

Chickpea Leaf Exudates: A green Bronsted acid type biosurfactant for bis(indole)methanes and bis(pyrazolyl)methanes synthesis

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Electronic Supplemental Information (ESI)

Sr. No.	Table of Contents	Pages
1	Experimental section	1-2
2	HPLC-MS spectra of all acids are present in <i>Chickpea leaf exudates</i>	3-18
3	IR, ¹ H and ¹³ C NMR spectroscopic data of all products	19-25
4	IR, ¹ H and ¹³ C NMR spectrum of selected products	26-50

1. Experimental section:

1.1 Collection of catalyst

For quantitative collection of *CLE* as a catalytic medium we consider growing period of newly cultivated chickpea crops. At first, for the purpose of exudates collection cultivated crops on various lands were selected and then exudates were collected manually using clean and soft cotton cloth by absorption-wringing process. It was observed that good quantity of exudates was obtained from chickpea crops of two months old (just before flowering stage). It was also observed that early morning (5.00 am to 6.00 am) period gave good collection of exudates (ESI). The pH of collected exudates was measured using pH-meter before use and it was found to be 1.1. The collected catalyst was stored several days at 5 °C.



Fig. 1 (a) Cultivated *Chickpea crops* (b) absorption of *Chickpea exudates* by cotton cloth (c) wringing of *Chickpea exudates* (d) turbid *Chickpea leaf exudates*

1.2 General procedure for the synthesis of 3-((1H-indol-3-yl)(4-methoxyphenyl)methyl)-1H-indol

All the reactions were carried out under air atmosphere in pre-dried glassware. A mixtures of indoles (2.0 mmol), and aryl aldehydes (1.0 mmol) in solution of *CLE* (5.0 mL) and *iso*-PrOH (3.0 mL) were stirred at 60 °C in preheated oil bath till the completion of reaction as indicated by TLC (petroleum ether: ethyl acetate). After completion of reaction, 5.0 mL water was added in reaction mixture. The solid products were separated by simple filtration followed by washing with cold water 5.0 mL. The pure products were obtained by recrystallization with 96 % ethanol. All the products were confirmed by the spectroscopic method using NMR and FT-IR. The physical and spectroscopic data are in consistent with the proposed structures and are in harmony with the literature values.

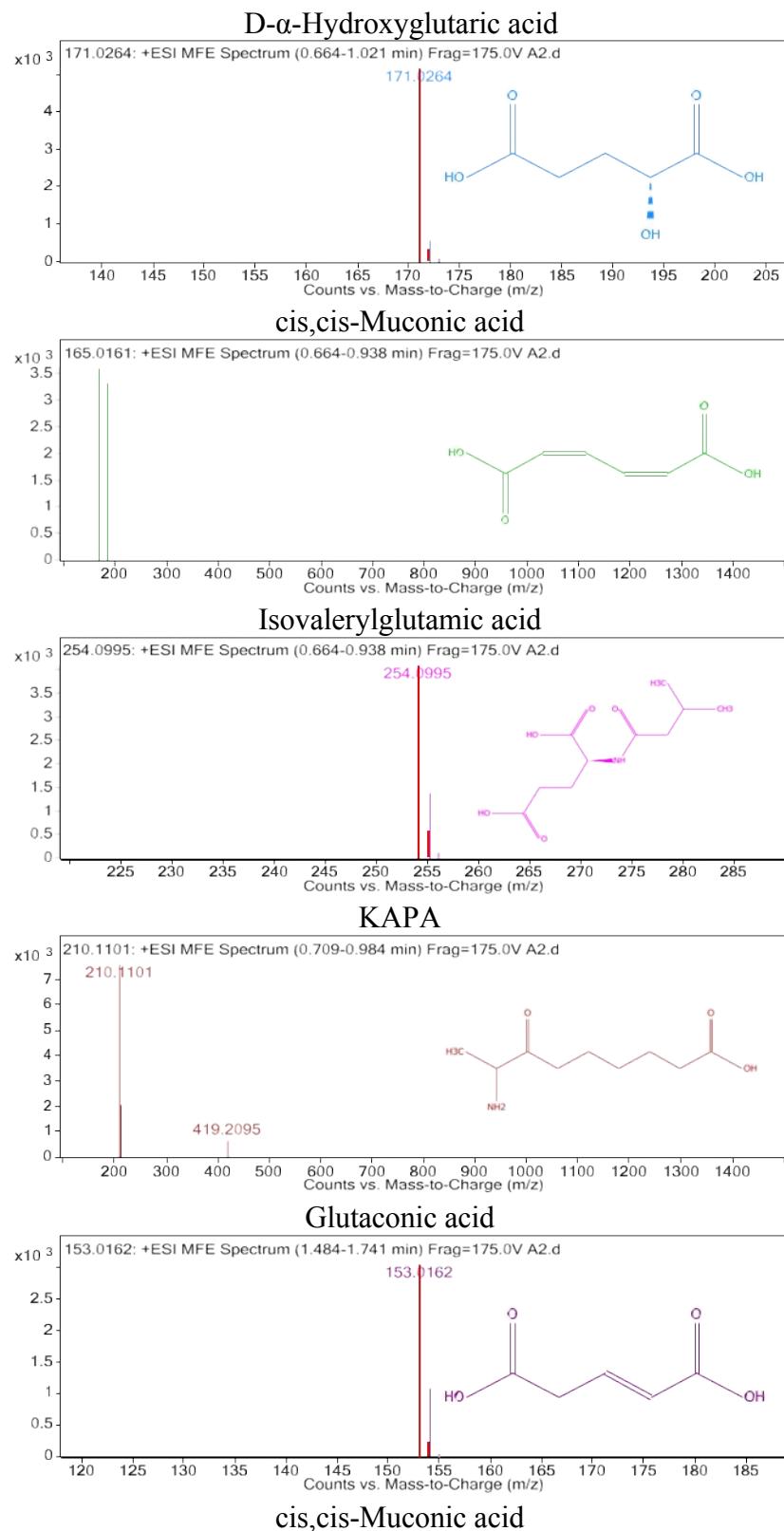
1.3 General procedure for synthesis of 4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(4-methoxyphenyl)methyl)-3-methyl-1H-pyrazol-5-ol

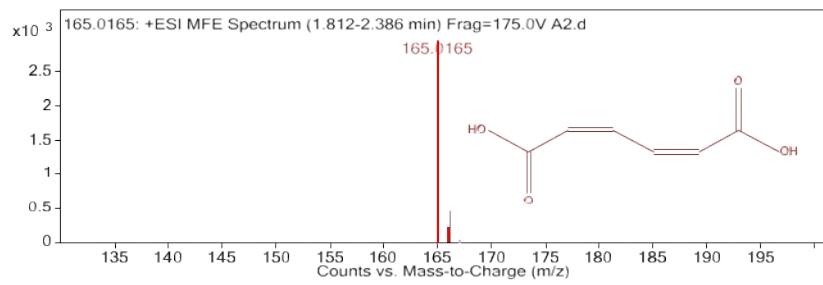
In a 25 mL round bottom flask aryl aldehyde (1.0 mmol), ethyl acetoacetate (2.0 mmol), hydrazine hydrate (2.0 mmol) were placed in solution of *CLE* (5.0 mL) in *iso*-PrOH (3.0 mL) and stirred at 60 °C in preheated oil bath till the completion of reaction as indicated by TLC (petroleum: ethyl acetate). After completion of reaction, 5.0 mL water was added in reaction mixture. The solid products were separated by simple filtration followed by washing with cold water 5.0 mL. The pure products were obtained by recrystallization with 96 % ethanol. Representative compounds were confirmed by physical constants and characterized by spectral analysis.

1.4 Recycle of catalyst

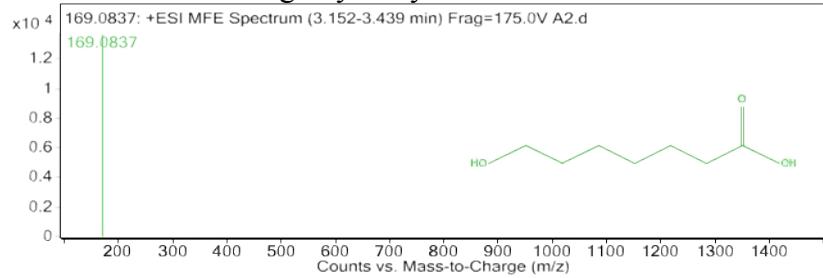
In order to investigate the recyclability and reusability of *CLE* catalyst, we synthesized compounds **3a** and **7a**. After completion of reaction, H₂O (5.0 mL) was added in reaction mixture and then it was filtered off. Whole filtrate containing *CLE* was concentrated under vacuum and directly used for the next cycle with fresh reactants for synthesis of **3a** and **7a** in *iso*-PrOH at 60°C. The recovered catalyst was employed for further five successful recycles without significant lose of efficiency. However, reaction times were found to be increased while reuse of the recovered catalyst (Fig. 9).

HPLC-MS spectra of all acids are present in *Chickpea Leaf Exudates*:

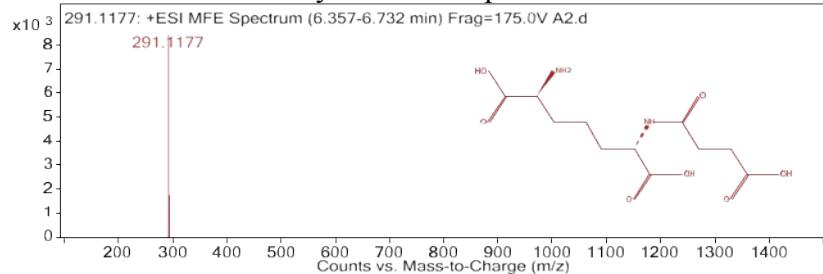




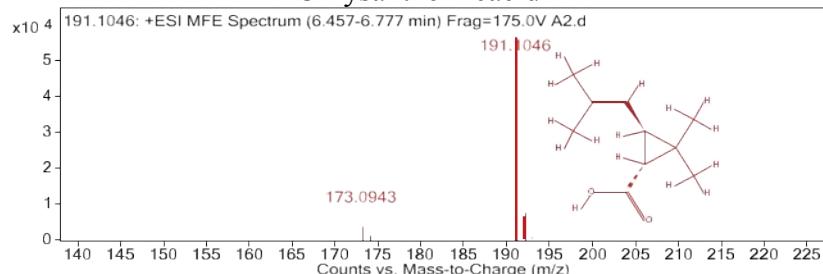
omega-hydroxyenanthoic acid



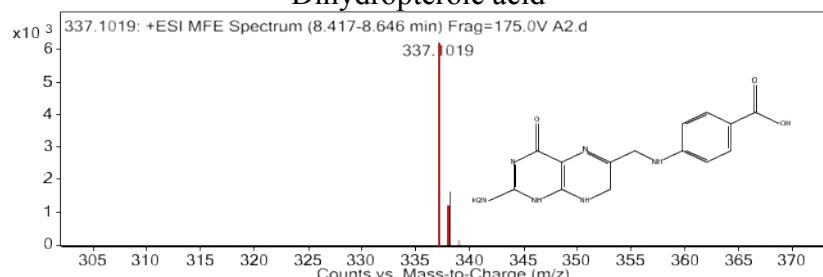
N-Succinyl-L-diaminopimelic acid



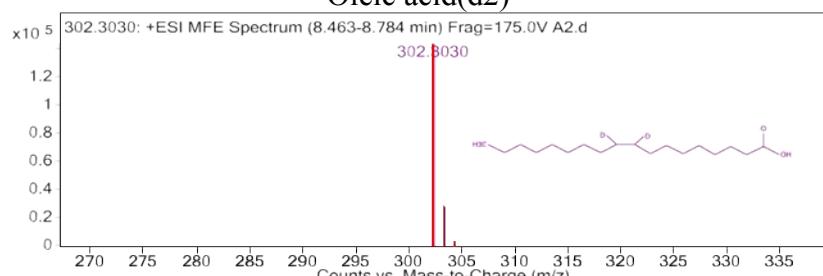
Chrysanthemic acid



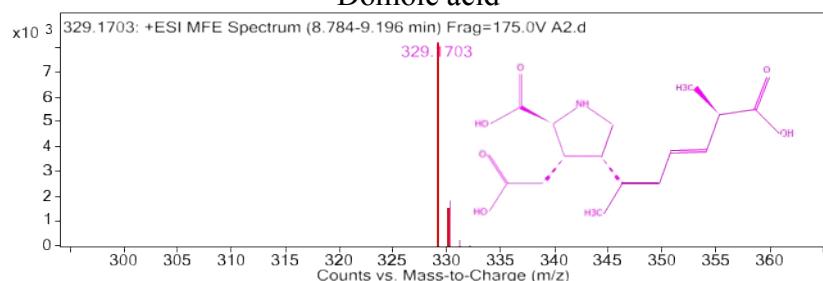
Dihydropteroic acid



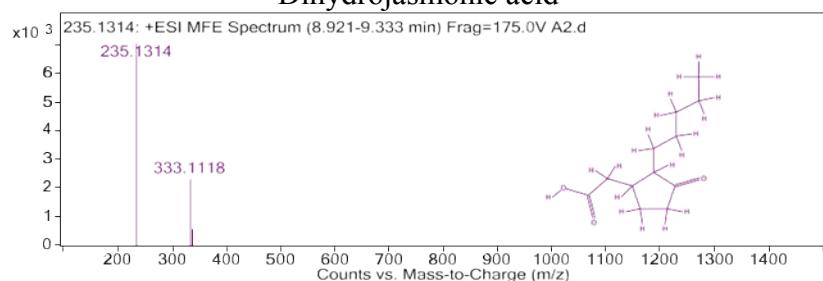
Oleic acid(d2)



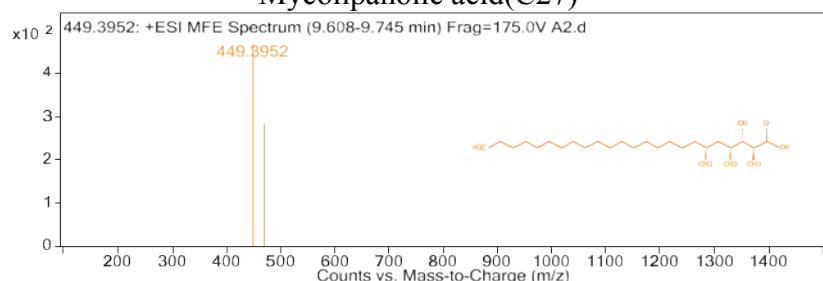
Domoic acid



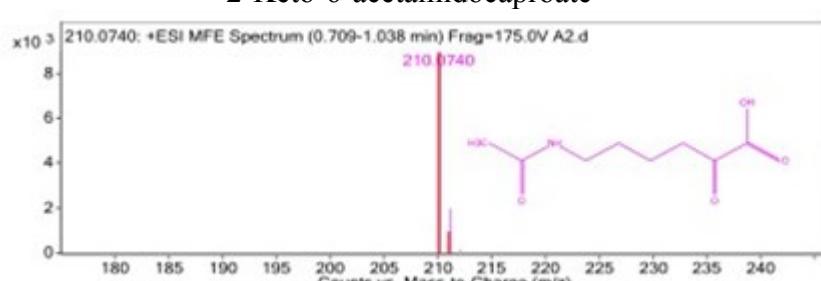
Dihydrojasmonic acid



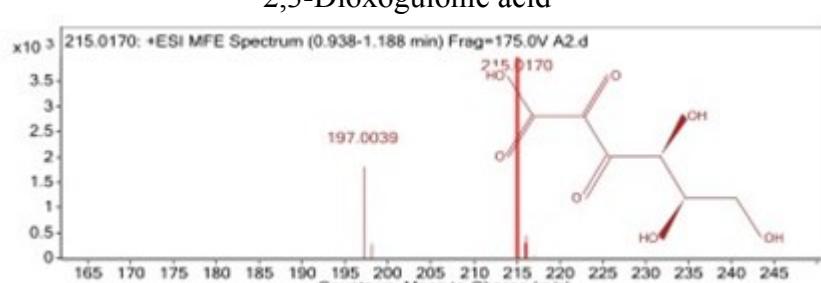
Mycolipanolic acid(C27)



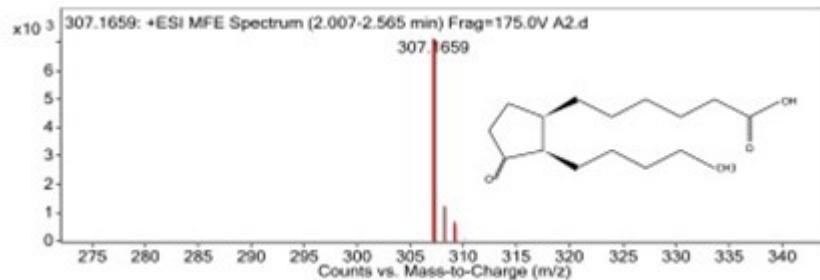
2-Keto-6-acetamidocaproate



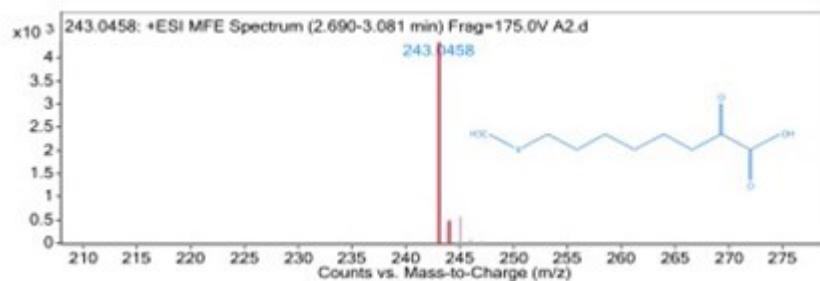
2,3-Dioxogulonic acid



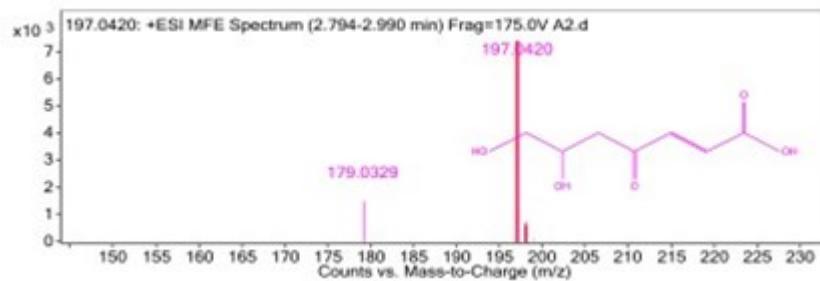
(1R,2R)-3-oxo-2-pentyl-cyclopentanehexanoic acid



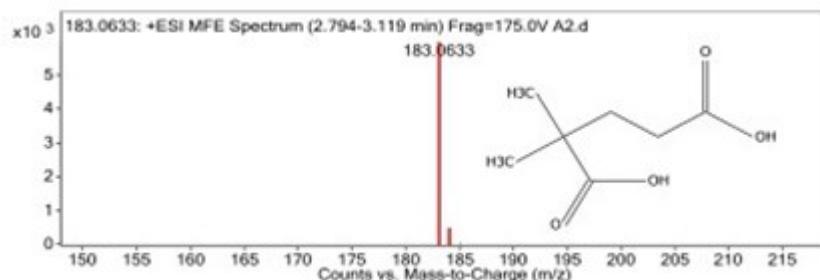
2-Oxo-8-methylthiooctanoic



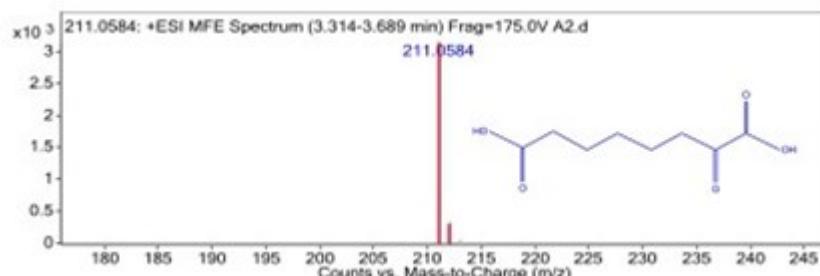
6,7-dihydroxy-4-oxo-2-heptenoic acid



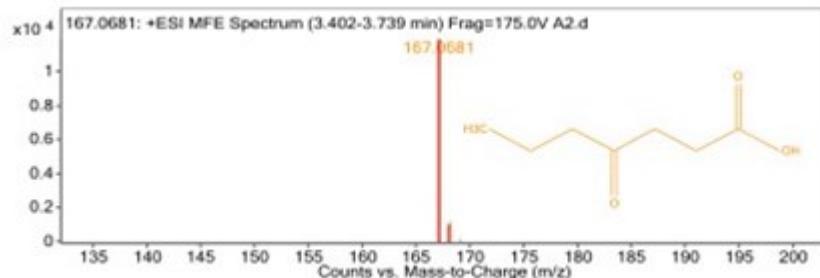
2,2-Dimethylglutaric acid



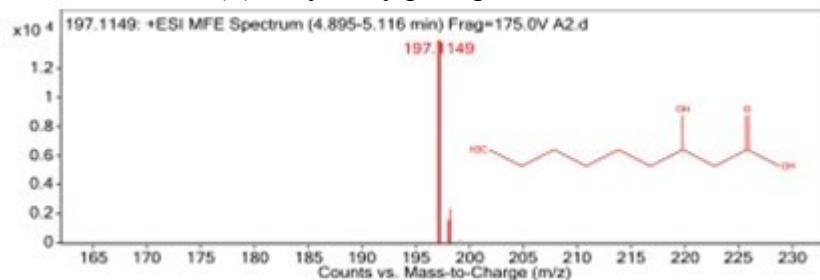
2-Oxosuberate



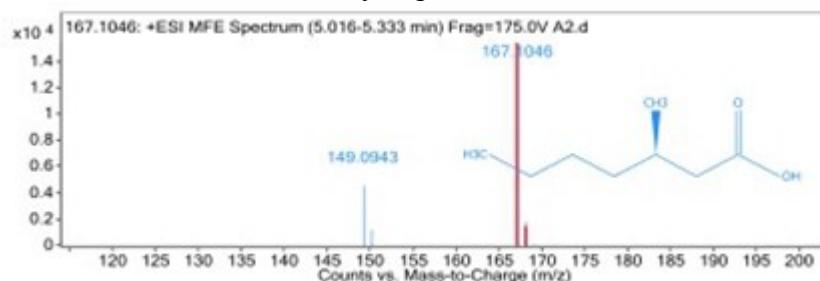
3-butyryl propionic acid



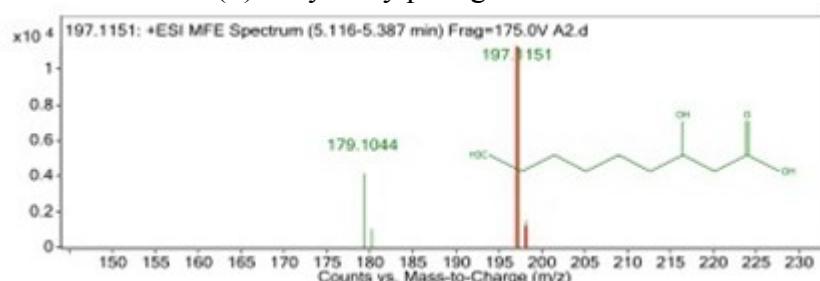
(+)-3-hydroxy pelargonic acid



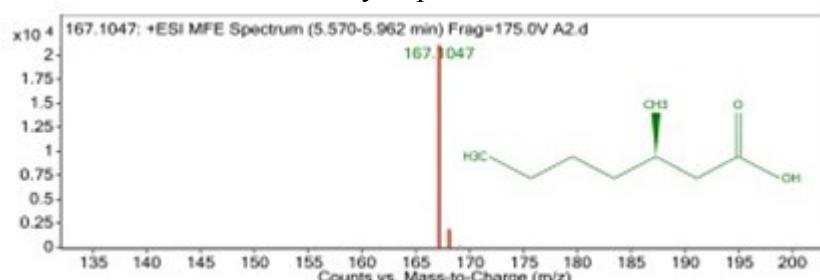
3R-Methylheptanoic acid



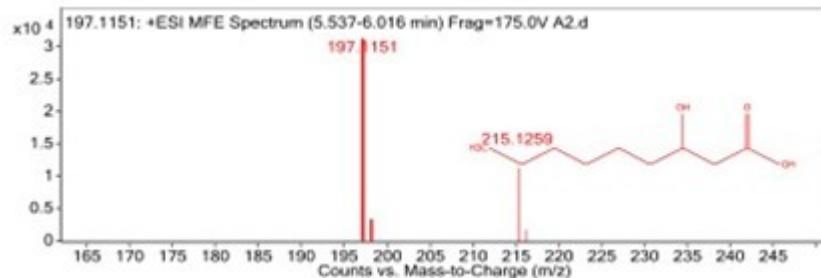
(+)-3-hydroxy pelargonic acid



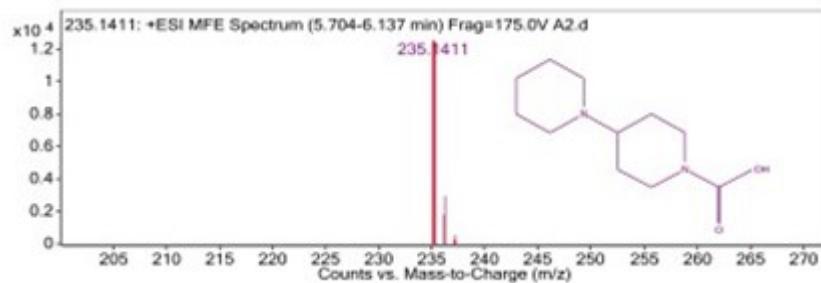
3R-Methylheptanoic acid



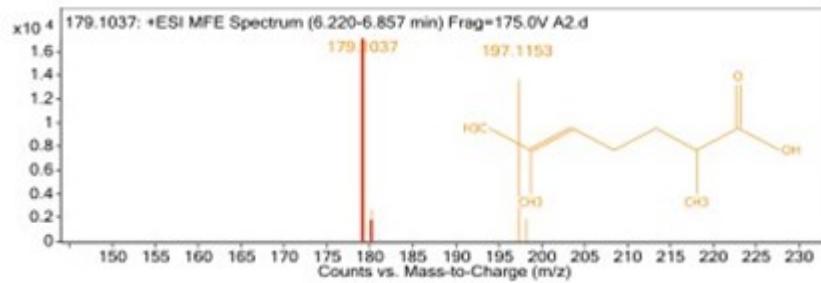
(+)-3-hydroxy pelargonic acid



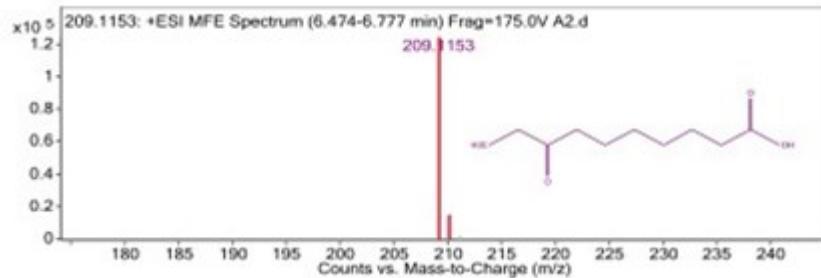
1,4'-Bipiperidine-1'-carboxylic acid



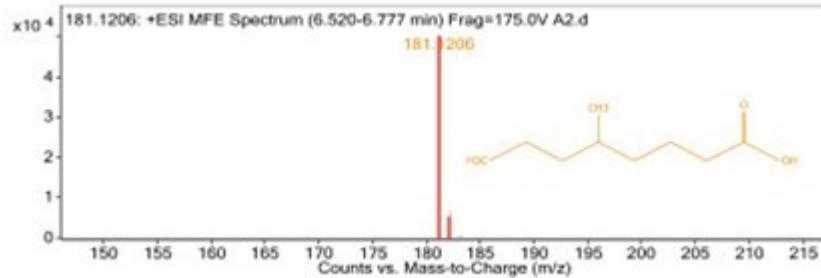
2,6-Dimethyl-5-heptenoic acid 156



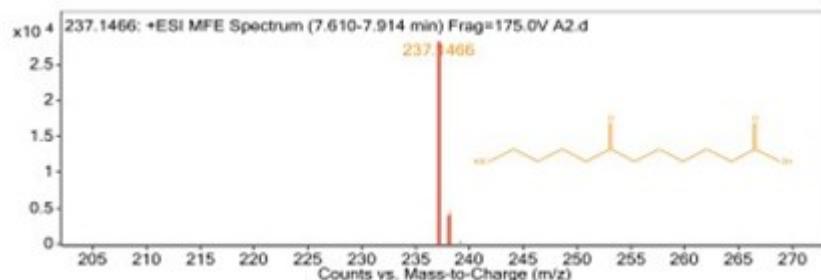
8-oxo capric acid 186



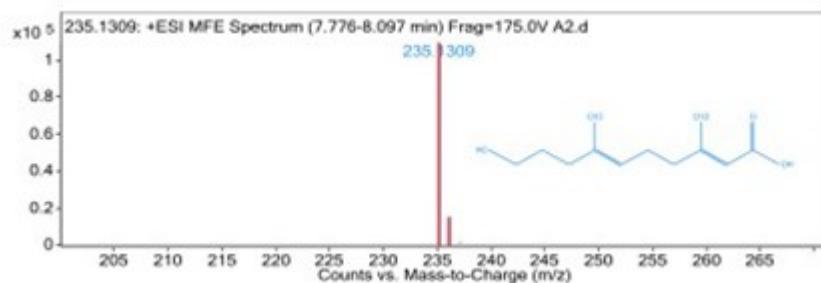
5-methyl-octanoic acid 158



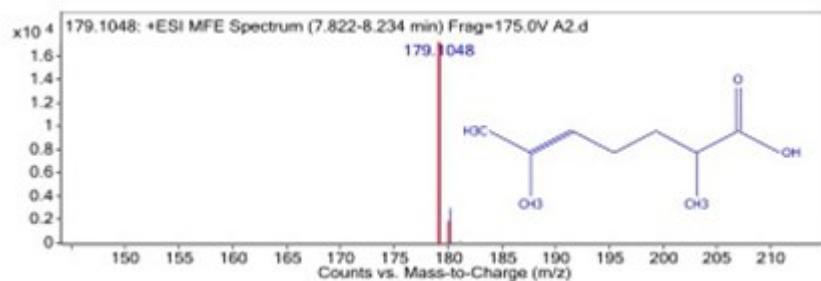
7-Oxododecanoic acid 214



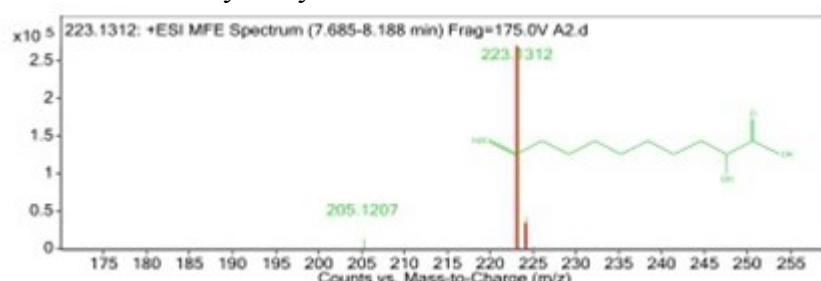
10-Hydroxy-3,7-dimethyl-2E,6E- decadienoic acid



