D(13,18,25,16)	0.0932
! D72	D(28,18,25,16)	-179.7543
! D73	D(14,20,29,22)	-0.071
! D74	D(14,20,29,35)	179.9949
! D75	D(30,20,29,22)	179.9229
! D76	D(30,20,29,35)	-0.0113
! D77	D(15,22,29,20)	0.0334
! D78	D(15,22,29,35)	179.9677
! D79	D(31,22,29,20)	-179.9443
! D80	D(31,22,29,35)	-0.0101
! D81	D(16,24,32,26)	0.0205
! D82	D(16,24,32,36)	-179.9551
! D83	D(33,24,32,26)	179.9778
! D84	D(33,24,32,36)	0.0022
! D85	D(17,26,32,24)	-0.0185
! D86	D(17,26,32,36)	179.9572
! D87	D(34,26,32,24)	-179.9155
! D88	D(34,26,32,36)	0.0601
! D89	D(17,26,34,37)	0.4968
! D90	D(17,26,34,38)	120.8388
! D91	D(17,26,34,39)	-119.745
! D92	D(32,26,34,37)	-179.6092
! D93	D(32,26,34,38)	-59.2672
! D94	D(32,26,34,39)	60.149

Geometrical Parameters for Structure –II

! Optimized Parameters of Structure II !		
! (Angstroms and Degrees) !		
! Name	Definition	Value
! R1	R(1,2)	1.5311
! R2	R(1,3)	1.506
! R3	R(1,6)	1.52
! R4	R(1,7)	1.0855
! R5	R(2,3)	1.5396
! R6	R(2,4)	1.4753
! R7	R(2,5)	1.4753
! R8	R(3,8)	1.5147
! R9	R(3,9)	1.0844
! R10	R(4,10)	1.1559
! R11	R(5,11)	1.1558
! R12	R(6,12)	1.4859
! R13	R(6,13)	1.3243
! R14	R(8,14)	1.3931
! R15	R(8,15)	1.3923
! R16	R(12,16)	1.3946
! R17	R(12,17)	1.4019
! R18	R(13,18)	1.5025
! R19	R(13,19)	1.0812
! R20	R(14,20)	1.385
! R21	R(14,21)	1.0826
! R22	R(15,22)	1.3855
! R23	R(15,23)	1.0814
! R24	R(16,24)	1.4022
! R25	R(16,25)	1.39
! R26	R(17,26)	1.3786
! R27	R(17,27)	1.081
! R28	R(18,25)	1.4042
! R29	R(18,28)	1.2185
! R30	R(20,29)	1.3866
! R31	R(20,30)	1.0827
! R32	R(22,29)	1.3865
! R33	R(22,31)	1.0827
! R34	R(24,32)	1.373
! R35	R(24,33)	1.0819
! R36	R(26,32)	1.4033
! R37	R(26,34)	1.5262
! R38	R(29,35)	1.0827
! R39	R(32,36)	1.0833
! R40	R(34,37)	1.0851
! R41	R(34,38)	1.0876
! R42	R(34,39)	1.0877
! A1	A(2,1,6)	122.4661
! A2	A(2,1,7)	113.197
! A3	A(3,1,6)	122.2926

! A4	A(3,1,7)	115.3078
! A5	A(6,1,7)	113.1153
! A6	A(1,2,4)	120.5013
! A7	A(1,2,5)	117.7975
! A8	A(3,2,4)	116.905
! A9	A(3,2,5)	119.6595
! A10	A(4,2,5)	113.0855
! A11	A(1,3,8)	124.4576
! A12	A(1,3,9)	114.4529
! A13	A(2,3,8)	122.7605
! A14	A(2,3,9)	111.8662
! A15	A(8,3,9)	113.0078
! A16	A(1,6,12)	118.9629
! A17	A(1,6,13)	122.1416
! A18	A(12,6,13)	118.8323
! A19	A(3,8,14)	118.192
! A20	A(3,8,15)	122.9493
! A21	A(14,8,15)	118.8587
! A22	A(6,12,16)	117.7829
! A23	A(6,12,17)	123.7513
! A24	A(16,12,17)	118.4612
! A25	A(6,13,18)	122.4833
! A26	A(6,13,19)	122.9185
! A27	A(18,13,19)	114.5981
! A28	A(8,14,20)	120.6932
! A29	A(8,14,21)	119.5561
! A30	A(20,14,21)	119.7507
! A31	A(8,15,22)	120.4265
! A32	A(8,15,23)	120.5578
! A33	A(22,15,23)	119.0157
! A34	A(12,16,24)	120.2175
! A35	A(12,16,25)	124.2769
! A36	A(24,16,25)	115.5055
! A37	A(12,17,26)	121.8796
! A38	A(12,17,27)	118.9626
! A39	A(26,17,27)	119.1575
! A40	A(13,18,25)	117.9612
! A41	A(13,18,28)	124.6418
! A42	A(25,18,28)	117.3958
! A43	A(14,20,29)	120.0378
! A44	A(14,20,30)	119.7929
! A45	A(29,20,30)	120.1693
! A46	A(15,22,29)	120.3017
! A47	A(15,22,31)	119.601
! A48	A(29,22,31)	120.0972
! A49	A(16,24,32)	119.9371
! A50	A(16,24,33)	118.6062
! A51	A(32,24,33)	121.4565
! A52	A(16,25,18)	118.5435
! A53	A(17,26,32)	118.5183
! A54	A(17,26,34)	121.3625
! A55	A(32,26,34)	120.1191
! A56	A(20,29,22)	119.6819
! A57	A(20,29,35)	120.1835

