# Supporting Information

## Inhibition of monoamine oxidases by heterocyclic derived conjugated dienones: synthesis, *in vitro*, and *in silico* investigations

Sunil Kumar[a#], Bishnu Prasad Pandey[b, c#], Mohamed A. Abdelgawad[d], Mohammed M. Ghoneim[e], Rania B. Bakr[f], Hoon Kim[b*], and Bijo Mathew[a*]

[a] Department of Pharmaceutical Chemistry, Amrita School of Pharmacy, Amrita Vishwa Vidyapeetham, AIMS Health Sciences Campus, Kochi 682 041, India

[b] Department of Pharmacy, and Research Institute of Life Pharmaceutical Sciences, Sunchon National University, Suncheon 57922, Republic of Korea

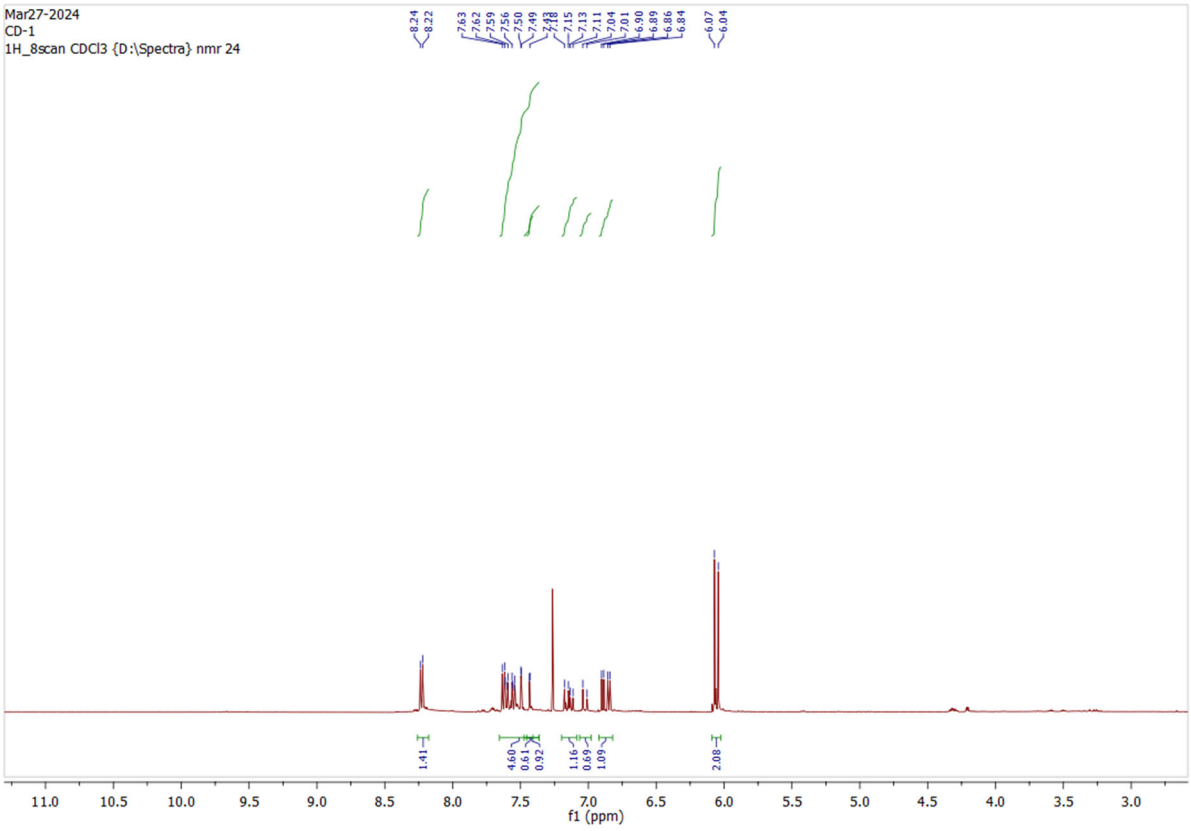
[c] Department of Chemical Science and Engineering, Kathmandu University, PO Box No. 6250, Dhulikhel, 45200, Nepal

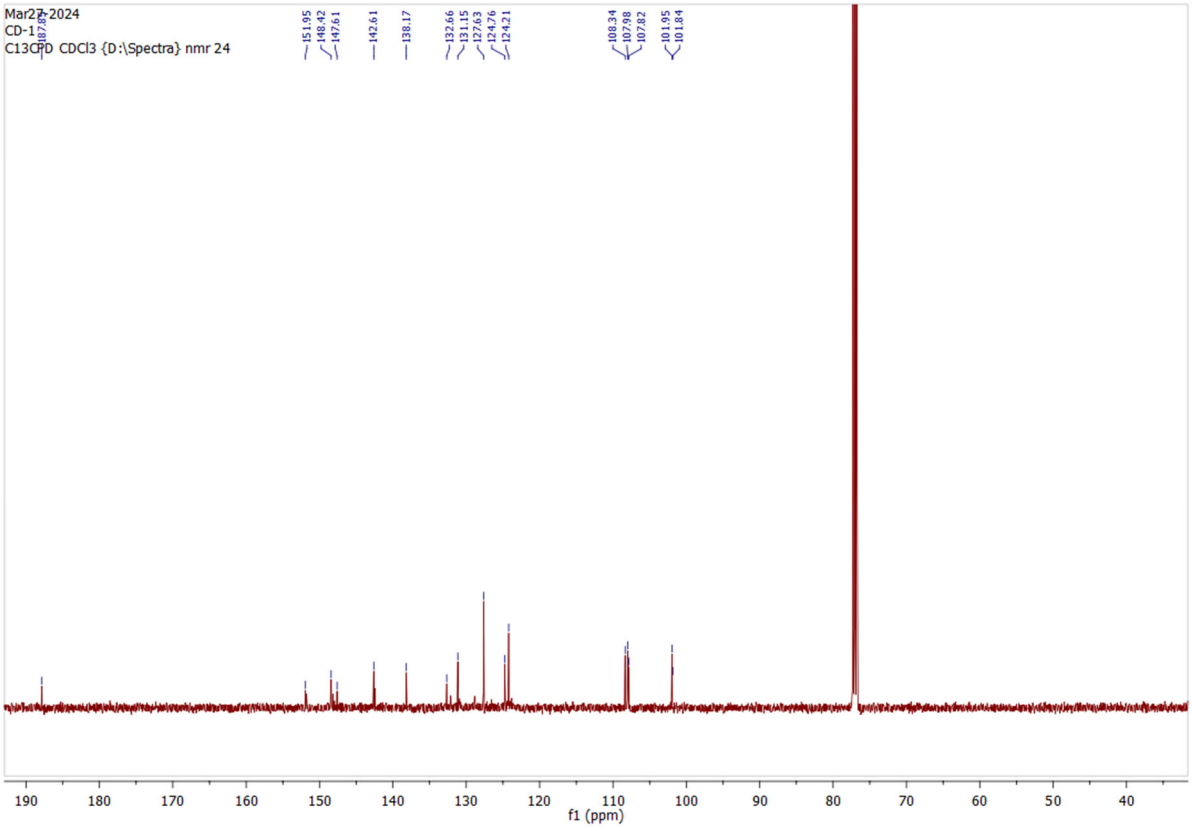
[d] Department of pharmaceutical chemistry, college of pharmacy, Jouf University, Sakaka 72341, Aljouf, Saudi Arabia

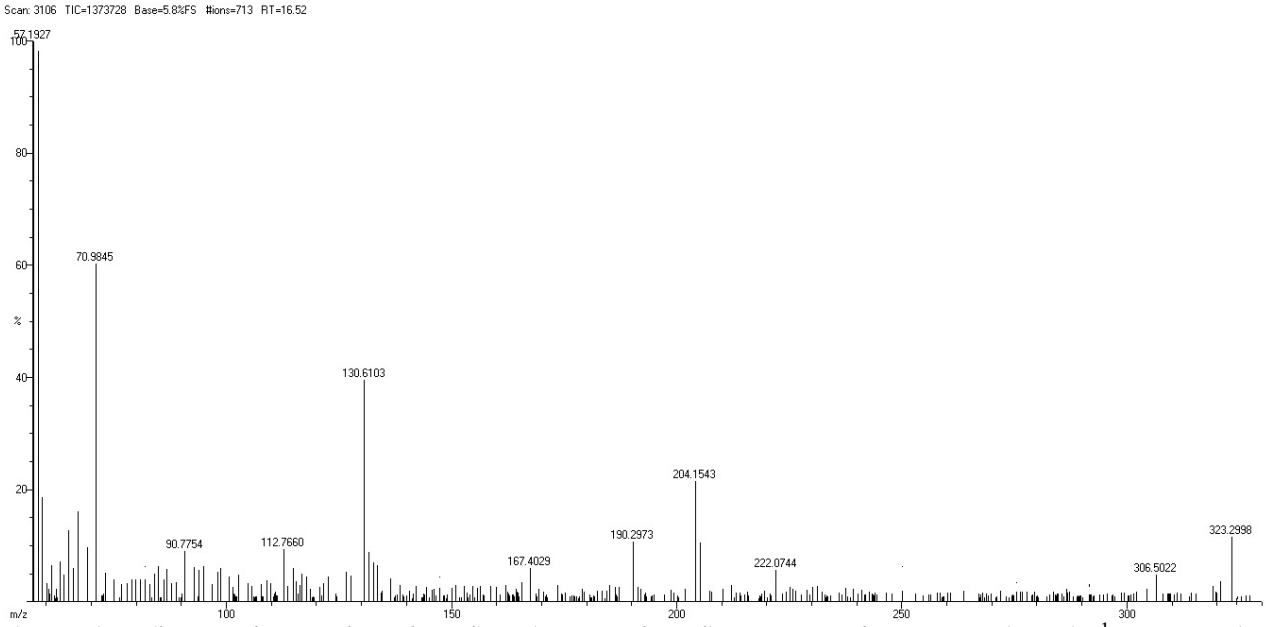
[e] Department of Pharmacy Practice, College of Pharmacy, AlMaarefa University, Ad Diriyah, Riyadh, 13713, Saudi Arabia

[f] Pharmaceutical Organic Chemistry Department, Faculty of Pharmacy, Beni-Suef University, Beni-Suef, 62514, Egypt

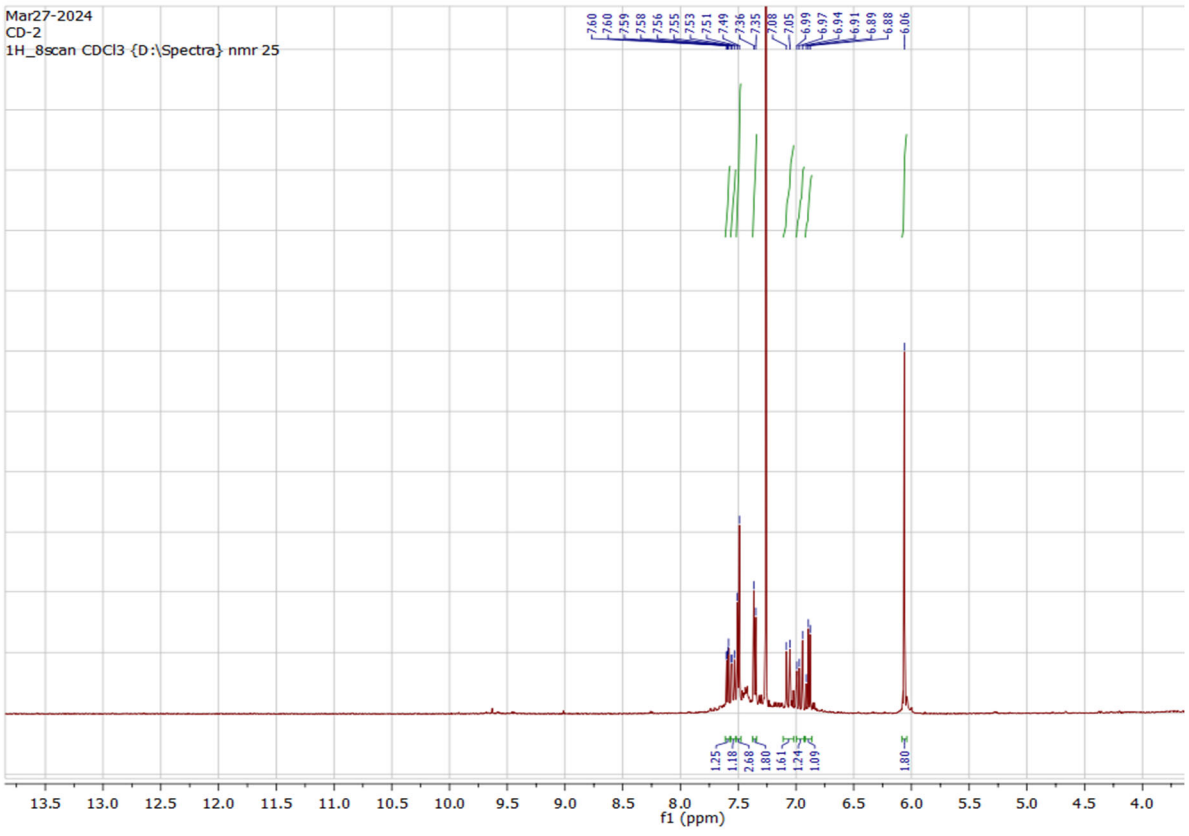
**Contents**

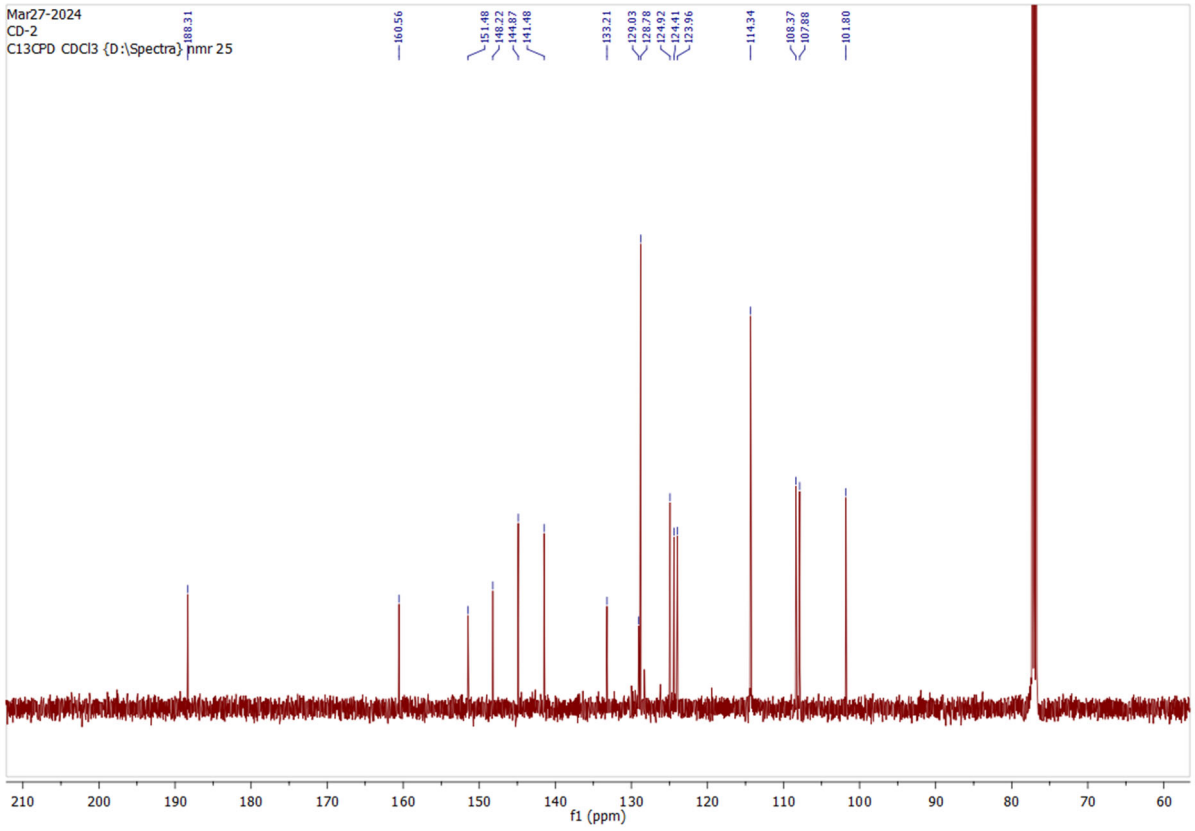

Mar27-2024
CD-1
1H_8scan CDCl3 {D:\Spectra} nmr 24
8.24
8.22
7.63
7.62
7.59
7.56
7.50
7.49
7.18
7.15
7.13
7.11
7.04
7.01
6.90
6.89
6.86
6.84
6.07
6.04
1.41
4.60
0.61
0.92
1.16
0.69
1.09
2.08
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)

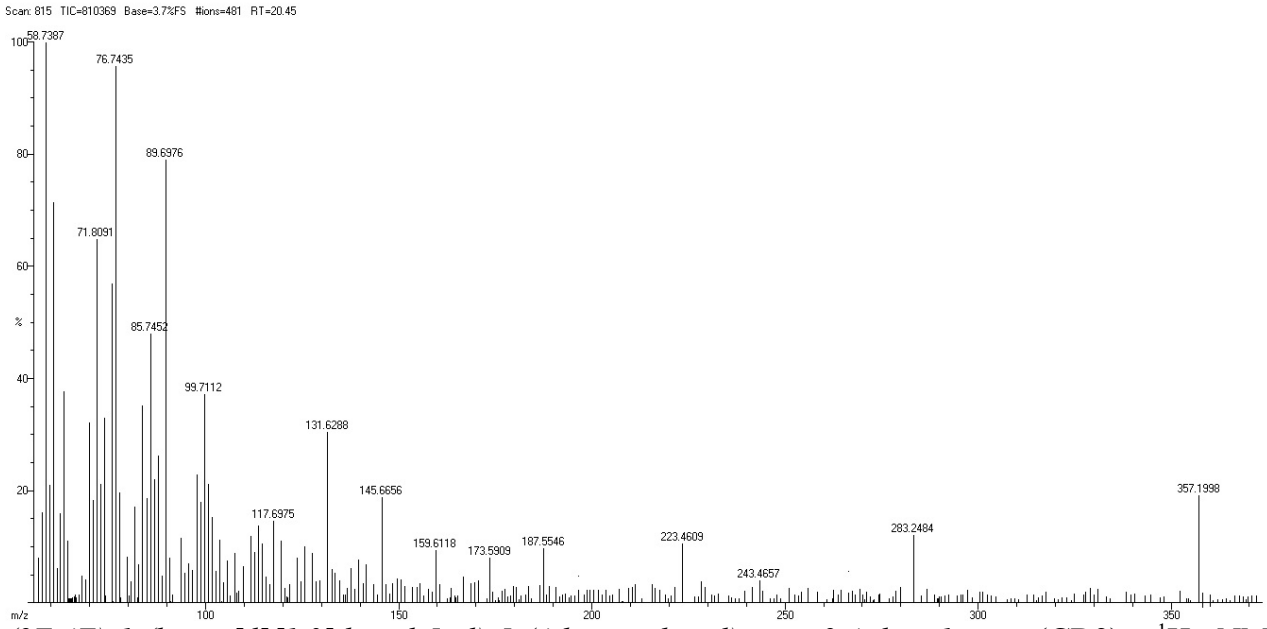

Mar27-2024
CD-1
C13CPD CDCl3 {D:\Spectra} nmr 24
187.70
151.95
148.42
147.61
142.61
138.17
132.66
131.15
127.63
124.76
124.21
108.34
107.98
107.82
101.95
101.84
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)



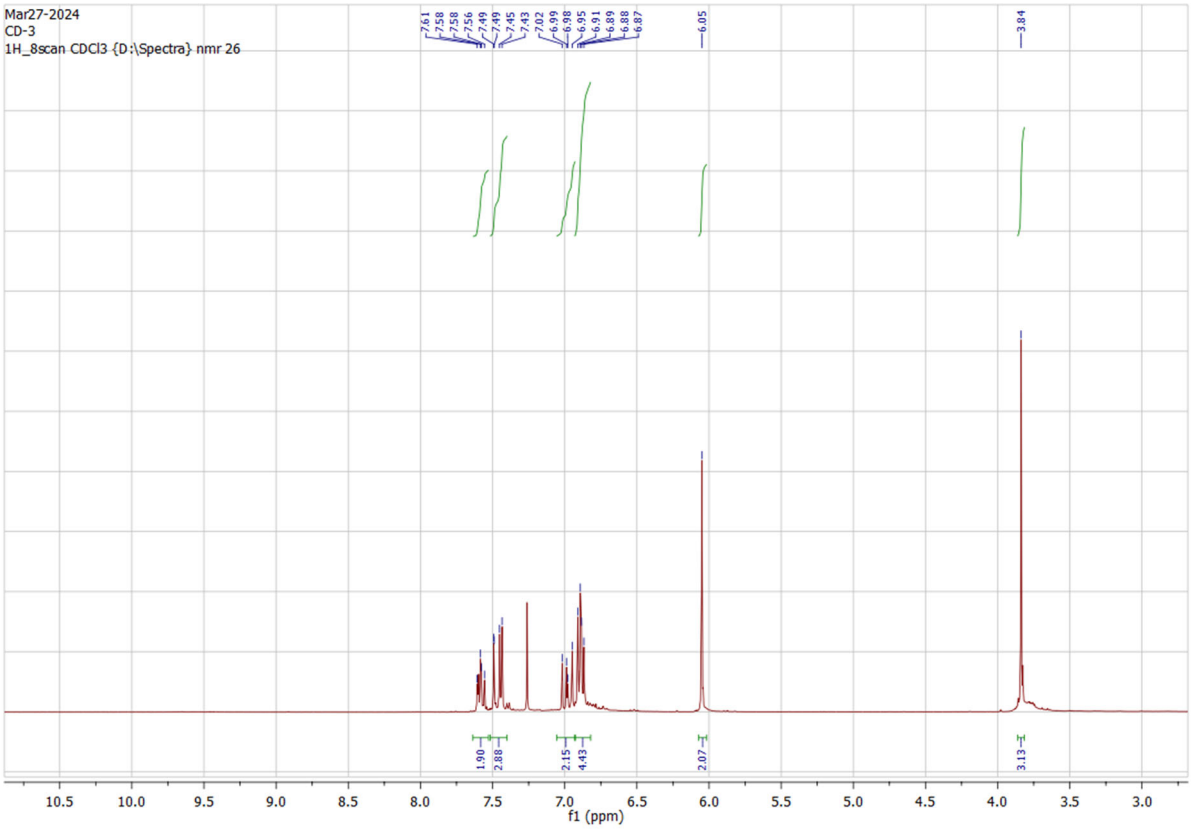

*(2E,4E)-1-(benzo[d][1,3]dioxol-5-yl)-5-(4-nitrophenyl)penta-2,4-dien-1-one* (**CD1**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.23 (d, *J* = 8.8 Hz, 1H), 7.65 – 7.36 (m, 5H), 7.43 (d, *J* = 1.7 Hz, 1H), 7.43 (d, *J* = 1.7 Hz, 1H), 7.14 (dd, *J* = 18.9, 12.7 Hz, 1H), 7.03 (d, *J* = 15.6 Hz, 1H), 6.87 (dd, *J* = 22.9, 8.1 Hz, 1H), 6.06 (d, *J* = 13.8 Hz, 2H). $^{13}$C NMR 500 MHz, $CDCl_3$) δ: 187.85 (s), 151.95 (s), 148.42 (s), 147.61 (s), 142.61 (s), 138.17 (s), 132.66 (s), 131.15 (s), 127.63 (s), 124.76 (s), 124.21 (s), 108.34 (s), 107.98 (s), 107.82 (s), 101.90. Molecular Formula $C_{18}H_{13}NO_5$ (ESI) Calculated= 323.2995, Observed= 323.2998.

