

Supporting Information

Synthesis of 2-Amino-*N'*-aroyl(het)arylhydrazides, DNA Photocleavage, Molecular Docking and Cytotoxicity Studies Against Melanoma CarB Cell Lines

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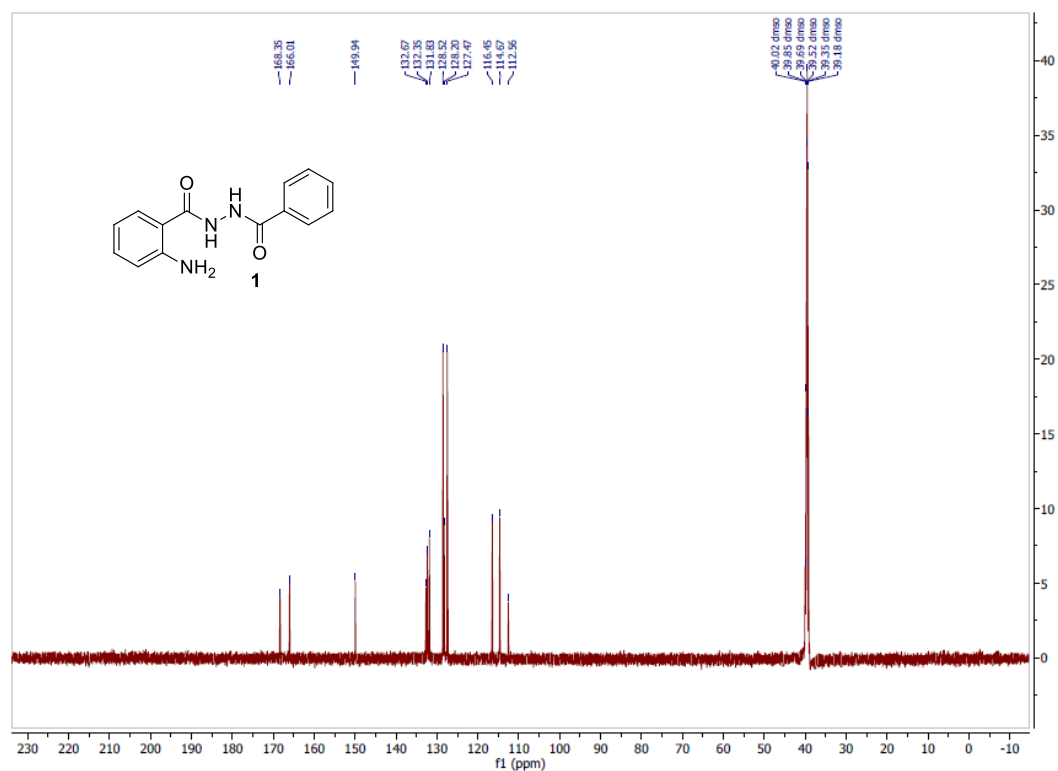
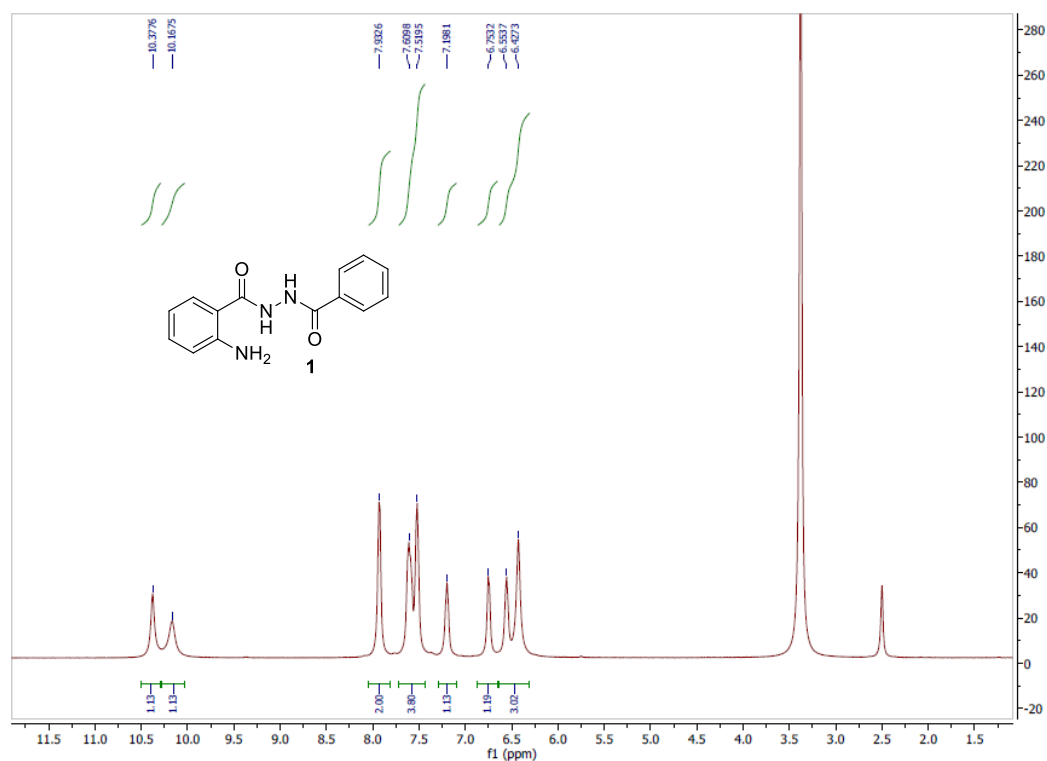
* Correspondence: kfylakta@chem.auth.gr

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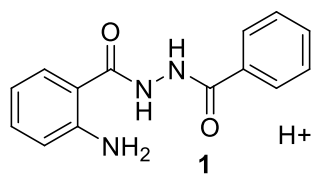
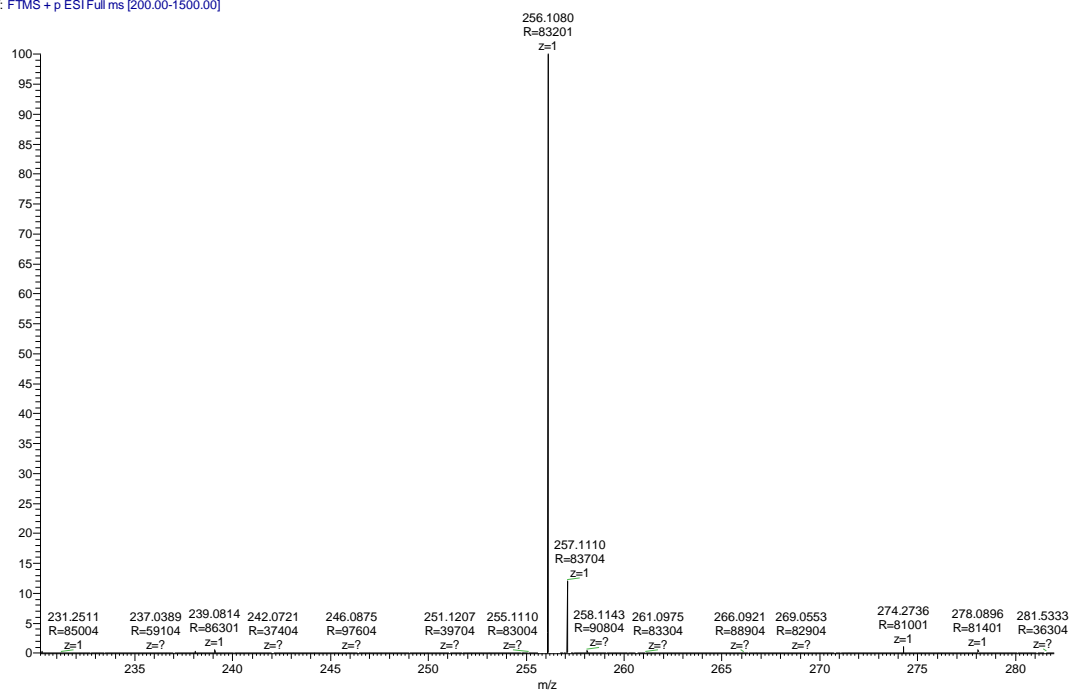
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S.1. Copies of NMR spectra of compounds 1-24 and HRMS measurements

2-amino-*N'*-benzoylbenzohydrazide (1)

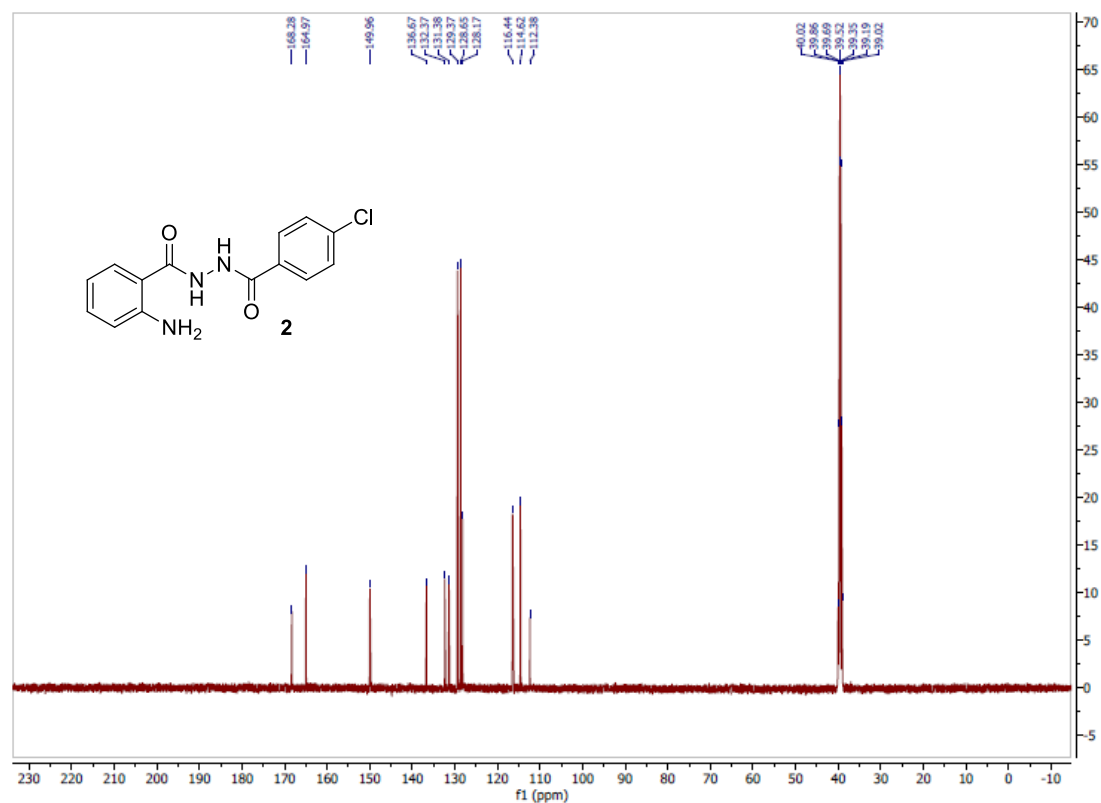
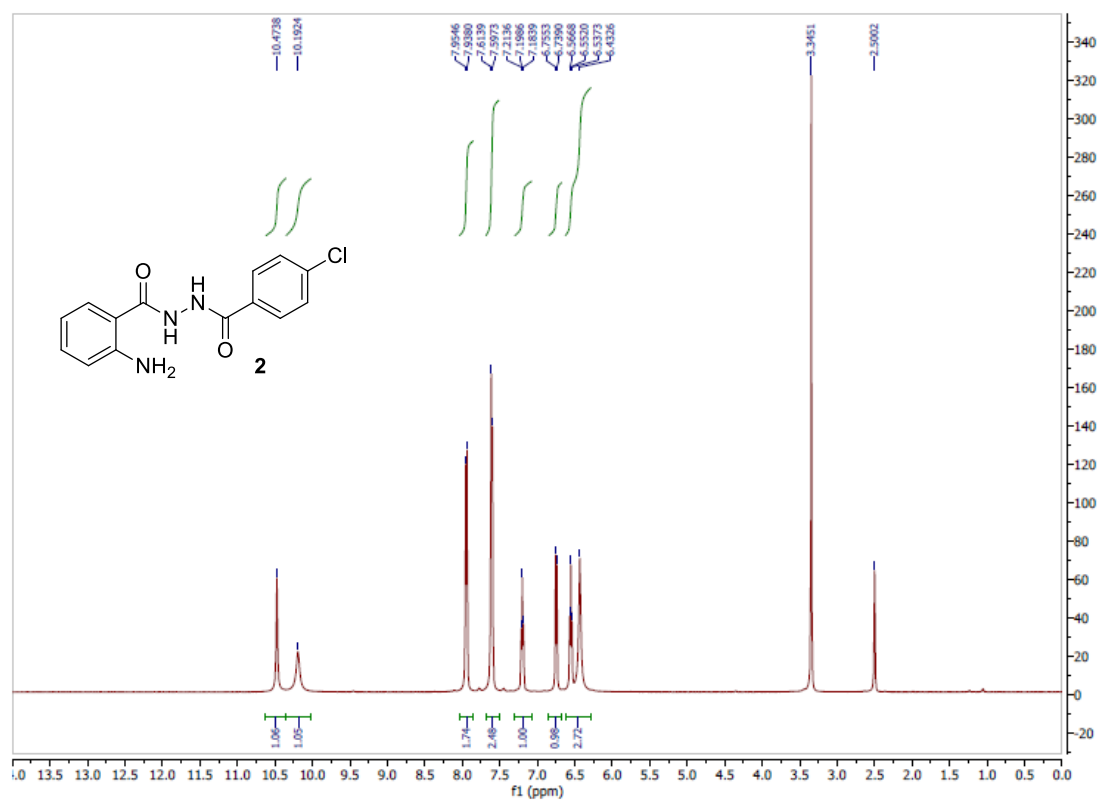


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T: FTMS + p ESI Full ms [200.00-1500.00]

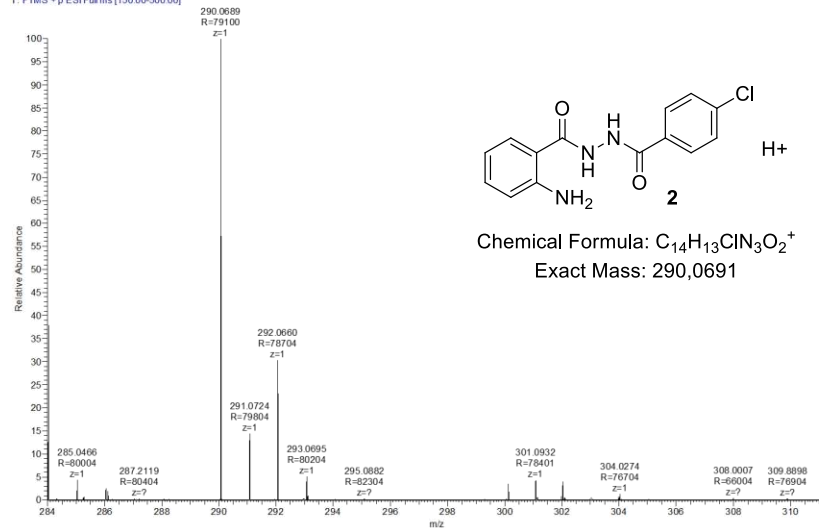


Chemical Formula: $C_{14}H_{14}N_3O_2^+$
Exact Mass: 256,1081

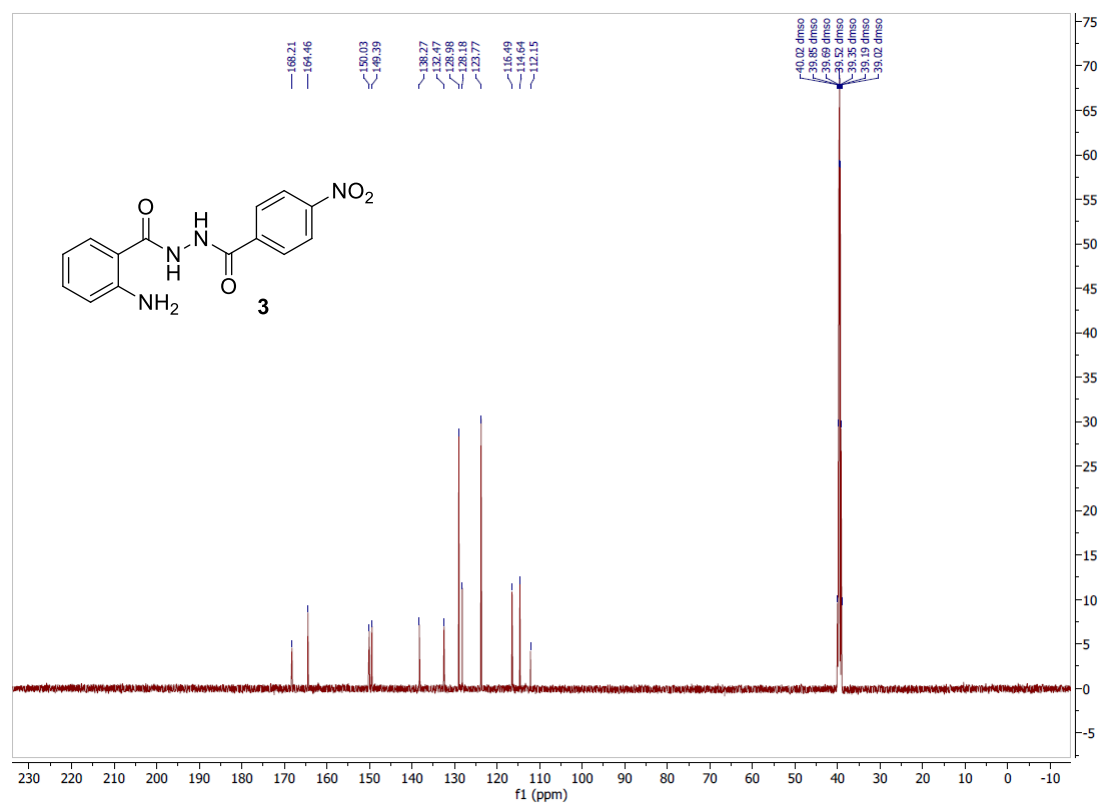
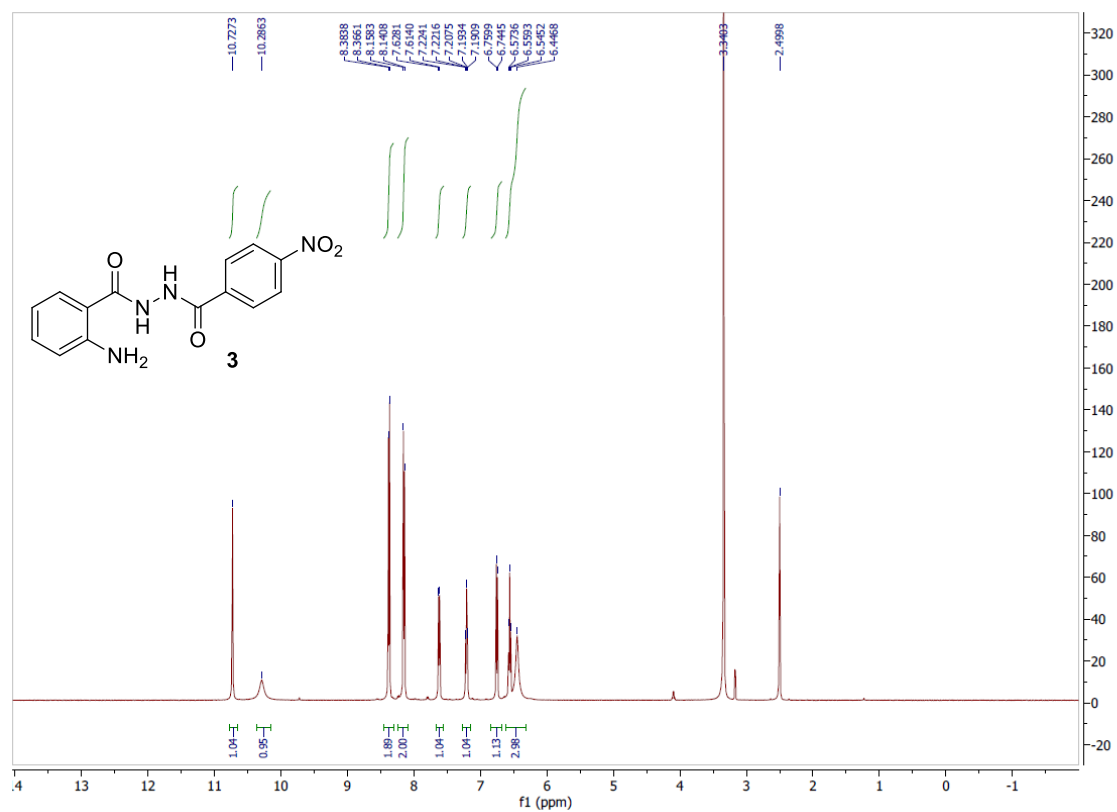
2-amino-*N'*-(4-chlorobenzoyl)benzohydrazide (**2**)

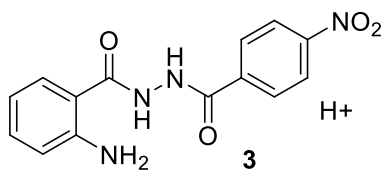


7: 181210123101 #249 RT: 3.65 AV: 1 NL: 3.09E6
T: FTMS • p ESI Full ms [150.00-500.00]



2-amino-*N'*-(4-nitrobenzoyl)benzohydrazide (**3**)

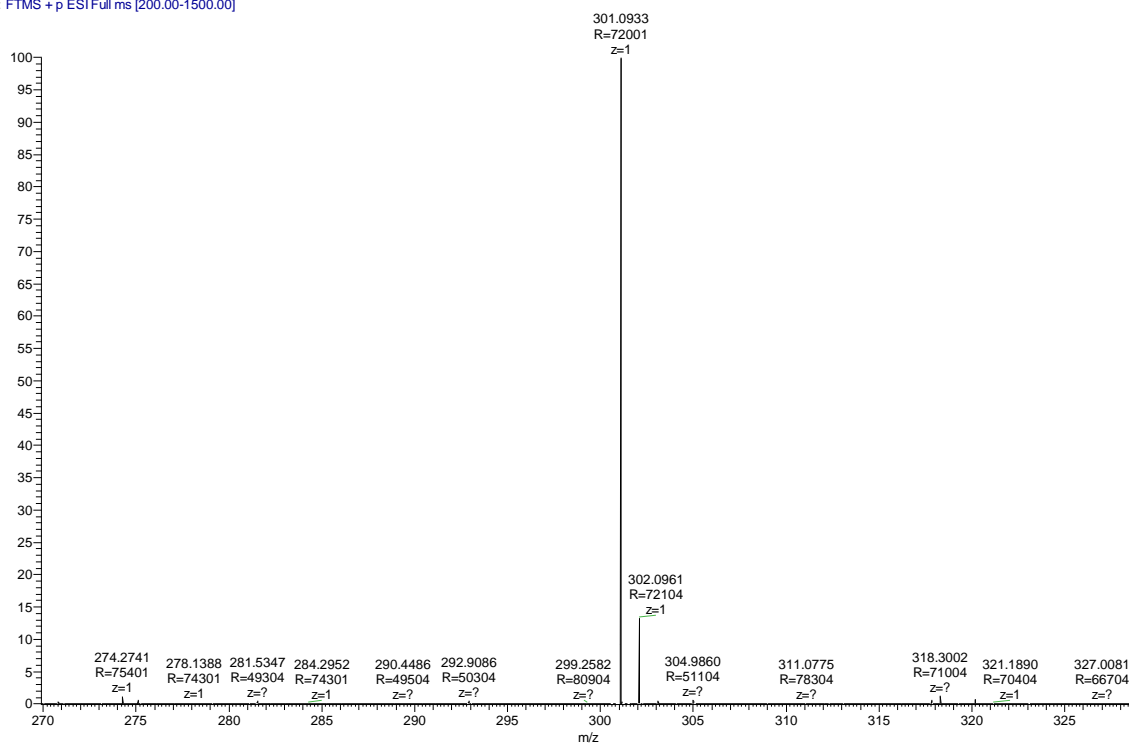




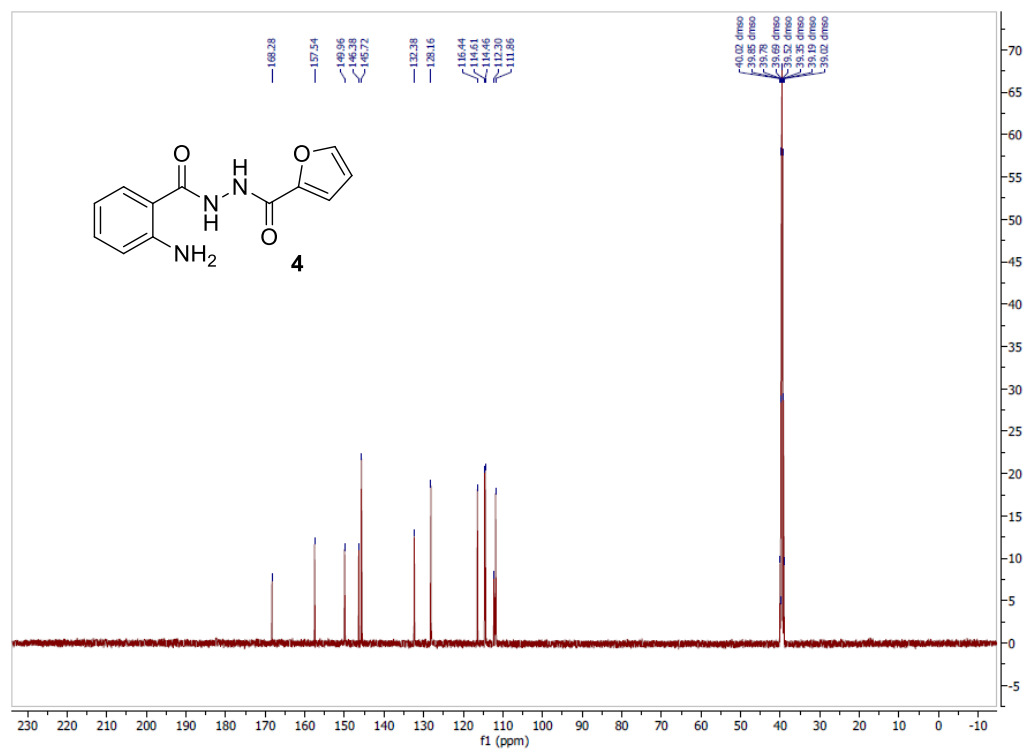
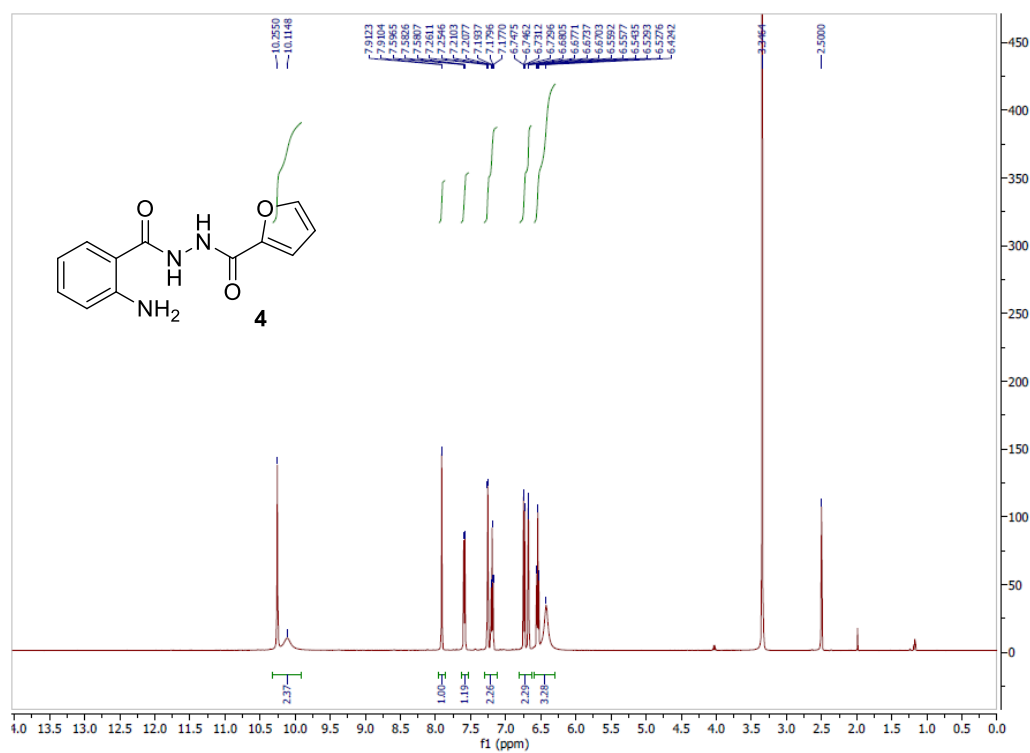
Chemical Formula: $C_{14}H_{13}N_4O_4^+$

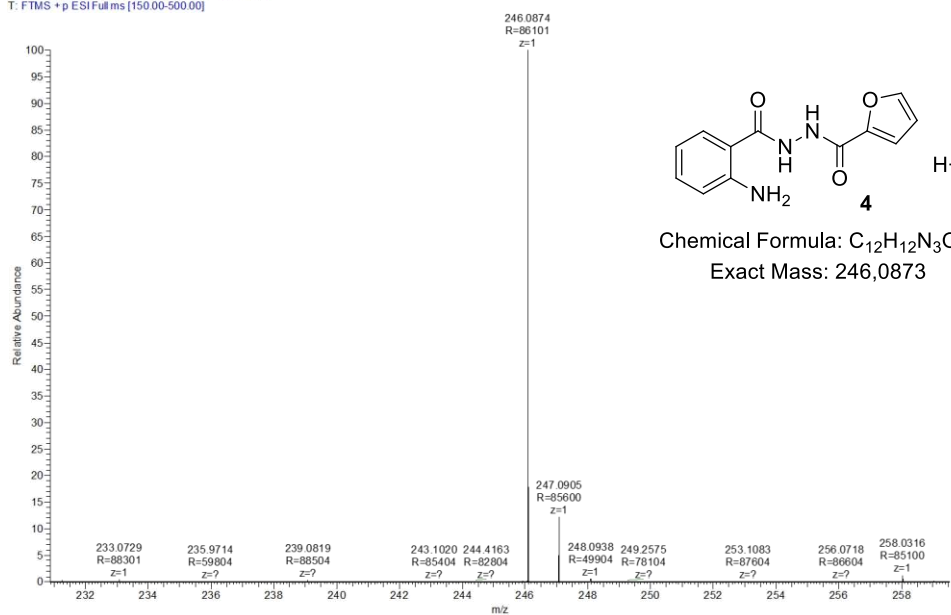
Exact Mass: 301,0931

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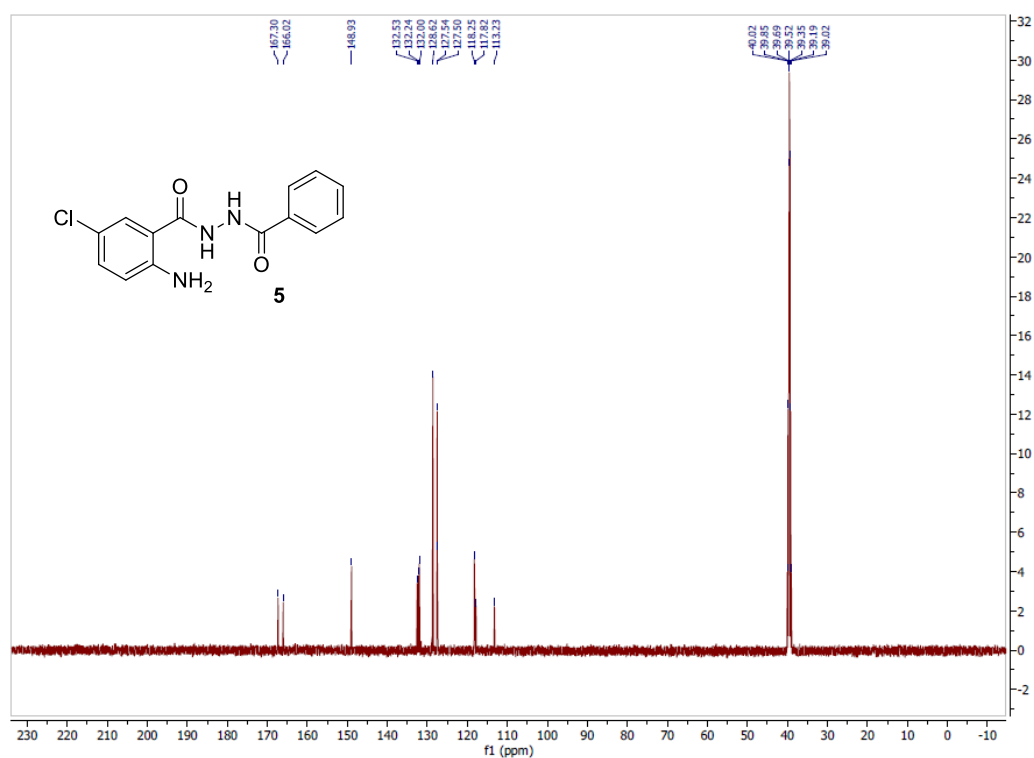
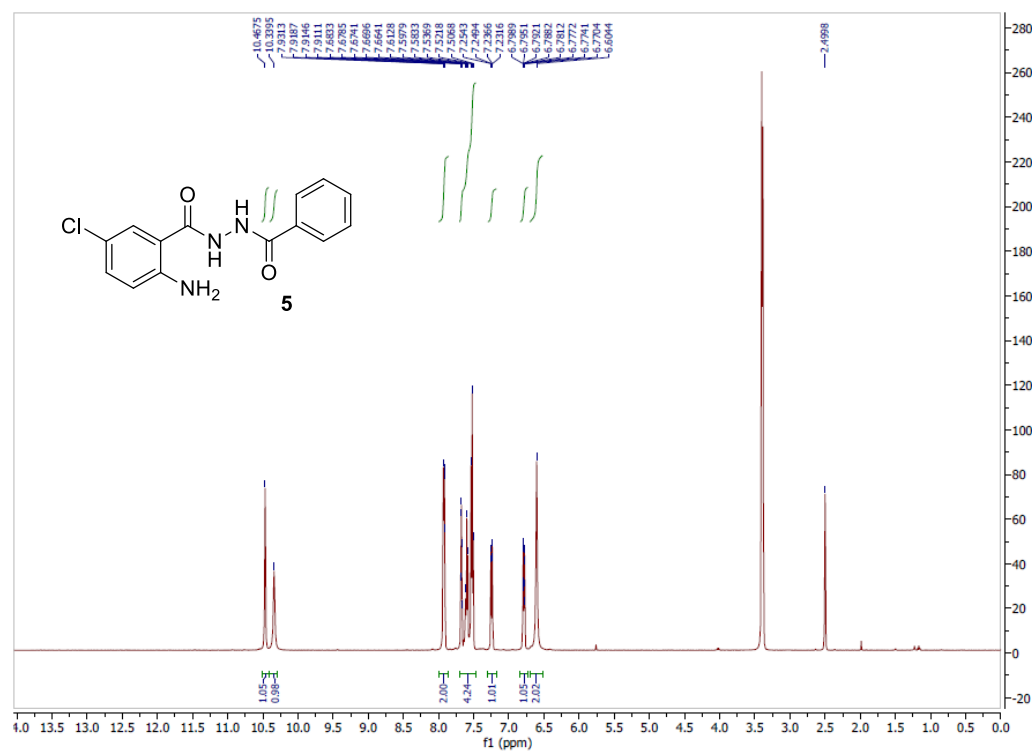


N'-(2-aminobenzoyl)furan-2-carbohydrazide (**4**)

