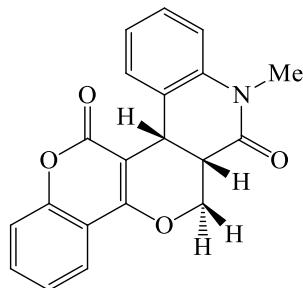
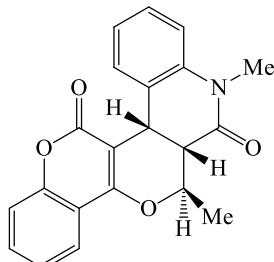


داده‌های طیفی برخی از فرآورده‌ها

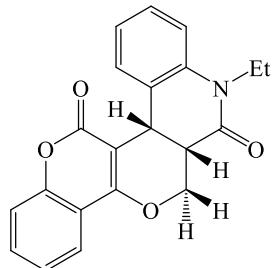


(6bS,14aS*)-2-methyl-14,14a-dihydrochromeno[3',4':5,6]pyrano[3,4-c]quinolone-1,7(2H,6bH)-dione (11a).* Yellow solid, mp 191–193 °C, yield 92%. ^1H NMR (300 MHz, CDCl_3): δ 3.20–3.29 (1H, m, H_{b}), 3.42 (3H, s, NCH_3), 4.13 (1H, t, $J = 11.30$ Hz, H_{a}), 4.55 (1H, d, $J = 4.3$ Hz, H_{c}), 4.54–4.60 (1H, m, H_{R^2}), 7.01–7.04 (1H, m, Ar-H), 7.09 (1H, dd, $J = 7.5, 0.9$ Hz, Ar-H), 7.16–7.39 (4H, m, Ar-H), 7.58 (1H, td, $J = 8.5, 1.5$ Hz, Ar-H), 7.79 (1H, dd, $J = 8.0, 1.5$ Hz, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): δ 30.1 (NCH_3), 30.9 (CH), 40.2 (CH), 63.8 (OCH_2), 99.8 (C), 114.4 (C), 115.1 (CH), 116.7 (CH), 122.8 (CH), 122.9 (CH), 124.1 (CH), 125.3 (C), 128.2 (CH), 129.6 (CH), 132.4 (CH), 137.0 (C), 152.8 (C), 160.5 (C), 163.0 (COO), 166.9 (CON). HRMS (ESI): calcd for $\text{C}_{20}\text{H}_{15}\text{NO}_4$ (M^+) 333.0996, found 333.0992.

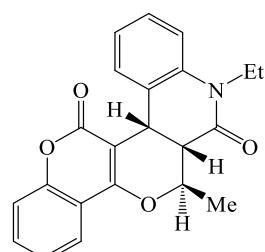


(6bS,14R*,14aS*)-2,14-dimethyl-14,14a-dihydrochromeno[3',4':5,6]pyrano[3,4-c]quinoline-1,7(2H,6bH)-dione (11b).* Yellow solid, mp 199–201 °C, yield 95%. ^1H NMR (250 MHz, CDCl_3): δ 1.57 (3H, d, $J = 6.3$ Hz, CH_3), 2.87 (1H, dd, $J = 10.4, 4.9$ Hz, H_{b}), 3.44 (3H, s, NCH_3), 4.31 (1H, qd, $J = 10.6, 6.3$ Hz, H_{a}), 4.57 (1H, d, $J = 4.8$ Hz, H_{c}), 7.00–7.13 (2H, m, Ar-H), 7.21–7.36 (4H, m, Ar-H), 7.58 (1H, td, $J = 8.5, 1.5$ Hz, Ar-H), 7.80 (1H, dd, $J = 7.9, 1.4$ Hz, Ar-H); ^{13}C NMR (62.5 MHz, CDCl_3): δ 19.0 (CH_3), 30.1 (NCH_3), 31.7 (CH), 46.2 (CH), 70.6 (OCH), 99.6 (C), 115.2 (CH), 115.9 (C), 116.7 (CH), 122.8 (CH), 124.0 (CH), 124.1 (CH), 126.4 (C), 128.1

(CH), 129.0 (CH), 132.3 (CH), 138.1 (C), 153.0 (C), 160.4 (C), 163.0 (COO), 166.8 (CON). HRMS (ESI): calcd for $\text{C}_{21}\text{H}_{17}\text{NO}_4$ (M^+) 347.1152, found 347.1151.

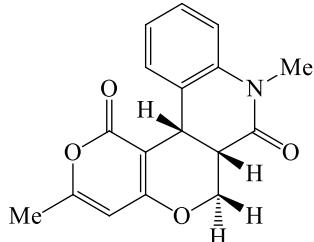


(6bS,14aS*)-2-ethyl-14,14a-dihydrochromeno[3',4':5,6]pyrano[3,4-c]quinoline-1,7(2H,6bH)-dione (11c).* Yellow solid, mp 198–200 °C, yield 90%. ^1H NMR (300 MHz, CDCl_3): δ 1.28 (3H, t, $J = 7.1$ Hz, CH_3), 3.22 (1H, ddd, $J = 11.6, 4.9, 4.3$ Hz, H_{b}), 3.97–4.15 (3H, m, NCH_2 , H_{a}), 4.53–4.59 (2H, m, $\text{H}_{\text{c}}, \text{H}_{\text{R}^2}$), 7.02–7.19 (3H, m, Ar-H), 7.26–7.32 (2H, m, Ar-H), 7.38 (1H, d, $J = 8.5$ Hz, Ar-H), 7.58 (1H, td, $J = 8.8, 1.6$ Hz, Ar-H), 7.79 (1H, dd, $J = 7.9, 1.4$ Hz, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): δ 12.7 (CH_3), 30.9 (CH), 37.5 (NCH_2), 40.2 (CH), 63.8 (OCH_2), 99.9 (C), 115.1 (C), 115.2 (CH), 116.7 (CH), 122.9 (CH), 124.0 (CH), 124.1 (CH), 125.7 (C), 128.2 (CH), 129.8 (CH), 132.4 (CH), 136.9 (C), 152.8 (C), 160.5 (C), 163.1 (COO), 166.2 (CON). HRMS (ESI): calcd for $\text{C}_{21}\text{H}_{17}\text{NO}_4$ (M^+) 347.1152, found 347.1152.