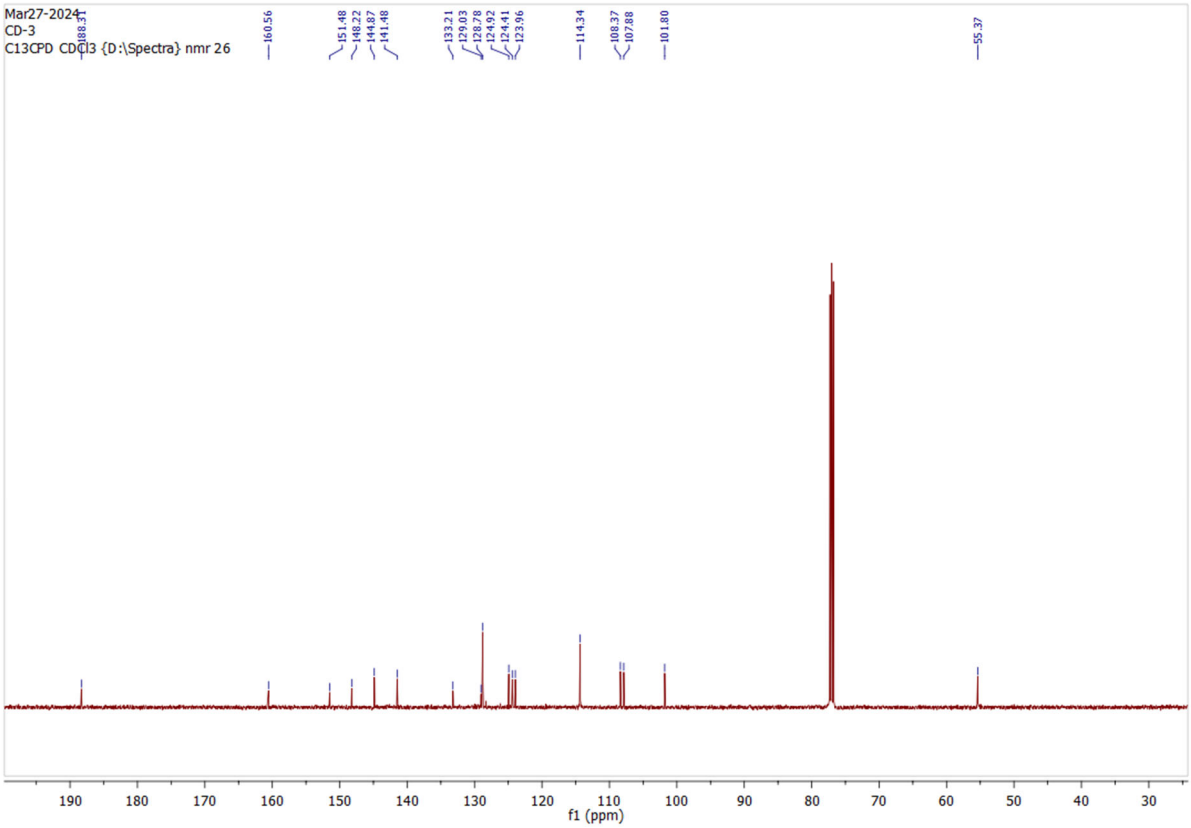


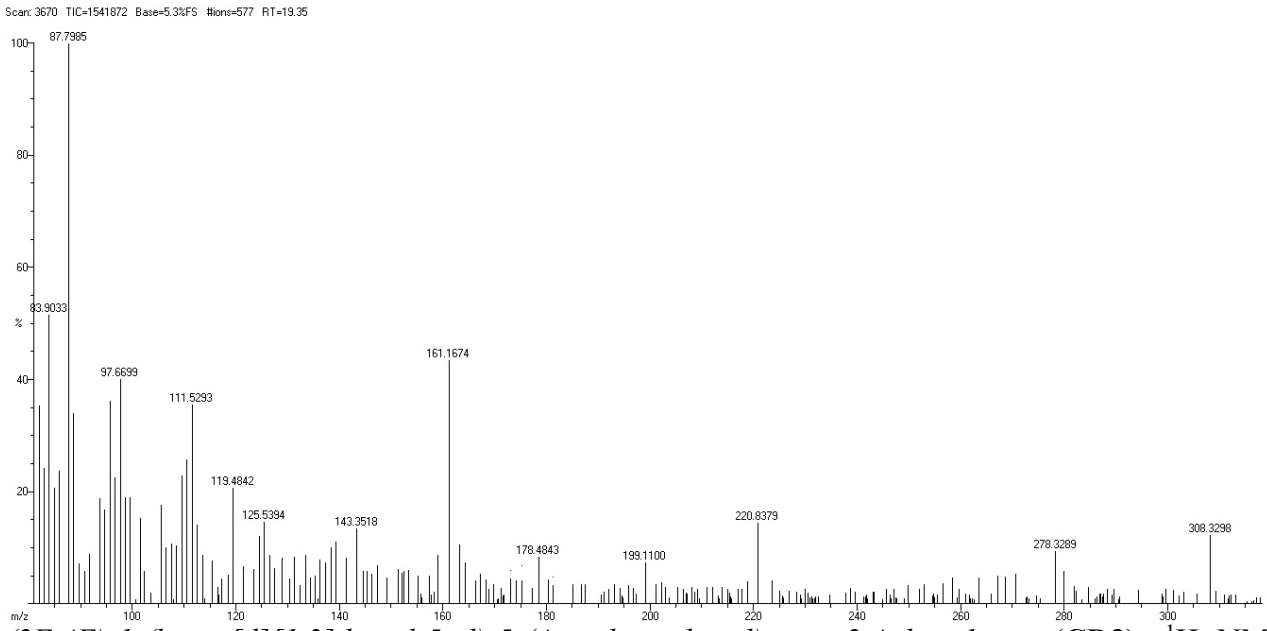


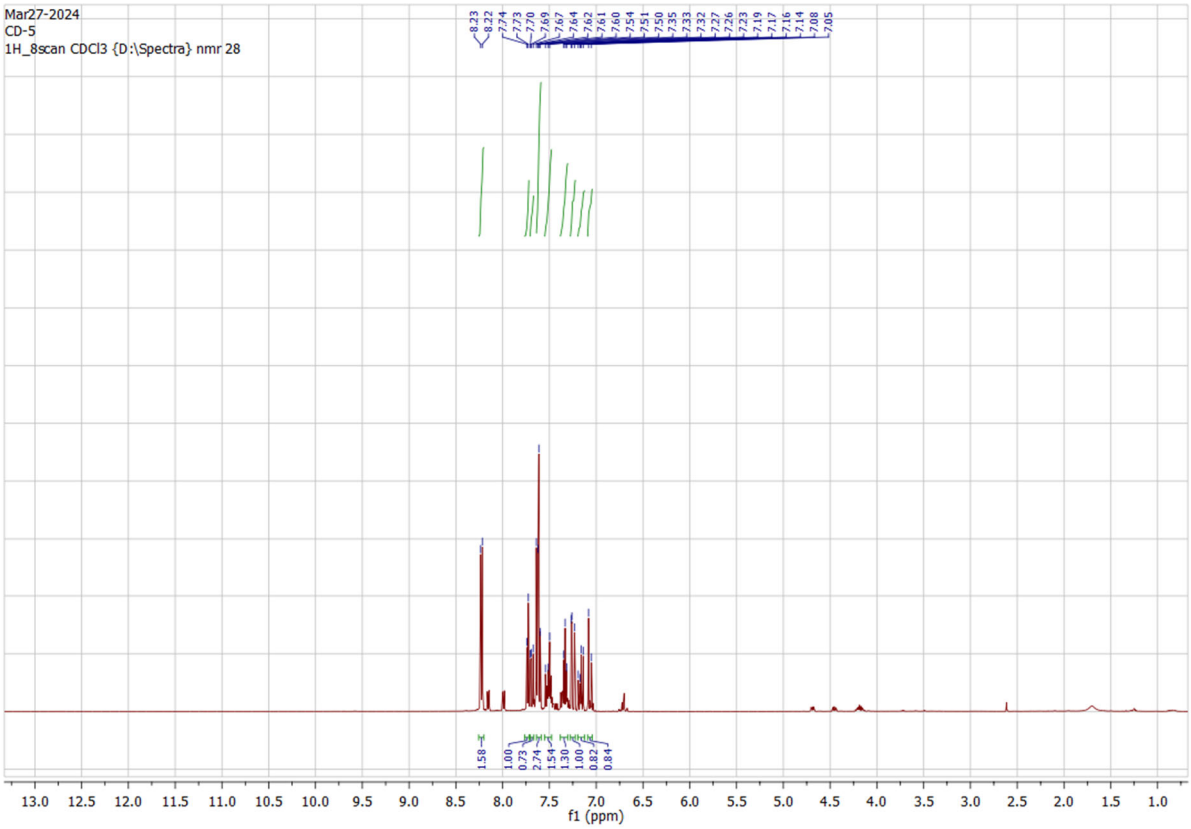

*(2E,4E)-1-(benzo[d][1,3]dioxol-5-yl)-5-(4-bromophenyl)penta-2,4-dien-1-one* (**CD2**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.59 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.57 – 7.52 (m, 2H), 7.50 (d, *J* = 8.7 Hz, 5H), 7.36 (d, *J* = 8.5 Hz, 3H), 7.07 (d, *J* = 14.8 Hz, 3H), 7.00 – 6.93 (m, 2H), 6.89 (t, *J* = 8.9 Hz, 2H), 6.06 (s, 3H). $^{13}$C NMR (500 MHz, CDCl3) δ: 188.31 (s), 160.56 (s), 151.48 (s), 148.22 (s), 144.87 (s), 141.48 (s), 133.21 (s), 129.03 (s), 128.78 (s), 124.92 (s), 124.41 (s), 123.96 (s), 114.34 (s), 108.37 (s), 107.88 (s), 101.80 (s). Molecular Formula $C_{18}H_{13}BrO_3$ (ESI) Calculated= 357.1980, Observed= 357.1998.

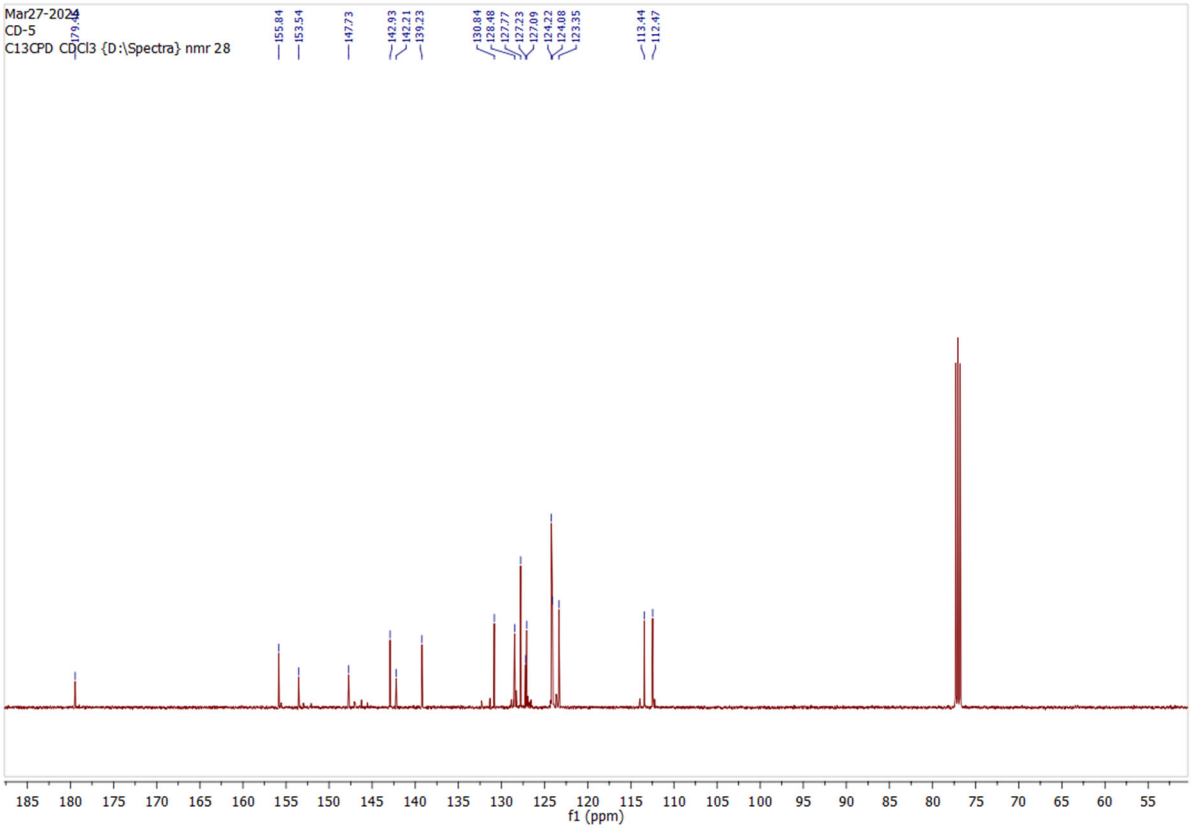

Mar27-2024
CD-3
1H_8scan CDCl3 {D:\Spectra} nmr 26
7.61
7.58
7.58
7.56
7.49
7.49
7.45
7.43
7.02
6.99
6.98
6.95
6.91
6.89
6.88
6.87
6.05
3.84
1.90
2.88
2.15
4.43
2.07
3.13
f1 (ppm)

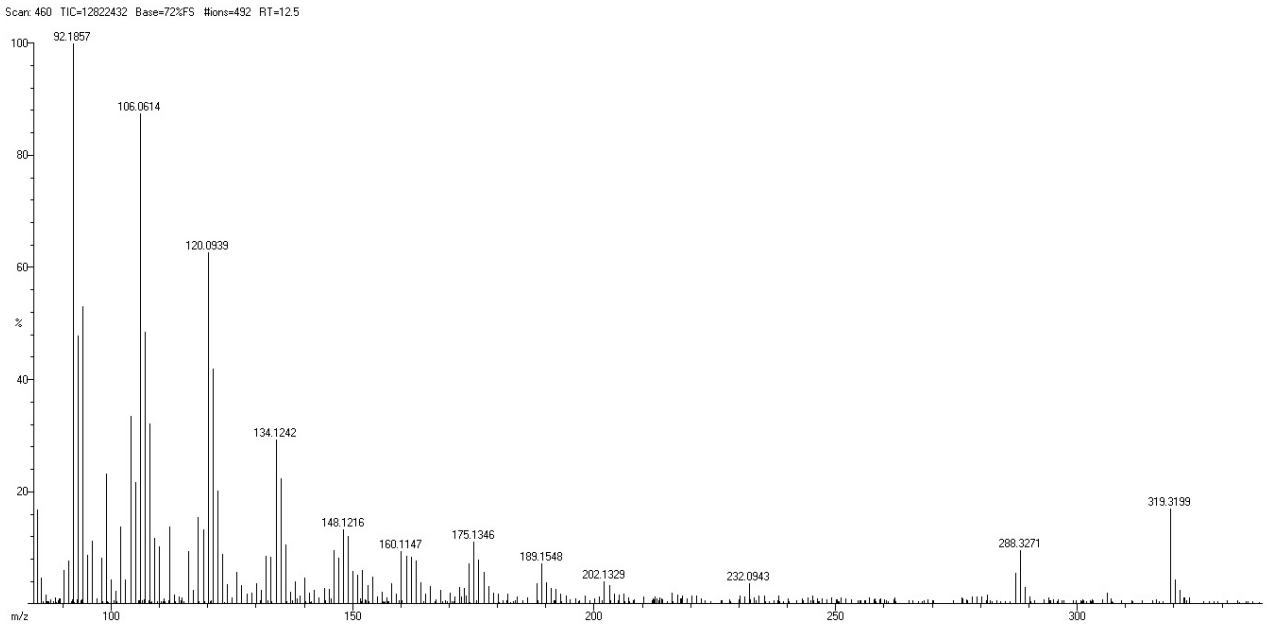

Mar27-2024
CD-3
C13CPD CDCl3 {D:\Spectra} nmr 26
188.31
160.56
151.48
148.22
144.87
141.48
133.21
129.03
128.78
124.92
124.41
123.96
114.34
108.37
107.88
101.80
55.37
f1 (ppm)



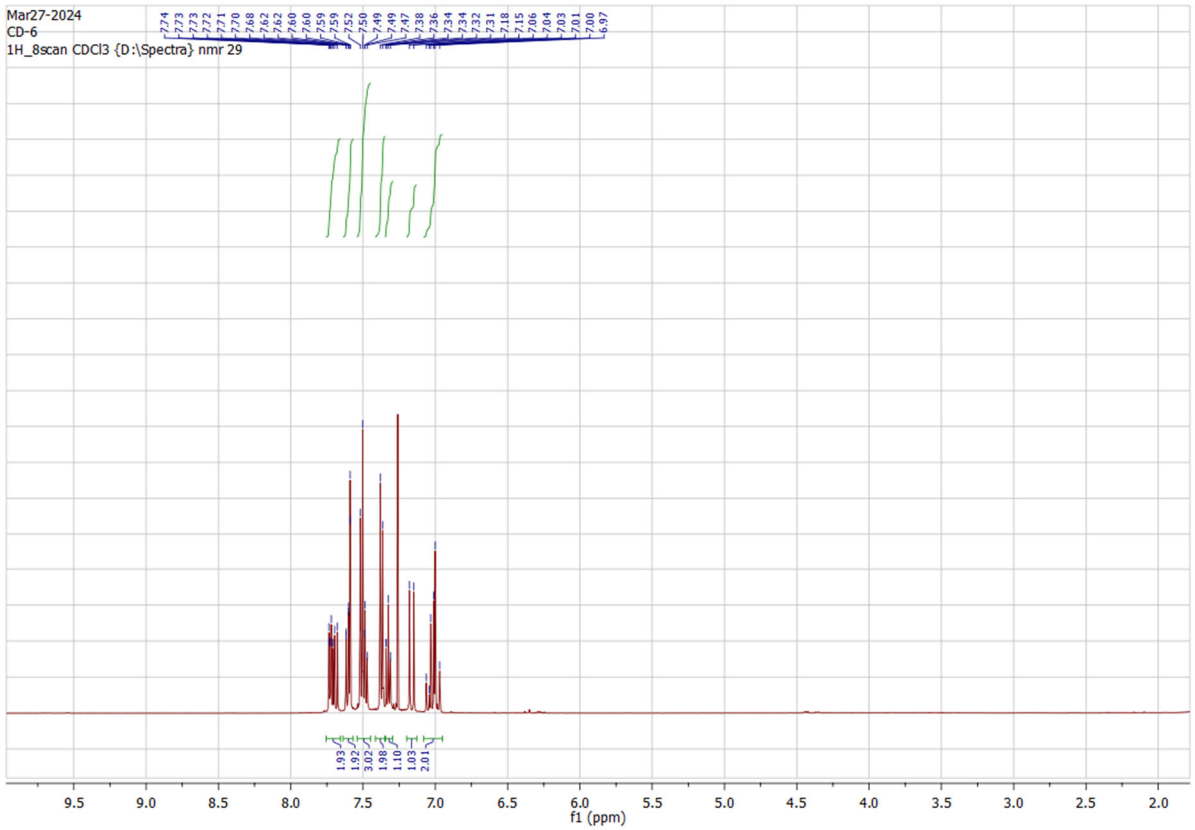

*(2E,4E)-1-(benzo[d][1,3]dioxol-5-yl)-5-(4-methoxyphenyl)penta-2,4-dien-1-one* (**CD3**): $^{1}$H NMR (500 MHz, $CDCl_3$) :δ 7.58 (dd, *J* = 14.3, 11.2 Hz, 2H), 7.47 (dd, *J* = 23.7, 5.2 Hz, 3H), 6.98 (dd, *J* = 19.4, 15.2 Hz, 2H), 6.89 (dd, *J* = 12.7, 8.5 Hz, 4H), 6.05 (s, 2H), 3.84 (s, 3H). $^{13}$C NMR (500 MHz, $CDCl_3$) δ: 188.31 (s), 160.56 (s), 151.48 (s), 148.22 (s), 144.87 (s), 141.48 (s), 133.21 (s), 129.03 (s), 128.78 (s), 124.92 (s), 124.41 (s), 123.96 (s), 114.34 (s), 108.37 (s), 107.88 (s), 101.80 (s), 55.37 (s). Molecular Formula $C_{19}H_{16}NO_4$ (ESI) Calculated= 308.3279, Observed= 308.3298

