Electronic Supplementary information

N-Heterocyclic carbene catalyzed 1,3-dipolar cycloaddition reactions: A facile synthesis of 3,5-di and 3,4,5-trisubstituted isoxazoles

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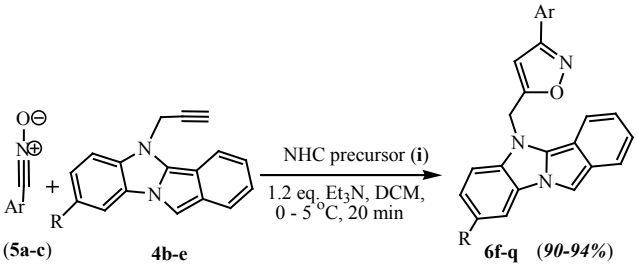
Table S_1. Results of organo-NHC catalyzed cycloaddtion of terminal alkyne of isoindole (**4b-e**) with nitrile oxides (**5a-c**).[a]



(**5a-c**) **4b-e** **6f-q** (***90-94%***)

Entry	Ar	R	Product	Time (min.) (Yield, %)[b]
1	4-OMeC_6H_4 (**5a**)	Cl (**4b**)	**6f**	20 (90)
2	4-MeC_6H_4 (**5b**)	**4b**	**6g**	18 (94)
3	2-$NO_2C_6H_4$ (**5c**)	**4b**	**6h**	20 (90)
4	**5a**	Br (**4c**)	**6i**	20 (92)
5	**5b**	**4c**	**6j**	20 (90)
6	**5c**	**4c**	**6k**	20 (90)
7	**5a**	CH_3 (**4d**)	**6l**	18 (90)
8	**5b**	**4d**	**6m**	20 (90)
9	**5c**	**4d**	**6n**	20 (91)
10	**5a**	OCH_3 (**4e**)	**6o**	15 (92)
11	**5b**	**4e**	**6p**	20 (94)
12	**5c**	**4e**	**6q**	20 (92)

[a] All products were characterized by NMR and mass spectral analysis.
[b] Isolated yields after column chromatography.

Spectral data of compounds 6f-q:

8-Chloro-5-(3-(4-methoxyphenyl)isoxazol-5-ylmethyl)-5*H* benzo(4,5)imidazo(2,1a) isoindole (6f). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 3.85 (s, 3H), 4.56 (s, 2H), 6.40 (s, 1H), 6.85-7.29 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 428 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}ClN_3O_2$ (427.88): calcd. C 70.18, H 4.24, N 9.82; found C 70.16, H 4.23, N 9.80.

8-Chloro-5-(3-(4-methylphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6g). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.35 (s, 3H), 4.56 (s, 2H), 6.38 (s, 1H), 6.95-7.21 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 412 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}ClN_3O$ (411.11): calcd. C 72.90, H 4.40, N 10.20; found C 72.89, H 4.38, N 10.18.

8-Chloro-5-(3-(2-nitrophenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6h). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 4.56 (s, 2H), 6.41 (s, 1H), 6.98-7.62 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 443 $[M + H]^+$. EA calcd (%) for $C_{24}H_{15}ClN_4O_3$ (442.08): calcd. C 65.09, H 3.41, N 12.65; found C 65.08, H 3.40, N 12.63.

8-Bromo-5-(3-(4-methoxyphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6i). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 3.86 (s, 3H), 4.56 (s, 2H), 6.40 (s, 1H), 6.88-7.27 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 472 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}BrN_3O_2$ (471.06): calcd. C 63.57, H 3.84, N 8.90; found C 63.55, H 3.83, N 8.87.

8-Bromo-5-(3-(4-methylphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6j). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.35 (s, 3H), 4.56 (s, 2H), 6.38 (s, 1H), 6.95-7.21 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 455 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}BrN_3O$ (455.06): calcd. C 65.80, H 3.98, N 9.21; found C 65.78, H 3.96, N 9.20.

8-Bromo-5-(3-(2-nitrophenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6k). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 4.56 (s, 2H), 6.41 (s, 1H), 6.96-7.64 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 487 $[M + H]^+$. EA calcd (%) for $C_{24}H_{15}BrN_4O_3$ (486.03): calcd. C 59.15, H 3.10, N 11.50; found C 59.13, H 3.08, N 11.47.

5-(3-(4-Methoxyphenyl)isoxazol-5-ylmethyl)-8-methyl-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6l). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.42 (s, 3H), 3.84 (s, 3H), 4.56 (s, 2H), 6.38 (s, 1H), 6.95-7.26 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 408 $[M + H]^+$. EA calcd (%) for $C_{26}H_{21}N_3O_2$ (407.16): calcd. C 76.64, H 5.19, N 10.31; found C 76.63, H 5.16, N 10.30.

8-Methyl-5-(3-(4-methylphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6m). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.36 (s, 3H), 2.42 (s, 3H), 4.56 (s, 2H), 6.36 (s, 1H), 6.96-7.21 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 392 $[M + H]^+$. EA calcd (%) for $C_{26}H_{21}N_3O$ (391.17): calcd. C 79.77, H 5.41, N 10.73; found C 79.76, H 5.40, N 10.70.

8-Methyl-5-(3-(2-nitrophenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6n). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.43 (s, 3H), 4.56 (s, 2H), 6.36 (s, 1H), 6.92-7.64 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 423 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}N_4O_3$ (422.14): calcd. C 71.08, H 4.29, N 13.26; found C 71.05, H 4.27, N 13.25.

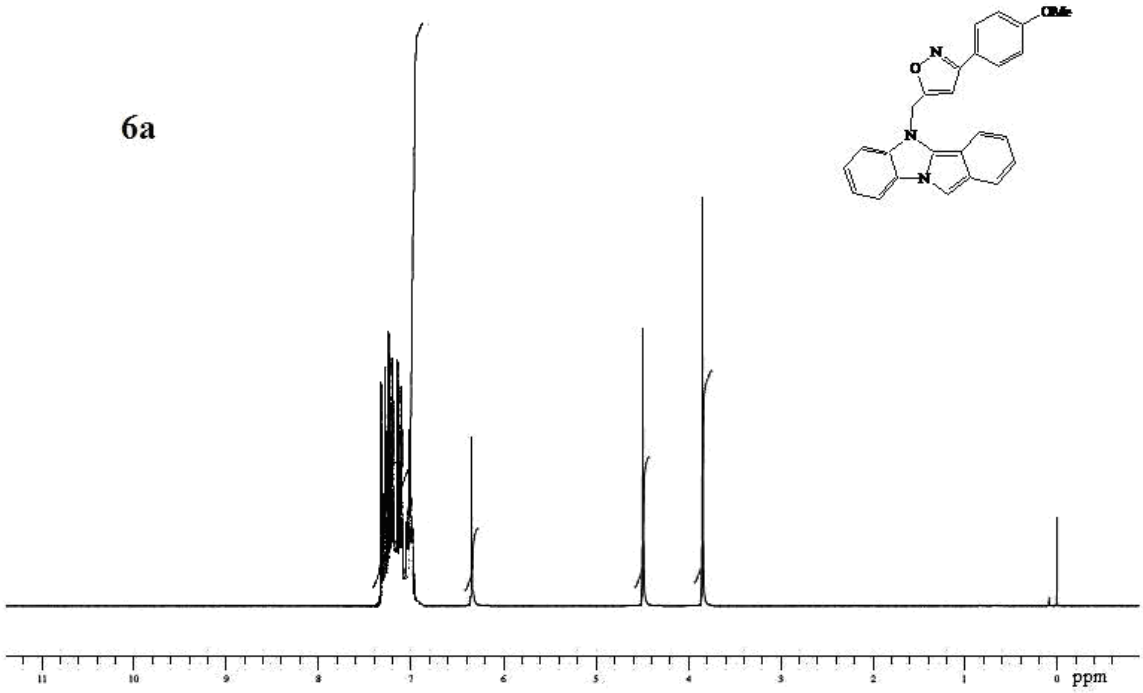
8-Methoxy-5-(3-(4-methoxyphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6o). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 3.84 (s, 3H), 3.92 (s, 3H), 4.56 (s, 2H), 6.38 (s, 1H), 6.95-7.26 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 424 $[M + H]^+$. EA calcd (%) for $C_{26}H_{21}N_3O_3$ (423.16): calcd. C 73.74, H 5.00, N 9.92; found C 73.72, H 4.98, N 9.90.