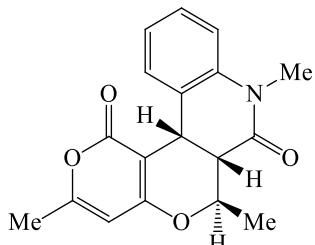


(6bS,14R*,14aS*)-2-ethyl-14-methyl-14,14a-dihydrochromeno[3',4':5,6]pyrano[3,4-c]quinoline-1,7(2H,6bH)-dione (11d).* Yellow solid, mp 206–208 °C, yield 88%. ^1H NMR (300 MHz, CDCl_3): δ 1.28 (3H, t, $J = 7.1$ Hz, CH_3), 1.56 (3H, d, $J = 6.3$ Hz, CH_3), 2.83 (1H, dd, $J = 10.5, 4.8$ Hz, H_{b}), 3.94–4.17 (2H, m, NCH_2), 4.30 (1H, qd, $J = 10.3, 6.3$ Hz, H_{a}), 4.55 (1H, d, $J = 4.5$ Hz, H_{c}), 6.99–7.39 (6H, m, Ar-H), 7.58 (1H, td, $J = 8.5, 1.3$ Hz, Ar-H), 7.80 (1H, dd, $J = 7.8, 1.3$ Hz, Ar-H); ^{13}C NMR (75 MHz, CDCl_3): δ 12.8 (CH_3), 18.9 (CH_3), 31.8 (CH), 37.7

(NCH₂), 46.2 (CH), 70.6 (OCH), 99.8 (C), 115.1 (C), 115.2 (CH), 116.8 (CH), 122.8 (CH), 123.9 (CH), 124.1 (CH), 126.8 (C), 128.2 (CH), 129.3 (CH), 132.3 (CH), 137.0 (C), 153.0 (C), 160.5 (C), 163.2 (COO), 166.3 (CON). HRMS (ESI): calcd for C₂₂H₁₉NO₄ (M+H) 362.1387, found 362.1387.

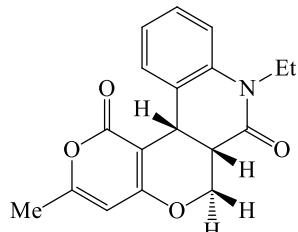


(6aS*,12bS*)-3,8-dimethyl-6,6a-dihydropyrano[3',4':5,6]pyrano[3,4-c]quinoline-1,7(8H,12bH)-dione (11e). Yellow solid, mp 144–146 °C, yield 93%. ¹H NMR (300 MHz, CDCl₃): δ 2.26 (3H, s, CH₃), 3.12 (1H, ddd, J = 11.4, 5.1, 4.2 Hz, H_b), 3.33 (3H, s, NCH₃), 3.95 (1H, t, J = 11.0 Hz, H_a), 4.29–4.33 (2H, m, H_c, H_R²), 5.82 (1H, s, Ar-H), 6.98 (1H, dd, J = 8.1, 0.6 Hz, Ar-H), 7.07 (1H, dt, J = 7.5, 0.9 Hz, Ar-H), 7.15–7.18 (1H, m, Ar-H), 7.26–7.30 (1H, m, Ar-H); ¹³C NMR (75 MHz, CDCl₃): δ 30.0 (CH₃), 30.3 (NCH₃), 38.0 (CH), 40.2 (CH), 60.5 (OCH₂), 97.1 (C), 100.1 (CH), 115.0 (CH), 124.1 (CH), 125.3 (C), 128.1 (CH), 129.3 (CH), 135.8 (C), 161.9 (C), 163.8 (C), 164.8 (COO), 169.2 (CON). HRMS (ESI): calcd for C₁₇H₁₅NO₄ (M⁺) 297.0996, found 297.0993.

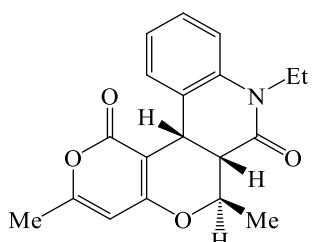


(6R*,6aS*,12bS*)-3,6,8-trimethyl-6,6a-dihydropyrano[3',4':5,6]pyrano[3,4-c]quinoline-1,7(8H,12bH)-dione (11f). Yellow solid, mp 150–152 °C, yield 95%. ¹H NMR (300 MHz, CDCl₃): δ 1.42 (3H, d, J = 6.3 Hz, CH₃), 2.26 (3H, s, CH₃), 2.74 (1H, dd, J = 10.3, 5.0 Hz, H_b), 3.40 (3H, s, NCH₃), 4.12 (1H, qd, J = 10.8, 6.3 Hz, H_a), 4.38 (1H, d, J = 4.9 Hz, H_c), 5.81 (1H, s, Ar-H), 6.97–7.11 (3H, m, Ar-H), 7.23–7.29 (1H, m, Ar-H); ¹³C NMR (75 MHz, CDCl₃): δ 18.9 (CH₃), 19.9 (CH₃), 30.1 (NCH₃), 31.1 (CH), 46.2 (CH), 70.1 (OCH), 96.9 (C),

100.1 (CH), 115.2 (CH), 124.0 (CH), 126.4 (C), 128.0 (CH), 129.0 (CH), 138.1 (C), 161.9 (C), 164.9 (C), 165.2 (COO), 167.0 (CON). HRMS (ESI): calcd for C₁₈H₁₇NO₄ (M⁺) 311.1152, found 311.1153.