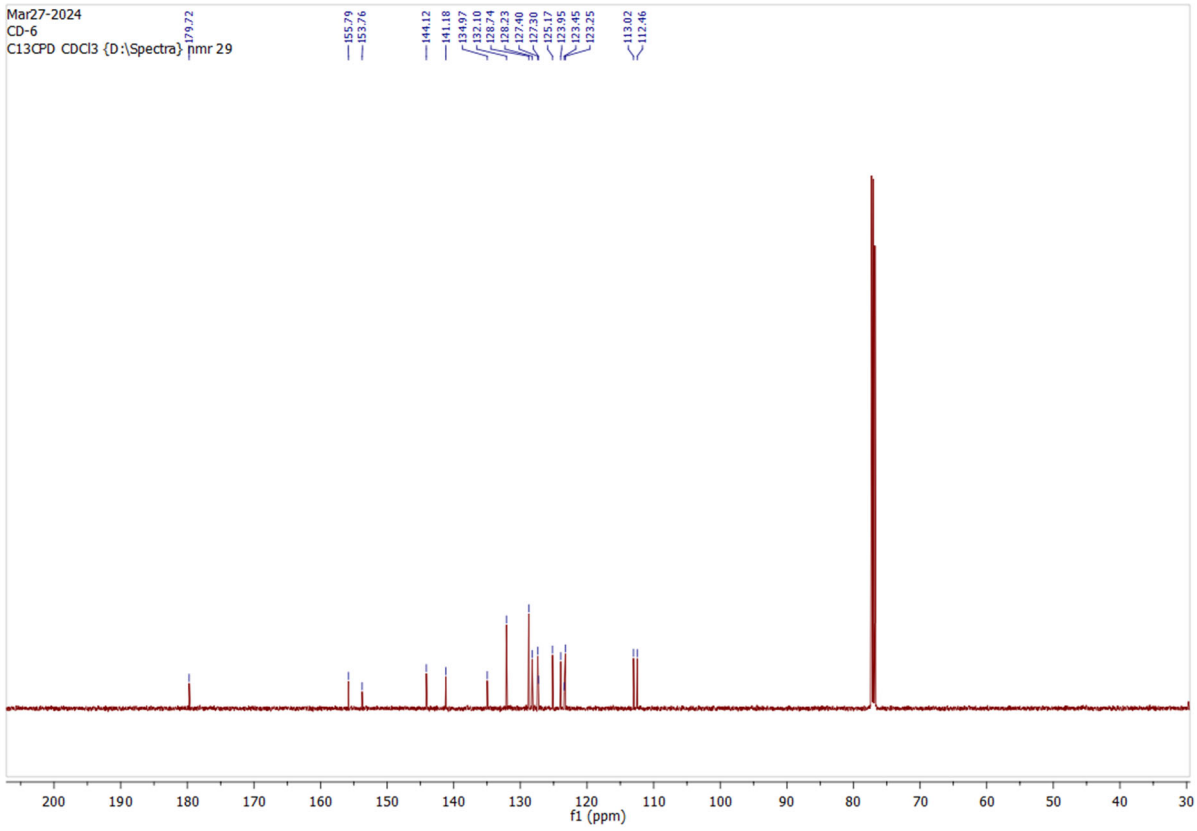

Mar27-2024
CD-5
1H_8scan CDCl3 {D:\Spectra} nmr 28
8.33
8.22
7.74
7.73
7.70
7.69
7.67
7.64
7.62
7.61
7.60
7.54
7.51
7.50
7.35
7.33
7.32
7.27
7.26
7.23
7.19
7.17
7.16
7.14
7.08
7.05
1.58
1.00
0.73
2.74
1.54
1.30
1.00
0.82
0.84
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

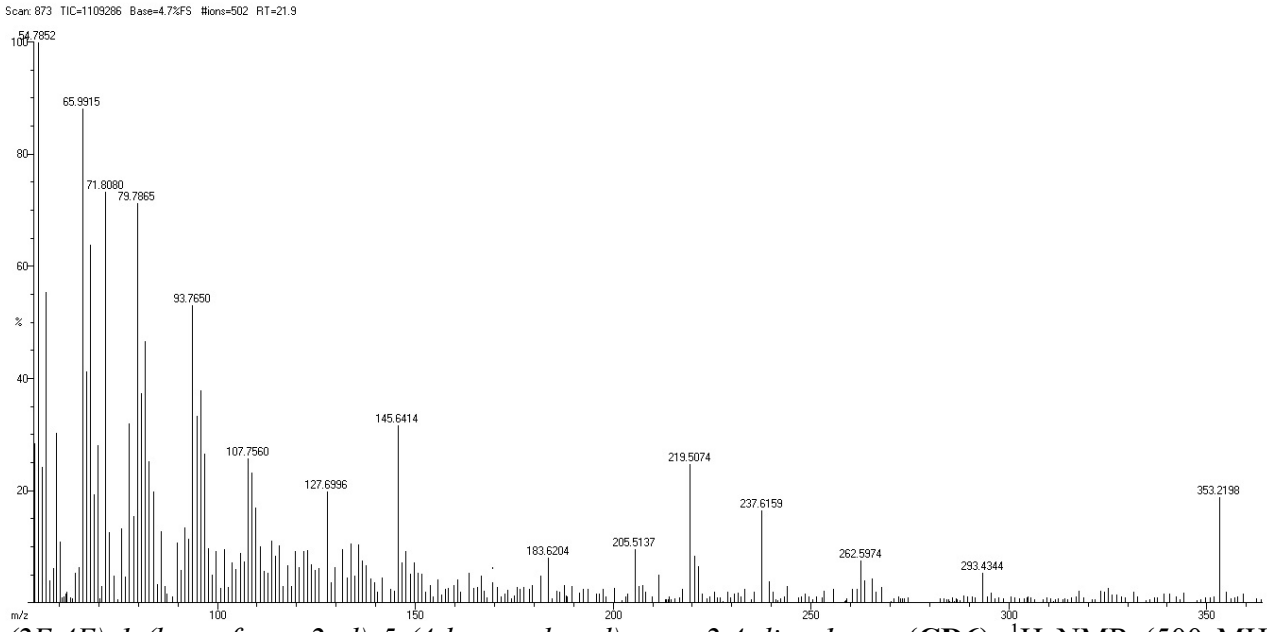

Mar27-2024
CD-5
C13CPD CDCl3 {D:\Spectra} nmr 28
179.44
155.84
153.54
147.73
142.93
142.21
139.23
130.84
128.48
127.77
127.23
127.09
124.22
124.08
123.35
113.44
112.47
185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55
f1 (ppm)



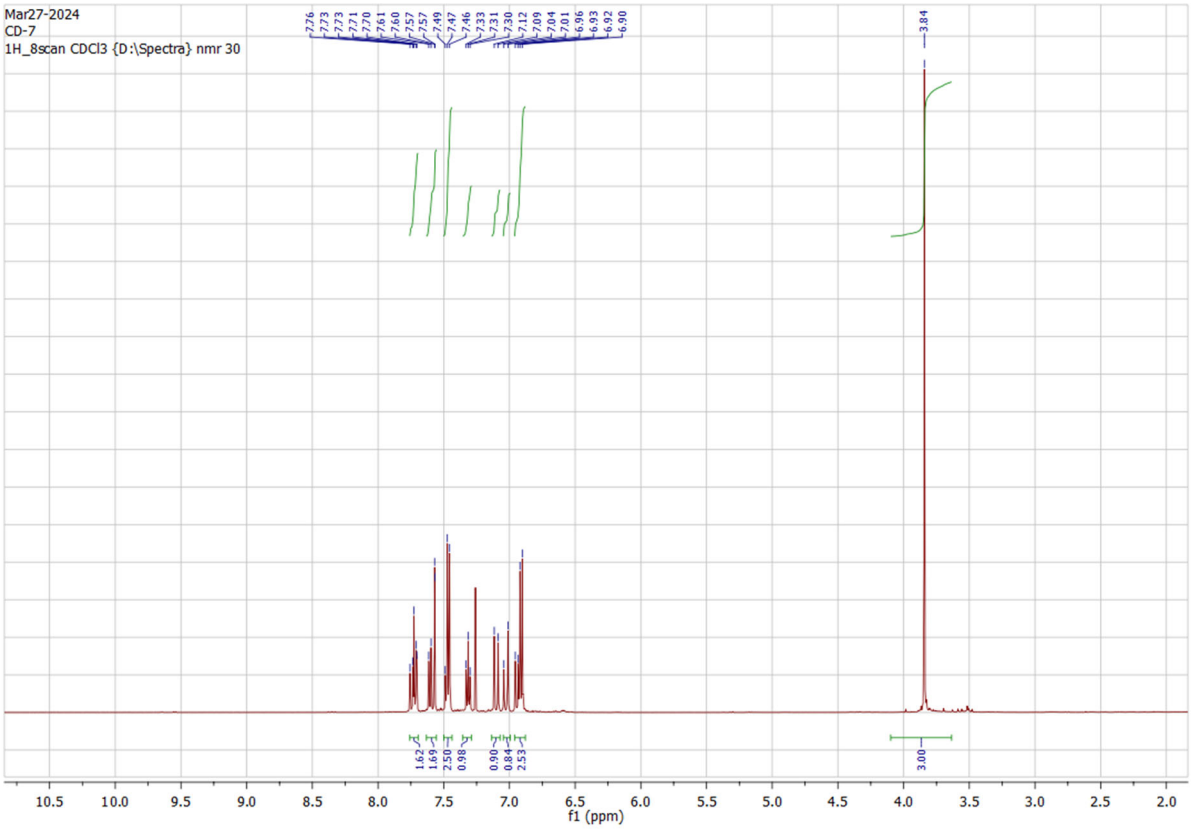

*(2E,4E)-1-(benzofuran-2-yl)-5-(4-nitrophenyl)penta-2,4-dien-1-one* (**CD5**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.23 (d, *J* = 8.8 Hz, 2H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.61 (t, *J* = 6.4 Hz, 3H), 7.55 – 7.48 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.17 (dd, *J* = 15.6, 10.9 Hz, 1H), 7.07 (d, *J* = 15.6 Hz, 1H). $^{13}$C NMR (500 MHz, $CDCl_3$) δ: 179.45 (s), 155.84 (s), 153.54 (s), 147.73 (s), 142.93 (s), 142.21 (s), 139.23 (s), 130.84 (s), 128.48 (s), 127.77 (s), 127.16 (d, J = 17.0 Hz), 124.15 (d, J = 16.9 Hz), 123.35 (s), 113.44 (s), 112.47 (s). Molecular Formula $C_{19}H_{13}NO_4$ (ESI) Calculated= 319.3108, Observed= 319.3199

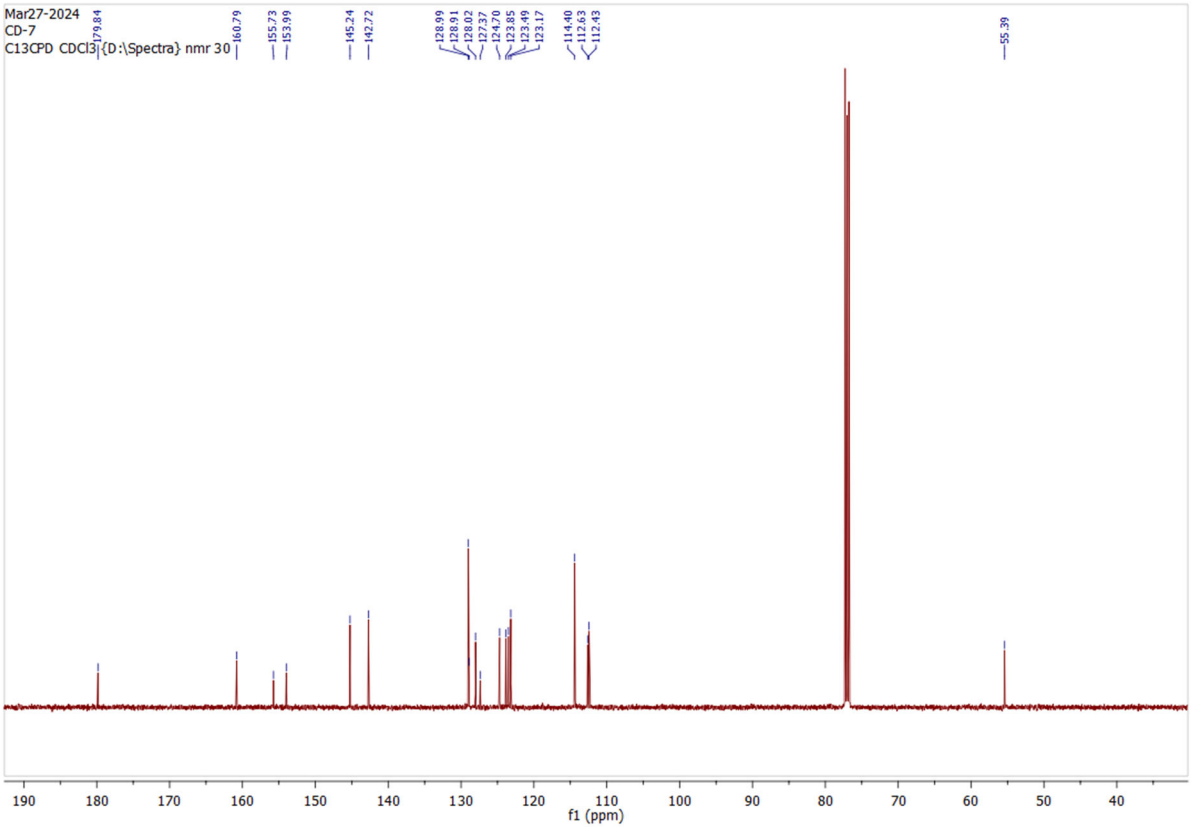


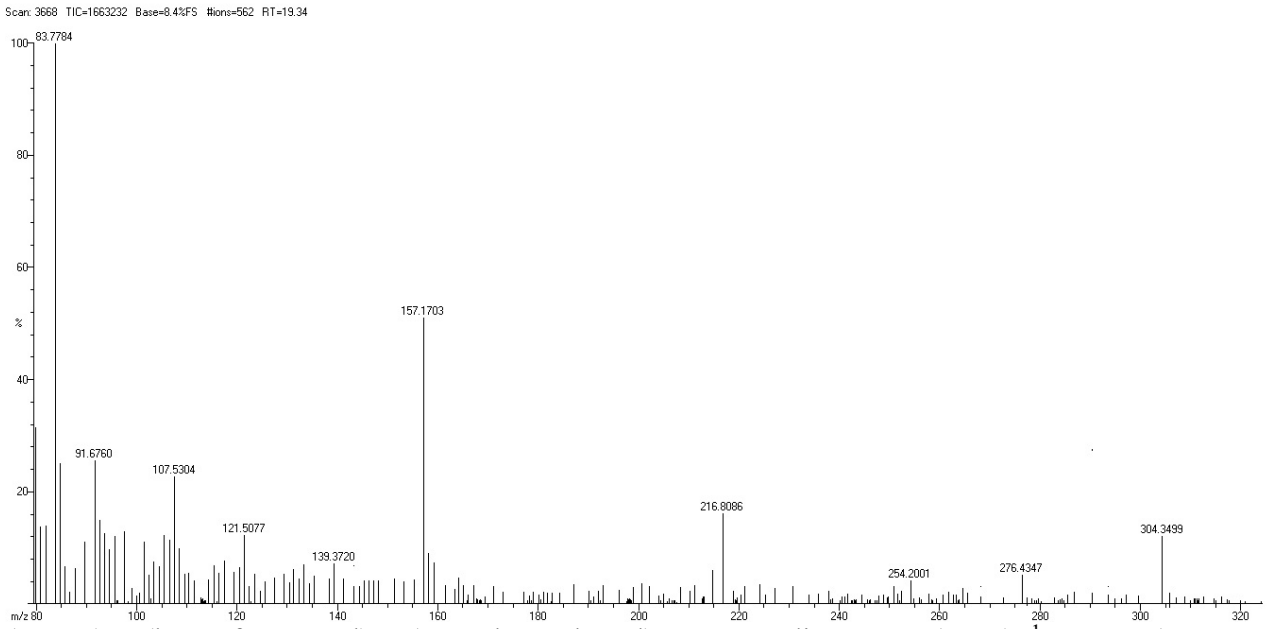


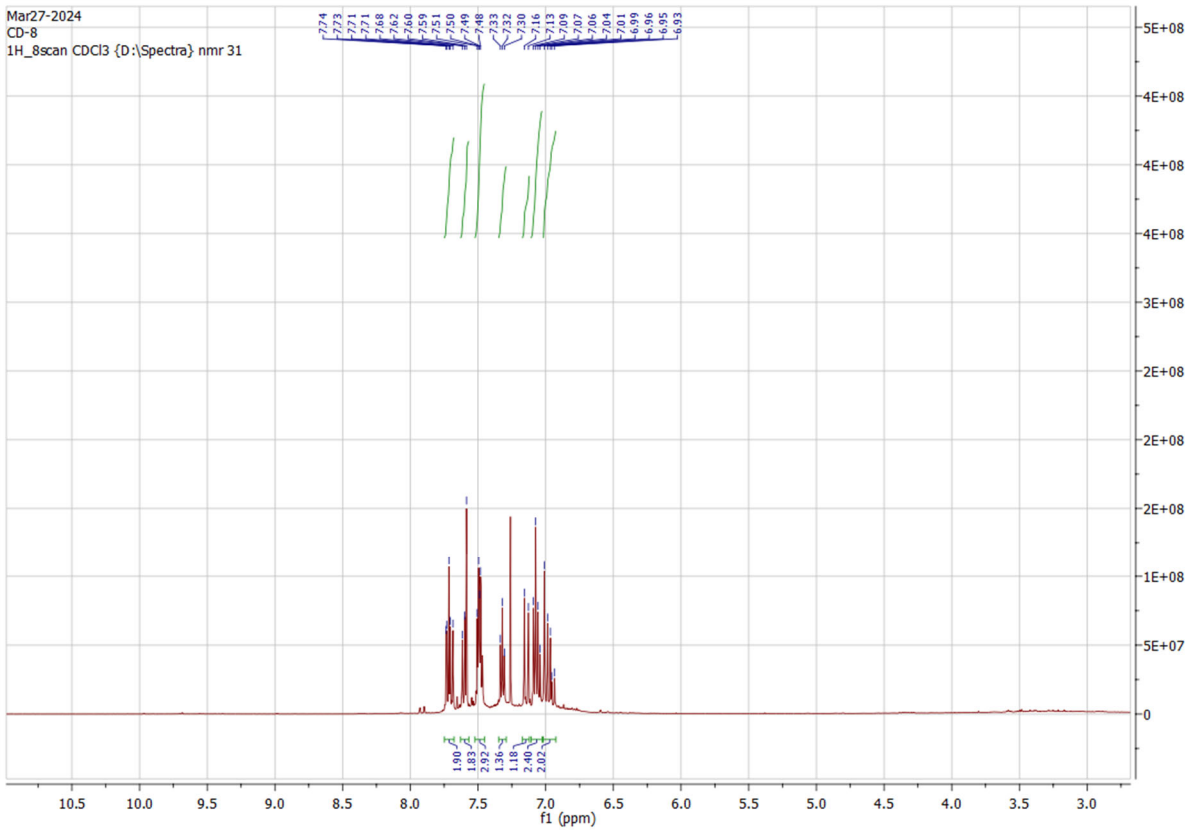

*(2E,4E)-1-(benzofuran-2-yl)-5-(4-bromophenyl)penta-2,4-dien-1-one* (**CD6**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.76 – 7.66 (m, 2H), 7.64 – 7.57 (m, 2H), 7.54 – 7.45 (m, 3H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.40 – 7.29 (m, 3H), 7.33 (dd, *J* = 11.5, 4.4 Hz, 1H), 7.16 (d, *J* = 15.0 Hz, 1H), 7.08 – 6.95 (m, 2H). $^{13}$C NMR (500 MHz, $CDCl_3$) δ: 179.72 (s), 155.79 (s), 153.76 (s), 144.12 (s), 141.18 (s), 134.97 (s), 132.10 (s), 128.74 (s), 128.23 (s), 127.35 (d, J = 12.3 Hz), 125.17 (s), 123.95 (s), 123.45 (s), 123.25 (s), 113.02 (s), 112.46 (s). Molecular Formula $C_{19}H_{13}BrO_2$ (ESI) Calculated= 353.2093, Observed= 353.2198.