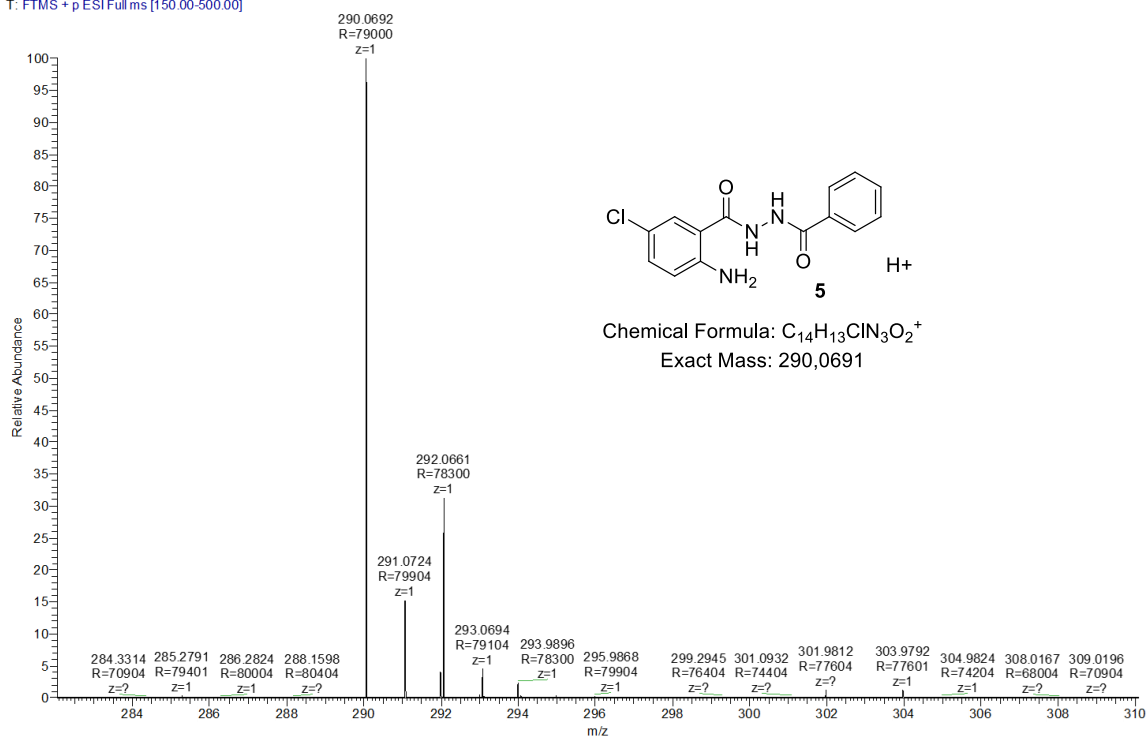




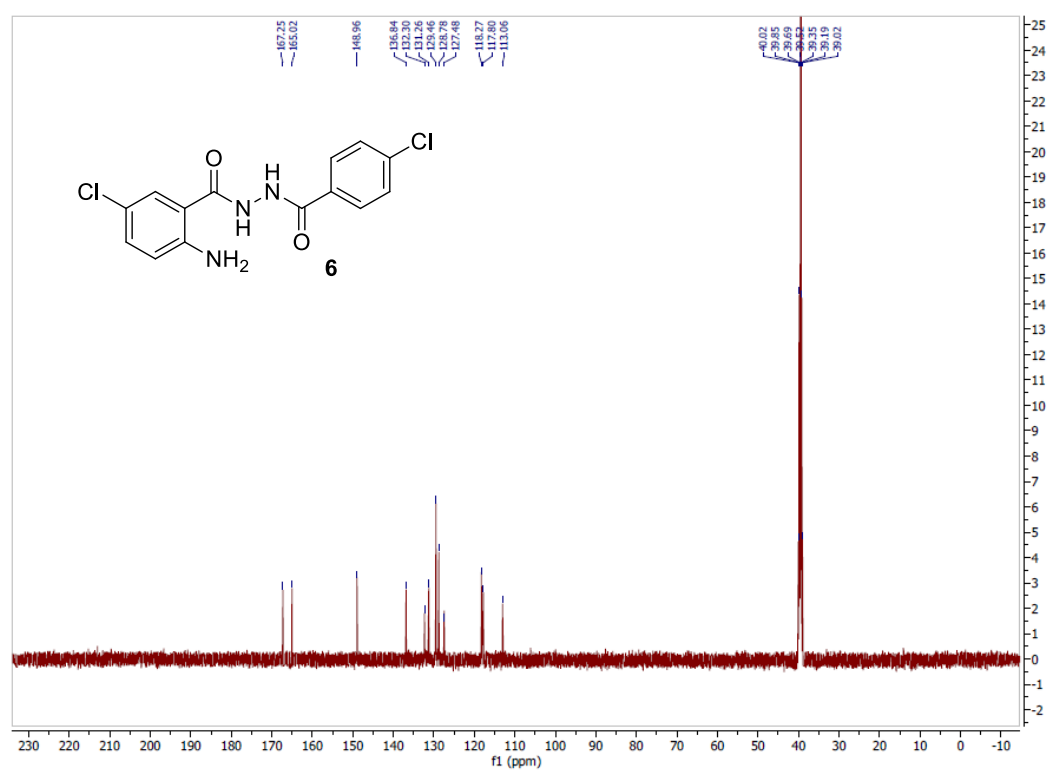
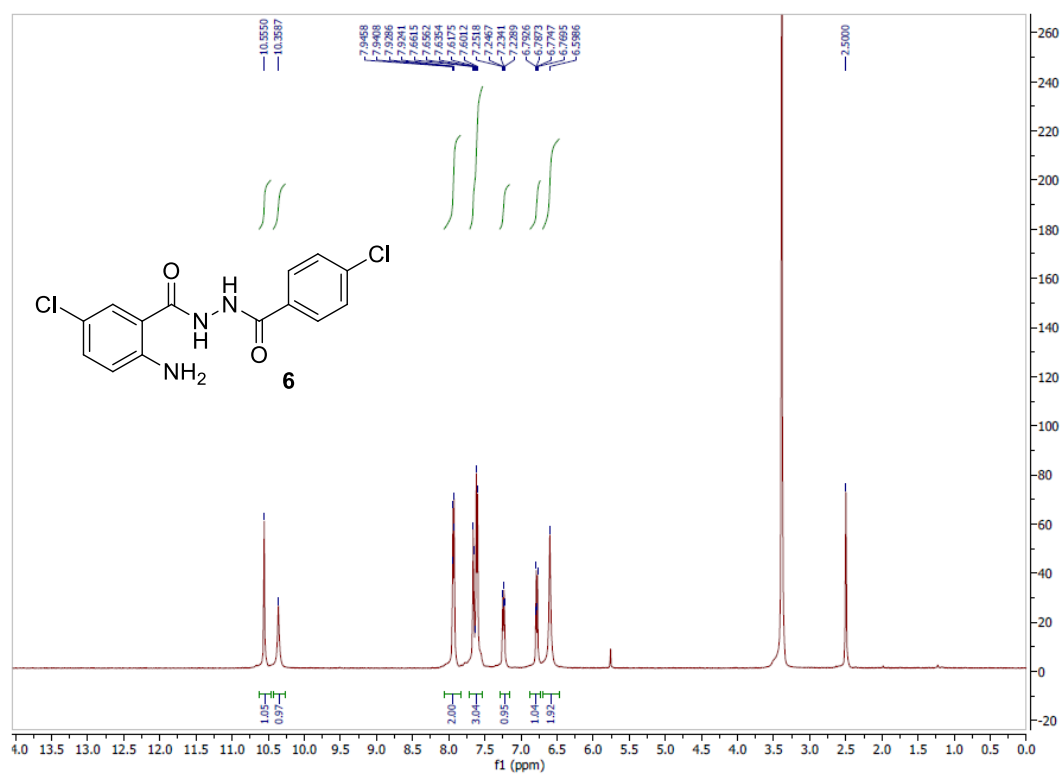
2-amino-*N'*-benzoyl-5-chlorobenzohydrazide (5)



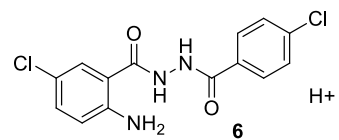
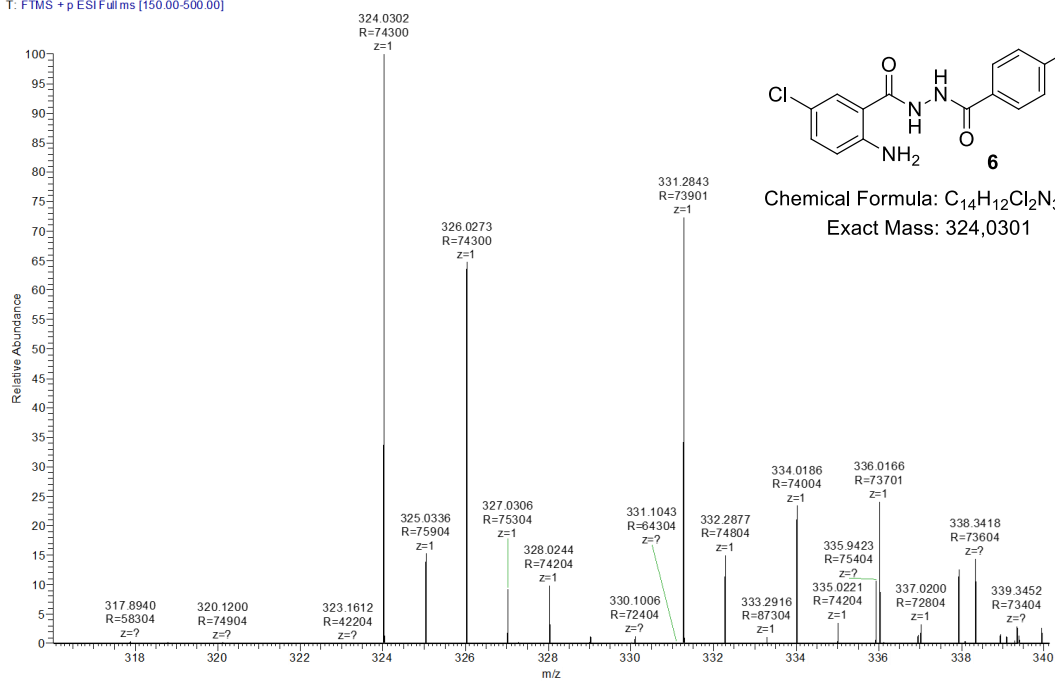
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T: FTMS + p ESI Full ms [150.00-500.00]



2-amino-5-chloro-*N'*-(4-chlorobenzoyl)benzohydrazide (**6**)

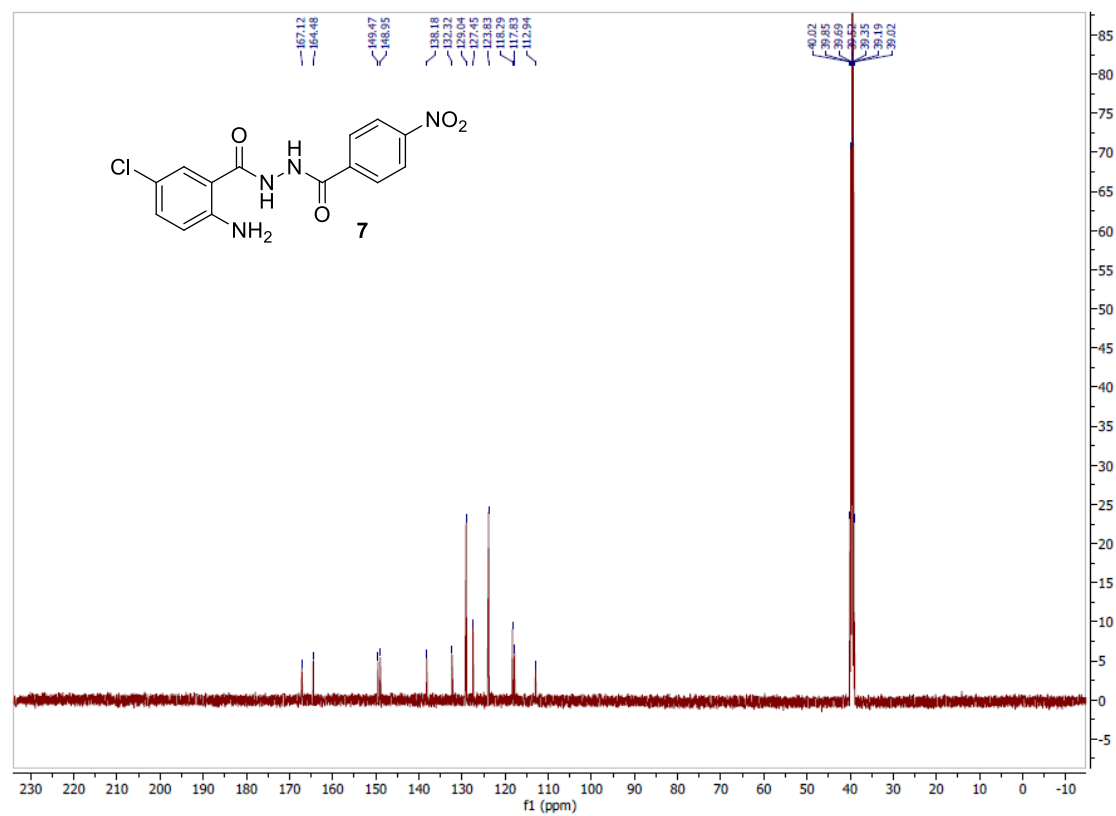
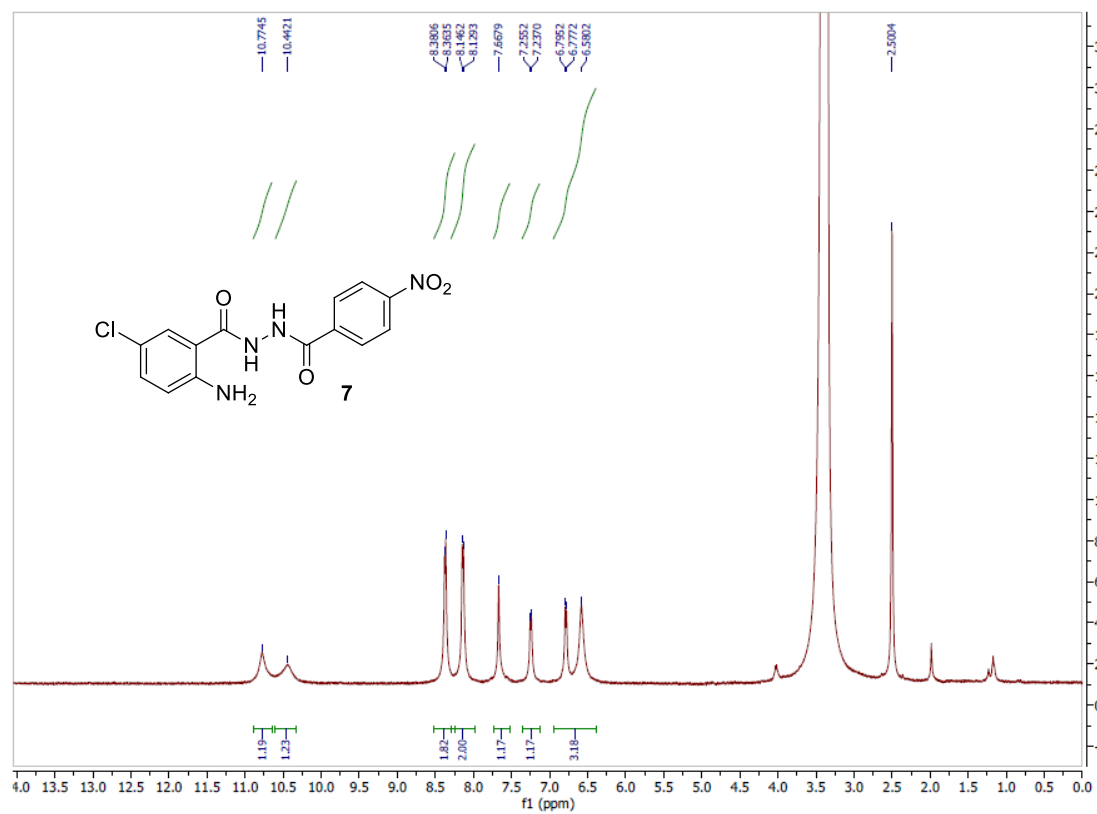


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T: FTMS + p ESI Full ms [150.00-500.00]

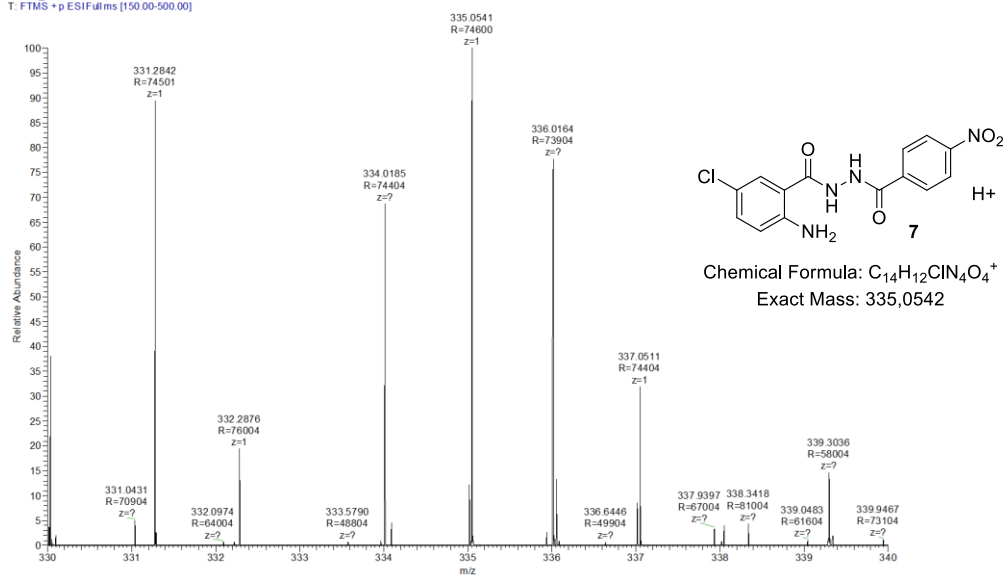


Chemical Formula: $C_{14}H_{12}Cl_2N_3O_2^+$
Exact Mass: 324,0301

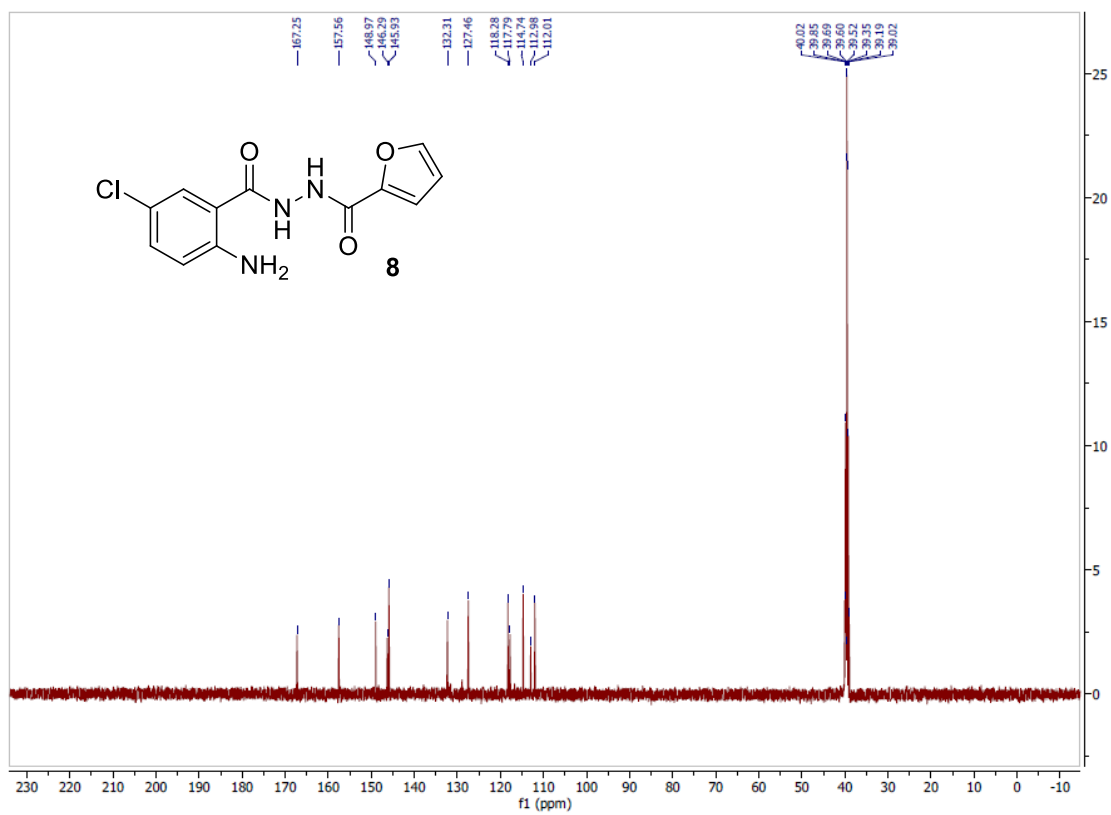
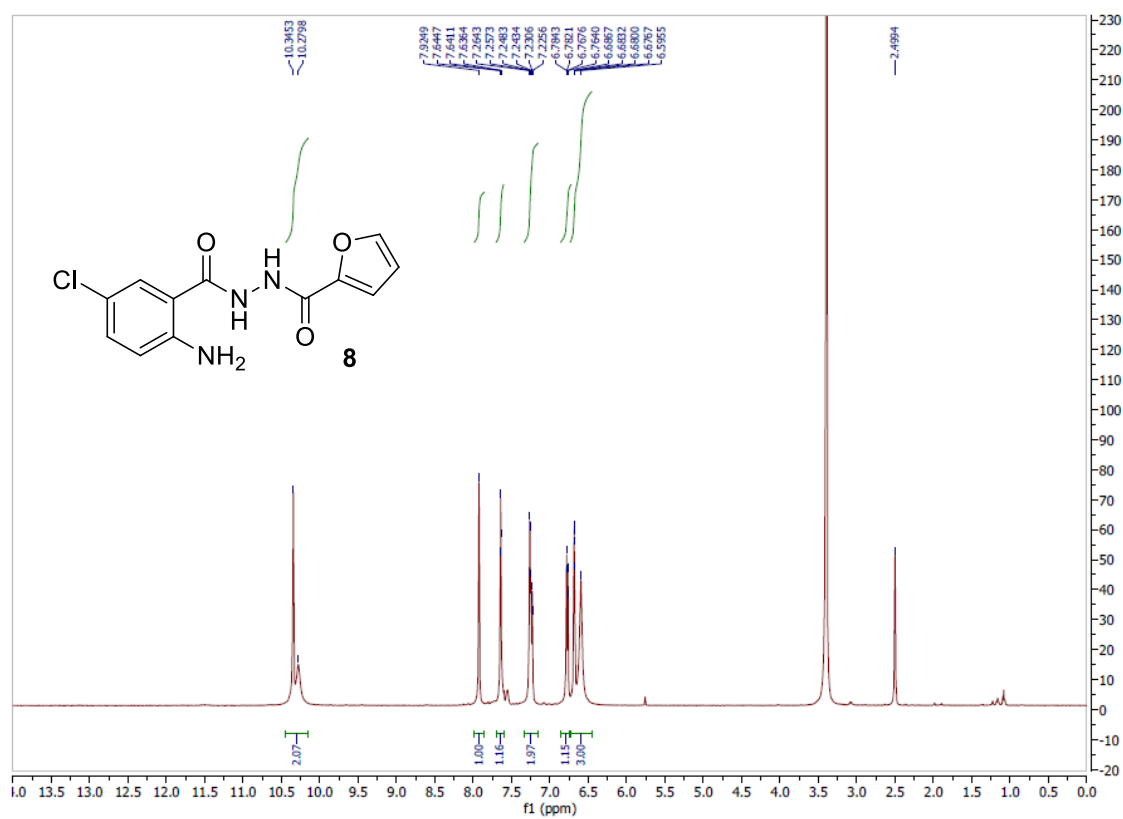
2-amino-5-chloro-*N'*-(4-nitrobenzoyl)benzohydrazide (7)



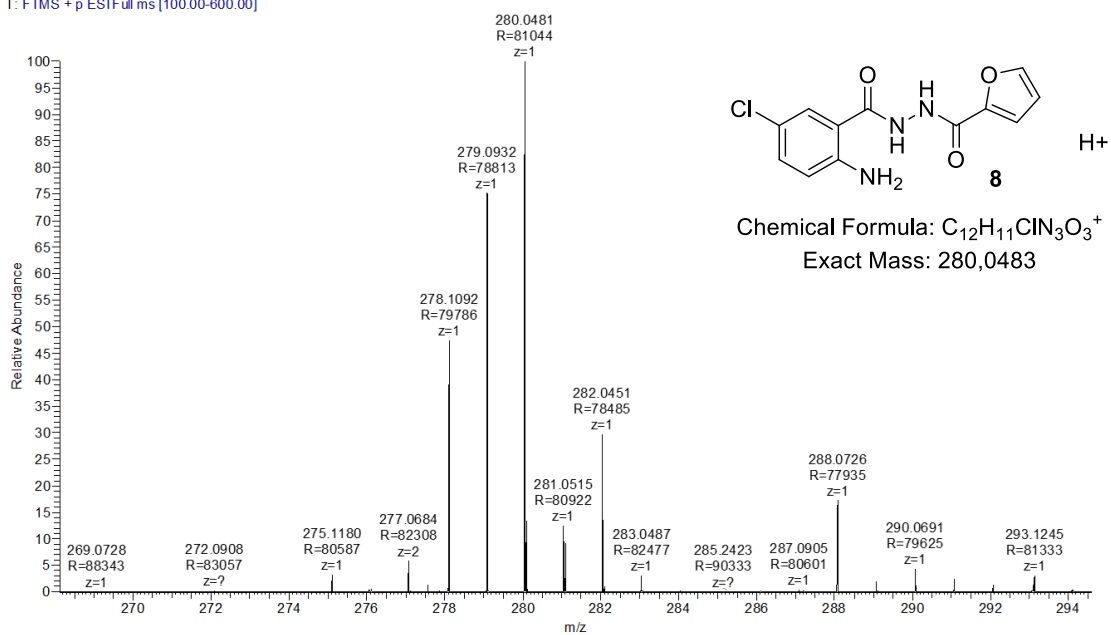
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T: FTMS +p ESIFulms [150.00-500.00]



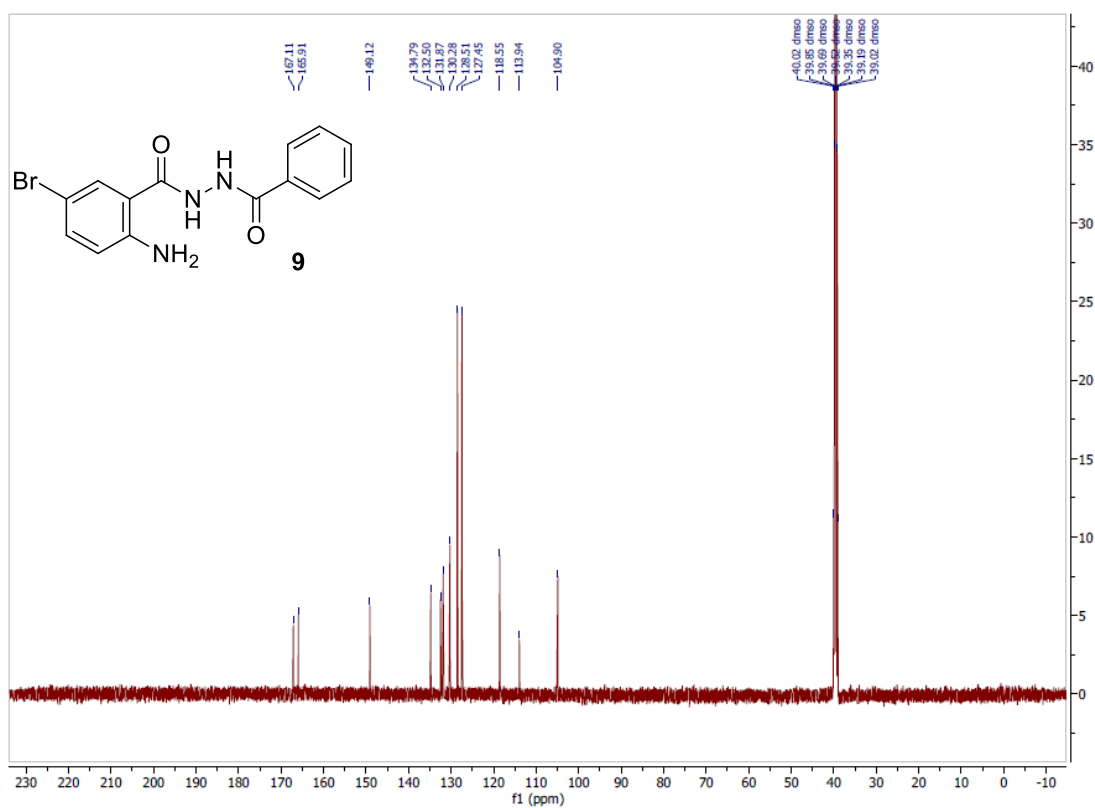
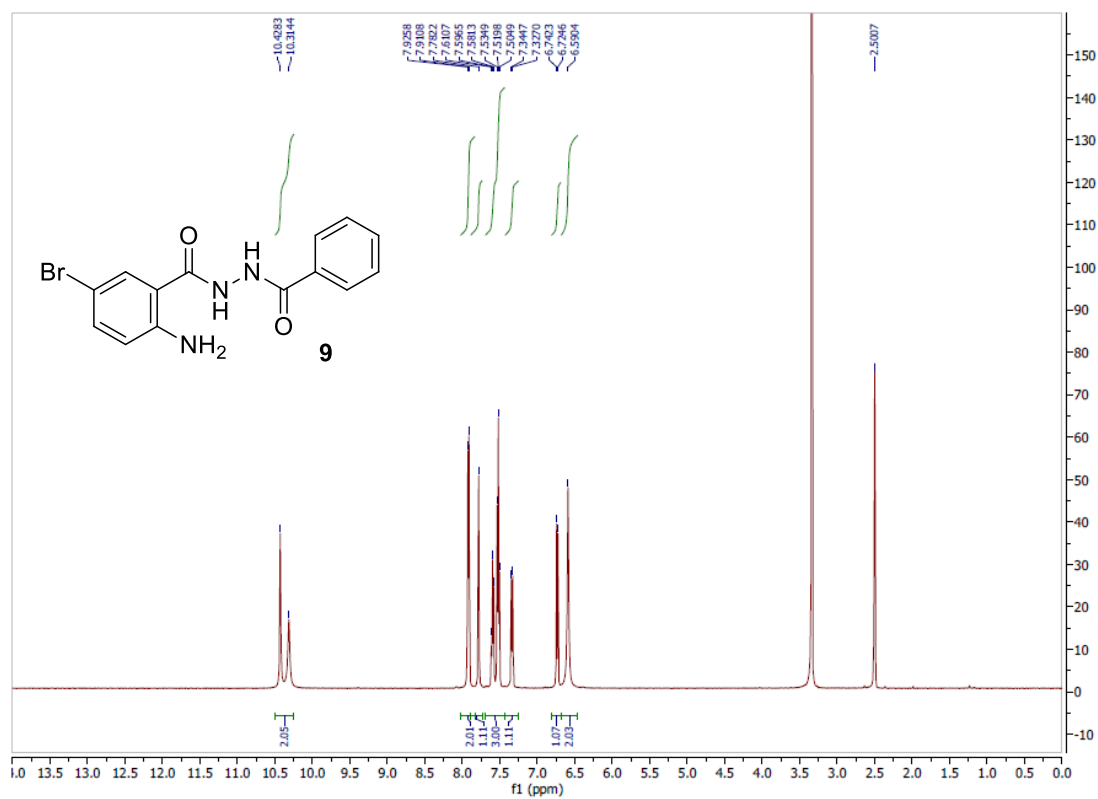
N'-(2-amino-5-chlorobenzoyl)furan-2-carbohydrazide (**8**)



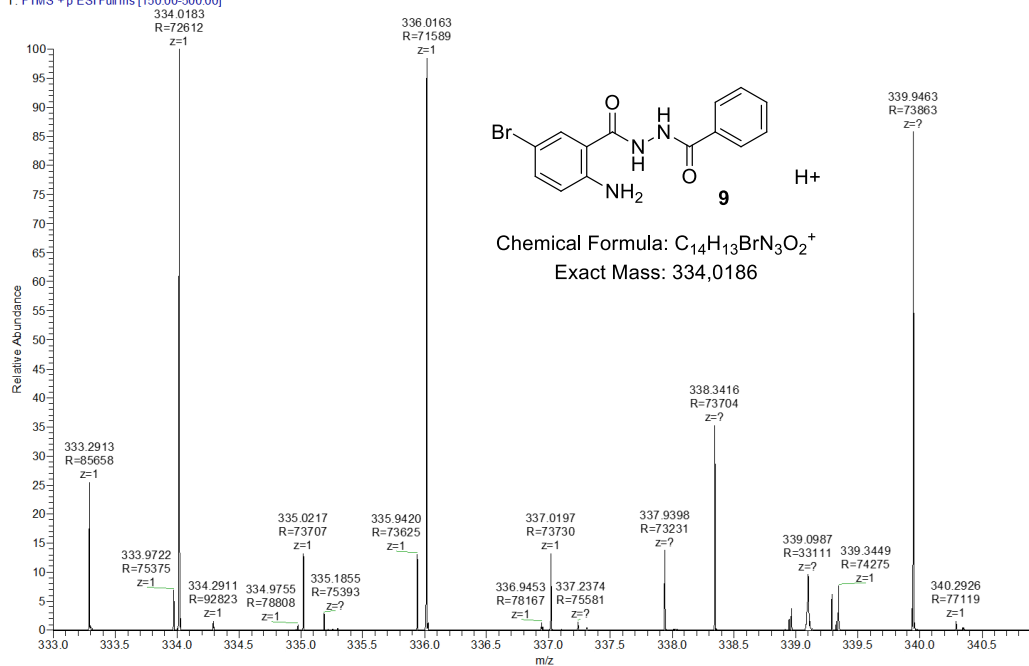
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T: FTMS + p ESIFull ms [100.00-600.00]