8-Methoxy-5-(3-(4-methylphenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6p). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 2.36 (s, 3H), 3.92 (s, 3H), 4.56 (s, 2H), 6.36 (s, 1H), 6.96-7.21 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 408 $[M + H]^+$. EA calcd (%) for $C_{26}H_{21}N_3O_2$ (407.16): calcd. C 76.64, H 5.19, N 10.31; found C 76.63, H 5.16, N 10.29.

8-Methoxy-5-(3-(2-nitrophenyl)isoxazol-5-ylmethyl)-5*H*-benzo(4,5)imidazo(2,1a) isoindole (6q). ^{1}H NMR (200 MHz, $CDCl_3$, 25 °C): δ = 3.93 (s, 3H), 4.56 (s, 2H), 6.36 (s, 1H), 6.92-7.64 (m, 12H, Ar-H) ppm. MS (EI, 70 eV): *m*/*z* (%) = 439 $[M + H]^+$. EA calcd (%) for $C_{25}H_{18}N_4O_4$ (438.13): calcd. C 68.49, H 4.14, N 12.78; found C 68.47, H 4.12, N 12.76.

^{1}H, ^{13}C NMR and Mass Spectra

6a



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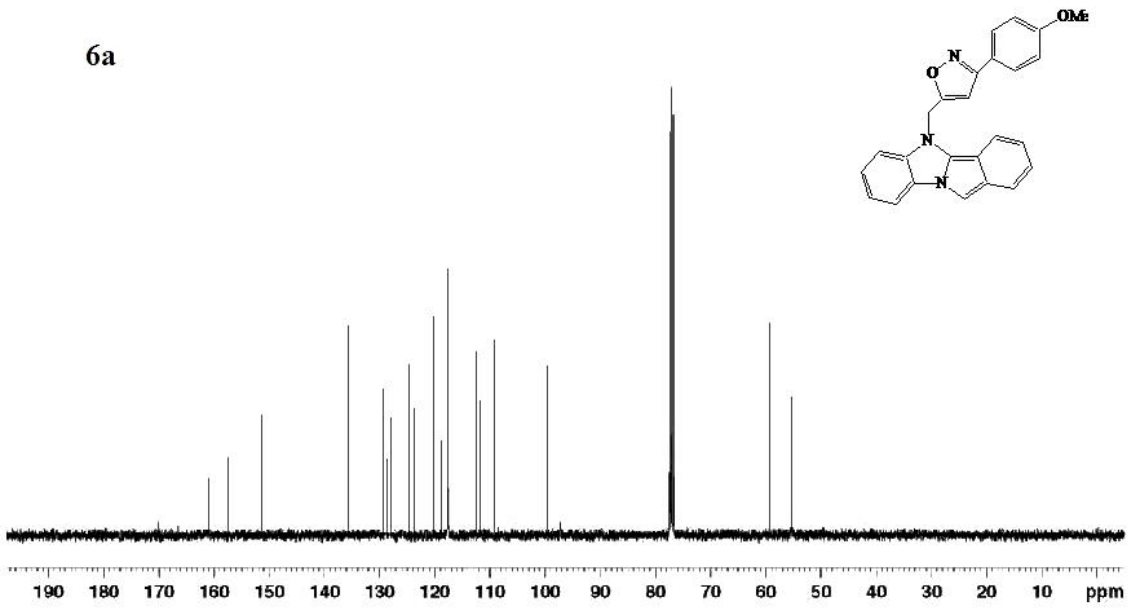