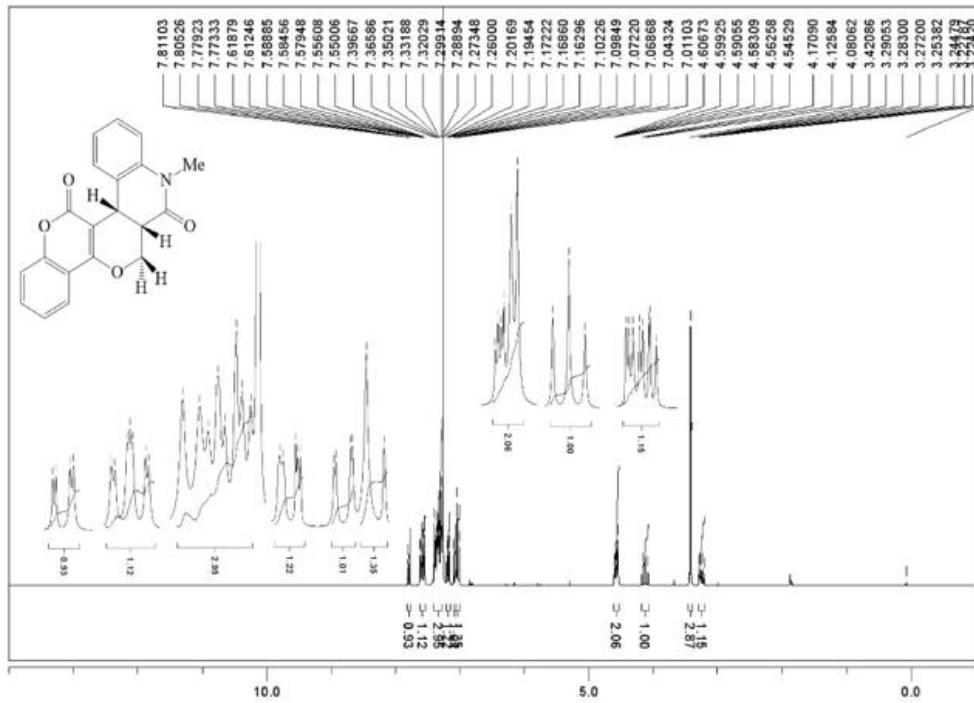


(6aS*,12bS*)-8-ethyl-3-methyl-6,6a-dihydropyrano[3',4':5,6]pyrano[3,4-c]quinoline-1,7(8H,12bH)-dione (11g). Yellow solid, mp 147–179 °C, yield 85%. ¹H NMR (300 MHz, CDCl₃): δ 1.28 (3H, t, J = 7.1 Hz, CH₃), 2.17 (3H, s, CH₃), 3.22 (1H, m, H_b), 3.97–4.15 (3H, m, NCH₂, H_a), 4.53–4.59 (2H, m, H_c, H_R²), 5.18 (1H, s, Ar-H), 7.02–7.29 (4H, m, Ar-H); ¹³C NMR (75 MHz, CDCl₃): δ 12.7 (CH₃), 19.8 (CH₃), 30.3 (CH), 37.5 (NCH₂), 40.2 (CH), 63.3 (OCH₂), 97.2 (C), 100.2 (CH), 115.0 (CH), 123.9 (CH), 126.8 (C), 128.1 (CH), 129.3 (CH), 136.9 (C), 161.9 (C), 165.0 (C), 165.2 (COO), 166.4 (CON). HRMS (ESI): calcd for C₁₈H₁₇NO₄ (M⁺) 311.1152, found 311.1150.



(6R*,6aS*,12bS*)-8-ethyl-3,6-dimethyl-6,6a-dihydropyrano[3',4':5,6]pyrano[3,4-c]quinoline-1,7(8H,12bH)-dione (11h). Yellow solid, mp 159–161 °C, yield 90%. ¹H NMR (300 MHz, CDCl₃): δ 1.26 (3H, t, J = 7.1 Hz, CH₃), 1.42 (3H, d, J = 6.3 Hz, CH₃), 2.26 (3H, s, CH₃), 2.71 (1H, dd, J = 10.4, 4.9 Hz, H_b), 3.91–4.16 (3H, m, NCH₂, H_a), 4.37 (1H, d, J = 4.7 Hz, H_c), 5.81 (1H, s, Ar-H), 7.00–7.10 (3H, m, Ar-H), 7.22–7.27 (1H, m, Ar-H); ¹³C NMR (75 MHz, CDCl₃): δ 12.8 (CH₃), 18.8 (CH₃), 19.9 (CH₃), 31.2 (CH), 37.7 (NCH₂), 46.2 (CH), 70.1 (OCH), 97.1 (C), 100.1 (CH), 115.0 (CH), 123.9 (CH), 126.8 (C), 128.0 (CH), 129.3 (CH), 136.9 (C), 161.9 (C), 165.0 (C), 165.2 (COO), 166.4 (CON). HRMS (ESI): calcd for C₁₉H₁₉NO₄ (M⁺) 326.1387, found 326.1385.

دادهای طیفی محصول‌ها



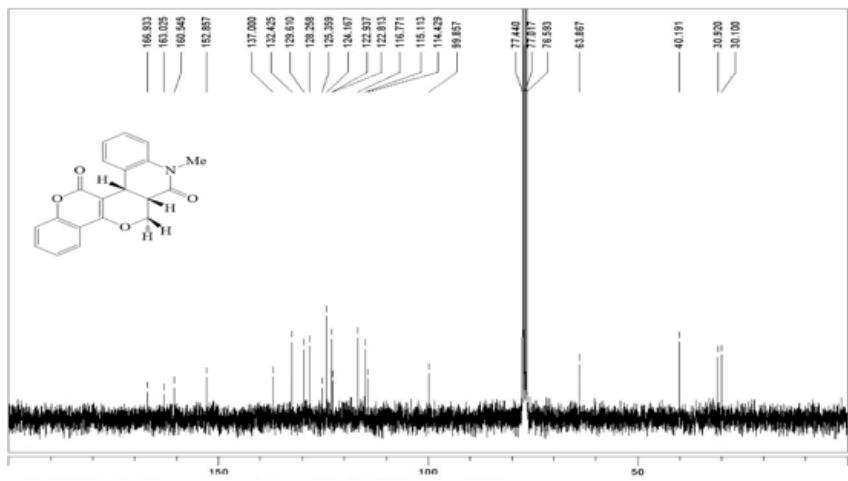
طیف ^1H NMR ترکیب 11a

Jan/2011 LM-3

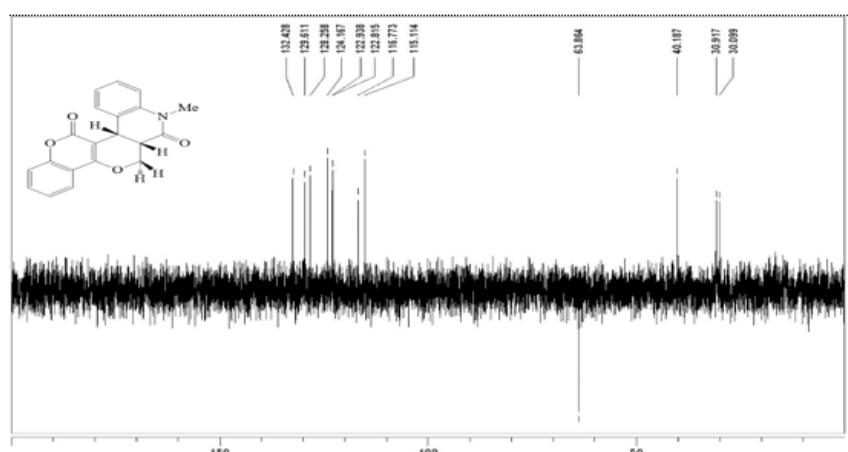
File : D:\Xcalibur\data\1612\16121306hrei-av2.RAW
Full ms [315.500 - 347.500] - Range: 333.000 - 333.500
Scan No. 1 of 1