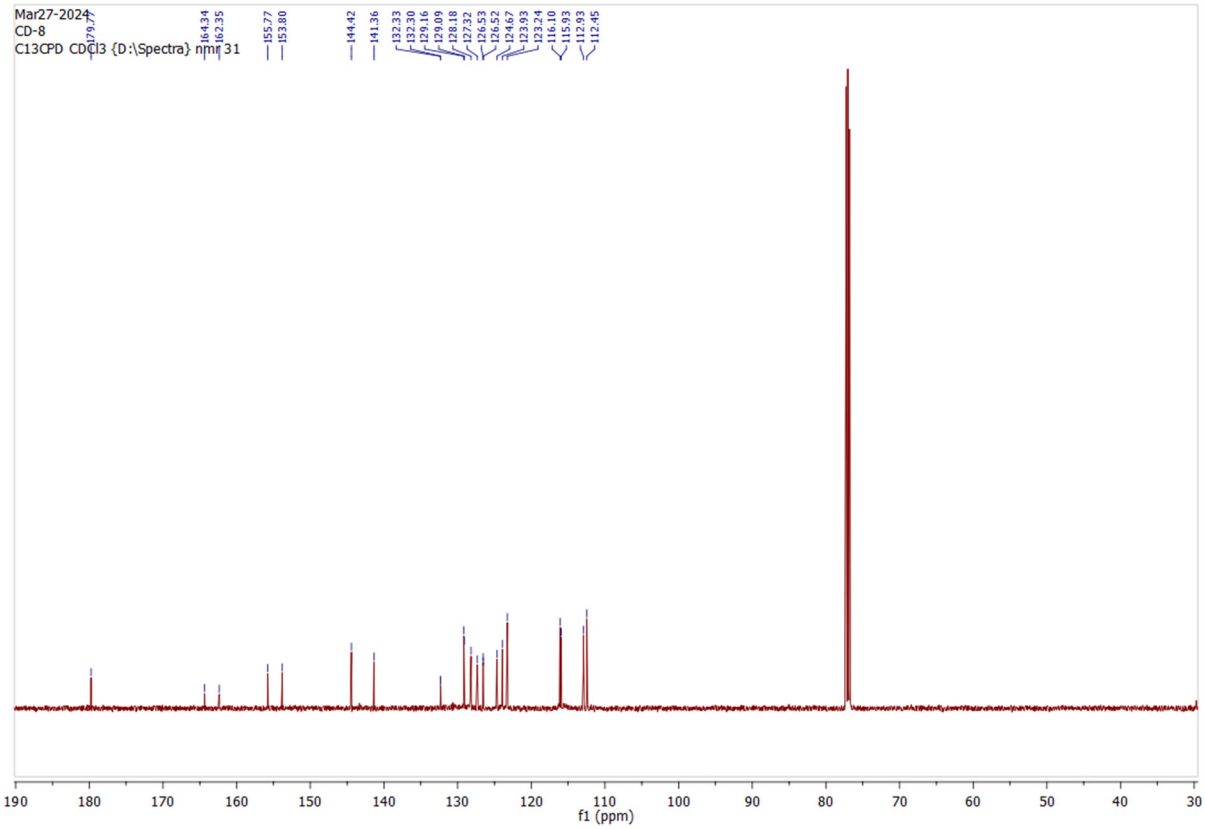

Mar27-2024
CD-7
1H_8scan CDCl3 {D:\Spectra} nmr 30
7.76
7.73
7.73
7.71
7.70
7.61
7.60
7.57
7.57
7.49
7.47
7.46
7.33
7.31
7.30
7.12
7.09
7.04
7.01
6.96
6.93
6.92
6.90
3.84
1.62
1.69
2.50
0.98
0.90
0.84
2.53
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)

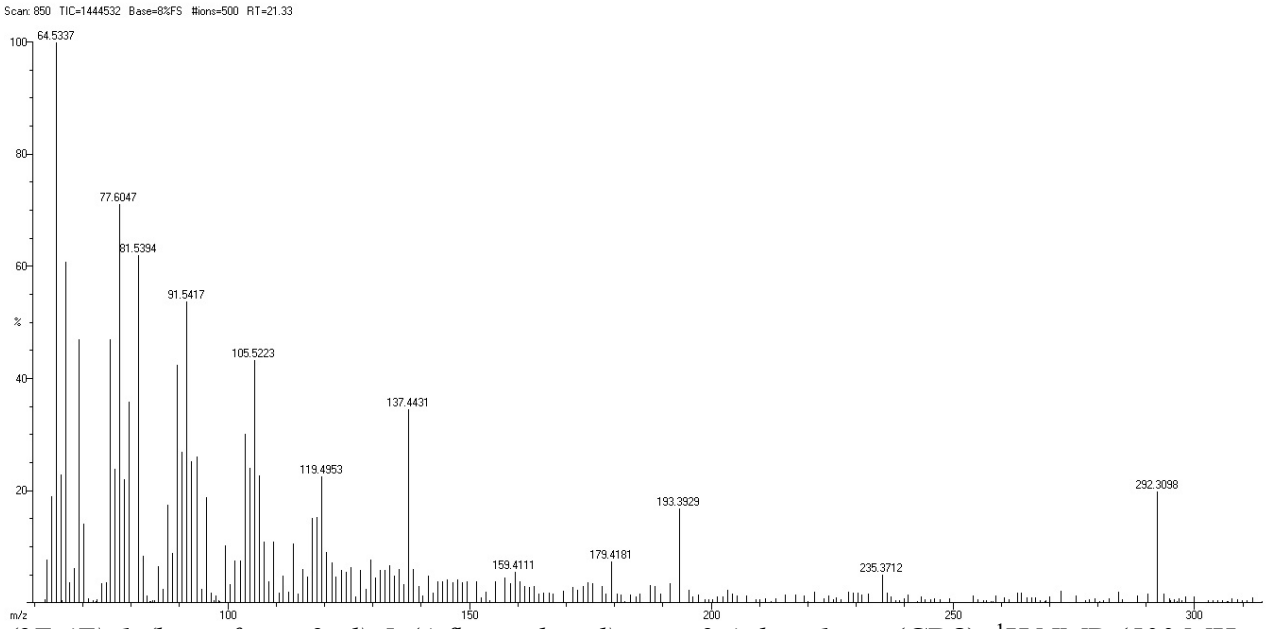

Mar27-2024
CD-7
C13CPD CDCl3 {D:\Spectra} nmr 30
179.84
160.79
155.73
153.99
145.24
142.72
128.99
128.91
128.02
127.37
124.70
123.85
123.49
123.17
114.40
112.63
112.43
55.39
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)



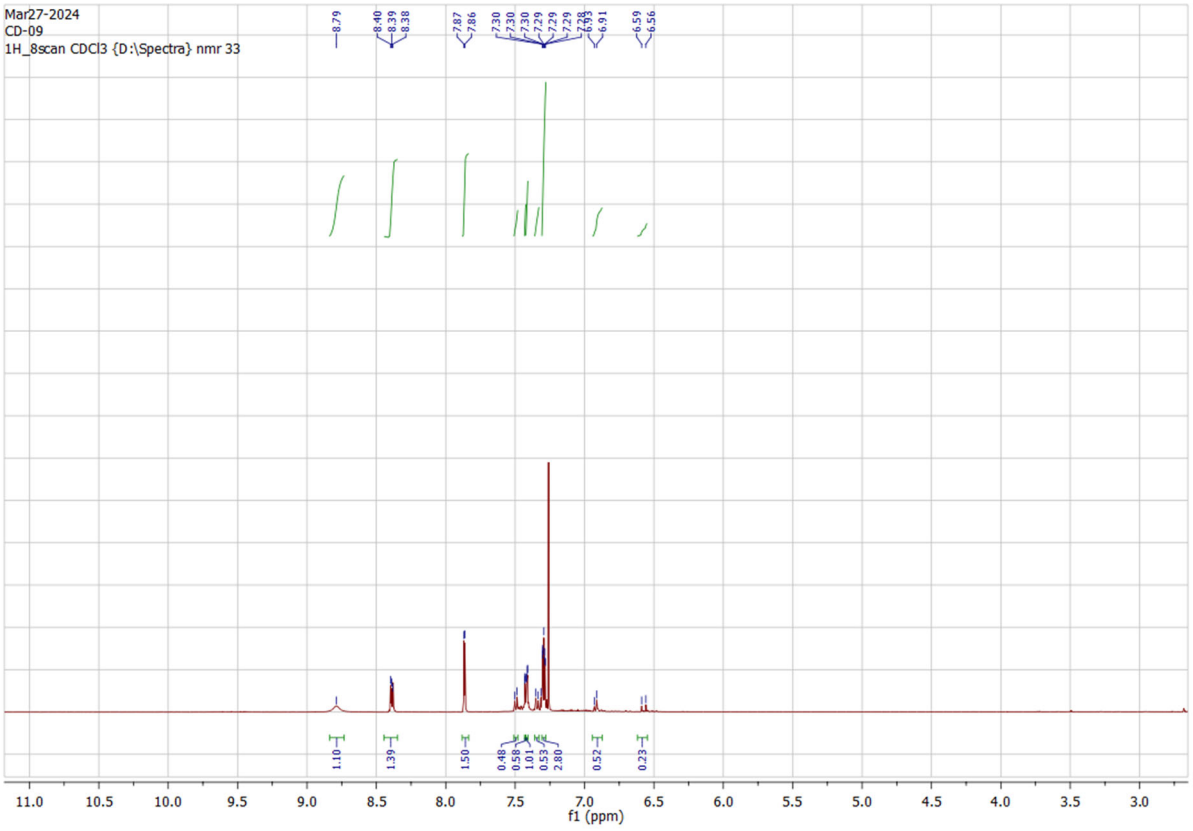

(2E,4E)-1-(benzofuran-2-yl)-5-(4-methoxyphenyl)penta-2,4-dien-1-one (**CD7**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.76 – 7.69 (m, 2H), 7.59 (dd, *J* = 18.3, 5.0 Hz, 2H), 7.47 (t, *J* = 8.3 Hz, 3H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 14.9 Hz, 1H), 7.03 (d, *J* = 15.5 Hz, 1H), 6.93 (dd, *J* = 16.7, 10.0 Hz, 3H), 3.84 (s, 3H). $^{13}$C NMR (500 MHz, $CDCl_3$) δ: 179.84 (s), 160.79 (s), 155.73 (s), 153.99 (s), 145.24 (s), 142.72 (s), 128.95 (d, J = 11.1 Hz), 128.02 (s), 127.37 (s), 124.70 (s), 123.85 (s), 123.49 (s), 123.17 (s), 114.40 (s), 112.63 (s), 112.43 (s), 55.39 (s). Molecular Formula $C_{20}H_{16}O_3$ (ESI) Calculated= 304.3392, Observed= 304.3499.

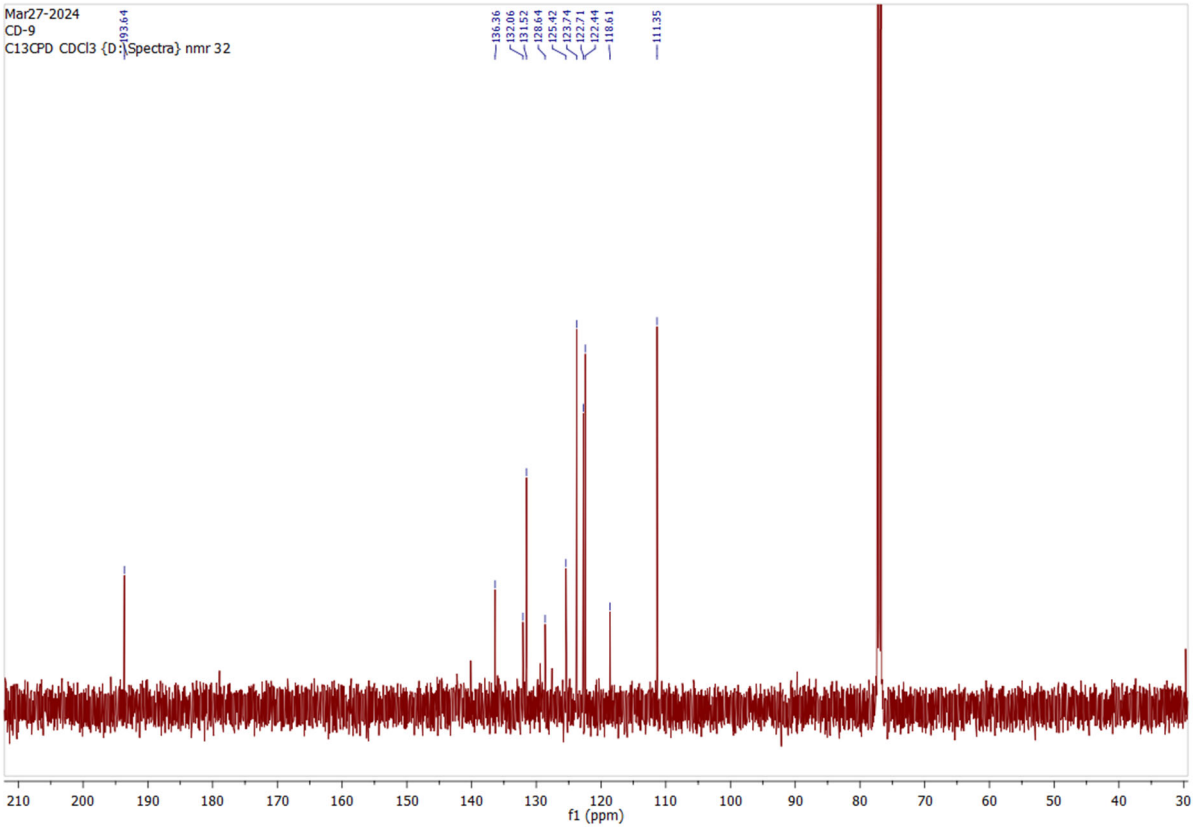


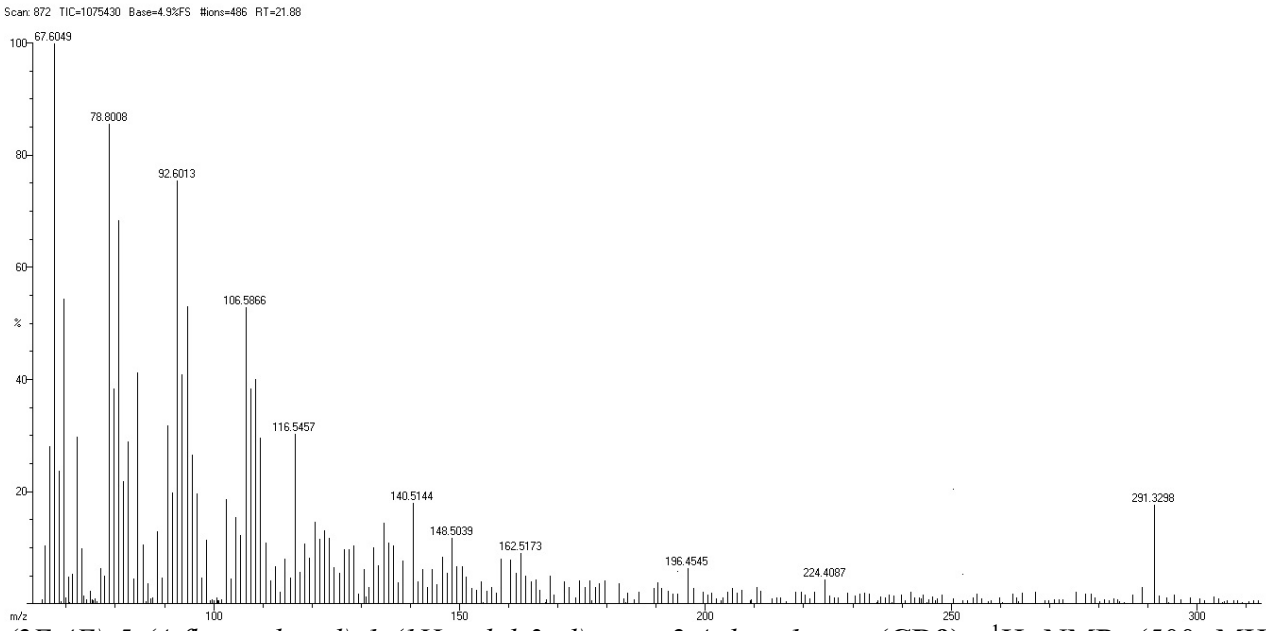


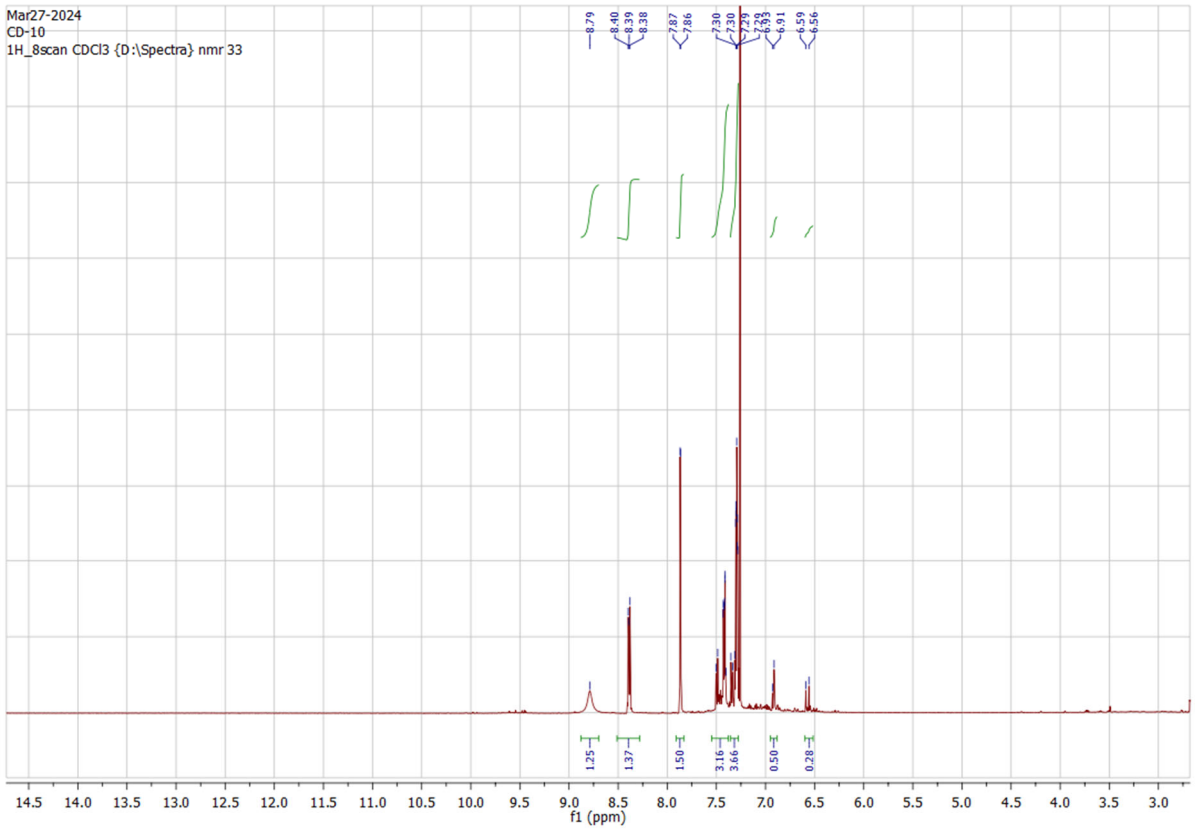

*(2E,4E)-1-(benzofuran-2-yl)-5-(4-fluorophenyl)penta-2,4-dien-1-one* (**CD8**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.75 – 7.68 (m, 2H), 7.63 – 7.57 (m, 2H), 7.49 (dd, *J* = 7.9, 4.4 Hz, 3H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.14 (d, *J* = 15.0 Hz, 1H), 7.07 (dd, *J* = 16.8, 8.2 Hz, 2H), 7.02 – 6.92 (m, 2H). 13C NMR (500 MHz, $CDCl_3$) δ: 179.77 (s), 164.34 (s), 162.35 (s), 155.77 (s), 153.80 (s), 144.42 (s), 141.36 (s), 132.32 (d, J = 3.3 Hz), 129.12 (d, J = 8.6 Hz), 128.18 (s), 127.32 (s), 126.52 (d, J = 2.2 Hz), 124.67 (s), 123.93 (s), 123.24 (s), 116.10 (s), 115.93 (s), 112.93 (s), 112.45 (s). Molecular Formula $C_{19}H_{13}FO_2$ (ESI) Calculated= 292.3037, Observed= 292.3098