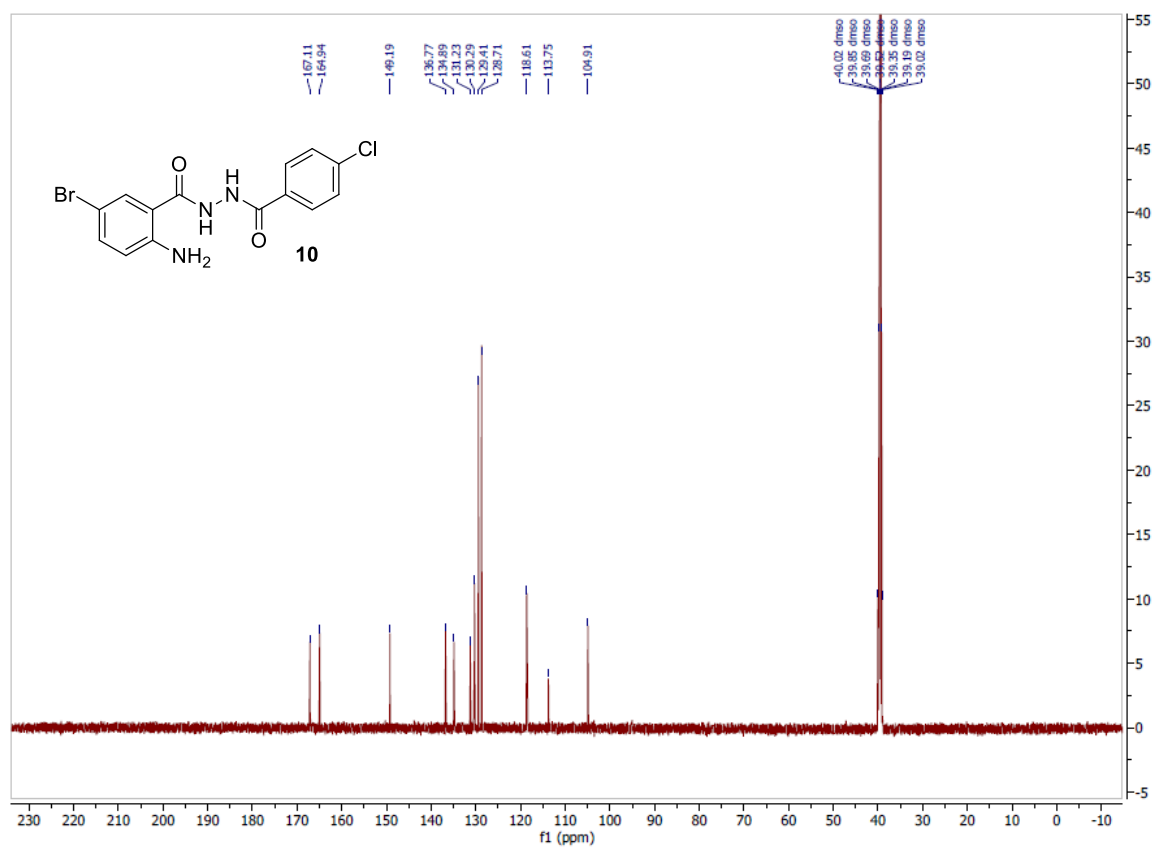
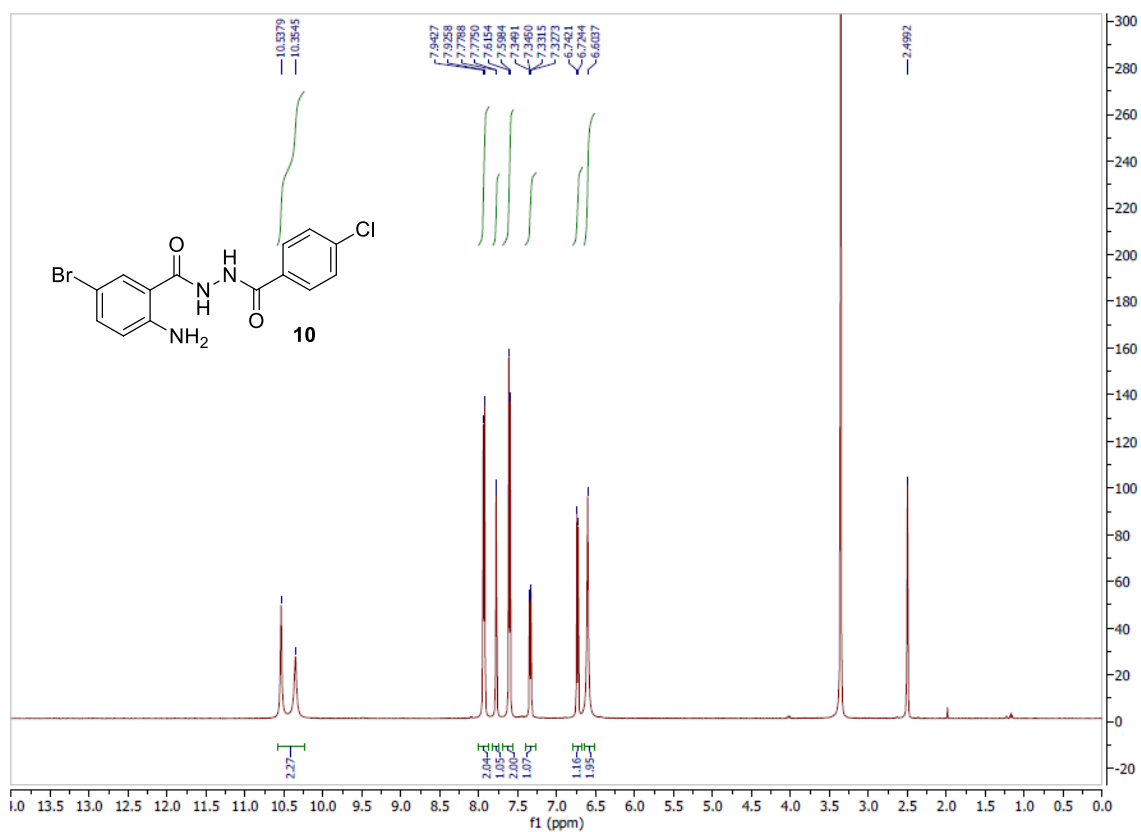
2-amino-*N'*-benzoyl-5-bromobenzohydrazide (**9**)



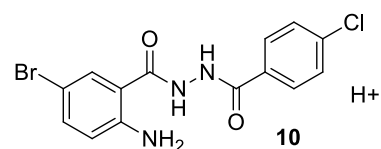
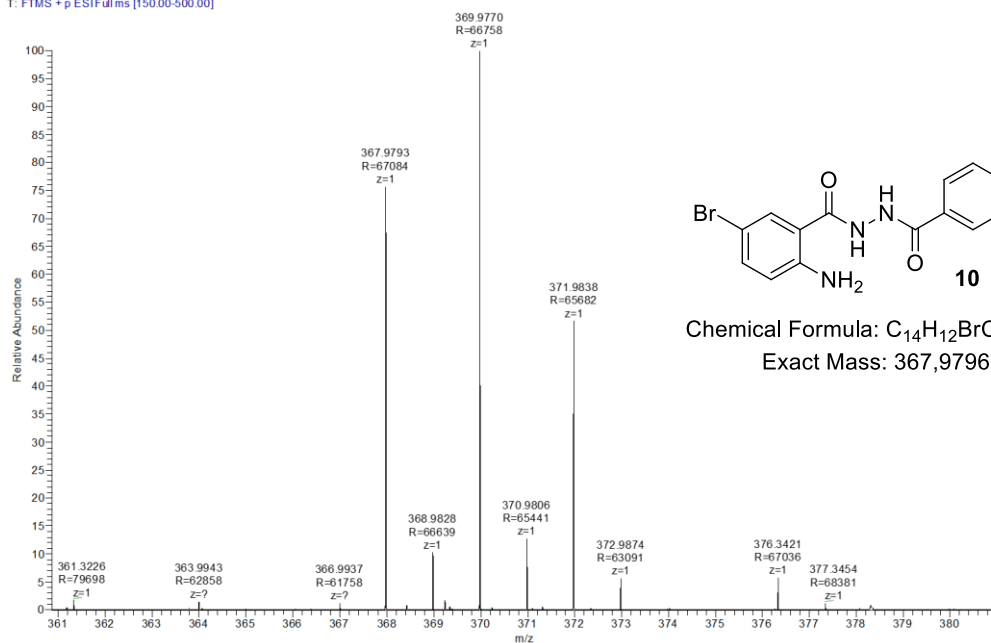
5_181210123101 #492-501 RT: 8.51-8.64 AV: 10 NL: 5.71E5
T: FTMS + p ESI Full ms [150.00-500.00]



2-amino-5-bromo-*N'*-(4-chlorobenzoyl)benzohydrazide (**10**)

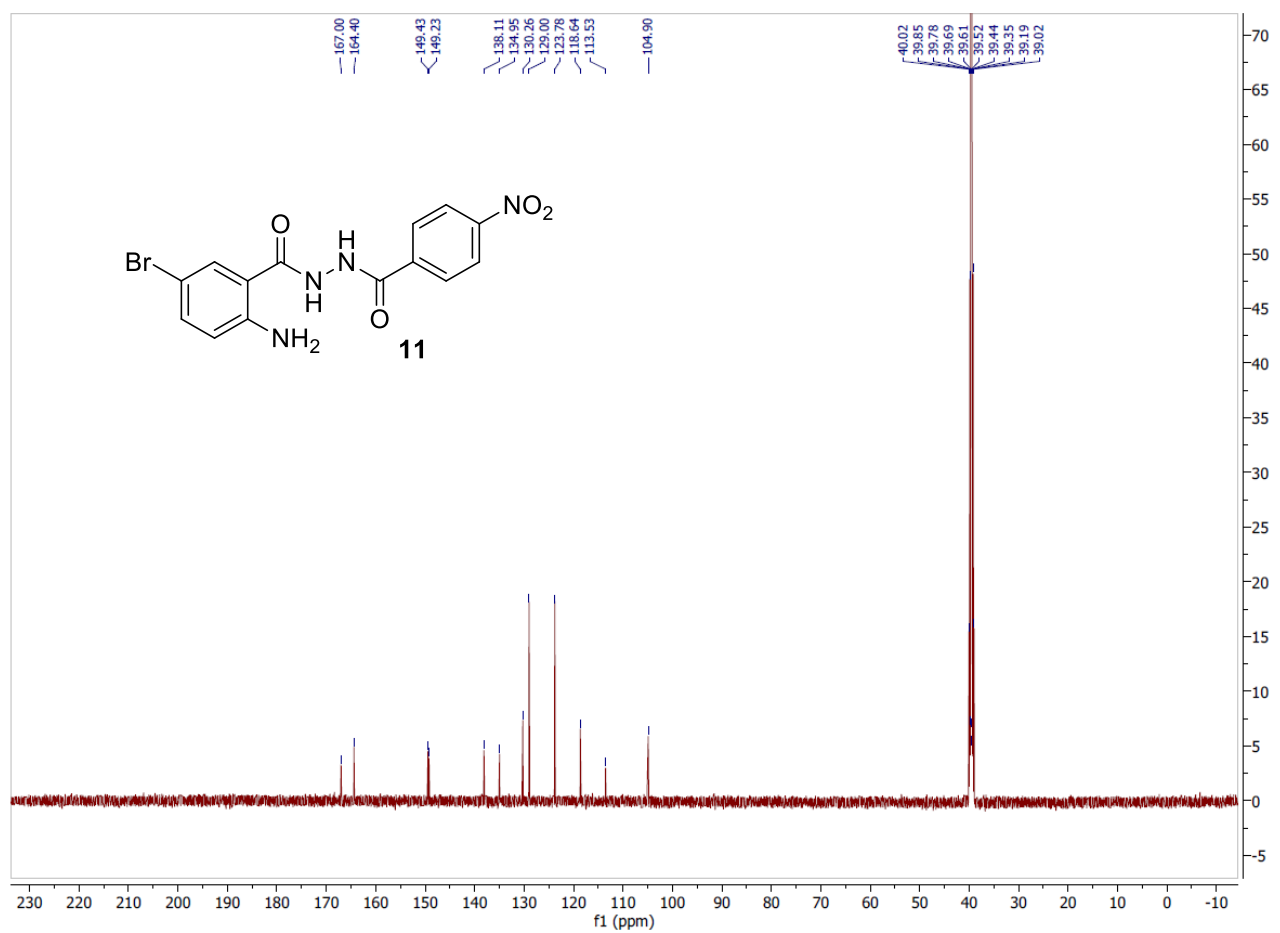
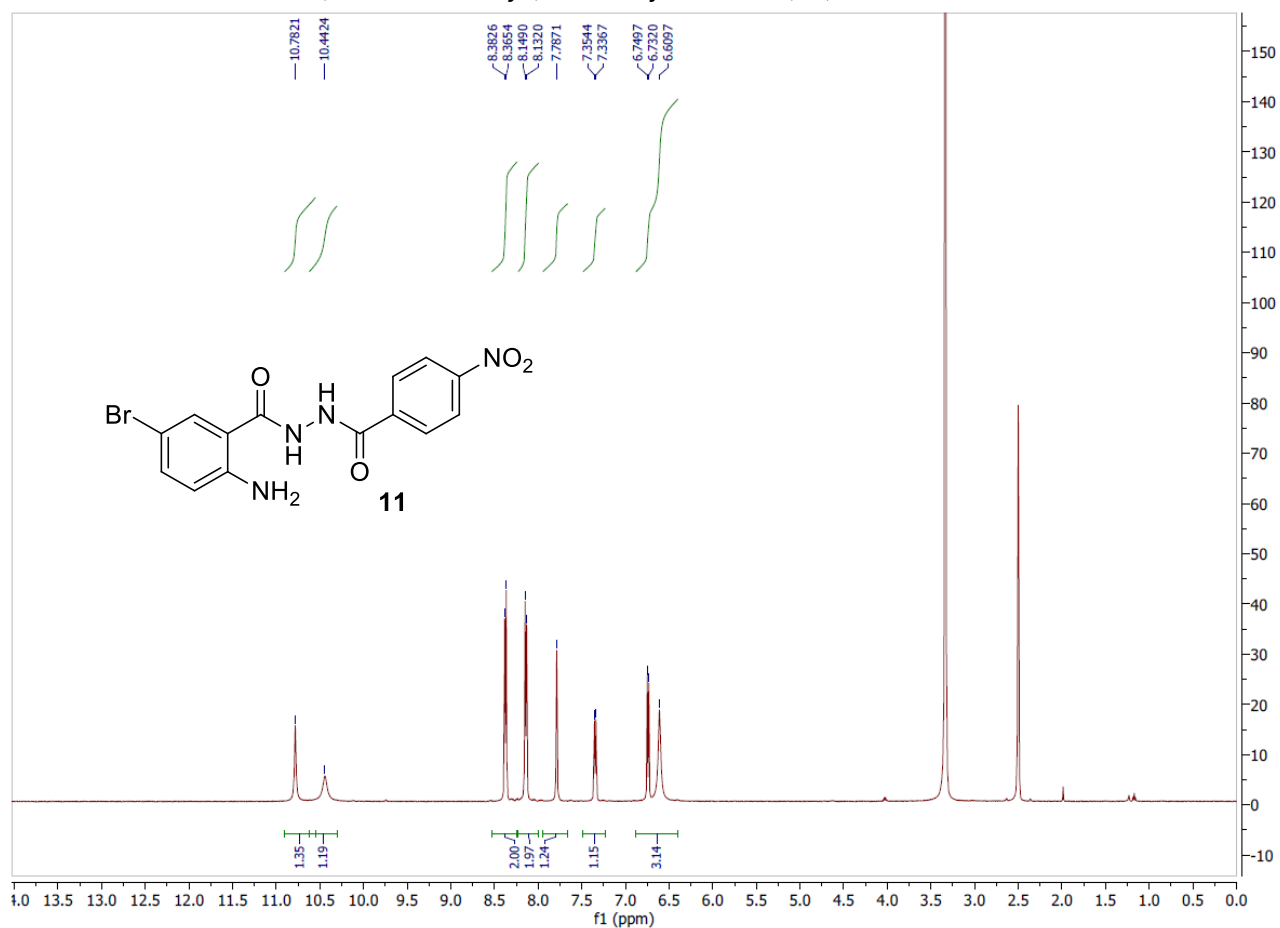


5#144-147 RT: 3.54-3.67 AV: 4 NL: 8.86E5
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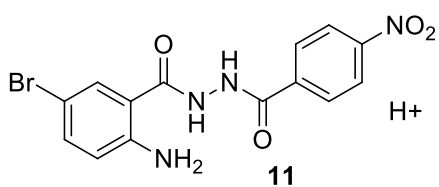
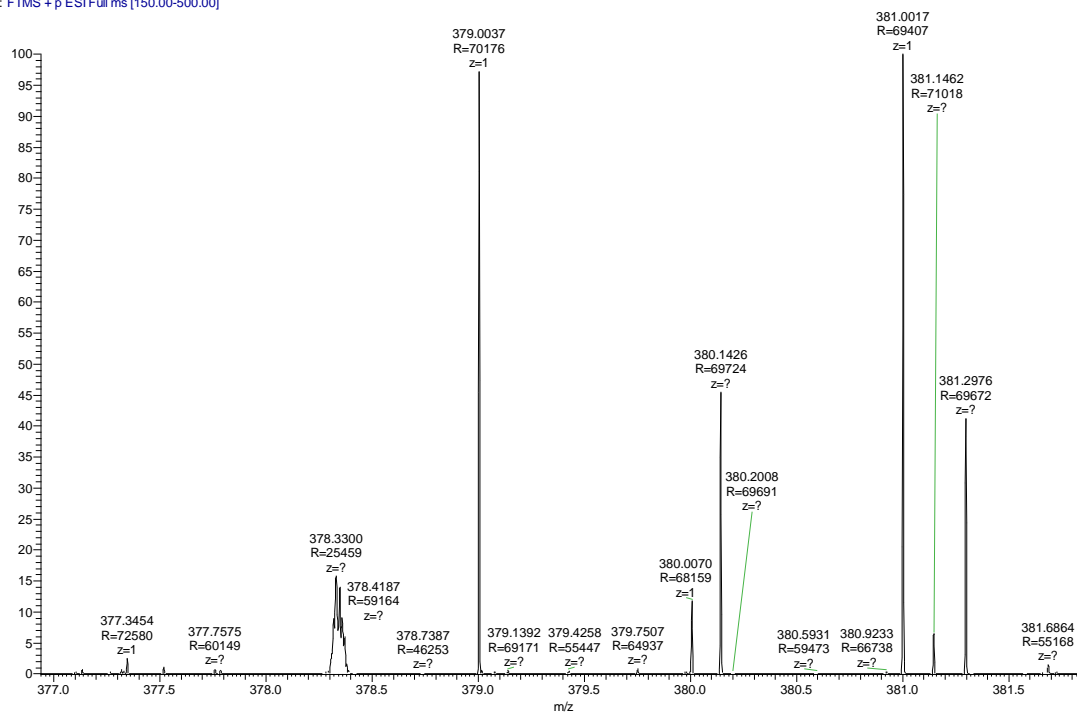


Chemical Formula: $C_{14}H_{12}BrClN_3O_2^+$
Exact Mass: 367,9796

2-amino-5-bromo-*N'*-(4-nitrobenzoyl)benzohydrazide (**11**)



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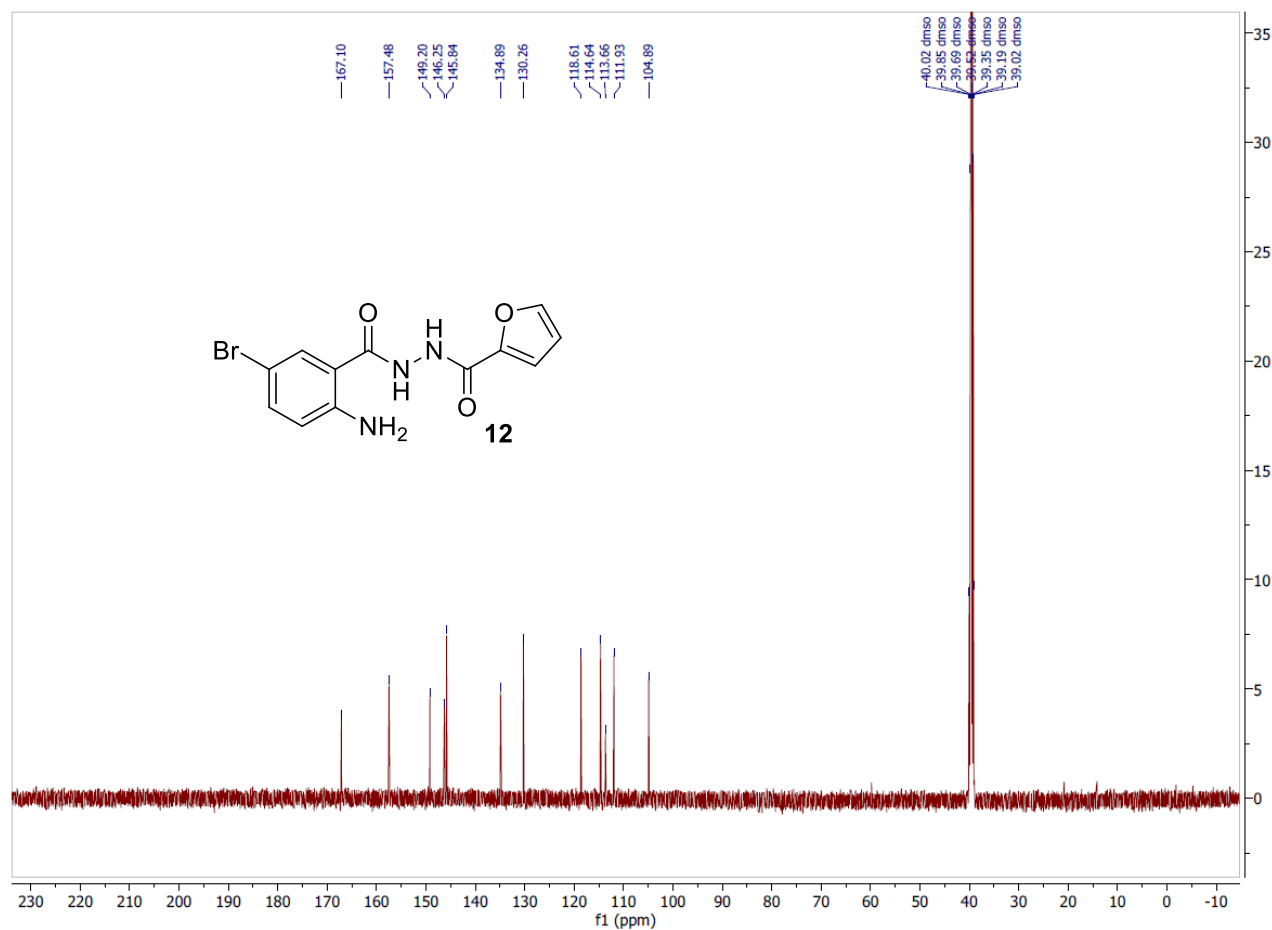
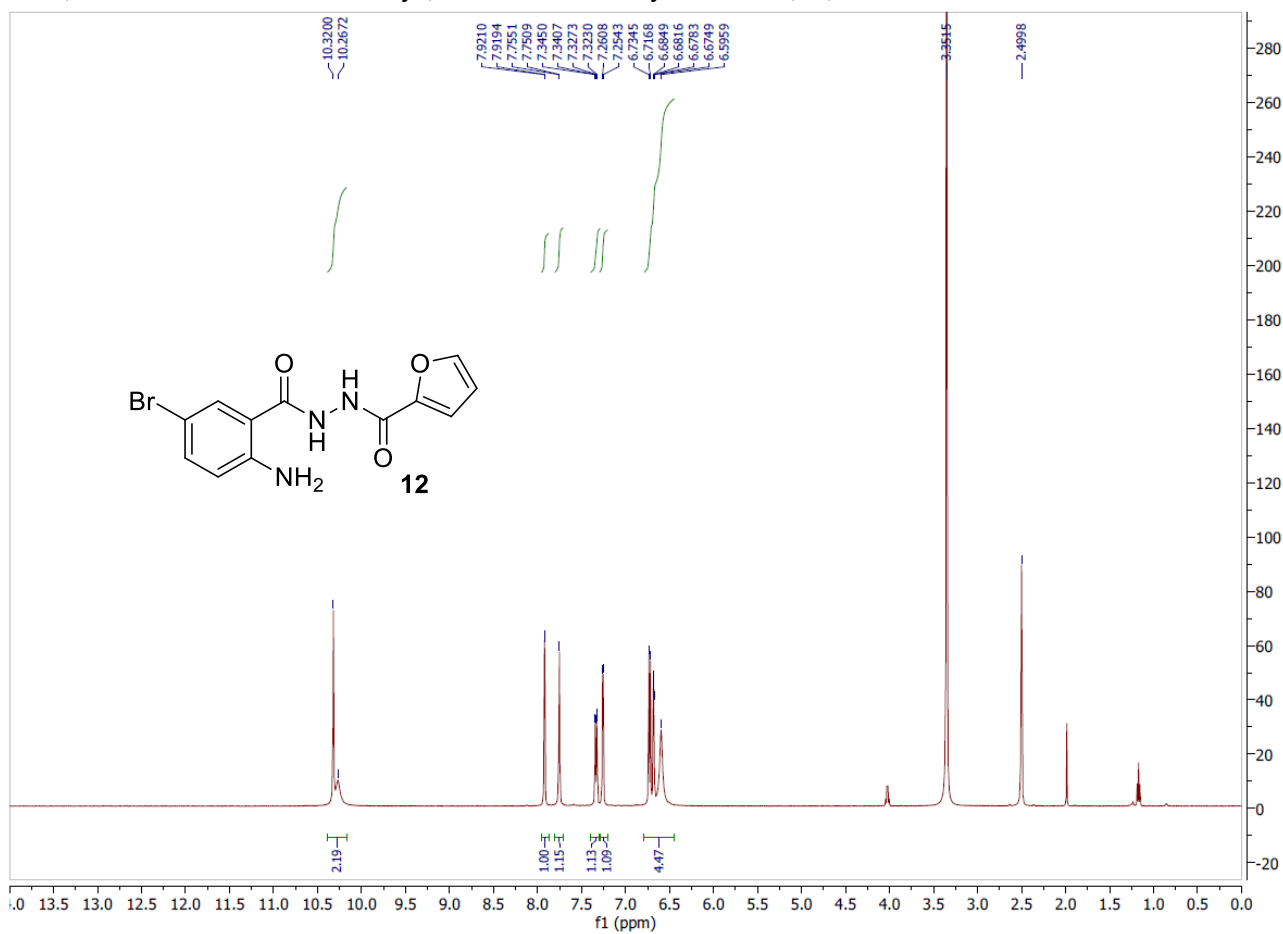


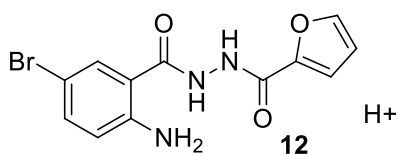
Chemical Formula: $C_{14}H_{12}BrN_4O_4^+$

Exact Mass: 379,0036

Molecular Weight: 380,1729

N'-(2-amino-5-bromobenzoyl)furan-2-carbohydrazide (**12**)



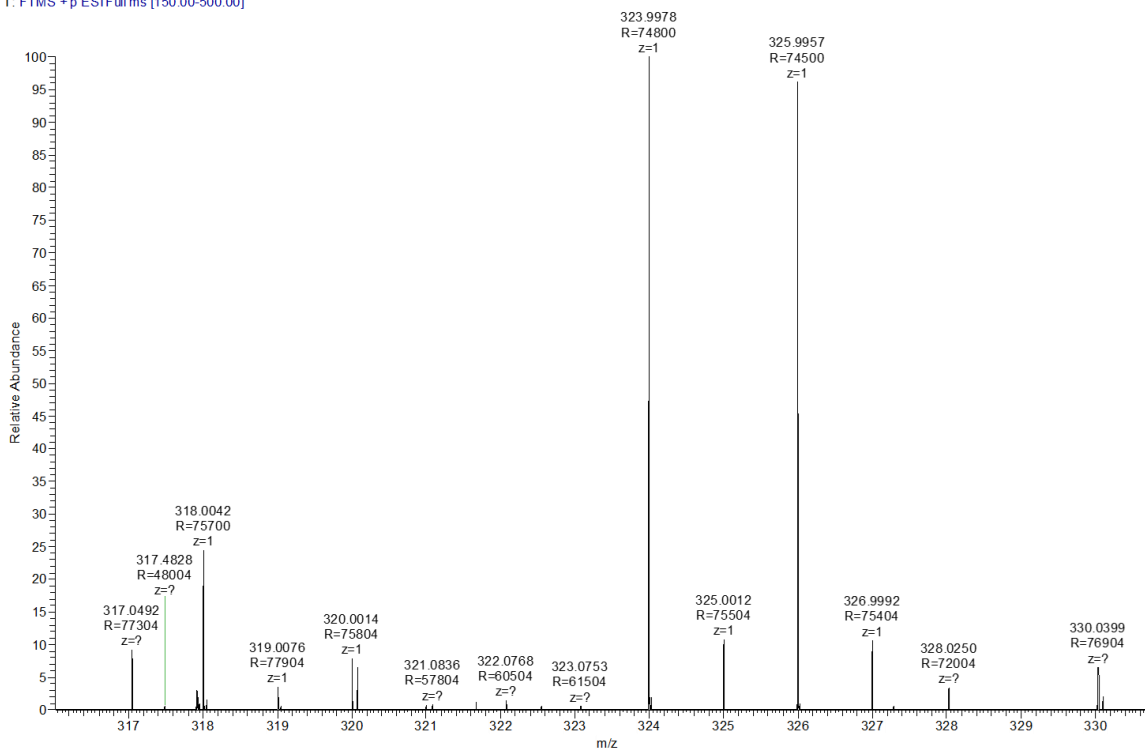


Chemical Formula: $\text{C}_{12}\text{H}_{11}\text{BrN}_3\text{O}_3^+$

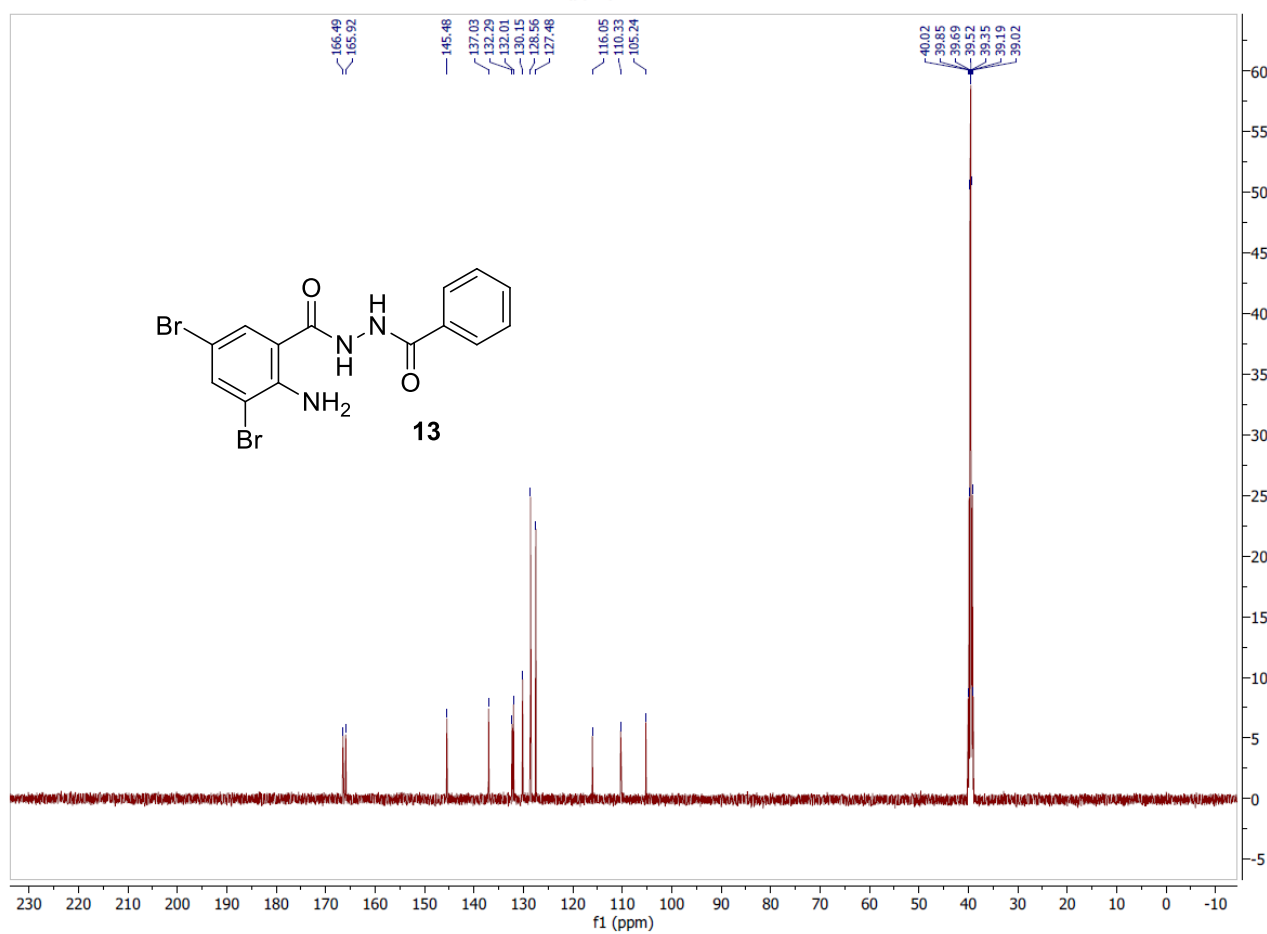
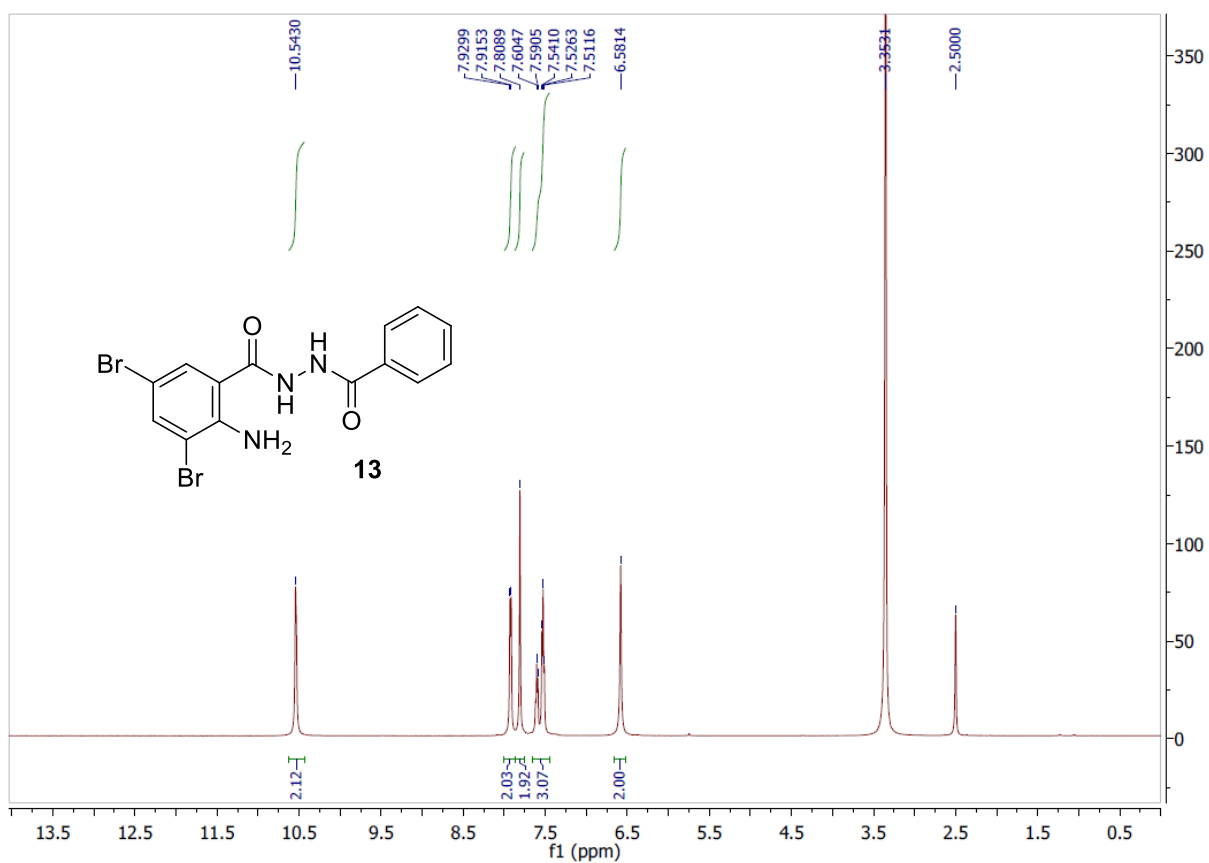
Exact Mass: 323,9978