Scan No.	T	For I	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [amu]	RDB	Composition
333.09925	1525845		53.3		333.09956	-0.9	-0.3	14.0	C ₂₀ H ₁₅ O ₄ N ₁

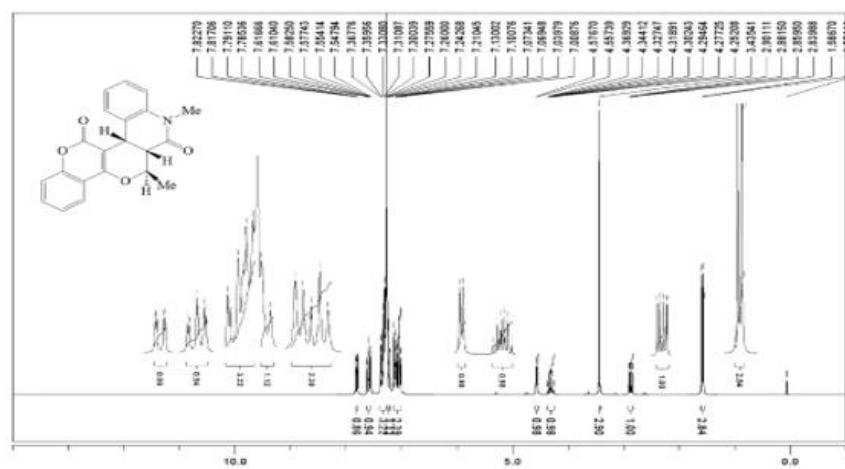
طیف HRMs ترکیب 11a



طیف ^{13}C NMR ترکیب 11a



طیف DEPT 135 ترکیب 11a



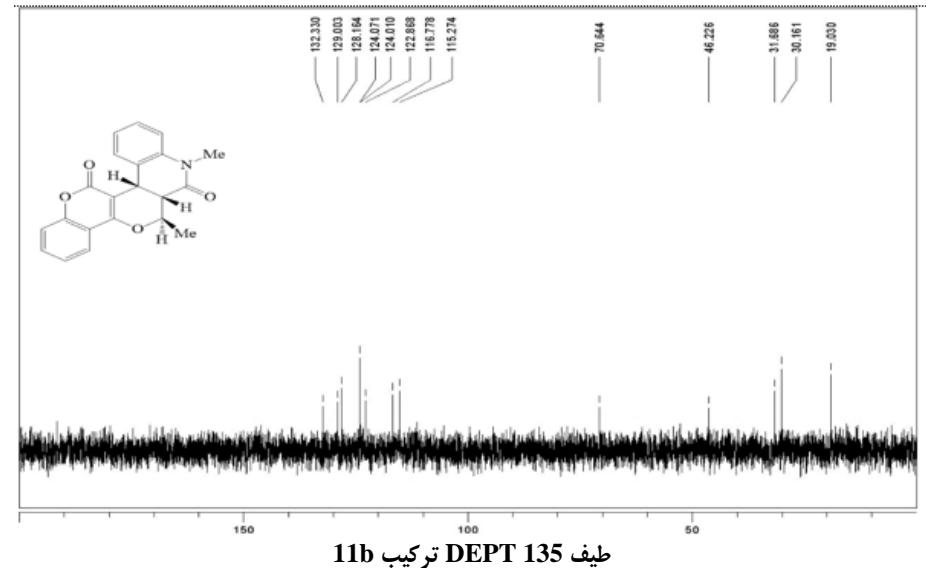
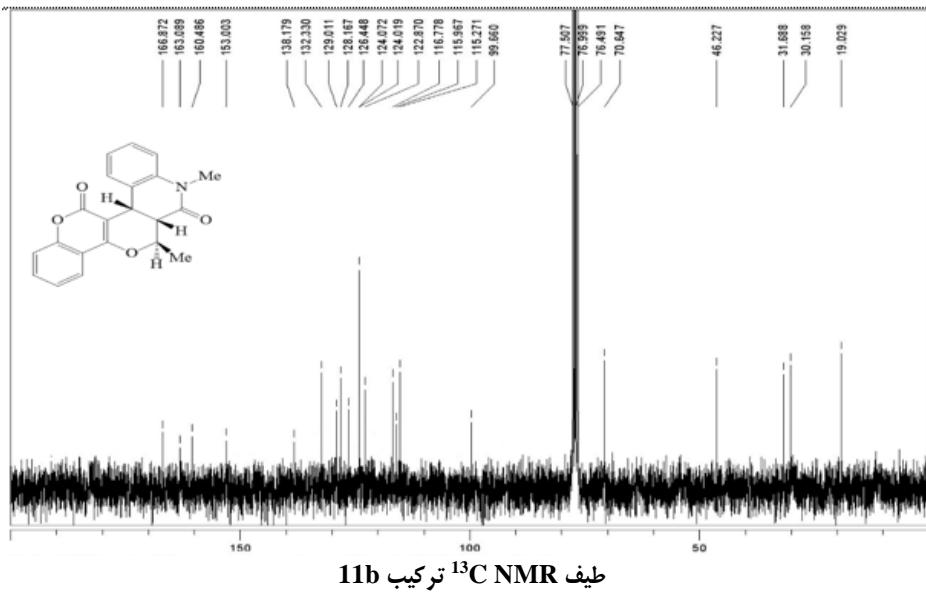
طیف ^1H NMR ترکیب 11b