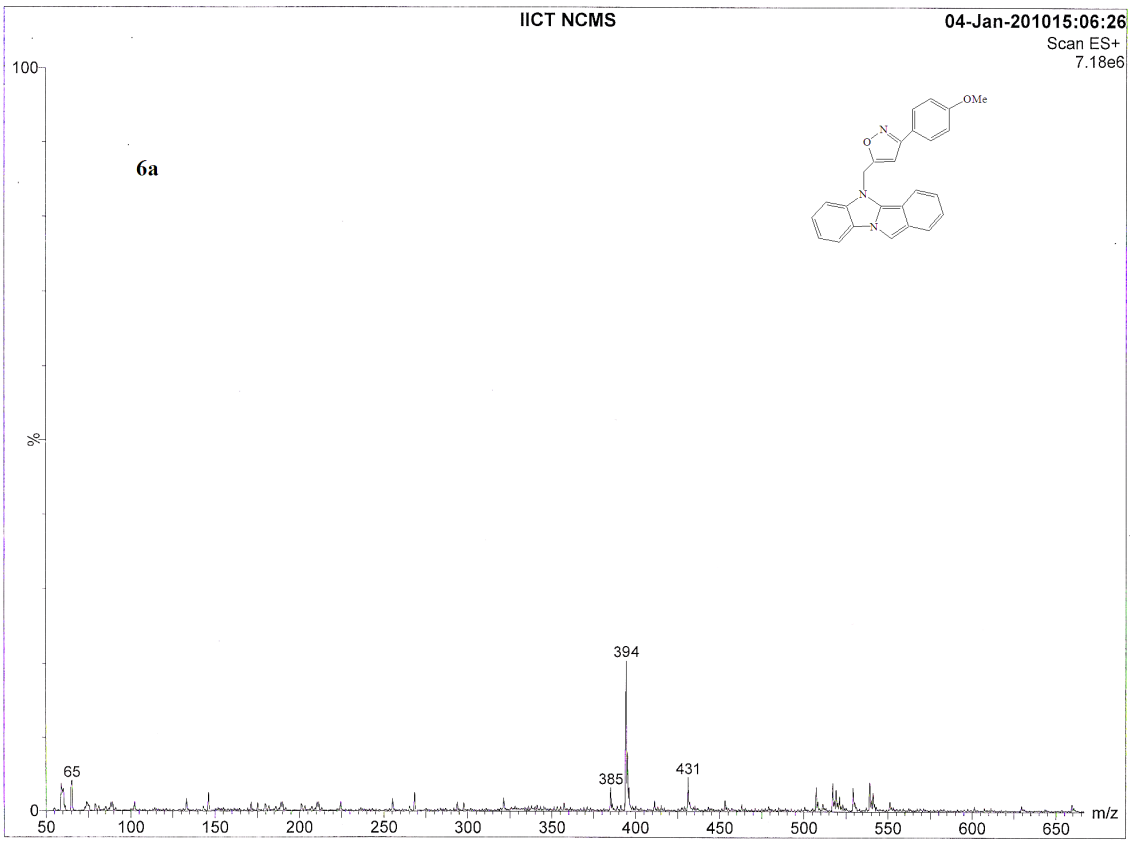

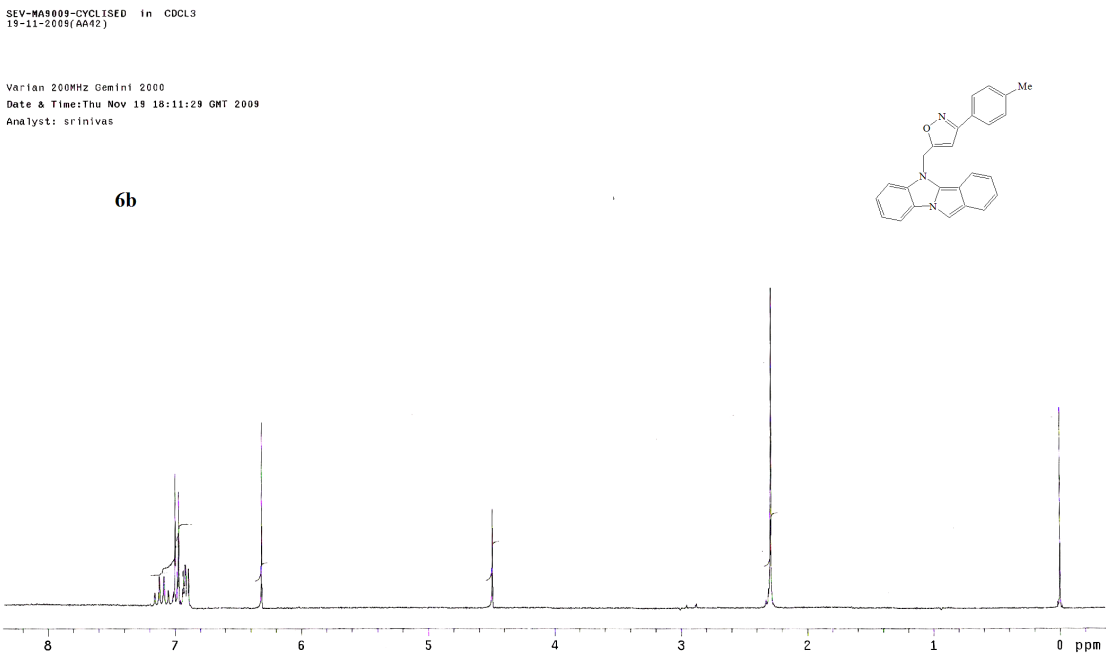

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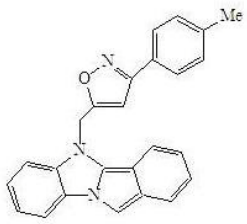

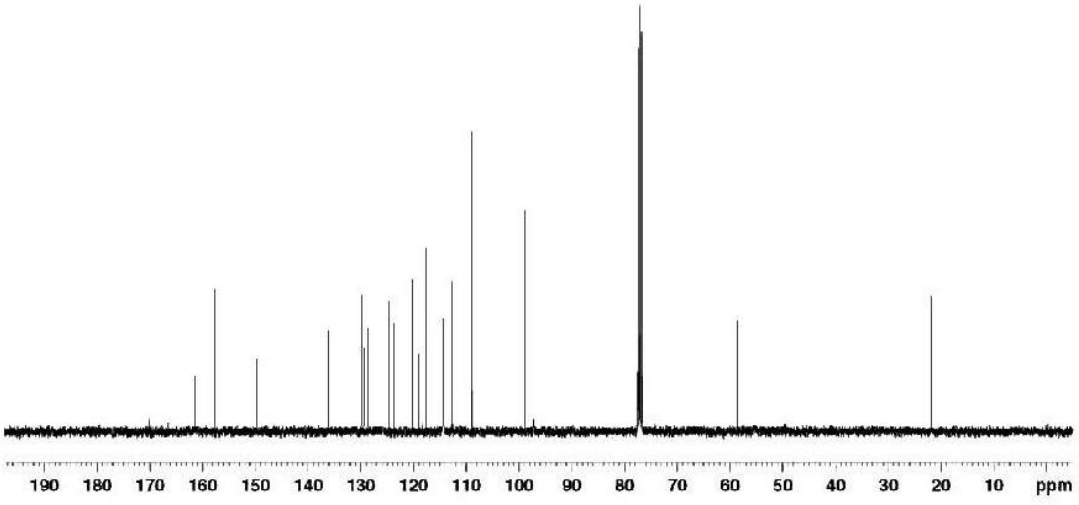

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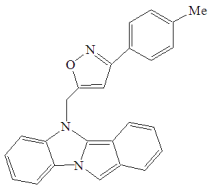

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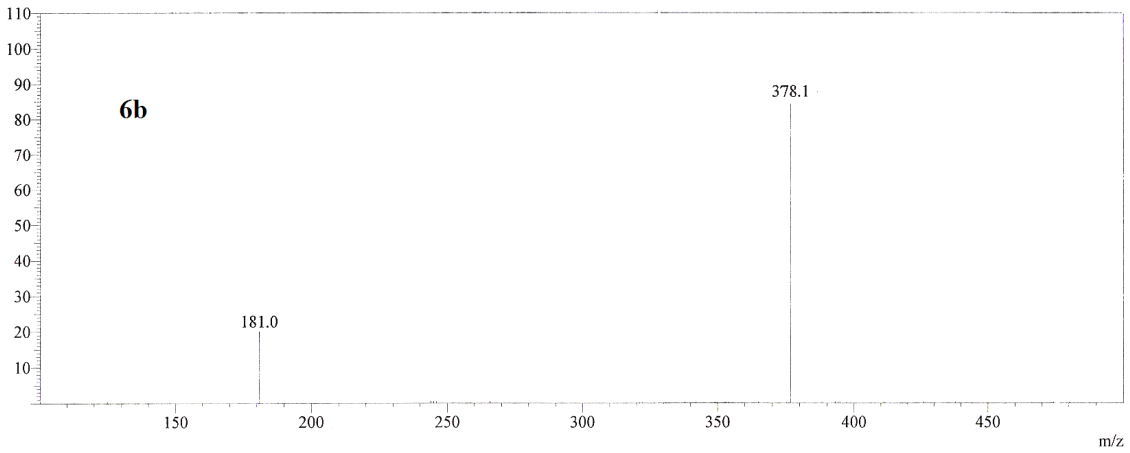

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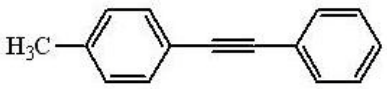

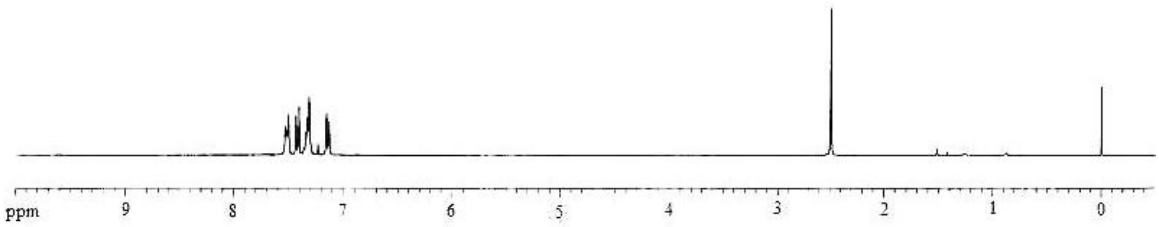

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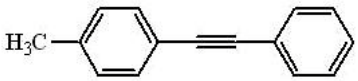