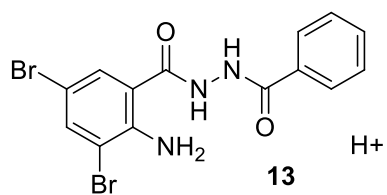
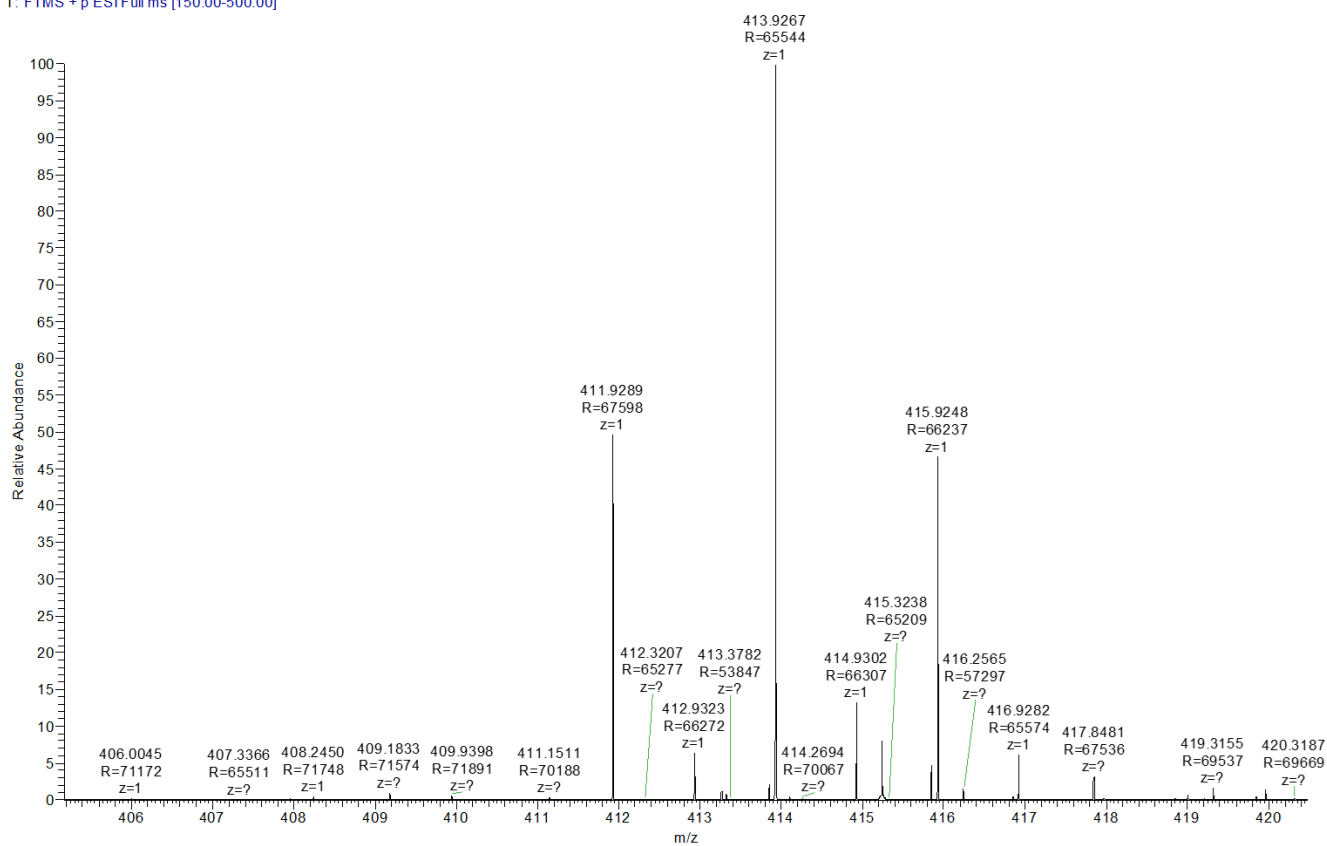
Molecular Weight: 325,1375

7_181210123101 #498 RT: 7.23 AV: 1 NL: 8.91E5
T: FTMS + p ESIFullms [150.00-500.00]



2-amino-*N'*-benzoyl-3,5-dibromobenzohydrazide (**13**)



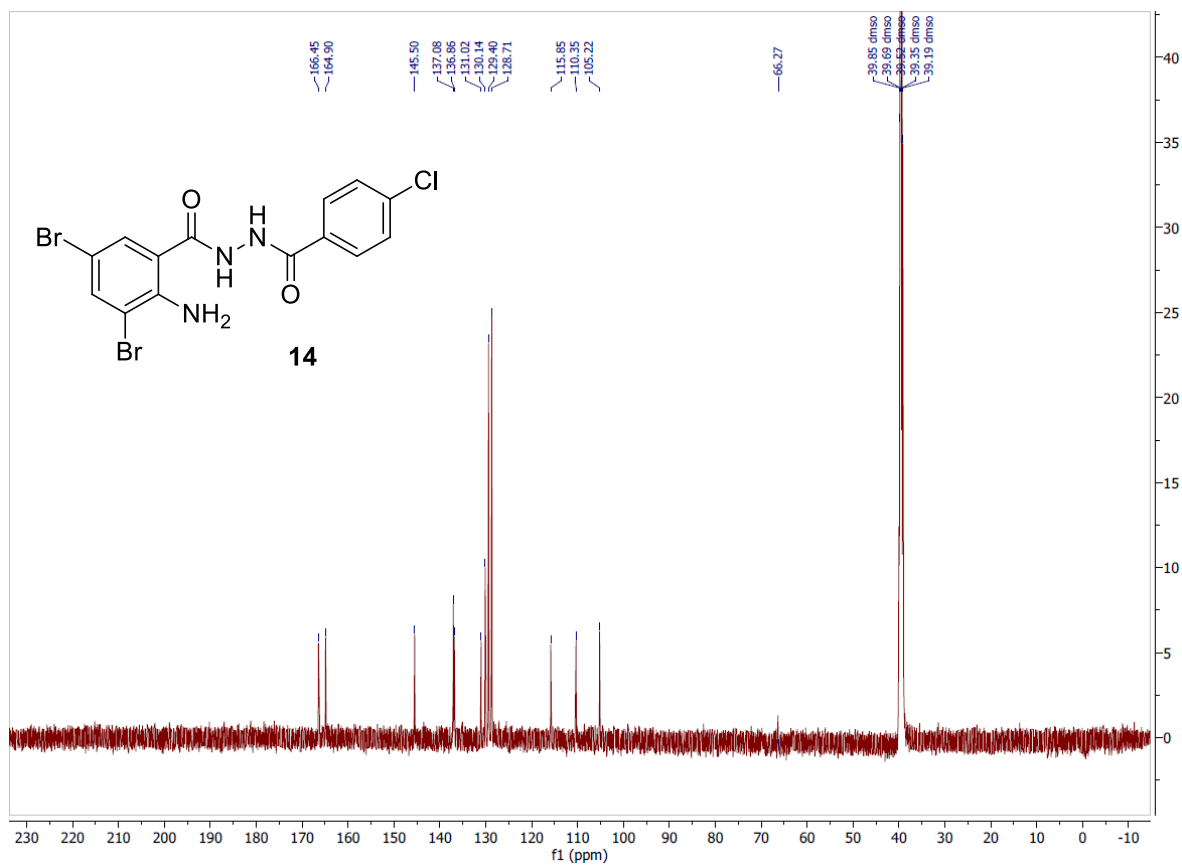
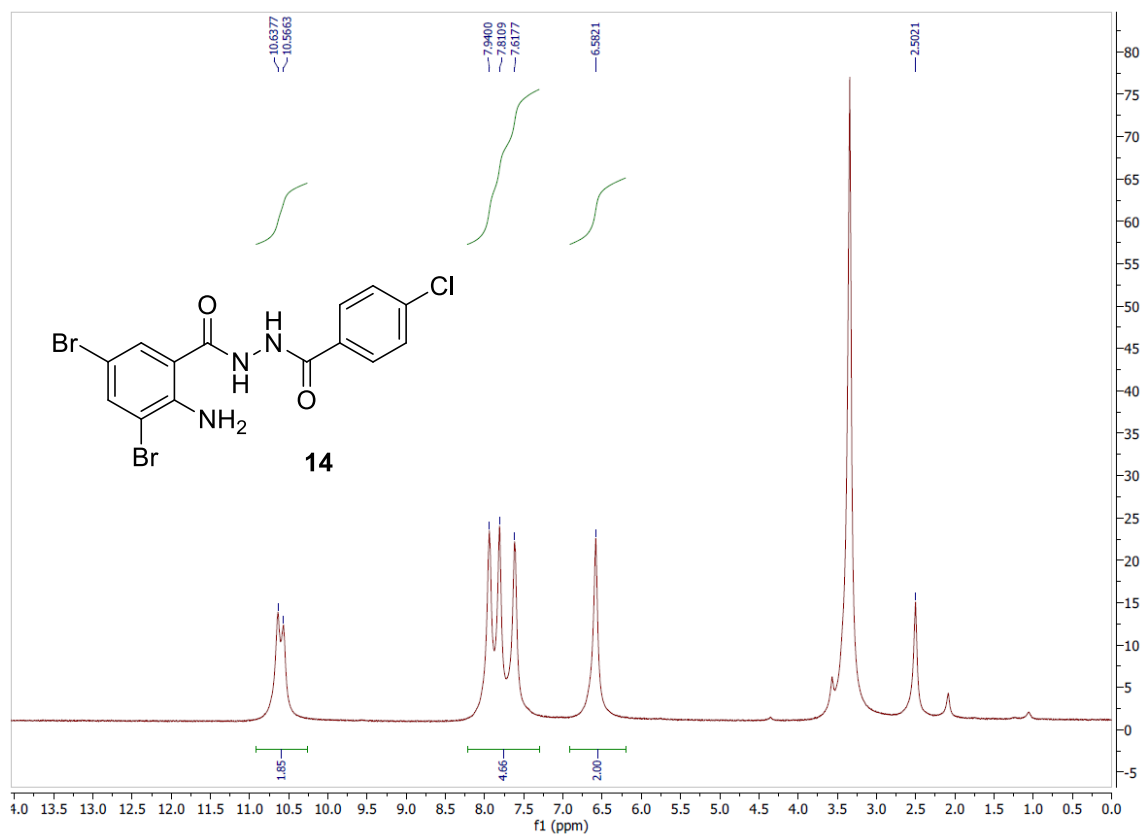


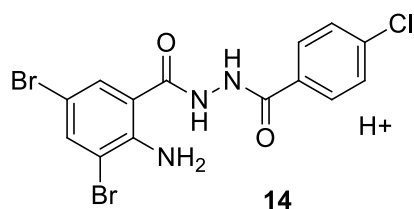
Chemical Formula: C₁₄H₁₂Br₂N₃O₂⁺

Exact Mass: 411,9291

Molecular Weight: 414,0714

2-amino-3,5-dibromo-*N*'-(4-chlorobenzoyl)benzohydrazide (**14**)



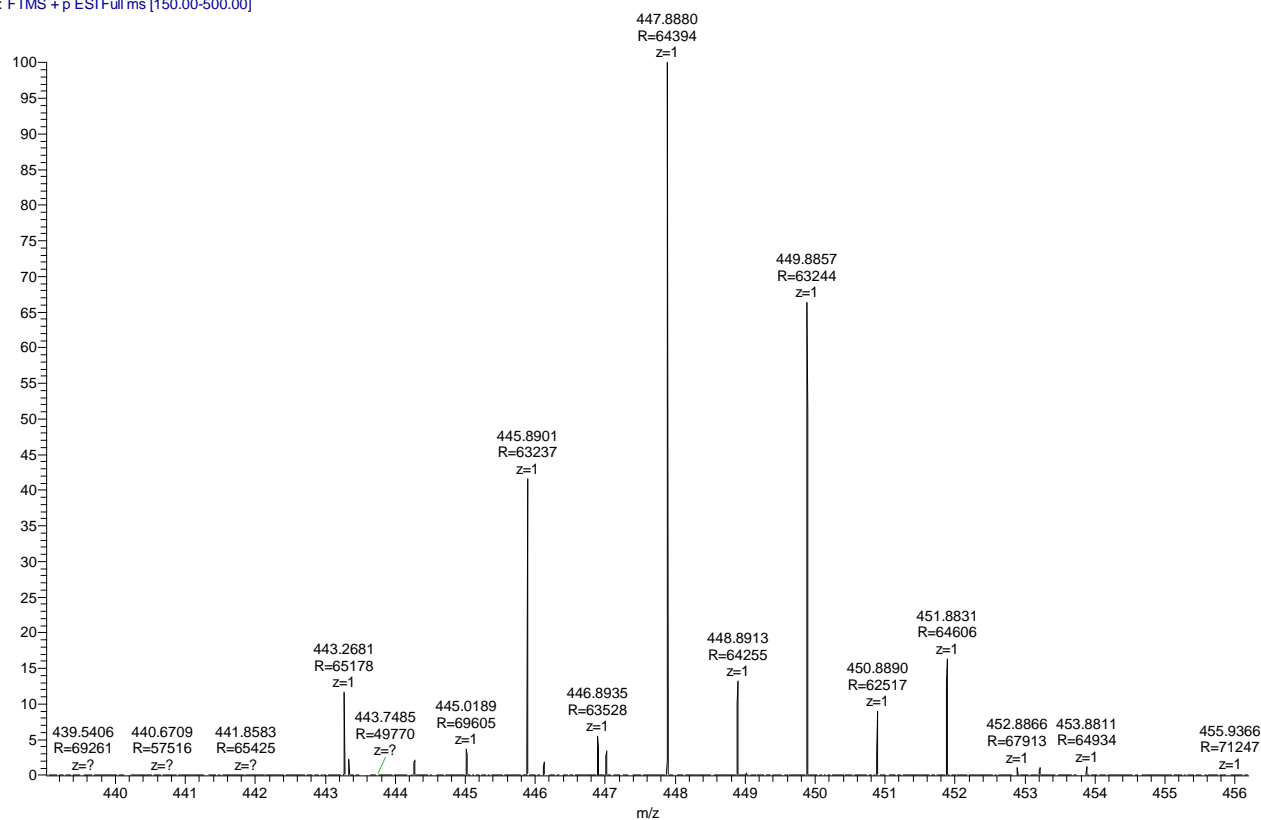


Chemical Formula: $C_{14}H_{11}Br_2ClN_3O_2^+$

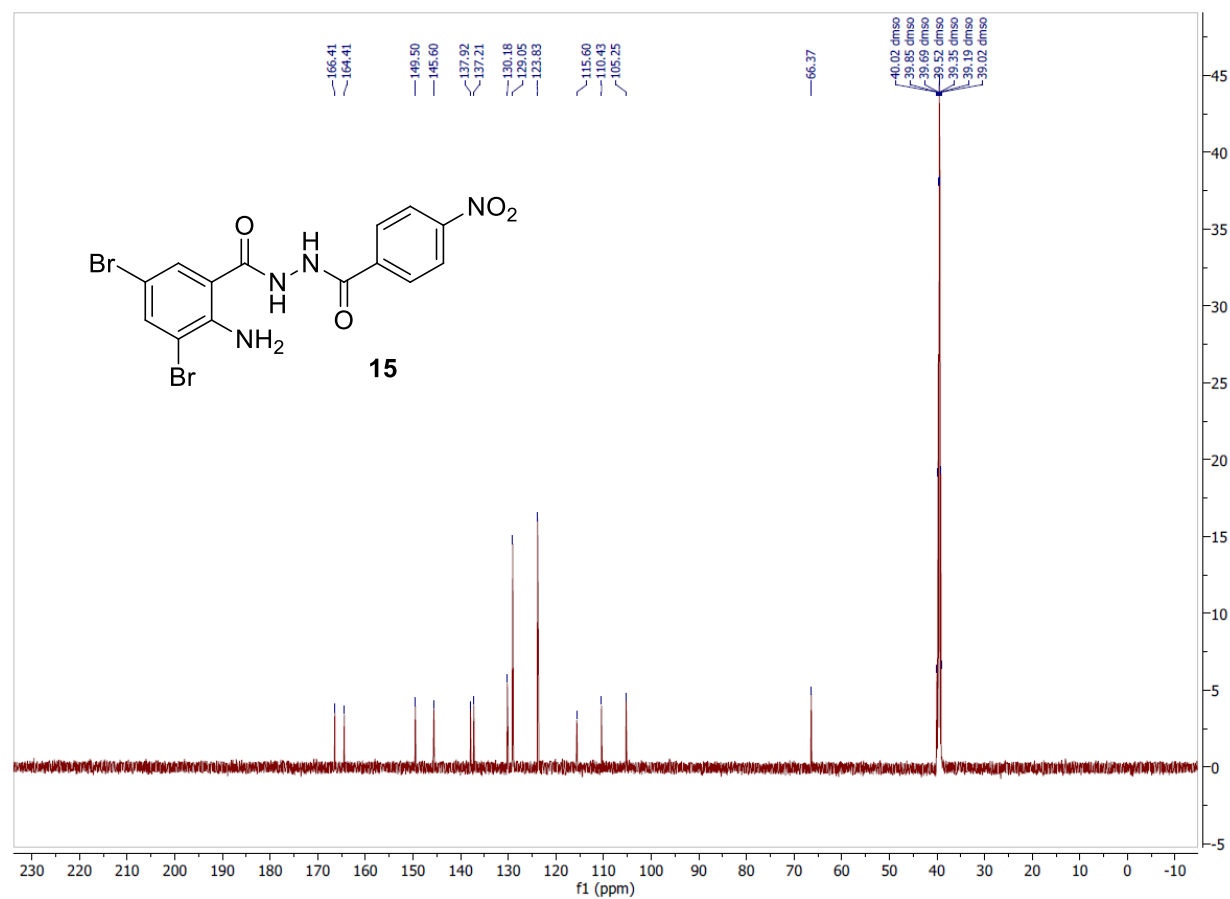
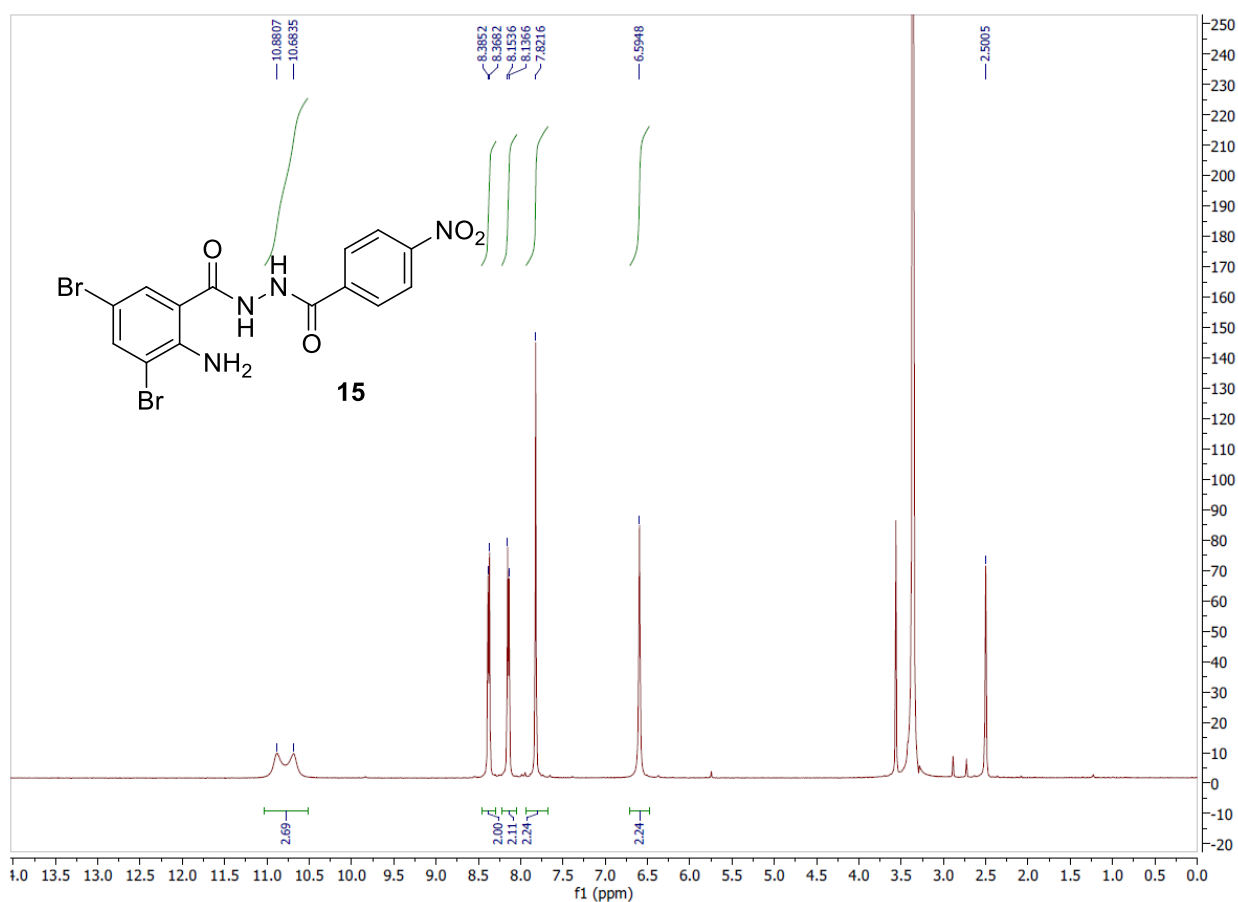
Exact Mass: 445,8901

Molecular Weight: 448,5165

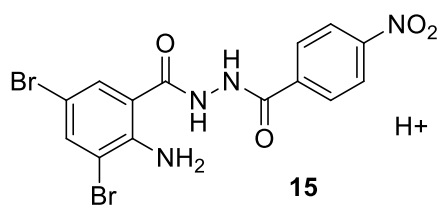
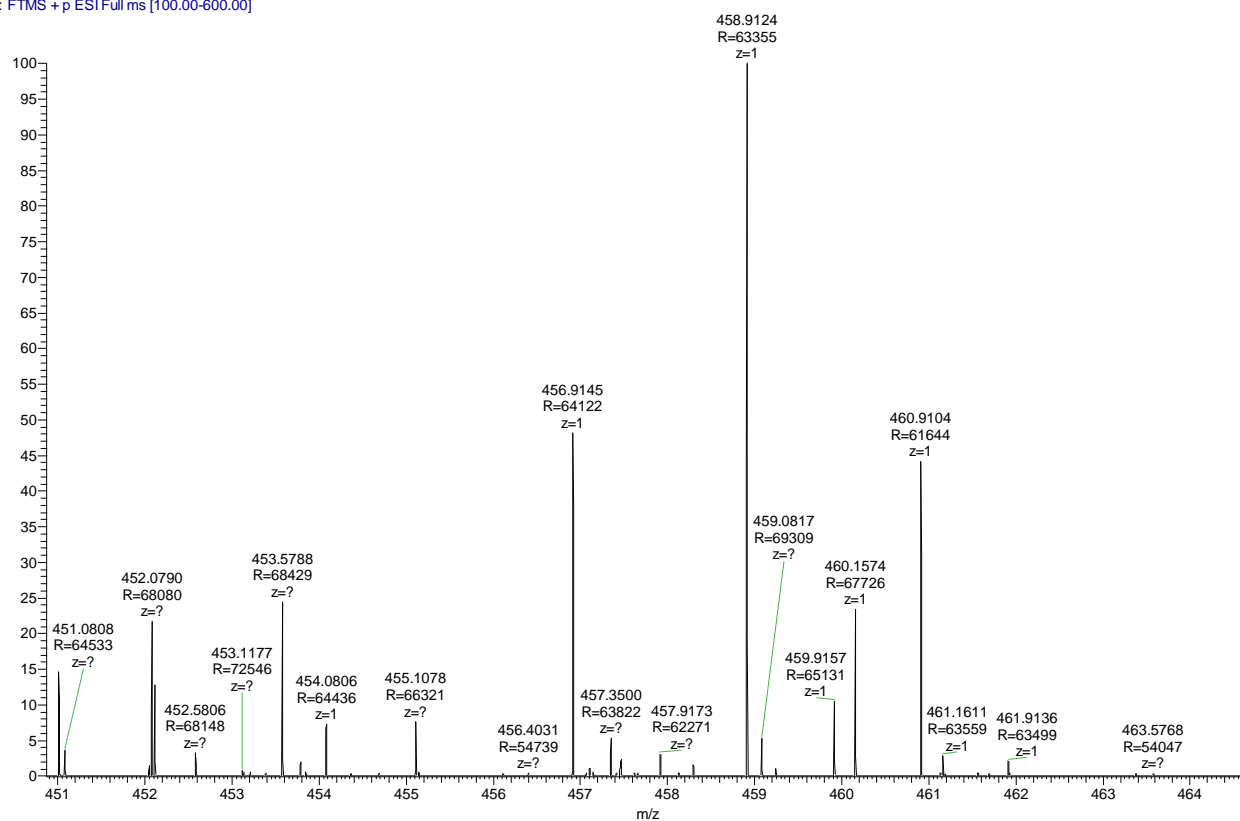
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2-amino-3,5-dibromo-*N'*-(4-nitrobenzoyl)benzohydrazide (**15**)



1 #34-48 RT: 1.39-1.97 AV: 15 NL: 1.80E5
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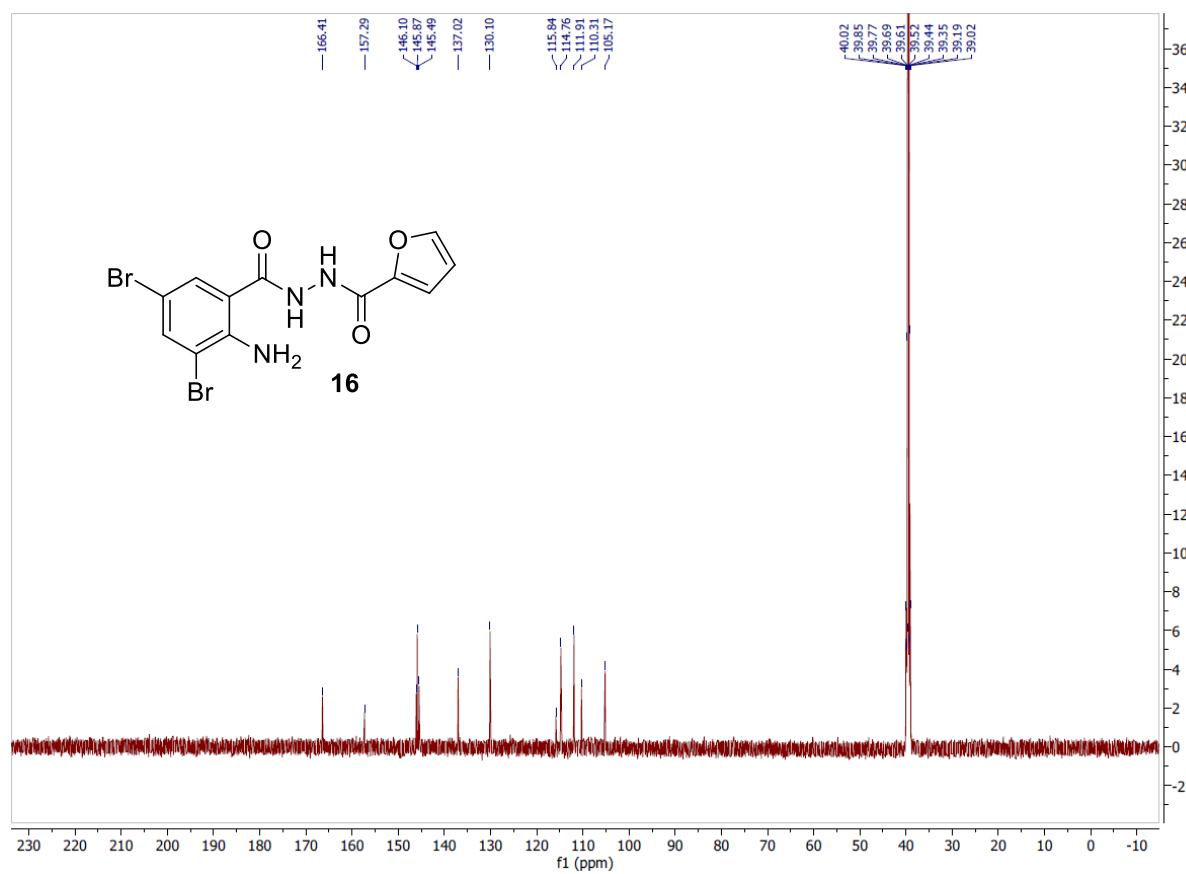
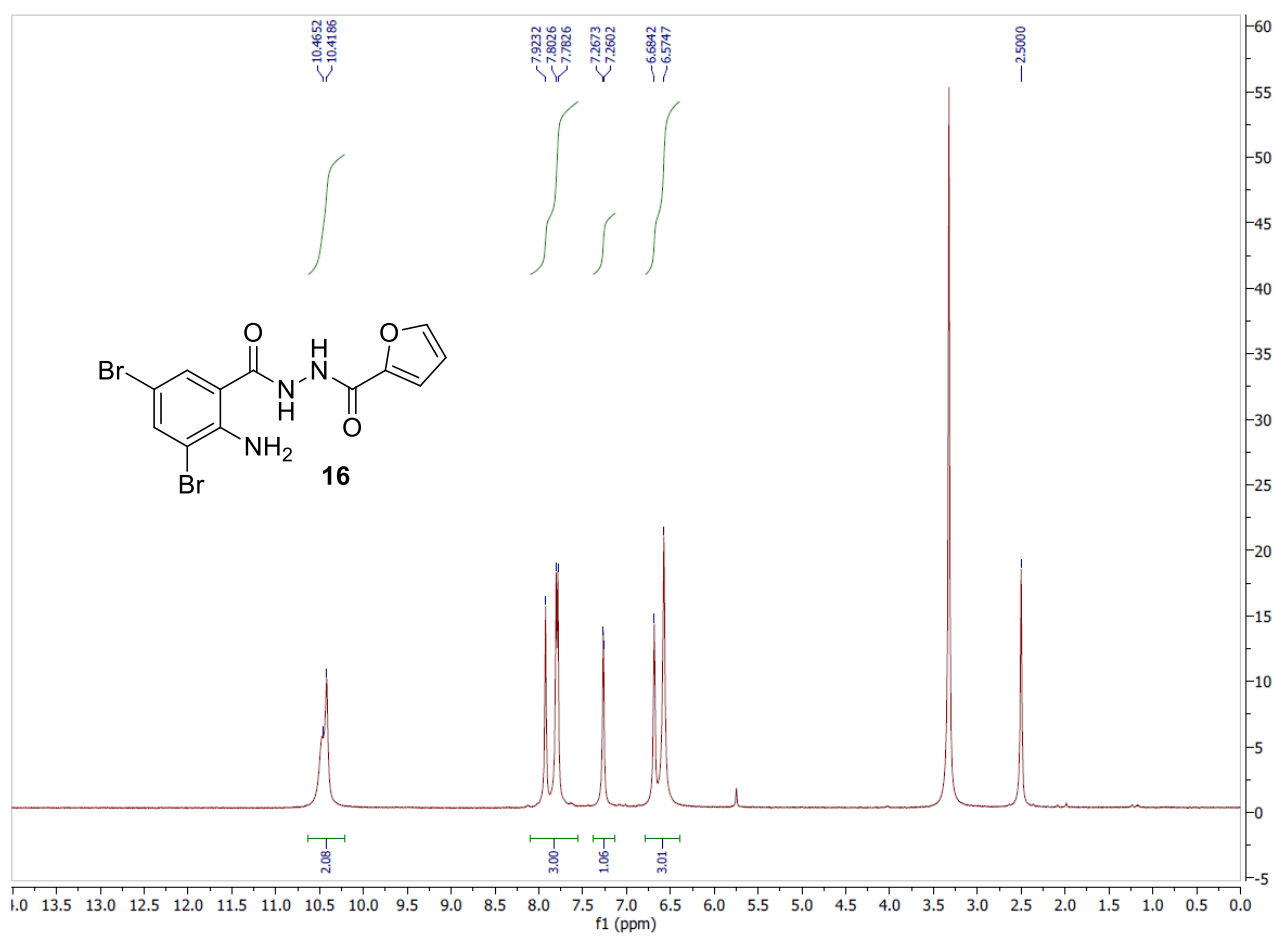


Chemical Formula: $C_{14}H_{11}Br_2N_4O_4^+$

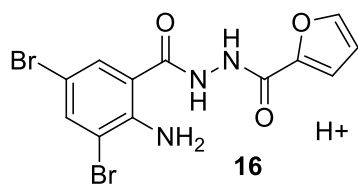
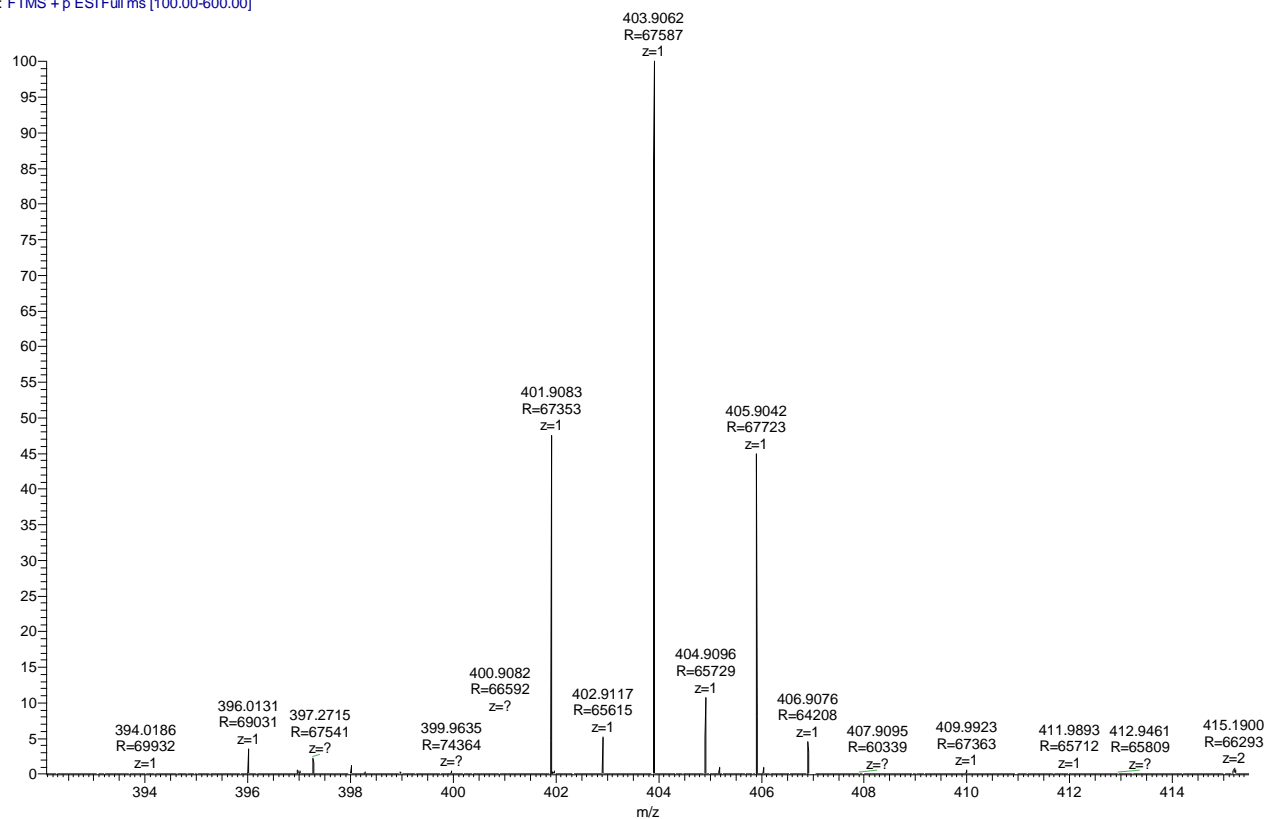
Exact Mass: 456,9142

Molecular Weight: 459,0690

N'-(2-amino-3,5-dibromobenzoyl)furan-2-carbohydrazide (**16**)