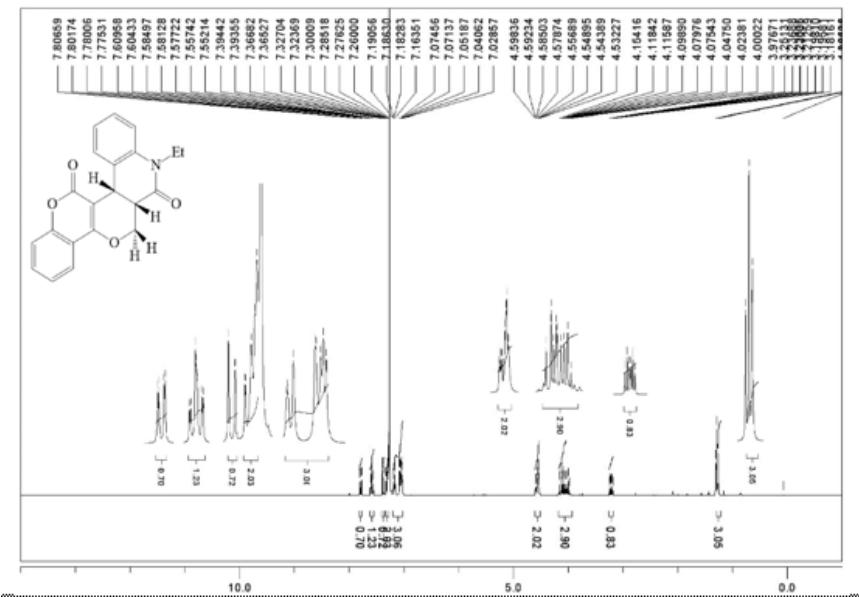
garfasi CH-14

File : D:\Xcalibur\data\1612\16121307brei-av2.RAW
 Full ms [327.500 - 359.500] - Range: 347.000 - 347.500
 Scan No. 1 of 1

Mass	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
347.11511	1257967	41.8	347.11521	-0.3	-0.1	14.0	C ₂₁ H ₁₇ O ₄ N ₁

طيف ترکيب HRMs 11b

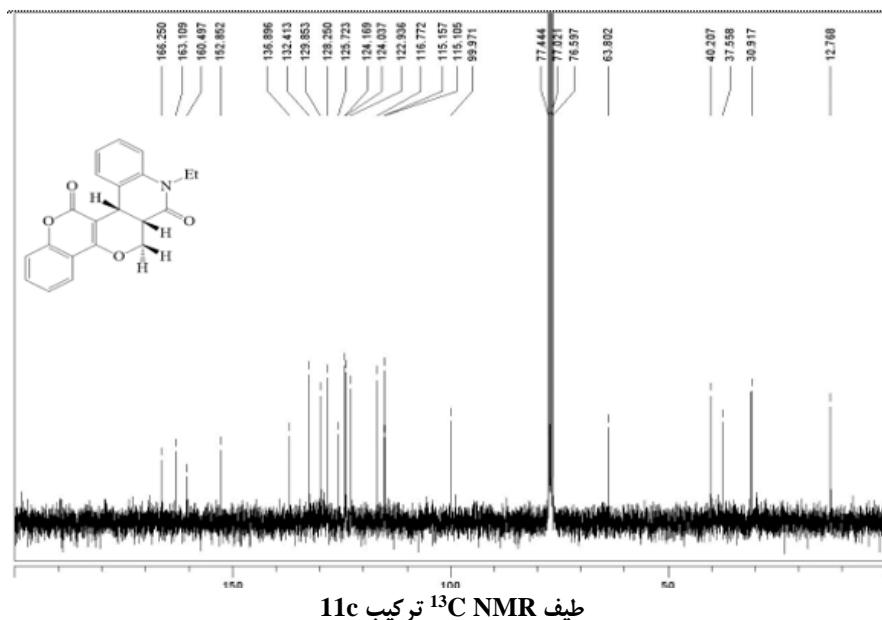




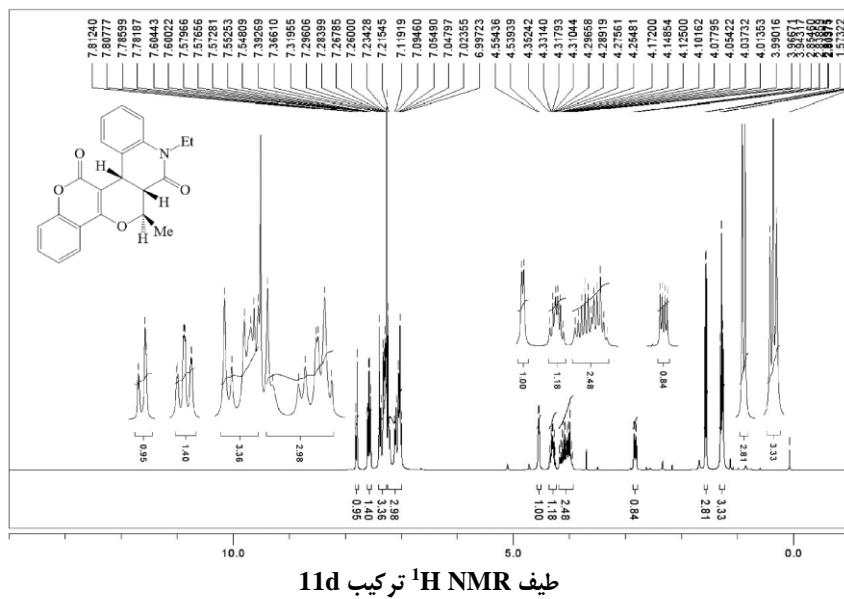
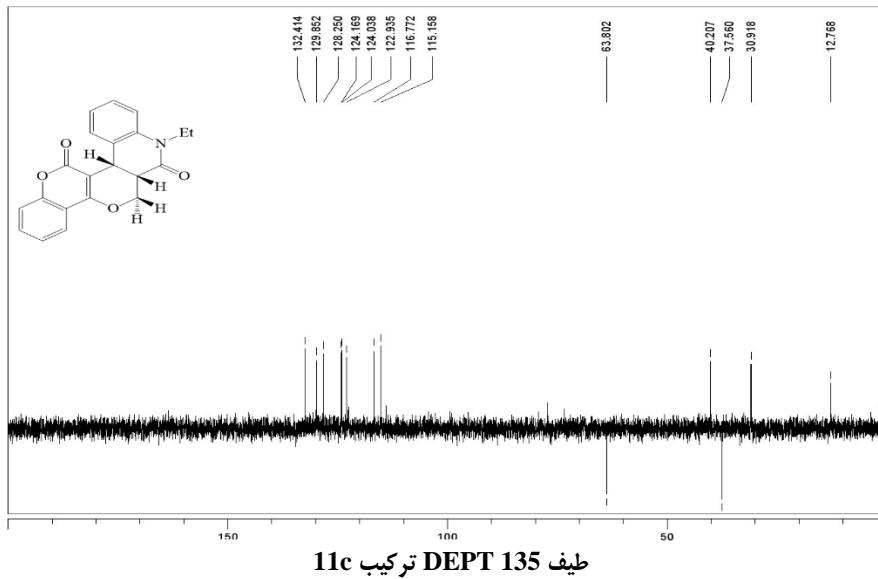
11c ترکیب ۱H NMR طیف