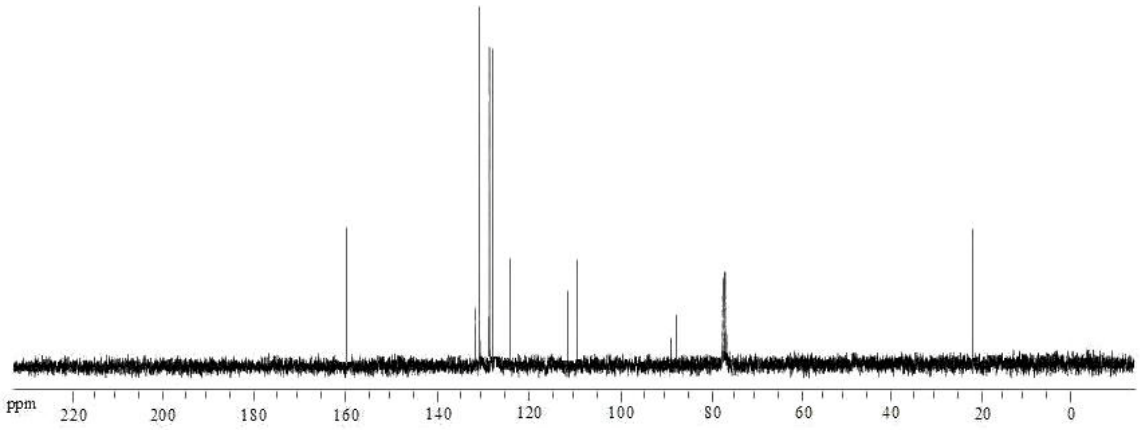

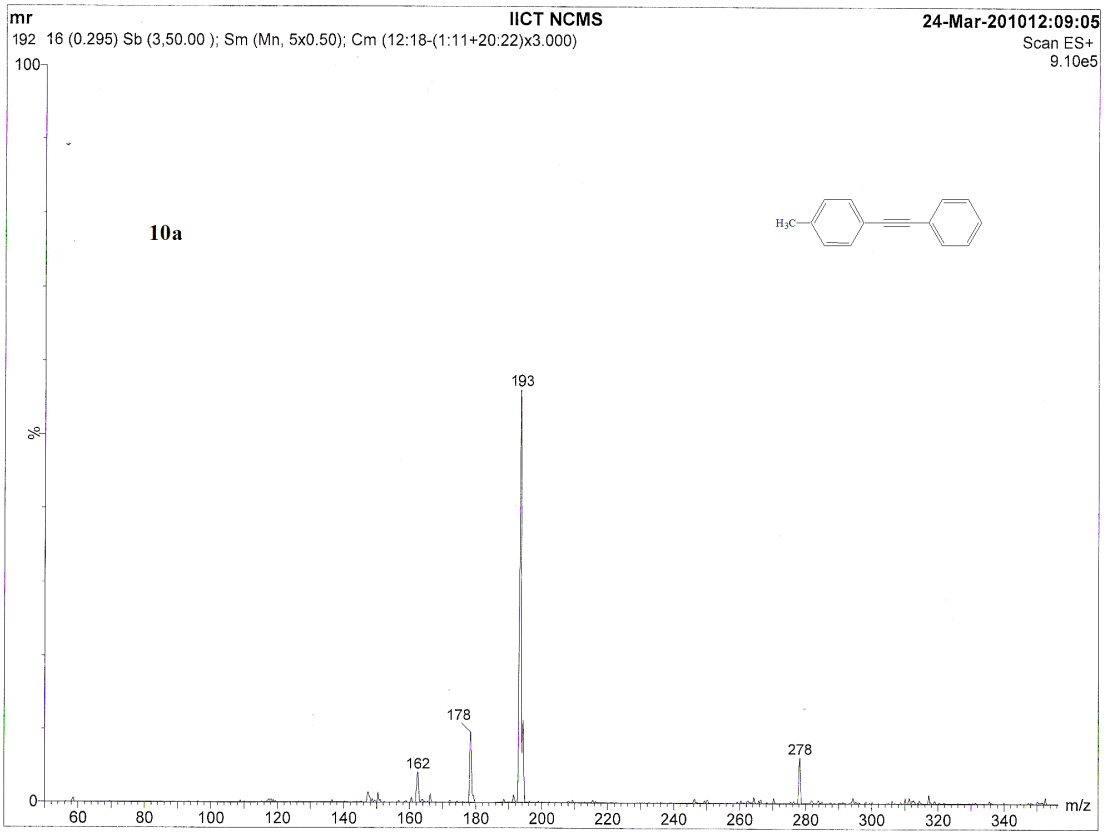

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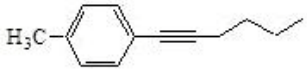

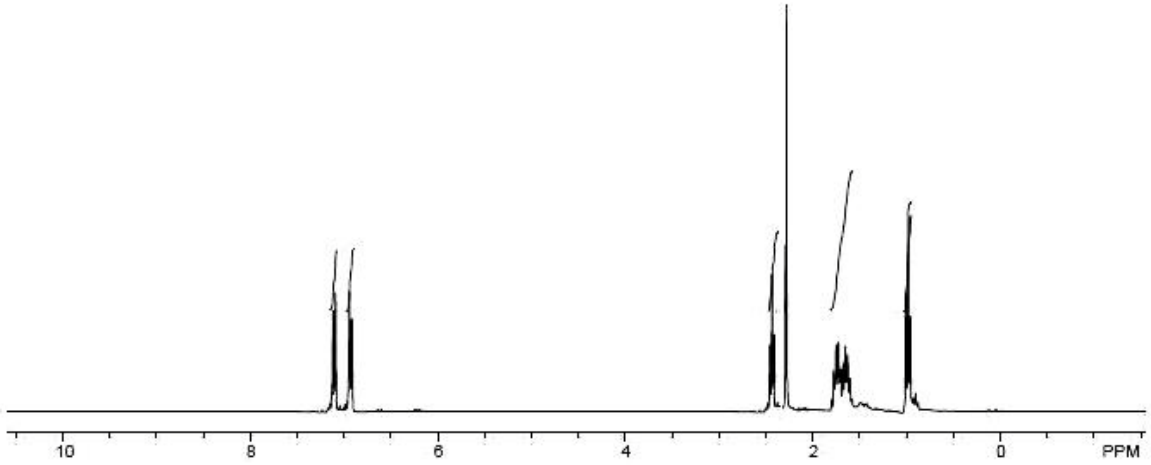

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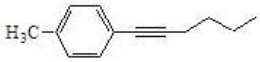