8_2#137-143 RT: 1.96-2.04 AV: 7 NL: 3.08E6
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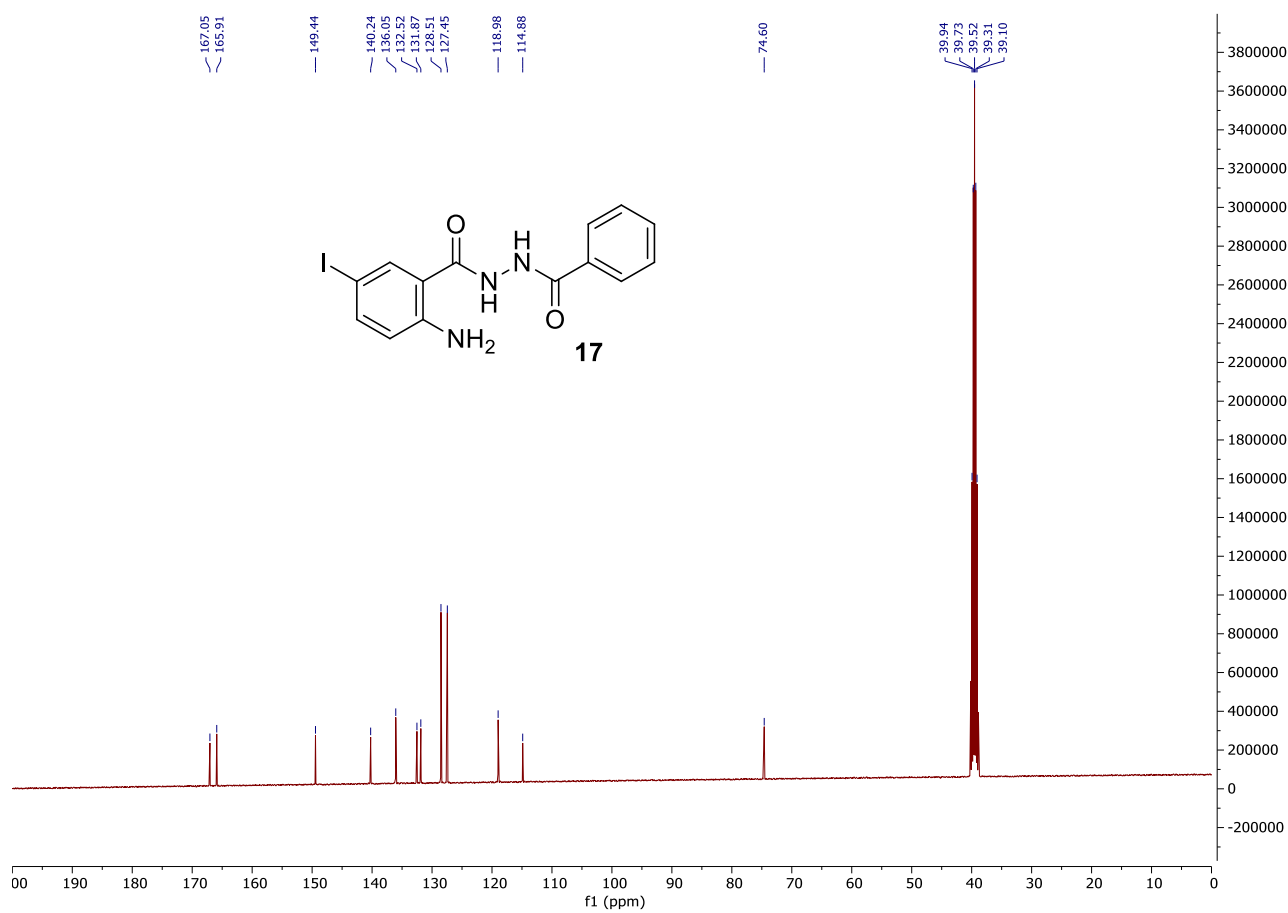
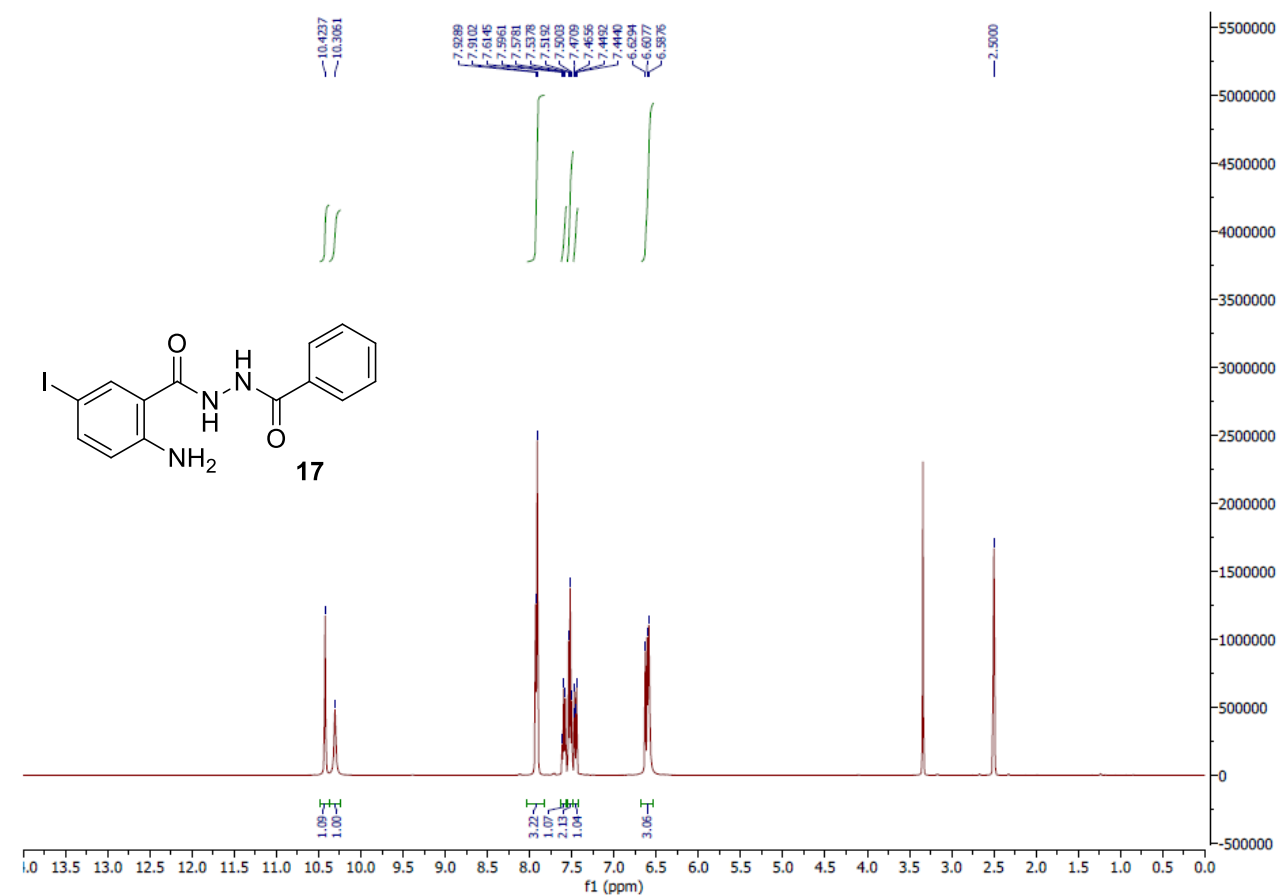


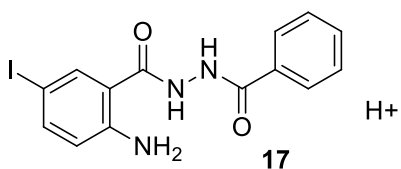
Chemical Formula: $C_{12}H_{10}Br_2N_3O_3^+$

Exact Mass: 401,9083

Molecular Weight: 404,0336

2-amino-*N'*-benzoyl-5-iodobenzohydrazide (**17**)



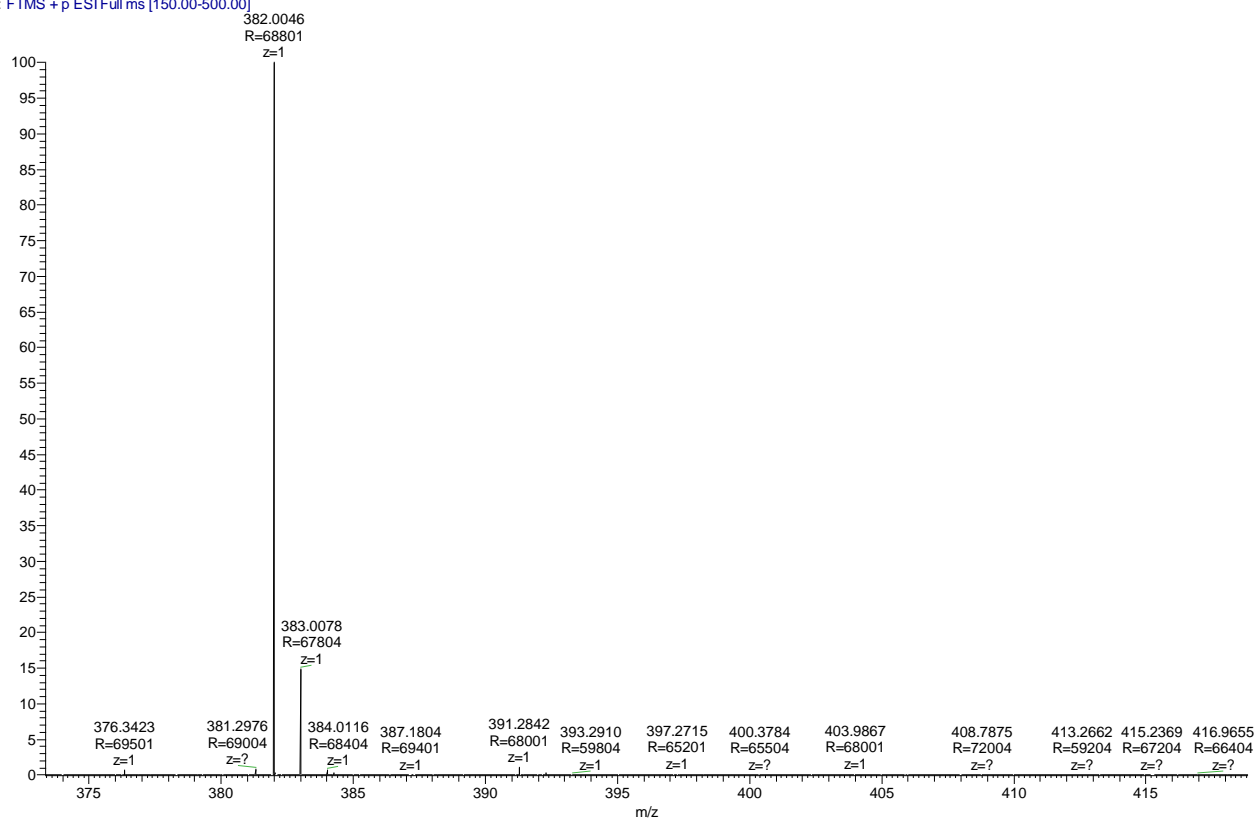


Chemical Formula: $C_{14}H_{13}IN_3O_2^+$

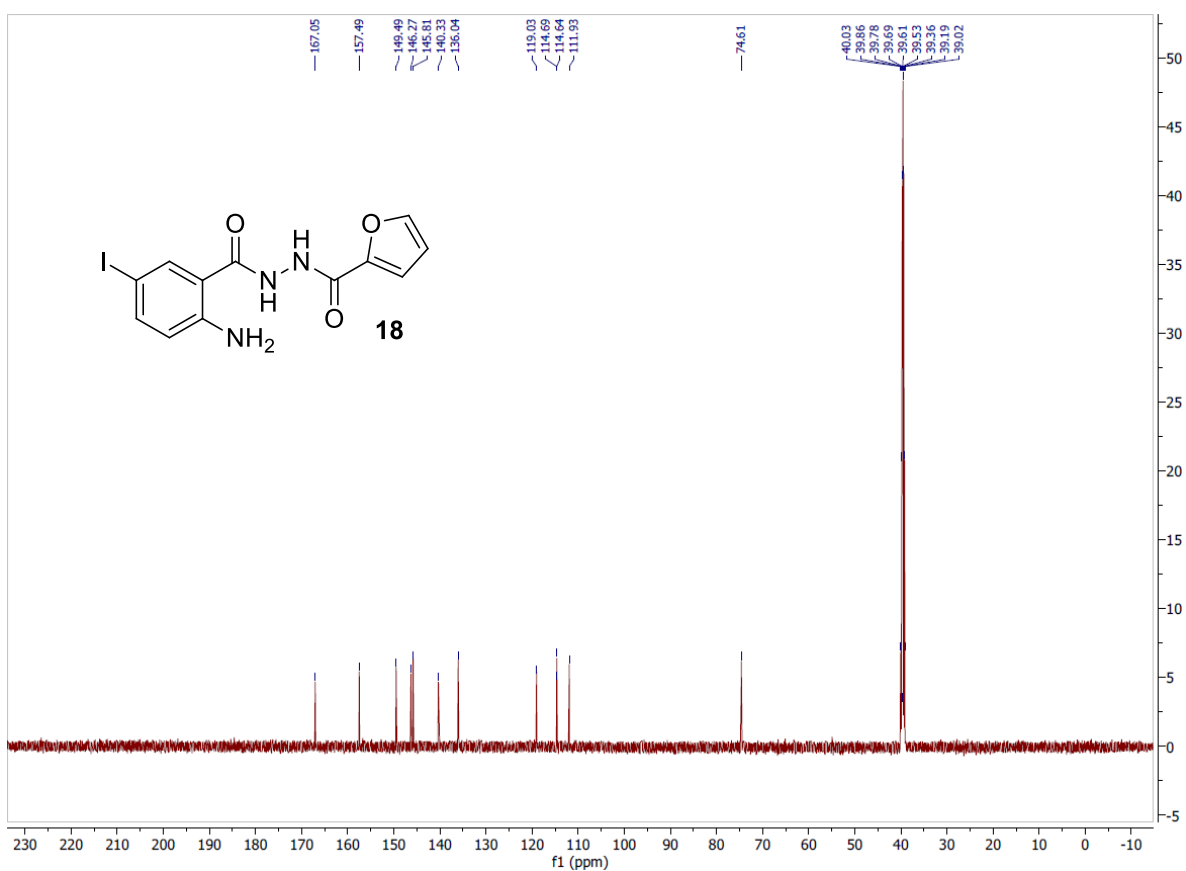
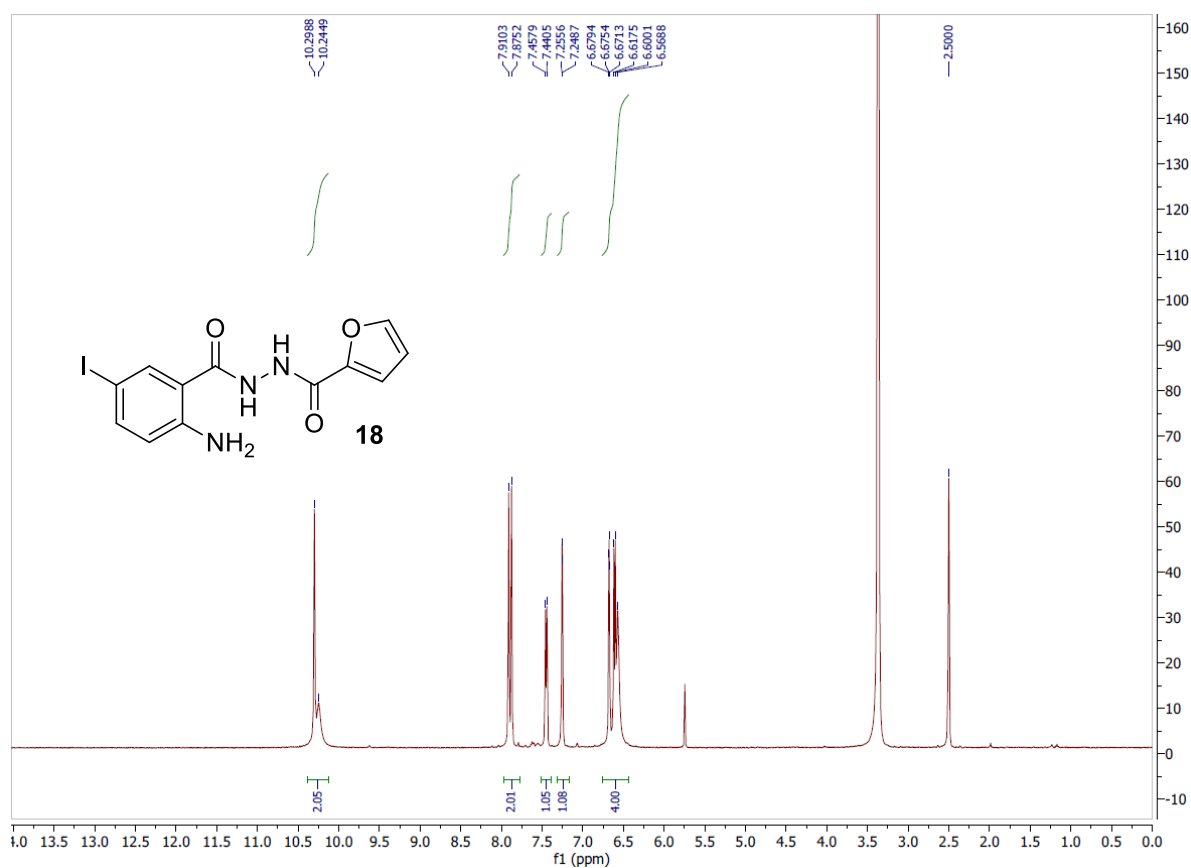
Exact Mass: 382,0047

Molecular Weight: 382,1758

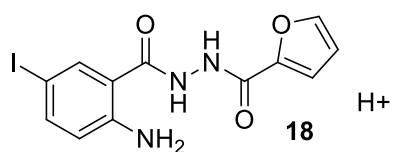
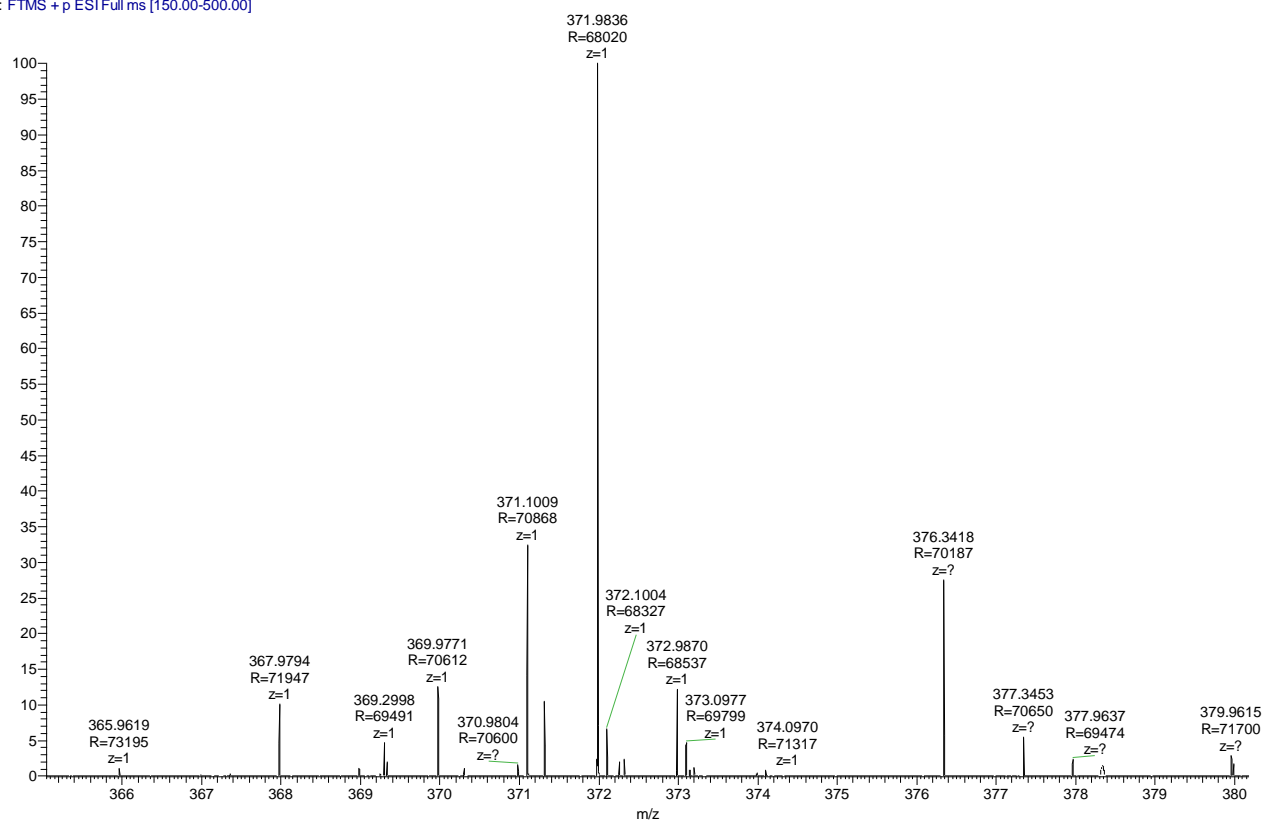
5 #145 RT: 3.59 AV: 1 NL: 8.61E6
T: FTMS + p ESI Full ms [150.00-500.00]



N'-(2-amino-5-iodobenzoyl)furan-2-carbohydrazide (**18**)



5_181210123101 #492-501 RT: 8.51-8.64 AV: 10 NL: 1.26E6
T: FTMS + p ESI Full ms [150.00-500.00]

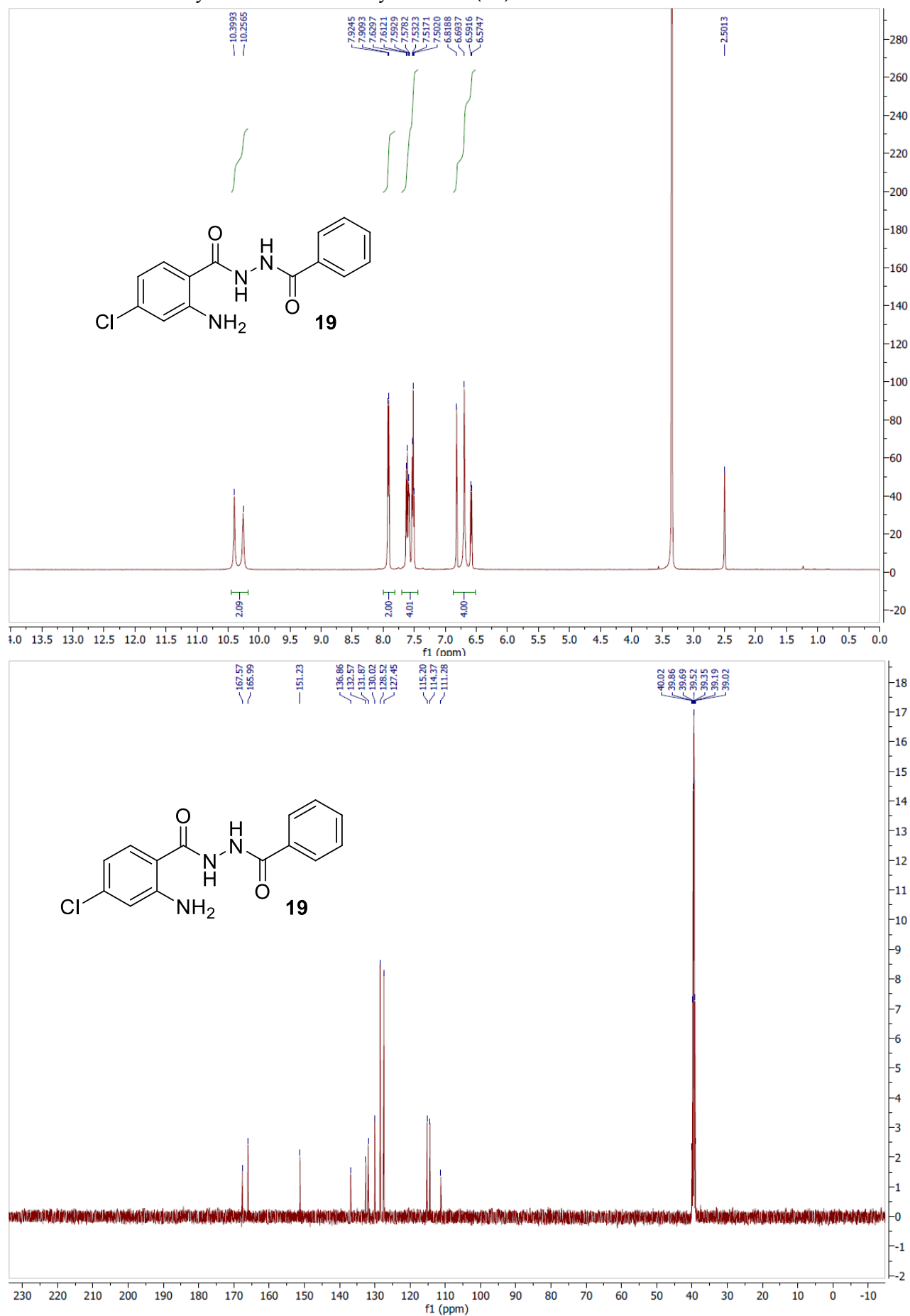


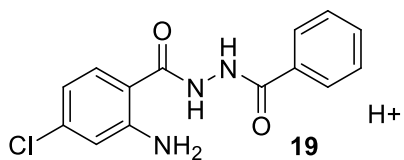
Chemical Formula: C₁₂H₁₁IN₃O₃⁺

Exact Mass: 371,9840

Molecular Weight: 372,1380

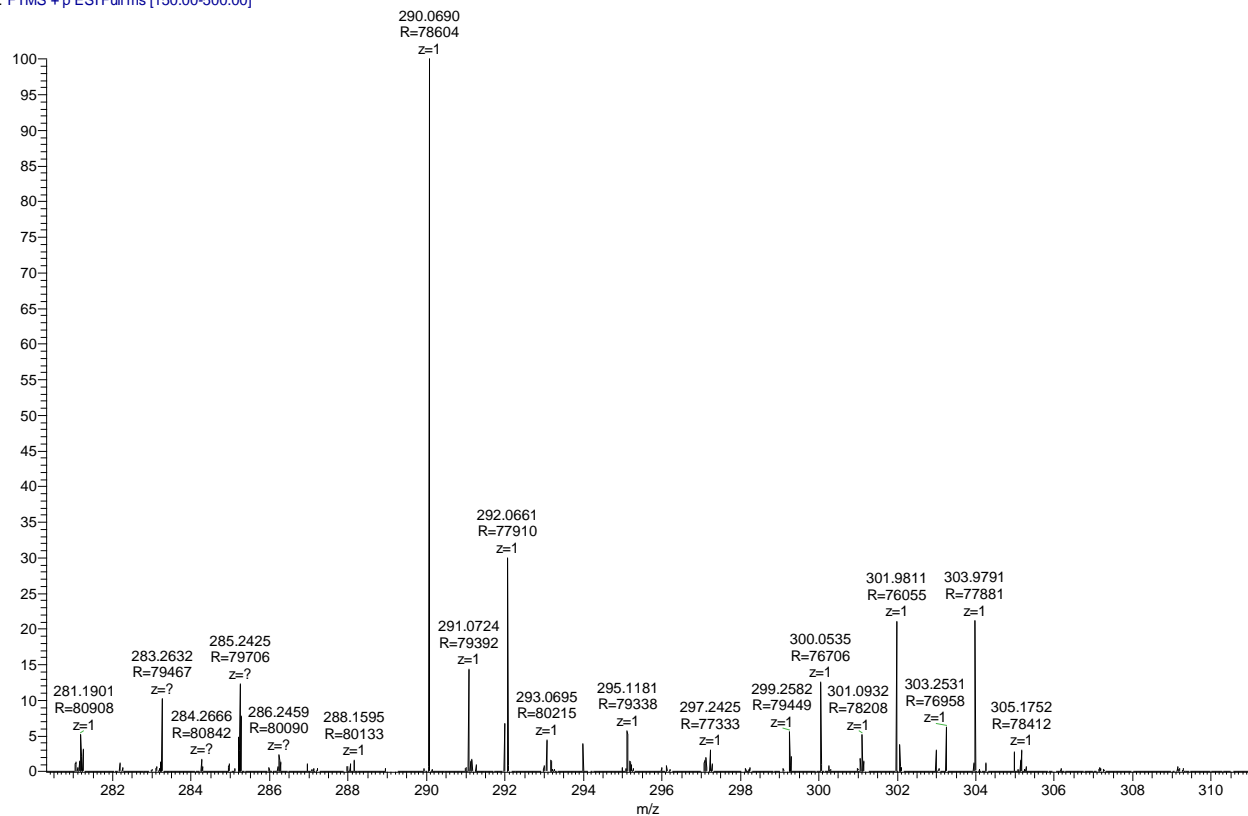
2-amino-*N'*-benzoyl-4-chlorobenzohydrazide (**19**)



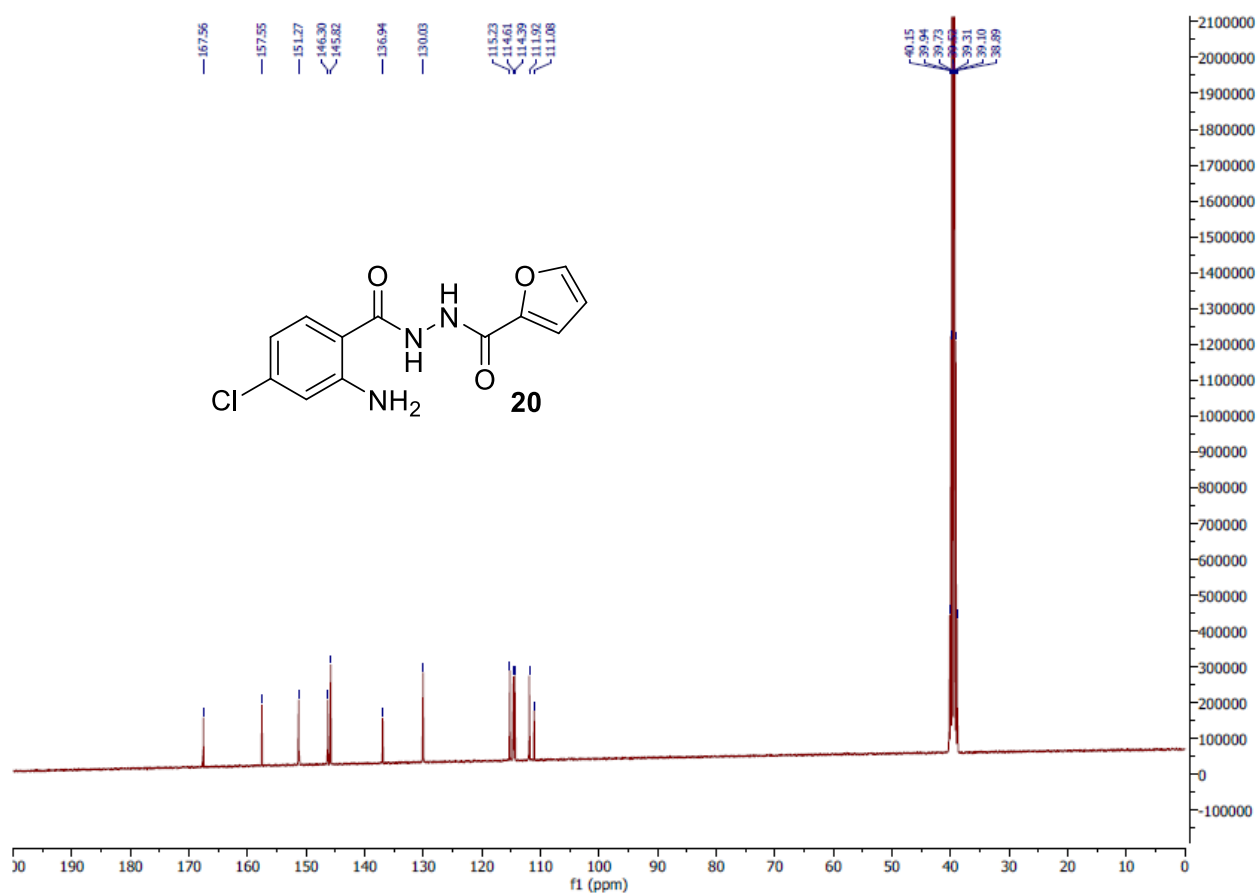
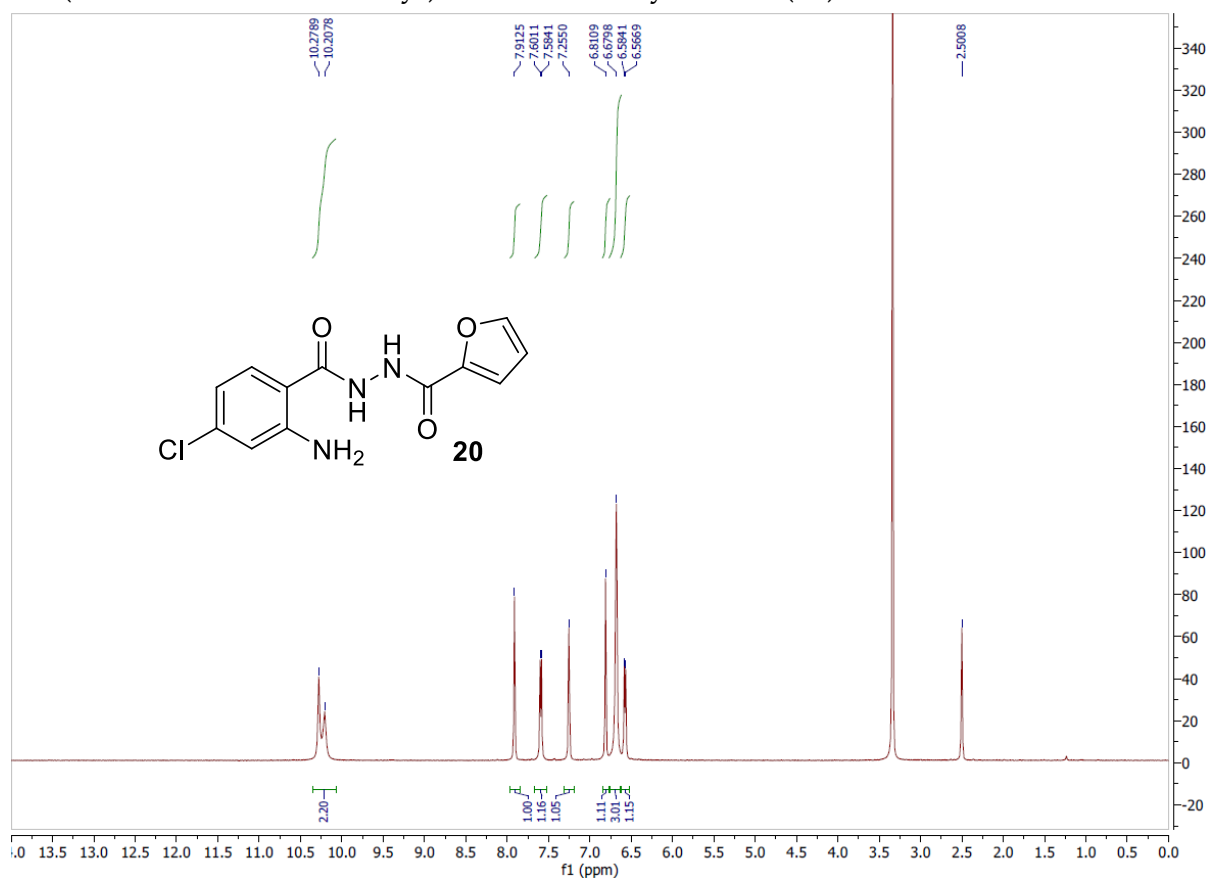