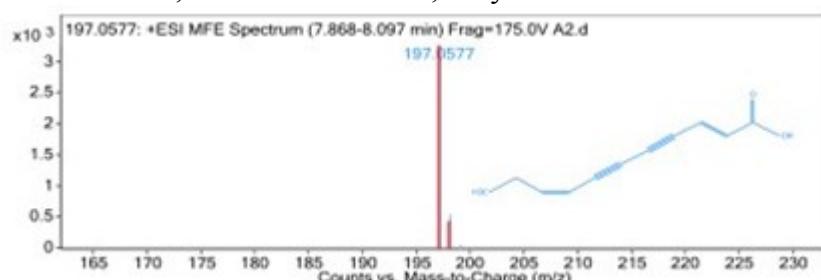
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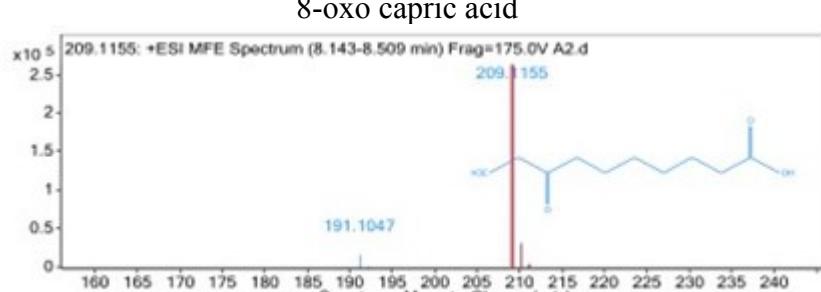
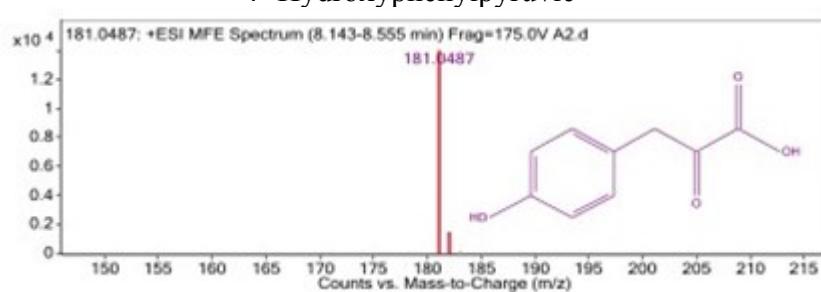
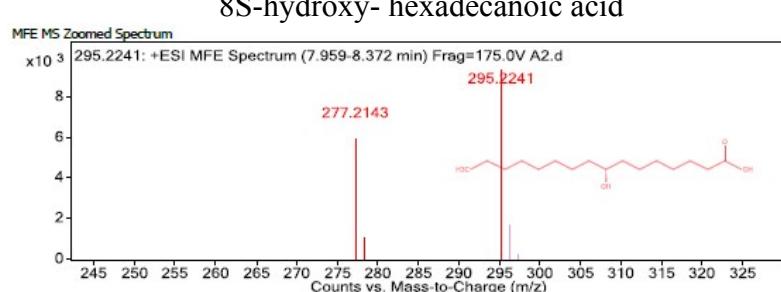
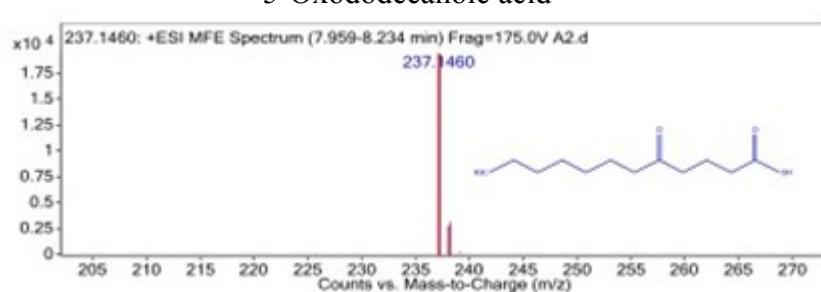
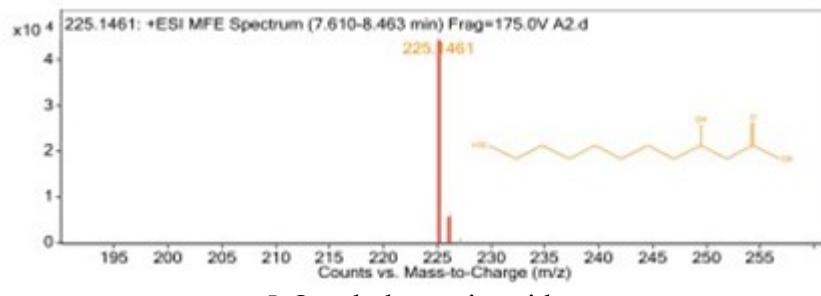
2-hydroxy-10- undecenoic acid 200

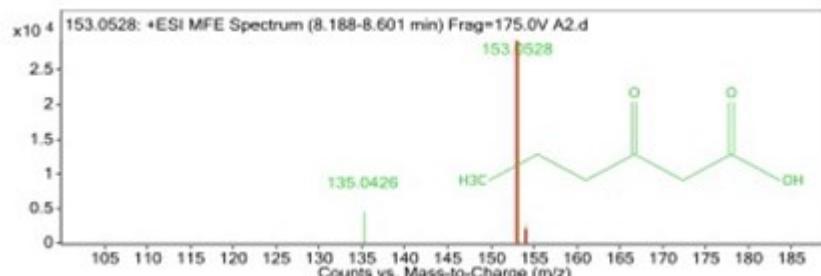


2E,8Z-Undecadiene- 4,6-diynoic acid 174

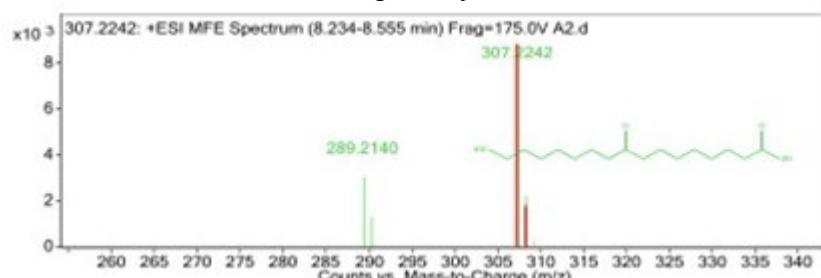


3-hydroxy-undecanoic acid 202

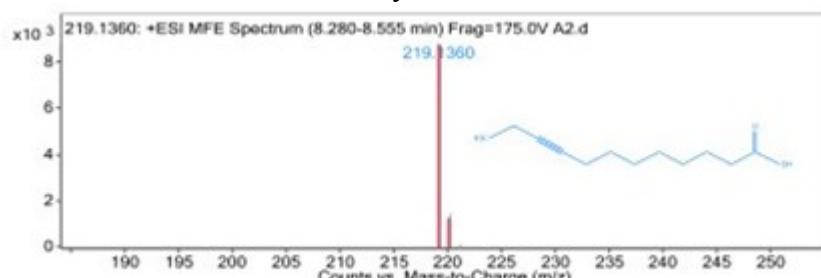




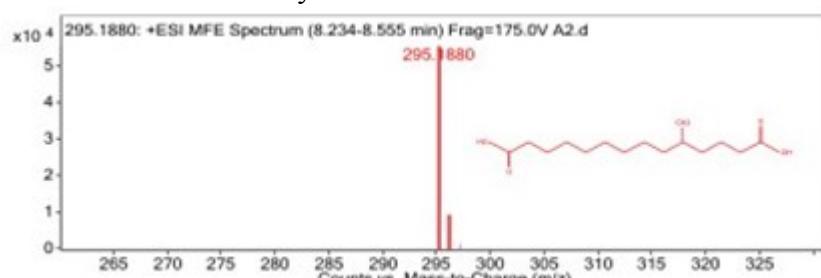
9-Keto heptadecylic acid



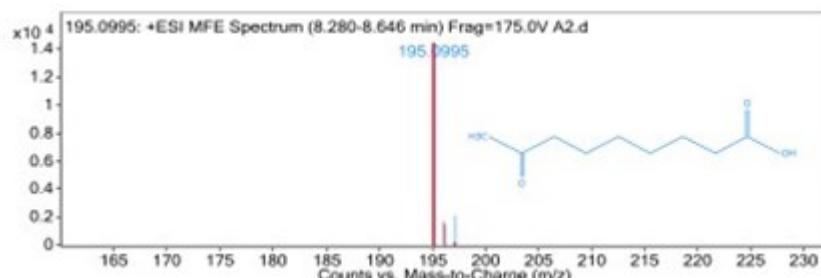
9-dodecynoic acid



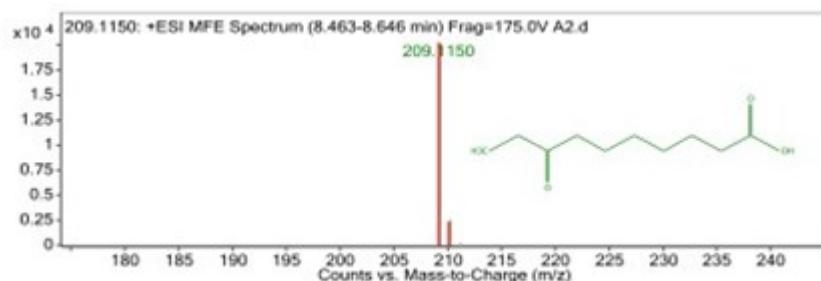
5-methyl-tetradecanedioic acid



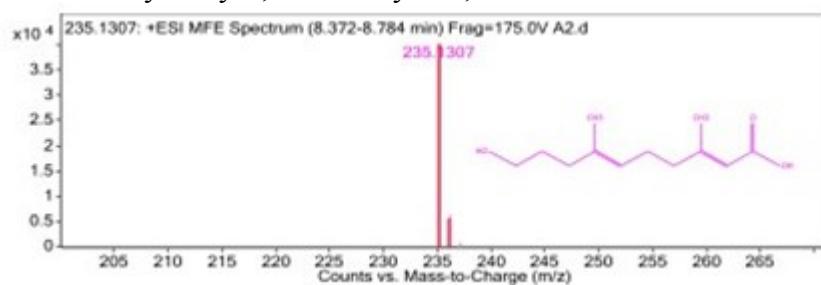
8-oxo-nonanoic acid



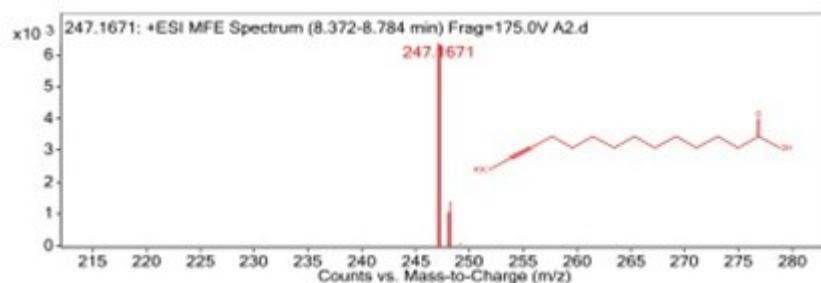
8-oxo capric acid



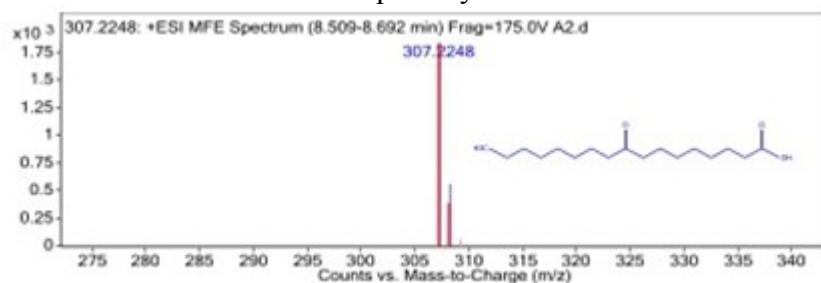
10-Hydroxy-3,7-dimethyl-2E,6E-decadienoic acid



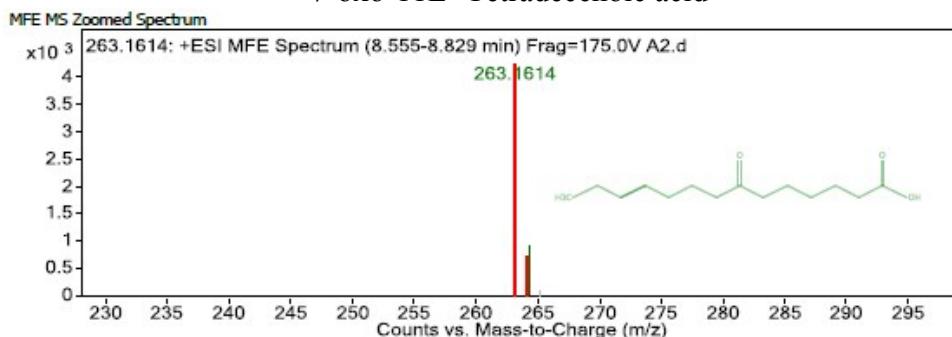
12-tetradecynoic acid



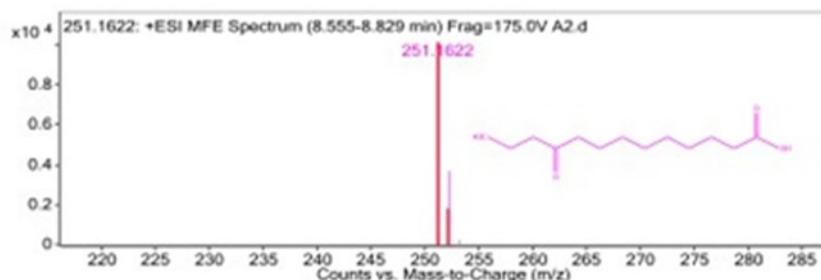
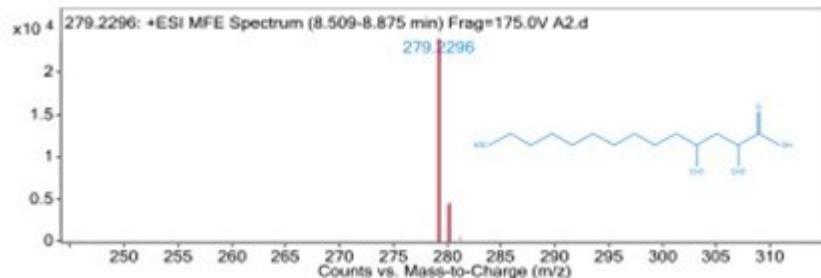
9-Keto heptadecyclic acid



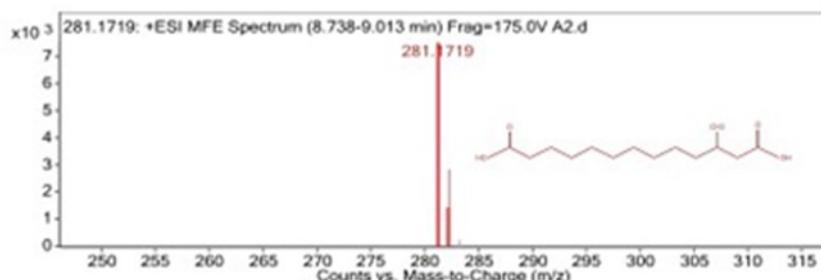
7-oxo-11E- Tetradecenoic acid



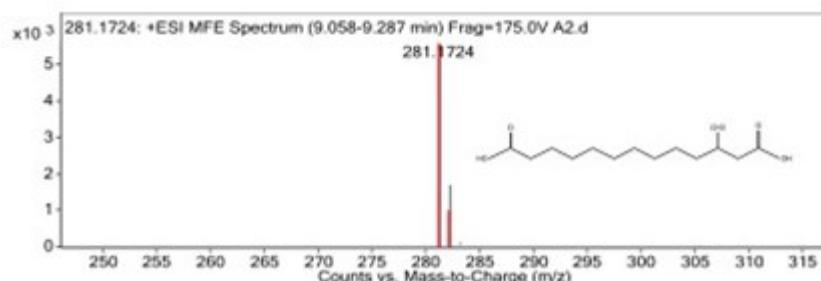
2,4-dimethyl-tetradecanoic acid



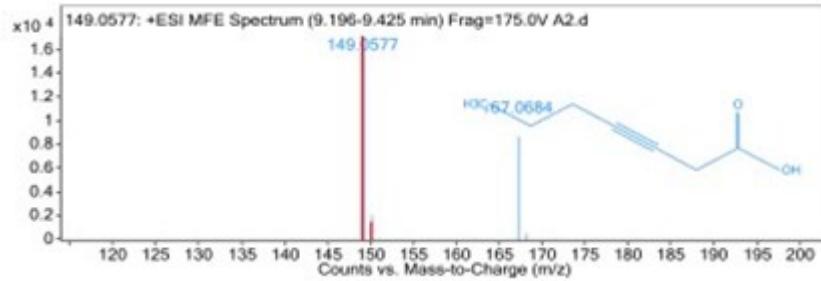
3-methyl-tridecanedioic acid



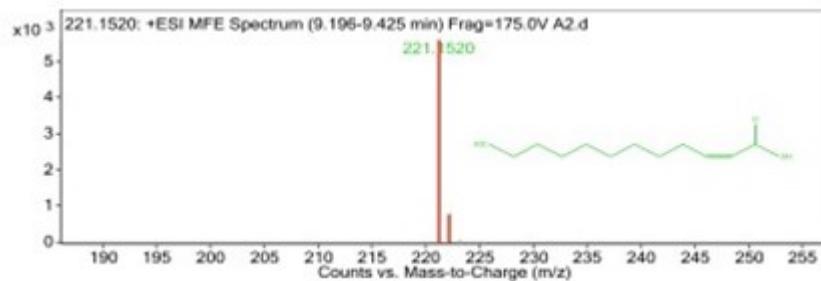
3-methyl-tridecanedioic acid



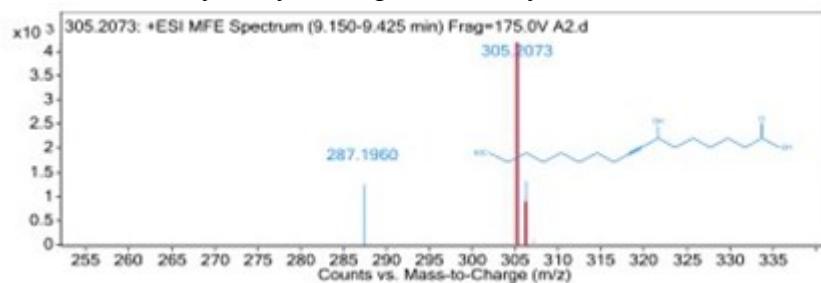
3-heptynoic acid



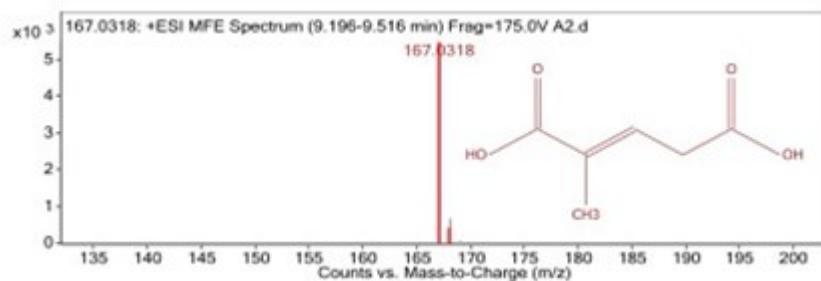
2Z-dodecenoic acid



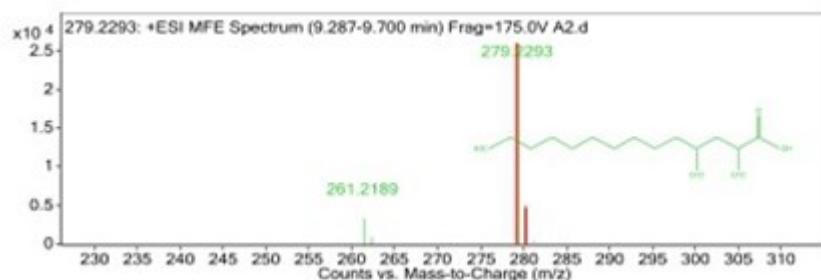
7-hydroxy-10-heptadecen-8-yonic acid



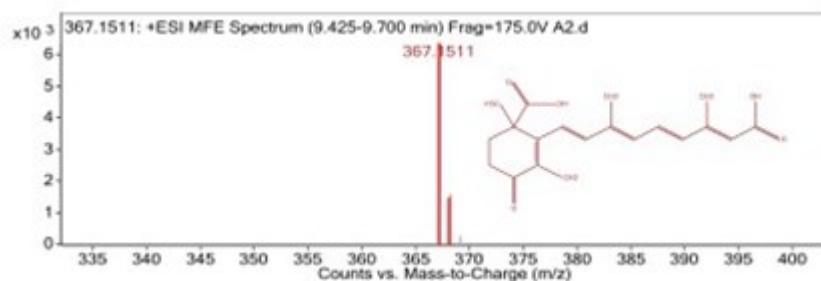
(E)-2-Methylglutaconic acid



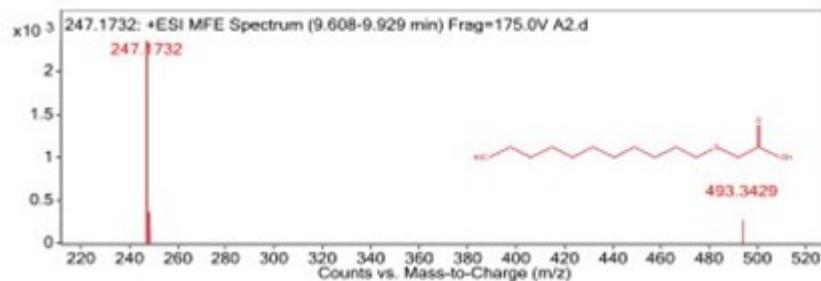
2,4-dimethyl-tetradecanoic acid



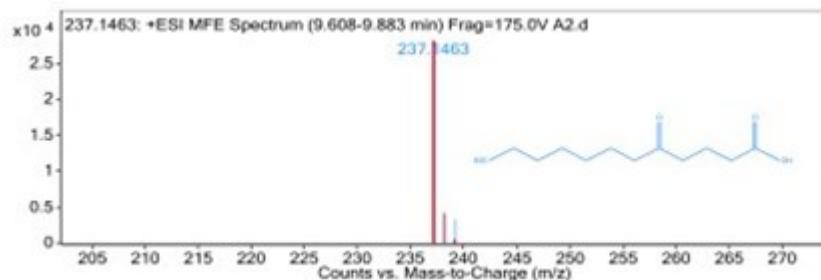
16-Hydroxy-4-carboxyretinoic acid



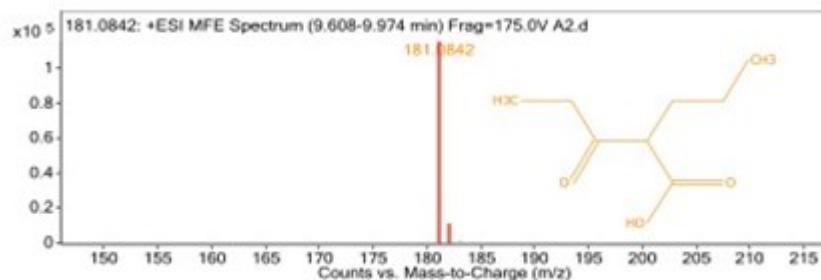
3-Thiatetradecanoic Acid



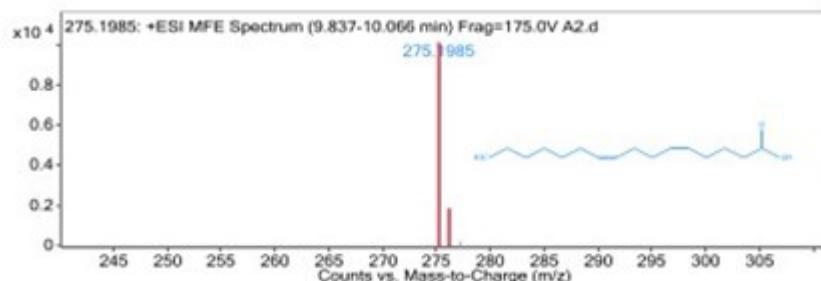
5-Oxododecanoic acid



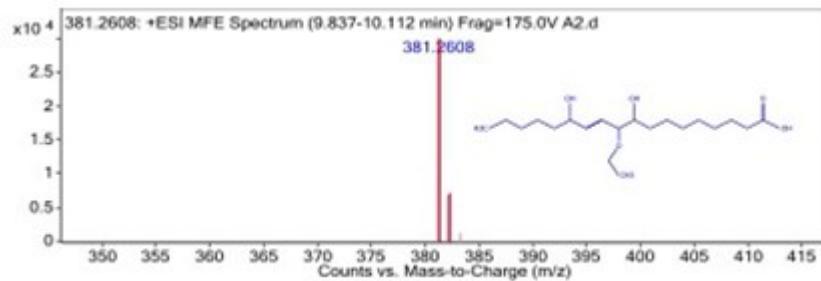
3-Oxoalproic acid



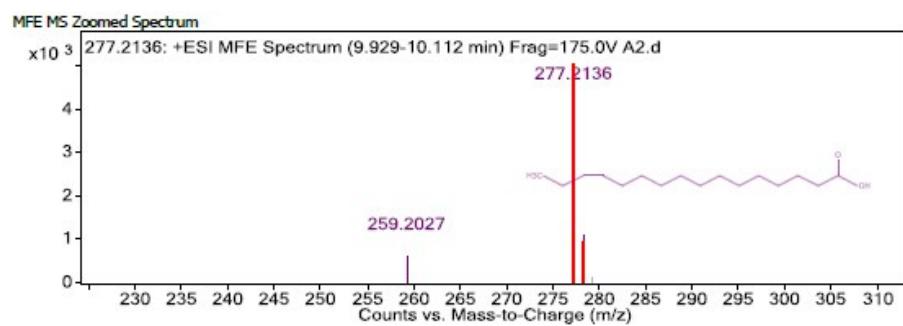
5Z,9Z-hexadecadienoic acid



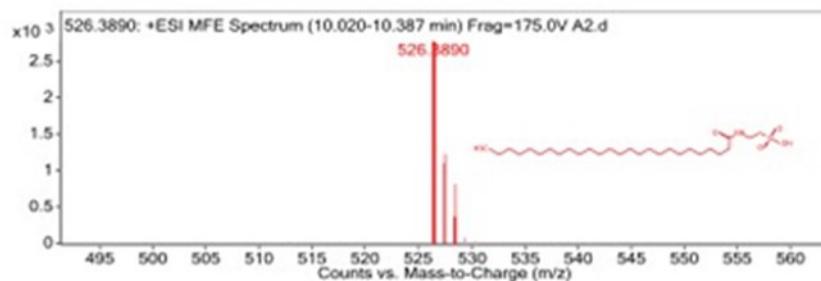
9,13-dihydroxy-10- ethoxy-11- octadecenoic acid