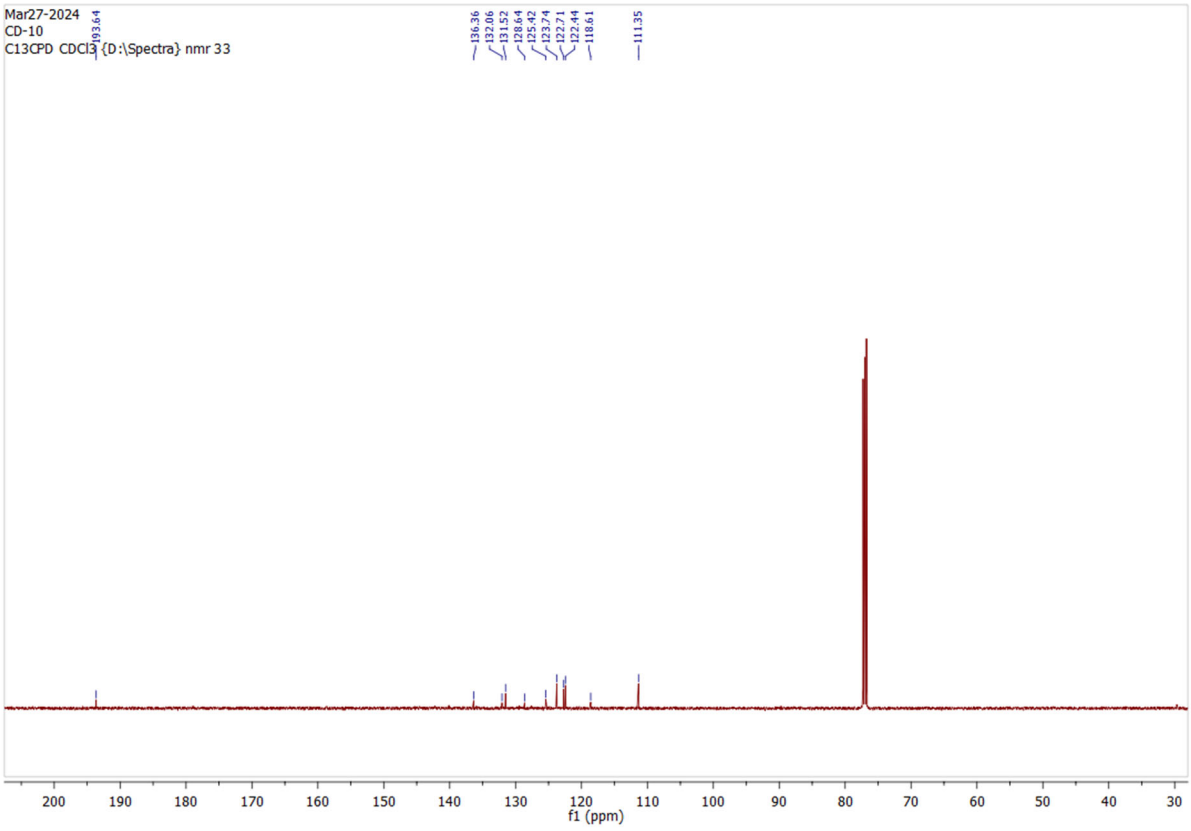

Mar27-2024
CD-09
1H_8scan CDCl3 {D:\Spectra} nmr 33
8.79
8.40
8.39
8.38
7.87
7.86
7.30
7.30
7.30
7.29
7.29
7.29
7.28
6.93
6.91
6.59
6.56
1.10
1.39
1.50
0.48
0.58
1.01
0.53
2.80
0.52
0.23
f1 (ppm)

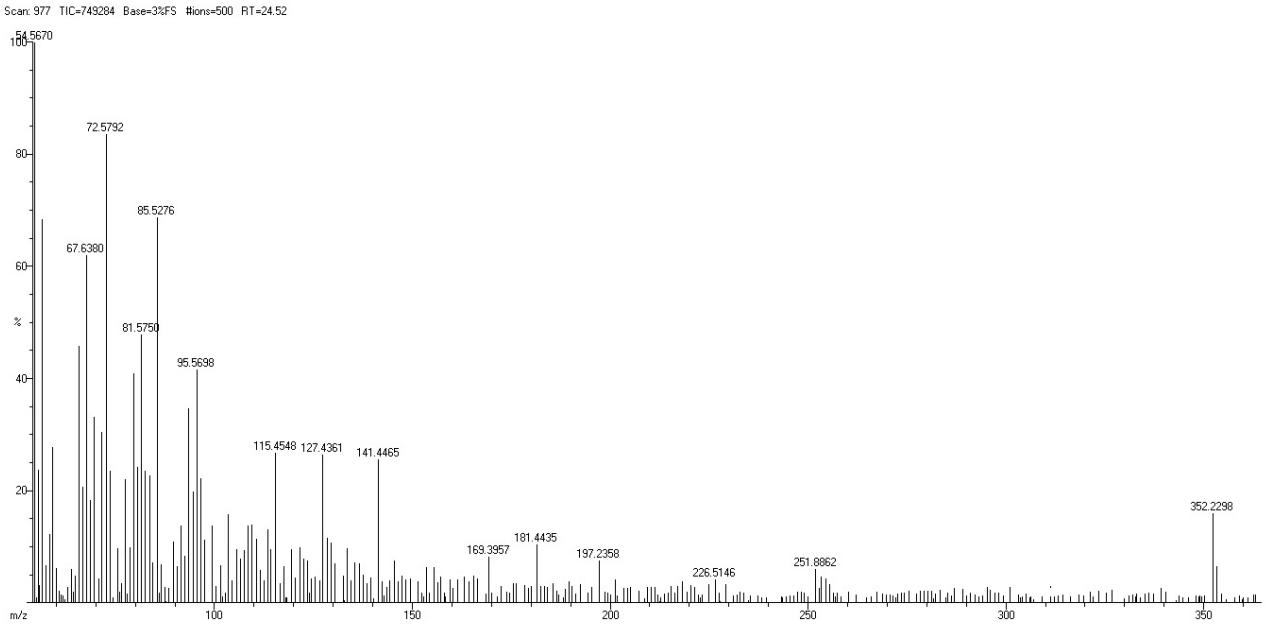

Mar27-2024
CD-9
C13CPD CDCl3 {D:\Spectra} nmr 32
193.64
136.36
132.06
131.52
128.64
125.42
123.74
122.71
122.44
118.61
111.35
f1 (ppm)



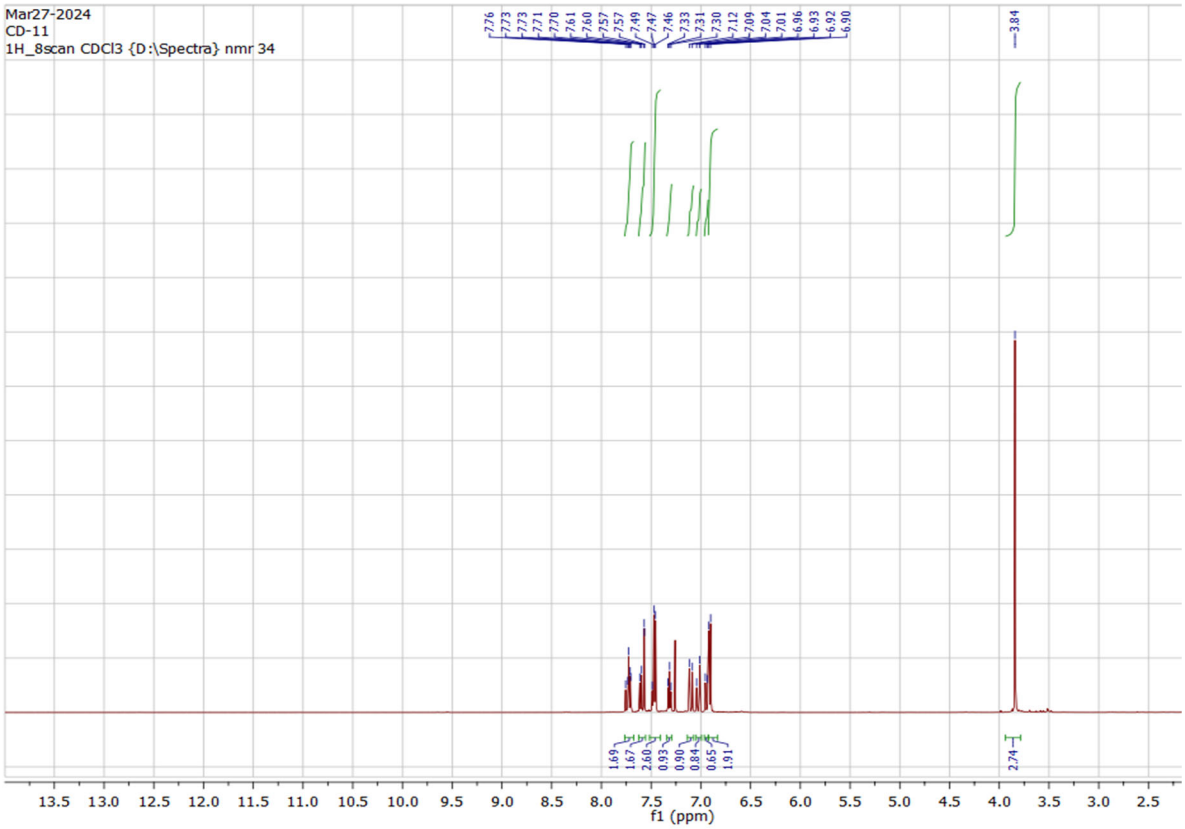

*(2E,4E)-5-(4-fluorophenyl)-1-(1H-indol-3-yl)penta-2,4-dien-1-one* (**CD9**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.79 (s, 1H), 8.44 – 8.35 (m, 1H), 7.87 (d, *J* = 3.0 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.43 – 7.42 (m, 1H), 7.41 (dd, *J* = 3.2, 1.0 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.31 – 7.28 (m, 3H), 6.92 (d, *J* = 8.5 Hz, 1H), 6.57 (d, *J* = 15.2 Hz, 1H). 13C NMR (500 MHz, $CDCl_3$) δ: 193.64 (s), 136.36 (s), 132.06 (s), 131.52 (s), 128.64 (s), 125.42 (s), 123.74 (s), 122.71 (s), 122.44 (s), 118.61 (s), 111.35 (s). Molecular Formula $C_{19}H_{14}FNO$ (ESI) Calculated= 291.3189, Observed= 291.3298.

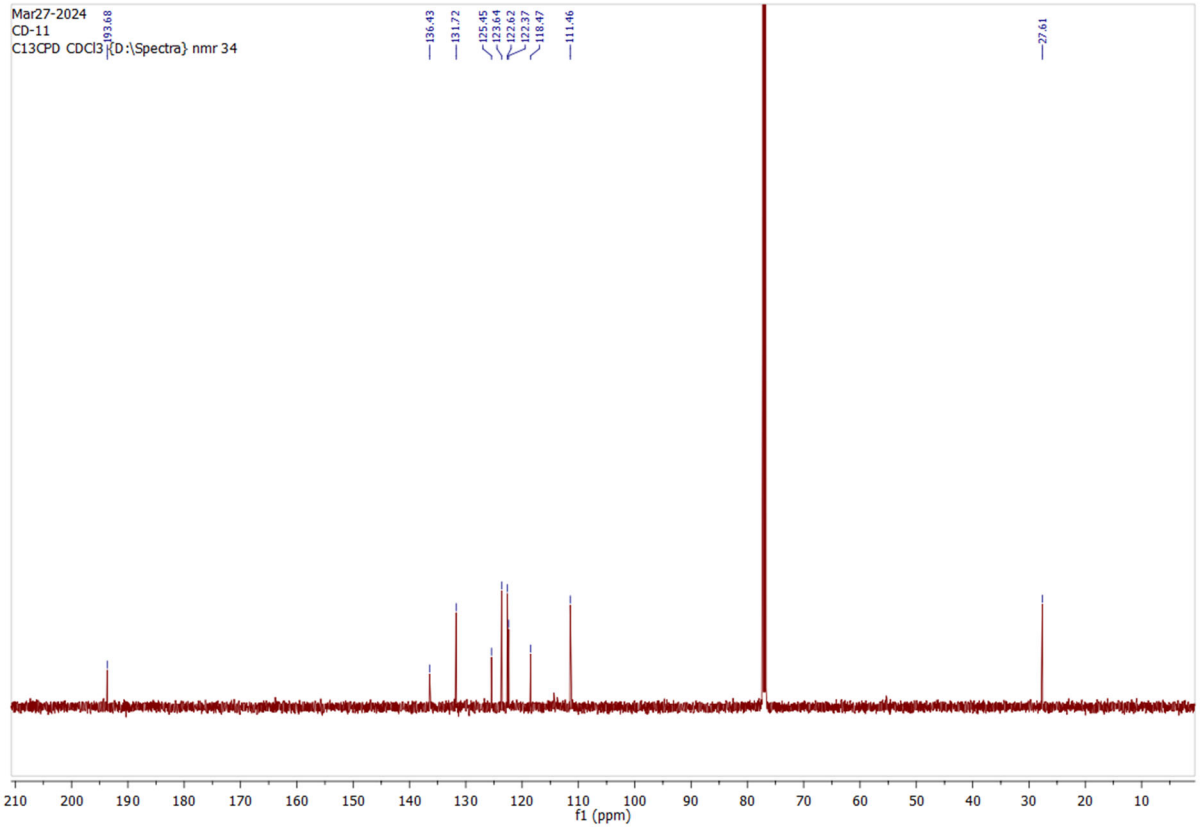


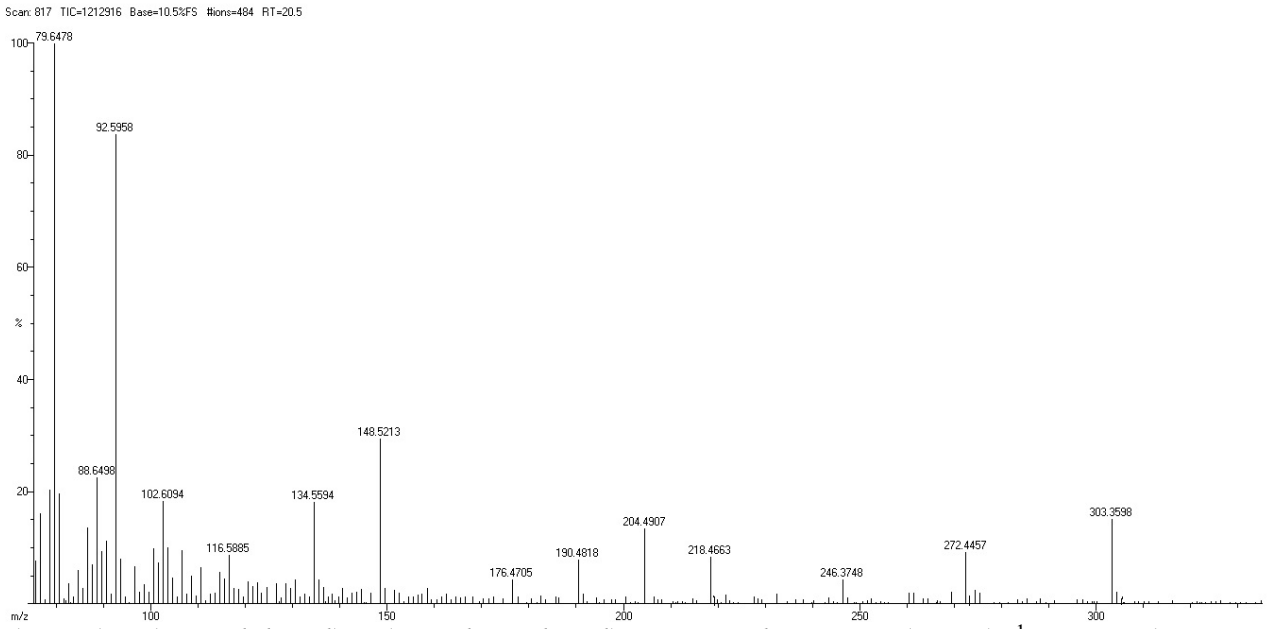


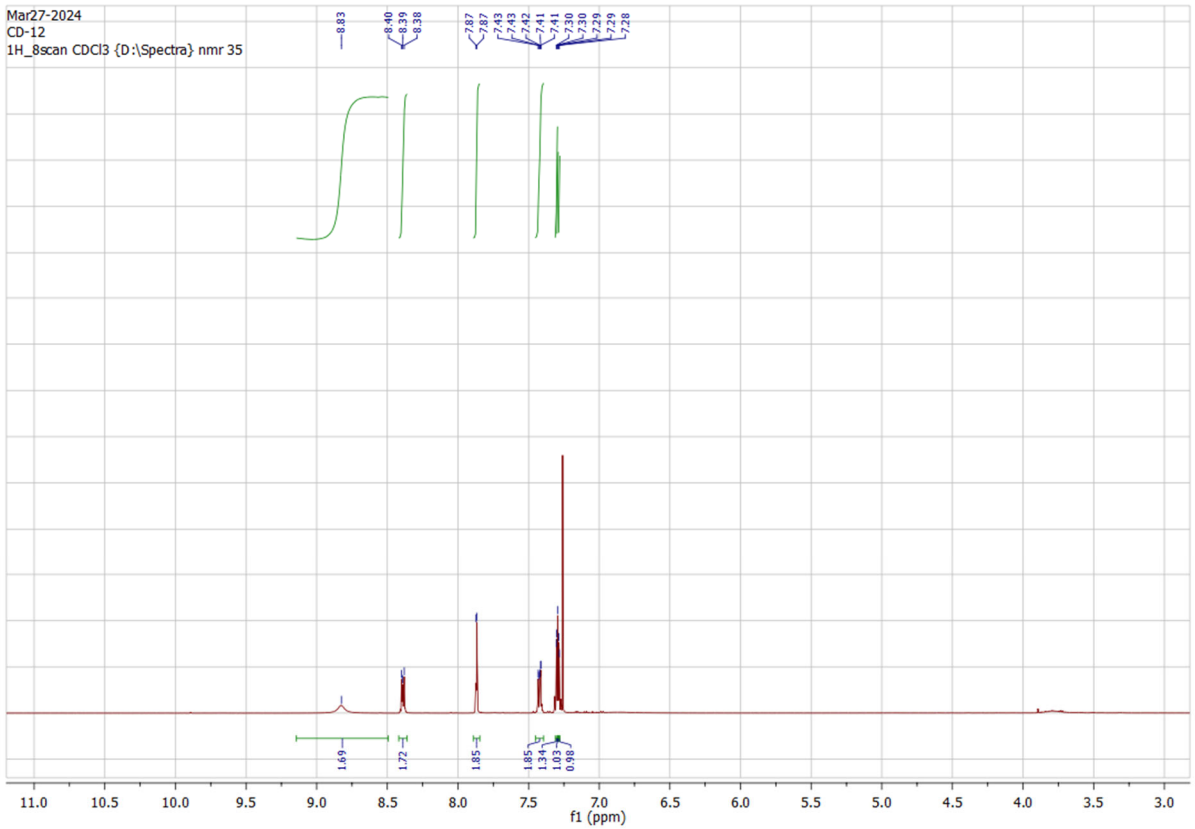

*(2E,4E)-5-(4-bromophenyl)-1-(1H-indol-3-yl)penta-2,4-dien-1-one* (**CD10**): 1H NMR (500 MHz, CDCl3) δ: 8.79 (s, 1H), 8.51 – 8.28 (m, 1H), 7.87 (d, J = 3.0 Hz, 2H), 7.55 – 7.38 (m, 3H), 7.36 – 7.28 (m, 4H), 6.92 (d, J = 8.5 Hz, 1H), 6.57 (d, J = 15.2 Hz, 1H). 13C NMR (500 MHz, CDCl3) δ: 193.64 (s), 136.36 (s), 132.06 (s), 131.52 (s), 128.64 (s), 125.42 (s), 123.74 (s), 122.71 (s), 122.44 (s), 118.61 (s), 111.35 (s). Molecular Formula $C_{19}H_{14}BrNO$ (ESI) Calculated= 352.2245, Observed= 352.2298.