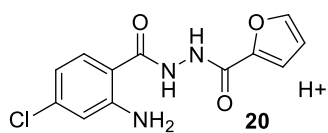
Chemical Formula: $C_{14}H_{13}ClN_3O_2^+$
 Exact Mass: 290,0691

5_181210123101 #419-428 RT: 7.47-7.60 AV: 10 NL: 2.05E6
 T: FTMS + p ESI Full ms [150.00-500.00]



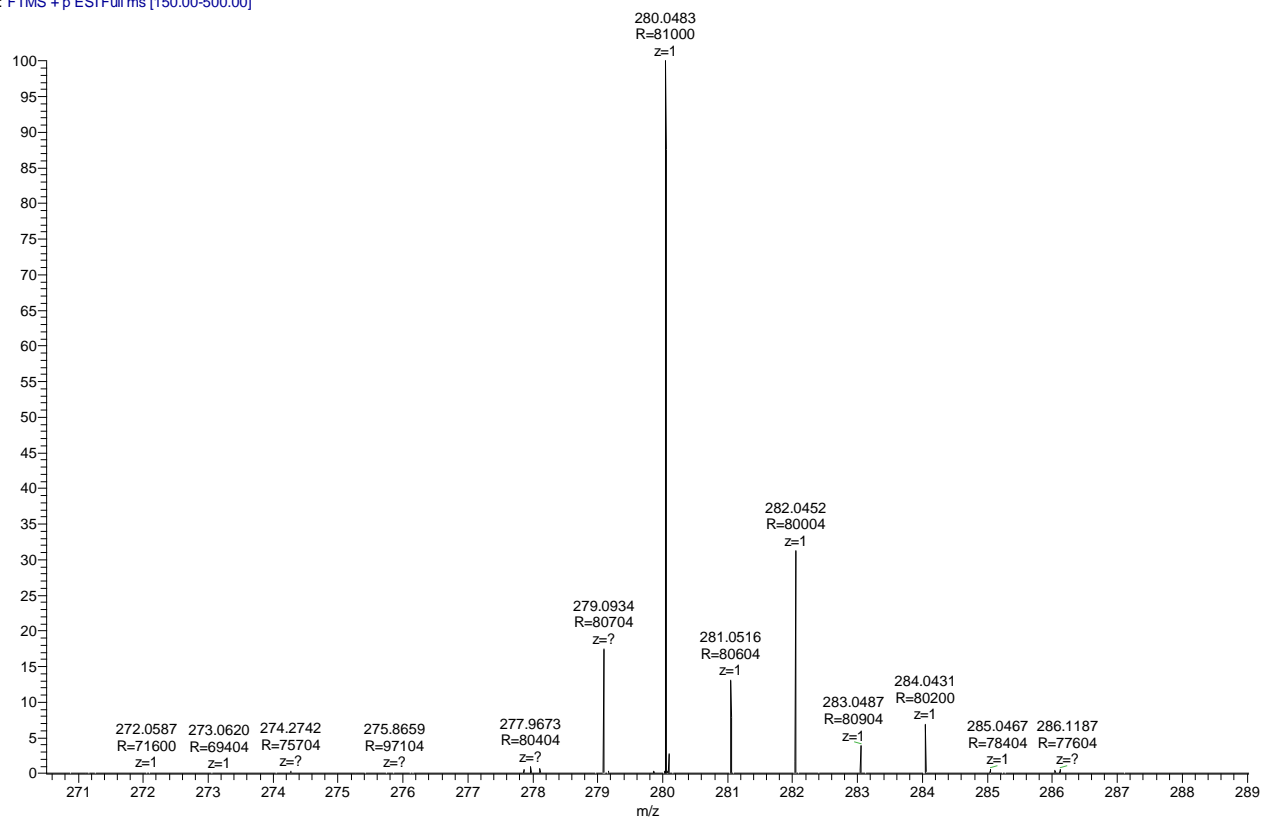
N'-(2-amino-4-chlorobenzoyl)furan-2-carbohydrazide (**20**)



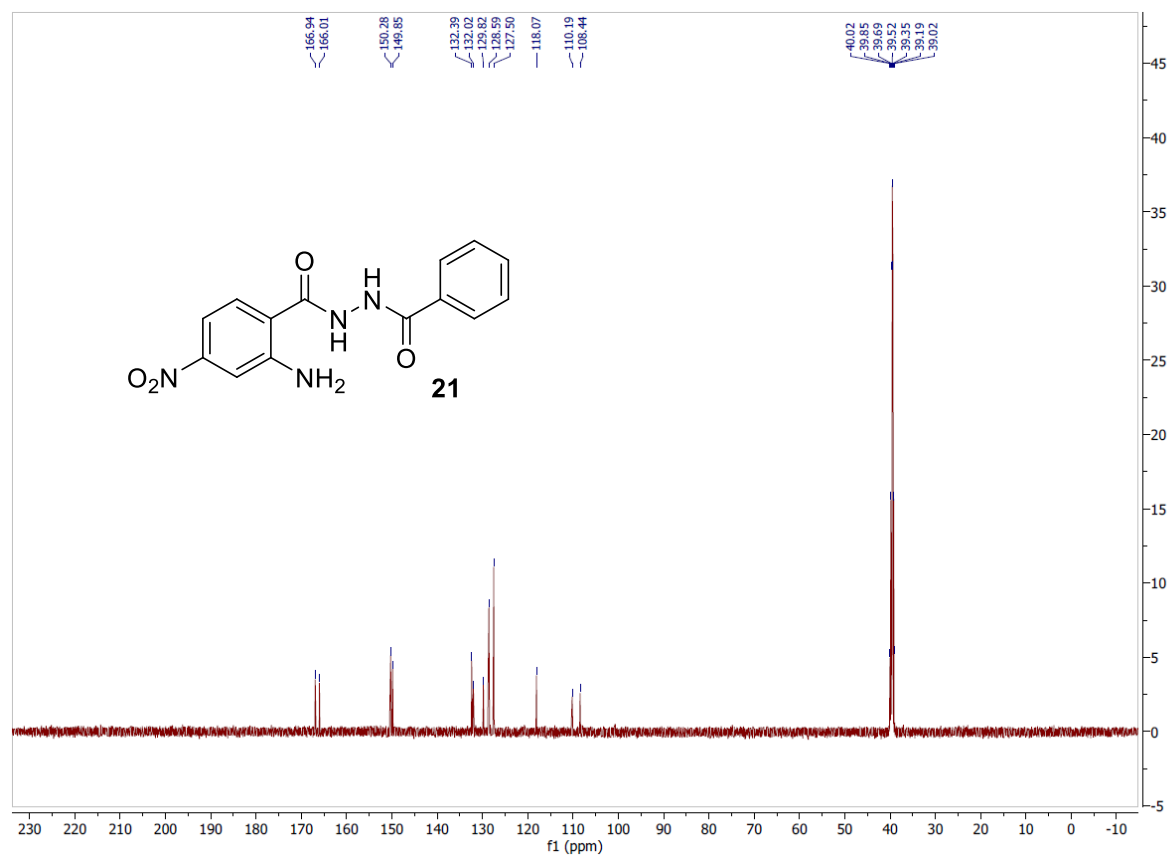
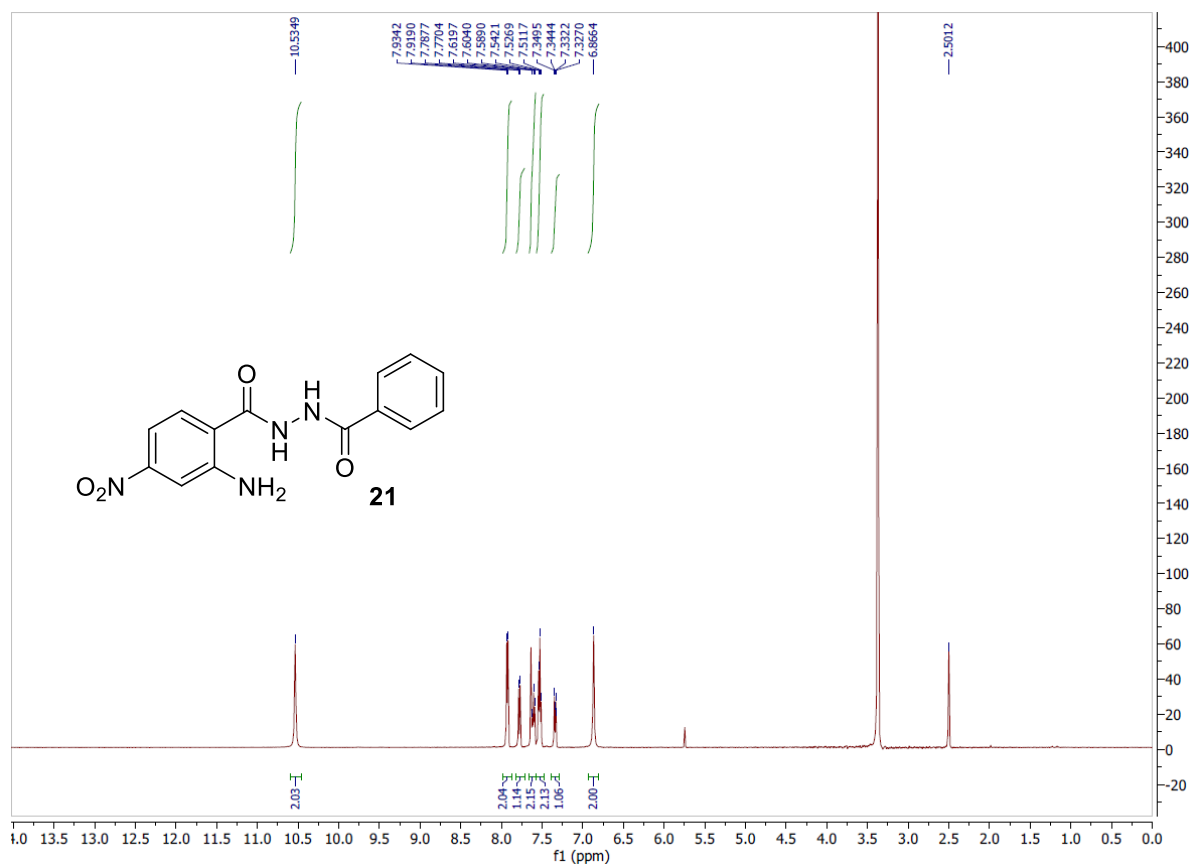


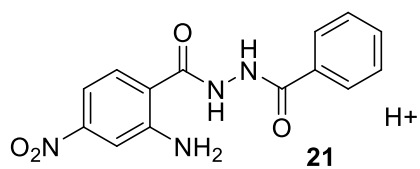
Chemical Formula: $C_{12}H_{11}ClN_3O_3^+$
Exact Mass: 280,0483

WASH_181210123101 #616 RT: 8.82 AV: 1 NL: 5.50E7
T: FTMS + p ESI Full ms [150.00-500.00]



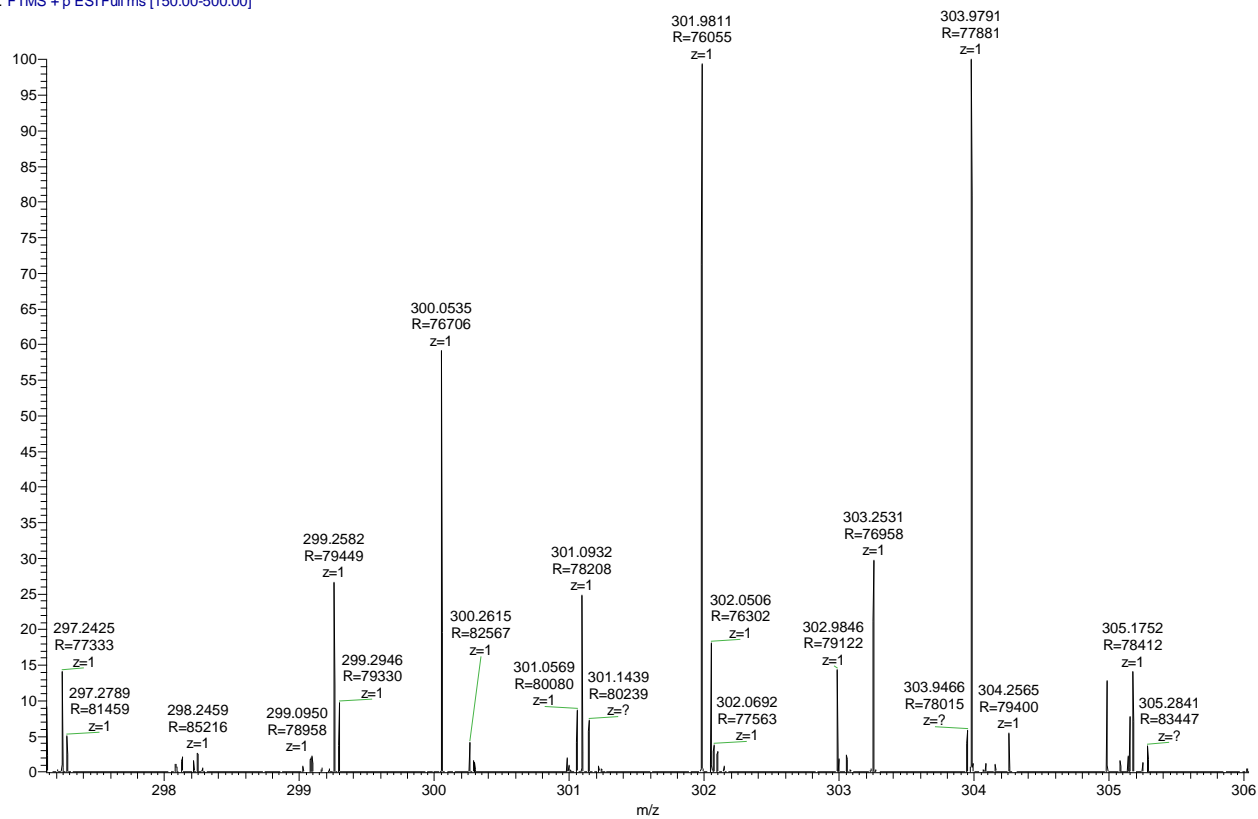
2-amino-*N'*-benzoyl-4-nitrobenzohydrazide (**21**)



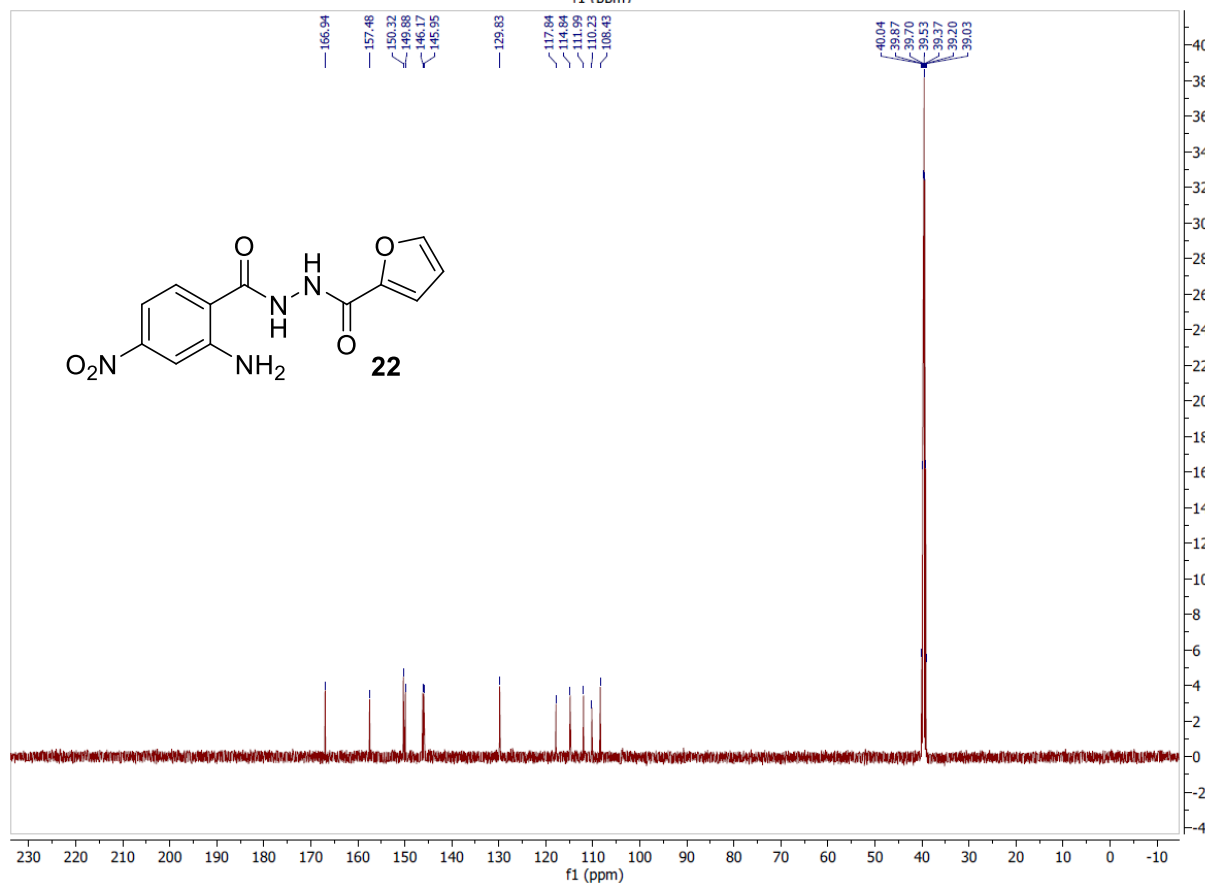
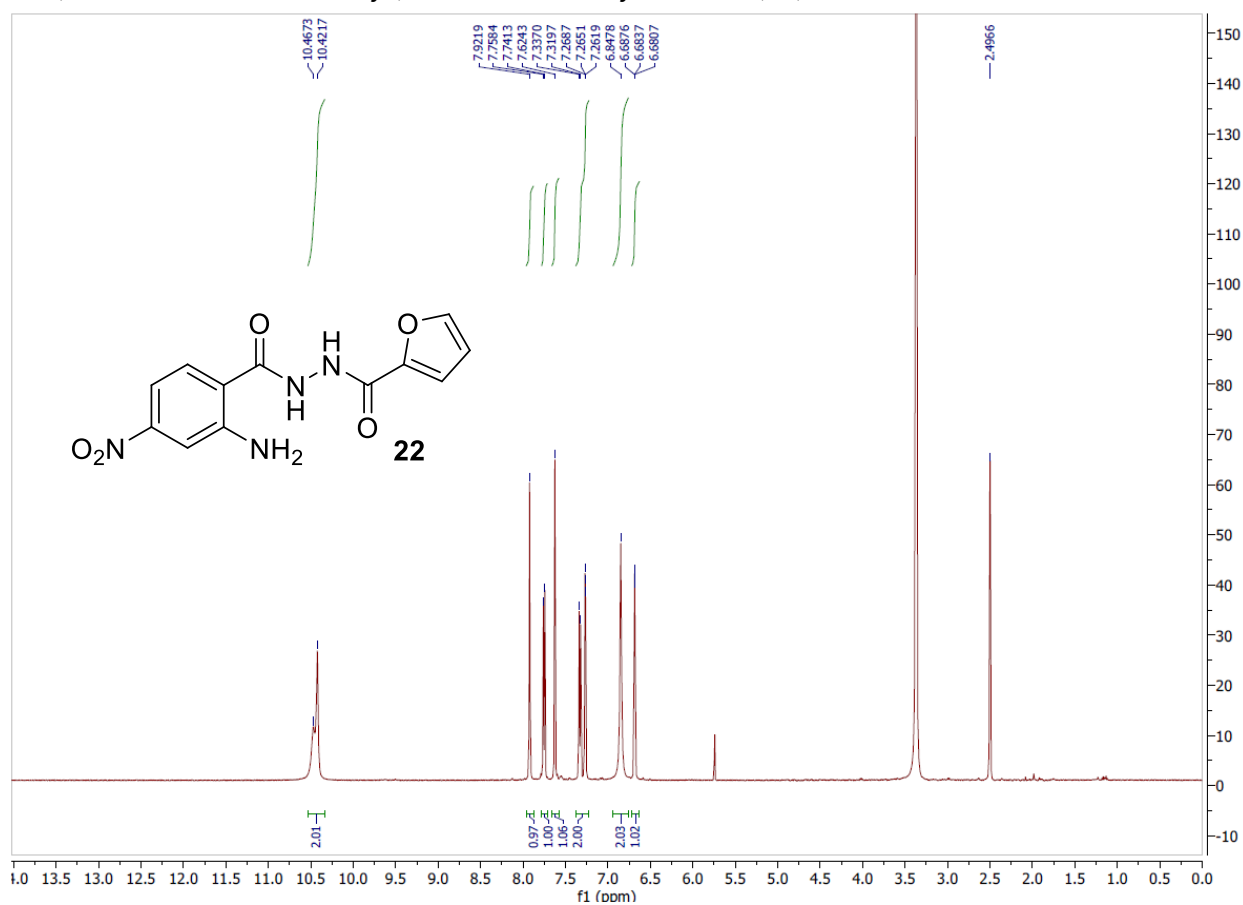


Chemical Formula: $\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_4^+$
Exact Mass: 301,0931

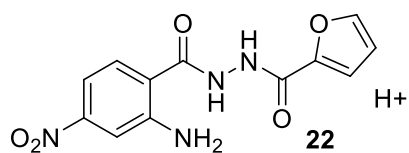
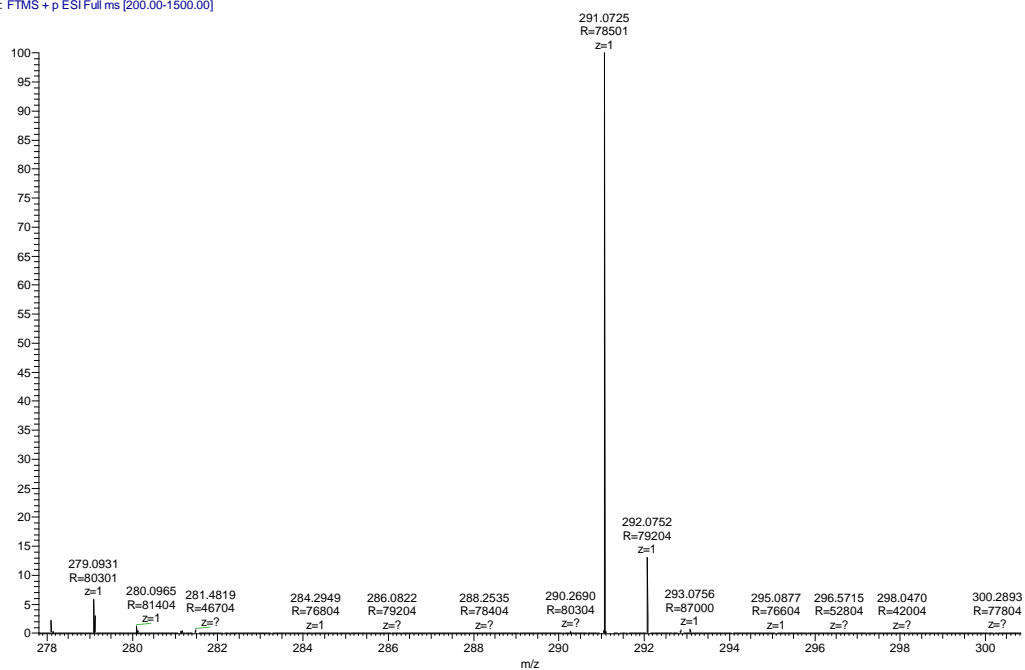
5_181210123101 #419-428 RT: 7.47-7.60 AV: 10 NL: 4.36E5
T: FTMS + p ESI Full ms [150.00-500.00]



N'-(2-amino-4-nitrobenzoyl)furan-2-carbohydrazide (**22**)

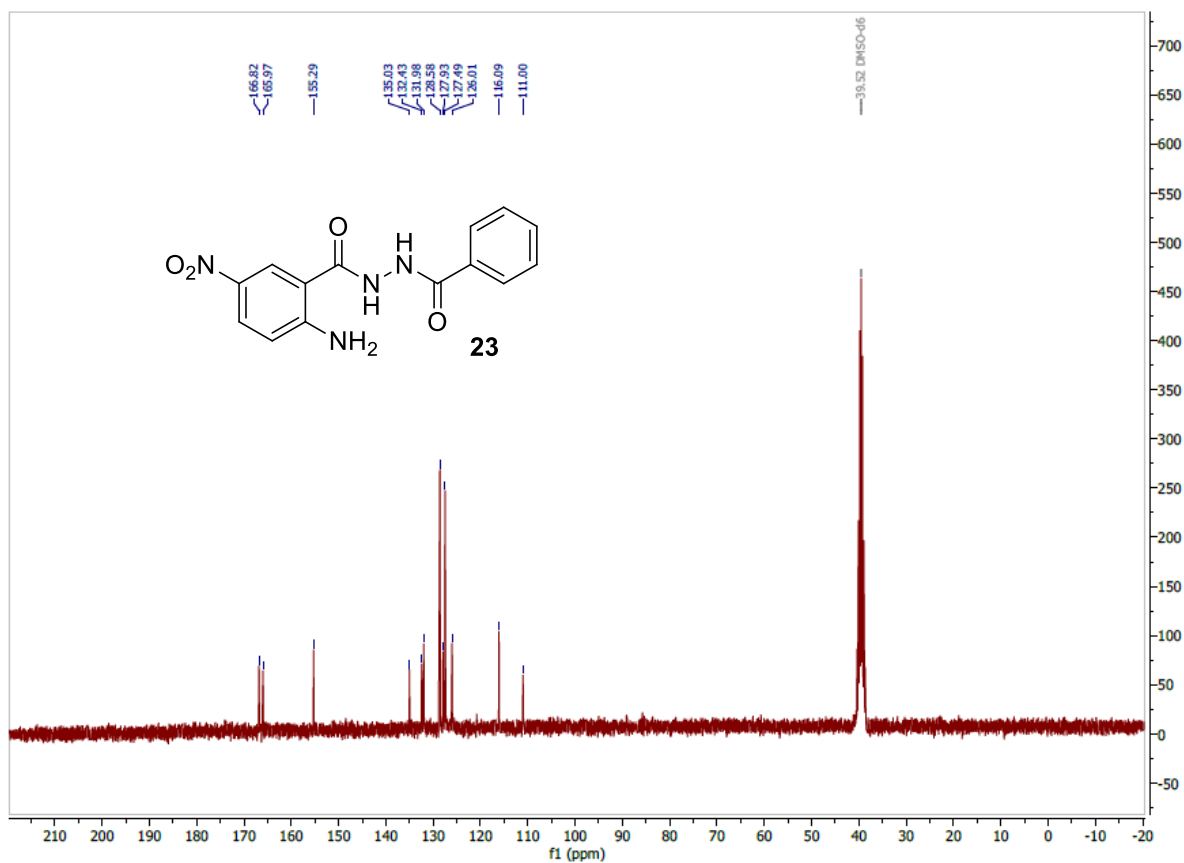
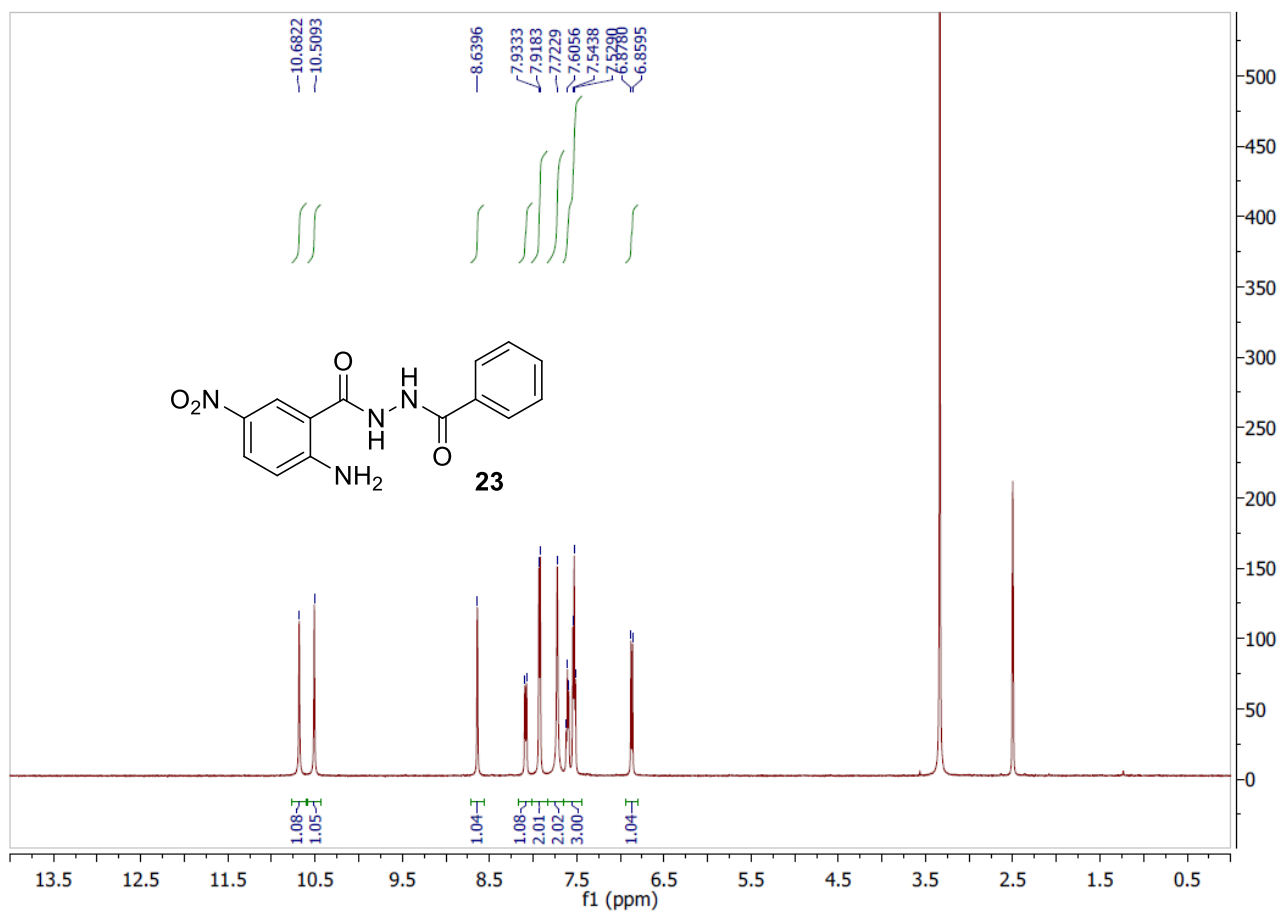


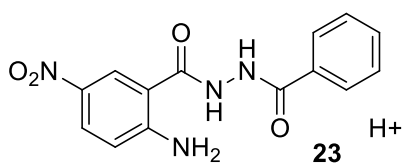
KX24_02_Recal#425 RT: 6.57 AV: 1 NL: 3.94E7
T: FTMS + p ESI Full ms [200.00-1500.00]



Chemical Formula: $C_{12}H_{11}N_4O_5^+$
Exact Mass: 291,0724

2-amino-*N'*-benzoyl-5-nitrobenzohydrazide (**23**):