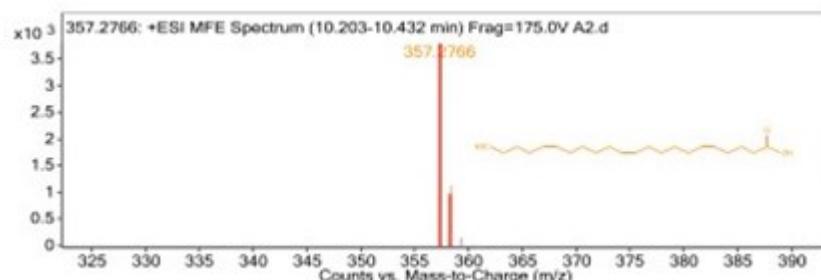
13Z-hexadecenoic acid



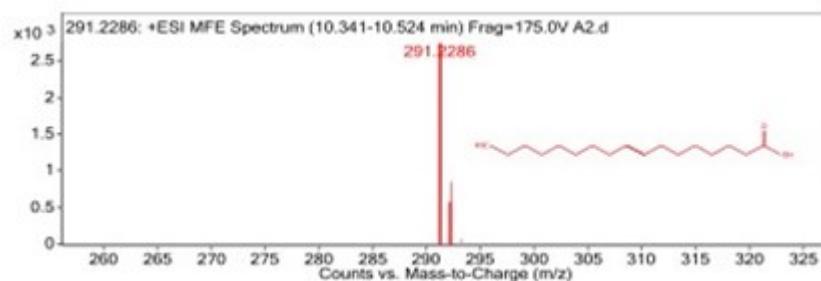
2-hexacosanamidoethanesulfonic acid



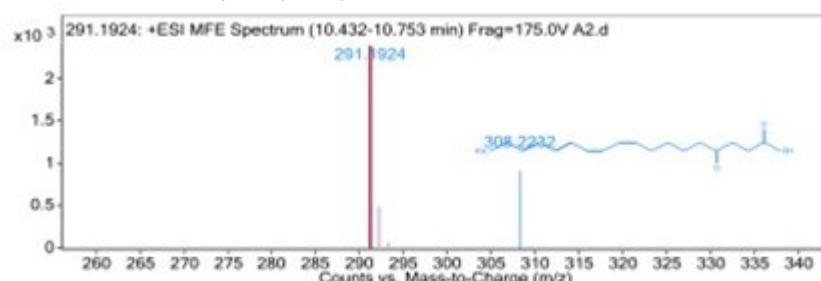
5Z,11Z,17Z-docosatrienoic acid



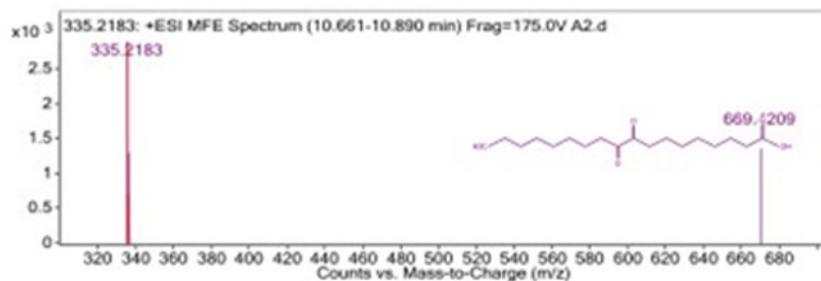
8E-heptadecenoic acid



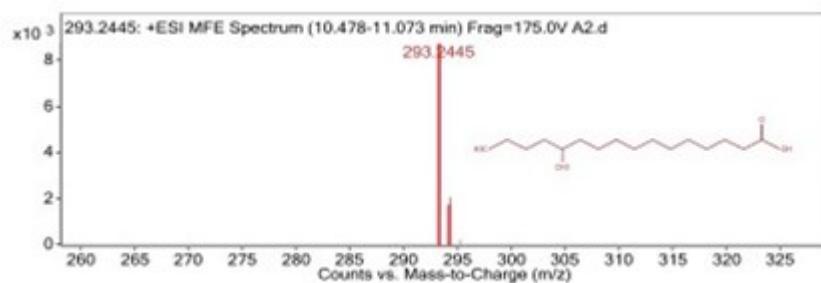
4-oxo-9Z,11Z,13E,15E-octadecatetraenoic acid



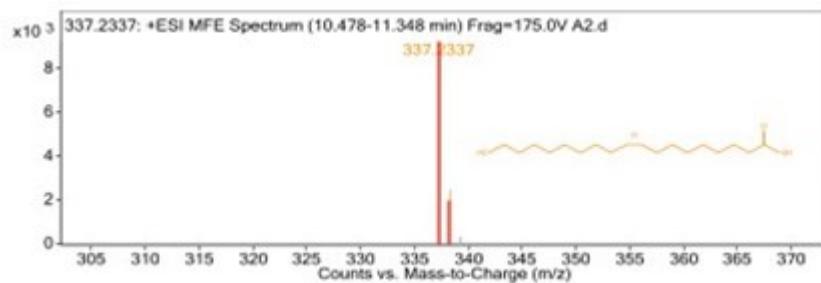
9,10-dioxo-octadecanoic acid



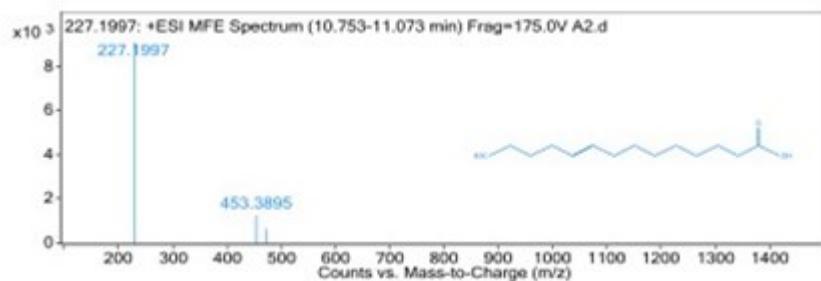
12-methyl-hexadecanoic acid



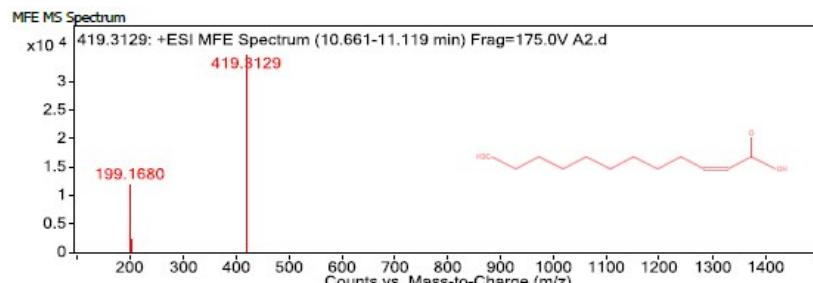
18-hydroxy-9S,10R- epoxy-stearic acid



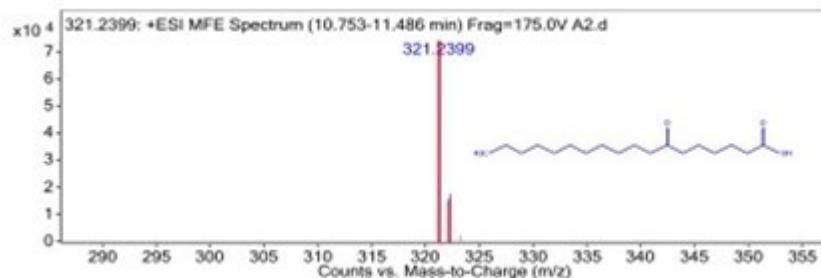
9E-tetradecenoic acid



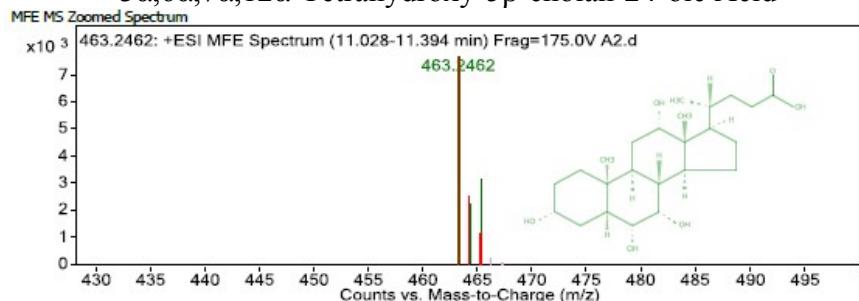
2Z-dodecenoic acid



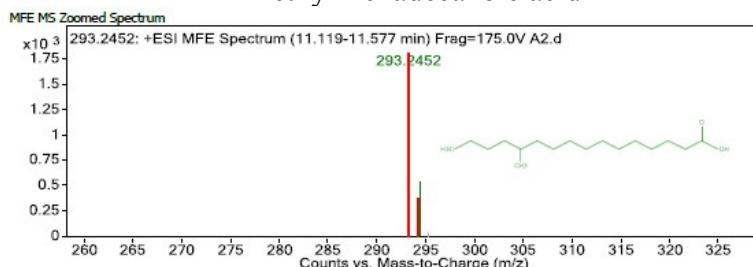
7-keto-stearic acid



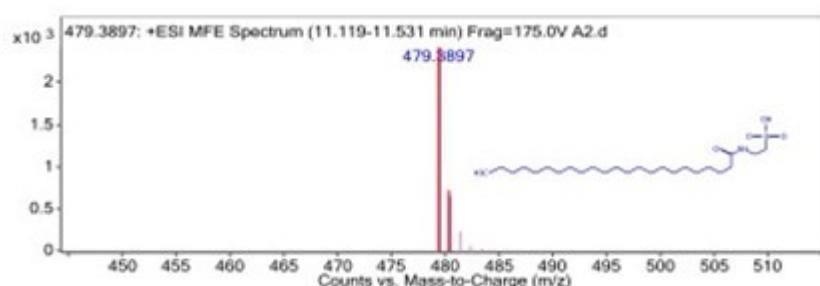
3 α ,6 α ,7 α ,12 α -Tetrahydroxy-5 β -cholan-24-oic Acid



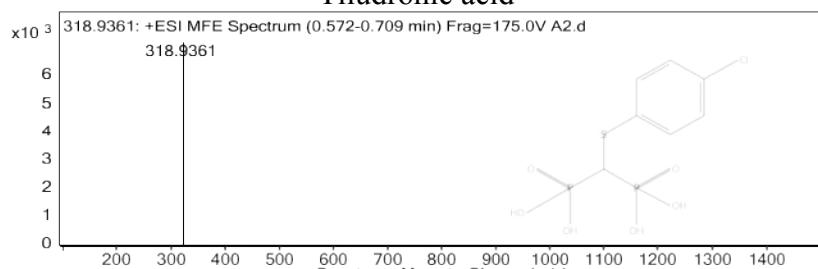
12-methyl-hexadecanoic acid



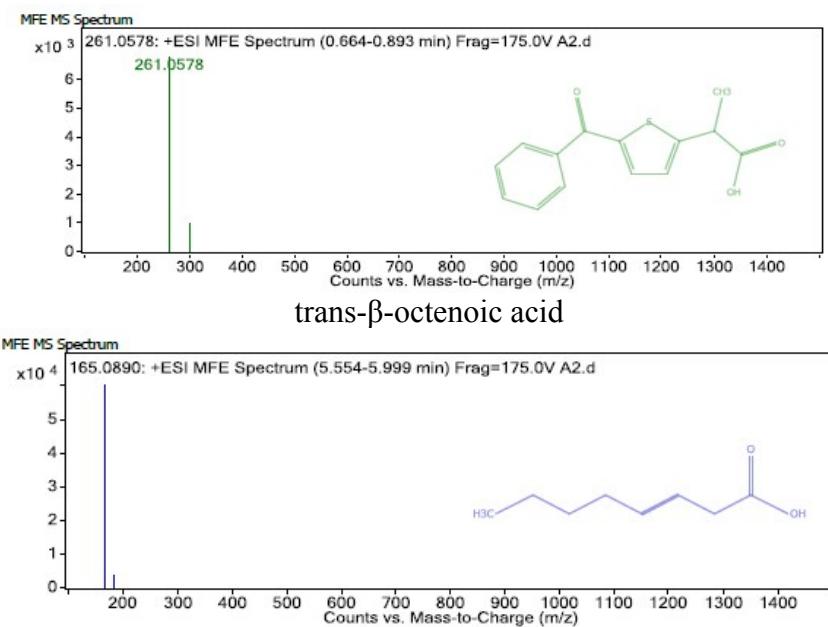
2-Tricosanamidoethanesulfonic acid



Tiludronic acid

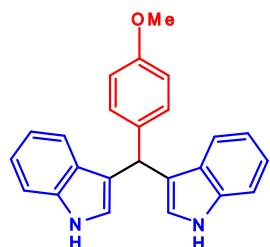


Tiaprofenic acid



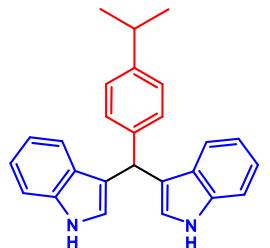
Spectroscopic data and copies of FT-IR, ¹H NMR & ¹³C NMR of isolated compounds:

3, 3`-(4-Methoxyphenyl)methylenebisindole (table 2, entry 3a)



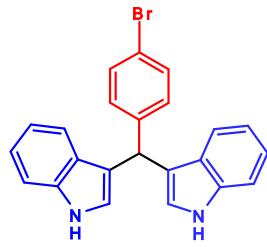
FTIR ν_{\max} = 3399, 3052, 2929, 2835, 1606, 1505, 1450, 1420, 1340, 1302, 1015, 739 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.85 (s, 2H, -NH), 7.31-7.39 (m, 4H, Ar-H), 7.25 (s, 1H, Ar-H), 7.23 (d, J = 2.2 Hz, 1H, Ar-H), 7.14 (ddd, J = 8.1 Hz, 7.0 Hz & 1.1 Hz, 2H, Ar-H), 6.98 (ddd, J = 8.1 Hz, 7.0 Hz & 1.1 Hz, 2H, Ar-H), 6.8 (m, 2H, Ar-H), 6.61 (dd, J = 2.5 Hz & 1.1 Hz, 2H, Ar-H), 5.82 (s, 1H, -CH), 3.76 (s, 3H, -OCH₃) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 157.8, 136.6, 136.2, 129.5, 127.0, 123.4, 121.8, 120.0, 119.9, 119.1, 113.5, 110.9, 55.2, 39.3 ppm.

3, 3`-(4-Isopropylphenyl)methylenebisindole (table 2, entry 3b)



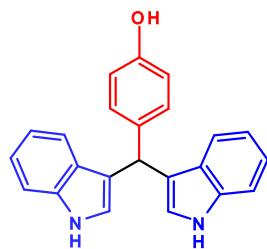
FTIR ν_{\max} = 3402, 3051, 2956, 2838, 1606, 1548, 1453, 1244, 1089, 795, 745, 597 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.7 (s, 2H, -NH), 7.38 (d, J = 4.5 Hz, 2H, Ar-H), 7.30 (d, J = 4.5 Hz, 2H, Ar-H), 7.23 (d, J = 3.0 Hz, 2H, Ar-H), 7.09-7.17 (m, 4H, Ar-H), 6.9-7.01 (m, 2H, Ar-H), 6.60 (d, J = 1.5 Hz, 2H, Ar-H), 5.8 (s, 1H, -CH), 2.8 (m, 1H, -CH), 1.21 (d, 6H, -CH₃) ppm; ¹³C NMR (100 MHz, CDCl₃): 145.4, 141.2, 136.6, 128.4, 127.0, 126.3, 123.5, 121.5, 121.8, 119.9, 119.1, 110.9, 54.1, 36.4, 22.4 ppm.

3,3`-((4-Bromophenyl)methylene)bis(1H-indole) (table 2, entry 3c)



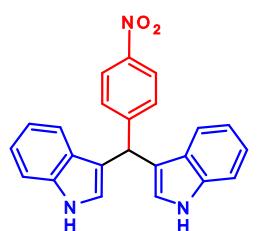
FTIR ν_{max} = 3402, 3058, 2924, 2854, 1617, 1457, 1010 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.9 (s, 2H, -NH), 7.45 (d, J = 2.2 Hz, 2H, Ar-H), 7.43 (d, J = 8Hz, 2H, Ar-H), 7.35 (d, J = 8.1Hz, 2H, Ar-H), 7.0 (ddd, J = 8.0 Hz, 6.9 Hz & 1.1 Hz, 2H, Ar-H), 6.62 (d, J = 2.3 Hz, 2H, Ar-H), 5.83 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 143.0, 136.6, 131.2, 130.5, 126.8, 123.6, 122.1, 119.9, 119.8, 119.3, 119.0, 111.0, 39.6 ppm.

3,3'-(4-Hydroxyphenyl)methylenabisindole (table 2, entry 3d)



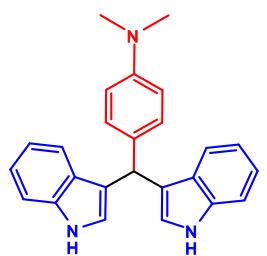
FTIR ν_{max} = 3435, 3398, 3051, 2838, 1605, 1508, 1171, 1086, 1046, 792, 744 cm⁻¹; ¹H NMR (300 MHz, CDCl₃+DMSO-d₆): δ 10.4 (brs, 1H, -OH), 9.36 (s, 2H, -NH), 7.25-7.35 (m, 4H, Ar-H), 6.86-7.08 (m, 4H, Ar-H), 6.84 (d, J = 8.2 Hz, 2H, Ar-H), 6.67-6.82 (d, J = 8.2 Hz, 2H, Ar-H), 6.60 (s, 2H, Ar-H), 5.69 (s, 1H, -CH) ppm; ¹³C NMR (75.5 MHz, CDCl₃): δ 154.1, 134.2, 131.7, 131.0, 127.3, 123.5, 122.6, 121.2, 118.4, 114.8, 113.5, 110.7, 57.7 ppm.

3,3'-(4-Nitrophenyl)methylenabisindole (table 2, entry 3e)



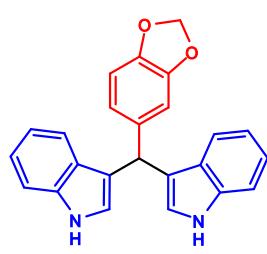
FTIR ν_{max} = 3429, 3055, 1599, 1519, 1457, 1359 cm⁻¹; ¹H NMR (400 MHz, CDCl₃+DMSO-d₆): δ 10.2 (s, 2H, -NH), 8.01 (dd, J = 8.3 Hz & 2.7 Hz, 2H, Ar-H), 7.48 (dd, J = 8.4 Hz, 2H, Ar-H), 7.36 (dd, J = 8 Hz, 2H, Ar-H), 7.19 (d, J = 7.1 Hz, 2H, Ar-H), 6.98-7.03 (m, 2H, Ar-H), 6.6-6.8 (m, 4H, Ar-H), 5.88 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 145.1, 137.1, 127.6, 128.0, 127.2, 126.7, 125.1, 121.8, 119.9, 118.1, 111.7, 110.9, 31.6 ppm.

3,3'-(P-dimethylaminophenyl)methylenabisindole (table 2, entry 3f)



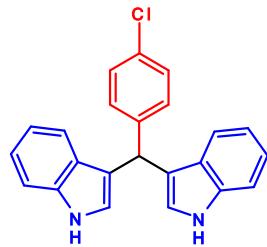
FTIR ν_{max} = 3402, 3049, 2956, 1652, 1595, 1451, 1420, 1228, 1166, 1088, 1011, 931, 849, 742cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.90 (s, 2H, -NH), 7.41 (d, J = 7.9 Hz, 2H, Ar-H), 7.34 (d, J = 7.9 Hz, 2H, Ar-H), 7.13-7.25 (m, 4H, Ar-H), 7.00 (d, J = 8.3 Hz, 2H, Ar-H), 6.66 (d, J = 8.4 Hz, 4H, Ar-H), 5.8 (s, 1H, -CH), 3.9 (s, 6H, -NCH₃); ¹³C NMR (100 MHz, CDCl₃): δ 149.0, 136.7, 132.3, 129.2, 127.2, 123.5, 121.7, 120.4, 120.0, 119.0, 112.6, 110.9, 110.9, 40.8, 40.0, 39.1 ppm.

3,3'-(benzo[d][1,3]dioxol-5-ylmethylene)bis(1H-indole) (table 2, entry 3g)



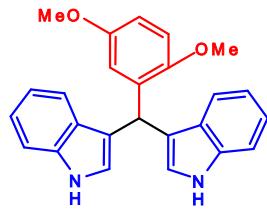
FTIR ν_{max} = 3410, 3055, 1485, 1336, 1242, 1093, 1037, 741 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.8 (brs, 2H, -NH), 7.25-7.34 (m, 4H, Ar-H), 7.08-7.20 (m, 2H, Ar-H), 6.91-6.93 (m, 2H, Ar-H), 6.72-6.78 (m, 2H, Ar-H), 6.58-6.68 (m, 3H, Ar-H), 5.6 (s, 2H, -OCH₂-), 3.2 (s, 1H, -CH) ppm; ¹³C NMR (75 MHz, CDCl₃): δ 147.8, 145.8, 138.2, 136.7, 126.7, 123.5, 121.1, 121.0, 119.7, 119.2, 119.0, 110.8, 110.4, 108.0, 101.8, 39.3 ppm.

3,3'-(4-Chlorophenyl)methylenabisindole (table 2, entry 3h)



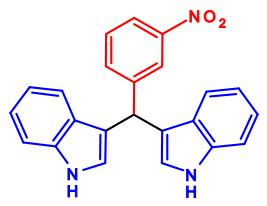
FTIR ν_{max} = 3420, 3054, 1499, 1460, 1093 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.79 (brs, 2H, -NH), 7.34 (d, J = 8.1 Hz, 4H, Ar-H), 7.25 (d, J = 5.1 Hz, 4H, Ar-H), 7.13 (m, J = 7.7 Hz, 2H, Ar-H), 6.99 (m, 2H, Ar-H), 6.55 (s, 2H, Ar-H), 5.8 (s, 1H, -CH) ppm; ¹³C NMR (75.5 MHz, CDCl₃): δ 146.0, 136.2, 133.2, 129.5, 129.4, 127.6, 123.4, 121.8, 120.7, 119.6, 119.0, 112.3, 40.2 ppm.

3, 3'-(2, 5 dimethoxyphenyl)methylenebisindole (table 2, entry 3i)



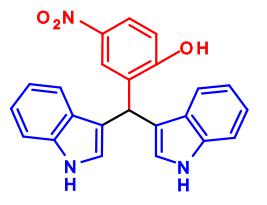
FTIR ν_{max} = 3410, 2838, 1512, 1466, 1241, 1088, 848 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.8 (s, 2H, -NH), 7.39 (d, J = 7.9 Hz, 2H, Ar-H), 7.26 (d, J = 8.1 Hz, 2H, Ar-H), 7.11 (t, J = 7.5 Hz, 2H, Ar-H), 6.97 (t, J = 7.5 Hz, 2H, Ar-H), 6.85 (d, J = 8.7 Hz, 1H, Ar-H), 6.73 (d, J = 3.1 Hz, 1H, Ar-H), 6.69 (dd, J = 8.7 Hz & 5.6 Hz, 1H, Ar-H), 6.5 (s, 2H, Ar-H), 6.3 (s, 1H, -CH), 3.76 (s, 3H, -OCH₃), 3.62 (s, 3H, -OCH₃) ppm; ¹³C NMR (75.5 MHz, CDCl₃): δ 153.4, 151.4, 136.7, 133.9, 127.2, 123.5, 121.7, 119.9, 119.3, 118.9, 116.7, 111.8, 110.9, 110.6, 56.6, 55.5, 32.1 ppm.