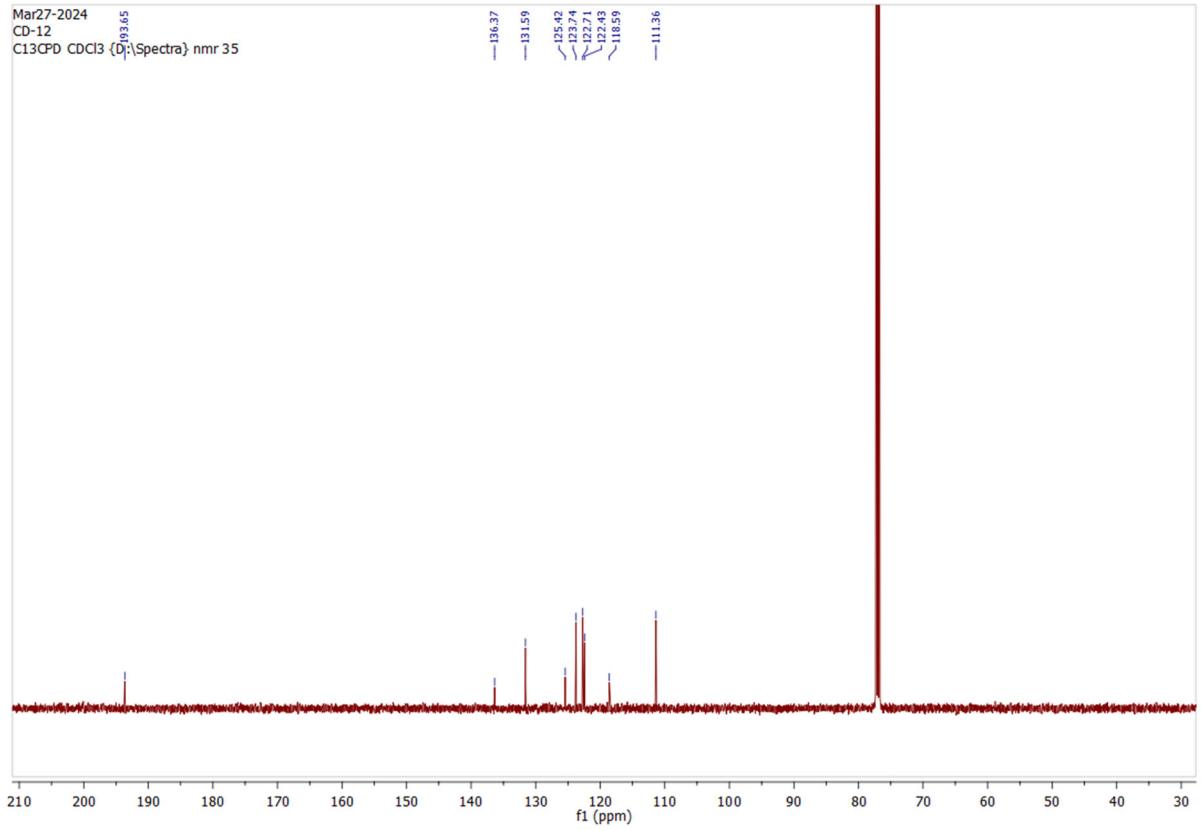

Mar27-2024
CD-11
1H_8scan CDCl3 {D:\Spectra} nmr 34
7.76
7.73
7.73
7.71
7.70
7.61
7.60
7.57
7.57
7.49
7.47
7.46
7.33
7.31
7.30
7.12
7.09
7.04
7.01
6.96
6.93
6.92
6.90
3.84
1.69
1.67
2.60
0.93
0.90
0.84
0.65
1.91
2.74
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
f1 (ppm)

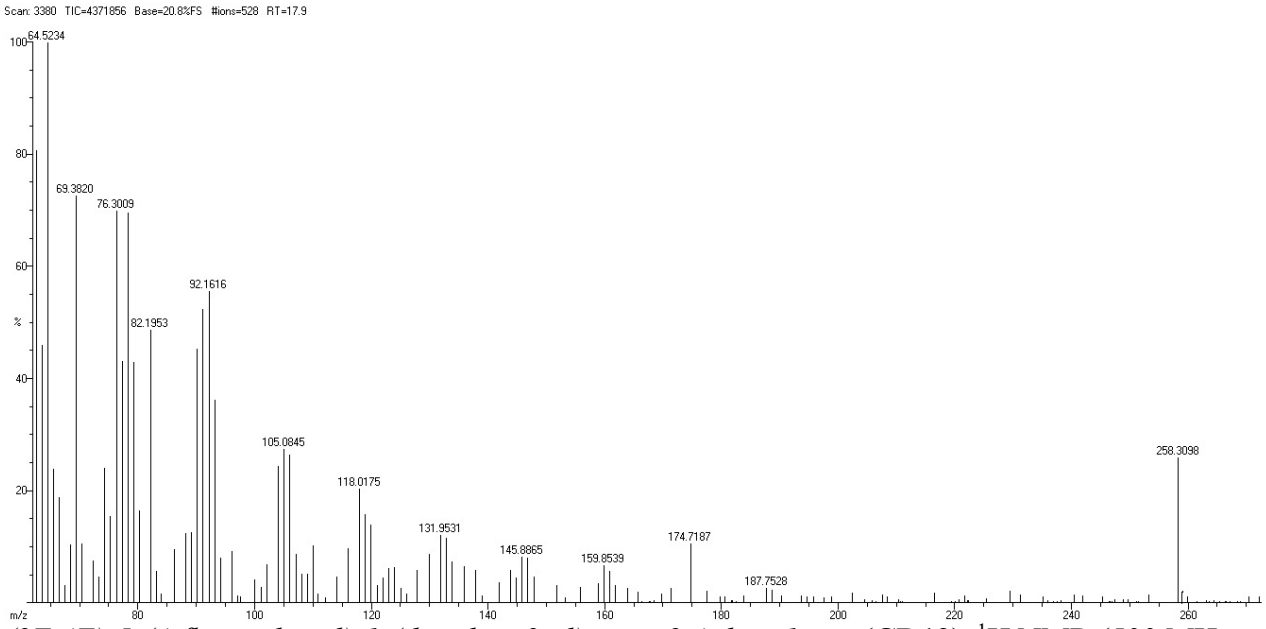

Mar27-2024
CD-11
C13CPD CDCl3 {D:\Spectra} nmr 34
193.68
136.43
131.72
125.45
123.64
122.62
122.37
118.47
111.46
27.61
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)



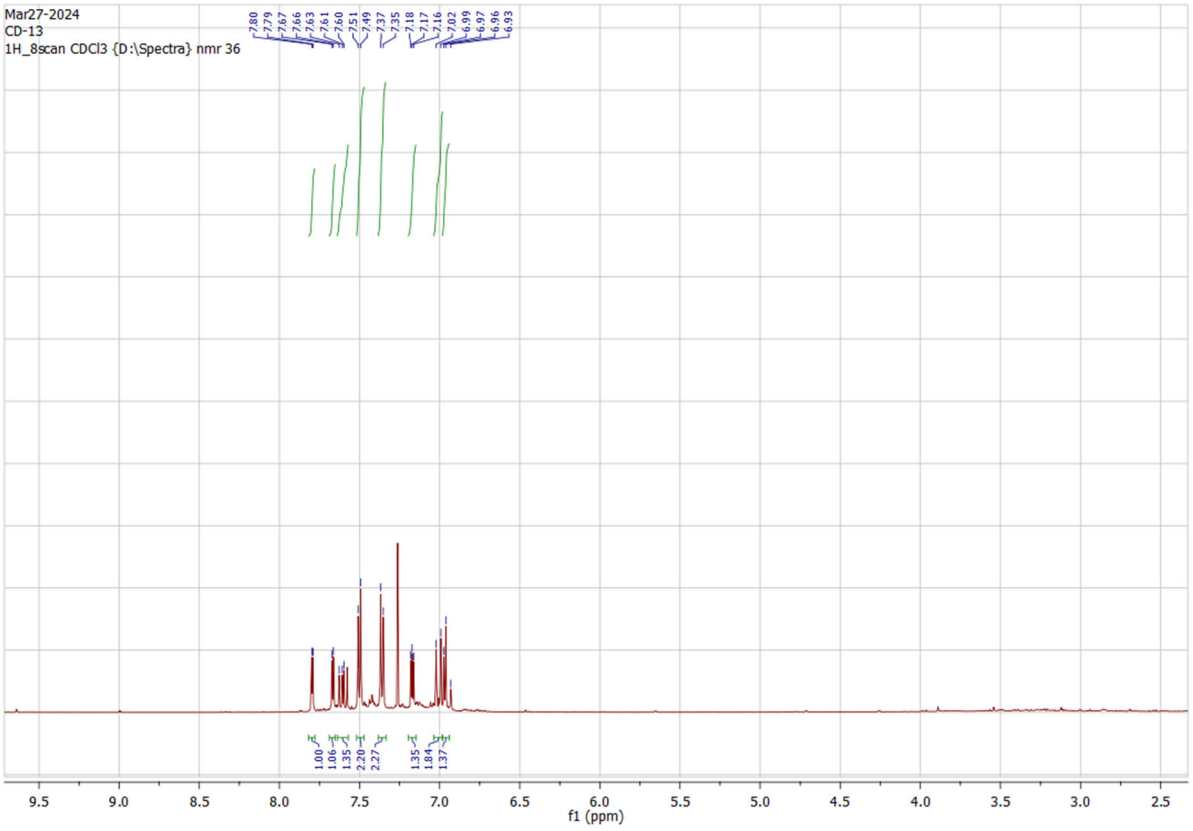

*(2E,4E)-1-(1H-indol-3-yl)-5-(4-methoxyphenyl)penta-2,4-dien-1-one* (**CD11**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.77 – 7.68 (m, 2H), 7.59 (dd, *J* = 18.3, 5.0 Hz, 2H), 7.47 (t, *J* = 8.3 Hz, 3H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 14.9 Hz, 1H), 7.03 (d, *J* = 15.5 Hz, 1H), 6.94 (d, *J* = 11.3 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H). 13C NMR (500 MHz, $CDCl_3$) δ: 193.68 (s), 136.43 (s), 131.72 (s), 125.45 (s), 123.64 (s), 122.62 (s), 122.37 (s), 118.47 (s), 111.46 (s), 27.61 (s). Molecular Formula $C_{20}H_{17}NO_2$ (ESI) Calculated= 303.3544, Observed= 303.3598.

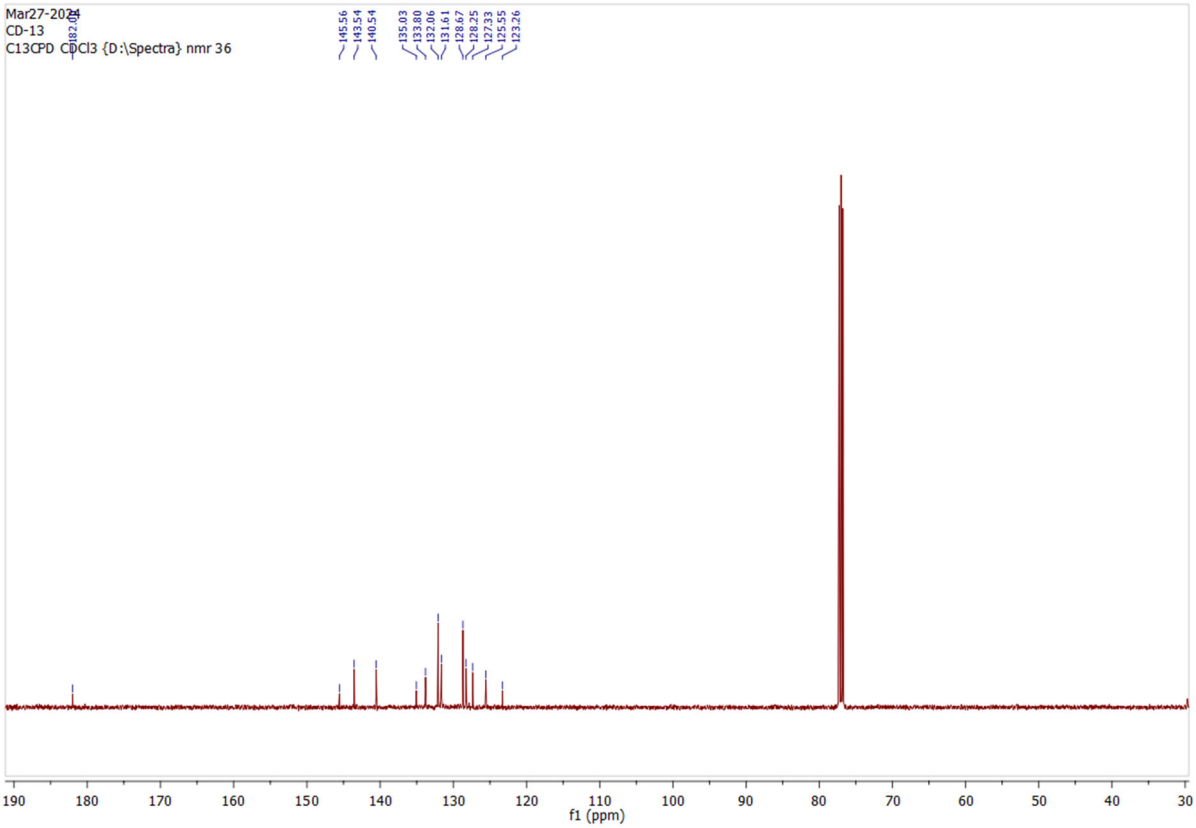


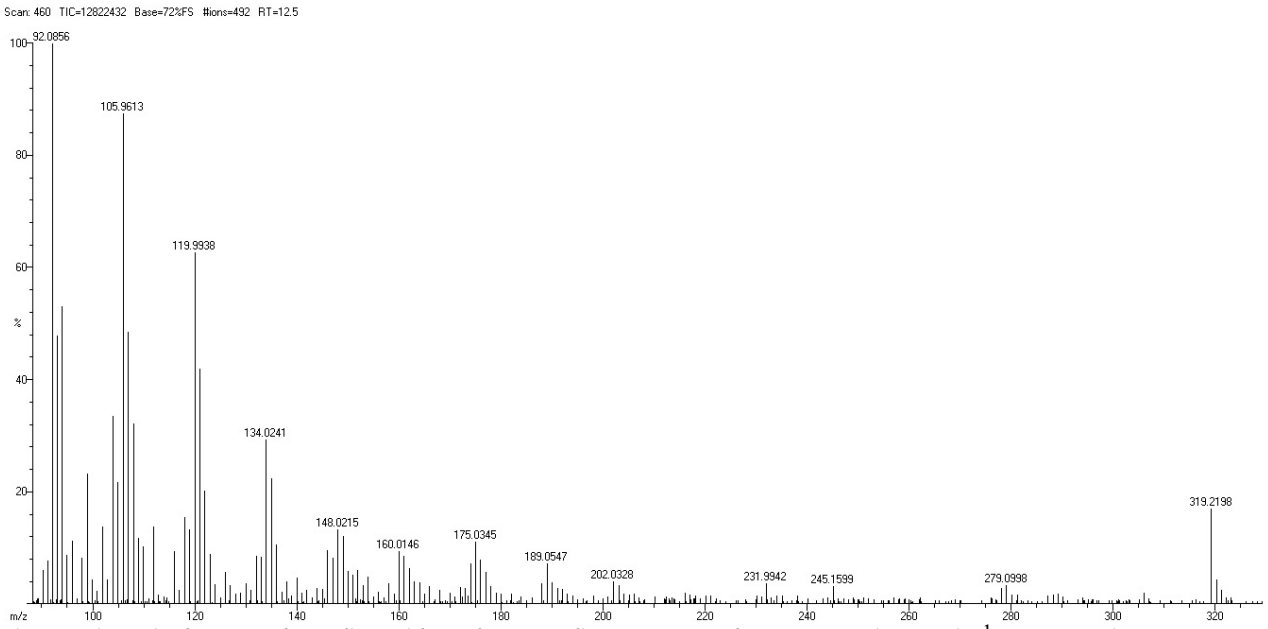


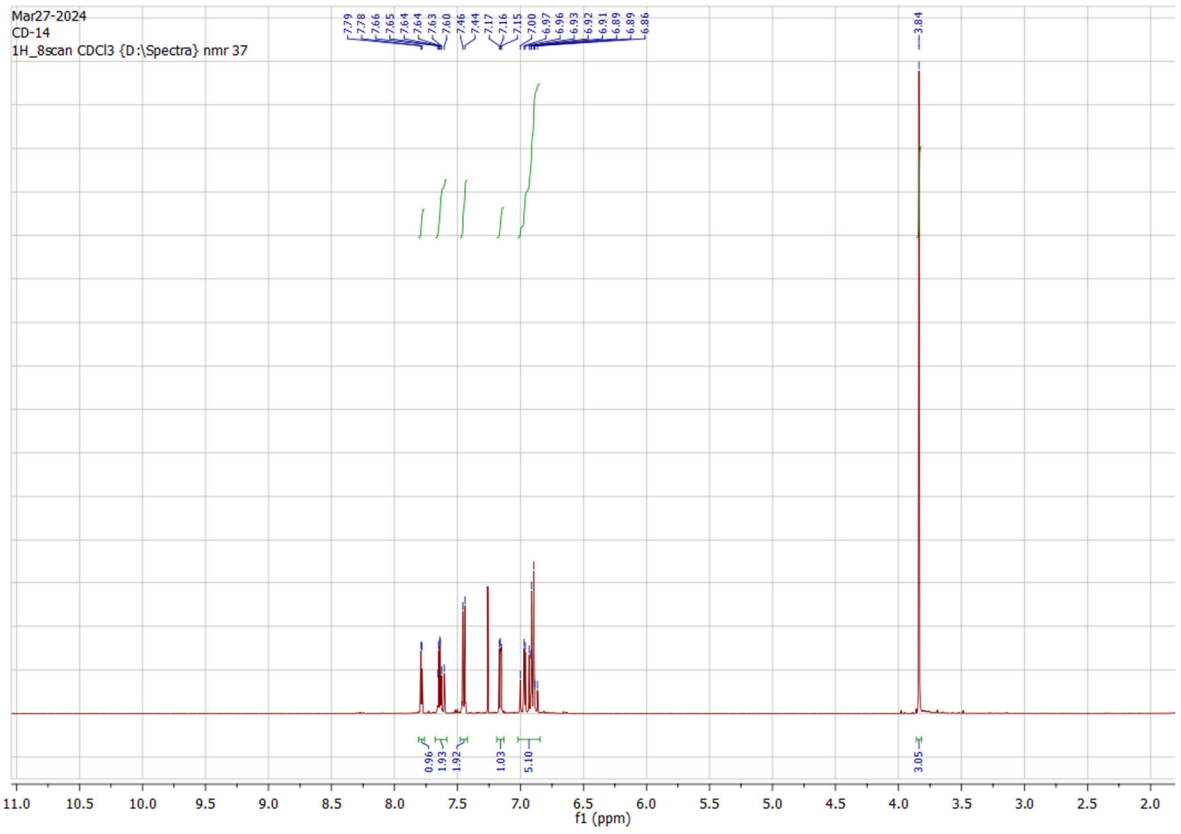

*(2E,4E)-5-(4-fluorophenyl)-1-(thiophen-2-yl)penta-2,4-dien-1-one* (**CD12**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.83 (s, 2H), 8.42 – 8.36 (m, 2H), 7.87 (d, $J$ = 3.0 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.30 (d, $J$ = 1.4 Hz, 1H), 7.29 (s, 1H), 7.28 (d, $J$ = 1.5 Hz, 1H). 13C NMR (500 MHz, $CDCl_3$) δ: 193.65 (s), 136.37 (s), 131.59 (s), 125.42 (s), 123.74 (s), 122.71 (s), 122.43 (s), 118.59 (s), 111.36 (s). Molecular Formula $C_{15}H_{11}FSO_2$ (ESI) Calculated= 258.3106, Observed= 258.3098.

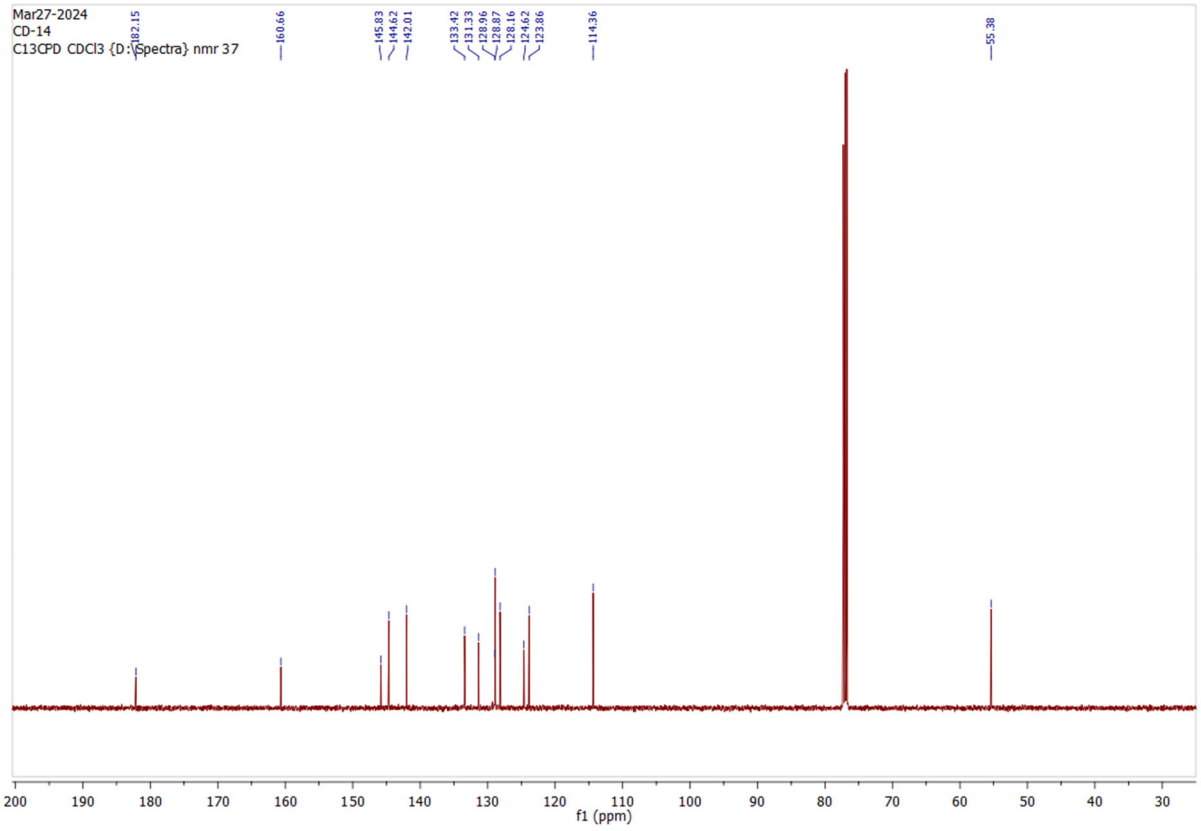

Mar27-2024
CD-13
1H_8scan CDCl3 {D:\Spectra} nmr 36
7.80
7.79
7.67
7.66
7.63
7.61
7.60
7.51
7.49
7.37
7.35
7.18
7.17
7.16
7.02
6.99
6.97
6.96
6.93
1.00
1.06
1.35
2.20
2.27
1.35
1.84
1.37
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)

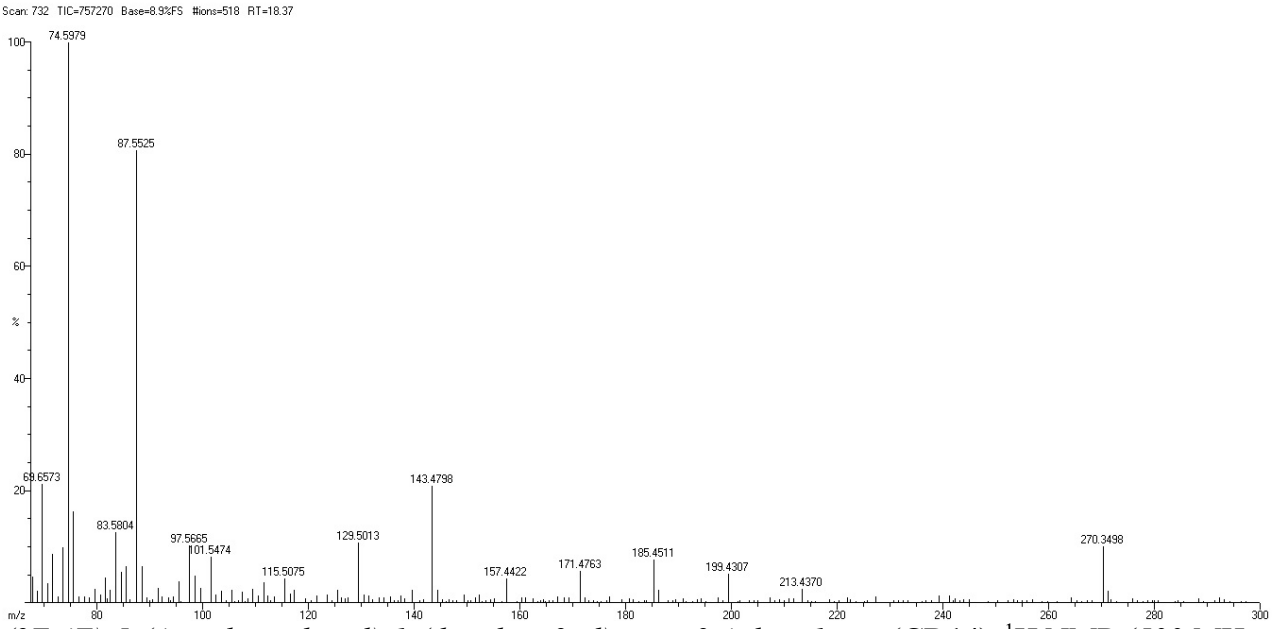

Mar27-2024
CD-13
C13CPD CDCl3 {D:\Spectra} nmr 36
182.04
145.56
143.54
140.54
135.03
133.80
132.06
131.61
128.67
128.25
127.33
125.55
123.26
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)