! A58	A(22,29,35)	120.1345
! A59	A(24,32,26)	120.9818
! A60	A(24,32,36)	119.5915
! A61	A(26,32,36)	119.4262
! A62	A(26,34,37)	110.8556
! A63	A(26,34,38)	110.7326
! A64	A(26,34,39)	110.7378
! A65	A(37,34,38)	108.3518
! A66	A(37,34,39)	108.3439
! A67	A(38,34,39)	107.7113
! A68	L(2,4,10,13,-1)	181.1216
! A69	L(2,5,11,22,-1)	180.1803
! A70	L(2,4,10,13,-2)	179.103
! A71	L(2,5,11,22,-2)	179.6126
! D1	D(6,1,2,4)	6.8775
! D2	D(6,1,2,5)	-138.7106
! D3	D(7,1,2,4)	148.0361
! D4	D(7,1,2,5)	2.4479
! D5	D(6,1,3,8)	136.5906
! D6	D(6,1,3,9)	-9.7939
! D7	D(7,1,3,8)	-7.7566
! D8	D(7,1,3,9)	-154.1411
! D9	D(2,1,6,12)	-139.7028
! D10	D(2,1,6,13)	43.2248
! D11	D(3,1,6,12)	-65.9349
! D12	D(3,1,6,13)	116.9928
! D13	D(7,1,6,12)	79.1105
! D14	D(7,1,6,13)	-97.9619
! D15	D(4,2,3,8)	-134.9639
! D16	D(4,2,3,9)	4.4169
! D17	D(5,2,3,8)	7.6872
! D18	D(5,2,3,9)	147.068
! D19	D(1,3,8,14)	-160.8738
! D20	D(1,3,8,15)	19.1644
! D21	D(2,3,8,14)	124.9032
! D22	D(2,3,8,15)	-55.0586
! D23	D(9,3,8,14)	-14.0703
! D24	D(9,3,8,15)	165.9679
! D25	D(1,6,12,16)	-179.5506
! D26	D(1,6,12,17)	-0.3377
! D27	D(13,6,12,16)	-2.3802
! D28	D(13,6,12,17)	176.8327
! D29	D(1,6,13,18)	178.7867
! D30	D(1,6,13,19)	-1.3392
! D31	D(12,6,13,18)	1.7107
! D32	D(12,6,13,19)	-178.4153
! D33	D(3,8,14,20)	-179.8763
! D34	D(3,8,14,21)	0.1816
! D35	D(15,8,14,20)	0.0871
! D36	D(15,8,14,21)	-179.8551
! D37	D(3,8,15,22)	179.8371
! D38	D(3,8,15,23)	-0.1263
! D39	D(14,8,15,22)	-0.1244
! D40	D(14,8,15,23)	179.9122

! D41	D(6,12,16,24)	-179.9733
! D42	D(6,12,16,25)	0.02
! D43	D(17,12,16,24)	0.7711
! D44	D(17,12,16,25)	-179.2356
! D45	D(6,12,17,26)	-179.7868
! D46	D(6,12,17,27)	0.0302
! D47	D(16,12,17,26)	-0.5789
! D48	D(16,12,17,27)	179.2381
! D49	D(6,13,18,25)	1.2732
! D50	D(6,13,18,28)	-179.1426
! D51	D(19,13,18,25)	-178.6105
! D52	D(19,13,18,28)	0.9737
! D53	D(8,14,20,29)	0.0116
! D54	D(8,14,20,30)	180.0008
! D55	D(21,14,20,29)	179.9537
! D56	D(21,14,20,30)	-0.0571
! D57	D(8,15,22,29)	0.0635
! D58	D(8,15,22,31)	-179.9393
! D59	D(23,15,22,29)	-179.9725
! D60	D(23,15,22,31)	0.0247
! D61	D(12,16,24,32)	-0.4176
! D62	D(12,16,24,33)	179.7471
! D63	D(25,16,24,32)	179.5885
! D64	D(25,16,24,33)	-0.2468
! D65	D(12,16,25,18)	2.9867
! D66	D(24,16,25,18)	-177.0196
! D67	D(12,17,26,32)	0.023
! D68	D(12,17,26,34)	179.984
! D69	D(27,17,26,32)	-179.7936
! D70	D(27,17,26,34)	0.1674
! D71	D(13,18,25,16)	-3.5541
! D72	D(28,18,25,16)	176.8312
! D73	D(14,20,29,22)	-0.074
! D74	D(14,20,29,35)	179.9788
! D75	D(30,20,29,22)	179.9368
! D76	D(30,20,29,35)	-0.0103
! D77	D(15,22,29,20)	0.0367
! D78	D(15,22,29,35)	179.9839
! D79	D(31,22,29,20)	-179.9604
! D80	D(31,22,29,35)	-0.0132
! D81	D(16,24,32,26)	-0.1558
! D82	D(16,24,32,36)	-179.915
! D83	D(33,24,32,26)	179.6747
! D84	D(33,24,32,36)	-0.0845
! D85	D(17,26,32,24)	0.3512
! D86	D(17,26,32,36)	-179.8891
! D87	D(34,26,32,24)	-179.6103
! D88	D(34,26,32,36)	0.1494
! D89	D(17,26,34,37)	0.3777
! D90	D(17,26,34,38)	120.6733
! D91	D(17,26,34,39)	-119.9114
! D92	D(32,26,34,37)	-179.6619
! D93	D(32,26,34,38)	-59.3663
! D94	D(32,26,34,39)	60.049