3, 3'-(3-Nitrophenyl)methylenebisindole (table 2, entry 3j)



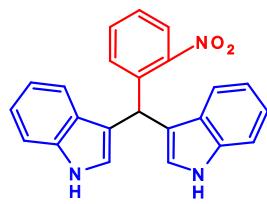
FTIR ν_{max} = 3402, 2957, 2839, 1669, 1589, 1366, 1248, 1165, 796, 742, 591 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.19 (brs, 1H, -NH), 8.05 (s, 1H, NH), 7.97 (s, 2H, Ar-H), 7.68 (d, J = 7.4 Hz, 1H, Ar-H), 7.33-7.46 (m, 4H, Ar-H), 7.17-7.26 (m, 3H, Ar-H), 7.03 (m, J = 7.4 Hz, 2H, Ar-H), 6.63 (s, 2H, Ar-H), 6.0 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃+DMSO): δ 147.6, 146.6, 136.4, 134.4, 128.5, 126.0, 123.5, 122.6, 120.8, 120.5, 118.5, 118.1, 116.6, 111.0, 39.2 ppm.

3, 3'-(2-Hydroxyl, 5-Nitrophenyl)methylenebisindole (table 2, entry 3k)



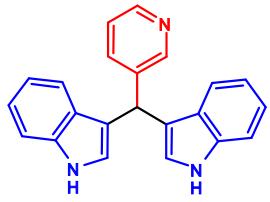
FTIR ν_{max} = 3426, 3312, 3047, 1590, 1531, 1460, 1363 cm⁻¹; ¹H NMR (300 MHz, CDCl₃+DMSO-*d*₆): δ 10.4 (brs, 1H, -OH), 9.9 (s, 2H, -NH), 7.82-7.87 (m, 2H, Ar-H), 7.47-7.48 (m, 4H, Ar-H), 7.27 (d, J = 7.2 Hz, 2H, Ar-H), 6.80-7.02 (m, 3H, Ar-H), 6.63 (s, 2H, Ar-H), 6.2 (s, 1H, -CH) ppm; ¹³C NMR (75.5 MHz, CDCl₃): δ 150.0, 140.9, 136.5, 127.4, 125.8, 125.4, 122.9, 122.4, 120.4, 119.5, 119.1, 116.7, 112.1, 111.0, 49.8 ppm.

3, 3'-(2-Nitrophenyl)methylenebisindole (table 2, entry 3l)



FTIR ν_{max} = 3413, 3055, 1521, 1456, 1352, 1095 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.0 (brs, 2H, -NH), 7.82 (m, 2H, Ar-H), 7.32-7.42 (m, 2H, Ar-H), 7.14 (d, J = 7.9 Hz, 2H, Ar-H), 7.28 (d, J = 7.9 Hz, 2H, Ar-H), 7.08-7.17 (m, 4H, Ar-H), 6.66 (s, 2H, Ar-H), 6.7 (s, 1H, -CH) ppm; ¹³C NMR (75.5 MHz, CDCl₃): δ 150.0, 138.5, 136.1, 132.5, 130.7, 128.2, 127.7, 124.4, 124.0, 121.9, 120.1, 120.0, 118.7, 111.2, 35.7 ppm.

3,3'-(3-pyridyl)methylenebis(1H-indole) (table 2, entry 3m)



FTIR ν_{max} = 3448, 3029, 2780, 1677, 1699, 904, 718 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ 9.1 (brs, 2H, -NH); 8.60-8.61 (m, 1H, Ar-H), 8.37-8.39 (m, 1H, Ar-H), 7.25-7.37 (m, 6H, Ar-H), 7.02-7.06 (m, 2H, Ar-H), 6.84-6.88 (m, 4H, Ar-H), 5.9 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 155.1, 137.8, 137.8, 132.7, 130.9, 128.0, 127.4, 124.8, 121.7, 119.5, 118.7, 112.4, 33.6 ppm.

3-[(Furan-2-yl)(1H-indol-3-yl)methyl]-1H-indole (table 2, entry 3n)



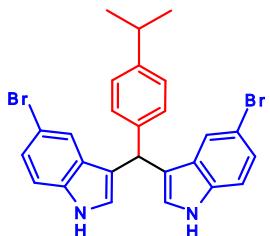
FTIR ν_{max} = 742, 783, 1008, 1454, 3053, 3412 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.9 (brs, 2H, -NH), 7.48 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.35-6.96 (m, 7H, Ar-H), 6.83 (s, 2H, Ar-H), 6.28 (s, 1H, Ar-H), 6.0 (s, 1H, Ar-H), 5.93 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 157.0, 141.8, 136.3, 126.4, 122.1, 120.8, 118.8, 117.1, 115.6, 111.4, 110.2, 105.7, 33.6 ppm.

3, 3'-Phenylmethylenebisindole (table 2, entry 3o)



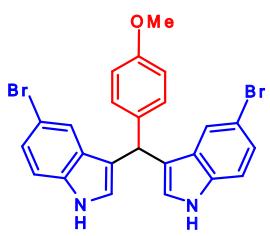
FTIR ν_{max} = 3412, 3056, 1616, 1455, 1417, 1337, 1093, 1010, 744 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.36 (brs, 2H, -NH), 7.25-7.32 (d, *J* = 2.4 Hz, 2H, Ar-H), 7.19-7.24 (m, 2H, Ar-H), 7.17-7.19 (m, 4H, Ar-H), 7.11-7.16 (m, 3H, Ar-H), 6.97 (ddd, *J* = 8.0 Hz, 6.7 Hz & 1.3 Hz, 2H, Ar-H), 6.5 (dd, *J* = 2.4 Hz & 1.3 Hz, 2H, Ar-H), 5.8 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 144.7, 136.2, 128.9, 127.8, 127.6, 127.5, 124.1, 123.8, 122.7, 120.5, 119.9, 119.5, 111.7, 40.7 ppm.

5-bromo-3-((5-bromo-1H-indol-3-yl)(4-isopropylphenyl)methyl)-1H-indole (table 2, entry 3p)



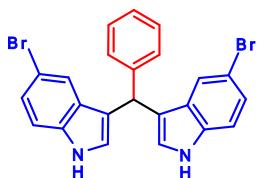
FTIR ν_{max} = 3400, 3100, 2841, 1679, 581 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 9.96 (s, 2H, -NH), 7.76 (s, 2H, Ar-H), 7.28 (d, *J* = 8.2 Hz, 2H, Ar-H), 7.25 (d, *J* = 8.2 Hz, 2H, Ar-H), 7.22 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.18 (d, *J* = 8.0 Hz, 2H, Ar-H), 6.48 (s, 2H, Ar-H), 5.7 (s, 1H, -CH), 2.8-2.9 (m, 1H, -CH), 1.26 (d, *J* = 6.9 Hz, -CH₃, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 141.9, 134.8, 133.2, 128.3, 127.4, 126.5, 123.8, 122.1, 121.7, 116.3, 112.7, 111.6, 38.4, 32.5, 22.8 ppm.

5-bromo-3-((5-bromo-1H-indol-3-yl)(4-methoxyphenyl)methyl)-1H-indole (table 2, entry 3q)



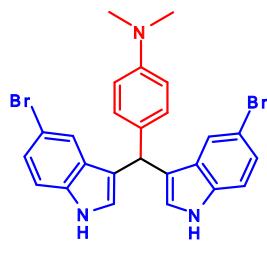
FTIR ν_{max} = 3400, 3100, 2840, 1681, 580 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.0 (s, 2H, -NH), 7.45 (s, 2H, Ar-H), 7.22-7.25 (m, 2H, Ar-H), 7.21 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.18 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.82 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.61 (s, Ar-H, 2H), 5.68 (s, 1H, -CH), 3.78 (s, 3H, -OCH₃) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 142.4, 134.6, 133.3, 129.2, 128.4, 125.8, 124.5, 123.5, 120.3, 117.7, 111.8, 108.6, 55.6, 40.3 ppm.

5-bromo-3-((5-bromo-1H-indol-3-yl)(phenyl)methyl)-1H-indole (table 2, entry 3r)



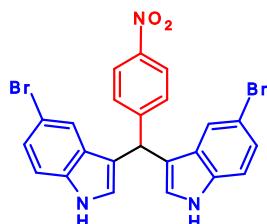
FTIR ν_{max} = 3405, 2910, 2370, 1718, 1560, 1441, 1217, 1099, 872, 704 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.0 (s, 2H, -NH), 7.52 (d, *J* = 2.1 Hz, 2H, Ar-H), 7.50 (m, Ar-H, 3H), 7.20-7.30 (m, 6H, Ar-H), 6.64 (d, *J* = 2.1 Hz, 2H, Ar-H), 5.75 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 138.4, 135.2, 129.7, 129.1, 128.7, 126.8, 123.9, 121.5, 121.3, 116.0, 113.3, 112.8, 55.3 ppm.

4-(bis(5-bromo-1H-indol-3-yl)methyl)-N,N-dimethylbenzenamine (table 2, entry 3s)



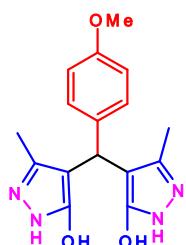
FTIR ν_{max} = 3415, 3142, 2856, 2903, 1679, 581 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.0 (s, 2H, -NH), 7.74 (m, 2H, Ar-H), 7.49 (m, 2H, Ar-H), 7.12-7.26 (d, J = 7.5 Hz, 1H, Ar-H), 6.64-6.71 (m, 5H, Ar-H), 6.49 (s, 1H, Ar-H), 5.7 (s, 1H, Ar-H), 3.08 (d, -NCH₃, 3H), 2.92 (s, -NCH₃, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 146.0, 135.5, 130.2, 129.9, 128.9, 127.1, 121.9, 121.4, 117.3, 114.1, 113.3, 112.5, 55.2, 40.2 ppm.

5-bromo-3-((5-bromo-1H-indol-3-yl)(4-nitrophenyl)methyl)-1H-indole (table 2, entry 3t)



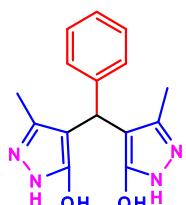
FTIR ν_{max} = 3390, 3167, 2822, 2900, 1686, 1534, 1330, 587 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 8.15 (s, 2H, -NH), 8.08 (d, J = 8.0 Hz, 2H, Ar-H), 7.42-7.45 (m, Ar-H, 4H), 7.24-7.29 (m, 4H, Ar-H), 6.65 (s, 2H, Ar-H), 5.85 (s, 1H, -CH) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 145.2, 144.1, 135.3, 130.2, 129.7, 128.7, 121.9, 121.6, 121.3, 116.2, 113.1, 112.3, 54.9 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(4-methoxyphenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7a)



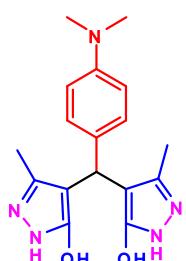
FTIR ν_{max} = 3661, 3261, 2624, 2361, 1589, 1508, 1234, 1020, 788, 740 cm⁻¹; ¹H NMR (300 MHz, DMSO-d₆): δ 10.2-12.5 (brs, 4H, -NH,-OH), 7.00-7.03 (d, J = 8.4 Hz, 2H, Ar-H), 6.74-6.77 (d, J = 8.4 Hz, 2H, Ar-H), 4.79 (s, 1H, -CH), 3.67 (s, 3H, -OCH₃), 2.05 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-d₆): δ 161.1, 157.2, 139.6, 135.3, 128.4, 113.1, 104.5, 54.9, 31.9, 10.4 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(phenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7b)



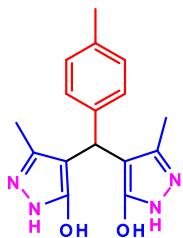
FTIR ν_{max} = 3051, 2908, 2723, 2528, 1626, 1531, 1492, 1380, 1202 cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆): δ 11.26 (brs, 4H, -NH,-OH), 7.19-7.27 (m, 2H, Ar-H), 7.07-7.18 (m, 3H, Ar-H), 4.84 (s, 1H, -CH), 2.07 (s, 6H, CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-d₆): δ 161.4, 143.8, 140.5, 128.3, 127.9, 126.0, 104.3, 33.2, 10.9 ppm.

4-((4-(dimethylamino)phenyl)(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7c)



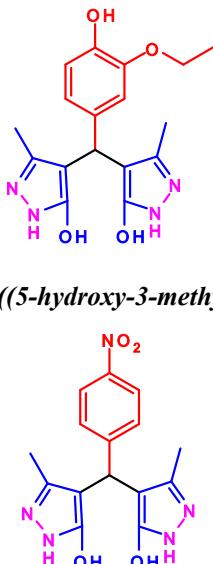
FTIR ν_{max} = 3639, 3106, 2362, 2324, 1699, 1511, 1467, 1124, 786, 745 cm⁻¹; ¹H NMR (300 MHz, DMSO-d₆): δ 11.36 (brs, 4H, -NH, -OH), 6.92 (d, J = 7.5 Hz, 2H, Ar-H), 6.56 (d, J = 7.5 Hz, 2H, Ar-H), 4.67 (s, 1H, -CH), 2.79 (s, -NCH₃, 3H), 2.64 (s, -NCH₃, 3H), 2.04 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-d₆): δ 161.0, 148.6, 139.7, 131.5, 127.9, 112.3, 104.6, 46.5, 26.7, 10.5 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(p-tolyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7d)



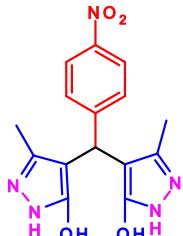
FTIR ν_{max} = 3449, 3124, 2920, 2729, 1703, 1600, 1516, 1464, 1393 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 9.5-12.5 (brs, 4H, -OH, -NH), 6.99 (d, *J* = 8.0 Hz, 4H, Ar-H), 4.75 (s, 1H, -CH), 2.21 (s, 6H, CH₃), 2.05 (s, 3H, -CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 161.3, 141.2, 140.3, 133.9, 127.9, 127.1, 105.5, 32.2, 21.6, 10.8 ppm.

4-((3-ethoxy-4-hydroxyphenyl)(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7e)



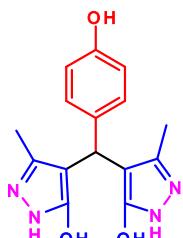
FTIR ν_{max} = 3616, 2992, 2364, 1703, 1604, 1511, 1427, 1262, 1202, 1125, 1041, 825, 752 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 11.23 (brs, 4H, -NH, -OH), 8.54 (brs, 1H -OH), 6.71 (m, 1H, Ar-H), 6.60 (d, *J* = 8.4 Hz, Ar-H) 6.49 (d, 1H, *J* = 8.4 Hz, Ar-H), 4.68 (s, 1H, -CH), 3.84 (q, 2H, *J* = 6.9 Hz, -OCH₂), 2.03 (s, 6H, 2x CH₃), 1.25 (t, *J* = 6.9 Hz, 3H, -CH₂-) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 148.1, 142.8, 139.2, 135.1, 122.1, 120.1, 116.3, 114.3, 63.9, 25.3, 14.7, 10.4 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(4-hydroxyphenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7f)



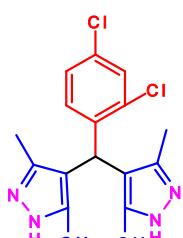
FTIR ν_{max} = 3420, 2961, 1602, 1510, 1444, 1345, 1178, 881, 802, 772 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 11.36 (brs, 4H, -NH, -OH), 8.0 (d, *J* = 8.2 Hz, 2H, Ar-H), 7.5 (d, *J* = 8.2 Hz, 2H, Ar-H), 4.99 (s, 1H, -CH), 2.10 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 160.4, 151.4, 148.1, 138.0, 127.2, 125.5, 104.3, 33.3, 11.8 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(4-hydroxyphenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7g)



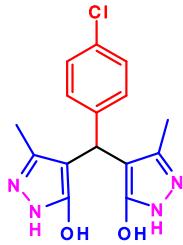
FTIR ν_{max} = 3267, 1559, 1514, 1467, 1401, 1174, 872, 788, 730 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 11.7 (brs, 4H, -NH, -OH), 9.04 (s, 1H, -OH), 6.91 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.59 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.70 (s, 1H, -CH), 2.06 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 161.4, 155.5, 139.2, 135.4, 130.4, 116.0, 115.7, 25.3, 11.8 ppm.

4-((2,4-dichlorophenyl)(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7h)



FTIR ν_{max} = 3578, 3095, 2362, 2118, 1699, 1469, 1348, 1212, 783, 693 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 7.21 (d, 1H, *J* = 4.8 Hz, Ar-H), 6.83 (dd, *J* = 8.4 Hz & *J* = 4.8 Hz, 1H, Ar-H), 6.58 (d, *J* = 7.2 Hz, 1H, Ar-H), 4.96 (s, 1H, -CH), 2.08 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 155.7, 139.2, 136.1, 135.8, 132.6, 131.4, 130.2, 125.9, 116.3, 22.4, 11.7 ppm.

4-((4-chlorophenyl)(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7i)



FTIR ν_{max} = 3225, 3089, 2975, 1604, 1540, 1496, 1302 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 11.0 (brs, 4H, -NH, -OH), 7.27 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.13 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.80 (s, 1H, -CH), 2.05 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 158.2, 144.3, 136.3, 129.8, 129.3, 127.5, 108.5, 33.6, 11.9 ppm.

4-((benzo[d][1,3]dioxol-6-yl)(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7j)



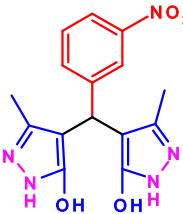
FTIR ν_{max} = 3614, 3320, 3141, 2886, 2360, 1593, 1489, 1230, 1027, 753, 662 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 9.8-12.3 (brs, 4H, -NH, -OH), 6.56-6.64 (m, 3H, Ar-H), 5.91 (s, 2H, -O-CH₂-O-), 4.70 (s, 1H, -CH), 2.06 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 148.6, 145.4, 139.1, 135.0, 131.2, 122.4, 120.2, 108.0, 107.4, 100.5, 32.5, 10.3 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(thiophen-2-yl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7k)



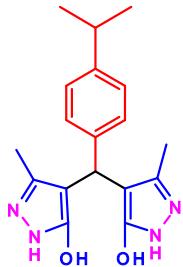
FTIR ν_{max} = 3580, 3112, 2926, 1607, 1482 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 11.36 (brs, 4H, -NH, -OH), 7.30 (d, *J* = 5.2 Hz, 1H, Ar-H), 7.05 (m, 1H, Ar-H), 6.55 (m, 1H, Ar-H), 5.27 (s, 1H, CH), 2.24 (s, 6H, CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 159.9, 136.8, 135.4, 134.9, 125.6, 118.4, 101.1, 30.8, 11.3 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(3-nitrophenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7l)



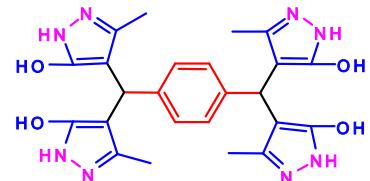
FTIR ν_{max} = 3419, 2961, 1603, 1515, 1444, 1343, 1178, 881, 806, 773 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 10.4-12.2 (brs, 4H, -NH, -OH), 8.02 (dd, 1H, *J* = 7.6 Hz & 4.0 Hz, Ar-H), 7.95 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.55-7.58 (m, 2H, Ar-H), 4.81 (s, 1H, -CH), 2.06 (s, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 148.2, 139.2, 139.0, 135.7, 135.2, 129.6, 124.2, 118.2, 116.4, 25.9, 11.4 ppm.

4-((5-hydroxy-3-methyl-1H-pyrazol-4-yl)(4-isopropylphenyl)methyl)-3-methyl-1H-pyrazol-5-ol (table 4, entry 7m)



FTIR ν_{max} = 3276, 2954, 2360, 1599, 1506, 1445, 1202, 754, 609 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 10.7-12.2 (brs, 4H, -NH, -OH), 7.01-7.07 (m, 2H, Ar-H), 4.74 (s, 1H, -CH), 2.79 (m, 1H, -CH(CH₃)), 2.07 (s, 6H, 2CH₃), 1.14 (d, 6H, 2CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 145.6, 139.02, 135.8, 135.3, 128.6, 126.2, 116.3, 36.4, 25.4, 23.5, 11.8 ppm.

4,4',4'',4'''-(1,4-phenylenebis(methanetriyl)) tetrakis (3-methyl-1H-pyrazol-5-ol) (table 4, entry 7n)



FTIR ν_{max} = 3615, 3260, 2885, 2360, 1687, 1505, 1122, 868, 735, 601 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆): δ 10.6-12.4 (brs, 8H, -NH, -OH), 6.95 (s, 4H, Ar-H), 4.68 (s, 2H, -CH), 2.05 (s, 12H, -CH₃) ppm; ¹³C NMR (75.5 MHz, DMSO-*d*₆): δ 139.3, 135.1, 135.0, 129.2, 116.4, 25.4, 11.8 ppm.

Spectral characterization of selected compounds

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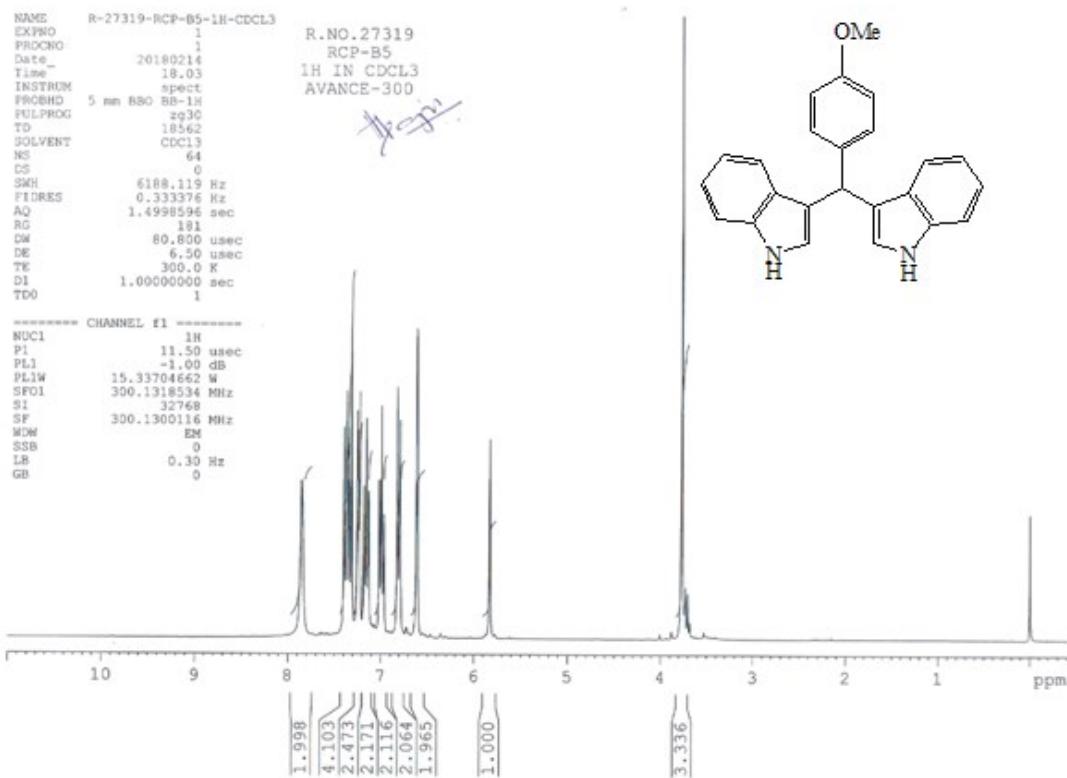
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DE      6.50 usec
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DI      1.0000000 sec
TD0      1

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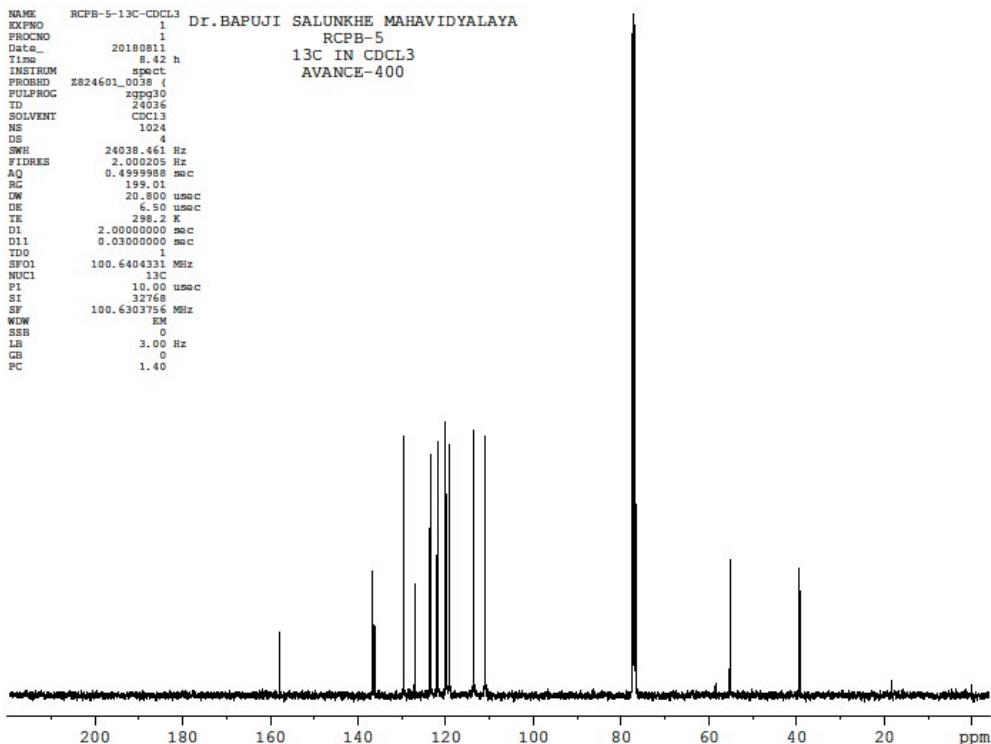
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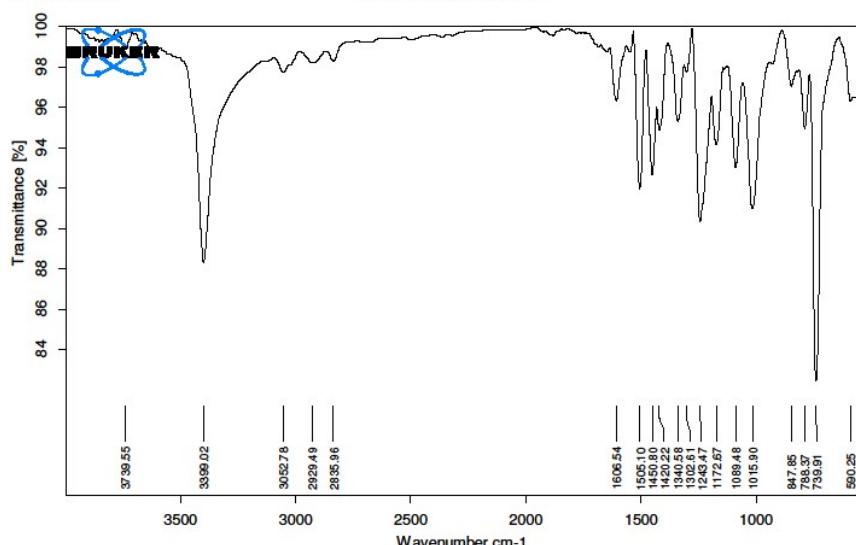
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¹³C NMR spectrum of compound 3a