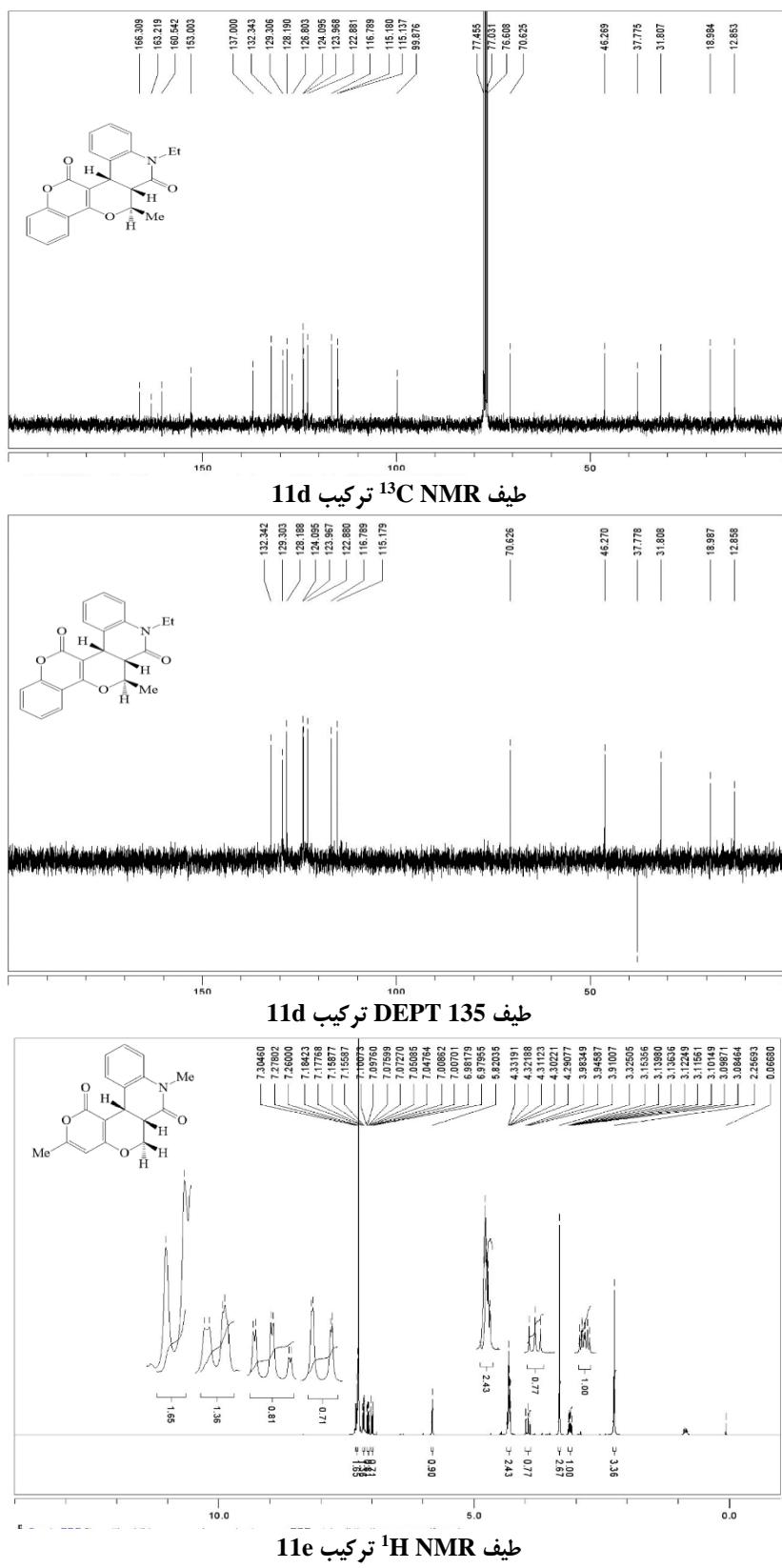
File : D:\Xcalibur\data\1701\17010502hrei-av2.RAW
 Full ms [327.500 - 359.500] - Range: 347.000 - 347.500
 Scan No. 1 of 1
 Mass Absolute Relative Theoretical Delta Delta RDB Composition
 Intensity Intensity Mass [ppm] [mmu] [mmu]
 347.11521 136557 21.7 347.11521 0.0 0.0 14.0 C₂₁H₁₇O₄N₁