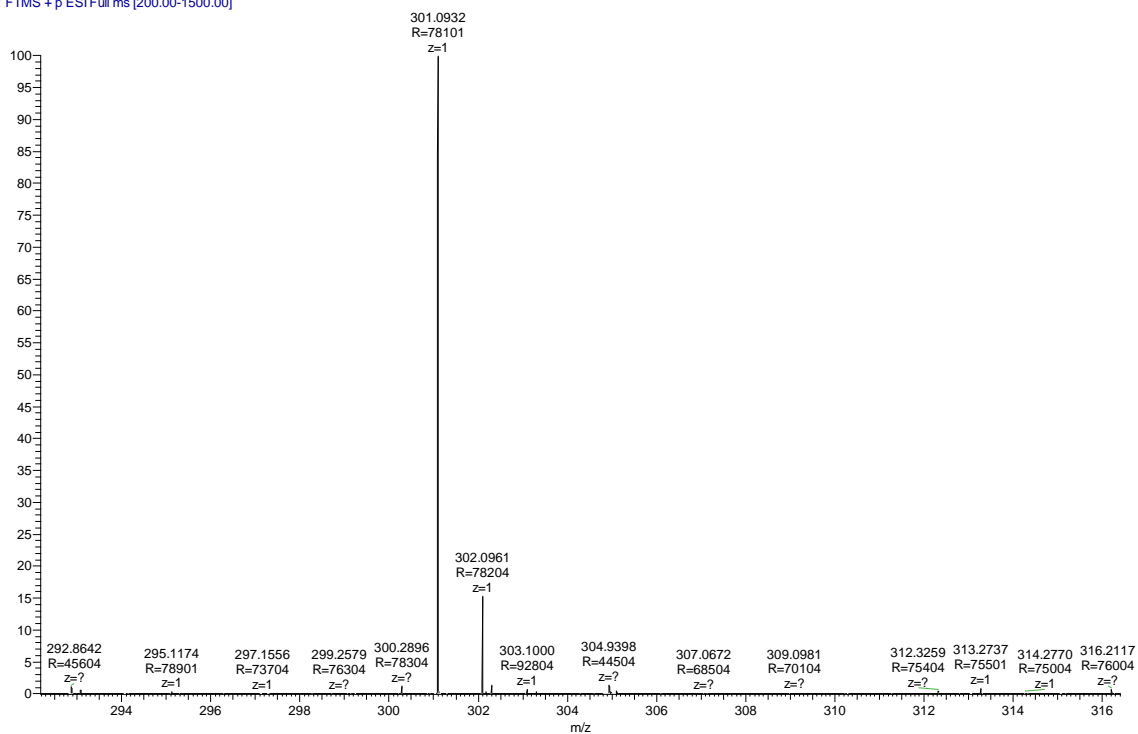


Chemical Formula: $C_{14}H_{13}N_4O_4^+$

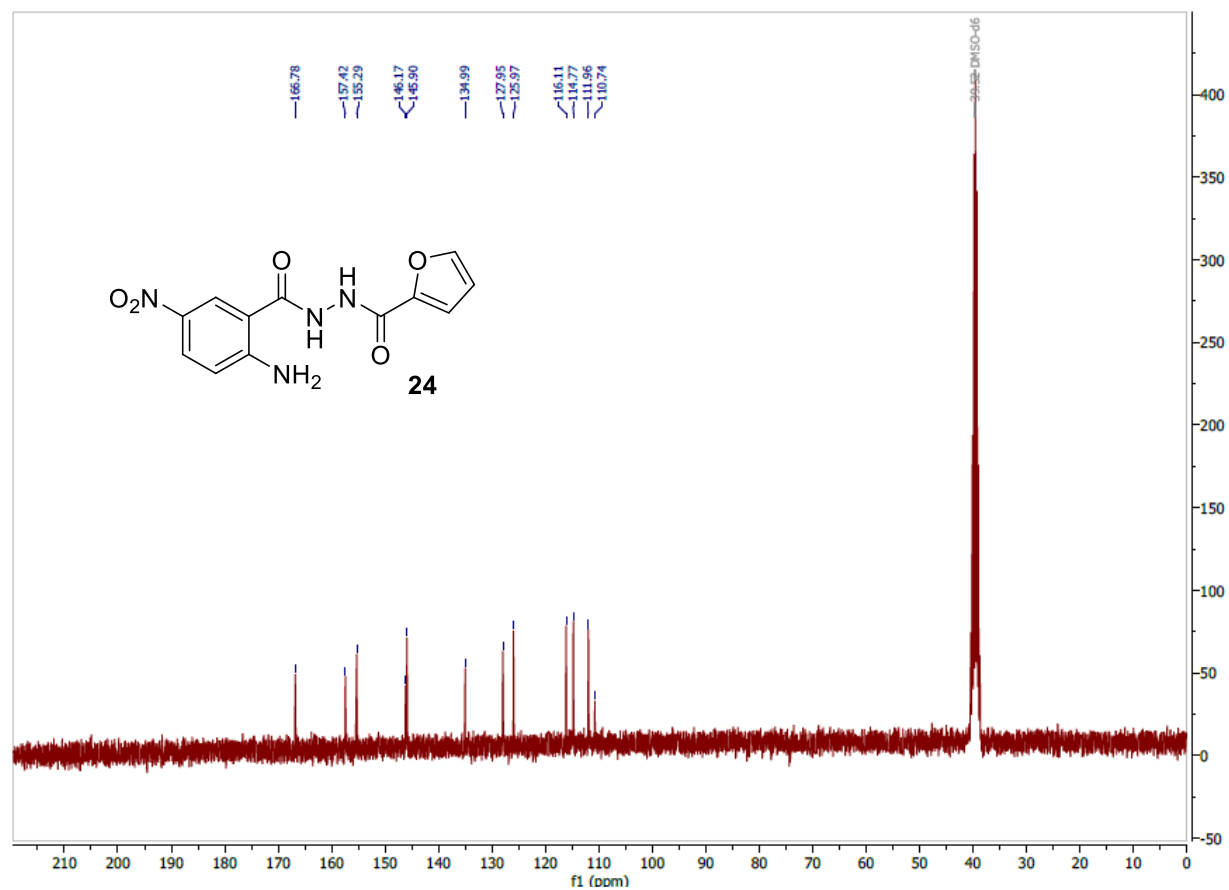
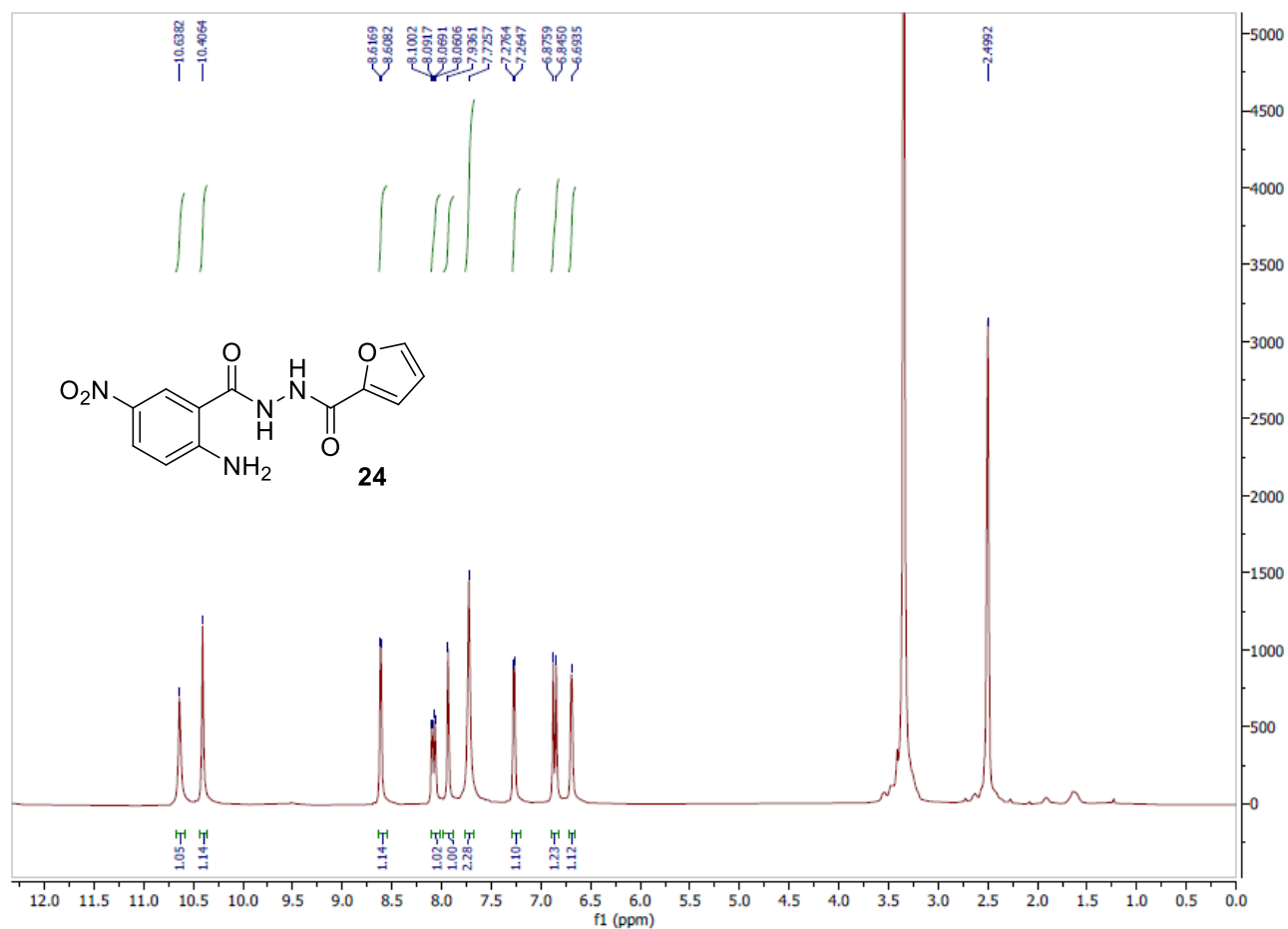
Exact Mass: 301,0931

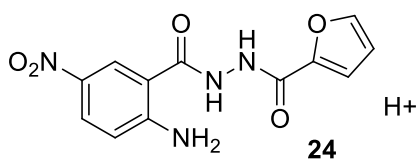
Molecular Weight: 301,2769

KX27 #422 RT: 6.84 AV: 1 NL: 5.91E6
T: FTMS +p ESI Full ms [200.00-1500.00]



N'-(2-amino-5-nitrobenzoyl)furan-2-carbohydrazide (**24**)



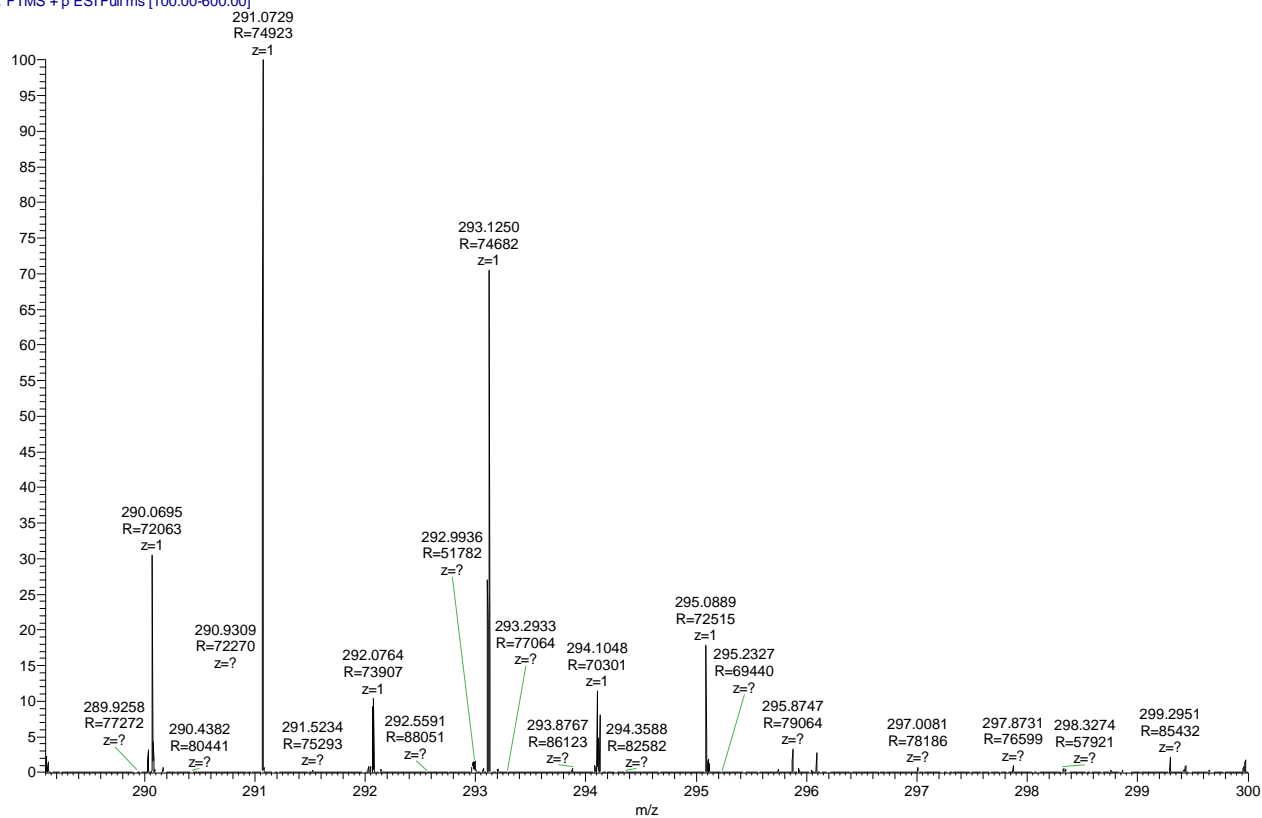


Chemical Formula: $C_{12}H_{11}N_4O_5^+$

Exact Mass: 291,0724

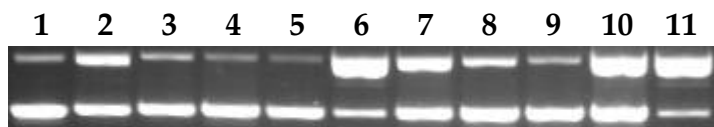
Molecular Weight: 291,2390

8 #482-488 RT: 9.89-10.16 AV: 7 NL: 5.07E5
T: FTMS + p ESI Full ms [100.00-600.00]



S.2. Gel electrophoresis pictures of AA DACHZs 1-24 and AA II a-h

S.2.1.



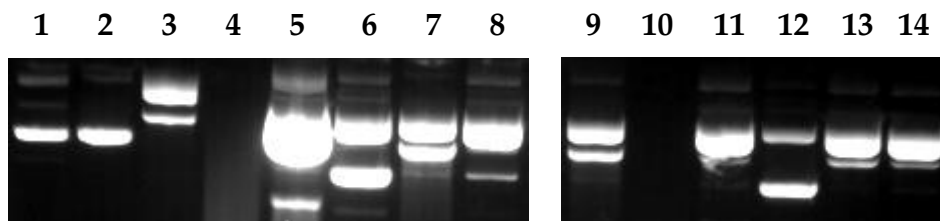
Form II% : 37 20 16 16 55 42 28 21 42 59

Form III% : 0 0 0 0 4 4 0 0 4 6

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C = 500 μ M | | | | |
|------|--|---------|------|------------|------|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | II d | 7 | DNA + UV + | II d |
| 3 | DNA + UV + | 13 | 8 | DNA + UV + | 13 |
| 4 | DNA + UV + | 14 | 9 | DNA + UV + | 14 |
| 5 | DNA + UV + | 15 | 10 | DNA + UV + | 15 |
| 6 | DNA + UV + | 16 | 11 | DNA + UV + | 16 |

Gel S.2.1: Compounds 13-16 and II d

S.2.2.



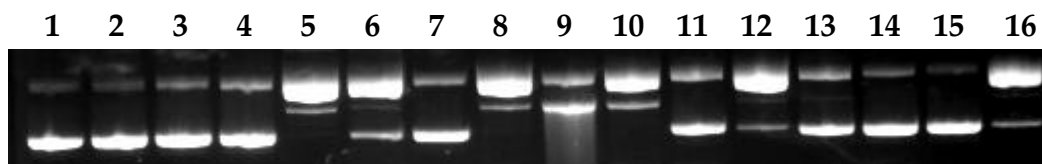
Form II% : 63 - 0 0 49 77 54 - 100 20 73 87

Form III% : 37 - 80 51 38 0 46 - 0 0 2 13

| lane | 312nm, 15cm, 30min, pH=6.8 DMSO, C = 500 μ M | | | | |
|------|---|---------|------|------------|------|
| 1 | DNA + UV | Control | | | |
| 2 | DNA | Control | lane | | |
| 3 | DNA + UV + | II c | 9 | DNA + UV + | II c |
| 4 | DNA + UV + | 9 | 10 | DNA + UV + | 9 |
| 5 | DNA + UV + | 10 | 11 | DNA + UV + | 10 |
| 6 | DNA + UV + | 11 | 12 | DNA + UV + | 11 |
| 7 | DNA + UV + | 12 | 13 | DNA + UV + | 12 |
| 8 | DNA + UV + | 8 | 14 | DNA + UV + | 8 |

Gel S.2.2: Compounds 8-12 and II c

S.2.3.

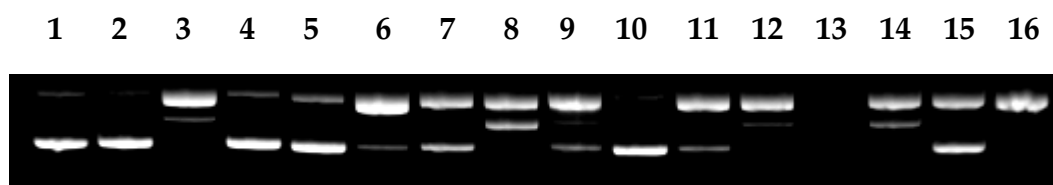


| | | | | | | | | | | | | | | | |
|-------------|---|----|----|----|----|----|----|----|----|----|----|----|---|---|----|
| Form II% : | 4 | 11 | 19 | 88 | 65 | 18 | 84 | 35 | 75 | 25 | 78 | 21 | 7 | - | 83 |
| Form III% : | 0 | 0 | 0 | 12 | 6 | 0 | 16 | 65 | 25 | 0 | 4 | 0 | 0 | - | 0 |

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C= 500 μ M | | lane | | |
|------|---|---------|------|------------|----|
| 1 | DNA + UV + | Control | 9 | DNA + UV + | 9 |
| 2 | DNA + UV + | 2 | 10 | DNA + UV + | 10 |
| 3 | DNA + UV + | 3 | 11 | DNA + UV + | 11 |
| 4 | DNA + UV + | 4 | 12 | DNA + UV + | 12 |
| 5 | DNA + UV + | 5 | 13 | DNA + UV + | 13 |
| 6 | DNA + UV + | 6 | 14 | DNA + UV + | 14 |
| 7 | DNA + UV + | 7 | 15 | DNA + UV + | 15 |
| 8 | DNA + UV + | 8 | 16 | DNA + UV + | 16 |

Gel S.2.3: Compounds 1-16

S.2.4.

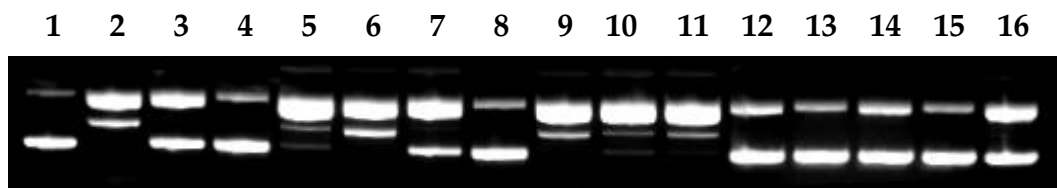


| | | | | | | | | | | | | | | | |
|-------------|---|----|---|----|----|----|----|----|---|----|----|---|----|----|-----|
| Form II% : | 0 | 92 | 5 | 13 | 90 | 56 | 64 | 77 | 0 | 80 | 95 | - | 80 | 42 | 100 |
| Form III% : | 0 | 8 | 0 | 0 | 0 | 0 | 36 | 2 | 0 | 0 | 5 | - | 20 | 0 | 0 |

| Σ ειqά | 312nm, 15cm, 30min, pH=6.8, DMSO, C= 500 μ M | | | | |
|---------------|---|------------|----|------------|------|
| 1 | DNA + UV + | Control | 9 | DNA + UV + | II d |
| 2 | DNA + UV + | II a | 10 | DNA + UV + | II g |
| 3 | DNA + UV + | irrelevant | 11 | DNA + UV + | II f |
| 4 | DNA + UV + | II h | 12 | DNA + UV + | II c |
| 5 | DNA + UV + | irrelevant | 13 | DNA + UV + | 9 |
| 6 | DNA + UV + | II e | 14 | DNA + UV + | 10 |
| 7 | DNA + UV + | irrelevant | 15 | DNA + UV + | 11 |
| 8 | DNA + UV + | II b | 16 | DNA + UV + | 12 |

Gel S.2.4: Compounds II a-g, 9-12

S.2.5.

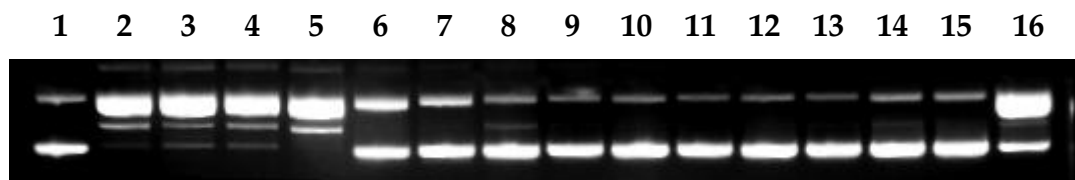


Form II% : 69 42 13 85 68 59 3 80 89 87 24 13 25 11 41
 Form III% : 31 0 0 9 32 0 0 20 7 13 0 0 0 0 0

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C= 500 μ M | | lane | | |
|------|--|---------|------|------------|------|
| 1 | DNA + UV + | Control | 10 | DNA + UV + | 17 |
| 2 | DNA + UV + | 5 | 11 | DNA + UV + | 18 |
| 3 | DNA + UV + | 6 | 12 | DNA + UV + | 19 |
| 4 | DNA + UV + | 7 | 13 | DNA + UV + | 20 |
| 5 | DNA + UV + | 8 | 14 | DNA + UV + | 19 |
| 6 | DNA + UV + | 5 | 15 | DNA + UV + | 20 |
| 7 | DNA + UV + | 6 | 16 | DNA + UV + | II f |
| 8 | DNA + UV + | 7 | | | |
| 9 | DNA + UV + | 8 | | | |

Gel S.2.5: Compounds II f, 5-8, 17-20

S.2.6.

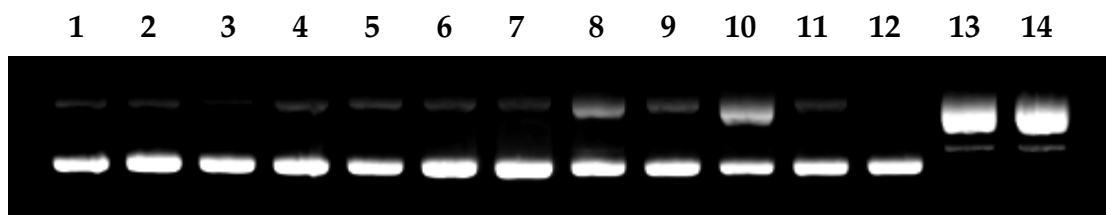


Form II% : 80 80 74 73 25 11 0 0 0 0 0 0 0 0 55
 Form III% : 17 11 15 27 0 0 7 0 0 0 0 0 0 3 4

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C $\tau\epsilon\lambda$ = 500 μ M | | lane | | |
|------|---|---------|------|------------|------|
| 1 | DNA + UV + | Control | 8 | DNA + UV + | 21 |
| 2 | DNA + UV + | 17 | 9 | DNA + UV + | 22 |
| 3 | DNA + UV + | 18 | 10 | DNA + UV + | 21 |
| 4 | DNA + UV + | 17 | 11 | DNA + UV + | 22 |
| 5 | DNA + UV + | 18 | 12 | DNA + UV + | 21 |
| 6 | DNA + UV + | 19 | 13 | DNA + UV + | 22 |
| 7 | DNA + UV + | 20 | 14 | DNA + UV + | II g |
| | | | 15 | DNA + UV + | II h |
| | | | 16 | DNA + UV + | II e |

Gel S.2.6: Compounds II e,g,h, 17-22

S.2.7.

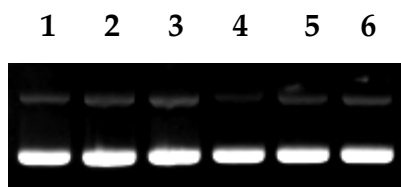


Form II% : 0 0 2 3 1 1 20 6 38 2 0 96 96
 Form III% : 0 0 0 0 0 0 0 0 0 0 0 4 4

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C=500 μ M | | | | |
|------|---|---------|------|------------|----|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 1 | 10 | DNA + UV + | 13 |
| 3 | DNA + UV + | 2 | 11 | DNA + UV + | 14 |
| 4 | DNA + UV + | 3 | 12 | DNA + UV + | 15 |
| 5 | DNA + UV + | 4 | 13 | DNA + UV + | 16 |
| 6 | DNA + UV + | 1 | 14 | DNA + UV + | 8 |
| 7 | DNA + UV + | 2 | | | |
| 8 | DNA + UV + | 3 | | | |
| 9 | DNA + UV + | 4 | | | |

Gel S.2.7: Compounds 1-4, 8, 13-16

S.2.8.



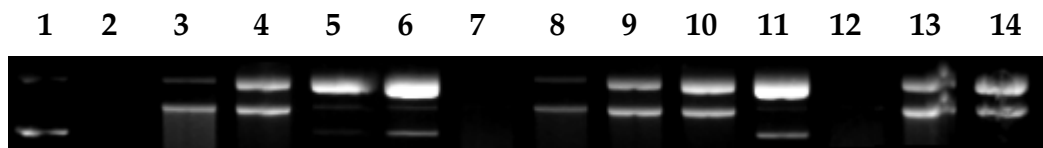
Form II% : 0 0 0 0 0 0
 Form III% : 0 0 0 0 0 0

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C=500 μ M | |
|------|---|----|
| 1 | DNA + UV + | 23 |
| 2 | DNA + UV + | 24 |
| 3 | DNA + UV + | 23 |
| 4 | DNA + UV + | 24 |
| 5 | DNA + UV + | 23 |
| 6 | DNA + UV + | 24 |

Gel S.2.8: Compounds 23-24

S.3. Gel electrophoresis pictures of 9 at various concentrations, pH studies and mechanistic studies

S.3.1

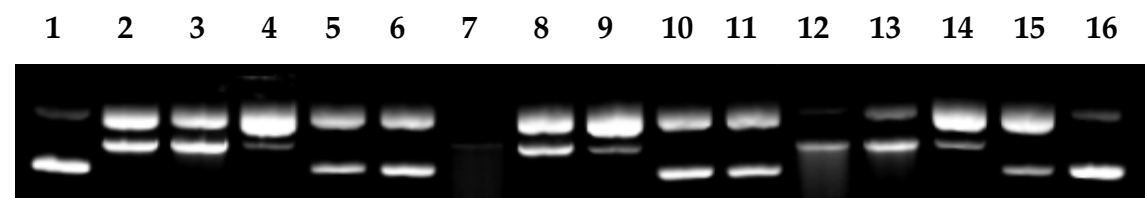


Form II% : - 7 50 92 84 - 14 46 60 85 - 41 62
 Form III% : - 93 50 4 3 - 86 54 40 2 - 59 38

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, compound 9 | | lane | | |
|------|--|-------------|------|------------|-------------|
| 1 | DNA + UV + | Control | 8 | DNA + UV + | 200 μ M |
| 2 | DNA + UV + | 400 μ M | 9 | DNA + UV + | 100 μ M |
| 3 | DNA + UV + | 200 μ M | 10 | DNA + UV + | 50 μ M |
| 4 | DNA + UV + | 100 μ M | 11 | DNA + UV + | 10 μ M |
| 5 | DNA + UV + | 50 μ M | 12 | DNA + UV + | 400 μ M |
| 6 | DNA + UV + | 10 μ M | 13 | DNA + UV + | 200 μ M |
| 7 | DNA + UV + | 400 μ M | 14 | DNA + UV + | 200 μ M |

Gel S.3.1: Compound 9 from 400 to 10 μ M

S.3.2

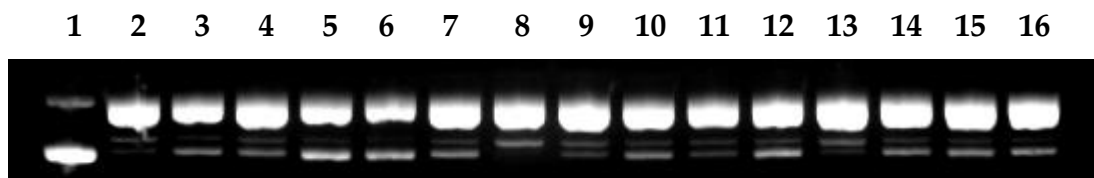


Form II% : 59 49 93 53 44 - 66 88 43 47 - 24 86 70 2
 Form III% : 41 51 7 0 0 - 34 12 0 0 - 76 14 0 0

| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, Compound 9 | | lane | | |
|------|--|-------------|------|------------|-------------|
| 1 | DNA + UV + | Control | 9 | DNA + UV + | 10 μ M |
| 2 | DNA + UV + | 100 μ M | 10 | DNA + UV + | 1 μ M |
| 3 | DNA + UV + | 50 μ M | 11 | DNA + UV + | 500nM |
| 4 | DNA + UV + | 10 μ M | 12 | DNA + UV + | 100 μ M |
| 5 | DNA + UV + | 1 μ M | 13 | DNA + UV + | 50 μ M |
| 6 | DNA + UV + | 500nM | 14 | DNA + UV + | 10 μ M |
| 7 | DNA + UV + | 100 μ M | 15 | DNA + UV + | 1 μ M |
| 8 | DNA + UV + | 50 μ M | 16 | DNA + UV + | 500nM |

Gel S.3.2: Compound 9 from 100 to 0.5 μ M

S.3.3

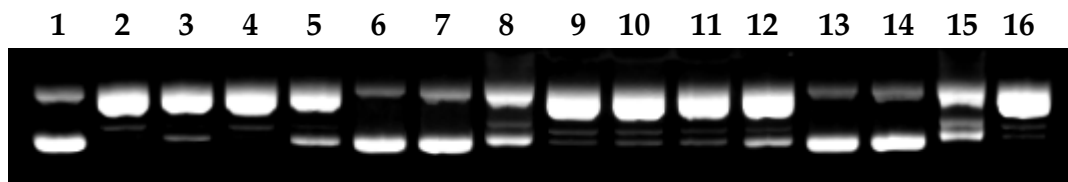


Form II% : 94 83 85 65 68 81 88 88 82 90 77 90 84 84 86
Form III% : 4 1 4 2 1 4 12 6 4 4 3 7 3 2 1

| lane | 312nm, 15cm, 30min, DMSO, C= 5μM | | lane | | |
|------|----------------------------------|--------|------|--------------|--------|
| 1 | DNA + UV Control | pH 6.8 | 8 | DNA + UV + 9 | pH 5 |
| 2 | DNA + UV + 9 | pH 5 | 9 | DNA + UV + 9 | pH 6.0 |
| 3 | DNA + UV + 9 | pH 6.0 | 10 | DNA + UV + 9 | pH 8.1 |
| 4 | DNA + UV + 9 | pH 6.8 | 11 | DNA + UV + 9 | pH 8.9 |
| 5 | DNA + UV + 9 | pH 8.1 | 12 | DNA + UV + 9 | pH 10 |
| 6 | DNA + UV + 9 | pH 8.9 | 13 | DNA + UV + 9 | pH 5 |
| 7 | DNA + UV + 9 | pH 10 | 14 | DNA + UV + 9 | pH 6.0 |
| | | | 15 | DNA + UV + 9 | pH 8.1 |
| | | | 16 | DNA + UV + 9 | pH 8.9 |

Gel S.3.3: Compound 9 from pH 5-10

S.3.4

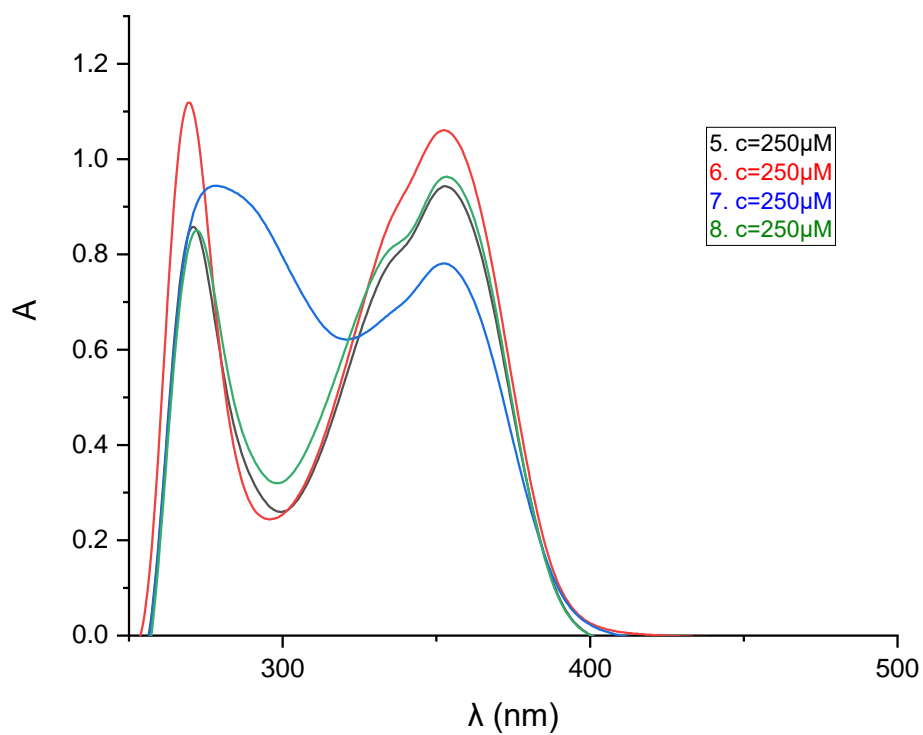
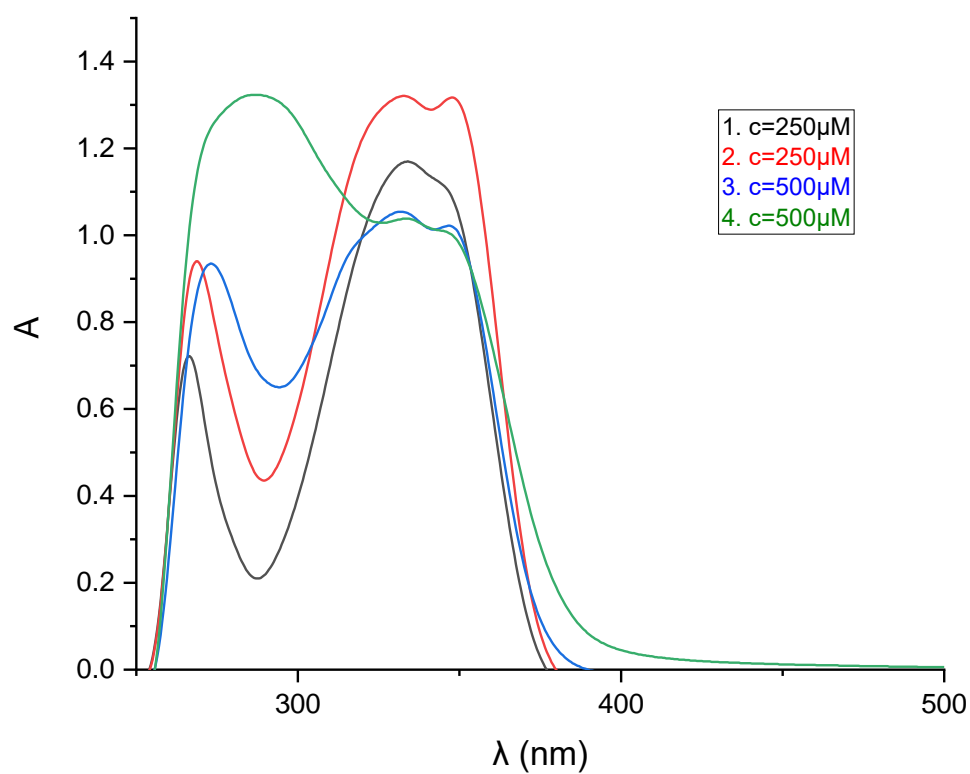


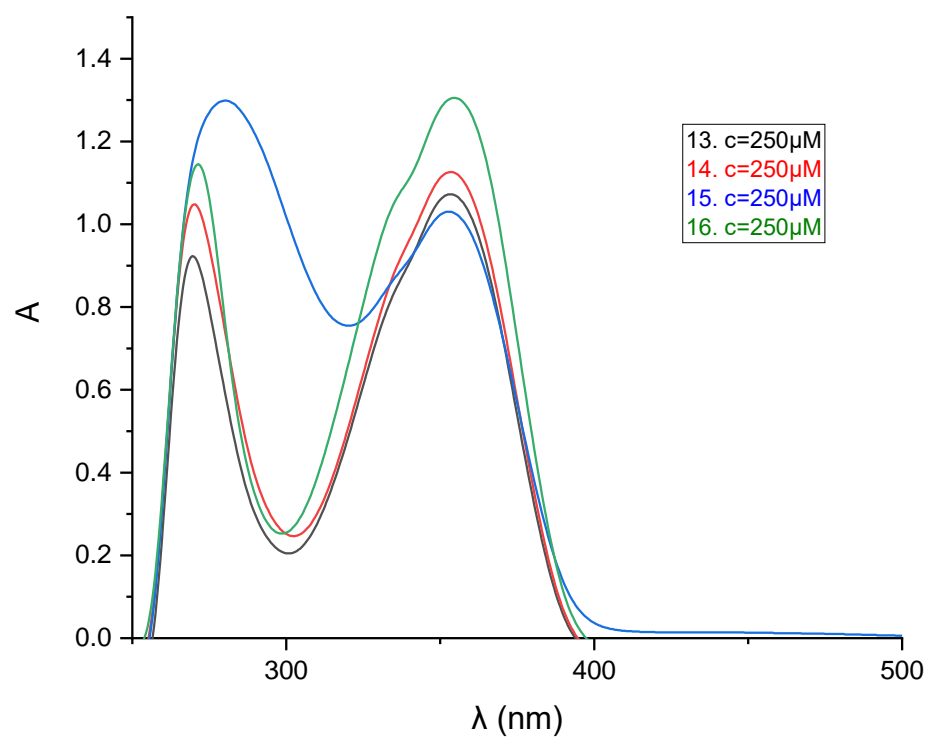
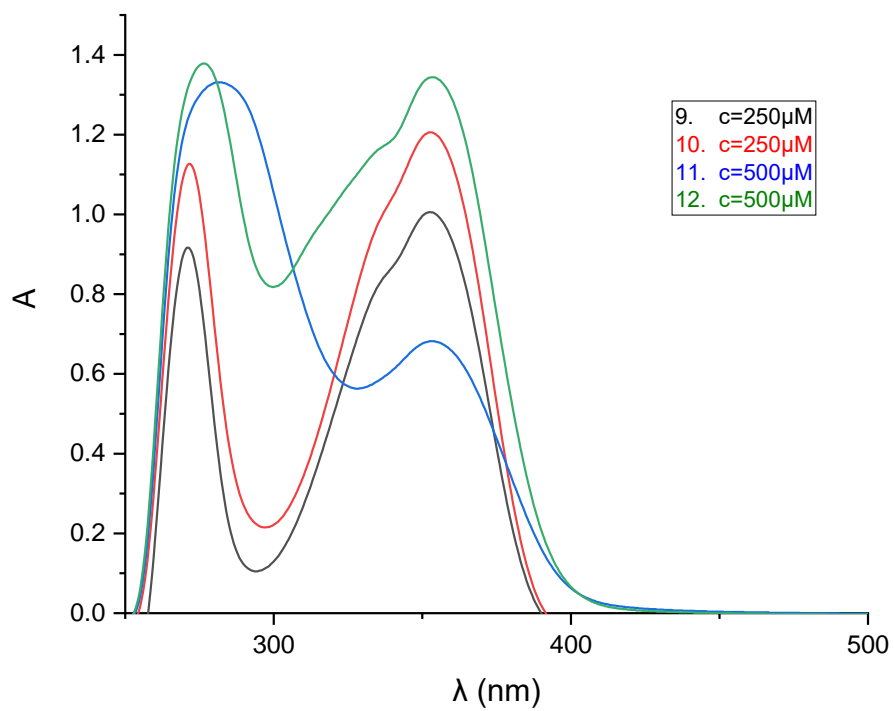
FII%: 97 89 97 65 0 0 41 92 90 90 72 0 0 42 96
FIII%: 3 0 3 1 0 0 6 4 3 2 2 0 0 16 2