ALPHA 100508

CFC SHIVAJI UNIVERSITY

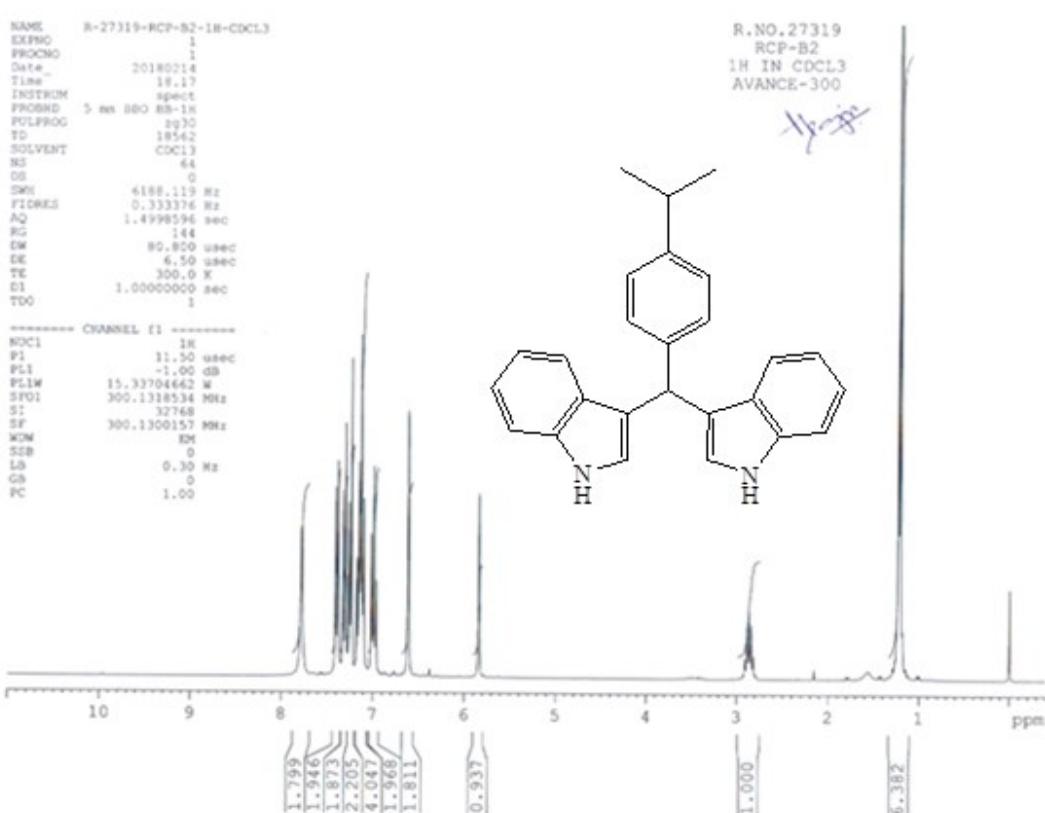


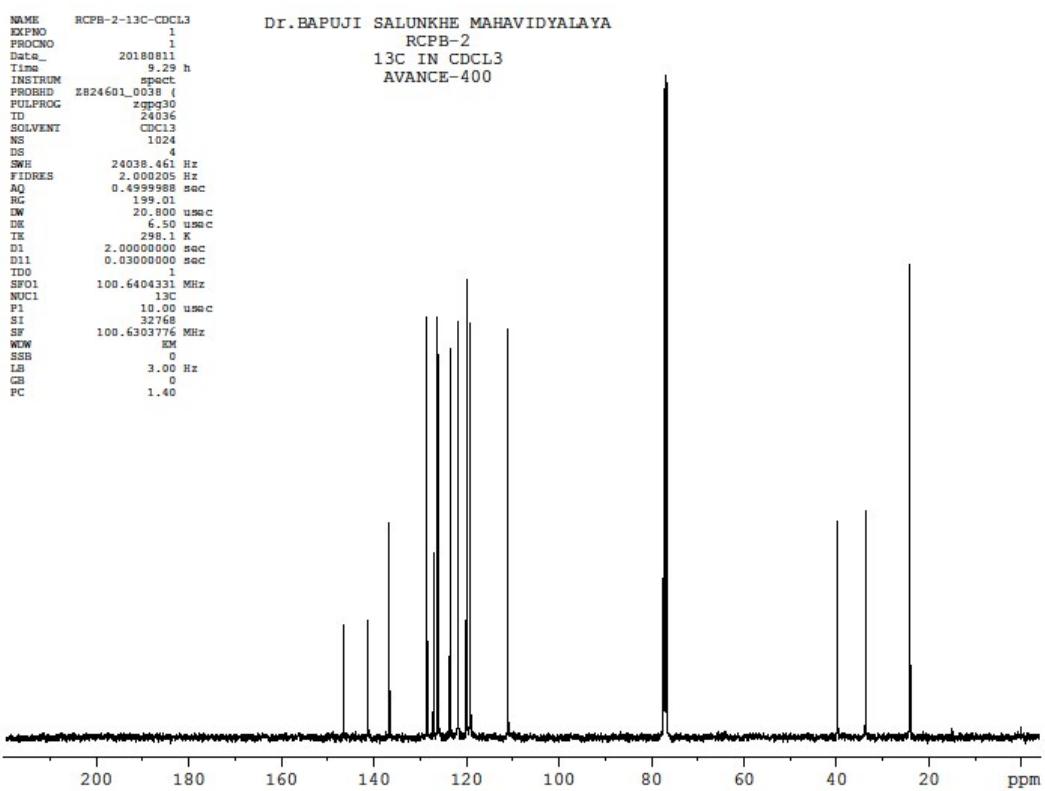
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8/4/2018

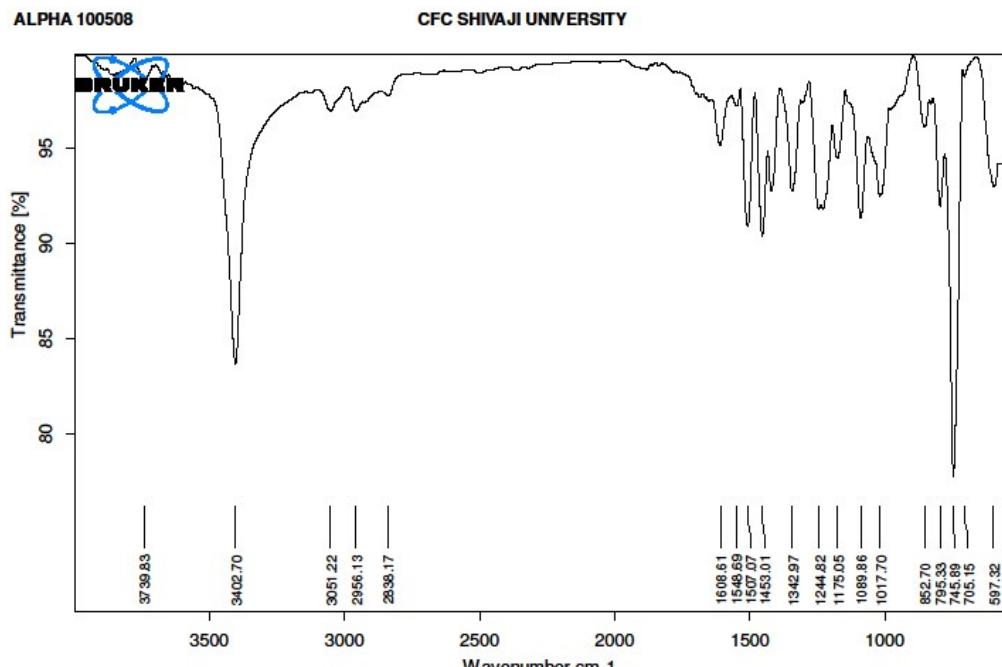
Page 1/1

FT-IR spectrum of compound 3a

¹H NMR spectrum of compound 3b

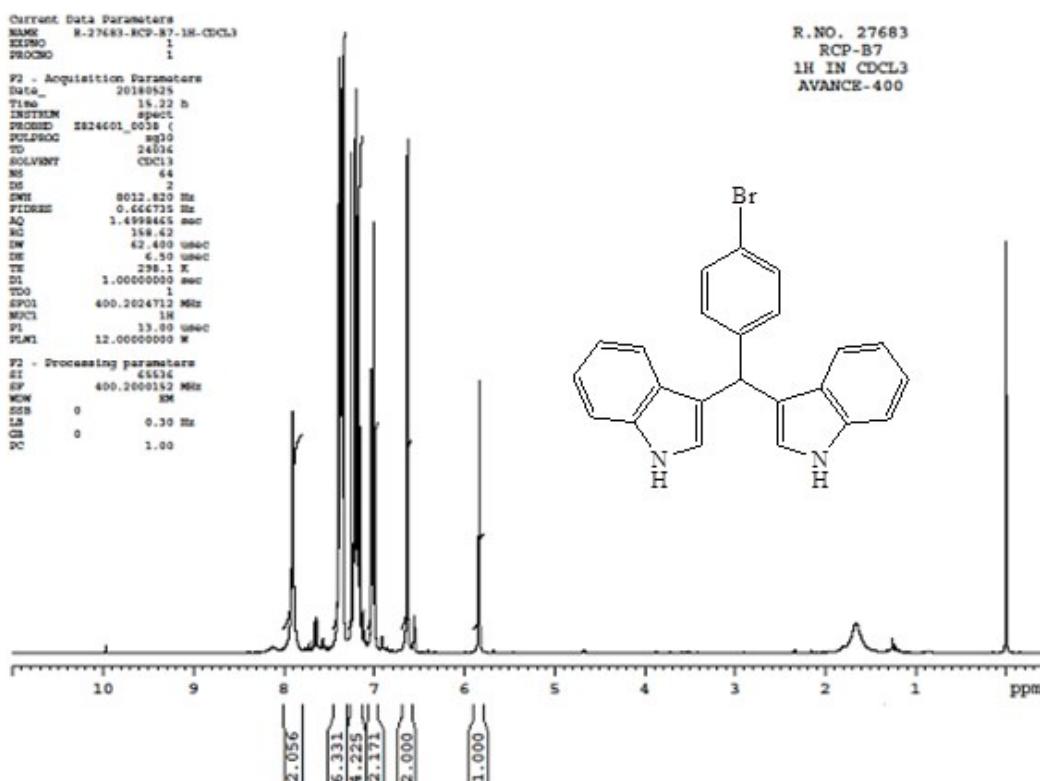


¹³C NMR spectrum of compound 3b

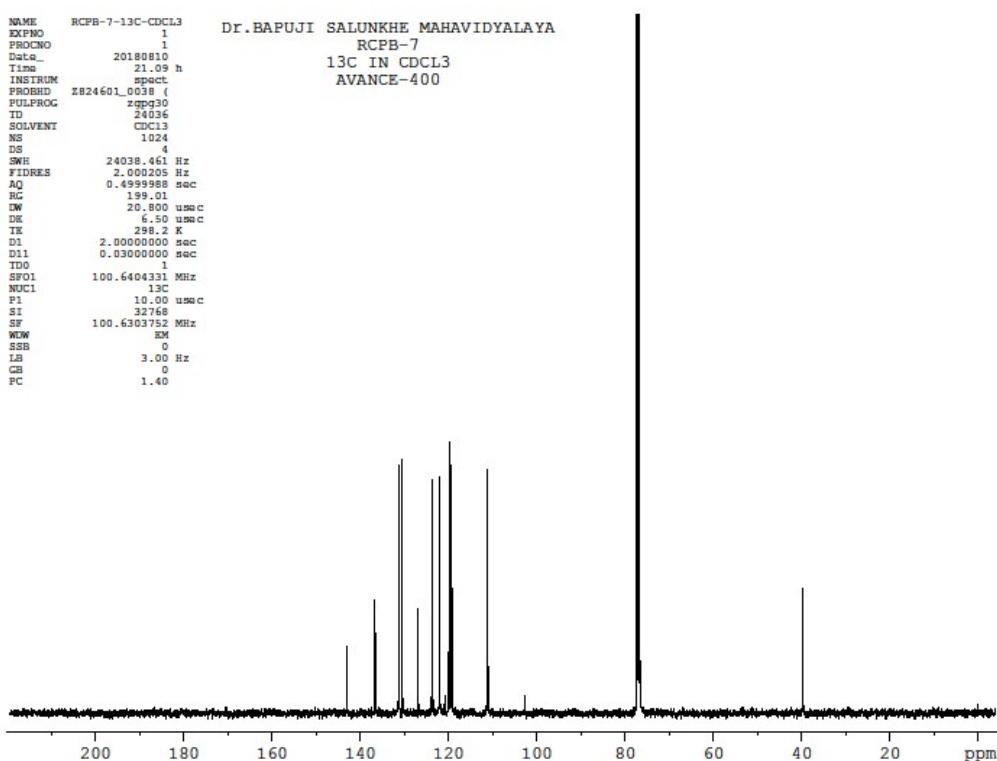


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FT-IR spectrum of compound 3b



¹H NMR spectrum of compound 3c

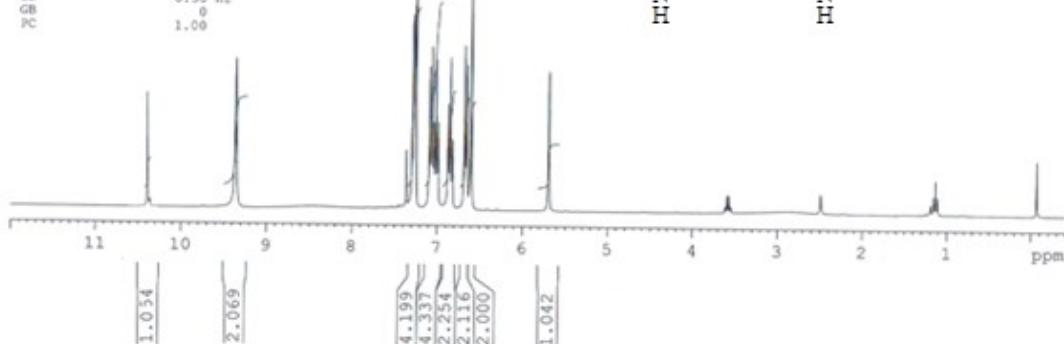
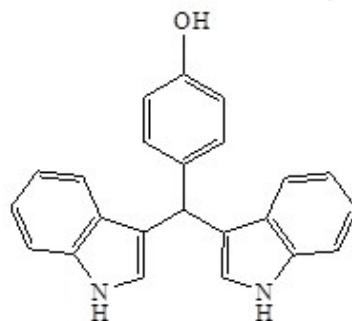


¹³C NMR spectrum of compound 3c

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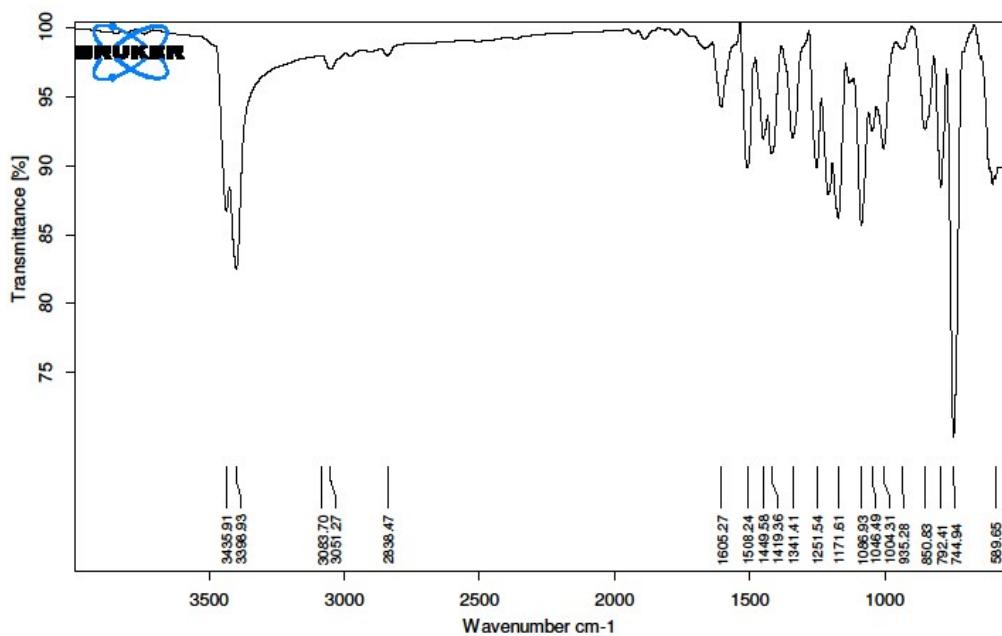
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AVANCE-300



¹H NMR spectrum of compound 3d

ALPHA 100508

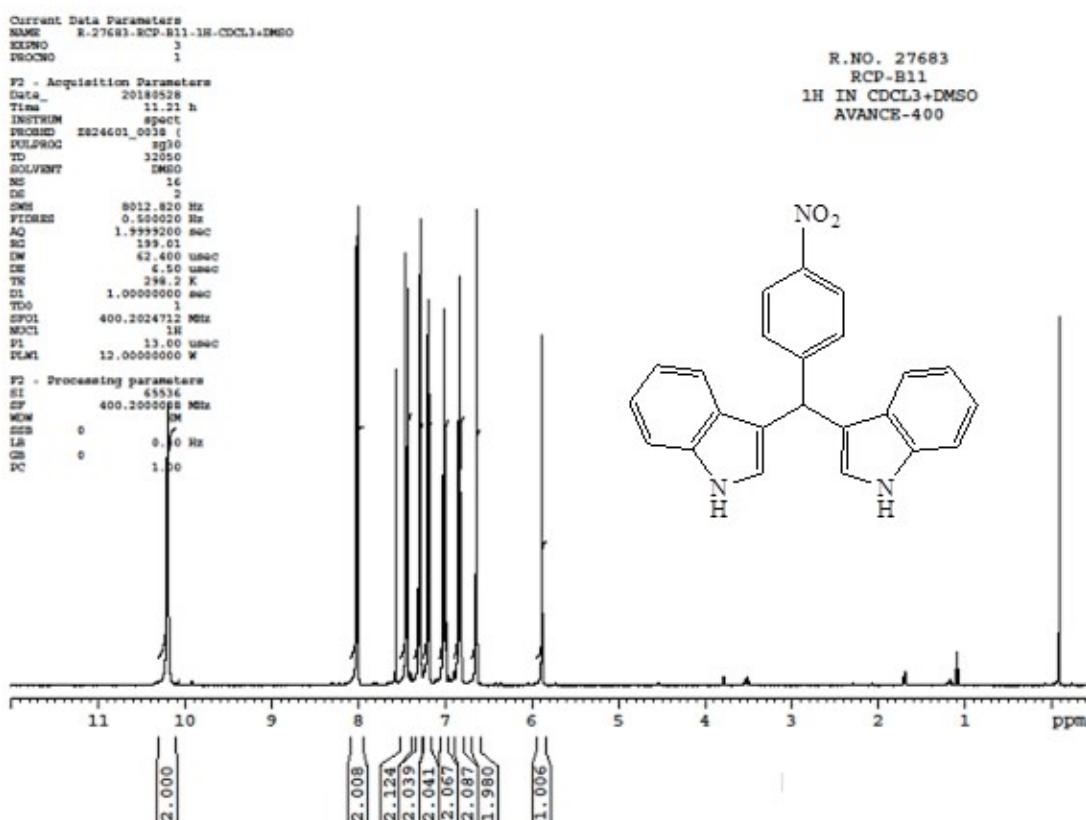
CFC SHIVAJI UNIVERSITY



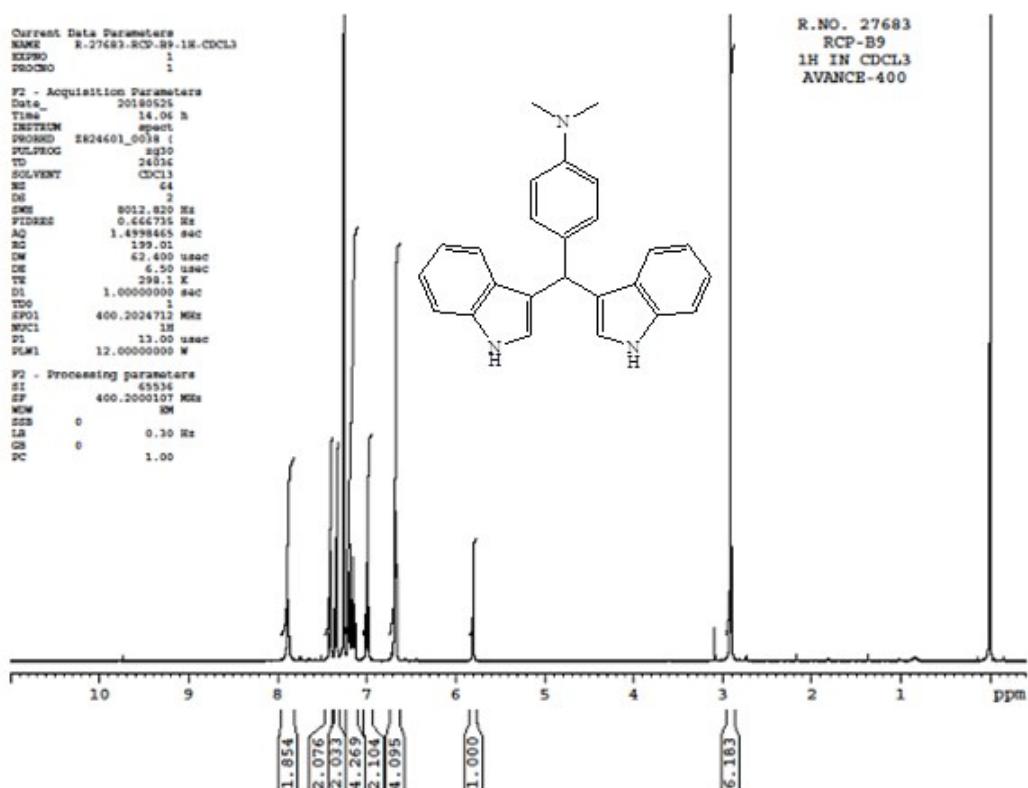
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8/4/2018

FT-IR spectrum of compound 3d



¹H NMR spectrum of compound 3e



¹H NMR spectrum of compound 3f

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DURATION 201200.1

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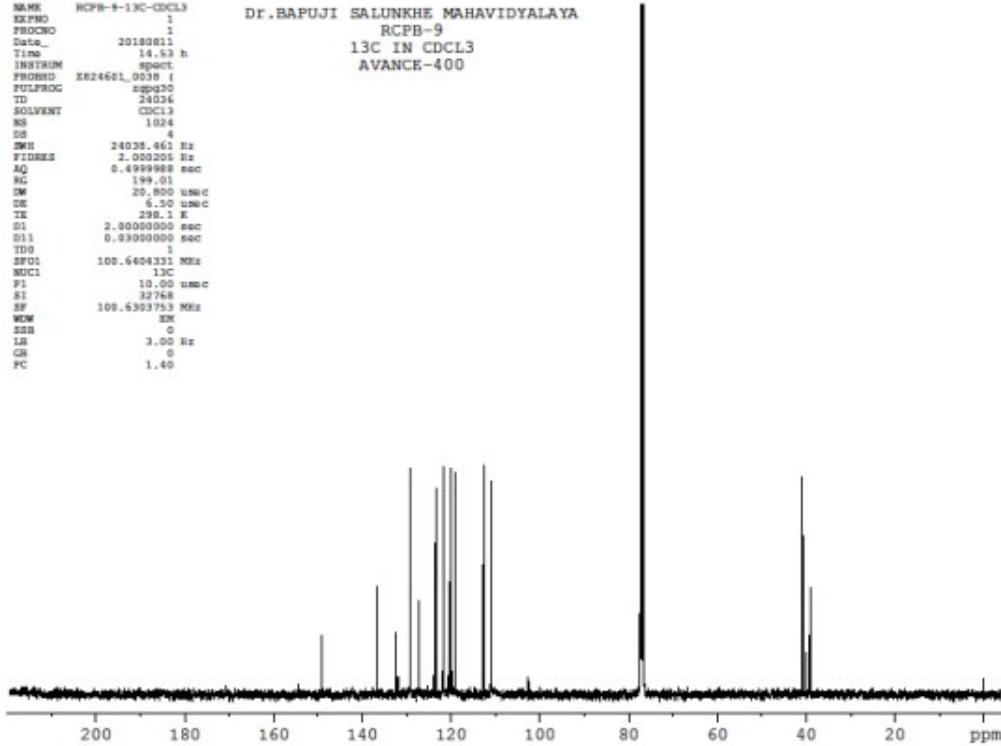
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DR.BAPUJI SALUNKHE MAHAVIDYALAYA