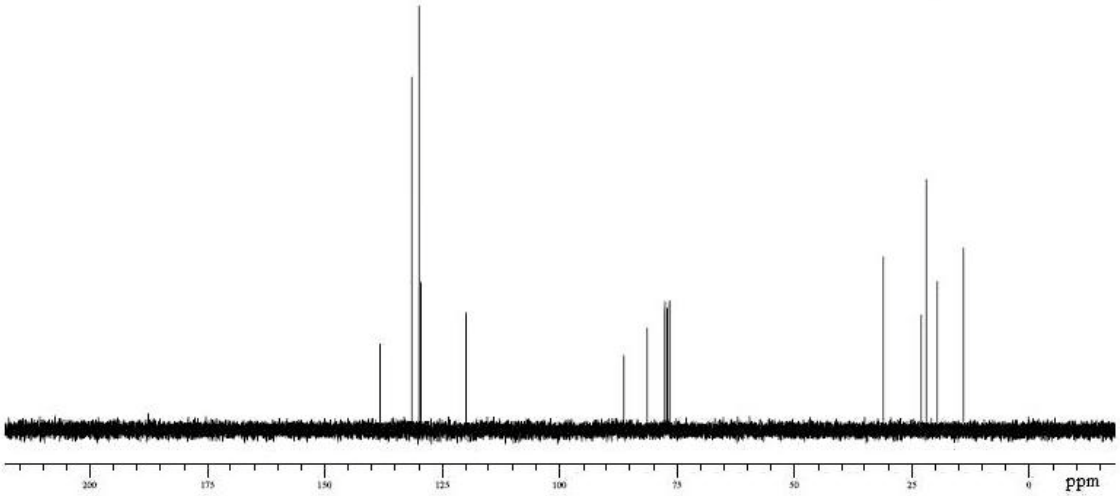

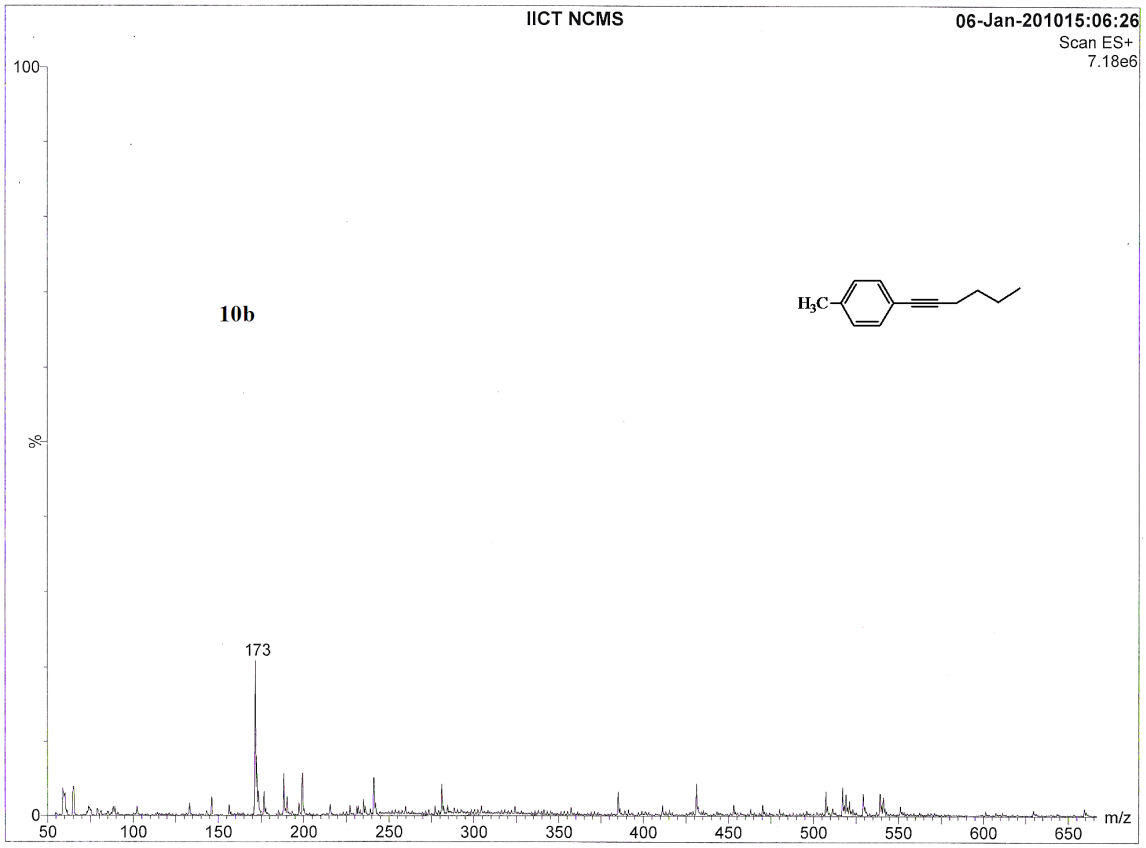

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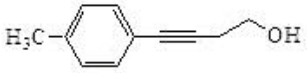

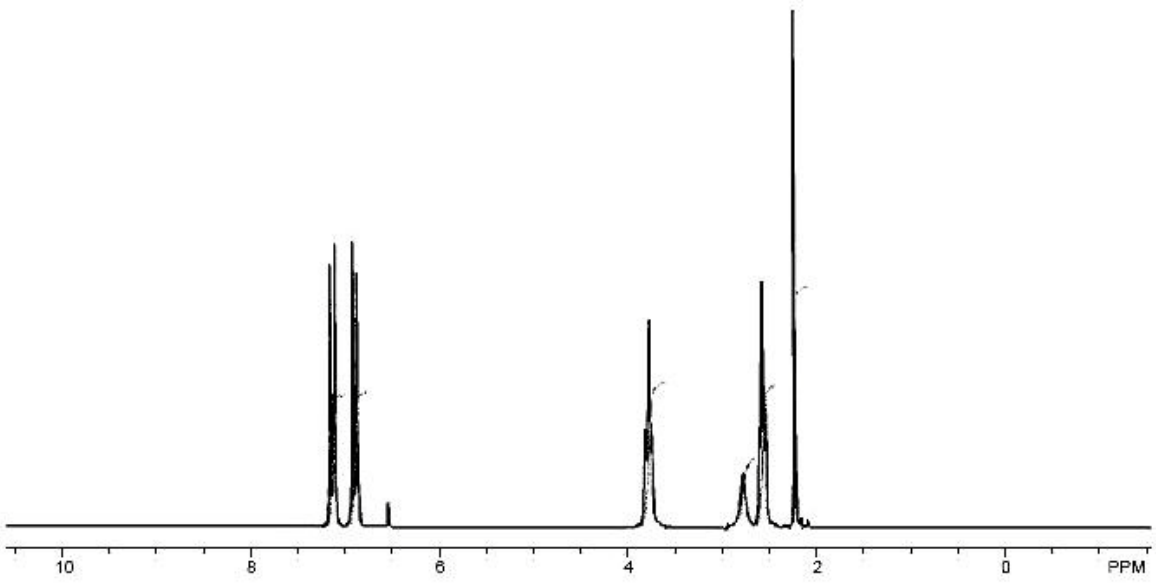

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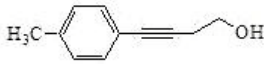