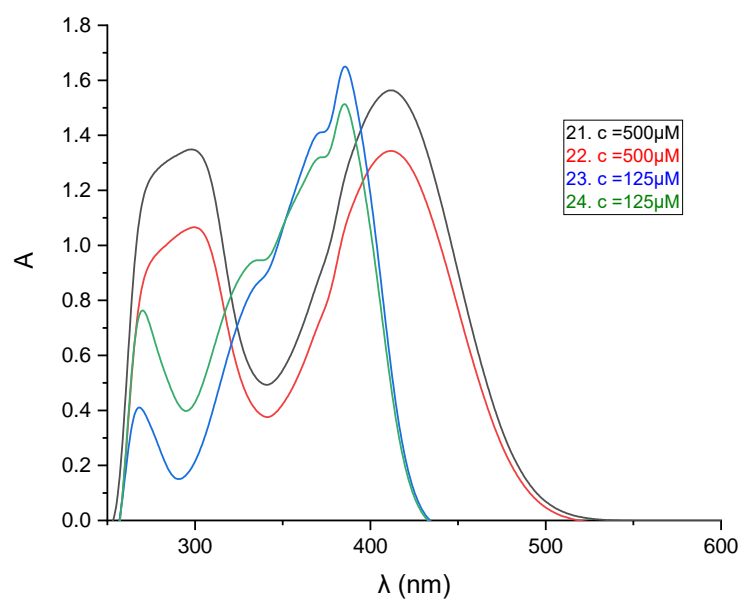
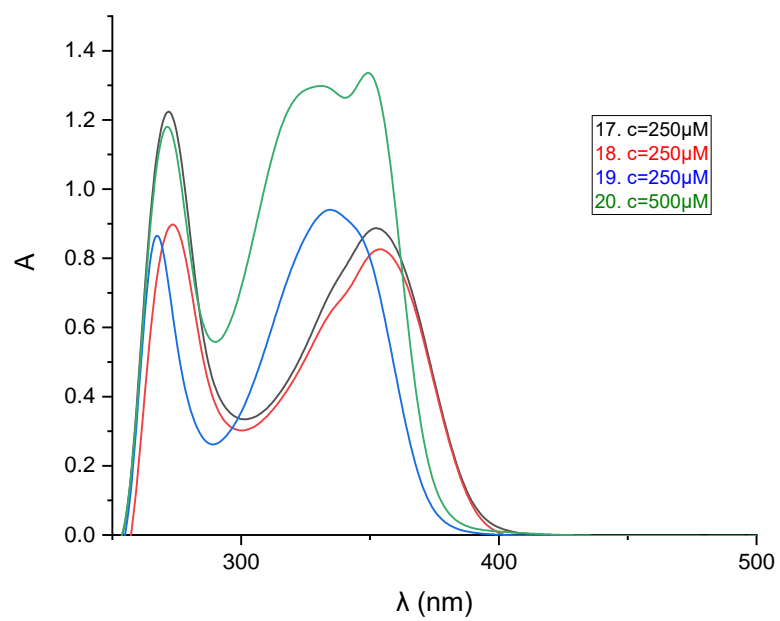
| lane | 312nm, 15cm, 30min, pH=6.8, DMSO, C=5μM | | lane | | |
|------|---|--------------------------|------|--------------|--------------------------|
| 1 | DNA + UV + | Control | 9 | DNA + UV + 9 | air |
| 2 | DNA + UV + 9 | air | 10 | DNA + UV + 9 | argon |
| 3 | DNA + UV + 9 | argon | 11 | DNA + UV + 9 | L-cyst (1500 μM) |
| 4 | DNA + UV + 9 | L-cyst (1500 μM) | 12 | DNA + UV + 9 | KI (250 μM) |
| 5 | DNA + UV + 9 | KI (250 μM) | 13 | DNA + UV + 9 | NaN ₃ (20 mM) |
| 6 | DNA + UV + 9 | NaN ₃ (20 mM) | 14 | DNA + UV + 9 | D ₂ O |
| 7 | DNA + UV + 9 | D ₂ O | 15 | DNA + UV + 9 | DMSO 20% |
| 8 | DNA + UV + 9 | DMSO 20% | 16 | DNA + UV + 9 | air |

Gel S.3.4: Compound 9, mechanistic studies

S.4. UV-vis spectra of AA DACHZs 1-24, in DMSO

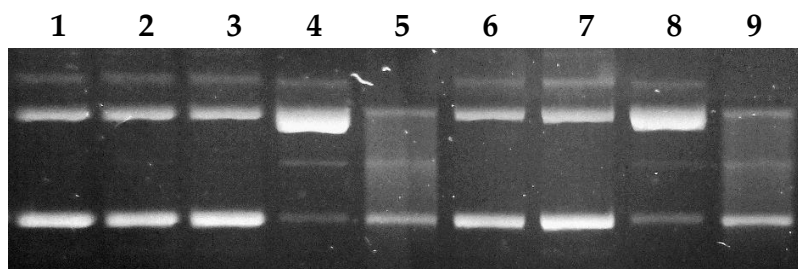






S.5. Gel electrophoresis pictures of compounds 1-24 (UV-A)

S.5.1

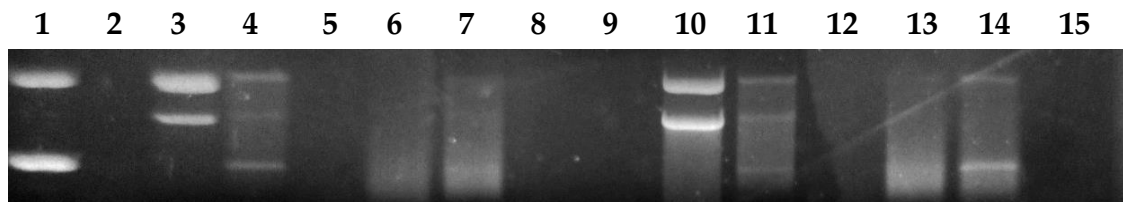


Form II% : 38 33 66 40 38 36 60 37
 Form III%: 12 23 14 24

| lane | 365nm, 10cm, 120min, DMSO, C = 500 μ M | | lane | | |
|------|---|---------|------|------------|---|
| 1 | DNA + UV + | Control | 6 | DNA + UV + | 1 |
| 2 | DNA + UV + | 1 | 7 | DNA + UV + | 2 |
| 3 | DNA + UV + | 2 | 8 | DNA + UV + | 3 |
| 4 | DNA + UV + | 3 | 9 | DNA + UV + | 4 |
| 5 | DNA + UV + | 4 | | | |

Gel S.5.1: Compounds 1-4

S.5.2

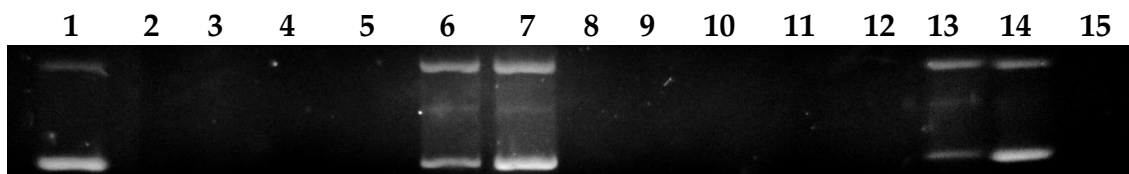


Form II%: 57 49 37 42
 Form III%: 29 23 49 31

| lane | 365nm, 10cm, 120min, DMSO, C = 500 μ M | | lane | | |
|------|---|---------|------|------------|----|
| 1 | DNA + UV + | Control | 9 | DNA + UV + | 5 |
| 2 | DNA + UV + | 5 | 10 | DNA + UV + | 6 |
| 3 | DNA + UV + | 6 | 11 | DNA + UV + | 7 |
| 4 | DNA + UV + | 7 | 12 | DNA + UV + | 8 |
| 5 | DNA + UV + | 8 | 13 | DNA + UV + | 19 |
| 6 | DNA + UV + | 19 | 14 | DNA + UV + | 20 |
| 7 | DNA + UV + | 20 | 15 | DNA + UV + | 9 |
| 8 | DNA + UV + | 9 | | | |

Gel S.5.2: Compounds 5-9 & 19-20

S.5.3

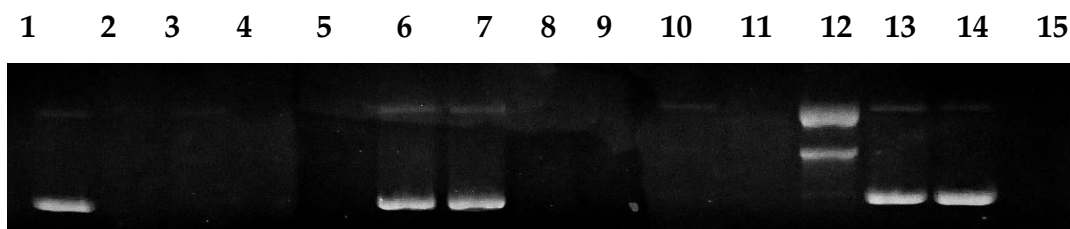


Form II% : 33 30 36 28
Form III%: 27 20 18 9

| lane | 365nm, 10cm, 120min, DMSO, C = 100 μ M | | | | |
|------|---|---------|------|------------|----|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 5 | 9 | DNA + UV + | 5 |
| 3 | DNA + UV + | 6 | 10 | DNA + UV + | 6 |
| 4 | DNA + UV + | 7 | 11 | DNA + UV + | 7 |
| 5 | DNA + UV + | 8 | 12 | DNA + UV + | 8 |
| 6 | DNA + UV + | 19 | 13 | DNA + UV + | 19 |
| 7 | DNA + UV + | 20 | 14 | DNA + UV + | 20 |
| 8 | DNA + UV + | 9 | 15 | DNA + UV + | 9 |

Gel S.5.3: Compounds 5-9 & 19-20

S.5.4

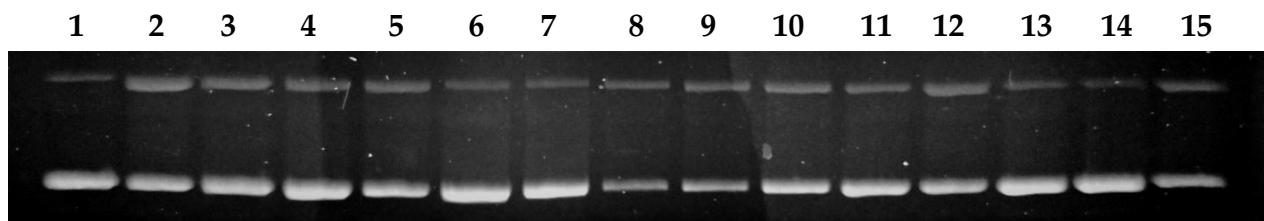


Form II% : 26 25 55 10 5
Form III%: 33

| lane | 365nm, 10cm, 120min, DMSO, C = 10 μ M | | | | |
|------|--|---------|------|------------|----|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 5 | 9 | DNA + UV + | 5 |
| 3 | DNA + UV + | 6 | 10 | DNA + UV + | 6 |
| 4 | DNA + UV + | 7 | 11 | DNA + UV + | 7 |
| 5 | DNA + UV + | 8 | 12 | DNA + UV + | 8 |
| 6 | DNA + UV + | 19 | 13 | DNA + UV + | 19 |
| 7 | DNA + UV + | 20 | 14 | DNA + UV + | 20 |
| 8 | DNA + UV + | 9 | 15 | DNA + UV + | 9 |

Gel S.5.4: Compounds 5-9 & 19-20

S.5.5

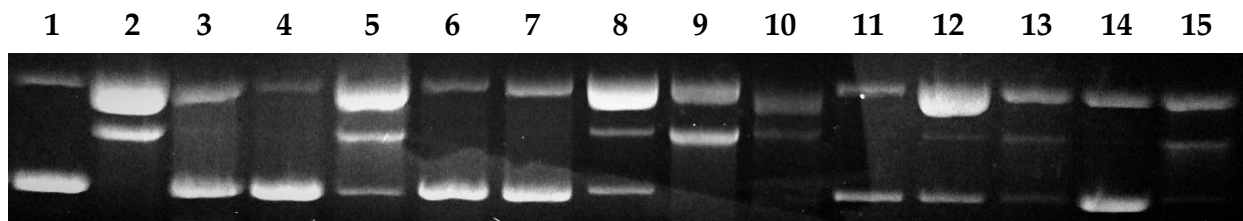


Form II% : 33 27 23 27 19 19 32 33 29 22 31 17 12 24
Form III%:

| lane | 365nm, 10cm, 120min, DMSO, C = 500 nM | | | | |
|------|--|---------|------|------------|----|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 5 | 9 | DNA + UV + | 5 |
| 3 | DNA + UV + | 6 | 10 | DNA + UV + | 6 |
| 4 | DNA + UV + | 7 | 11 | DNA + UV + | 7 |
| 5 | DNA + UV + | 8 | 12 | DNA + UV + | 8 |
| 6 | DNA + UV + | 19 | 13 | DNA + UV + | 19 |
| 7 | DNA + UV + | 20 | 14 | DNA + UV + | 20 |
| 8 | DNA + UV + | 9 | 15 | DNA + UV + | 9 |

Gel S.5.5: Compounds 5-9 & 19-20

S.5.6

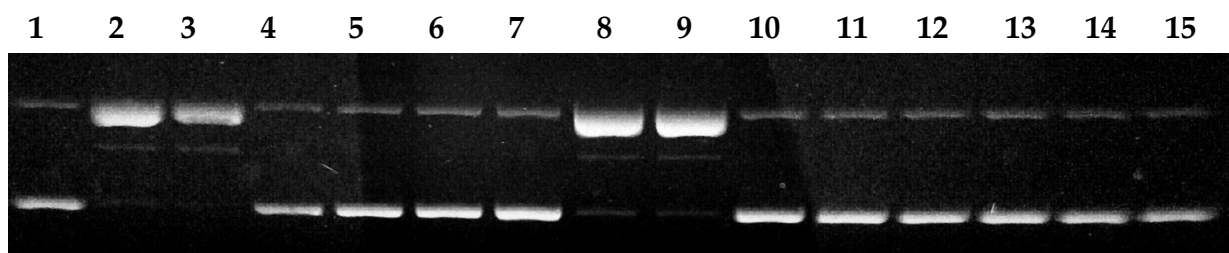


Form II% : 65 36 20 57 30 37 69 44 55 48 75 43 31 64
Form III%: 20 25 10 38 17 7 12 28

| lane | 365nm, 10cm, 120min, DMSO, C = 10 μ M | | | | |
|------|--|---------|------|------------|----|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 10 | 9 | DNA + UV + | 10 |
| 3 | DNA + UV + | 11 | 10 | DNA + UV + | 11 |
| 4 | DNA + UV + | 12 | 11 | DNA + UV + | 12 |
| 5 | DNA + UV + | 13 | 12 | DNA + UV + | 13 |
| 6 | DNA + UV + | 14 | 13 | DNA + UV + | 14 |
| 7 | DNA + UV + | 15 | 14 | DNA + UV + | 15 |
| 8 | DNA + UV + | 16 | 15 | DNA + UV + | 16 |

Gel S.5.6: Compounds 10-16

S.5.7

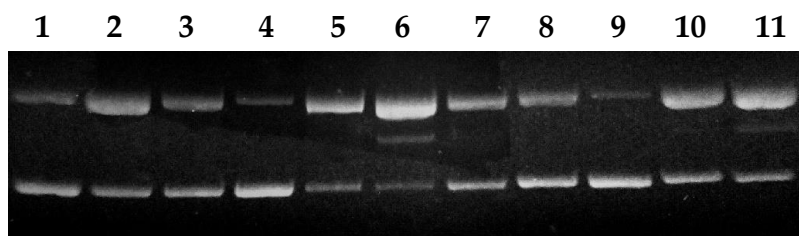


Form II% : 81 75 23 21 23 23 86 84 21 20 21 19 17 16
 Form III%: 11 14 9 11

| lane | 365nm, 10cm, 120min, DMSO, C = 10 μ M | | | | |
|------|--|---------|------|------------|----------------|
| 1 | DNA + UV + | Control | lane | | |
| 2 | DNA + UV + | 17 | 9 | DNA + UV + | 18 |
| 3 | DNA + UV + | 18 | 10 | DNA + UV + | 21 |
| 4 | DNA + UV + | 21 | 11 | DNA + UV + | 22 |
| 5 | DNA + UV + | 22 | 12 | DNA + UV + | 23 |
| 6 | DNA + UV + | 23 | 13 | DNA + UV + | 24 |
| 7 | DNA + UV + | 24 | 14 | DNA + UV + | 21 (5 μ M) |
| 8 | DNA + UV + | 17 | 15 | DNA + UV + | 22 (5 μ M) |

Gel S.5.7: Compounds 17-18 & 21-24

S.5.8

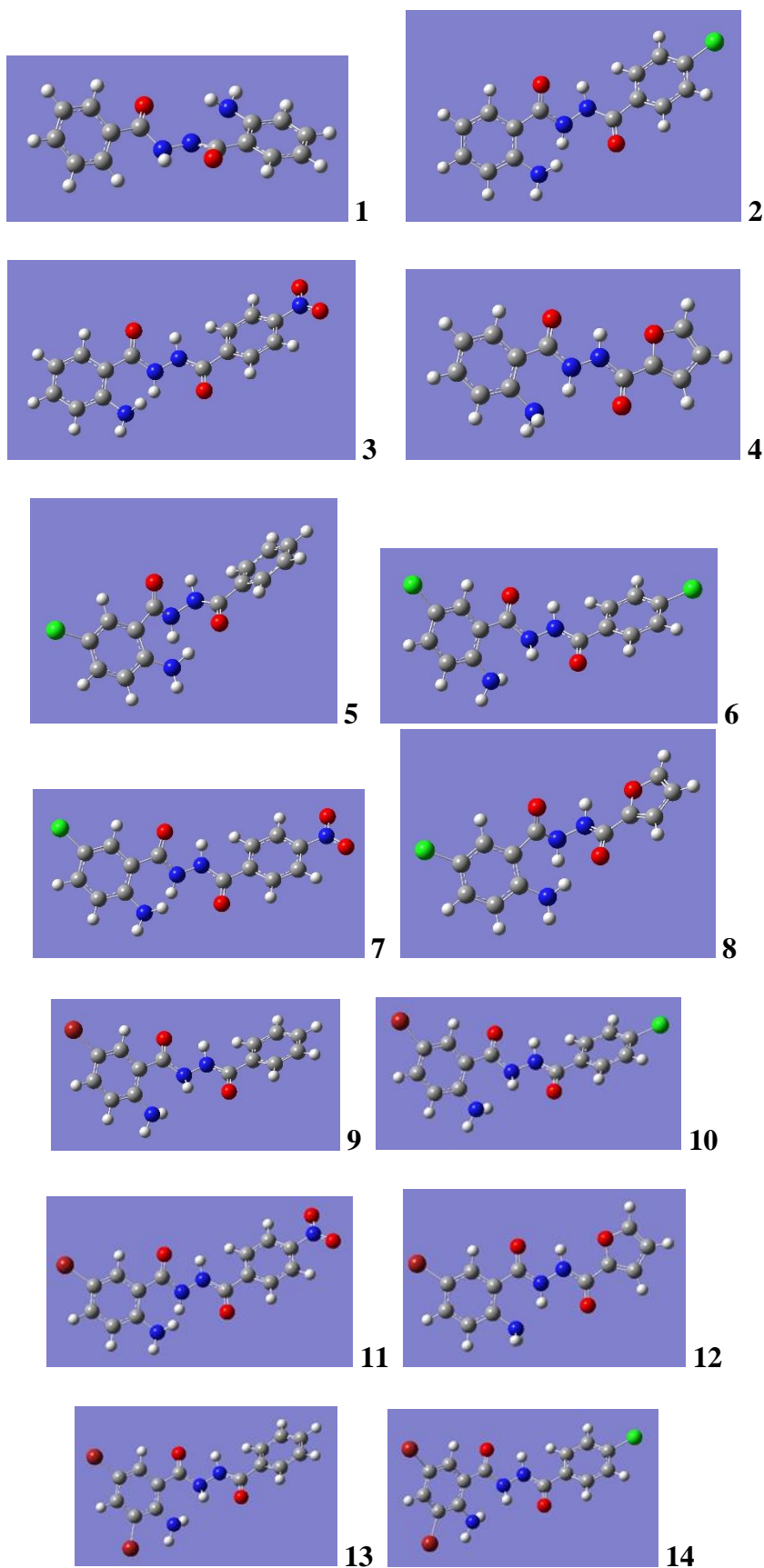


Form II%: 57 39 18 60 64 49 39 21 57 59
 Form III%: 15 11

| lane | 365nm, 10cm, 120min, DMSO, C = 2 μ M | | | | |
|------|---|---------|----|------------|---|
| 1 | DNA + UV + | Control | | | |
| 2 | DNA + UV + | 5 | 7 | DNA + UV + | 5 |
| 3 | DNA + UV + | 6 | 8 | DNA + UV + | 6 |
| 4 | DNA + UV + | 7 | 9 | DNA + UV + | 7 |
| 5 | DNA + UV + | 8 | 10 | DNA + UV + | 8 |
| 6 | DNA + UV + | 9 | 11 | DNA + UV + | 9 |

Gel S.5.8: Compounds 5-9

S.6. Optimized molecular geometries of compounds 1-24 at B3LYP/6-31g* level

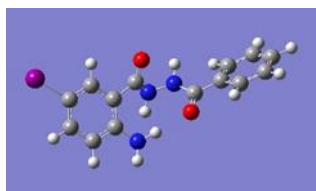




15



16



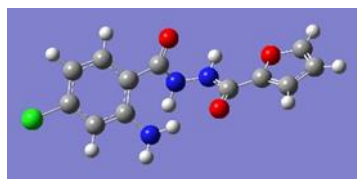
17



18



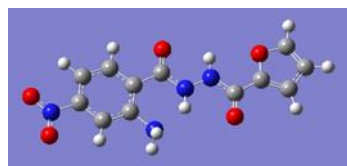
19



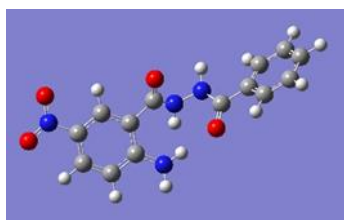
20



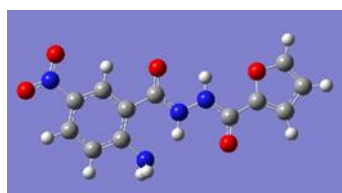
21



22

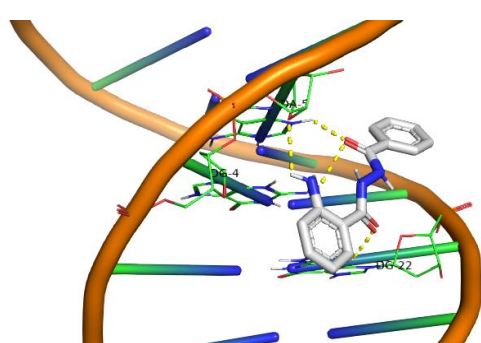


23

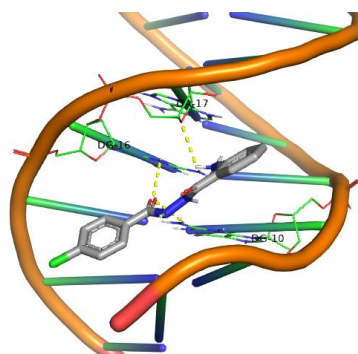


24

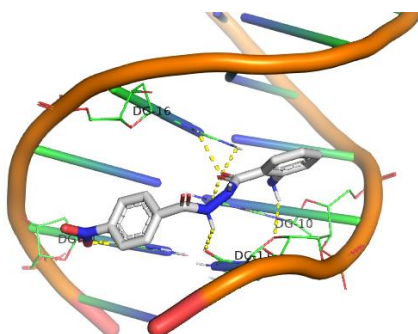
S.7. Molecular Docking Studies for the compounds 1-24



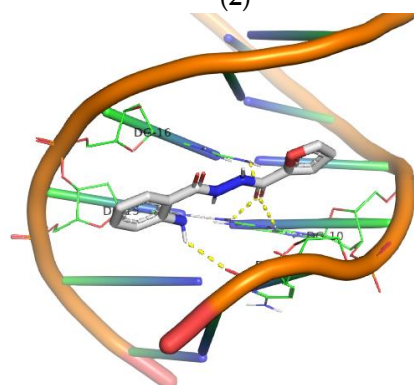
(1)



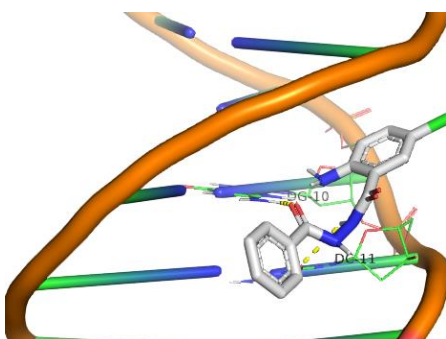
(2)



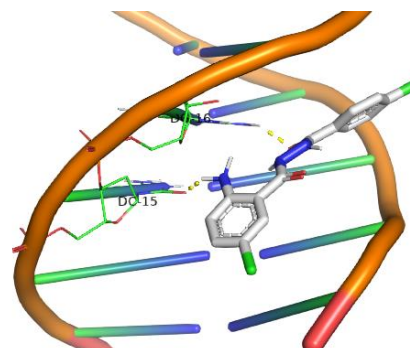
(3)



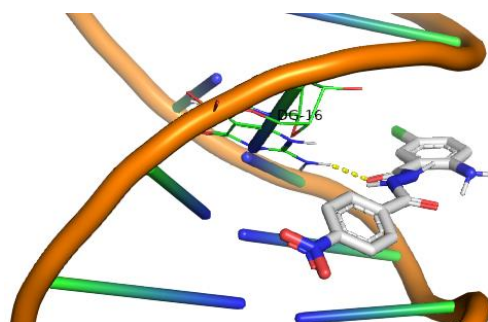
(4)



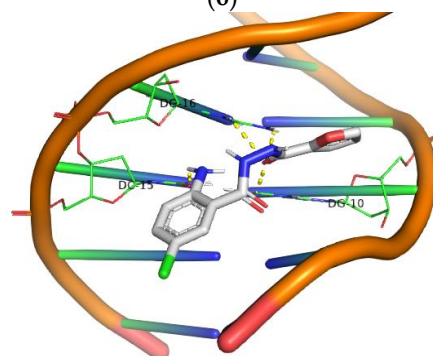
(5)



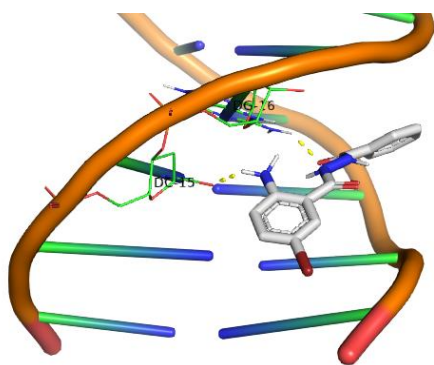
(6)



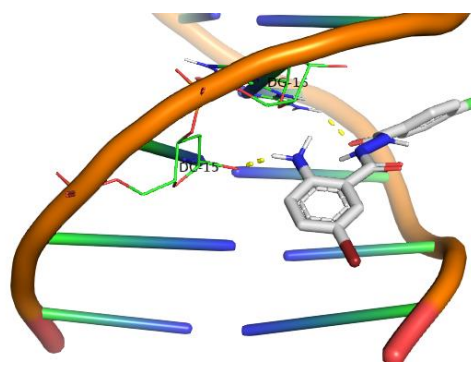
(7)



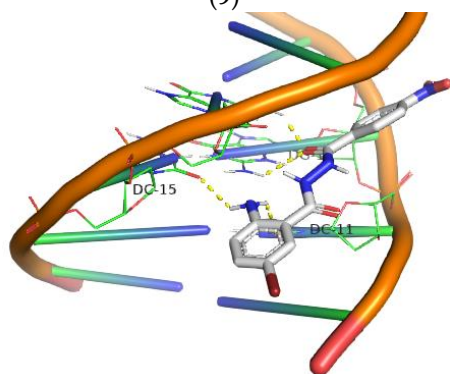
(8)



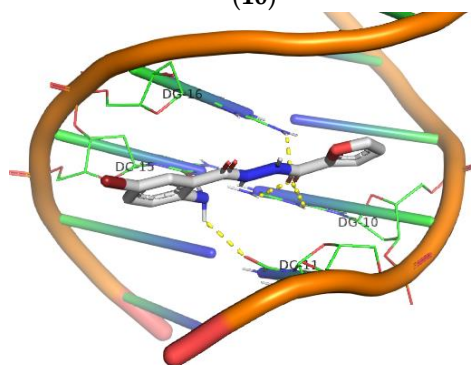
(9)



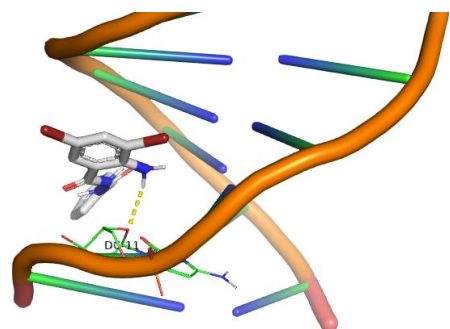
(10)



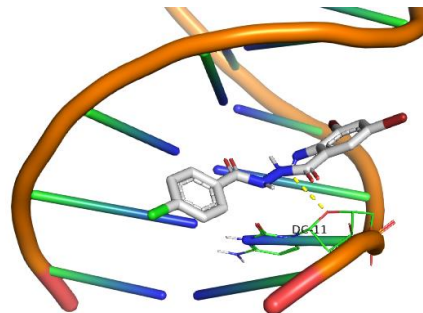
(11)



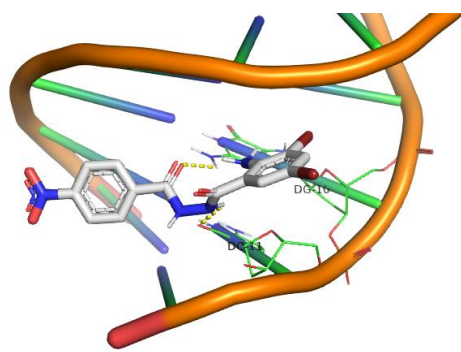
(12)



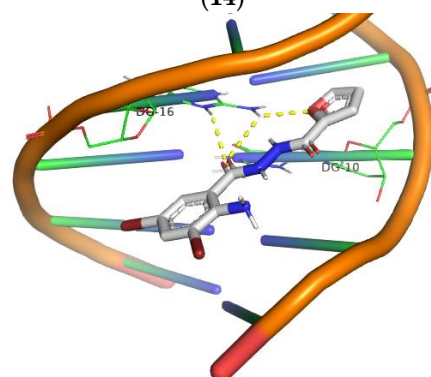
(13)



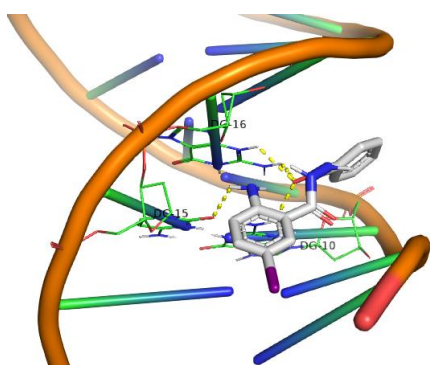
(14)



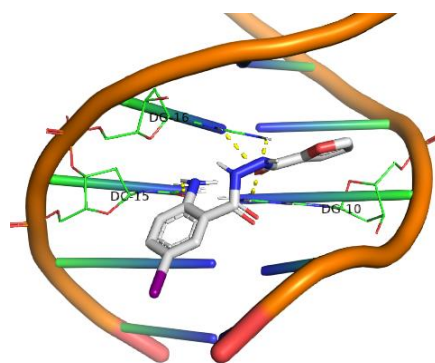
(15)



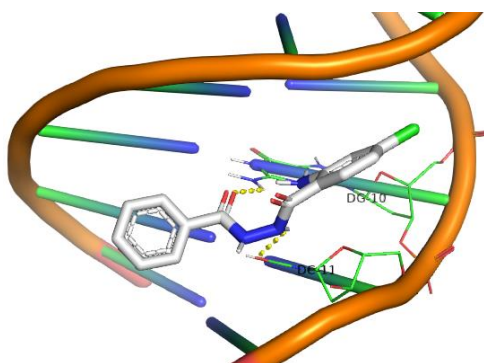
(16)



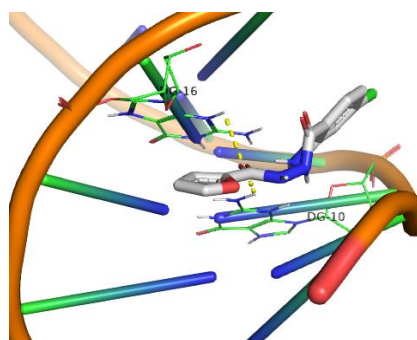
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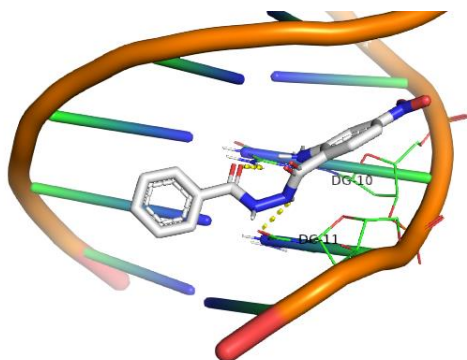
(18)



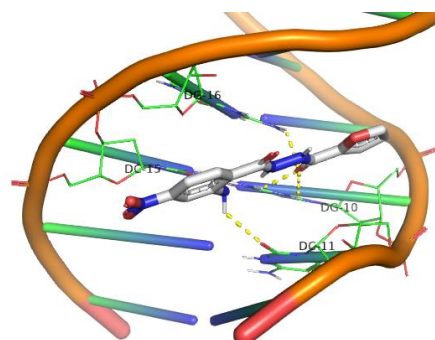
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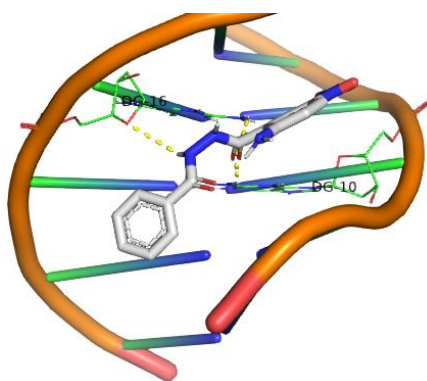
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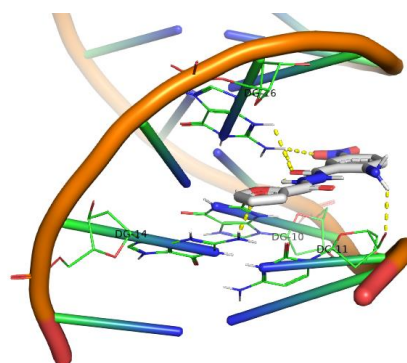
(21)



(22)



(23)



(24)