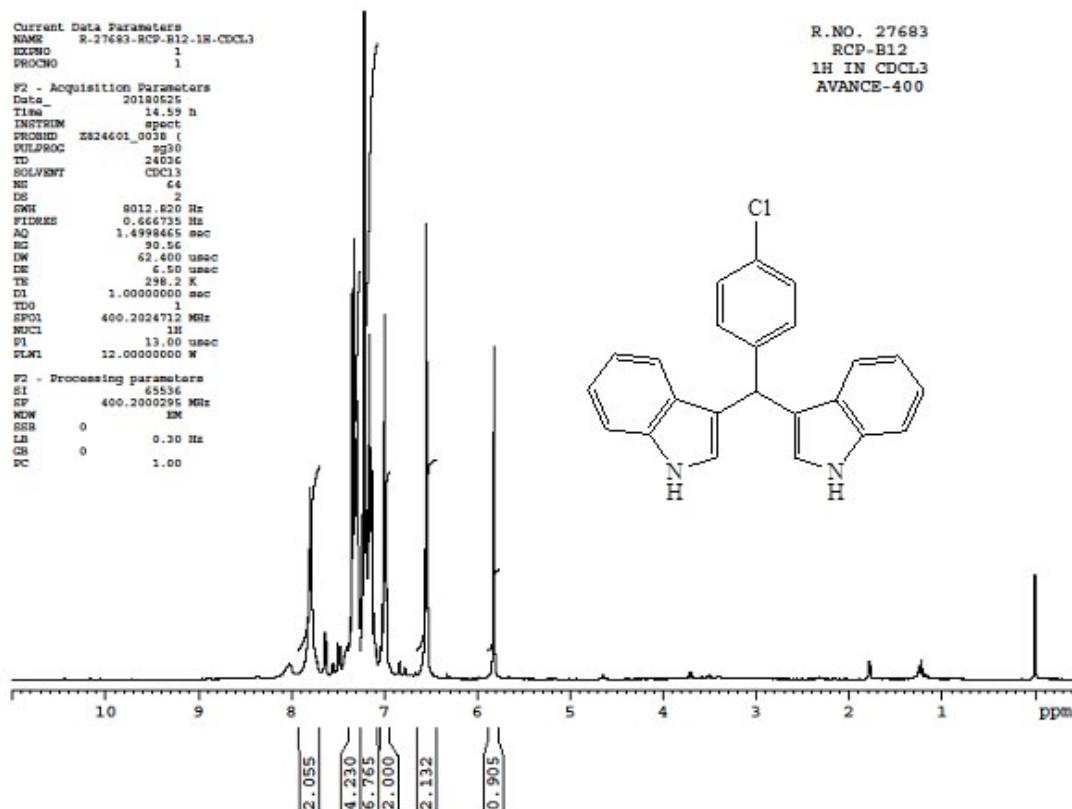
RCPB-9

¹³C IN CDCL₃

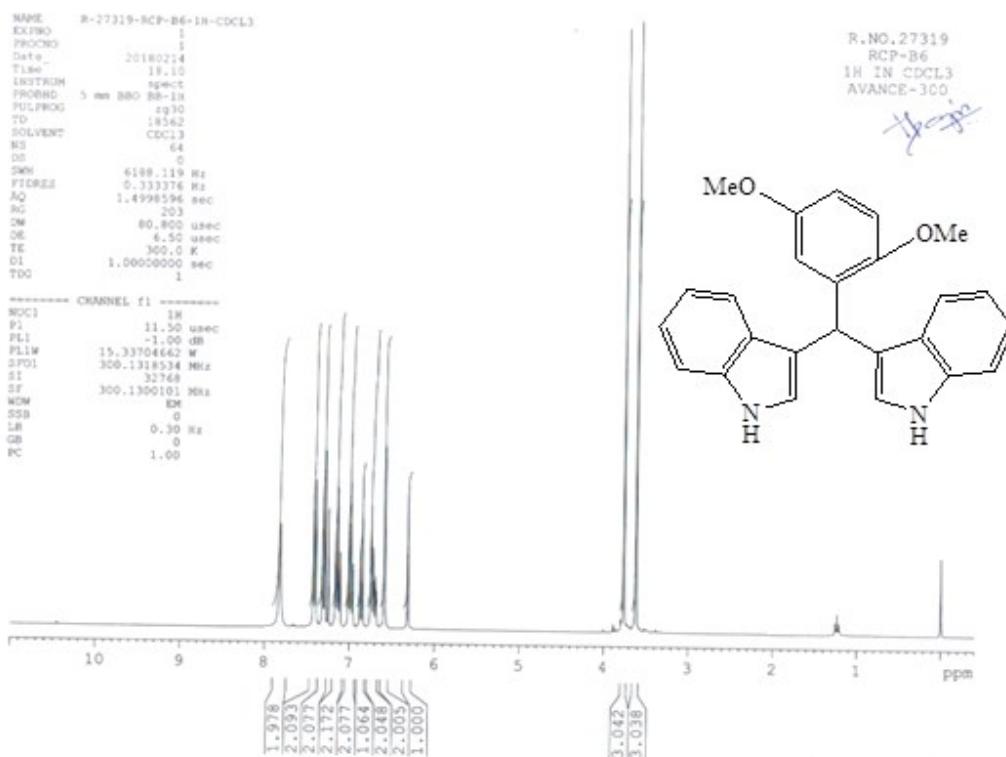
AVANCE-400



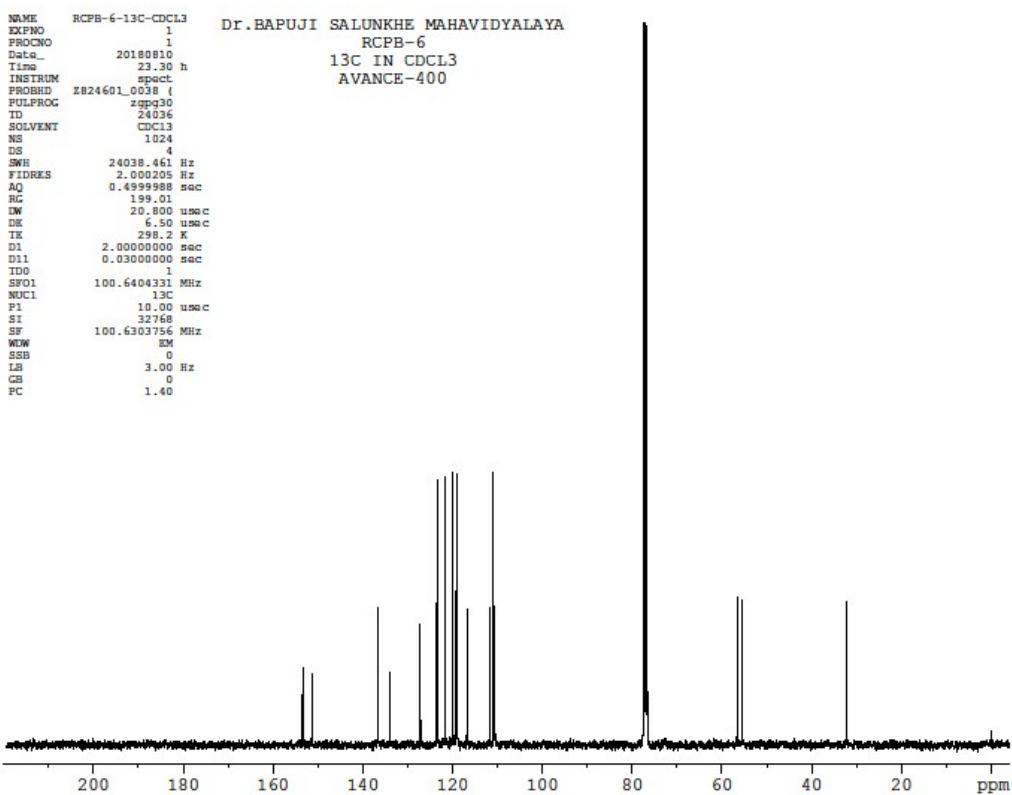
FT-IR spectrum of compound 3f



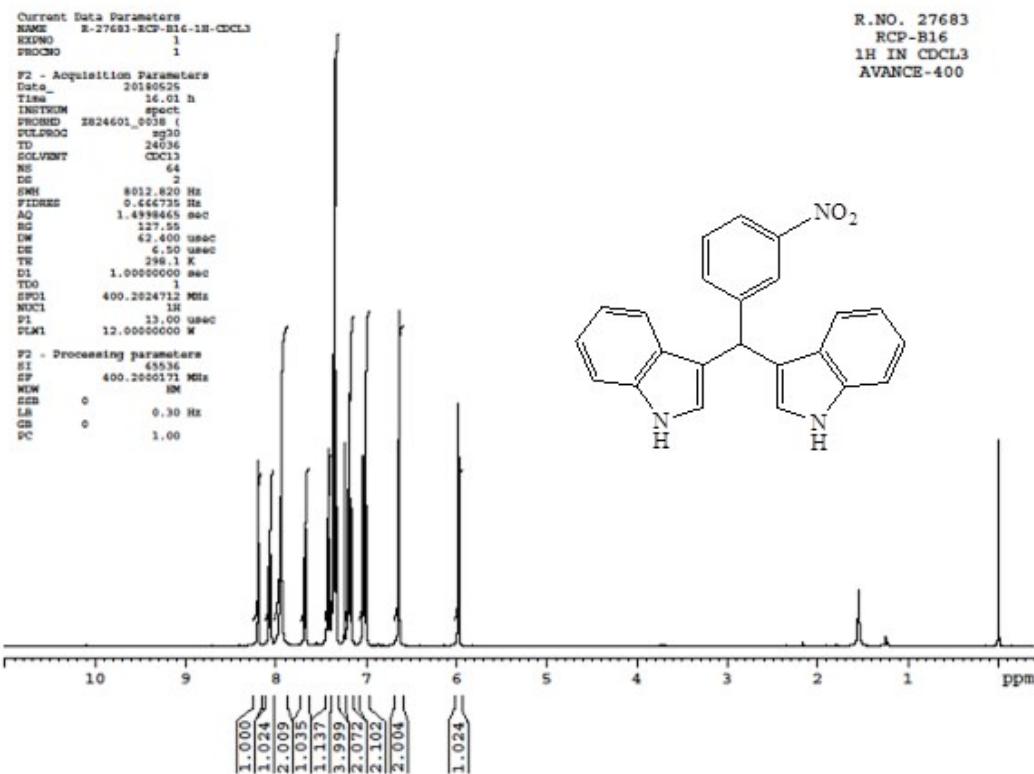
¹H NMR spectrum of compound 3h



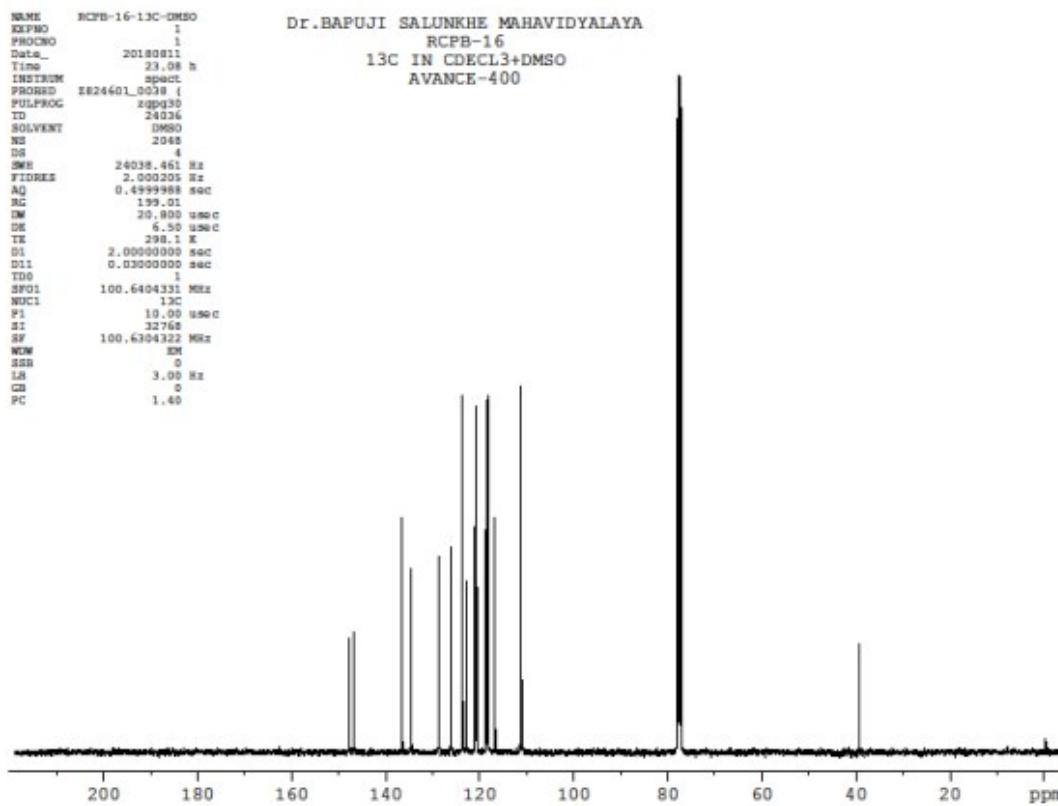
¹H NMR spectrum of compound 3i



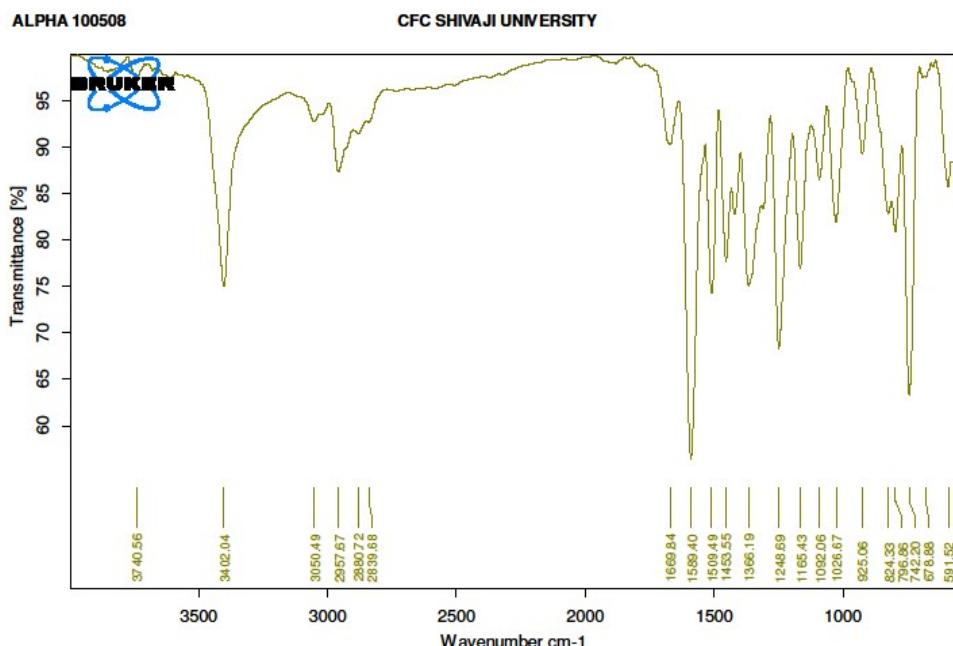
¹³C NMR spectrum of compound 3i



¹H NMR spectrum of compound 3j



¹³C NMR spectrum of compound 3j



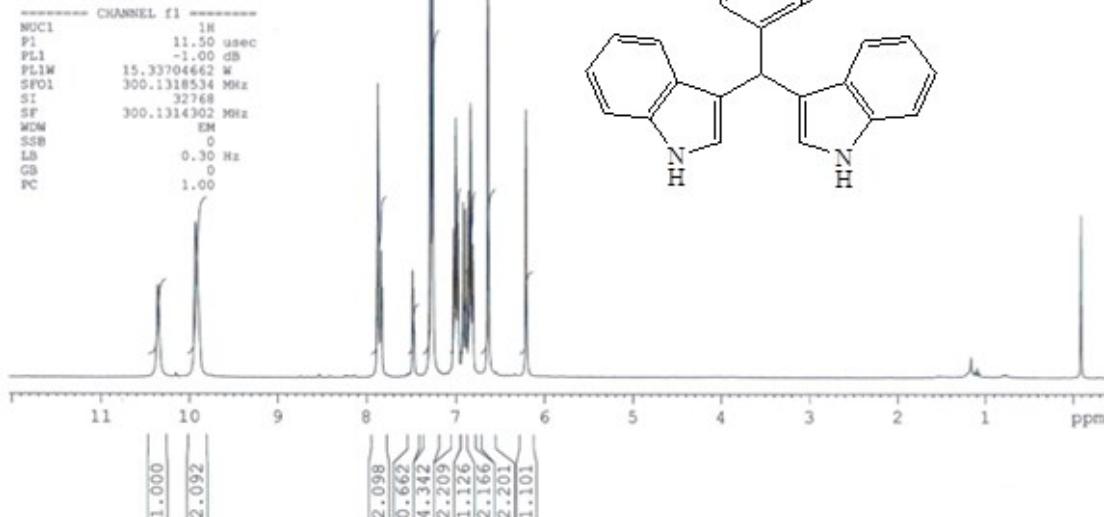
D:\FTIR DATA\Chemistry\SSP\Rupesh\RCF-B 16.0	RCP-B 16	Instrument type and / or accessory	8/4/2018
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Page 1/1

FT-IR spectrum of compound 3j

NAME R-27319-RCP-B8-1H-CDCl₃+DMSO
 EXPNO 1
 PROCN0 1
 Date 20180215
 Time 11.52
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 39998
 SOLVENT CDCl₃+DMSO
 NS 64
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.250012 Hz
 AQ 1.9999501 sec
 RG 228
 DW 50.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

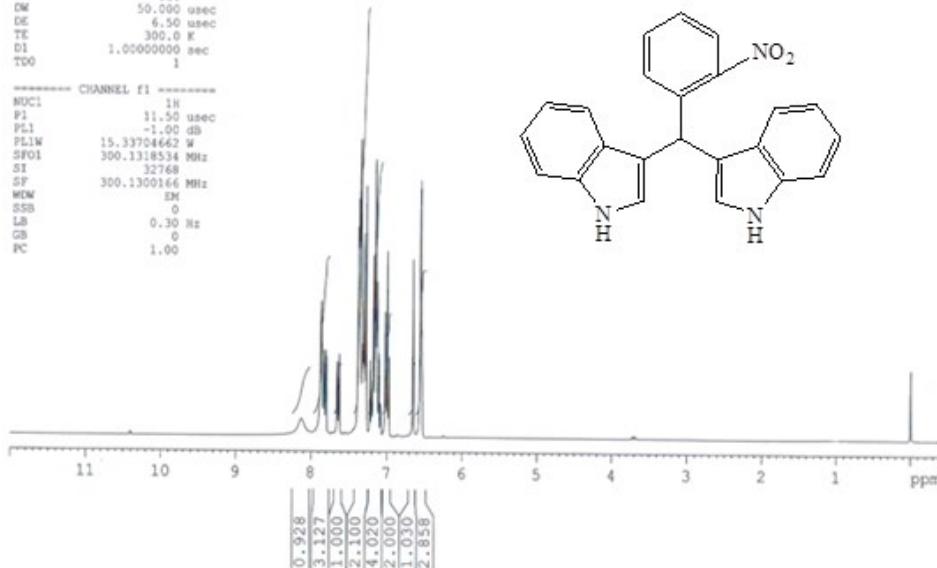
R.NO. 27319
 RCP-B8
 1H IN CDCl₃+DMSO
 AVANCE-300



¹H NMR spectrum of compound 3k

NAME R-27319-RCP-B4-1H-CDCl₃
 EXPNO 1
 PROCN0 1
 Date 20180215
 Time 11.37
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 39988
 SOLVENT CDCl₃
 NS 64
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.250012 Hz
 AQ 1.9999501 sec
 RG 128
 DW 50.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

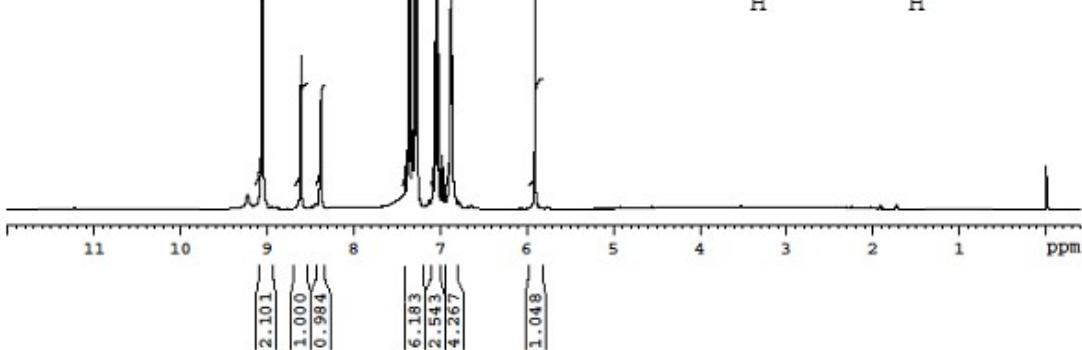
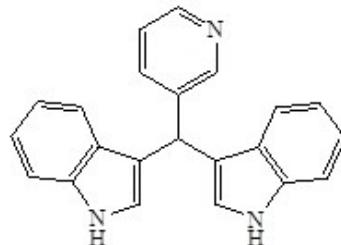
R.NO. 27319
 RCP-B4
 1H IN CDCl₃
 AVANCE-300



¹H NMR spectrum of compound 3l

Current Data Parameters
NAME R-27683-RCP-B14-1H-DMSO
EXPTNO 1
PROCNO 1
P2 - Acquisition Parameters
Date 20180525
TIME 13.44 h
INSTRUM spect
PROBHD Z824601_0038 (1H)
PULPROG zg30
TD 24096
SOLVENT DMSO
NS 64
DE 2
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 50.56
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDD 1
TD0 400.2024712 MHz
NUC1 1H
P1 13.00 usec
PLW1 12.0000000 W

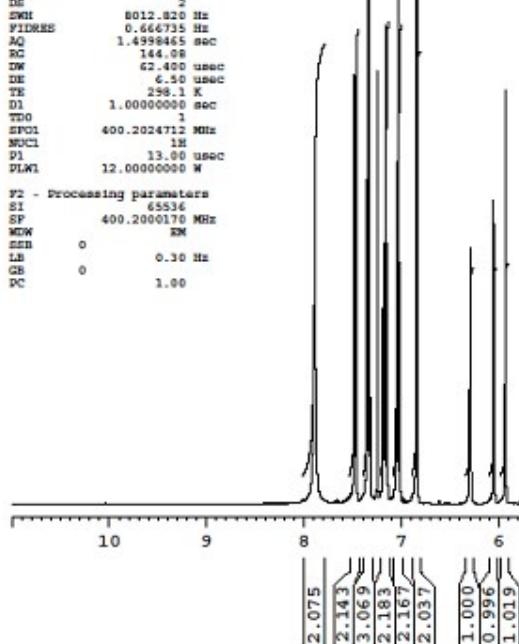
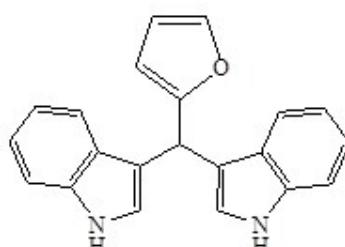
R.NO. 27683
RCP-B14
1H IN DMSO
AVANCE-400



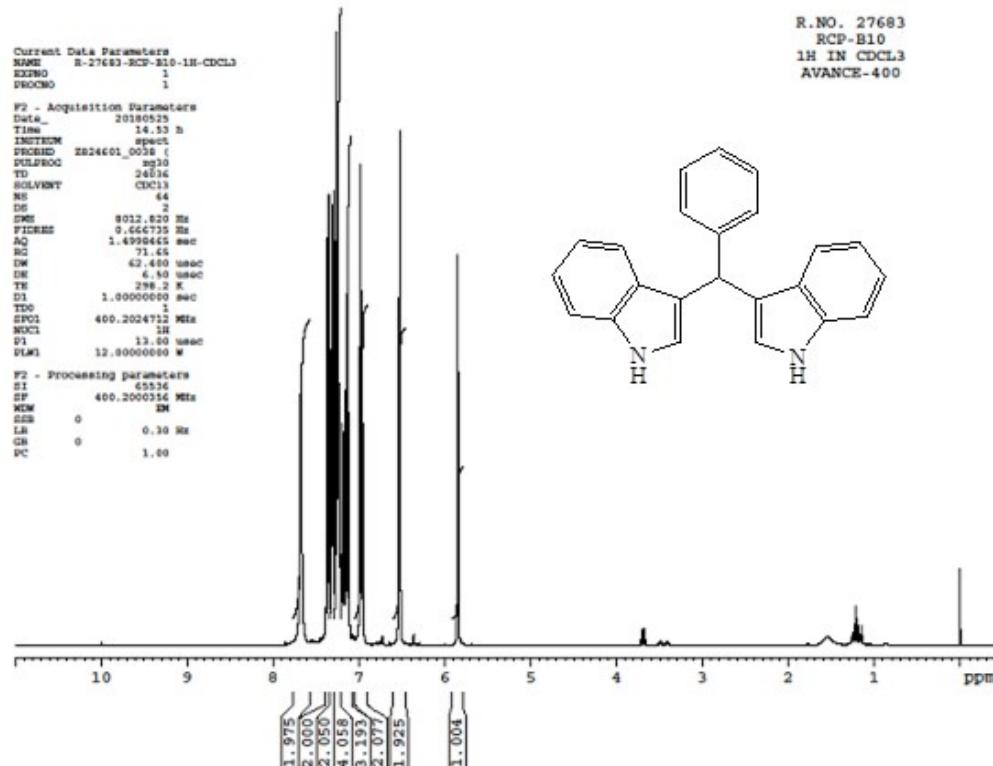
¹H NMR spectrum of compound 3m

Current Data Parameters
NAME R-27683-RCP-B13-1H-CDCL3
EXPTNO 1
PROCNO 1
P2 - Acquisition Parameters
Date 20180525
TIME 15.11 h
INSTRUM spect
PROBHD Z824601_0038 (1H)
PULPROG zg30
TD 24096
SOLVENT CDCl3
NS 64
DE 2
SWH 8012.820 Hz
FIDRES 0.666735 Hz
AQ 1.4998465 sec
RG 144.08
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TDD 1
TD0 400.2024712 MHz
NUC1 1H
P1 13.00 usec
PLW1 12.0000000 W

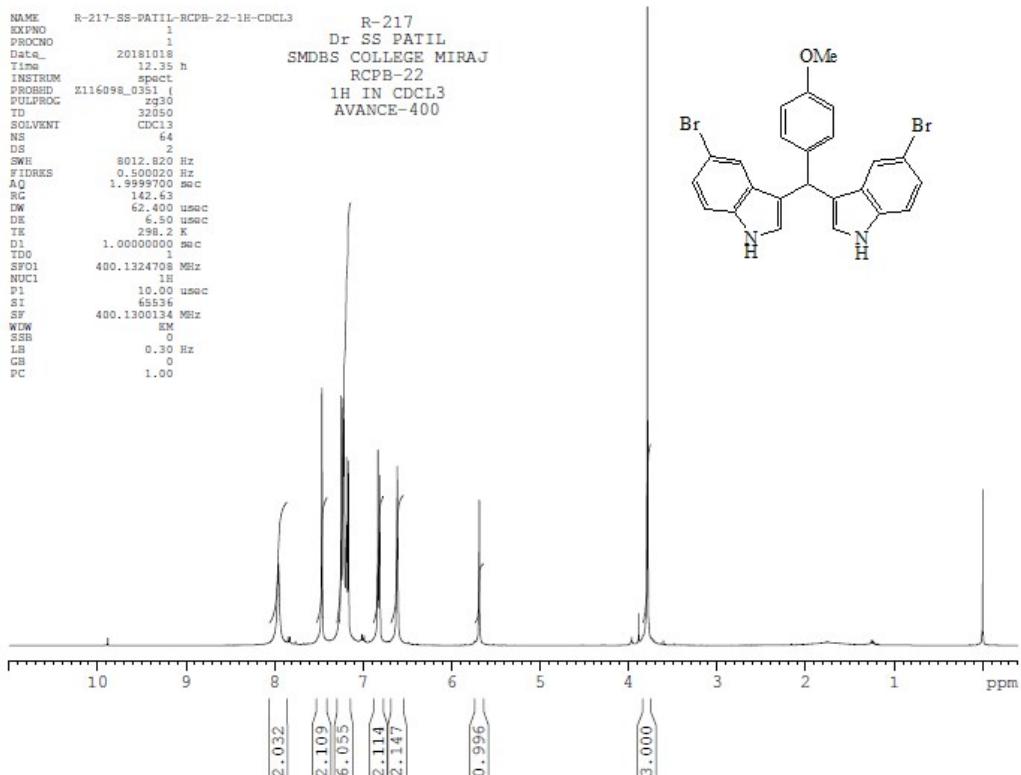
R.NO. 27683
RCP-B13
1H IN CDCL3
AVANCE-400



¹H NMR spectrum of compound 3n



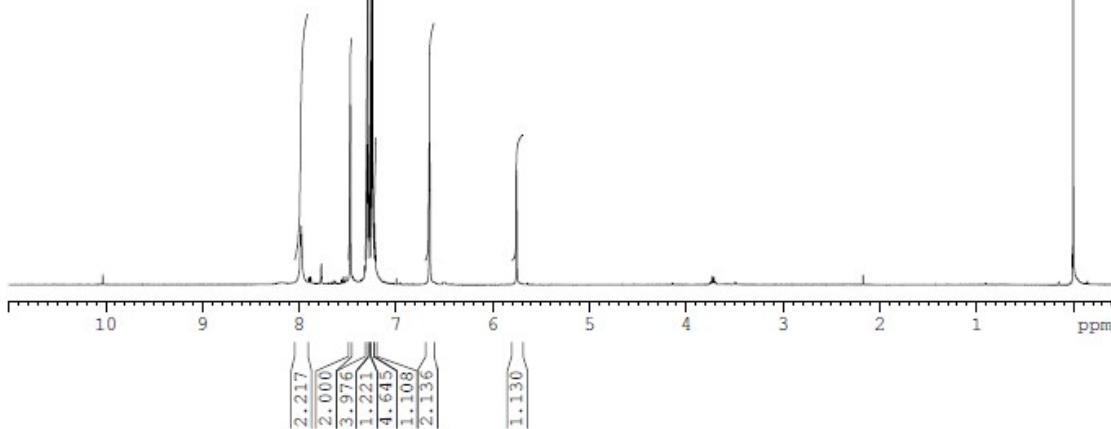
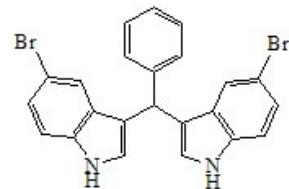
¹H NMR spectrum of compound 3o