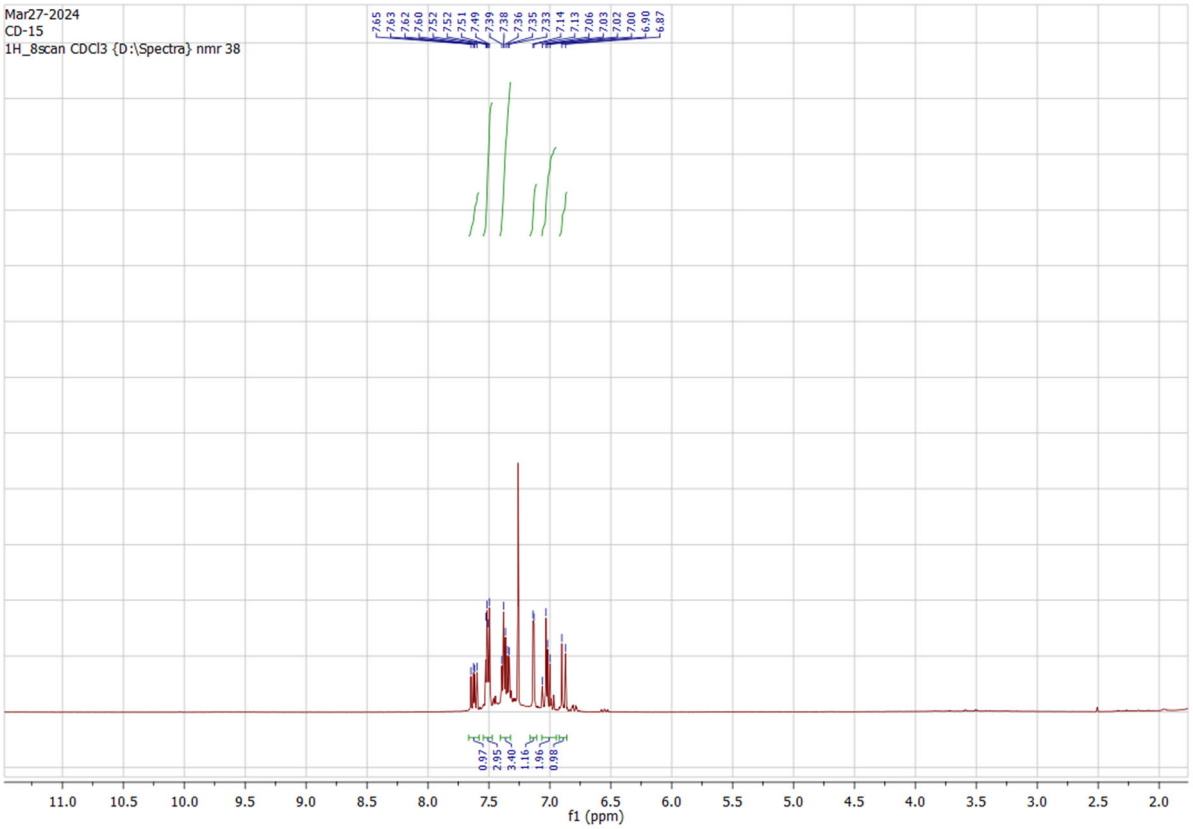

*(2E,4E)-5-(4-bromophenyl)-1-(thiophen-2-yl)penta-2,4-dien-1-one* (**CD13**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.79 (d, *J* = 3.8 Hz, 1H), 7.67 (d, *J* = 3.9 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.19 – 7.15 (m, 1H), 7.01 (d, *J* = 14.7 Hz, 2H), 6.97 (d, *J* = 6.3 Hz, 1H). 13C NMR (500 MHz, $CDCl_3$) δ: 182.00 (s), 145.56 (s), 143.54 (s), 140.54 (s), 135.03 (s), 133.80 (s), 132.06 (s), 131.61 (s), 128.67 (s), 128.25 (s), 127.33 (s), 125.55 (s), 123.26 (s). Molecular Formula $C_{15}H_{11}BrSO$ (ESI) Calculated= 319.2162, Observed= 319.2198

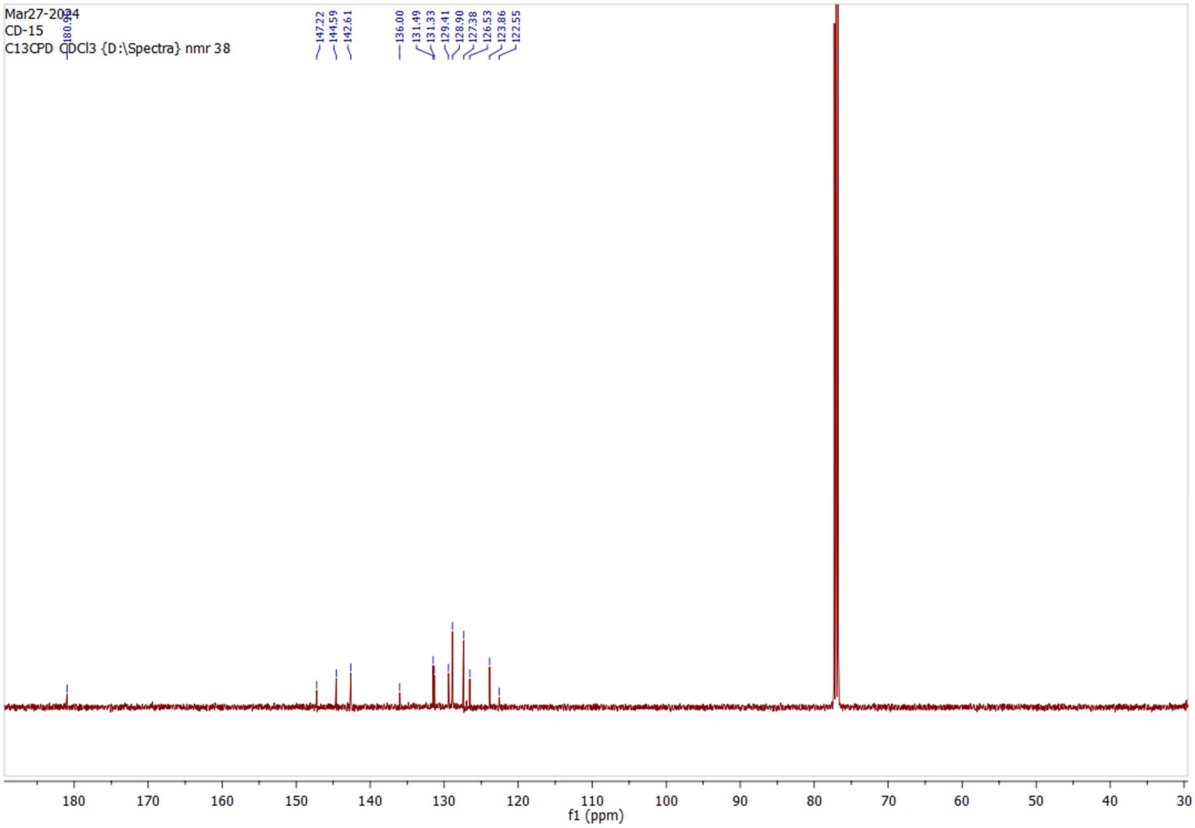


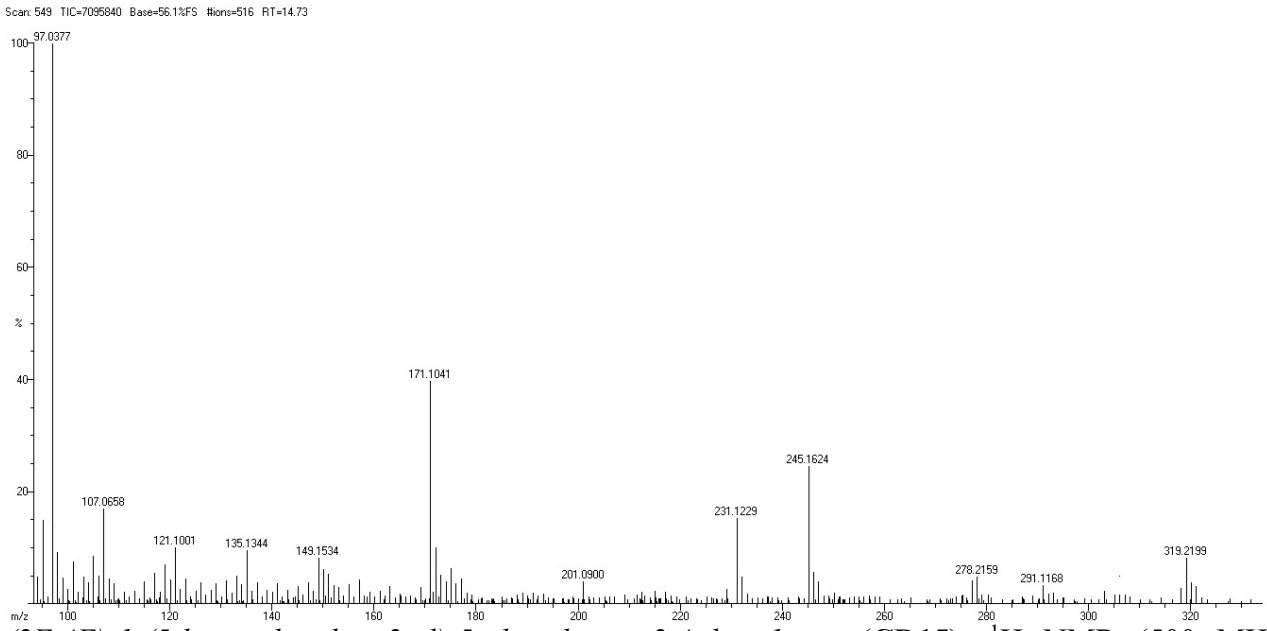


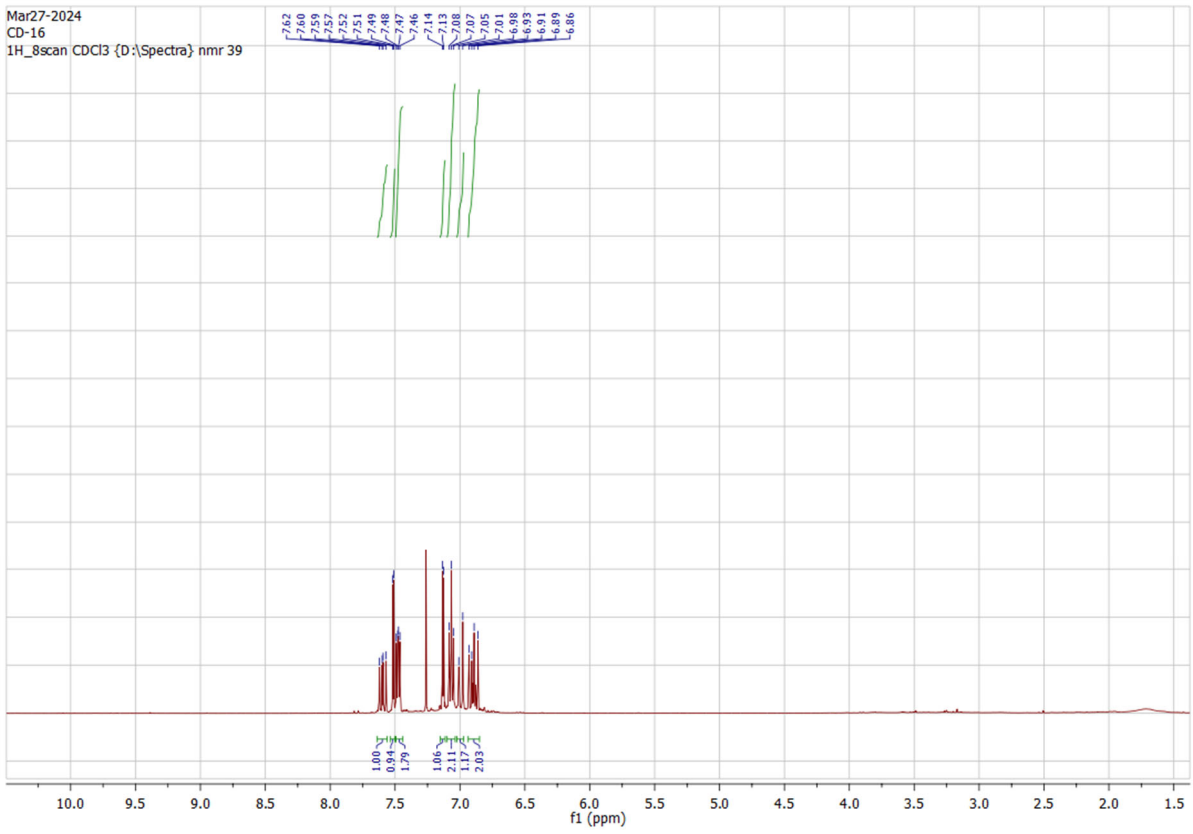

*(2E,4E)-5-(4-methoxyphenyl)-1-(thiophen-2-yl)penta-2,4-dien-1-one* (**CD14**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 3.8 Hz, 1H), 7.68 – 7.58 (m, 2H), 7.45 (d, *J* = 8.7 Hz, 2H), 7.19 – 7.13 (m, 1H), 7.02 – 6.84 (m, 5H), 3.84 (s, 3H). 13C NMR (500 MHz, $CDCl_3$) δ: 182.15 (s), 160.66 (s), 145.83 (s), 144.62 (s), 142.01 (s), 133.42 (s), 131.33 (s), 128.91 (d, J = 11.6 Hz), 128.16 (s), 124.62 (s), 123.86 (s), 114.36 (s), 55.38 (s). Molecular Formula $C_{16}H_{14}SO_2$ (ESI) Calculated= 270.3461, Observed= 270.3498.

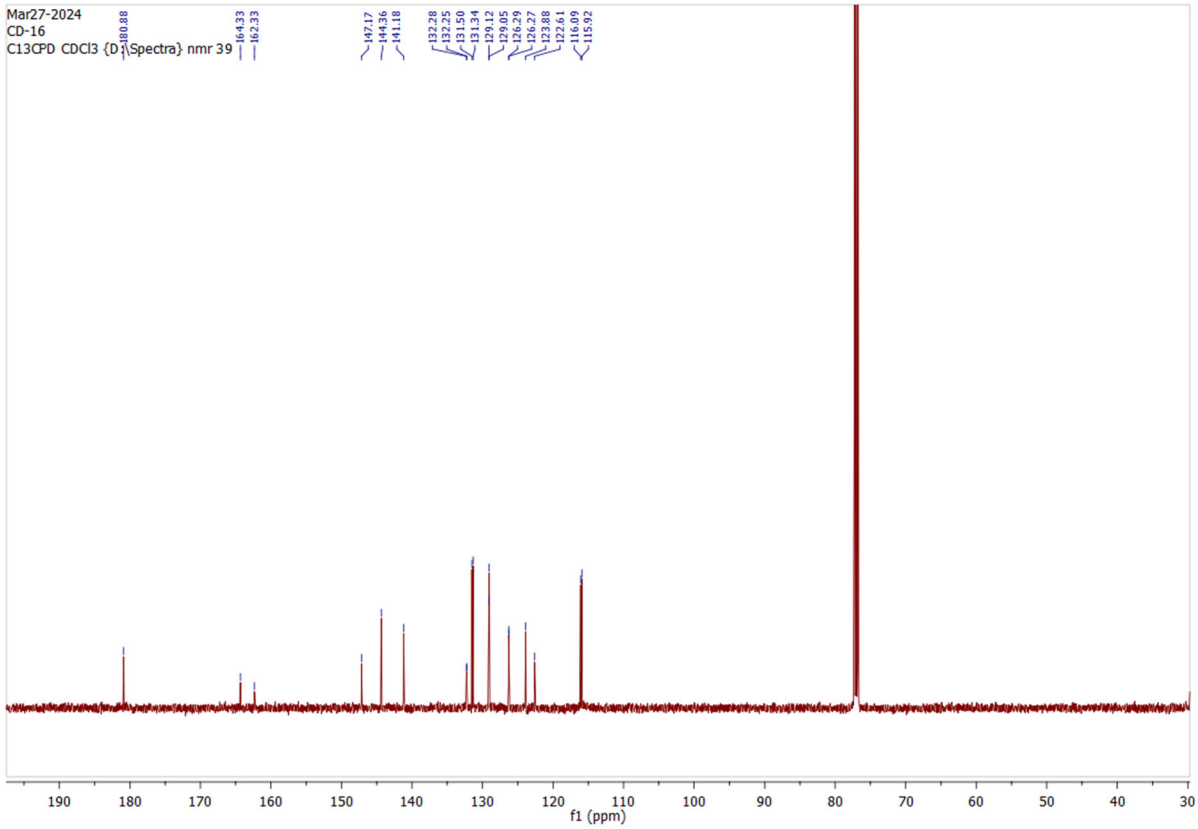

Mar27-2024
CD-15
1H_8scan CDCl3 {D:\Spectra} nmr 38
7.65
7.63
7.62
7.60
7.52
7.52
7.51
7.49
7.39
7.38
7.36
7.35
7.33
7.14
7.13
7.06
7.03
7.02
7.00
6.90
6.87
0.97
2.95
3.40
1.16
1.96
0.98
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)


Mar27-2024
CD-15
C13CPD CDCl3 {D:\Spectra} nmr 38
180.84
147.22
144.59
142.61
136.00
131.49
131.33
129.41
128.90
127.38
126.53
123.86
122.55
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