11c ترکیب HRMs طیف



11c ترکیب ۱3C NMR طیف

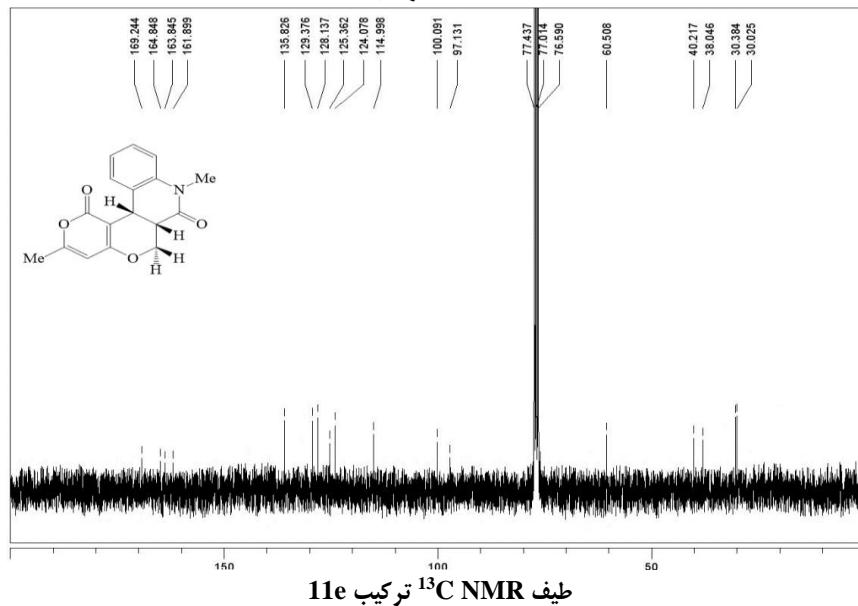




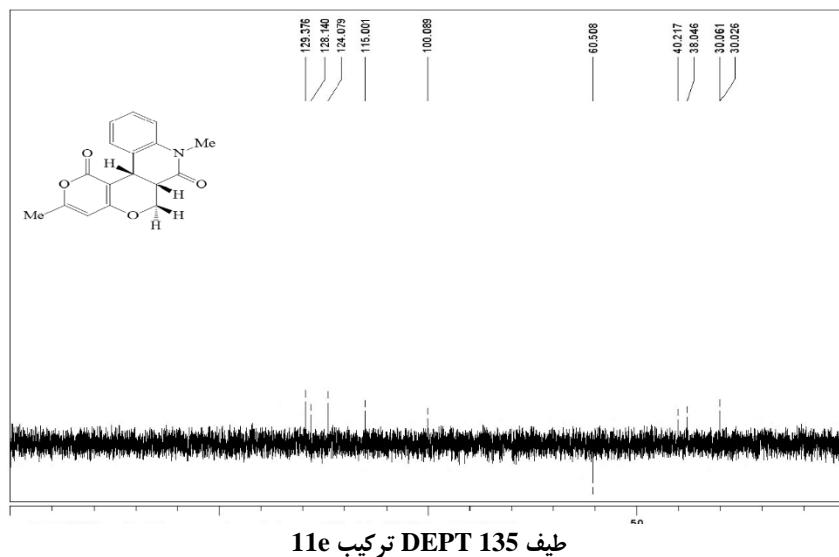
File : D:\Xcalibur\data\1701\17010501hrei-av2.RAW
 Full ms [277.500 - 309.500] - Range: 297.000 - 297.500
 Scan No. 1 of 1

Mass	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
297.09930	556364	41.3	297.09956	-0.9	-0.3	11.0	C ₁₇ H ₁₈ O ₄ N ₁

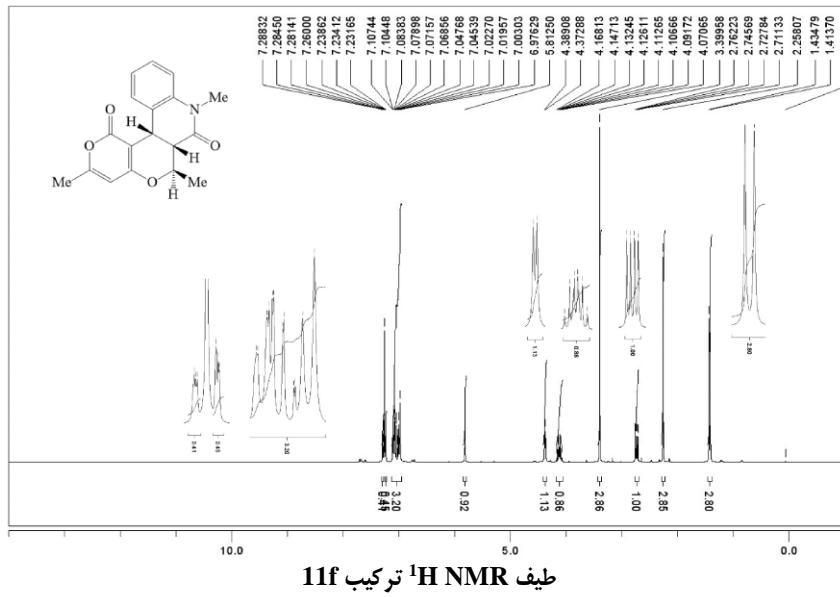
طيف ترکیب HRMs



طيف ترکیب ¹³C NMR

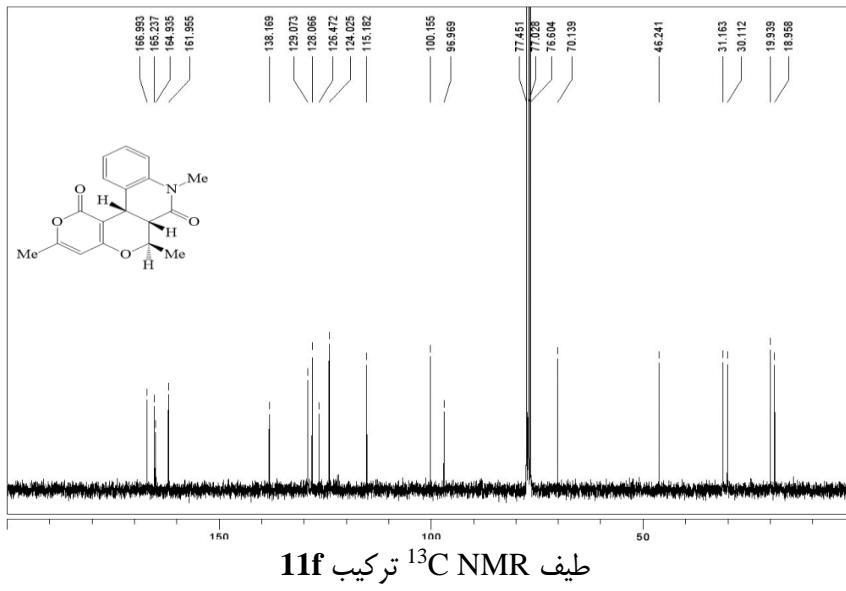


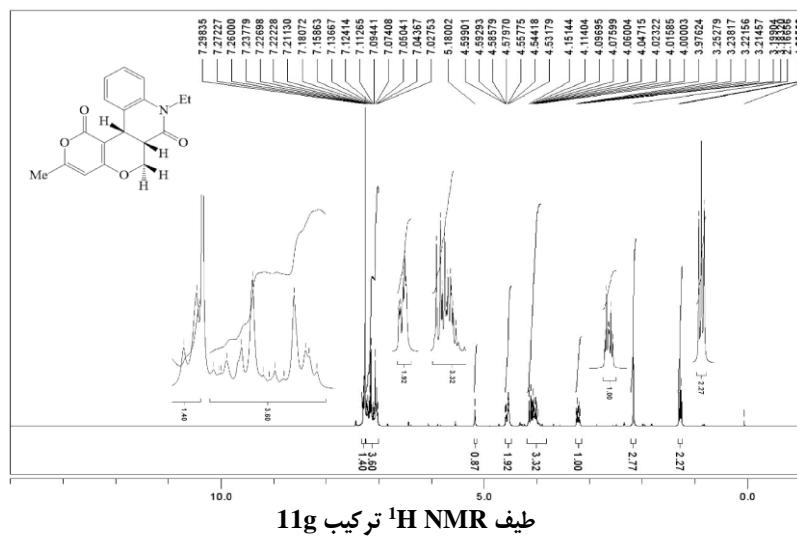
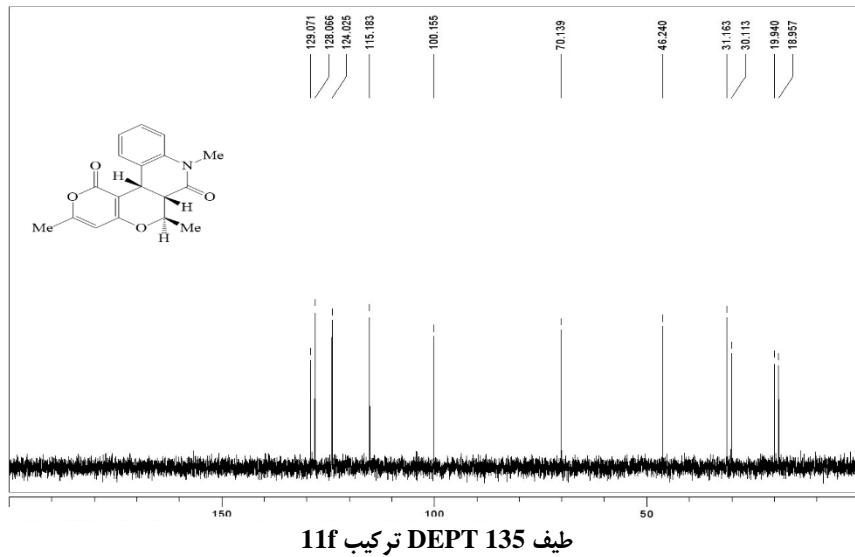
طيف ترکیب DEPT 135