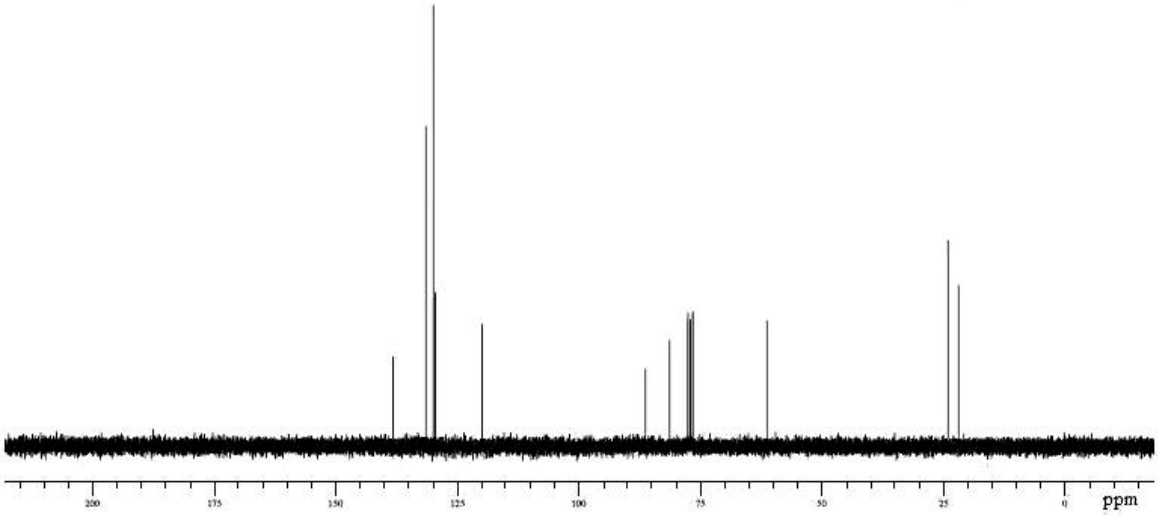

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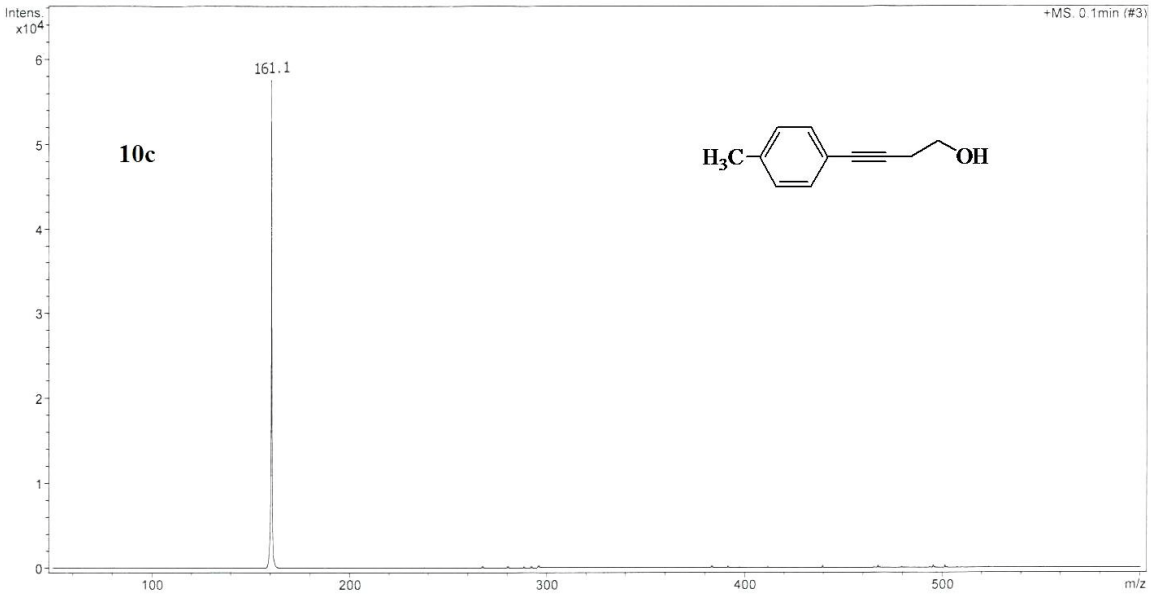

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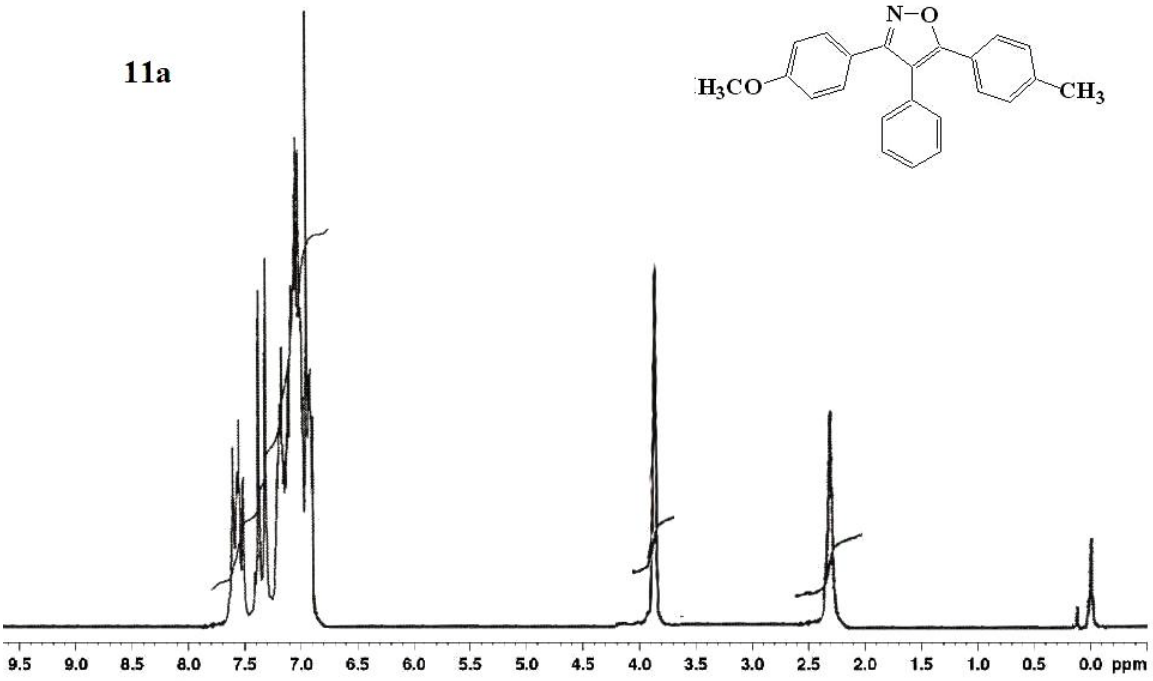

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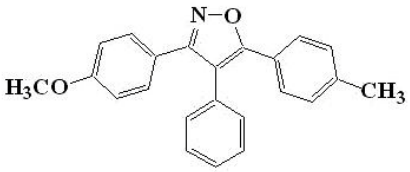