¹H NMR spectrum of compound 3q

NAME R-217-SSPATIL-RCPB-21-1H-CDCL3
 EXPNO 1
 PROCN0 1
 Data_ 20181018
 Time 12.29 h
 INSTRUM spect
 PROBHD Z116098_0351
 PULPROG zg3d30
 ID 32050
 SOLVENTI CDCl3
 NS 128
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.500020 Hz
 AQ 1.9999700 sec
 RG 186.53
 DW 62.400 usec
 DE 6.50 usec
 IR 298.1 K
 D1 1.0000000 sec
 TDO 1
 SF01 400.1324708 MHz
 NUC1 1H
 P1 10.00 usec
 SI 65536
 SF 400.1300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

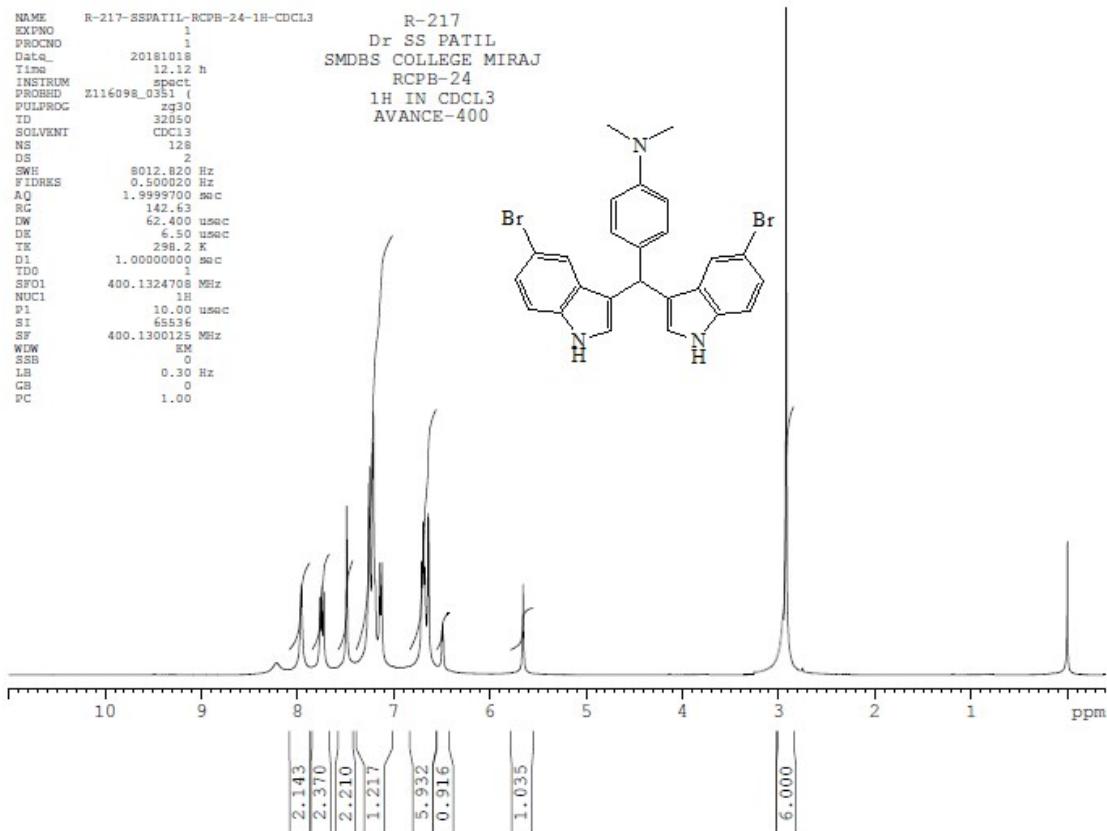
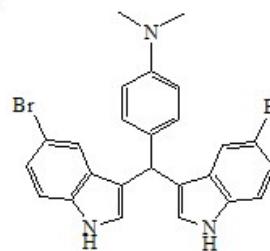
R-217
 Dr SS PATIL
 SMDBS COLLEGE MIRAJ
 RCPB-21
 1H IN CDCL3
 AVANCE-400



¹H NMR spectrum of compound 3r

NAME R-217-SSPATIL-RCPB-24-1H-CDCL3
 EXPNO 1
 PROCN0 1
 Data_ 20181018
 Time 12.12 h
 INSTRUM spect
 PROBHD Z116098_0351
 PULPROG zg3d30
 ID 32050
 SOLVENTI CDCl3
 NS 128
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.500020 Hz
 AQ 1.9999700 sec
 RG 142.63
 DW 62.400 usec
 DE 6.50 usec
 IR 298.2 K
 D1 1.0000000 sec
 TDO 1
 SF01 400.1324708 MHz
 NUC1 1H
 P1 10.00 usec
 SI 65536
 SF 400.1300125 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

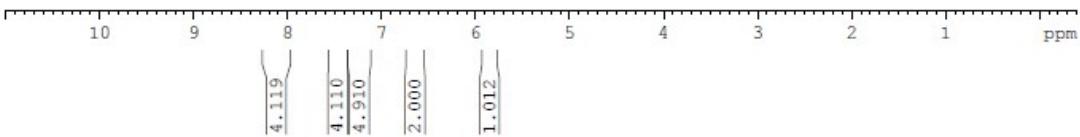
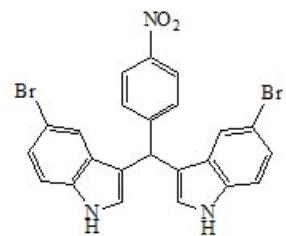
R-217
 Dr SS PATIL
 SMDBS COLLEGE MIRAJ
 RCPB-24
 1H IN CDCL3
 AVANCE-400



¹H NMR spectrum of compound 3Sk

NAME R-217-SSPATIL-RCPB-23-1H-CDCL3
 EXPNO 1
 PROCHNO 1
 Data_ 20181018
 Time 12:19 h
 INSTRUM spect
 PGMID Z116098_0351
 PULPROG zg30
 ID 32050
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.500020 Hz
 AQ 1.999800 sec
 RG 154.49
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1
 SF01 400.1324708 MHz
 NUC1 1H
 PI 10.00 usec
 SI 65536
 SF 400.1300116 MHz
 WDW KM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

R-217
 Dr SS PATIL
 SMDBS COLLEGE MIRAJ
 RCPB-23
 1H IN CDCl3
 AVANCE-400



¹H NMR spectrum of compound 3t

NAME R-1772-RCPR-4-1H-DMSO R.NO. 1772
 EXPNO 1 RCPR-4
 PROCHNO 1
 Data_ 20191122 1H IN DMSO
 Time 14.28
 INSTRUM spect
 PGMID 5 nm RHO BB-1H AVANCE-300
 PULPROG zg30
 TD 24780
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 6188,119 Hz
 FIDRES 0.250025 Hz
 AQ 1.999800 sec
 RG 144
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

----- CHANNEL F1 -----

NUC1 1H

PI 11.50 usec

PL1 -1.00 dB

P1LM 15.33704462 W

SF01 300.1300036 MHz

SI 32768

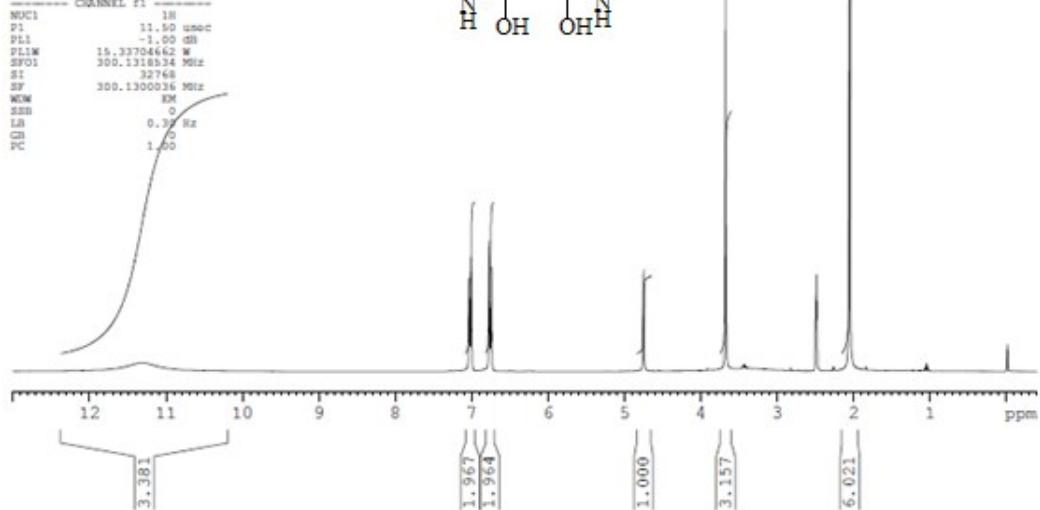
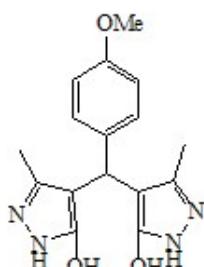
SF 300.1300036 MHz

WDM KM

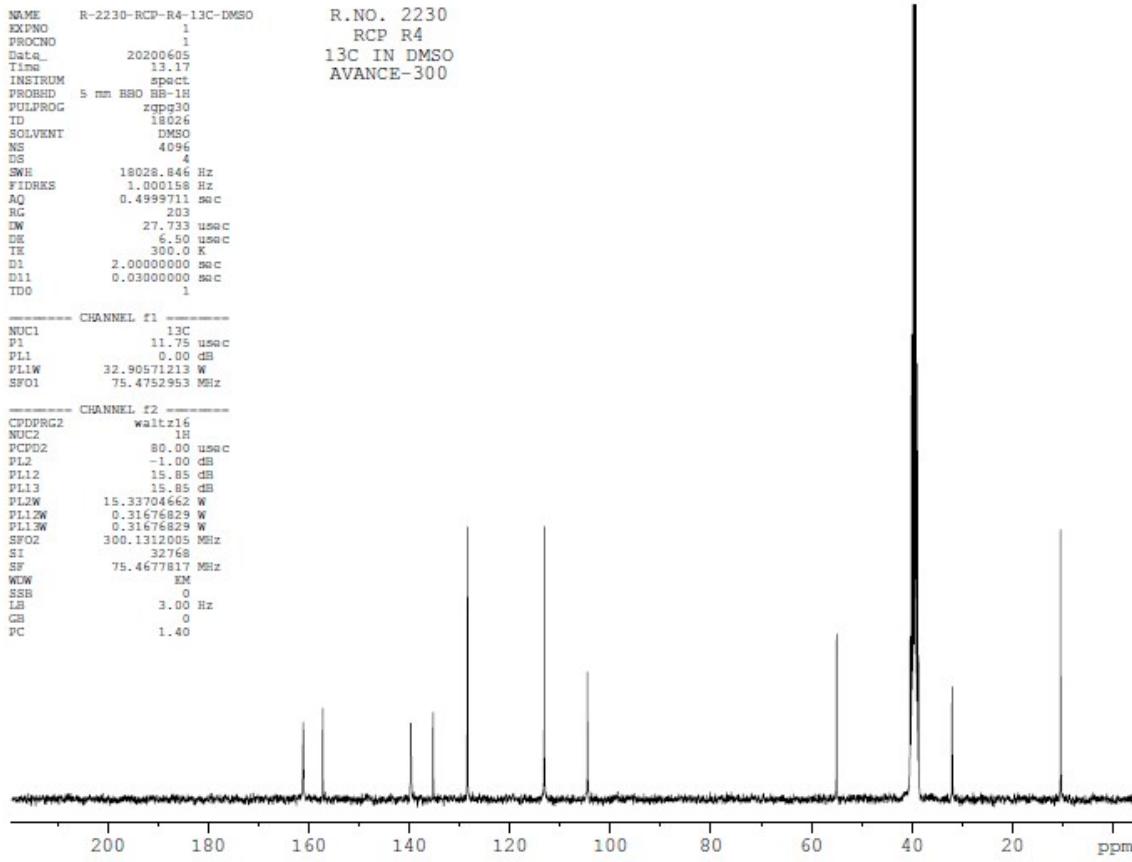
SSB 0

LB 0.30 Hz

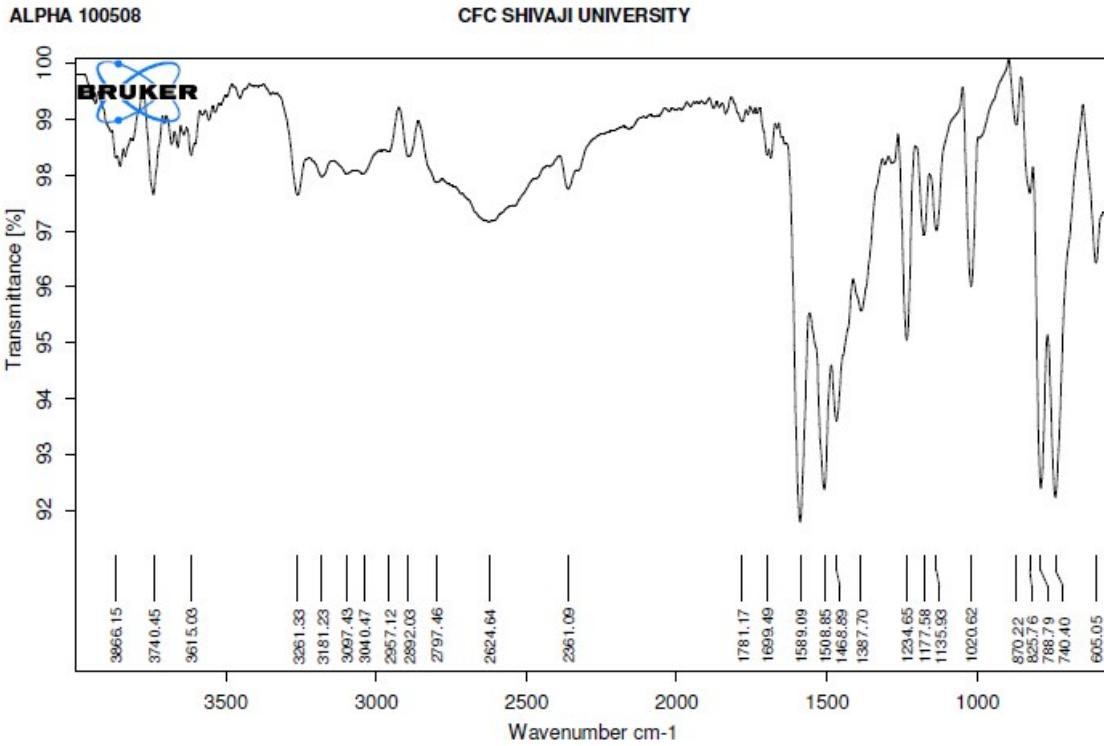
GB 1.00



¹H NMR spectrum of compound 7a



¹³C NMR spectrum of compound 7a

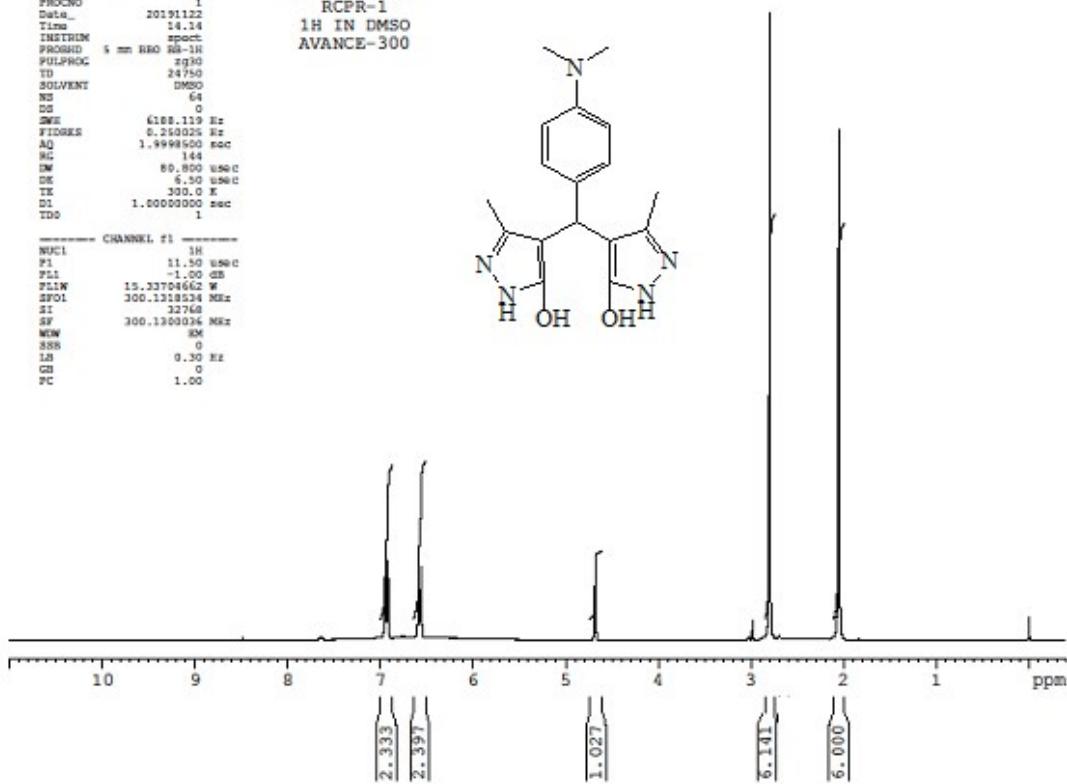
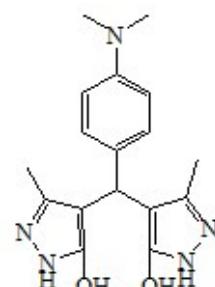


D:\FTIR DATA\Chemistry\SSP\Rupesh\R4.0	R4 Instrument type and / or accessory	2/24/2020
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FT-IR spectrum of compound 7a

NAME R-1772-RCPR-1-1H-DMSO
 EXPNO 1
 PROCNO 1
 Data_ 20191122
 Time 14.14
 INSTRUM spect
 PROBHD 5 mm BBP BB-1H
 PULPROG zgpp30
 TD 24750
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 6188.119 Hz
 FIDRES 0.250025 Hz
 AQ 1.999800 sec
 RG 144
 DW 80.800 usec
 DE 6.50 usec
 TM 300.0 K
 D1 1.0000000 sec
 TDO 1

----- CHANNEL #1 -----
 NUC1 1H
 F1 11.50 usec
 PL1 -1.00 dB
 PL1W 15.33704662 W
 SF01 300.1312005 MHz
 SI 32768
 SF 300.1300034 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GHA 0
 PC 1.00

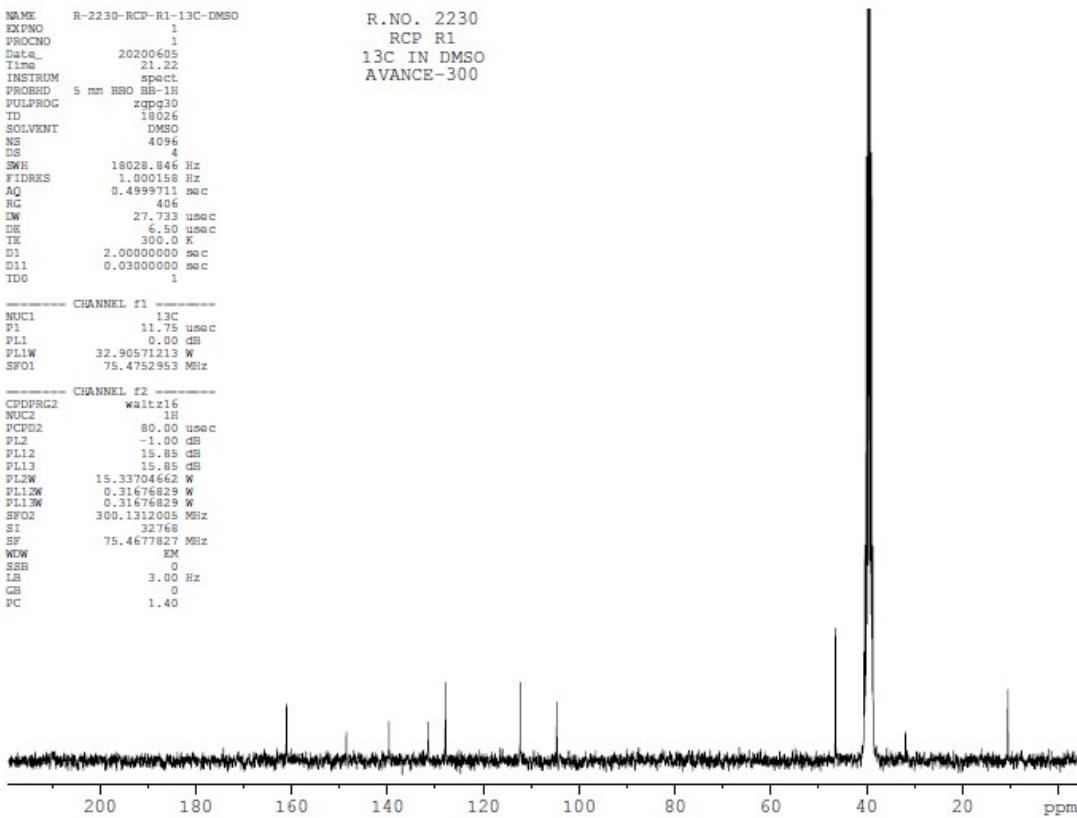


¹H NMR spectrum of compound 7c

NAME R-2230-RCP-R1-13C-DMSO
 EXPNO 1
 PROCNO 1
 Data_ 20200605
 Time 21.22
 INSTRUM spect
 PROBHD 5 mm BBP BB-1H
 PULPROG zgpp30
 TD 18026
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 18028.846 Hz
 FIDRES 1.000158 Hz
 AQ 0.4999711 sec
 RG 406
 DW 27.733 usec
 DE 6.50 usec
 TM 300.0 K
 D1 2.0000000 sec
 D1L 0.03000000 sec
 TDO 1

----- CHANNEL #1 -----
 NUC1 13C
 F1 11.75 usec
 PL1 0.00 dB
 PL1W 32.90571213 W
 SF01 75.4752953 MHz

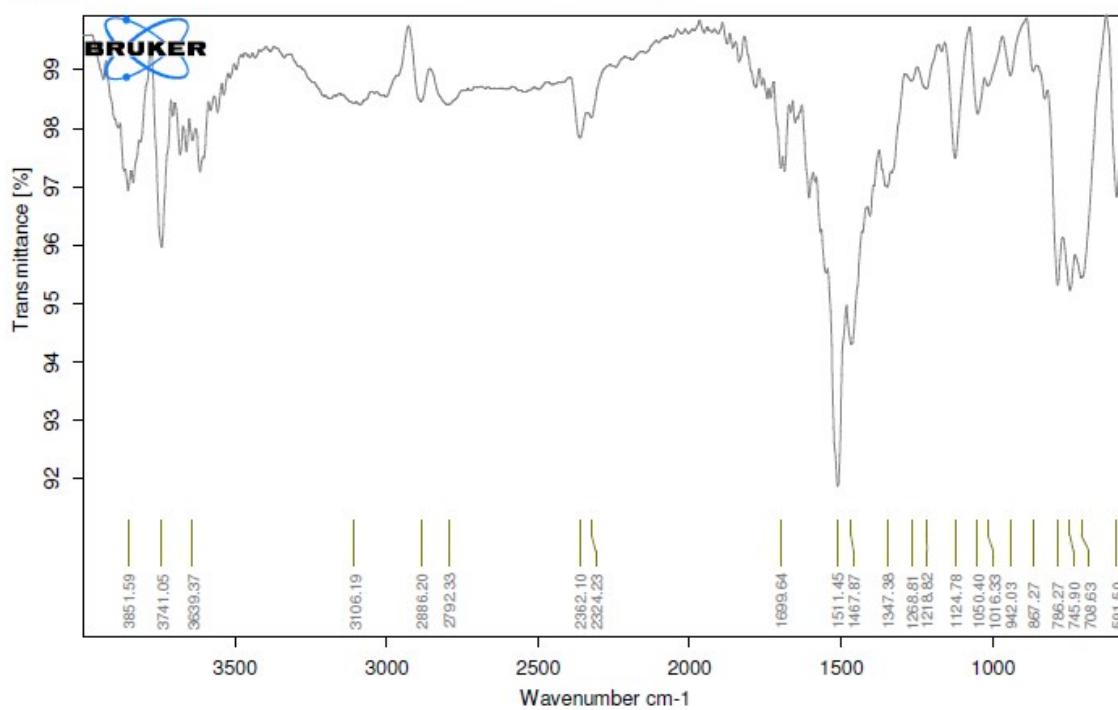
----- CHANNEL #2 -----
 CRDPG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 15.85 dB
 PL13 15.85 dB
 PL2W 15.33704662 W
 PL12W 0.31676828 W
 PL13W 0.31676829 W
 SF02 300.1312005 MHz
 SI 32768
 SF 75.4677827 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GHA 0
 PC 1.40



¹³C NMR spectrum of compound 7c

ALPHA 100508

CFC SHIVAJI UNIVERSITY

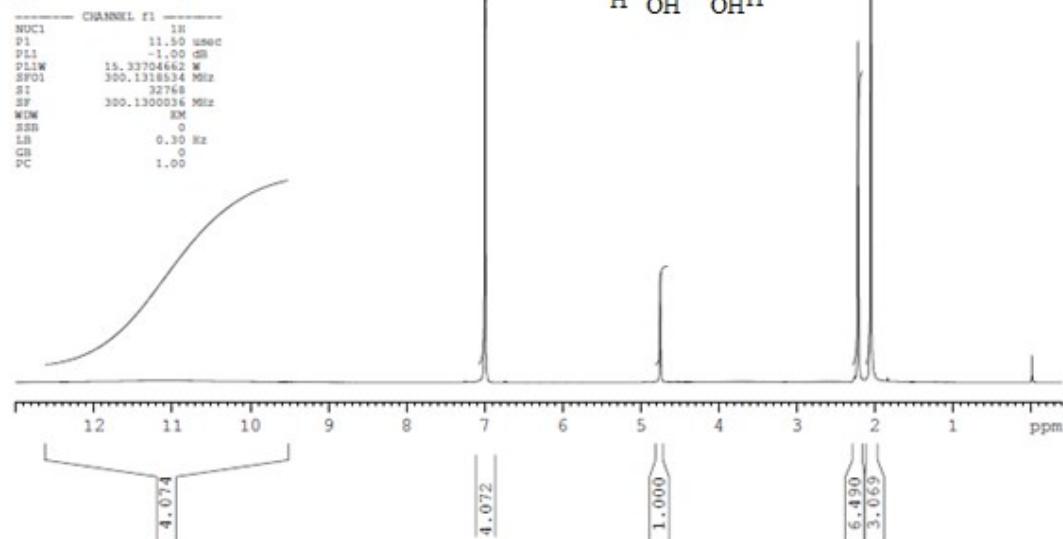
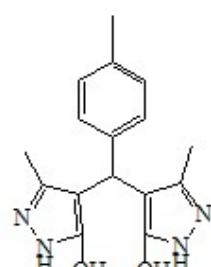