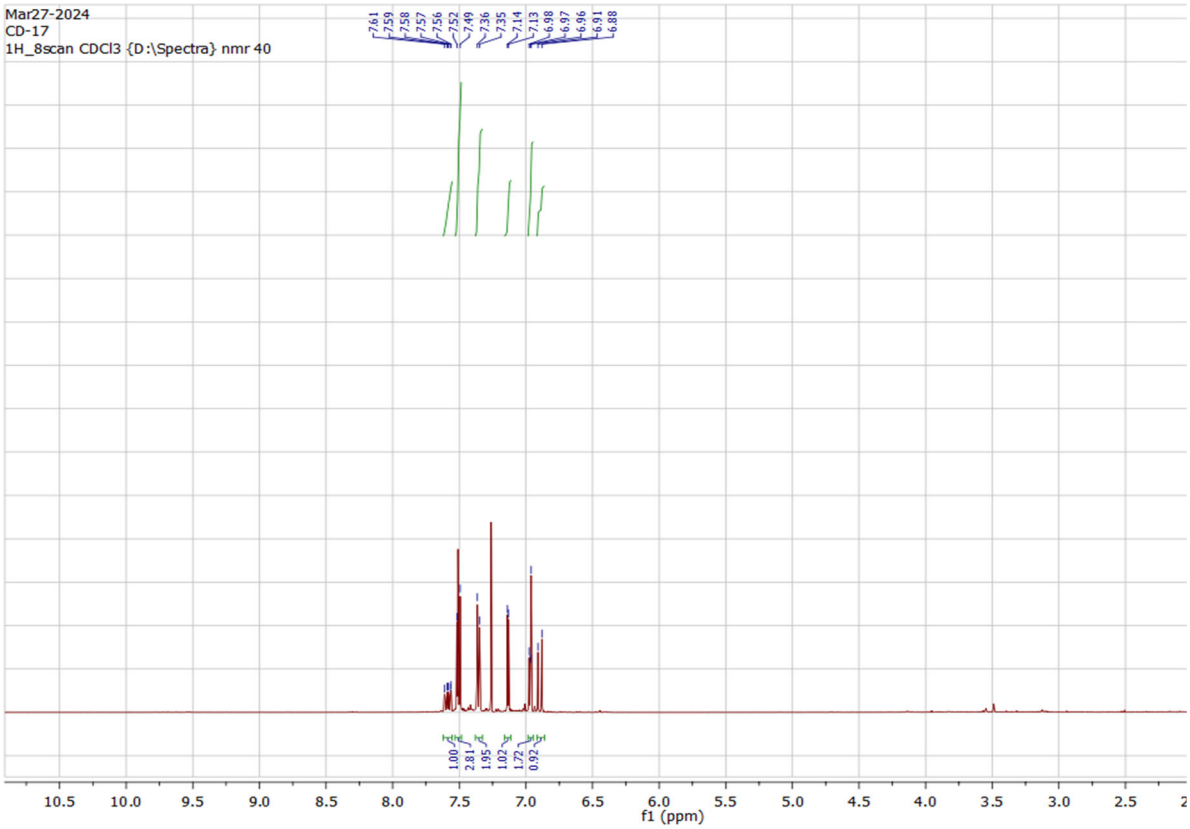


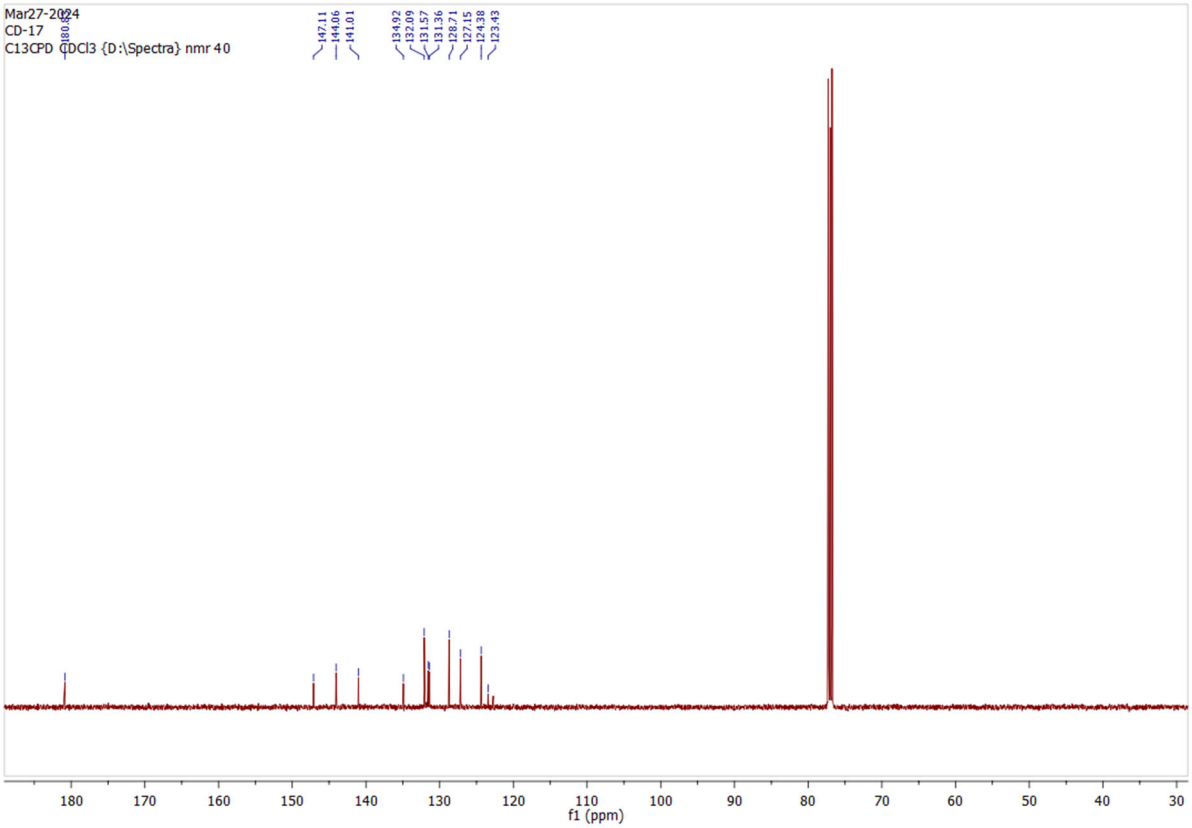

*(2E,4E)-1-(5-bromothiophen-2-yl)-5-phenylpenta-2,4-dien-1-one* (**CD15**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.62 (dd, *J* = 14.8, 10.1 Hz, 1H), 7.51 (dd, *J* = 9.1, 5.6 Hz, 3H), 7.41 – 7.32 (m, 3H), 7.13 (d, *J* = 4.0 Hz, 1H), 7.03 (dd, *J* = 18.8, 12.8 Hz, 2H), 6.89 (d, *J* = 14.8 Hz, 1H). 13C NMR (500 MHz, $CDCl_3$) δ: 180.95 (s), 147.22 (s), 144.59 (s), 142.61 (s), 136.00 (s), 131.41 (d, J = 19.4 Hz), 129.41 (s), 128.90 (s), 127.38 (s), 126.53 (s), 123.86 (s), 122.55 (s). Molecular Formula $C_{15}H_{11}BrSO$ (ESI) Calculated= 319.2162, Observed= 319.2199.

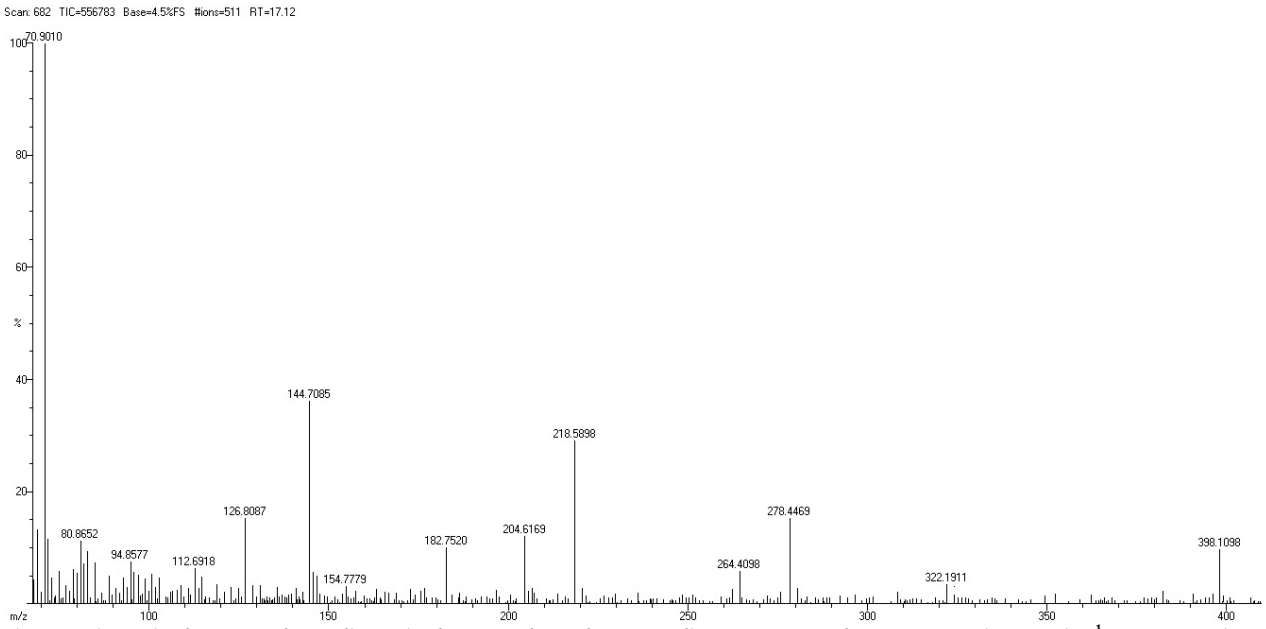




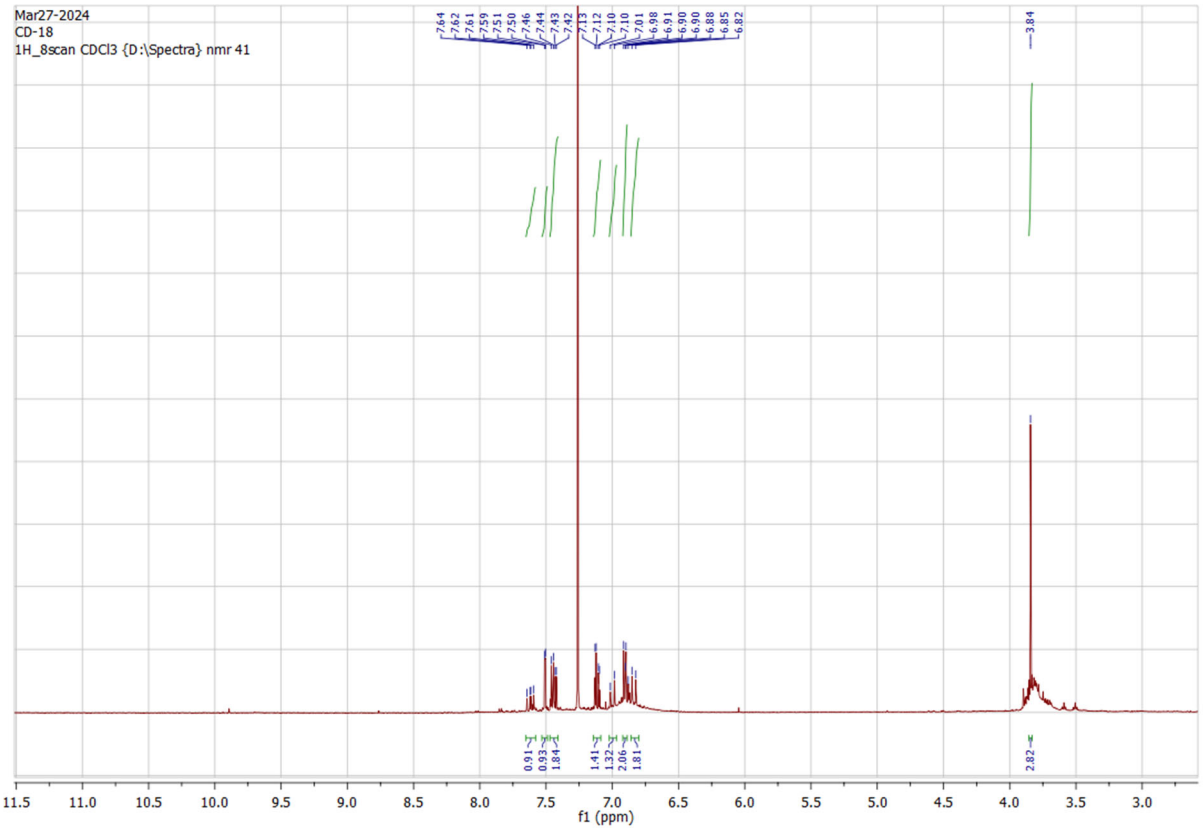

*(2E,4E)-1-(5-bromothiophen-2-yl)-5-(4-fluorophenyl)penta-2,4-dien-1-one* (**CD16**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 14.8, 10.8 Hz, 1H), 7.51 (d, *J* = 4.0 Hz, 1H), 7.48 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.13 (d, *J* = 4.0 Hz, 1H), 7.07 (t, *J* = 8.6 Hz, 2H), 6.99 (d, *J* = 15.5 Hz, 1H), 6.90 (dd, *J* = 22.1, 12.8 Hz, 2H). 13C NMR (500 MHz, $CDCl_3$) δ 180.88 (s), 164.33 (s), 162.33 (s), 147.17 (s), 144.36 (s), 141.18 (s), 132.26 (d, J = 3.3 Hz), 131.50 (s), 131.34 (s), 129.08 (d, J = 8.1 Hz), 126.28 (d, J = 2.2 Hz), 123.88 (s), 122.61 (s), 116.09 (s), 115.92 (s). Molecular Formula $C_{15}H_{10}BrFSO$ (ESI) Calculated= 337.2067, Observed= 337.2098

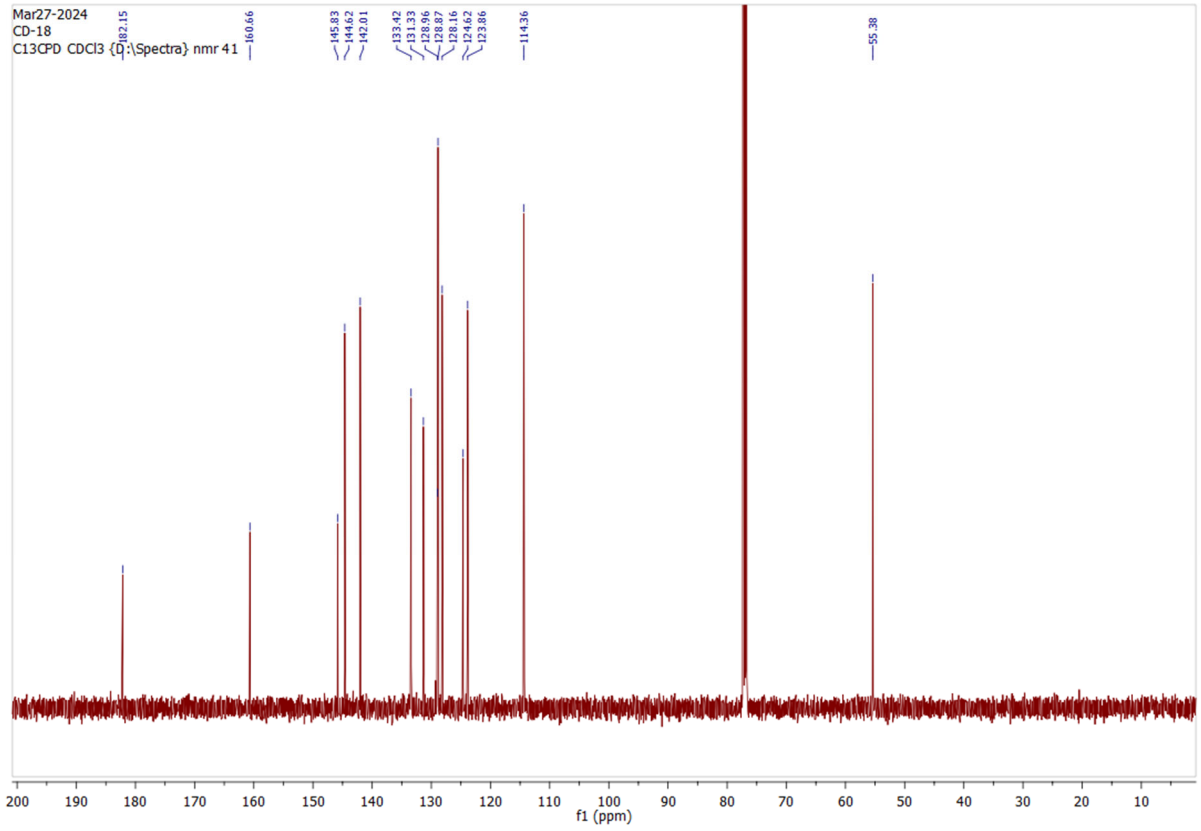

Mar27-2024
CD-17
1H_8scan CDCl3 {D:\Spectra} nmr 40
7.61
7.59
7.58
7.57
7.56
7.52
7.49
7.36
7.35
7.14
7.13
6.98
6.97
6.96
6.91
6.88
1.00
2.81
1.95
1.02
1.72
0.92
f1 (ppm)

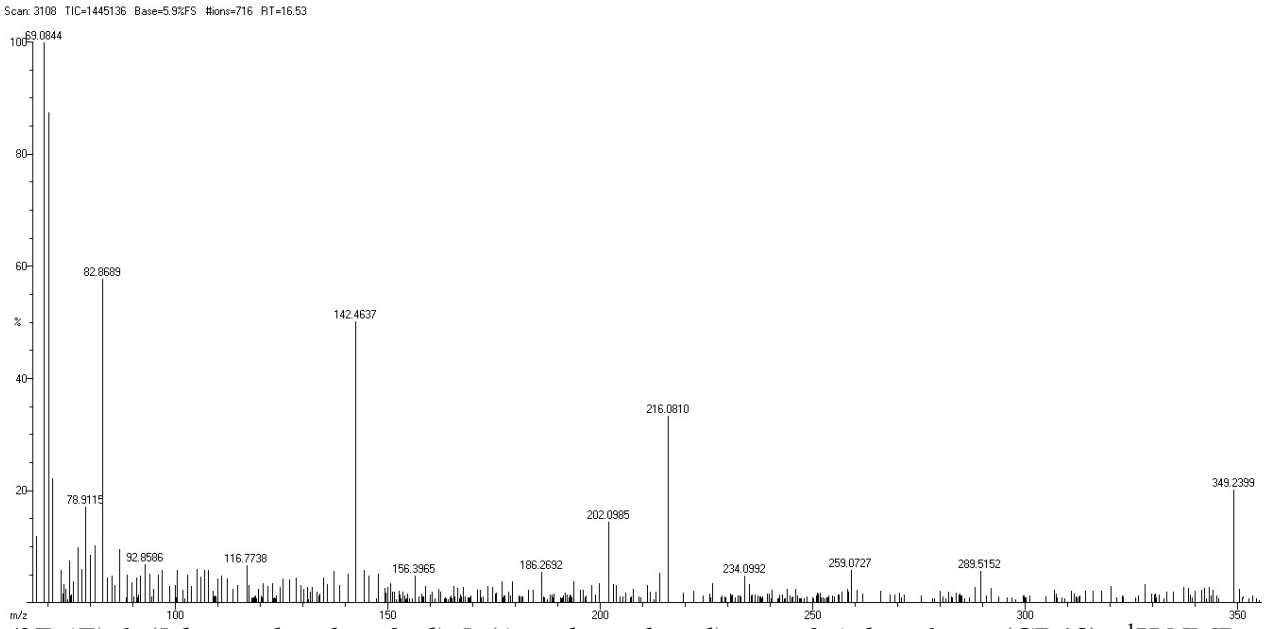

Mar27-2024
CD-17
C13CPD CDCl3 {D:\Spectra} nmr 40
180.64
147.11
144.06
141.01
134.92
132.09
131.57
131.36
128.71
127.15
124.38
123.43
f1 (ppm)




*(2E,4E)-5-(4-bromophenyl)-1-(5-bromothiophen-2-yl)penta-2,4-dien-1-one* (**CD17**): $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.62 – 7.55 (m, 1H), 7.51 (d, *J* = 12.3 Hz, 3H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.13 (d, *J* = 4.0 Hz, 1H), 6.98 – 6.95 (m, 2H), 6.89 (d, *J* = 14.8 Hz, 1H). 13C NMR (500 MHz, $CDCl_3$) δ: 180.83 (s), 147.11 (s), 144.06 (s), 141.01 (s), 134.92 (s), 132.09 (s), 131.57 (s), 131.36 (s), 128.71 (s), 127.15 (s), 124.38 (s), 123.43 (s). Molecular Formula $C_{15}H_{10}Br_2OS$ (ESI) Calculated= 398.1123, Observed= 398.1098.






*(2E,4E)-1-(5-bromothiophen-2-yl)-5-(4-methoxyphenyl)penta-2,4-dien-1-one* (**CD18**) : $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.62 (dd, *J* = 14.4, 11.1 Hz, 1H), 7.51 (d, *J* = 4.0 Hz, 1H), 7.44 (dd, *J* = 12.4, 6.4 Hz, 2H), 7.11 (dd, *J* = 12.5, 4.0 Hz, 1H), 7.00 (d, *J* = 15.5 Hz, 1H), 6.92 – 6.89 (m, 2H), 6.84 (d, *J* = 14.7 Hz, 2H), 3.84 (s, 3H). 13C NMR (500 MHz, $CDCl_3$) δ: 182.15 (s), 160.66 (s), 145.83 (s), 144.62 (s), 142.01 (s), 133.42 (s), 131.33 (s), 128.91 (d, J = 11.6 Hz), 128.16 (s), 124.62 (s), 123.86 (s), 114.36 (s), 55.38 (s). Molecular Formula $C_{16}H_{13}BrSO_2$ (ESI) Calculated= 349.2422, Observed= 349.2399

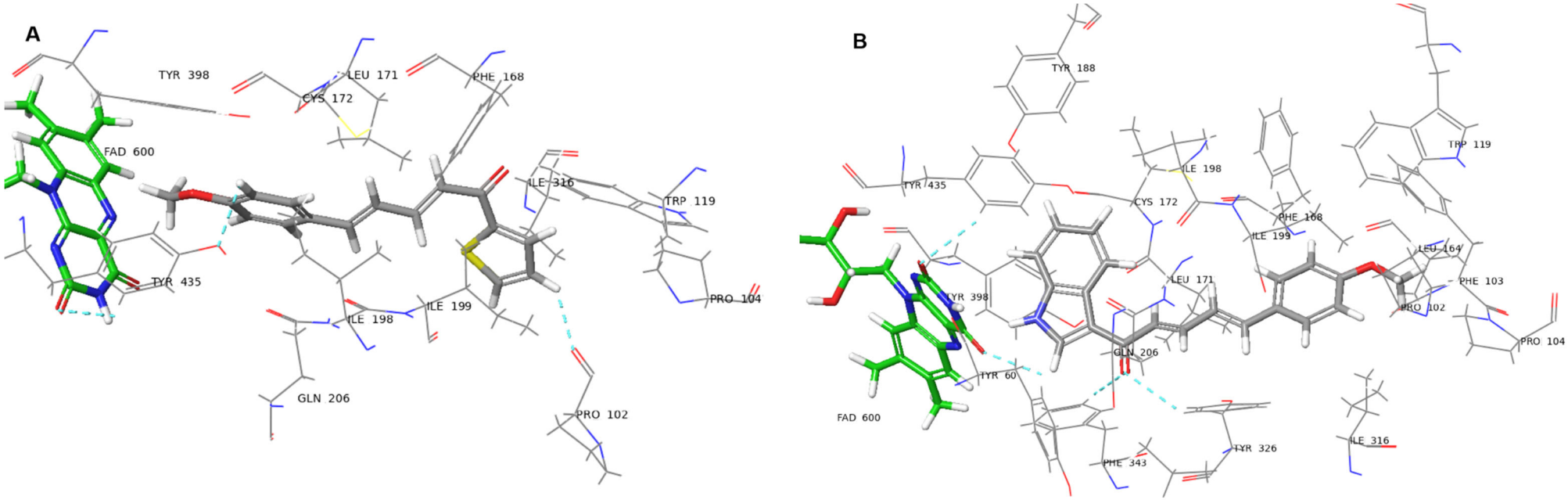



**Figure S1**. Representation of 3D-interactions of **CD14** and **CD11** in binding pocket of MAO-B