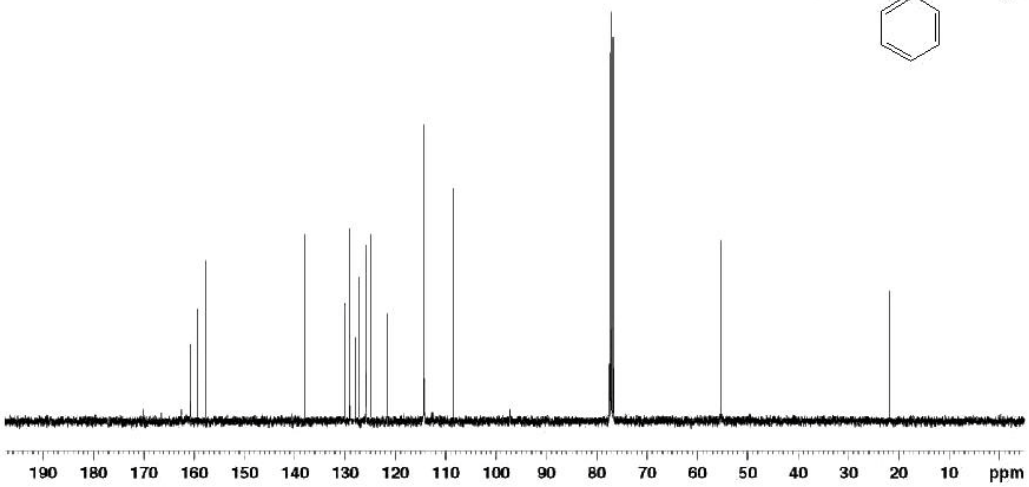

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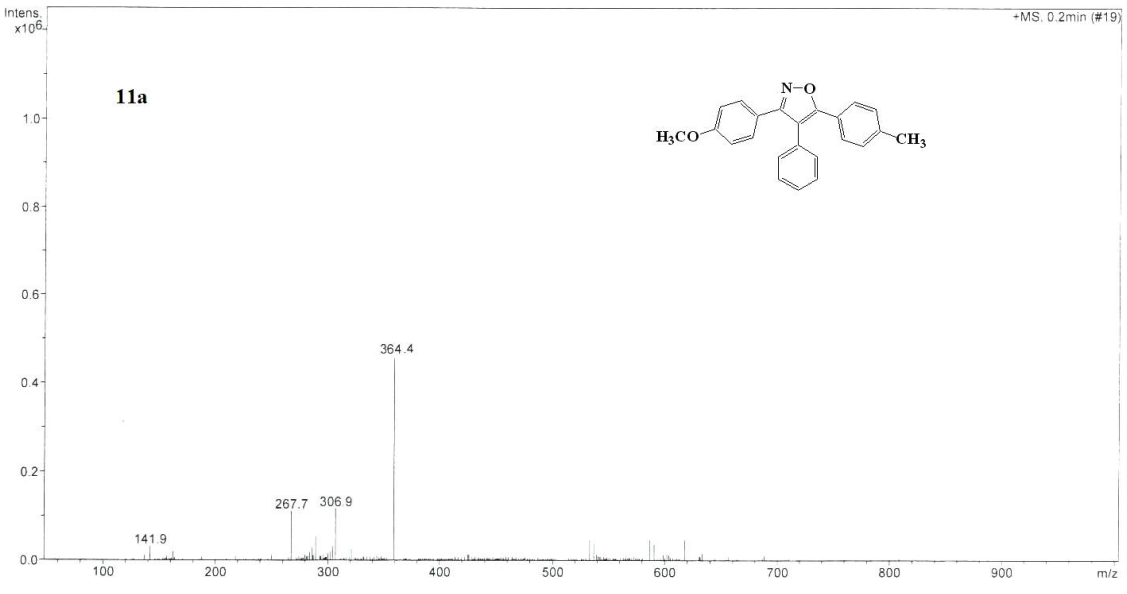

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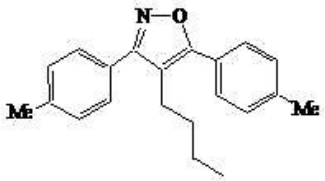

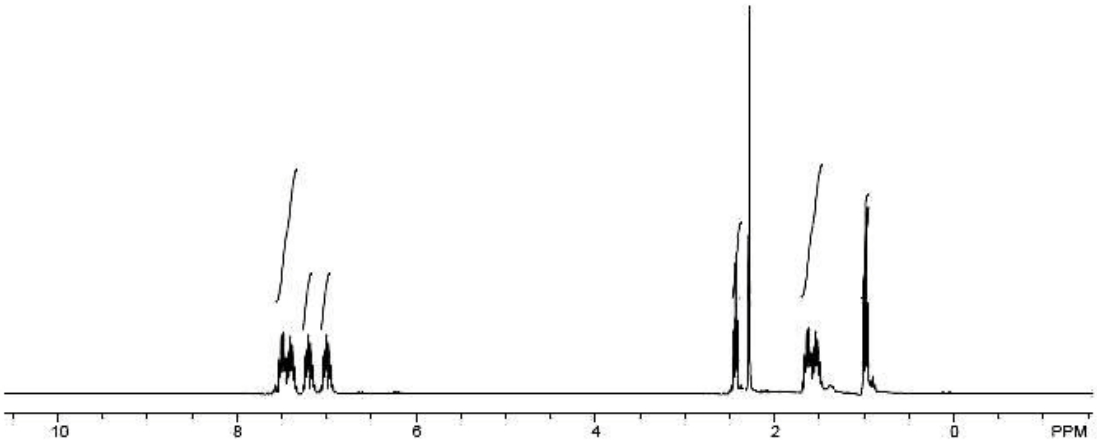

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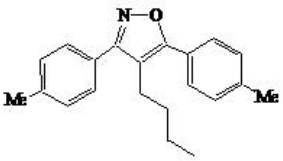