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FT-IR spectrum of compound 7c

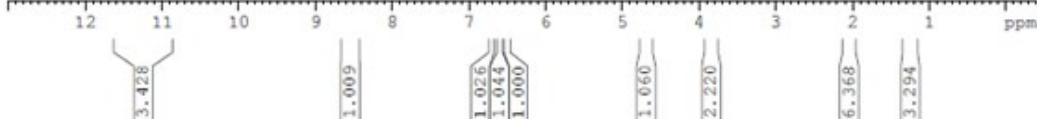
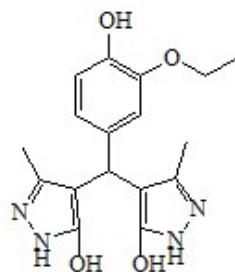
NAME R-1772-RCPR-5-1H-DMSO
 EXPNO 1
 PROCNO 1
 Date 20191122
 Time 14.35
 INSTRUM RCPR-5
 PROBOD 5 mm BBO
 PULPROG zg3D
 TD 24750
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 6188.119 Hz
 FIDRES 0.2500000 Hz
 AQ 1.9998500 sec
 RG 1K1
 DM 80.000 ussec
 DE 6.50 ussec
 TE 300.0 K
 D1 1.0000000 sec
 TDO :
 ----- CHANNEL f1 -----

R. NO. 1772
 RCPR-5
 1H IN DMSO
 AVANCE-300

¹H NMR spectrum of compound 7d

NAME R-1772-RCPR-3-1H-DMSO
 EXPNO 1
 PROCHN 1
 DATE 20191122
 TIME 14.21
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 24750
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 6188.119 Hz
 FIDRES 0.250025 Hz
 AQ 1.9998500 sec
 RG 228
 DW 80.000 usec
 DE 6.50 usec
 TM 30.00 K
 T1 1.0000000 sec
 TDO 1

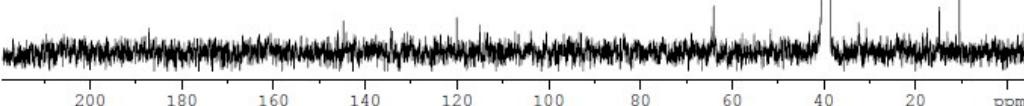
----- CHANNEL f1 -----
 NUC1 1H
 P1 11.00 usec
 PL1 -1.00 dB
 PLLW 15.33704662 W
 SF01 300.1318534 MHz
 SI 32768
 SF 300.1300036 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



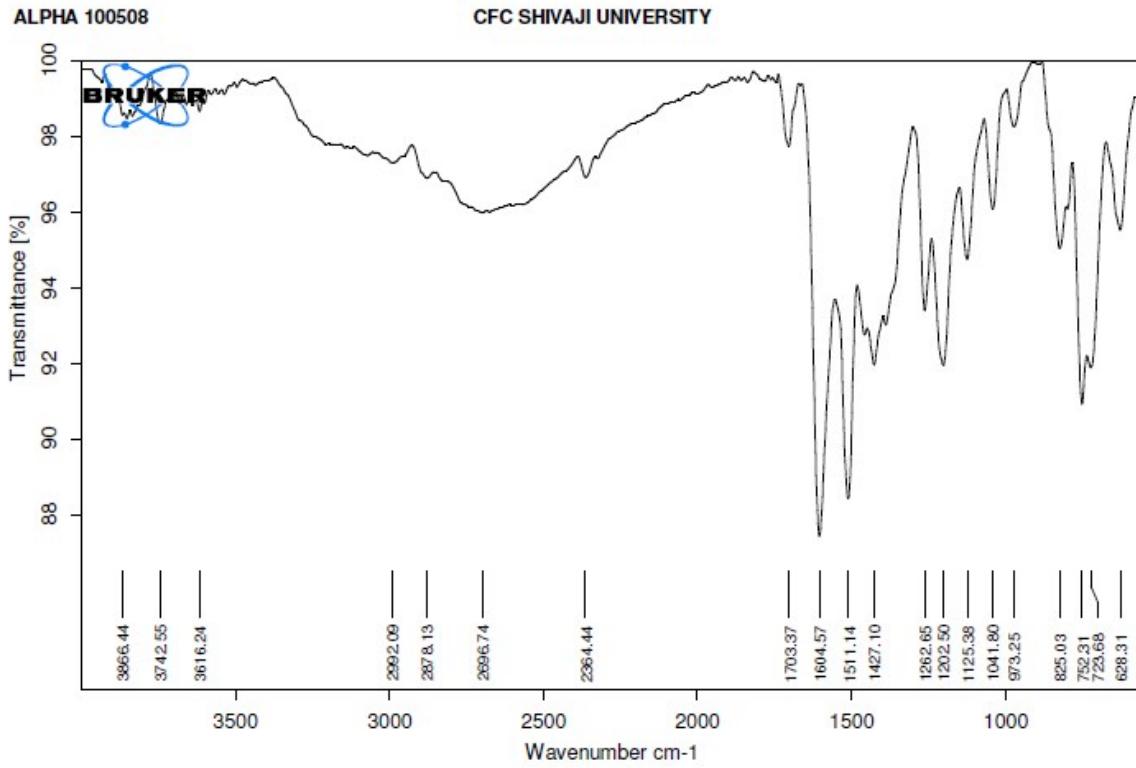
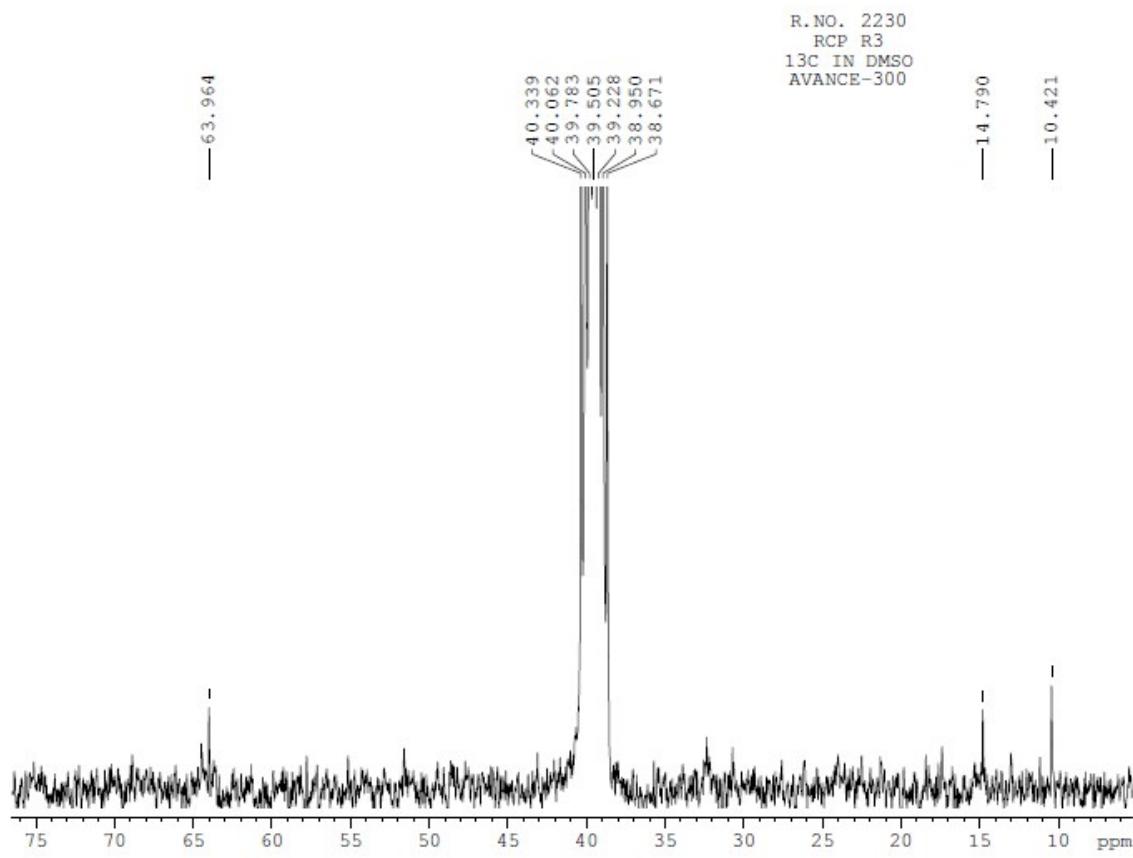
¹H NMR spectrum of compound 7e

NAME R-2230-RCP-R3-13C-DMSO
 EXPNO 1
 PROCHN 1
 DATE 20200605
 TIME 18.22
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgppg30
 TD 18026
 SOLVENT DMSO
 NS 4096
 DS 4
 SWH 18028.846 Hz
 FIDRES 1.000188 Hz
 AQ 0.4999711 sec
 RG 406
 DW 27.72 usec
 DE 4.50 usec
 TM 300.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 11.75 usec
 PL1 0.00 dB
 PLLW 32.90571213 W
 SF01 75.4752953 MHz
 ----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 P1 11.75 usec
 PL1 -1.00 dB
 PLL2 15.33704662 W
 PLL3 15.33704662 W
 PLL2W 0.31676829 W
 PLL3W 0.31676829 W
 SF02 300.1312005 MHz
 SI 32768
 SF 75.4677159 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



¹³C NMR spectrum of compound 7e



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FT-IR spectrum of compound 7e

NAME R-2230-RCP-R2-1H-DSO

EXPNO 1

PROCNO 1

Data_ 20200605

Time 12.08

INSTRUM spect

PROBHD 5 mm BBM BB-1H

PULPROG zg30

TD 24750

SOLVENT DMSO

NS 64

DS 0

SWH 6188.119 Hz

FIDRES 0.250025 sec

AQ 1.9998500 sec

RG 228

DM 80.000 usec

DE 6.50 usec

TE 300.0 K

D1 1.0000000 sec

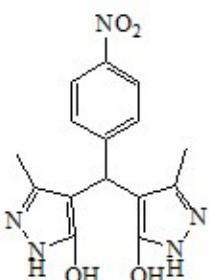
TDO 1

R.NO. 2230

RCP R2

1H IN DMSO

AVANCE-300



----- CHANNEL f1 -----

NUC1 1H

PL1 11.50 usec

PL1 11.50 usec

P1LW 15.33704462 MHz

SF01 300.1318534 MHz

SI 32768

SF 300.1300024 MHz

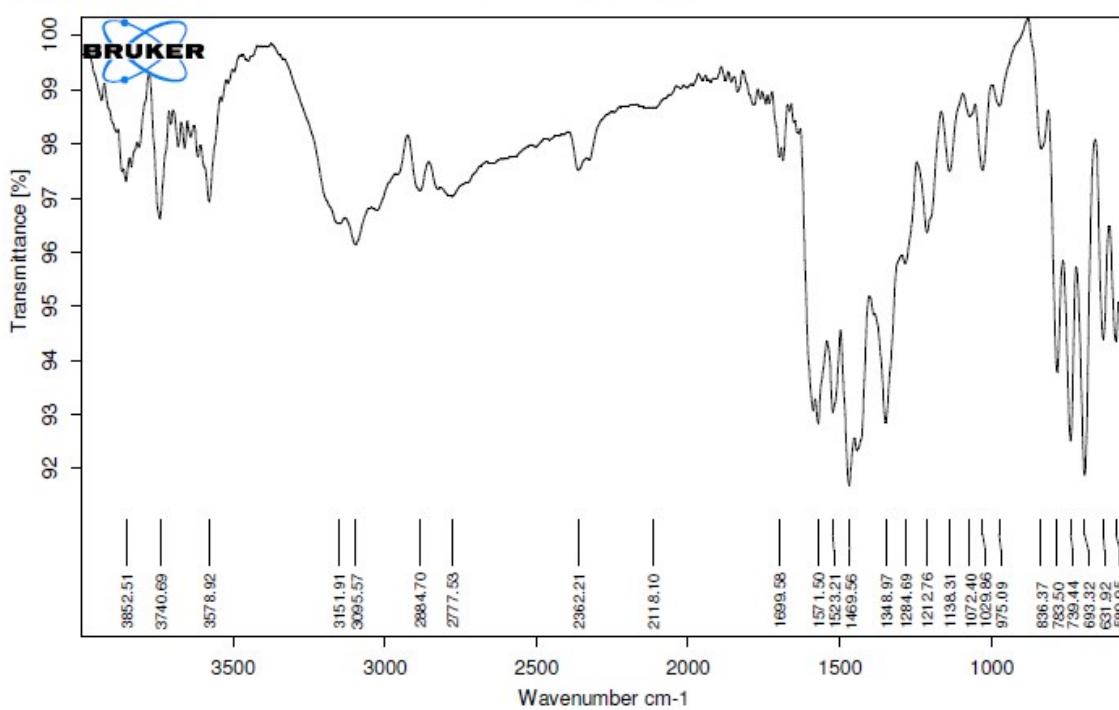
NEW EM

SSB 0

LB 0.30 Hz

GB 0

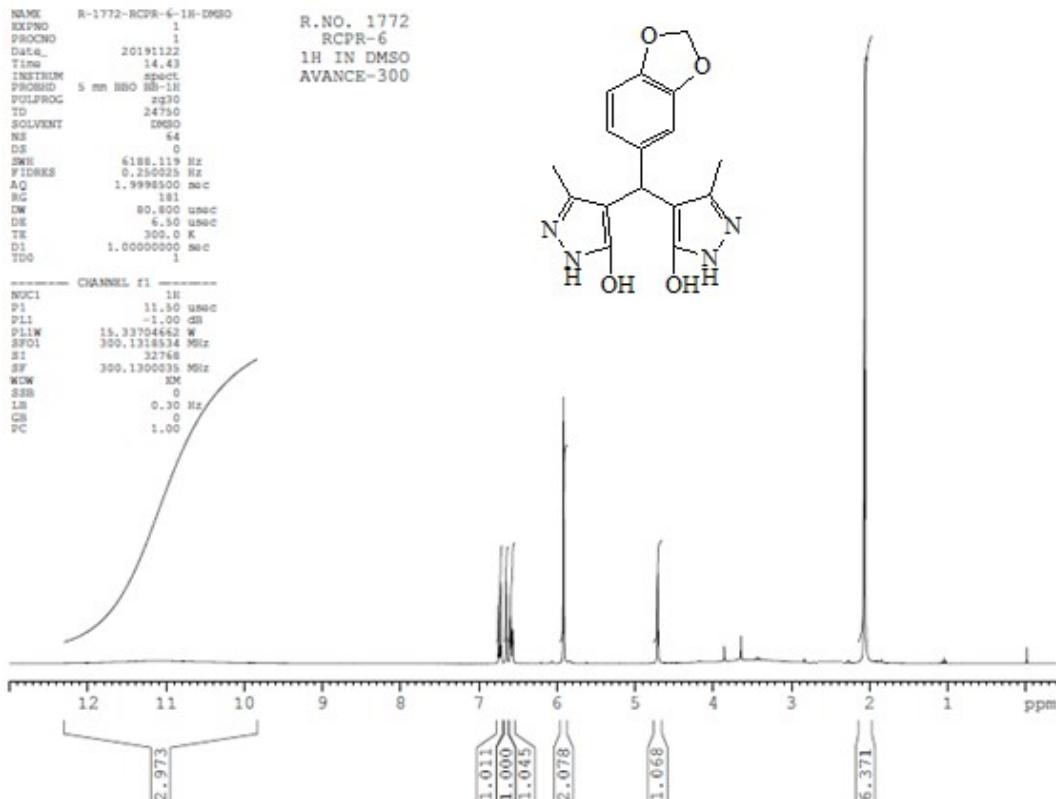
PC 1.00



D:\FTIR DATA\Chemistry\SSP\Rupesh\R8.0	R8	Instrument type and / or accessory
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2/24/2020

FT-IR spectrum of compound 7h

¹H NMR spectrum of compound 7j

NAME R-2230-RCP-R6-13C-DMSO

R. NO. 2230

EXPNO 1

RCP R6

PROCN0 1

13C IN DMSO

Data_ 20200606

1.50

Time 1.50

AVANCE-300

INSTRUM spect

PROBHD 5 mm BBO BB 1H

PULPROG rcp030

TD 18026

DMSO

SOLVENT DMSO

NS 6144

DS 4

SWH 18028.846 Hz

FIDRES 1.000158 Hz

AQ 0.4999711 sec

RG 362

DW 27.733 usec

DR 6.50 usec

IR 300.0 K

D1 2.0000000 sec

D11 0.03000000 sec

IDO 1

----- CHANNEL f1 -----

NUC1 13C

P1 11.75 usec

PL1 0.00 dB

PL1W 32.90571213 W

SF01 75.4752953 MHz

----- CHANNEL f2 -----

CPDPGR2 waltz16

NUC2 13C

PCPD2 80.00 usec

PL2 -1.00 dB

PL12 15.85 dB

PL13 15.85 dB

PL2W 15.33704662 W

PL12W 0.31676829 W

PL13W 0.31676829 W

SF02 300.1312005 MHz

SI 32768 MHz

SF 75.4677866 MHz

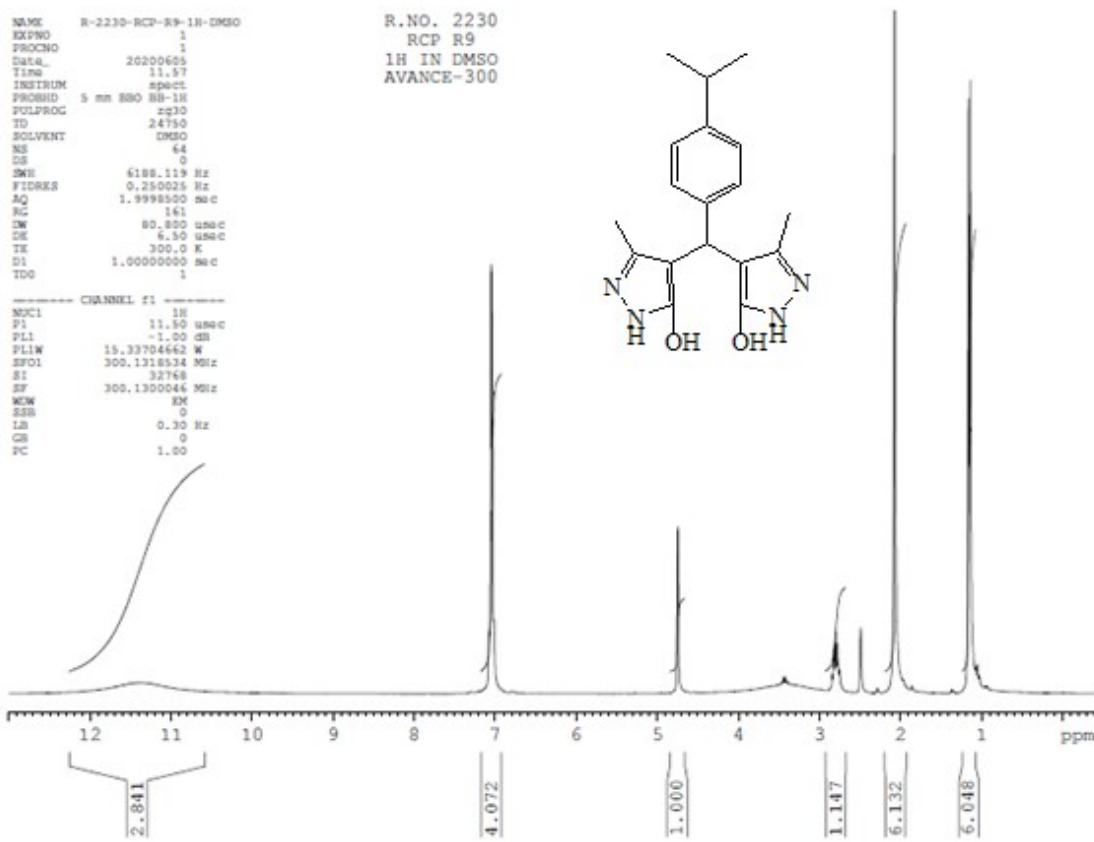
WOW EM

SSB 0

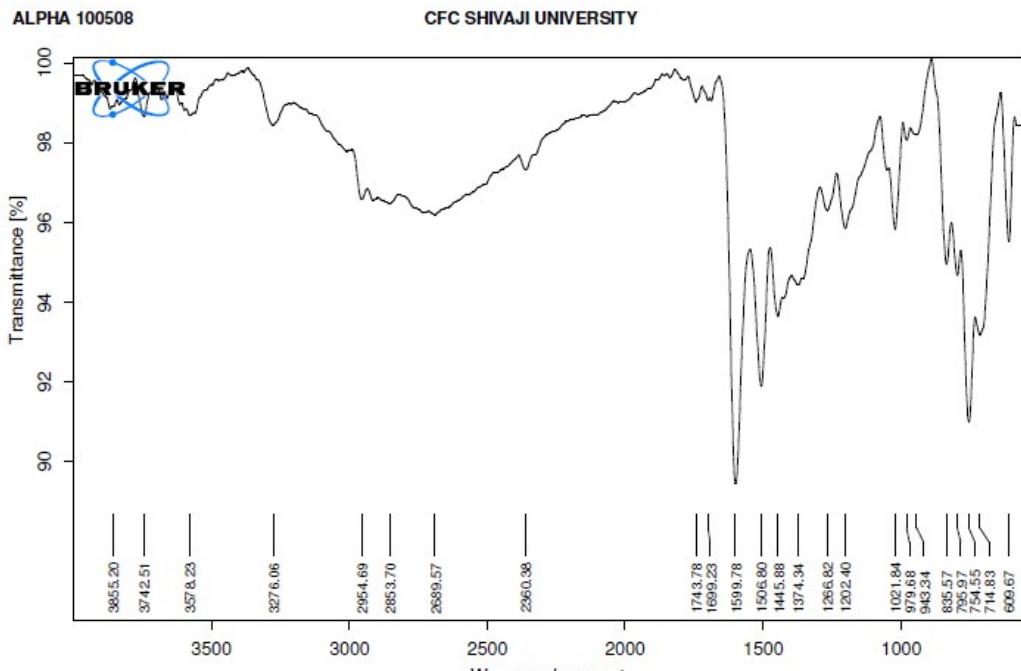
LB 3.00 Hz

GB 0

PC 1.40



¹H NMR spectrum of compound 7m



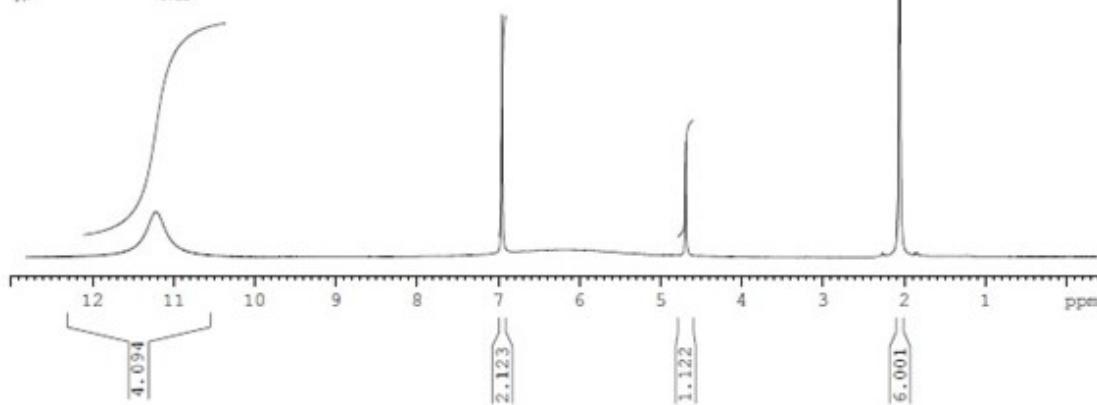
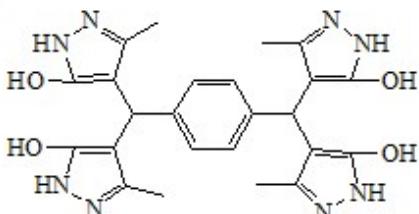
FT-IR spectrum of compound 7m

NAME R-2230-RCP-R7-1H-DMSO

R.NO. 2230
RCP R7
1H IN DMSO
AVANCE-300

EXPTNO. 1
PROCNO. 1
Date_ 20200605
Time_ 12.23
INSTRUM spect
PROBHD 5 mm RBO BB-1H
PULPROG zg30
TD 24750
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.250025 Hz
AQ 1.9999500 sec
RG 181
DM 80,000 usec
DR 8.50 usec
TE 300.0 K
D1 1.0000000 sec
TDS 1

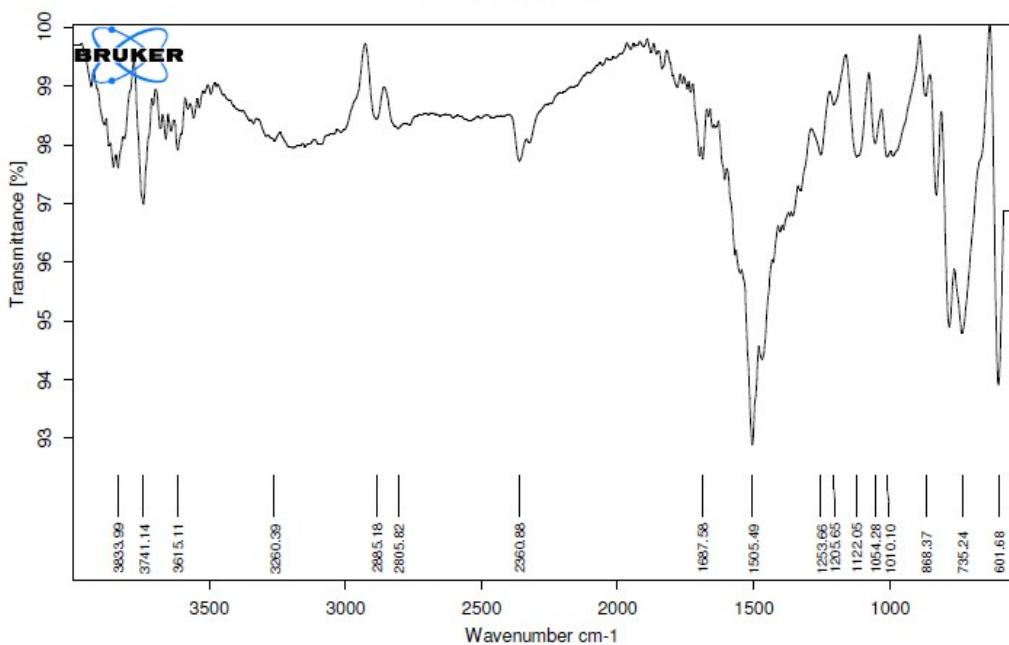
CHANNEL F1
NUC1 1H
P1 11.50 usec
PL1 -1.00 dB
PL1W 15.33704662 W
SF01 300.1318534 MHz
SI 32768
SF 300.1300046 MHz
WDW PC
SSB 0
LB 0.30 Hz
GB 0
PT 1.00



¹H NMR spectrum of compound 7n

ALPHA 100508

CFC SHIVAJI UNIVERSITY



D:\FTIR DATA\Chemistry\SSP\Rupesh\R7.0

R7 Instrument type and / or accessory

2/24/2020

FT-IR spectrum of compound 7n