File : D:\Xcalibur\data\1701\17011804hrei-av2.RAW
 Full ms [301.500 - 323.500] - Range: 311.000 - 311.500
 Scan No. 1 of 1
 Mass Absolute Relative Theoretical Delta RDB Composition
 Intensity Intensity Mass [ppm]
 311.11530 424786 57.0 311.11521 0.3 0.1 11.0 $\text{C}_{18}\text{H}_{17}\text{O}_4\text{N}_1$

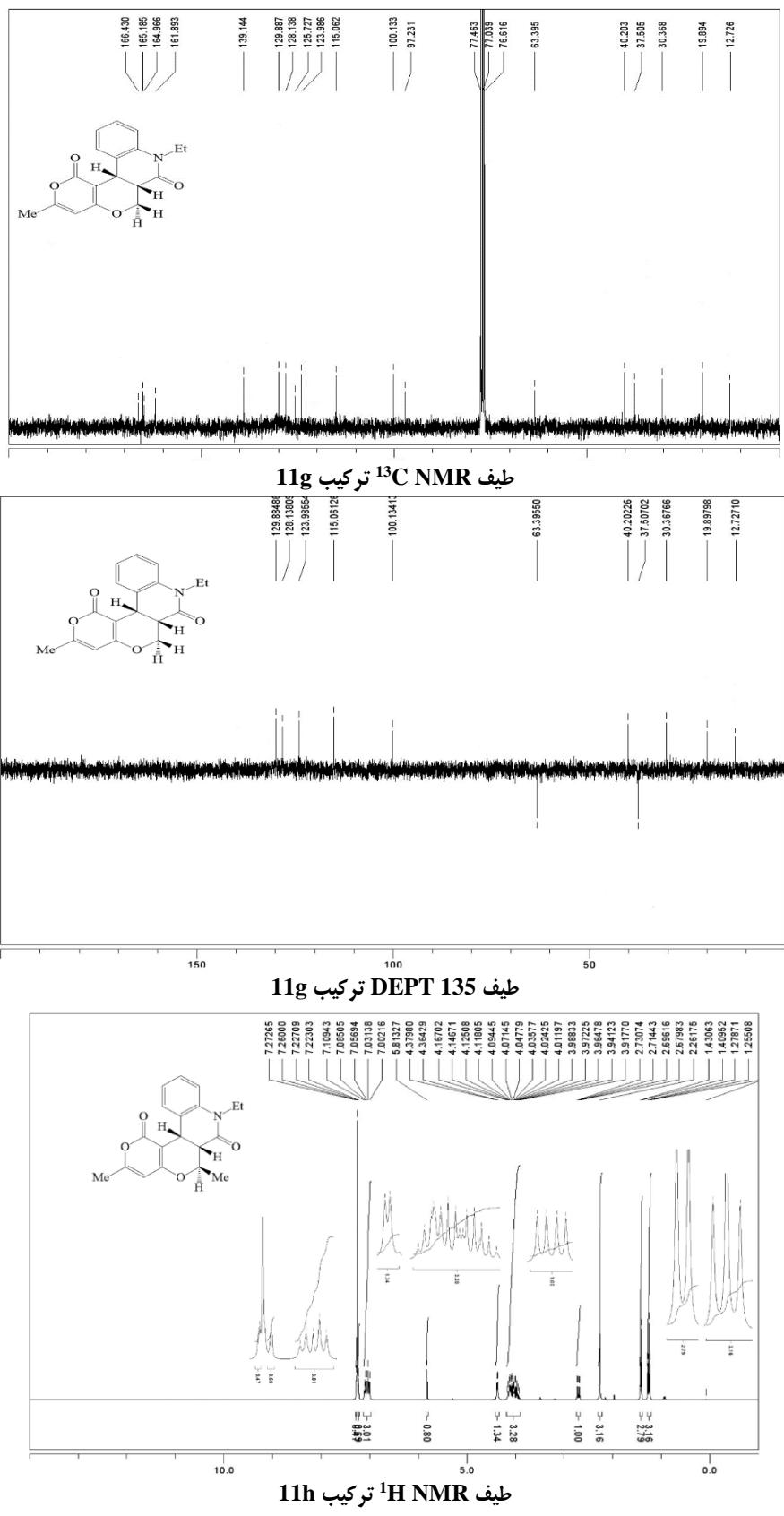
11f طيف HRMs





File : D:\Xcalibur\data\1701\17011804hrei-av2.RAW						2a-10		Composition	
Full ms [301.500 - 323.500] - Range: 311.000 - 311.500									
Scan No.	1 of 1	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition	
Mass	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition		
311.11530	424786	57.0	311.11521	0.3	0.1	11.0	C ₁₈ H ₁₇ O ₄ N ₁		

11g ترکیب HRMs طیف



MS Spectrum Peak List

Ion	Amund	Formula	Calculated Mass	Measured Mass	Difference	Diff (ppm)
(M+H)+	18786.29	C19H19NO4	326.13868	326.13847	0.21	0.65
(M+Na)+	52243	C19H19NO4	348.12063	348.12068	-0.05	-0.13

--- End Of Report ---

طيف HRMs تركيب 11h