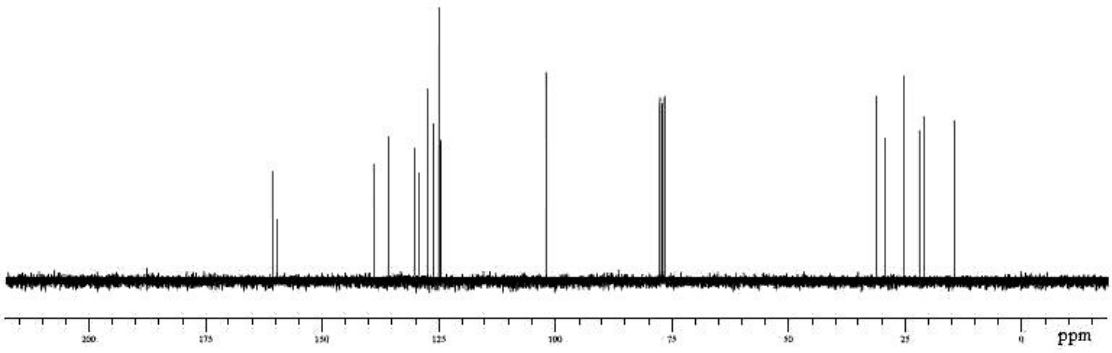

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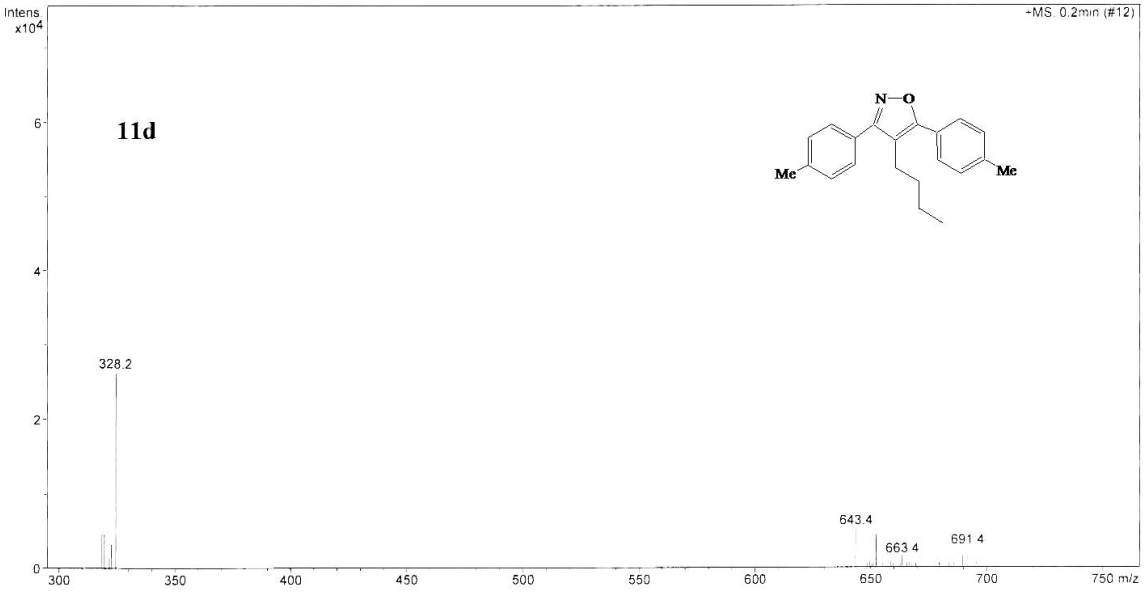

11d

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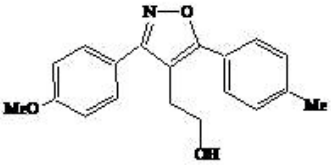
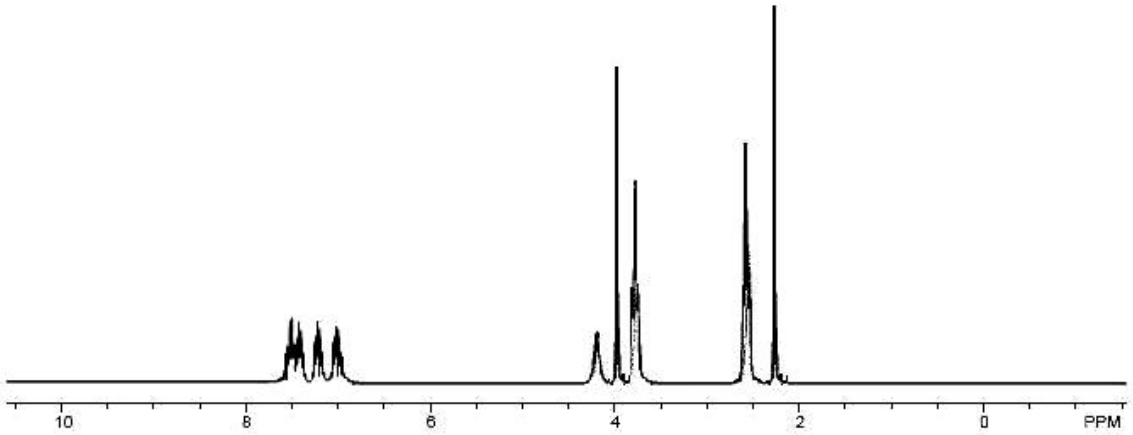
11f





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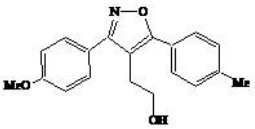

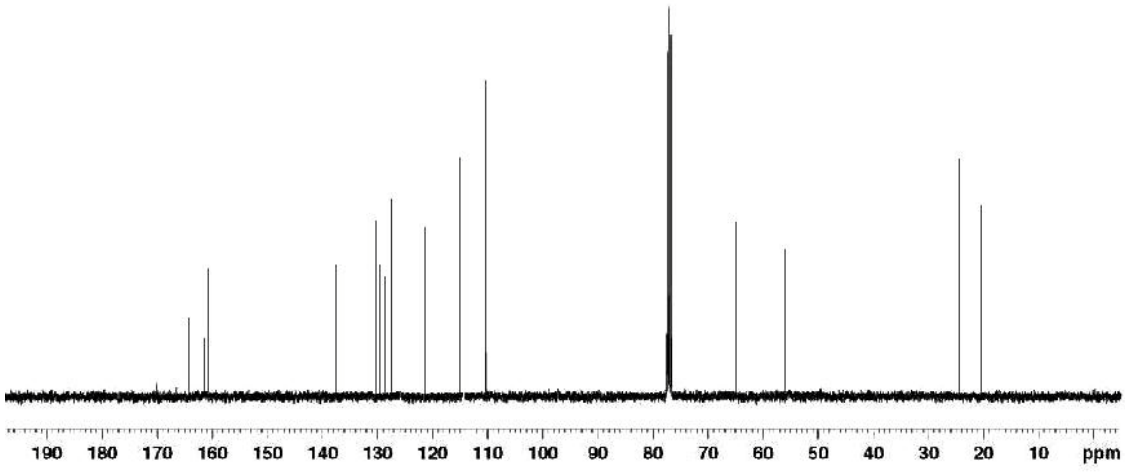

Display Report - Selected Window Selected Analysis

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Method:	Copy of ONLYMASS.M	**Operator:**	Administrator	**Acq. Date:**	10/05/09 03:23:05
Sample Name:	sa30				
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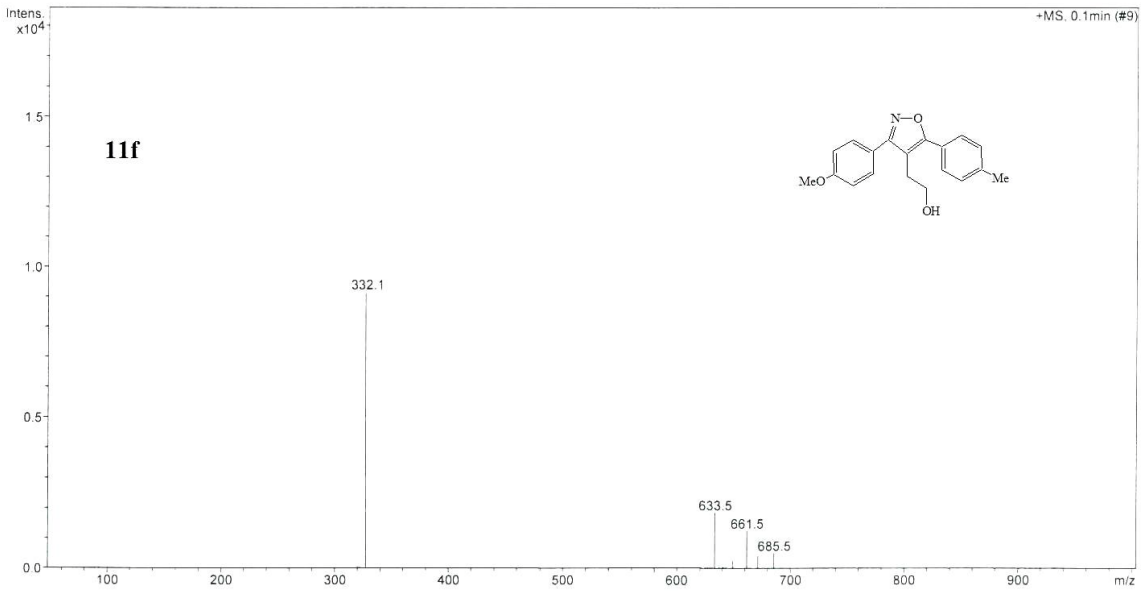

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry