

Synthesis of symmetric bis(N-alkylaniline)triarylmethanes via Friedel-Crafts catalyzed reaction between secondary anilines and aldehydes

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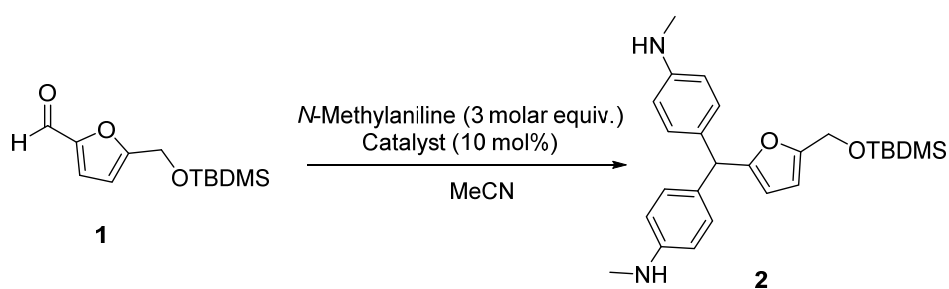
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Complete data of catalyst screening for TRAM formation



Entry	Catalyst	Conversion (%) ^a	Yield 2 (%) ^a
1	-	50	NO
2	BaCl ₂	52	NO
3	Ti(O ⁱ Pr) ₄	50	NO
4	FeCl ₃ ·6H ₂ O	93	Traces
5	RuCl ₃ ·xH ₂ O	94	6
6	NiCl ₂	60	12
7	Dy(OTf) ₃	91	15
8	ZnI ₂	55	17
9	AgOTf	61	19
10	CeCl ₃	63	24
11	ZrCl ₄	76	26
12	CoCl ₂ ·6H ₂ O	58	29
13	<i>p</i> TSOH	67	33
14	Cu(OTf) ₂	67	41
15	GdCl ₃ ·6H ₂ O	88	50
16	ZrCl ₄	82	52
17	Yb(OTf) ₃	100	61
18	LaCl ₃ ·7H ₂ O	100	72
19	AlCl ₃	94	82

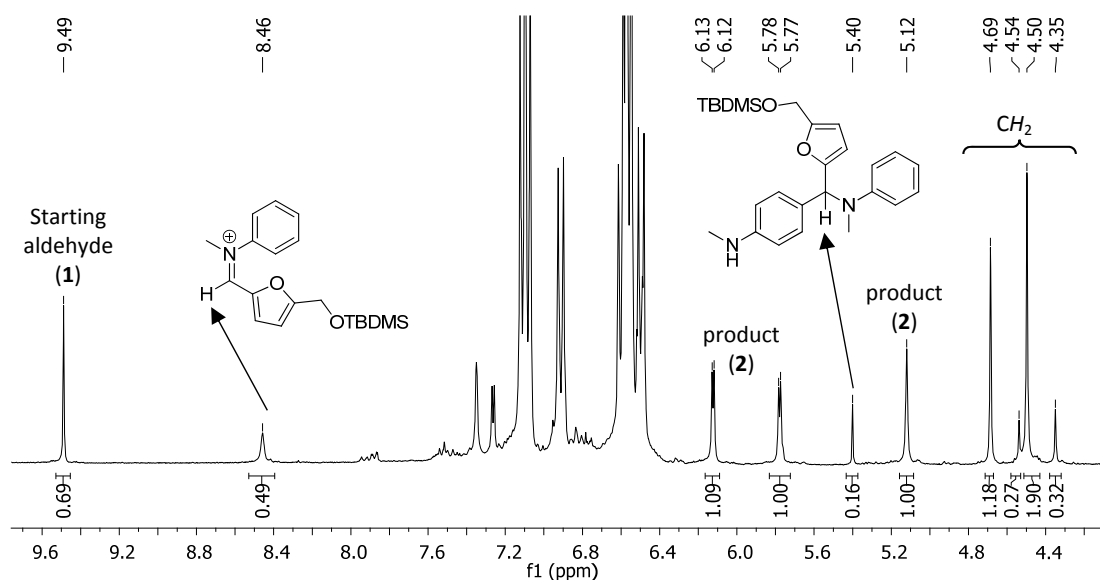
^aDetermined by HPLC analysis of crude reaction mixture.

NO = Not observed by HPLC analysis.

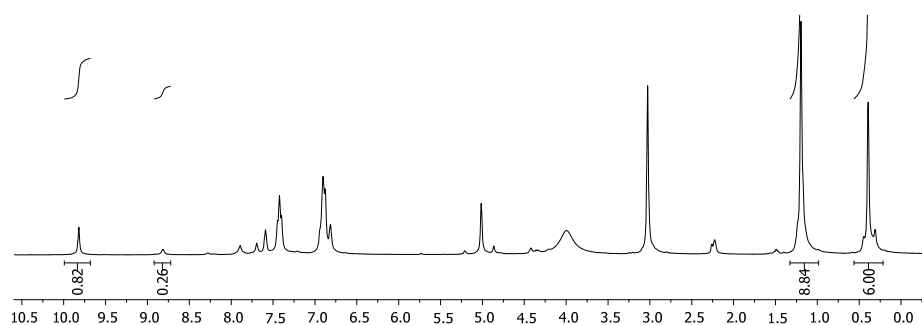
Protocol for stability of **2.** To a solution of **2** (54.5 mg, 0.125 mmol) in anhydrous acetonitrile (0.1 M), *N*-methylaniline (40 μ L, 3 equiv.) was added followed by the addition of Yb(OTf)₃ (10 mol%) in one portion. The reaction mixture was allowed to stir at 40 °C for 48 h under argon atmosphere. The solvent was then evaporated and the crude reaction mixture was filtered through a small pad of silica gel. The solvent was evaporated and hexane/2-propanol was used to dilute the mixture to the appropriate concentration for HPLC analysis.

Study of the reaction by NMR.

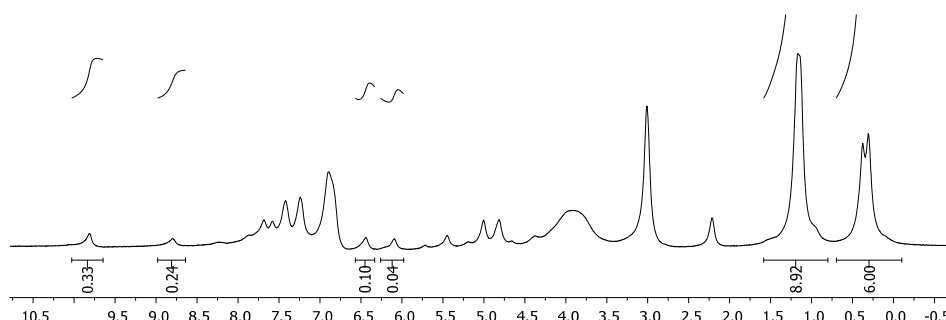
Protocol: The general protocol was followed using anhydrous acetonitrile- d_3 (dried under molecular sieves for overnight). For the time described in the next spectra, the reaction mixture was transfer from the round bottom flask to the NMR tube, and then back again to the flask, under argon atmosphere. Although the reaction was very slow and full conversion was not achieved after 4 days, plausible intermediates were observed as depicted bellow (the chemical shifts are in agreement with similar structures from iminium-ions¹ and tertiary anilines²)



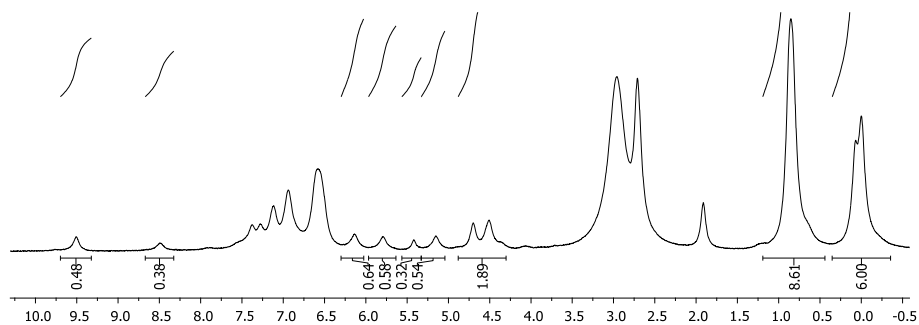
After 4 h:



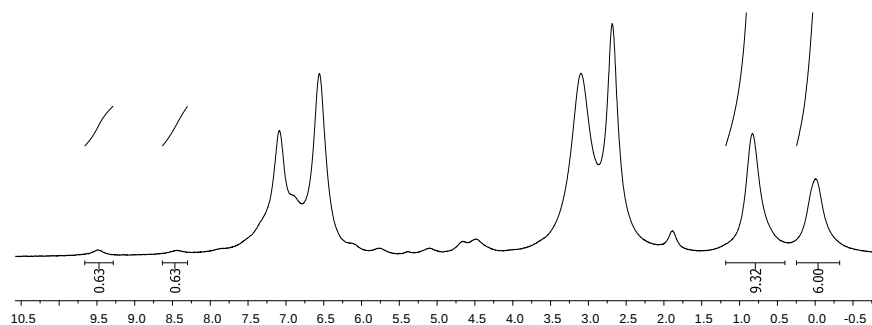
After 23 h:



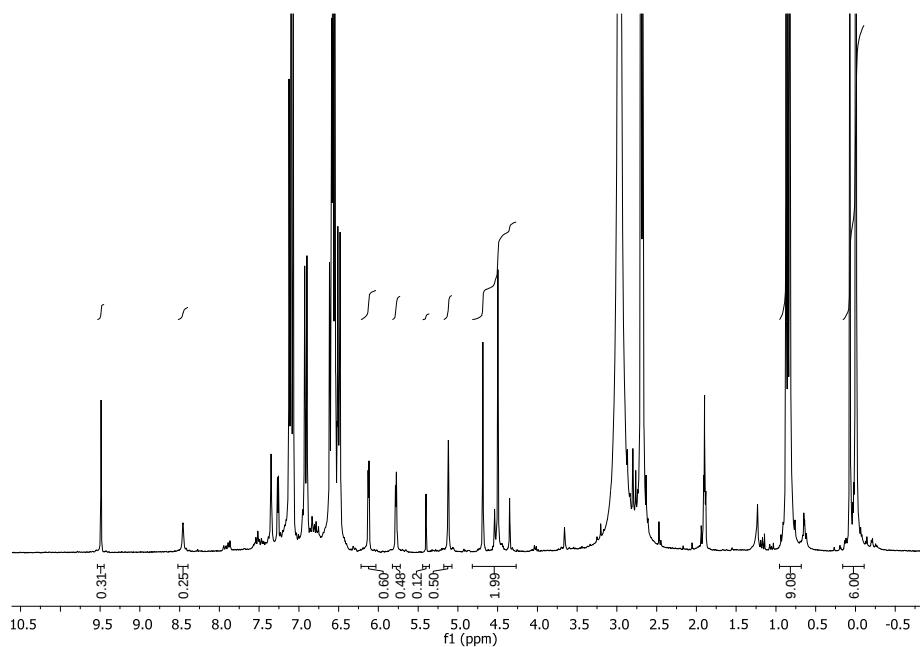
After 3 days:



After 5 days:

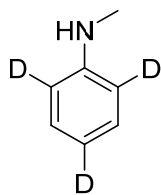


After filtration through a pad of celite and 1 week in the freezer:



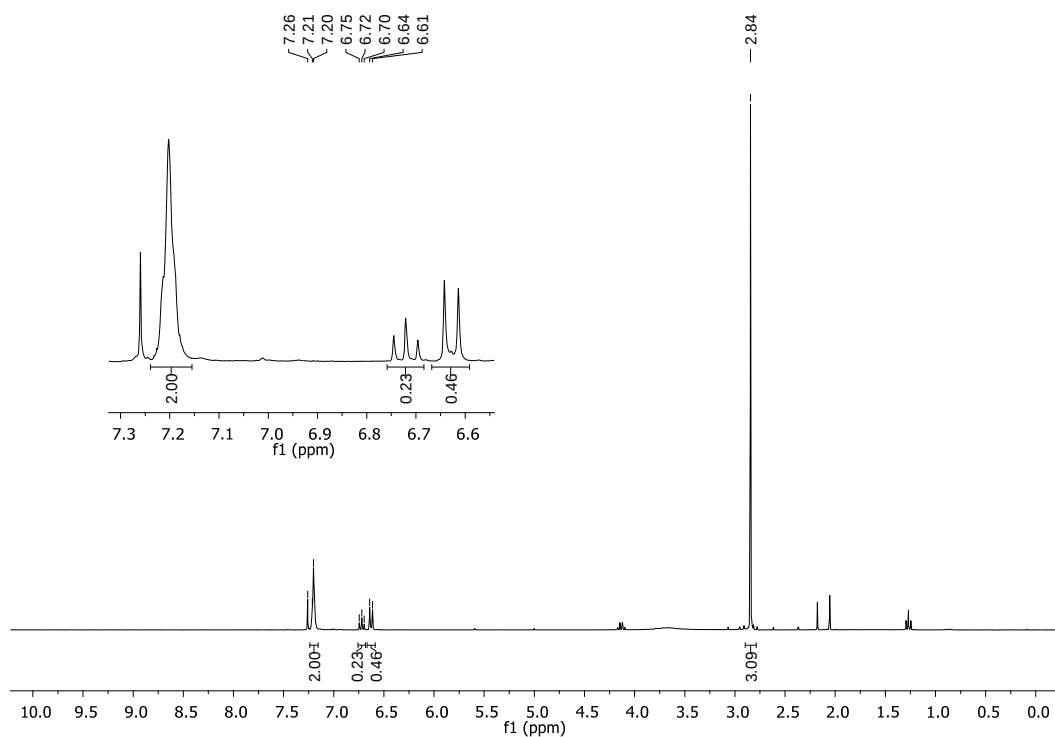
Kinetic isotope effect determination

Preparation of *N*-methylaniline-2,4,6-*d*₃



Acetyl chloride (1.5 mL) was slowly added to deuterium oxide (0.5 mL) with vigorous stirring at 0 °C. After 2 hours, *N*-methylaniline (0.2 mL) was slowly added and the reaction mixture was allowed to stir for 1 day at reflux. The reaction mixture was diluted and neutralized with NaHCO₃ sat. aq. solution and extracted with EtOAc.

After careful solvent evaporation (40 °C, 150 mbar) the product was purified by column chromatography using hexane/EtOAc to give the desired *N*-methylaniline with 80% D incorporation in *ortho* and *para* positions to the nitrogen (quantitative yield). **HRMS (ESI)**: *m/z* calculated for C₇H₇D₃N [M+H⁺] 111.09961, found 111.09903.



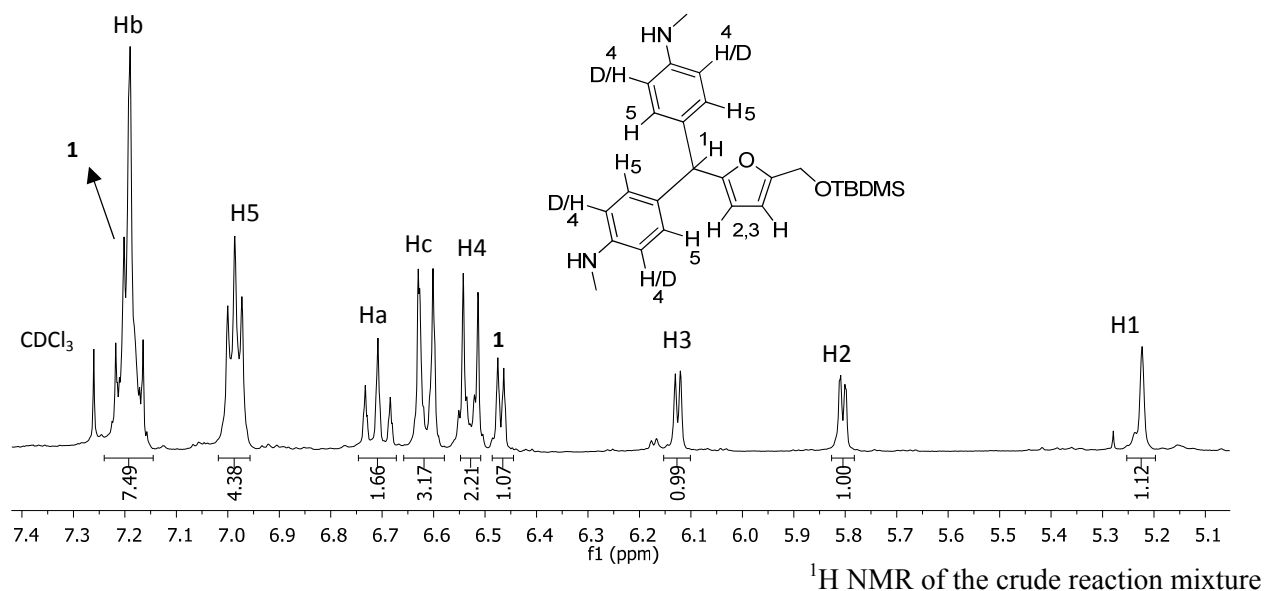
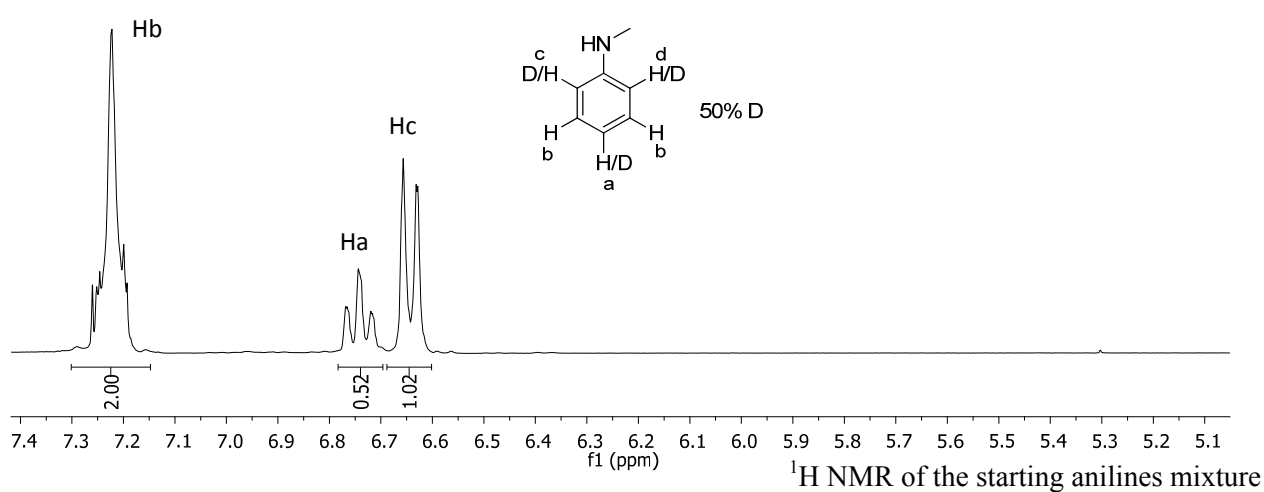
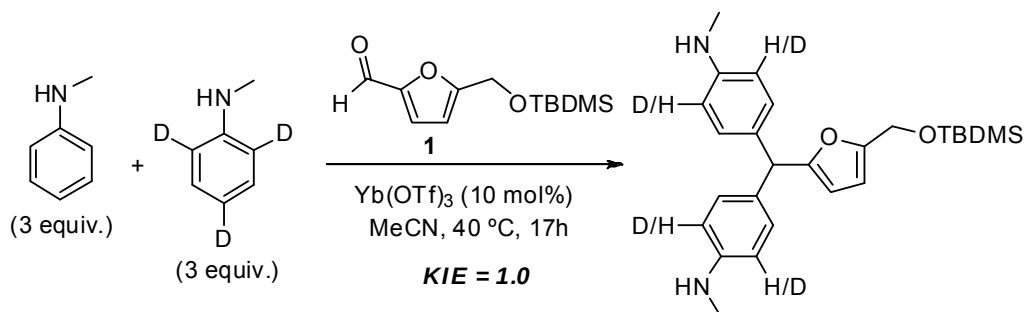
Protocol for intermolecular competition

To a 1:1 mixture of *N*-methylaniline and *N*-methylaniline-2,4,6-*d*₃ (6 equiv., ratio analyzed by ¹H NMR) and **1** (30 mg, 0.127 mmol, 1 equiv.) in anhydrous acetonitrile (1.3 mL, 0.1 M), Yb(OTf)₃ (10 mol%) was added. The reaction mixture was allowed to stir at 40 °C for 17 h under argon atmosphere. The solvent was evaporated and the crude reaction mixture was filtered through a pad of celite and analyzed by ¹H NMR.

Product **2-d4** was obtained from the reaction of *N*-methylaniline-2,4,6-*d*₃ (80% D) – **HRMS (ESI)**: *m/z* calculated for C₂₆H₃₂D₄N₂O₂Si [M+H⁺] 440.27971, found 440.27916.

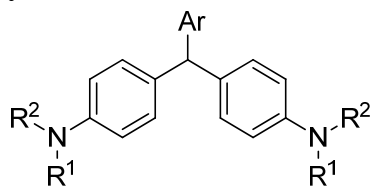
KIE determination

$$KIE = \frac{P_H}{P_D} = \frac{A(H4)}{A(H5) - A(H4)} = \frac{2.21}{(4.38 - 2.21)} = 1.02$$



Intermolecular competition reaction of *N*-methylaniline and *N*-methylaniline-2,4,6- d_3 for kinetic isotope effect study.

Complete data of biological activity of the new TRAM derivatives



Entry	Ar	R ¹	R ²	IC ₅₀ (μM)			
				NCI-H460	MCF-7	HT-29	CHOK1
1	2-furyl-5-CH ₂ OH	Me	H	>20	>20	>20	ND
2	Ph	Me	H	>20	>20	5.1 ± 3.3	>20
3	4-MeC ₆ H ₄	Me	H	>20	7.81 ± 1.02	1.74 ± 2.32	14.55 ± 1.06
4	4-OMeC ₆ H ₄	Me	H	>15	12.44 ± 1.11	12.80 ± 1.12	>20
5	4-NO ₂ C ₆ H ₄	Me	H	>20	12.08 ± 1.04	7.97 ± 3.13	>20
6	2-OHC ₆ H ₄	Me	H	>15	>15	>15	ND
7	2,4-Cl ₂ C ₆ H ₃	Me	H	13.85 ± 1.06	11.53 ± 1.07	10.77 ± 1.09	≥20
8	3-BrC ₆ H ₄	Me	H	11.25 ± 1.05	10.37 ± 1.05	12.66 ± 1.06	≥20
9	2-F,3-ClC ₆ H ₃	Me	H	12.91 ± 2.22	8.14 ± 1.03	9.52 ± 2.89	15.16 ± 1.05
10	4-FC ₆ H ₄	Me	H	21.58 ± 4.55	11.34 ± 1.05	10.71 ± 5.34	>20
11	4-ClC ₆ H ₄	Me	H	11.32 ± 2.62	9.16 ± 1.07	13.34 ± 3.14	10.60 ± 1.04
12	4-(CF ₃)C ₆ H ₄	Me	H	9.53 ± 1.02	8.07 ± 1.20	8.78 ± 1.15	10.16 ± 1.04
13	4-MeC ₆ H ₄	Bn	H	>20	>20	>20	ND
14	2-pyridyl	Me	H	>20	>20	>20	ND
15	4-(CHO)C ₆ H ₄	Me	H	>20	>20	>20	ND
16	4-(CH(MeNHC ₆ H ₄) ₂)C ₆ H ₄	Me	H	>20	>20	>20	ND

ND = Not determined

DFT calculations

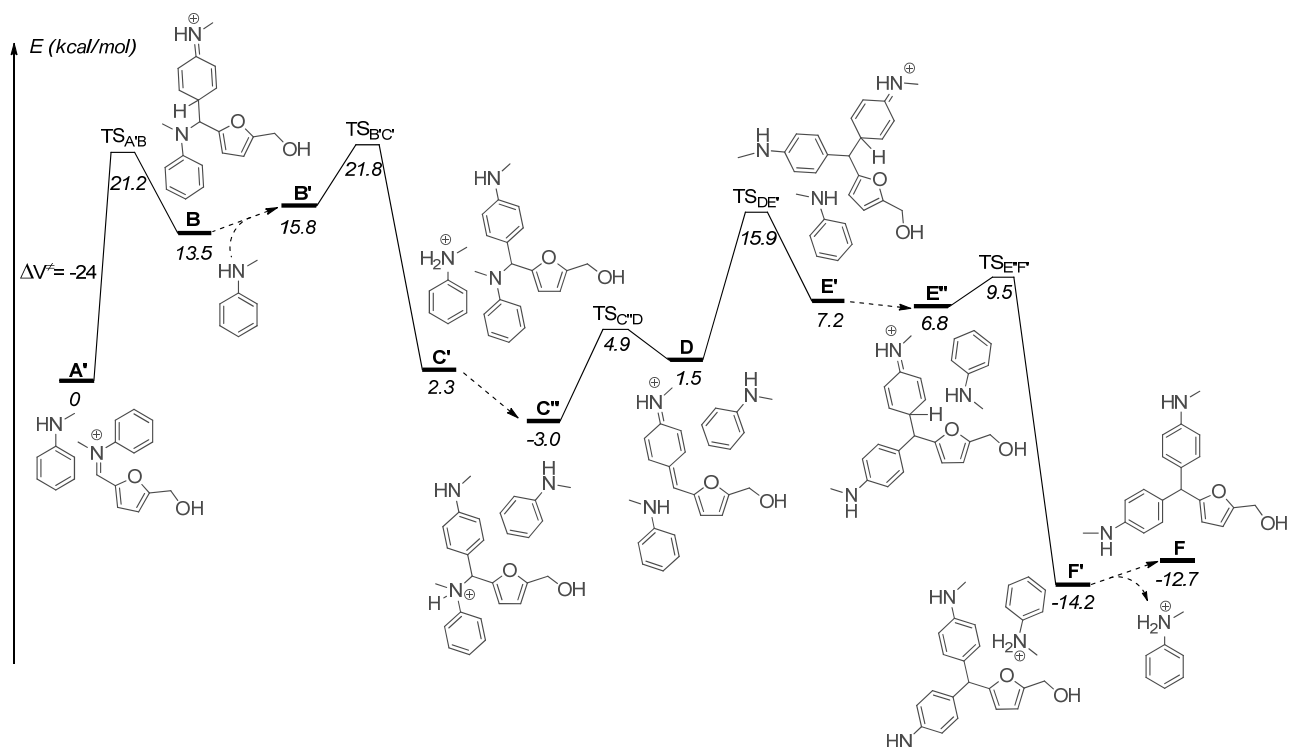
Computational Details

All calculations were performed using the Gaussian 09 software package.³ The optimized geometries were obtained using M06-2X functional and a standard 6-31G(d,p) basis set,⁴⁻⁸ without symmetry constraints, with solvent effects (acetonitrile) calculated by means of the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers,⁹⁻¹² with radii and non-electrostatic terms of the SMD solvation model, developed by Truhler *et al.*¹³ M06-2X is a hybrid meta-GGA functional developed by Truhlar and Zhao,¹⁴ and it was shown to perform very well for main-group kinetics, providing a good description of long range effects such as van der Waals interactions or π - π stacking.¹⁵⁻¹⁶

Transition state optimizations were performed with the Synchronous Transit-Guided Quasi-Newton Method (STQN) developed by Schlegel *et al.*,¹⁷⁻¹⁸ following extensive searches of the potential energy surface. Frequency calculations were performed to confirm the nature of the stationary points, yielding one imaginary frequency for the transition states and none for the minima. Each transition state was further confirmed by following its vibrational mode downhill on both sides and obtaining the minima presented on the energy profile.

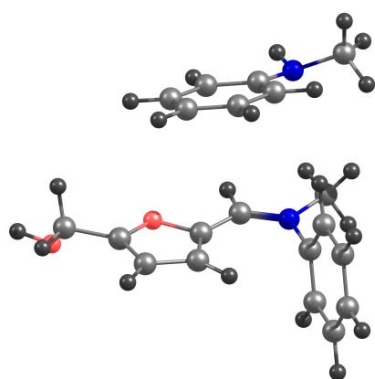
The electronic energies obtained at the M06-2X/6-31G(d,p) level of theory were converted to free energy (values presented) at 298.15 K and 1 atm by using zero point energy and thermal energy corrections based on structural and vibration frequency data calculated at the same level.

Molar volumes were determined at the M06-2X/6-31G(d,p) level of theory, without symmetry constraints, with solvent effects (acetonitrile) calculated by means of the Polarizable Continuum Model (PCM), using the keyword *Volume* and the option *tight* for an increased accuracy.

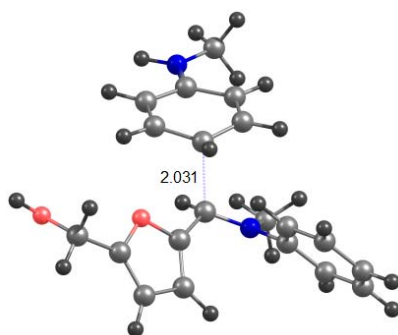


Free energy profile (kcal.mol⁻¹) calculated for the reaction of N-methyl aniline and 5-hydroxymethylfurfural. The minima and the transition states were optimized and the energy values are referred to A' after thermal correction to Gibbs Free Energy in acetonitrile.

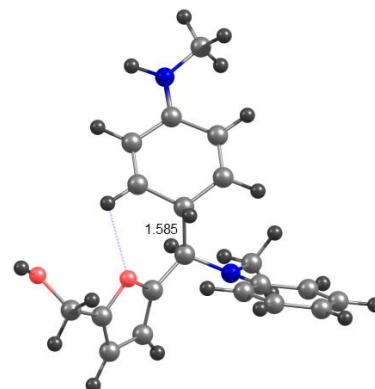
Energies (sum of electronic and thermal Free Energies) and molar volume of all the optimized species



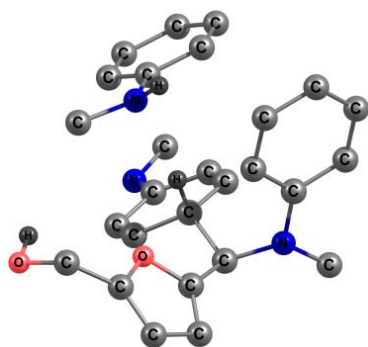
A'
-1035.004811 H
271.885 cm³mol⁻¹



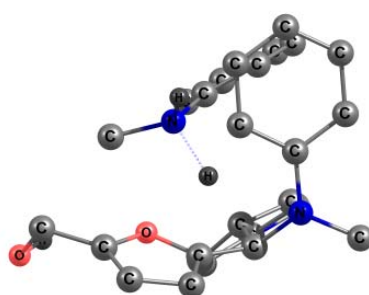
TSA'B
-1034.971059 H
247.738 cm³mol⁻¹



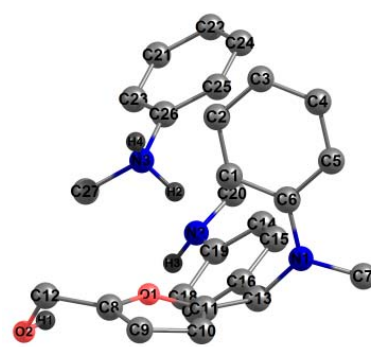
B
-1034.983373 H



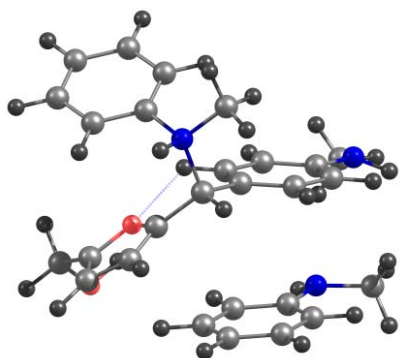
B'
-1361.646098 H
309.059 cm³mol⁻¹



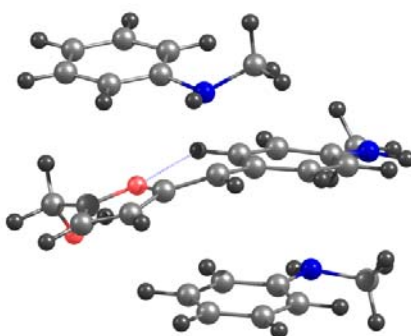
TSB'C'
-1361.636553 H
344.694 cm³mol⁻¹



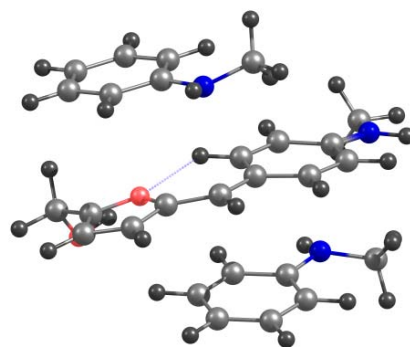
C'
-1361.667638 H



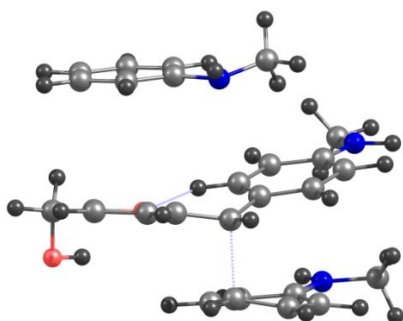
C''
-1361.676133 H
330.708 cm³mol⁻¹



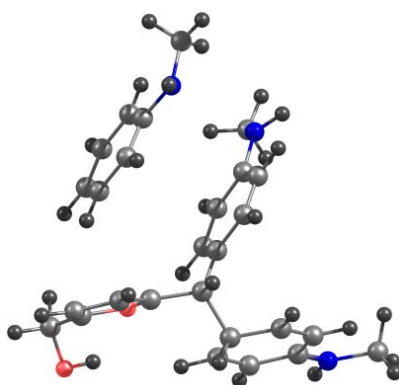
TSC''D
-1361.663525 H
348.658 cm³mol⁻¹



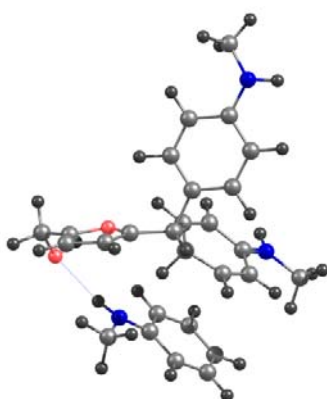
D
-1361.669099 H
334.277 cm³mol⁻¹



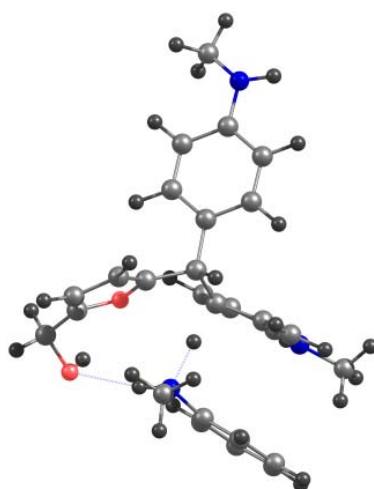
TSDE'
-1361.646084 H
335.595 cm³mol⁻¹



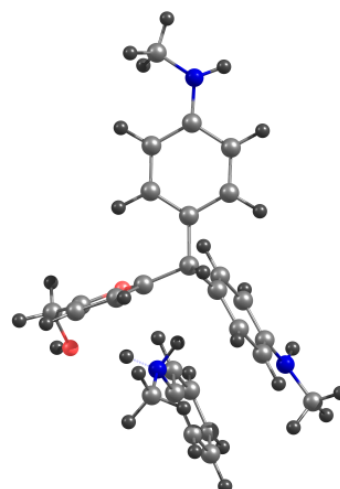
E'
-1361.659923 H



E''
-1361.660518 H
328.266 cm³mol⁻¹



TSE''F'
-1361.656243 H
329.311 cm³mol⁻¹



F'
-1361.69408 H

Atomic coordinates for all the optimized species

A'

6	-3.417551000	-2.095671000	1.997738000
6	-3.533725000	-2.594381000	3.292655000
6	-4.792606000	-2.750203000	3.872172000
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6	-4.479504000	1.095905000	0.781277000
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1	-6.724054000	-1.639345000	1.291951000
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TSA'B

6	-3.545735000	-0.951134000	2.704543000
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1	-4.785920000	5.379731000	1.923030000
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B

6	-3.779506000	-0.549771000	2.673983000
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6	-4.156933000	-3.164666000	3.528242000
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6	-3.790084000	4.503949000	1.862255000
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6	-4.334584000	0.093008000	-0.138435000
6	-1.700053000	-1.526418000	-1.913214000
6	-2.302435000	-1.245257000	-0.745660000
6	-2.764679000	0.114802000	-0.358361000
6	-2.402686000	1.169723000	-1.346437000
6	-1.811425000	0.899410000	-2.520952000
6	-1.461190000	-0.463511000	-2.867107000
7	-0.922310000	-0.708082000	-4.030969000
6	-0.508340000	-2.019031000	-4.521339000
1	-3.614797000	0.480197000	2.384523000
1	-2.909008000	-0.207861000	4.593834000
1	-3.242730000	-2.548300000	5.384345000
1	-4.307643000	-4.193373000	3.842870000
1	-5.012634000	-3.537962000	1.610333000
1	-6.228861000	-2.624156000	0.122784000
1	-5.695094000	-1.696027000	-1.280720000
1	-4.622298000	-2.925402000	-0.574829000
1	-6.704774000	3.666875000	1.908230000
1	-6.991222000	1.174240000	0.767620000
1	-2.997007000	4.183138000	2.550959000
1	-4.445529000	5.198808000	2.402231000
1	-2.594663000	5.752281000	0.977449000
1	-4.762374000	0.070298000	-1.144558000
1	-1.386449000	-2.536089000	-2.150263000
1	-2.472695000	-2.045971000	-0.029869000
1	-2.301801000	0.364912000	0.608417000
1	-2.649340000	2.197229000	-1.097403000
1	-1.576338000	1.683442000	-3.234511000
1	-0.772869000	0.083963000	-4.651245000
1	0.270533000	-2.433734000	-3.877672000
1	-0.116447000	-1.889087000	-5.527493000
1	-1.363334000	-2.697715000	-4.547097000

B'

6	-1.615730000	1.988743000	-0.651407000
6	-1.467148000	2.850525000	-1.733108000
6	-0.912911000	4.119796000	-1.574607000
6	-0.501610000	4.508431000	-0.302562000
6	-0.639138000	3.656219000	0.789732000
6	-1.209775000	2.375764000	0.641402000
7	-1.377175000	1.533453000	1.747150000
6	-1.023116000	2.051988000	3.060109000
6	-3.727798000	-1.569636000	-0.533220000
6	-4.594692000	-1.258012000	0.464516000
6	-3.832152000	-0.573116000	1.467637000

6	-2.554847000	-0.518285000	1.008559000
8	-2.478635000	-1.119265000	-0.213119000
6	-3.844010000	-2.295861000	-1.829634000
8	-3.100793000	-3.504355000	-1.844667000
6	-1.304422000	0.080920000	1.603111000
6	2.345696000	-0.250948000	1.661870000
6	1.190729000	0.335535000	1.294627000
6	-0.016335000	-0.413249000	0.857894000
6	0.142421000	-1.890566000	0.940865000
6	1.292428000	-2.486557000	1.298458000
6	2.453623000	-1.690016000	1.635193000
7	3.584311000	-2.292768000	1.901459000
6	4.839895000	-1.628015000	2.227200000
1	-2.058765000	1.016511000	-0.824983000
1	-1.799392000	2.518724000	-2.713264000
1	-0.804883000	4.788622000	-2.421927000
1	-0.057408000	5.487688000	-0.149200000
1	-0.289080000	3.991894000	1.758132000
1	-1.512514000	3.015394000	3.222068000
1	-1.386982000	1.360974000	3.821420000
1	0.060323000	2.186954000	3.199911000
1	-5.649035000	-1.494470000	0.483940000
1	-4.184646000	-0.173934000	2.408413000
1	-3.540344000	-1.636822000	-2.654550000
1	-4.893277000	-2.558808000	-1.981952000
1	-2.164000000	-3.270105000	-1.793660000
1	-1.238010000	-0.302539000	2.624332000
1	3.206298000	0.343700000	1.943584000
1	1.135648000	1.421160000	1.282658000
1	-0.161826000	-0.171293000	-0.216368000
1	-0.713150000	-2.506042000	0.677880000
1	1.388417000	-3.567732000	1.327761000
1	3.594712000	-3.308170000	1.860199000
1	5.110628000	-0.932869000	1.427938000
1	5.608637000	-2.391814000	2.321932000
1	4.748869000	-1.083555000	3.169953000
6	3.839460000	-0.883518000	-1.306024000
6	4.337474000	0.398252000	-1.078856000
6	2.533832000	-1.080257000	-1.752596000
6	3.501803000	1.496001000	-1.301903000
7	0.370574000	-0.132699000	-2.347478000
6	2.194408000	1.316812000	-1.731657000
6	1.690862000	0.021766000	-1.971232000
6	-0.150528000	-1.414755000	-2.764015000
1	4.474957000	-1.749594000	-1.137526000
1	5.359769000	0.541887000	-0.743774000
1	2.173026000	-2.088165000	-1.927574000
1	3.870987000	2.503642000	-1.133358000
1	-0.061390000	0.682054000	-2.762356000
1	1.542673000	2.173197000	-1.894579000
1	-1.189035000	-1.280999000	-3.072176000
1	-0.122588000	-2.123332000	-1.925565000
1	0.410125000	-1.856990000	-3.599491000

TSB'C'

6	-1.683264000	2.012179000	-0.713201000
6	-1.465475000	2.837015000	-1.812620000
6	-0.765323000	4.036161000	-1.686387000
6	-0.285291000	4.394604000	-0.430069000
6	-0.489432000	3.575469000	0.677845000
6	-1.194975000	2.362121000	0.561848000
7	-1.435729000	1.563069000	1.685924000
6	-1.136715000	2.120258000	2.996740000
6	-3.723004000	-1.548234000	-0.671829000
6	-4.659980000	-1.101848000	0.203609000
6	-3.953796000	-0.392434000	1.229390000
6	-2.636501000	-0.458001000	0.904579000
8	-2.480901000	-1.153941000	-0.256685000
6	-3.772036000	-2.393627000	-1.898821000
8	-3.097525000	-3.630683000	-1.729402000
6	-1.421398000	0.102411000	1.597429000
6	2.318929000	-0.383520000	1.678156000
6	1.112474000	0.223927000	1.481027000
6	-0.081185000	-0.493817000	1.087765000
6	0.046803000	-1.940281000	1.110802000
6	1.246400000	-2.560714000	1.274385000
6	2.429686000	-1.797161000	1.536460000
7	3.603109000	-2.415681000	1.629673000
6	4.865459000	-1.752511000	1.899439000
1	-2.249267000	1.099400000	-0.856856000
1	-1.860561000	2.534666000	-2.778633000
1	-0.602076000	4.676411000	-2.546814000
1	0.264330000	5.322578000	-0.300919000
1	-0.086799000	3.882778000	1.635953000
1	-1.580685000	3.115280000	3.083675000
1	-1.587744000	1.483993000	3.759913000
1	-0.060923000	2.204810000	3.211277000
1	-5.724827000	-1.271418000	0.130597000
1	-4.367617000	0.100894000	2.097712000
1	-3.374651000	-1.840831000	-2.761211000
1	-4.819115000	-2.622470000	-2.109675000
1	-2.155529000	-3.440481000	-1.622693000
1	-1.514463000	-0.226125000	2.636695000
1	3.196176000	0.208153000	1.913097000
1	1.053840000	1.304952000	1.573187000
1	-0.013724000	-0.334766000	-0.220711000
1	-0.838532000	-2.544811000	0.931203000
1	1.329559000	-3.642162000	1.218052000
1	3.613545000	-3.422646000	1.522613000
1	5.053830000	-0.969555000	1.157230000
1	5.658693000	-2.496042000	1.840445000
1	4.870879000	-1.303737000	2.897518000
6	4.017753000	-0.594508000	-1.485139000
6	4.383473000	0.719885000	-1.192480000
6	2.684137000	-0.930095000	-1.700659000
6	3.403355000	1.710662000	-1.133809000

7	0.320217000	-0.255230000	-1.652735000
6	2.066455000	1.386411000	-1.336781000
6	1.707583000	0.062408000	-1.608899000
6	-0.083338000	-1.498168000	-2.315795000
1	4.777116000	-1.368823000	-1.546065000
1	5.426201000	0.970627000	-1.025368000
1	2.411315000	-1.959105000	-1.910517000
1	3.676949000	2.739057000	-0.918912000
1	-0.212517000	0.539960000	-2.003440000
1	1.290772000	2.148134000	-1.271494000
1	-1.157821000	-1.449124000	-2.485706000
1	0.143829000	-2.352789000	-1.671797000
1	0.427397000	-1.624441000	-3.274987000

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6	-1.251907000	1.786366000	-0.470835000
6	-0.897629000	2.555618000	-1.574537000
6	-0.736893000	3.936382000	-1.473407000
6	-0.943499000	4.534479000	-0.232968000
6	-1.300778000	3.782386000	0.882213000
6	-1.469617000	2.384482000	0.790117000
7	-1.831158000	1.645759000	1.907668000
6	-1.780352000	2.288291000	3.211131000
6	-3.814493000	-1.329587000	-0.836176000
6	-4.860192000	-0.690597000	-0.250684000
6	-4.326053000	-0.001275000	0.887645000
6	-2.994284000	-0.273817000	0.913823000
8	-2.672055000	-1.079368000	-0.133670000
6	-3.663453000	-2.236159000	-2.009501000
8	-3.252371000	-3.542368000	-1.635554000
6	-1.914470000	0.187504000	1.870384000
6	1.871104000	-0.400833000	1.686854000
6	0.624610000	0.214220000	1.811320000
6	-0.563747000	-0.505770000	1.694274000
6	-0.468208000	-1.893328000	1.503632000
6	0.761256000	-2.517634000	1.366196000
6	1.960817000	-1.776206000	1.416171000
7	3.160550000	-2.391521000	1.129468000
6	4.417317000	-1.713942000	1.369687000
1	-1.347540000	0.715654000	-0.596665000
1	-0.739422000	2.056255000	-2.527341000
1	-0.457468000	4.528961000	-2.337887000
1	-0.824308000	5.608473000	-0.120276000
1	-1.450974000	4.290918000	1.826582000
1	-2.539669000	3.073420000	3.298707000
1	-1.974877000	1.544298000	3.983146000
1	-0.798189000	2.738912000	3.407908000
1	-5.886910000	-0.713321000	-0.587430000
1	-4.859392000	0.618287000	1.595034000
1	-2.962761000	-1.797967000	-2.733383000
1	-4.635140000	-2.330640000	-2.499424000

1	-2.366652000	-3.469175000	-1.255214000
1	-2.284032000	-0.092347000	2.862703000
1	2.768606000	0.201914000	1.767207000
1	0.590324000	1.284588000	1.992286000
1	0.784314000	-0.575420000	-0.536902000
1	-1.370393000	-2.495366000	1.446781000
1	0.811775000	-3.589122000	1.189365000
1	3.169800000	-3.393341000	1.269815000
1	4.480976000	-0.808664000	0.755475000
1	5.232165000	-2.377099000	1.076390000
1	4.556693000	-1.426032000	2.421436000
6	4.835525000	-0.413604000	-2.073737000
6	5.057585000	0.890286000	-1.642706000
6	3.552886000	-0.963932000	-2.039590000
6	3.994607000	1.661925000	-1.171779000
7	1.128488000	-0.689356000	-1.504701000
6	2.711242000	1.128994000	-1.133882000
6	2.512508000	-0.177264000	-1.568910000
6	0.900353000	-2.096632000	-1.937355000
1	5.660011000	-1.016753000	-2.439035000
1	6.058695000	1.307877000	-1.672847000
1	3.392076000	-1.981128000	-2.376708000
1	4.161972000	2.679294000	-0.834379000
1	0.530969000	-0.074309000	-2.073586000
1	1.869202000	1.711523000	-0.767233000
1	-0.154214000	-2.315603000	-1.777668000
1	1.523194000	-2.753047000	-1.331286000
1	1.153501000	-2.180108000	-2.992935000

C''

6	2.376415000	-2.782806000	-0.290169000
6	3.031139000	-3.054566000	-1.490548000
6	4.106221000	-2.271595000	-1.903081000
6	4.541115000	-1.210383000	-1.111189000
6	3.899751000	-0.929558000	0.090356000
6	2.821564000	-1.717251000	0.483237000
7	2.147196000	-1.363428000	1.743038000
6	1.685172000	-2.535703000	2.543275000
6	2.326934000	2.287203000	-0.560651000
6	2.697828000	2.859800000	0.616989000
6	2.243069000	1.980348000	1.650603000
6	1.621029000	0.944921000	1.022660000
8	1.675723000	1.118263000	-0.322645000
6	2.426486000	2.684056000	-1.994307000
8	1.152197000	2.938650000	-2.566335000
6	1.008989000	-0.292918000	1.578854000
6	-1.423841000	-1.590466000	-1.084081000
6	-0.290818000	-1.036865000	-0.502986000
6	-0.195791000	-0.863901000	0.885092000
6	-1.279866000	-1.280848000	1.672080000
6	-2.415101000	-1.835620000	1.107242000

6	-2.514825000	-1.994828000	-0.289801000
7	-3.643034000	-2.551274000	-0.837872000
6	-3.935743000	-2.405945000	-2.249781000
1	1.536150000	-3.393603000	0.019793000
1	2.694400000	-3.885347000	-2.101540000
1	4.609819000	-2.491781000	-2.838751000
1	5.383759000	-0.601850000	-1.421733000
1	4.230044000	-0.103361000	0.715364000
1	2.851323000	-0.884762000	2.319207000
1	2.529682000	-3.212364000	2.667490000
1	1.346141000	-2.161149000	3.508800000
1	0.865314000	-3.031371000	2.028403000
1	3.220143000	3.798861000	0.729968000
1	2.351244000	2.100128000	2.719811000
1	2.960588000	1.906522000	-2.556755000
1	3.002668000	3.609135000	-2.059927000
1	0.669601000	2.100643000	-2.583024000
1	0.752390000	-0.074733000	2.619049000
1	-1.466701000	-1.697380000	-2.162354000
1	0.524716000	-0.732539000	-1.149071000
1	-1.231955000	-1.155530000	2.751653000
1	-3.247759000	-2.139192000	1.736386000
1	-4.450404000	-2.552857000	-0.228634000
1	-3.873594000	-1.359145000	-2.579490000
1	-4.945315000	-2.775112000	-2.433494000
1	-3.243720000	-2.999618000	-2.855730000
6	-3.244786000	1.667453000	1.281691000
6	-2.287990000	2.341917000	2.038893000
6	-1.182876000	2.936695000	1.437319000
6	-1.041835000	2.848171000	0.048829000
6	-1.979850000	2.171965000	-0.717165000
6	-3.099680000	1.563330000	-0.113148000
7	-3.990206000	0.849874000	-0.888753000
6	-5.225873000	0.342399000	-0.339074000
1	-4.098234000	1.215745000	1.775779000
1	-2.419626000	2.405117000	3.115712000
1	-0.445435000	3.465906000	2.032039000
1	-0.191530000	3.306777000	-0.449527000
1	-1.861938000	2.098910000	-1.796466000
1	-4.011640000	1.103168000	-1.867049000
1	-5.017368000	-0.382071000	0.457002000
1	-5.775038000	-0.171602000	-1.130030000
1	-5.868916000	1.130002000	0.080911000

TSC''D

6	2.488971000	-2.383216000	-0.527155000
6	3.169266000	-2.203080000	-1.730066000
6	4.267069000	-1.349382000	-1.807452000
6	4.701074000	-0.682526000	-0.659765000
6	4.038679000	-0.861240000	0.547594000
6	2.918074000	-1.700550000	0.617040000

7	2.175011000	-1.739484000	1.809087000	1	-1.934415000	1.879864000	-2.012915000
6	1.424234000	-2.943062000	2.140995000	1	-4.058456000	0.868482000	-1.851569000
6	2.487475000	2.017834000	-0.611704000	1	-5.009987000	-0.292589000	0.669335000
6	2.955885000	2.568499000	0.549469000	1	-5.826496000	-0.234737000	-0.899010000
6	2.365894000	1.824504000	1.604332000	1	-5.824059000	1.201062000	0.154178000
6	1.558109000	0.881935000	1.014283000				
8	1.646878000	0.997327000	-0.340938000				
6	2.689030000	2.325984000	-2.058310000				
8	1.479045000	2.702328000	-2.694828000	D			
6	0.698454000	-0.091270000	1.611726000	6	2.145990000	2.627987000	0.121245000
6	-1.649764000	-1.555805000	-0.933879000	6	2.865709000	2.409869000	1.295589000
6	-0.547584000	-0.926646000	-0.408546000	6	4.048995000	1.677783000	1.288114000
6	-0.401066000	-0.742155000	0.993735000	6	4.511760000	1.156172000	0.075365000
6	-1.421047000	-1.265075000	1.835042000	6	3.805439000	1.361404000	-1.100032000
6	-2.538761000	-1.870153000	1.323333000	6	2.603256000	2.096563000	-1.096427000
6	-2.694016000	-2.010988000	-0.084129000	7	1.881086000	2.226983000	-2.266385000
7	-3.810622000	-2.565687000	-0.580450000	6	0.818769000	3.202030000	-2.381780000
6	-4.127488000	-2.611773000	-1.992207000	6	2.835681000	-1.705519000	0.457134000
1	1.629811000	-3.043960000	-0.487375000	6	3.269179000	-2.253935000	-0.723621000
1	2.832503000	-2.736263000	-2.613931000	6	2.411350000	-1.750675000	-1.725517000
1	4.787054000	-1.211411000	-2.750044000	6	1.497138000	-0.930844000	-1.091531000
1	5.564131000	-0.024919000	-0.702782000	8	1.777339000	-0.901974000	0.244714000
1	4.374944000	-0.348524000	1.444476000	6	3.258569000	-1.862084000	1.880271000
1	2.707768000	-1.385637000	2.600470000	8	2.190498000	-2.315113000	2.693940000
1	2.061142000	-3.833458000	2.112923000	6	0.357940000	-0.292105000	-1.626683000
1	1.007681000	-2.823835000	3.142146000	6	-1.651702000	1.502115000	0.955145000
1	0.597721000	-3.074457000	1.437638000	6	-0.615006000	0.816535000	0.395392000
1	3.637752000	3.402802000	0.625130000	6	-0.628682000	0.444249000	-0.992832000
1	2.494579000	1.961881000	2.669381000	6	-1.762715000	0.851365000	-1.776103000
1	3.145243000	1.459672000	-2.555269000	6	-2.811183000	1.519030000	-1.225919000
1	3.379143000	3.168015000	-2.139656000	6	-2.804580000	1.830183000	0.173394000
1	0.910914000	1.920075000	-2.732277000	7	-3.866443000	2.413885000	0.715043000
1	0.650315000	0.001109000	2.694762000	6	-4.036335000	2.654813000	2.136140000
1	-1.739488000	-1.674730000	-2.007593000	1	1.231889000	3.211008000	0.153346000
1	0.219711000	-0.567213000	-1.083157000	1	2.492807000	2.829357000	2.226027000
1	-1.316947000	-1.151047000	2.911411000	1	4.607364000	1.519478000	2.205286000
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1	-4.537640000	-2.817785000	0.075504000	1	4.168930000	0.953275000	-2.040205000
1	-4.090150000	-1.607765000	-2.431886000	1	2.414943000	2.070345000	-3.111200000
1	-5.134308000	-3.011677000	-2.106452000	1	1.153343000	4.227661000	-2.169425000
1	-3.430643000	-3.257820000	-2.536532000	1	0.421707000	3.165310000	-3.397462000
6	-3.130734000	1.790110000	1.169995000	1	0.000524000	2.963607000	-1.692715000
6	-2.132436000	2.540781000	1.790314000	1	4.094704000	-2.941163000	-0.836182000
6	-1.067871000	3.065142000	1.062543000	1	2.425216000	-1.965717000	-2.785286000
6	-1.009776000	2.826214000	-0.313889000	1	3.663858000	-0.910559000	2.246991000
6	-1.991159000	2.074012000	-0.943898000	1	4.050720000	-2.612305000	1.924644000
6	-3.070087000	1.535716000	-0.211879000	1	1.559319000	-1.587400000	2.780902000
7	-4.001659000	0.743310000	-0.850129000	1	0.236690000	-0.464671000	-2.694556000
6	-5.227328000	0.345861000	-0.195240000	1	-1.623854000	1.769013000	2.005260000
1	-3.949655000	1.395036000	1.761808000	1	0.239118000	0.554010000	1.006490000
1	-2.198079000	2.718957000	2.860258000	1	-1.776142000	0.596442000	-2.832705000
1	-0.294692000	3.647557000	1.553422000	1	-3.674577000	1.804253000	-1.819515000
1	-0.185683000	3.219678000	-0.904332000	1	-4.656993000	2.602958000	0.109962000

1	-3.935720000	1.717722000	2.694466000
1	-5.033193000	3.062296000	2.295591000
1	-3.296629000	3.370340000	2.506567000
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6	-2.080421000	-2.970652000	-1.257112000
6	-0.909197000	-3.306432000	-0.581127000
6	-0.722197000	-2.834211000	0.721233000
6	-1.681082000	-2.034995000	1.326709000
6	-2.865715000	-1.684293000	0.644820000
7	-3.773737000	-0.844368000	1.249712000
6	-5.090414000	-0.618295000	0.698311000
1	-3.956745000	-1.924010000	-1.210466000
1	-2.245326000	-3.333925000	-2.267873000
1	-0.153766000	-3.924063000	-1.056464000
1	0.188053000	-3.073933000	1.265721000
1	-1.528750000	-1.659254000	2.336179000
1	-3.692014000	-0.767544000	2.254140000
1	-5.020999000	-0.107997000	-0.270029000
1	-5.647900000	0.026824000	1.379656000
1	-5.656915000	-1.549064000	0.551953000

TSDE'

6	1.995036000	2.669167000	0.324262000
6	2.807408000	2.582484000	1.453894000
6	4.043627000	1.943867000	1.404671000
6	4.459780000	1.377410000	0.196239000
6	3.659453000	1.450415000	-0.934702000
6	2.408592000	2.095142000	-0.890704000
7	1.611477000	2.116666000	-2.022511000
6	0.499110000	3.039934000	-2.112549000
6	3.042539000	-1.695864000	0.422660000
6	3.504105000	-2.101217000	-0.792868000
6	2.433631000	-1.901566000	-1.715314000
6	1.390575000	-1.387146000	-0.994042000
8	1.760702000	-1.256469000	0.309496000
6	3.607007000	-1.689372000	1.802200000
8	2.929090000	-2.599257000	2.656035000
6	0.016856000	-1.116729000	-1.392660000
6	-1.568239000	1.404780000	0.945511000
6	-0.677459000	0.470075000	0.451183000
6	-0.809778000	-0.065389000	-0.850370000
6	-1.882762000	0.419362000	-1.640452000
6	-2.767767000	1.360207000	-1.171222000
6	-2.657976000	1.846210000	0.156678000
7	-3.577383000	2.717786000	0.633291000
6	-3.632826000	3.138378000	2.016319000
1	1.040601000	3.180354000	0.389784000
1	2.465583000	3.032117000	2.382108000
1	4.673167000	1.888128000	2.286839000
1	5.419974000	0.871762000	0.134152000
1	3.988904000	1.005544000	-1.870705000

1	2.124000000	1.991125000	-2.885901000
1	0.798457000	4.089383000	-1.973316000
1	0.035908000	2.934193000	-3.094924000
1	-0.257450000	2.798829000	-1.359040000
1	4.489542000	-2.495138000	-0.996524000
1	2.418985000	-2.120758000	-2.773846000
1	3.578649000	-0.669790000	2.208126000
1	4.651690000	-2.004653000	1.749466000
1	2.061070000	-2.221184000	2.849920000
1	-0.101552000	-1.266689000	-2.464256000
1	-1.438856000	1.785356000	1.952656000
1	0.136861000	0.141306000	1.086973000
1	-2.005937000	0.028264000	-2.647528000
1	-3.582033000	1.715139000	-1.796987000
1	-4.376672000	2.915193000	0.047619000
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1	-2.747426000	3.721764000	2.291008000
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6	-2.145525000	-2.785962000	-1.515123000
6	-0.869759000	-2.918198000	-0.878077000
6	-0.837399000	-2.803095000	0.551352000
6	-1.859201000	-2.195454000	1.211167000
6	-3.018656000	-1.758066000	0.483085000
7	-3.903175000	-0.969890000	1.082657000
6	-5.144852000	-0.490526000	0.499109000
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1	-2.246745000	-3.081195000	-2.555480000
1	-0.125894000	-3.542460000	-1.361443000
1	0.054355000	-3.106413000	1.091534000
1	-1.814664000	-2.001107000	2.278847000
1	-3.722009000	-0.723528000	2.049326000
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1	-5.517467000	0.324269000	1.119769000
1	-5.896607000	-1.285703000	0.462322000

E'

6	1.740308000	3.822564000	0.225183000
6	2.283918000	3.074283000	1.269153000
6	2.805146000	1.802104000	1.049261000
6	2.772244000	1.276666000	-0.245838000
6	2.225473000	2.004126000	-1.293628000
6	1.698887000	3.293755000	-1.077393000
7	1.125581000	3.981168000	-2.129028000
6	0.804723000	5.387914000	-2.012271000
6	3.061110000	-2.209453000	0.636677000
6	3.574296000	-2.515480000	-0.583575000
6	2.490002000	-2.405031000	-1.517521000
6	1.393428000	-2.047433000	-0.796101000
8	1.734072000	-1.918802000	0.517315000
6	3.609205000	-2.159834000	2.022691000

8	2.969258000	-3.087949000	2.885112000
6	-0.029589000	-1.811753000	-1.190715000
6	-0.972370000	1.382678000	0.720957000
6	-0.510808000	0.097999000	0.445439000
6	-0.547758000	-0.427286000	-0.848167000
6	-1.090582000	0.372761000	-1.862345000
6	-1.555197000	1.652510000	-1.605600000
6	-1.488349000	2.191133000	-0.306158000
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6	-2.031127000	4.014225000	1.257379000
1	1.350553000	4.815683000	0.422987000
1	2.304103000	3.503850000	2.267173000
1	3.237483000	1.232654000	1.865746000
1	3.182905000	0.288488000	-0.442016000
1	2.195291000	1.584623000	-2.296768000
1	1.435343000	3.683355000	-3.044377000
1	1.665962000	6.002756000	-1.713200000
1	0.442986000	5.742737000	-2.978024000
1	0.007187000	5.538489000	-1.276854000
1	4.599338000	-2.788392000	-0.790862000
1	2.516205000	-2.577172000	-2.584181000
1	3.530019000	-1.139436000	2.420986000
1	4.668424000	-2.424100000	1.984073000
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1	-0.913381000	1.761062000	1.735804000
1	-0.095565000	-0.489793000	1.258803000
1	-1.139541000	-0.015237000	-2.877398000
1	-1.954335000	2.264582000	-2.410369000
1	-2.511084000	3.874396000	-0.774239000
1	-2.721790000	3.416571000	1.869475000
1	-2.413825000	5.033557000	1.193681000
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6	-3.468816000	-2.657035000	-0.562240000
6	-2.334819000	-2.760115000	-1.275932000
6	-0.988843000	-2.953626000	-0.672611000
6	-1.012551000	-3.085519000	0.810007000
6	-2.138200000	-2.992912000	1.534843000
6	-3.409686000	-2.754790000	0.881309000
7	-4.484403000	-2.639980000	1.613967000
6	-5.836938000	-2.404615000	1.118605000
1	-4.425481000	-2.505318000	-1.047873000
1	-2.376098000	-2.680252000	-2.359832000
1	-0.565924000	-3.884607000	-1.082752000
1	-0.067899000	-3.271904000	1.312682000
1	-2.133720000	-3.095420000	2.615726000
1	-4.369905000	-2.724321000	2.620989000
1	-5.881337000	-1.457687000	0.576606000
1	-6.502505000	-2.362424000	1.977738000
1	-6.144180000	-3.219824000	0.460259000

E''

6	3.918248000	0.259293000	-1.457889000
6	4.575193000	-0.966479000	-1.365560000
6	4.673918000	-1.641381000	-0.151425000
6	4.105981000	-1.061703000	0.988661000
6	3.453071000	0.159986000	0.914948000
6	3.345138000	0.843652000	-0.313396000
7	2.612714000	2.009182000	-0.382016000
6	2.574973000	2.816158000	-1.581765000
1	3.848319000	0.760059000	-2.417603000
1	5.012340000	-1.396596000	-2.262354000
1	5.193221000	-2.592045000	-0.086275000
1	4.172364000	-1.570433000	1.946900000
1	3.006380000	0.601807000	1.802781000
1	2.418722000	2.491540000	0.489807000
1	2.065536000	2.285038000	-2.395403000
1	2.012186000	3.725163000	-1.364492000
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6	-0.366182000	3.711223000	0.492276000
6	-0.770060000	4.254613000	-0.685114000
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6	-0.970699000	2.025944000	-0.792776000
8	-0.504821000	2.357257000	0.444911000
6	0.223358000	4.243904000	1.754085000
8	1.434778000	3.570556000	2.086698000
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6	-2.353591000	-0.118468000	-0.746909000
6	-2.680115000	-1.337752000	-1.354963000
6	-3.837159000	-2.021895000	-1.022356000
6	-4.724028000	-1.507202000	-0.055269000
7	-5.895957000	-2.182196000	0.228081000
6	-6.666371000	-1.855429000	1.410575000
6	1.208612000	-2.411622000	-0.778175000
6	0.745357000	-1.254994000	-1.291085000
6	0.180538000	-0.159870000	-0.465772000
6	-0.020370000	-0.530269000	0.961265000
6	0.419902000	-1.686240000	1.483893000
6	1.105334000	-2.646971000	0.643712000
7	1.623999000	-3.714437000	1.194393000
6	2.372396000	-4.749248000	0.491740000
1	-0.762351000	5.305780000	-0.936528000
1	-1.517783000	3.198289000	-2.543449000
1	-0.492440000	4.165662000	2.581586000
1	0.458885000	5.300706000	1.610781000
1	1.190872000	2.717798000	2.473104000
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1	-3.001604000	1.328724000	0.707888000
1	-2.014445000	-1.754602000	-2.108475000
1	-4.077477000	-2.962595000	-1.511247000

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1	-6.064839000	-1.869208000	2.330972000
1	-7.473248000	-2.582037000	1.511046000
1	-7.117590000	-0.862446000	1.315918000
1	1.665206000	-3.161916000	-1.412718000
1	0.832043000	-1.070616000	-2.359766000
1	0.980081000	0.610958000	-0.453320000
1	-0.511172000	0.195743000	1.603157000
1	0.303397000	-1.922194000	2.537652000
1	1.509019000	-3.825672000	2.198076000
1	1.727074000	-5.271793000	-0.218229000
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1	3.214175000	-4.298982000	-0.040643000

TSE''F'

6	3.886332000	0.035020000	-1.458483000
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6	5.036613000	-1.605081000	-0.098700000
6	4.436815000	-1.070235000	1.045508000
6	3.562732000	0.003013000	0.942159000
6	3.268765000	0.546024000	-0.314537000
7	2.236566000	1.515804000	-0.403140000
6	2.163978000	2.345603000	-1.608096000
1	3.672799000	0.454744000	-2.435527000
1	5.238791000	-1.438252000	-2.234671000
1	5.721447000	-2.442974000	-0.015055000
1	4.649784000	-1.495451000	2.021843000
1	3.080168000	0.414445000	1.825403000
1	2.157711000	2.084548000	0.444434000
1	1.775759000	1.754353000	-2.443237000
1	1.479849000	3.172745000	-1.411402000
1	3.145699000	2.746111000	-1.881303000
6	-0.331353000	3.707909000	0.567045000
6	-0.908033000	4.283249000	-0.520941000
6	-1.363085000	3.205304000	-1.354017000
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8	1.608065000	3.483515000	1.970480000
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6	-3.321384000	0.454516000	0.187642000
6	-2.449352000	-0.042126000	-0.777960000
6	-2.810232000	-1.220834000	-1.443597000
6	-3.996329000	-1.875532000	-1.158476000
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7	-6.076910000	-2.020444000	0.058461000
6	-6.846975000	-1.718684000	1.248088000
6	1.292941000	-2.330836000	-0.729683000
6	0.664137000	-1.239439000	-1.259731000
6	0.051086000	-0.212382000	-0.448218000

6	-0.052563000	-0.531718000	0.966967000
6	0.559224000	-1.613418000	1.512674000
6	1.283962000	-2.531902000	0.682449000
7	1.935951000	-3.542259000	1.246670000
6	2.741377000	-4.508064000	0.523486000
1	-0.976563000	5.343425000	-0.719465000
1	-1.846688000	3.278200000	-2.317938000
1	-0.235159000	4.140003000	2.666806000
1	0.644522000	5.259320000	1.616694000
1	1.409111000	2.740168000	2.555809000
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1	-5.170897000	0.222153000	1.250422000
1	-3.071833000	1.366928000	0.724711000
1	-2.144311000	-1.631651000	-2.200285000
1	-4.262067000	-2.785464000	-1.690595000
1	-6.077379000	-2.996163000	-0.208805000
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1	-7.267666000	-0.709630000	1.190043000
1	1.800804000	-3.038175000	-1.374874000
1	0.670831000	-1.096171000	-2.338548000
1	1.031973000	0.614165000	-0.410784000
1	-0.600534000	0.151403000	1.610182000
1	0.518687000	-1.804419000	2.581210000
1	1.890572000	-3.626540000	2.254847000
1	2.132989000	-5.073335000	-0.188492000
1	3.174045000	-5.198799000	1.245127000
1	3.549023000	-4.003088000	-0.018546000

F'

6	4.476230000	-0.006503000	-0.159083000
6	5.512987000	-0.708929000	0.458559000
6	5.377412000	-1.164254000	1.766245000
6	4.202980000	-0.910408000	2.475527000
6	3.165192000	-0.206290000	1.875801000
6	3.316825000	0.230925000	0.563539000
7	2.163410000	0.922120000	-0.033817000
6	2.377393000	1.609031000	-1.334065000
1	4.588573000	0.337866000	-1.180724000
1	6.425950000	-0.901878000	-0.095343000
1	6.186590000	-1.713157000	2.236769000
1	4.093919000	-1.259243000	3.497077000
1	2.240856000	-0.004161000	2.411401000
1	1.828510000	1.649753000	0.641638000
1	2.682036000	0.880442000	-2.083235000
1	1.431126000	2.066617000	-1.626577000
1	3.143100000	2.372534000	-1.200431000
6	-0.445413000	3.161321000	0.031756000
6	-0.810829000	3.742612000	-1.139894000
6	-1.326659000	2.692096000	-1.969809000
6	-1.234273000	1.545640000	-1.243727000

8	-0.692606000	1.817321000	-0.021735000
6	0.156384000	3.671413000	1.287955000
8	1.491150000	3.159363000	1.401219000
6	-1.649012000	0.128128000	-1.500881000
6	-4.859177000	0.290353000	0.625081000
6	-3.662192000	0.654826000	0.006170000
6	-2.955072000	-0.234125000	-0.798569000
6	-3.488117000	-1.520863000	-0.970500000
6	-4.675563000	-1.897444000	-0.369222000
6	-5.391217000	-0.993934000	0.443484000
7	-6.596436000	-1.381817000	0.999411000
6	-7.198222000	-0.608235000	2.066542000
6	1.602187000	-1.873353000	-1.793609000
6	0.490412000	-1.088972000	-2.100525000
6	-0.503725000	-0.819384000	-1.158994000
6	-0.357166000	-1.375040000	0.121740000
6	0.741180000	-2.158699000	0.444971000
6	1.751672000	-2.420637000	-0.505447000
7	2.861575000	-3.139512000	-0.139732000
6	3.833334000	-3.591594000	-1.109793000
1	-0.720603000	4.792388000	-1.381022000
1	-1.724005000	2.776372000	-2.971131000
1	-0.440410000	3.353668000	2.149832000
1	0.170082000	4.764875000	1.251080000
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1	-1.816359000	0.064235000	-2.583137000
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1	-2.953922000	-2.240208000	-1.587539000
1	-5.072391000	-2.898415000	-0.519260000
1	-6.705414000	-2.383375000	1.090619000
1	-6.511935000	-0.430262000	2.907117000
1	-8.070552000	-1.148750000	2.435985000
1	-7.538162000	0.363959000	1.695185000
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1	1.392465000	0.244052000	-0.133329000
1	-1.113041000	-1.185390000	0.878989000
1	0.842145000	-2.570702000	1.445724000
1	2.768421000	-3.696010000	0.698440000
1	3.393627000	-4.228968000	-1.889956000
1	4.605431000	-4.158733000	-0.588391000
1	4.316143000	-2.737679000	-1.598014000

F

6	-0.508879000	3.252318000	0.113783000
6	-0.684227000	3.790380000	-1.121209000
6	-1.139104000	2.723047000	-1.966015000
6	-1.202145000	1.615063000	-1.180161000
8	-0.822142000	1.925905000	0.087936000
6	-0.059225000	3.809629000	1.415831000

8	1.192325000	3.231602000	1.757114000
6	-1.587995000	0.192832000	-1.450531000
6	-4.881263000	0.284137000	0.550435000
6	-3.685767000	0.682227000	-0.050394000
6	-2.882562000	-0.215437000	-0.749632000
6	-3.321571000	-1.545244000	-0.835534000
6	-4.509063000	-1.955041000	-0.255058000
6	-5.318937000	-1.043787000	0.452285000
7	-6.522147000	-1.470558000	0.988116000
6	-7.211540000	-0.663894000	1.974928000
6	1.514086000	-2.009943000	-1.889534000
6	0.414217000	-1.194273000	-2.154206000
6	-0.423094000	-0.740100000	-1.138525000
6	-0.129125000	-1.129553000	0.175250000
6	0.963072000	-1.933028000	0.457748000
6	1.812818000	-2.386901000	-0.571216000
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6	3.628894000	-3.883565000	-1.284408000
1	-0.507031000	4.821304000	-1.393679000
1	-1.386389000	2.768888000	-3.017090000
1	-0.812257000	3.593398000	2.186131000
1	0.008920000	4.899868000	1.308863000
1	1.403283000	3.515987000	2.655840000
1	-1.759890000	0.143177000	-2.533216000
1	-5.469898000	1.015433000	1.093716000
1	-3.384309000	1.722263000	0.041318000
1	-2.715749000	-2.273414000	-1.370245000
1	-4.830303000	-2.990332000	-0.338818000
1	-6.563580000	-2.466806000	1.159015000
1	-6.577988000	-0.398709000	2.833908000
1	-8.075020000	-1.223066000	2.337532000
1	-7.578053000	0.264559000	1.525783000
1	2.135307000	-2.349907000	-2.711104000
1	0.204246000	-0.910376000	-3.183201000
1	-0.769934000	-0.797776000	0.988457000
1	1.178185000	-2.223011000	1.483336000
1	2.849738000	-3.631704000	0.633763000
1	2.971896000	-4.536315000	-1.877512000
1	4.395451000	-4.497616000	-0.810217000
1	4.128217000	-3.193191000	-1.971787000

N-methylaniline

6	2.123420000	3.428829000	0.293704000
6	2.925019000	3.302269000	1.427038000
6	3.858039000	2.275736000	1.538688000
6	3.981132000	1.363183000	0.487514000
6	3.186986000	1.472214000	-0.644585000
6	2.239215000	2.507960000	-0.761373000
7	1.428845000	2.571049000	-1.881455000
6	0.684778000	3.777271000	-2.182884000
1	1.408361000	4.241925000	0.231936000

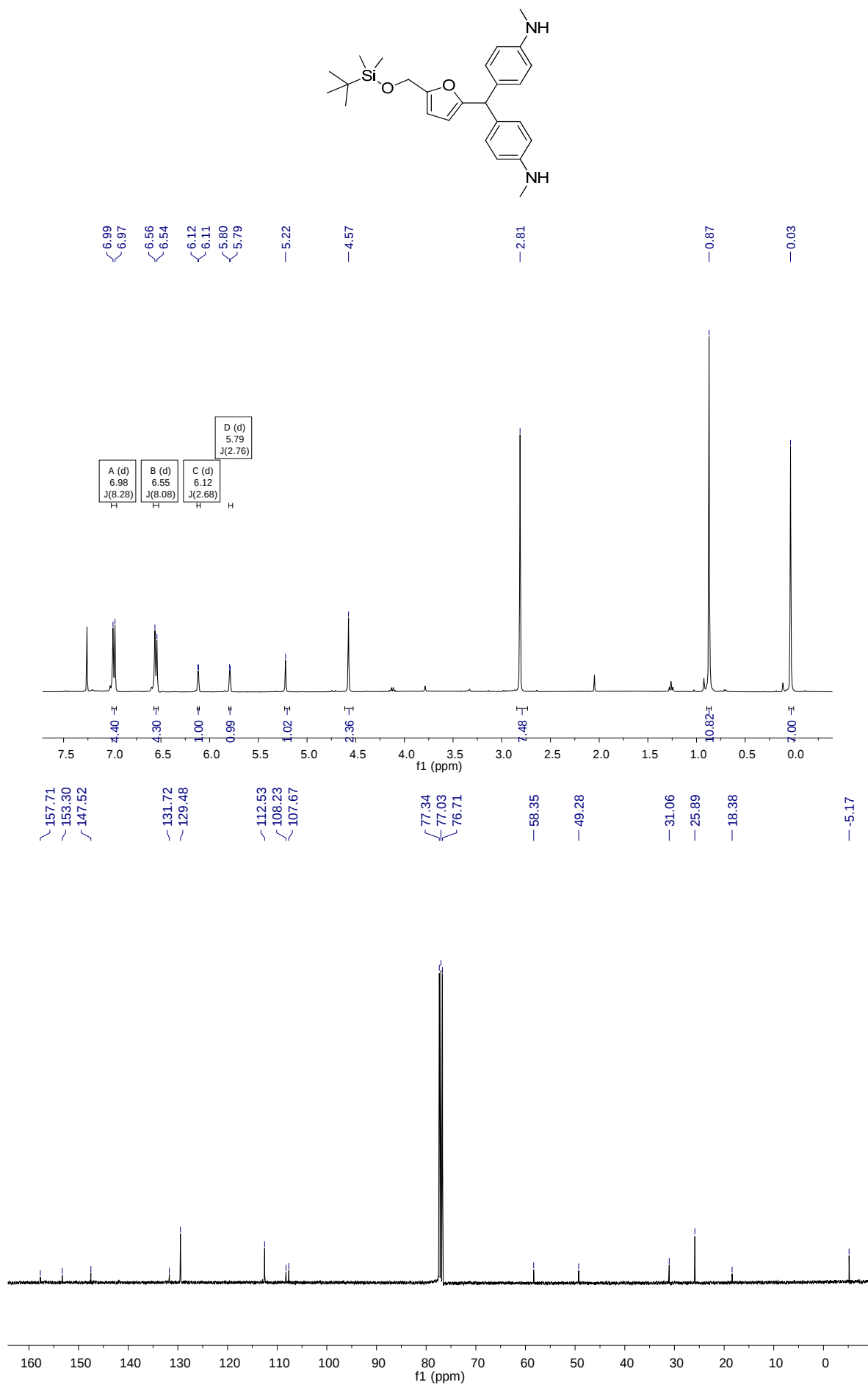
1	2.815894000	4.026160000	2.229859000
1	4.480552000	2.187241000	2.422851000
1	4.706243000	0.556448000	0.550023000
1	3.286343000	0.757394000	-1.457762000
1	1.808425000	2.096979000	-2.690487000
1	1.316204000	4.677222000	-2.210216000
1	0.207734000	3.656592000	-3.156196000
1	-0.103342000	3.940520000	-1.440881000

***N*-methylaniline-H⁺**

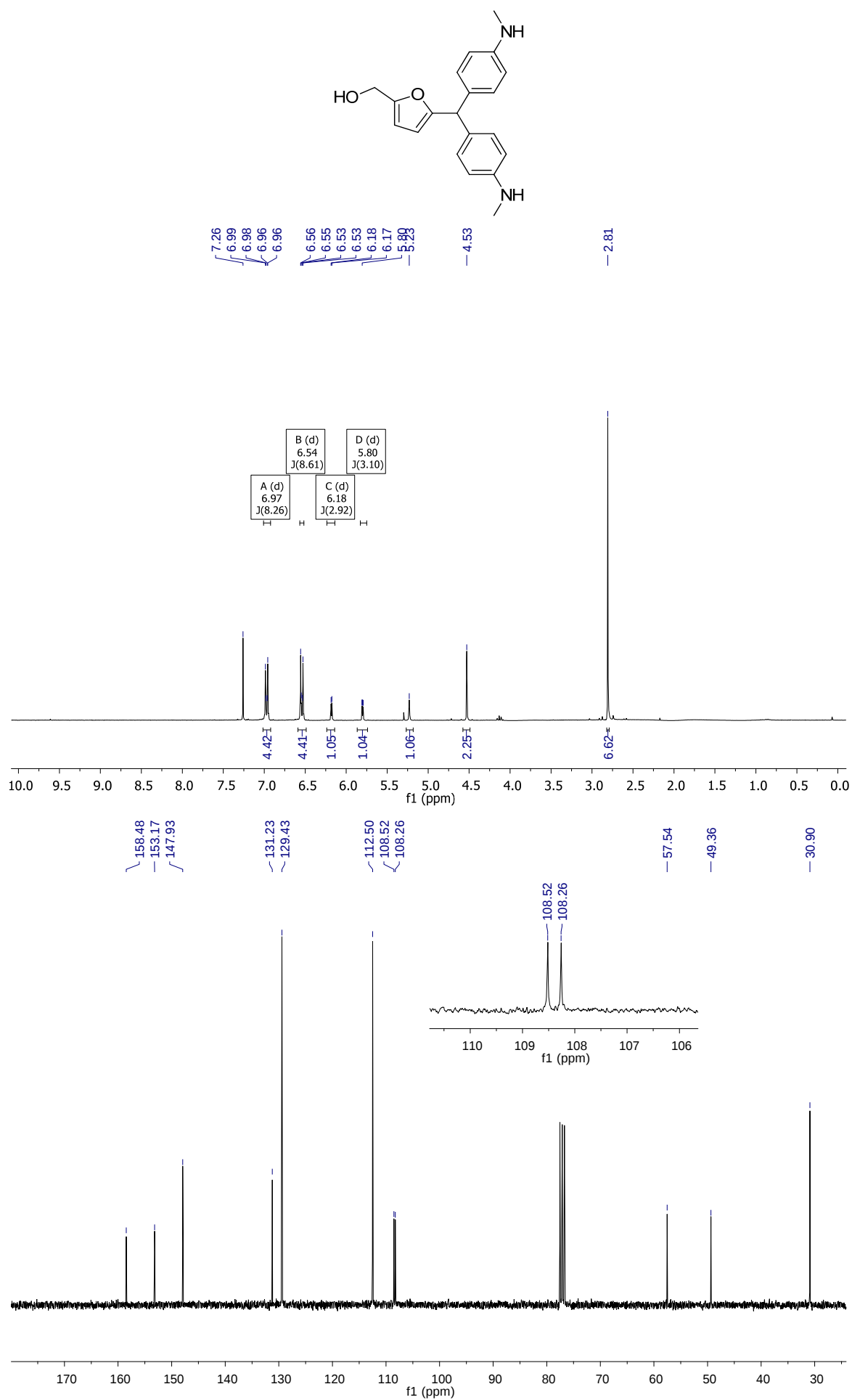
6	4.499345000	0.015024000	-0.165504000
6	5.526301000	-0.698233000	0.454266000
6	5.368115000	-1.185714000	1.747435000
6	4.176122000	-0.964139000	2.437008000
6	3.143952000	-0.254927000	1.833964000
6	3.325041000	0.223020000	0.540869000
7	2.194493000	0.964929000	-0.053787000
6	2.405607000	1.582517000	-1.393345000
1	4.631895000	0.392171000	-1.172565000
1	6.452373000	-0.868574000	-0.084493000
1	6.173323000	-1.737444000	2.221265000
1	4.048209000	-1.342090000	3.445740000
1	2.208848000	-0.071962000	2.356133000
1	1.913803000	1.704218000	0.603198000
1	2.608178000	0.793198000	-2.114404000
1	1.488869000	2.107872000	-1.653717000
1	3.239581000	2.278947000	-1.327225000
1	1.385383000	0.333069000	-0.111360000

Copies of NMR Spectra

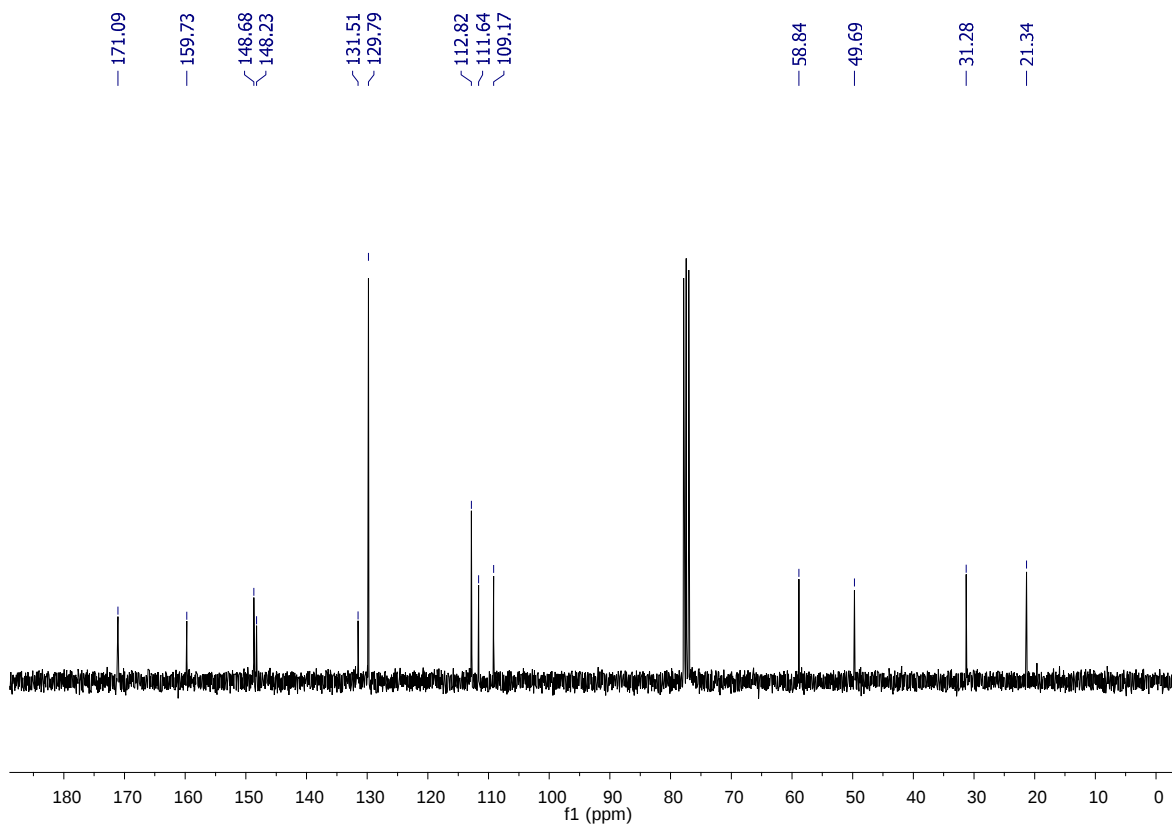
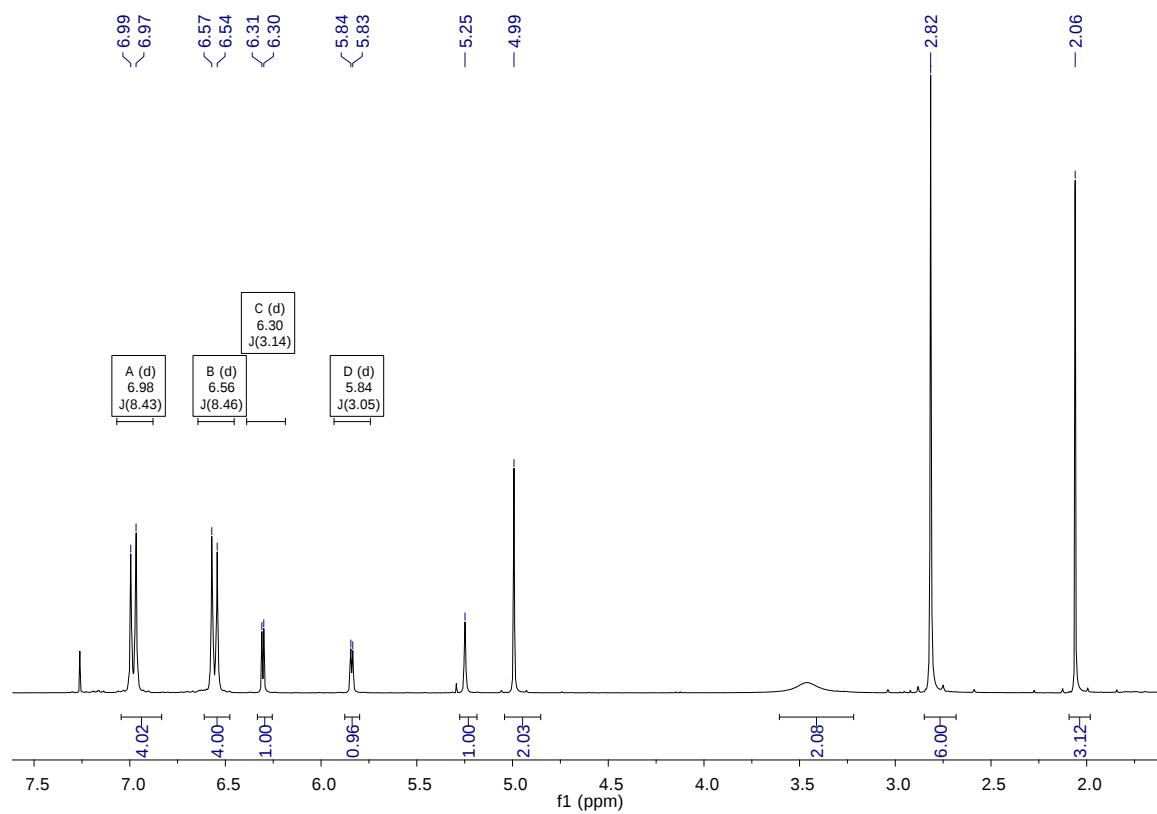
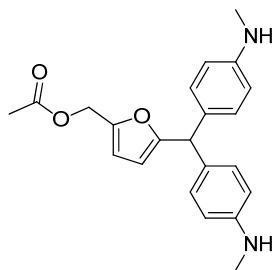
Compound 2



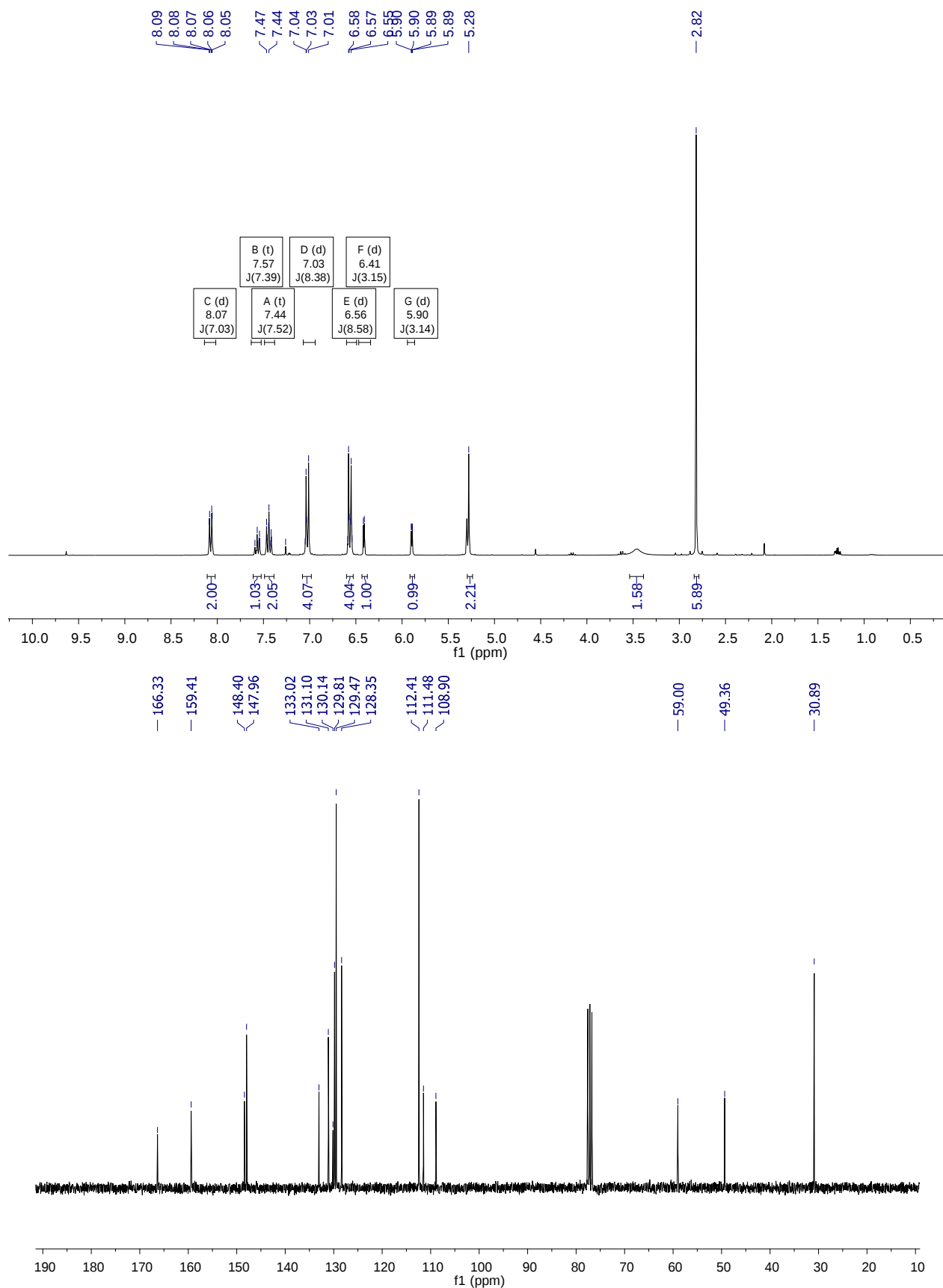
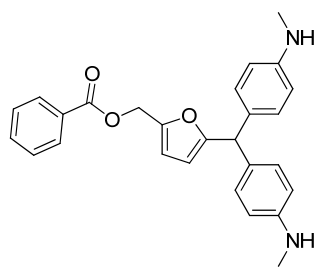
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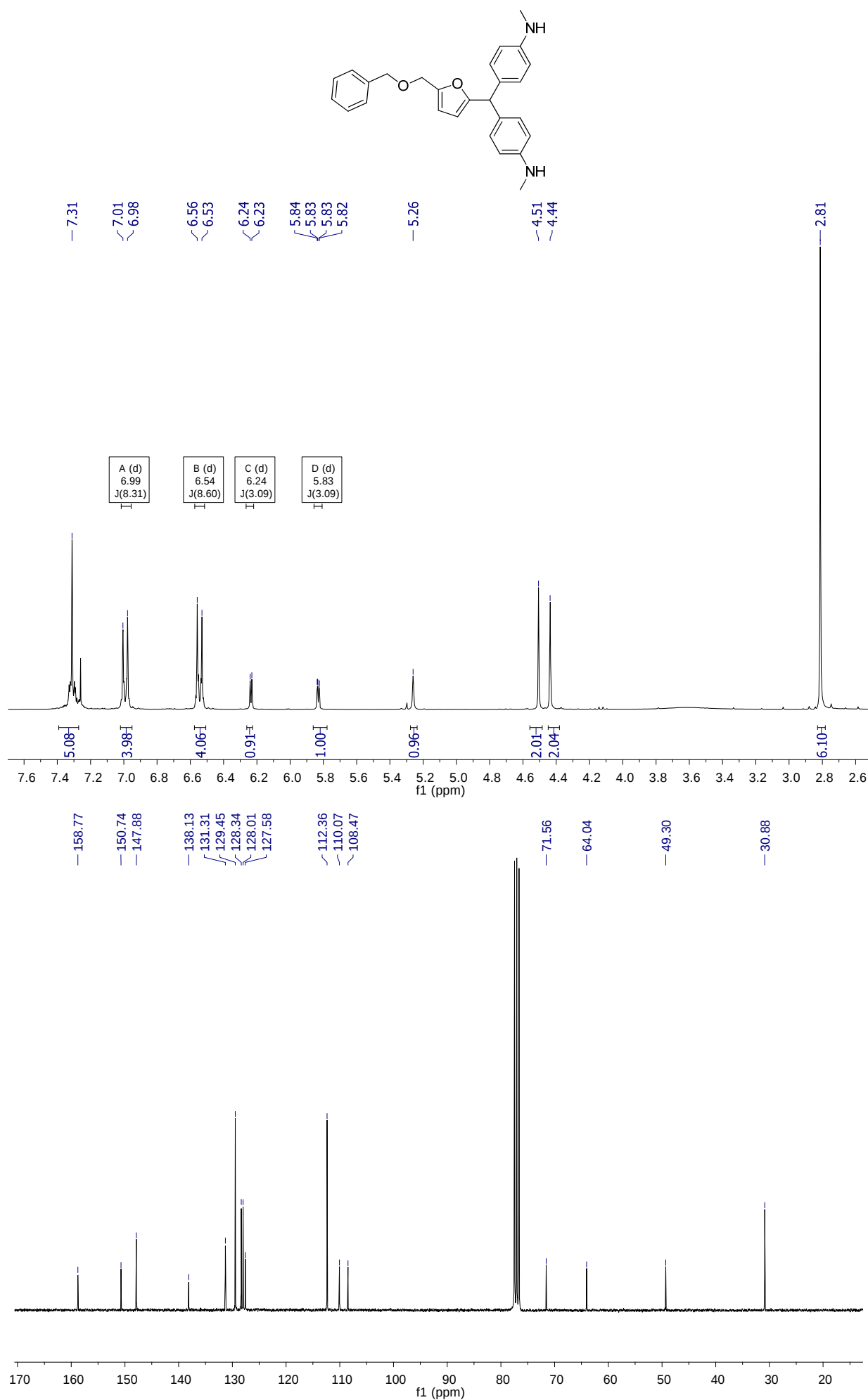
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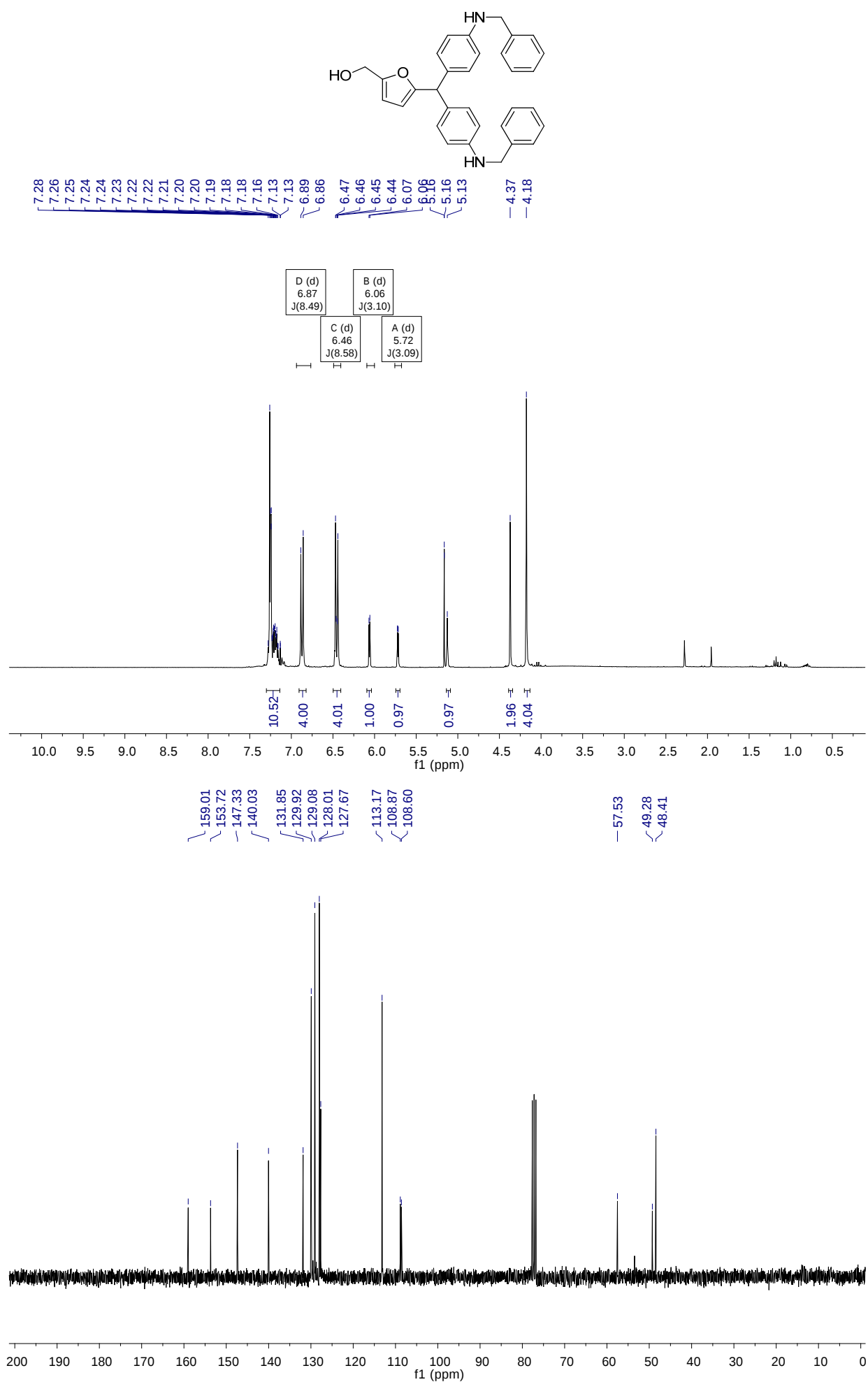
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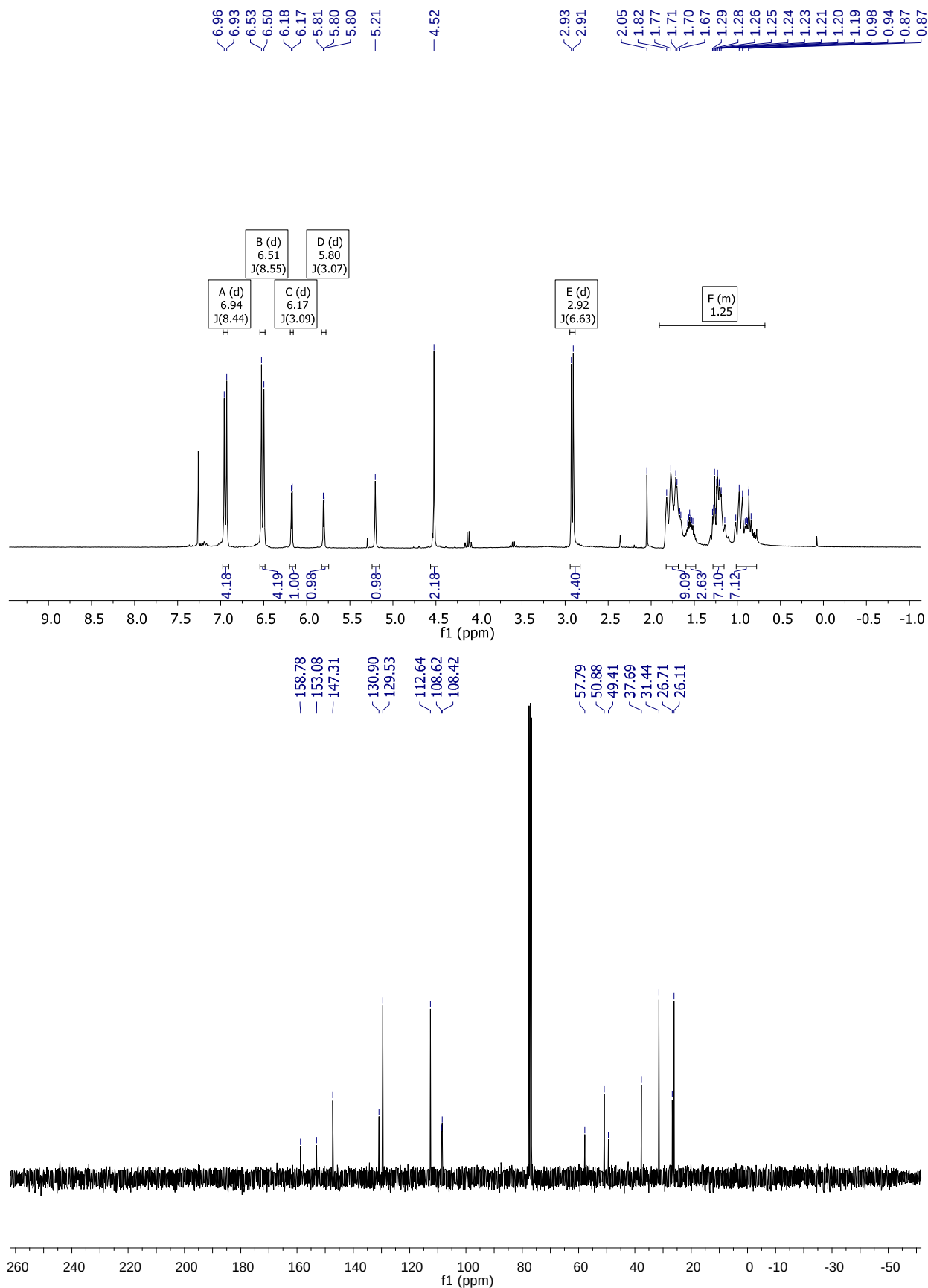
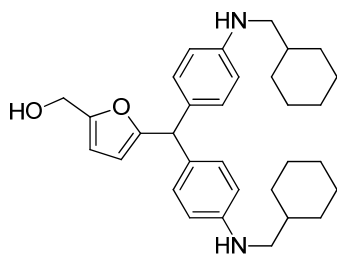
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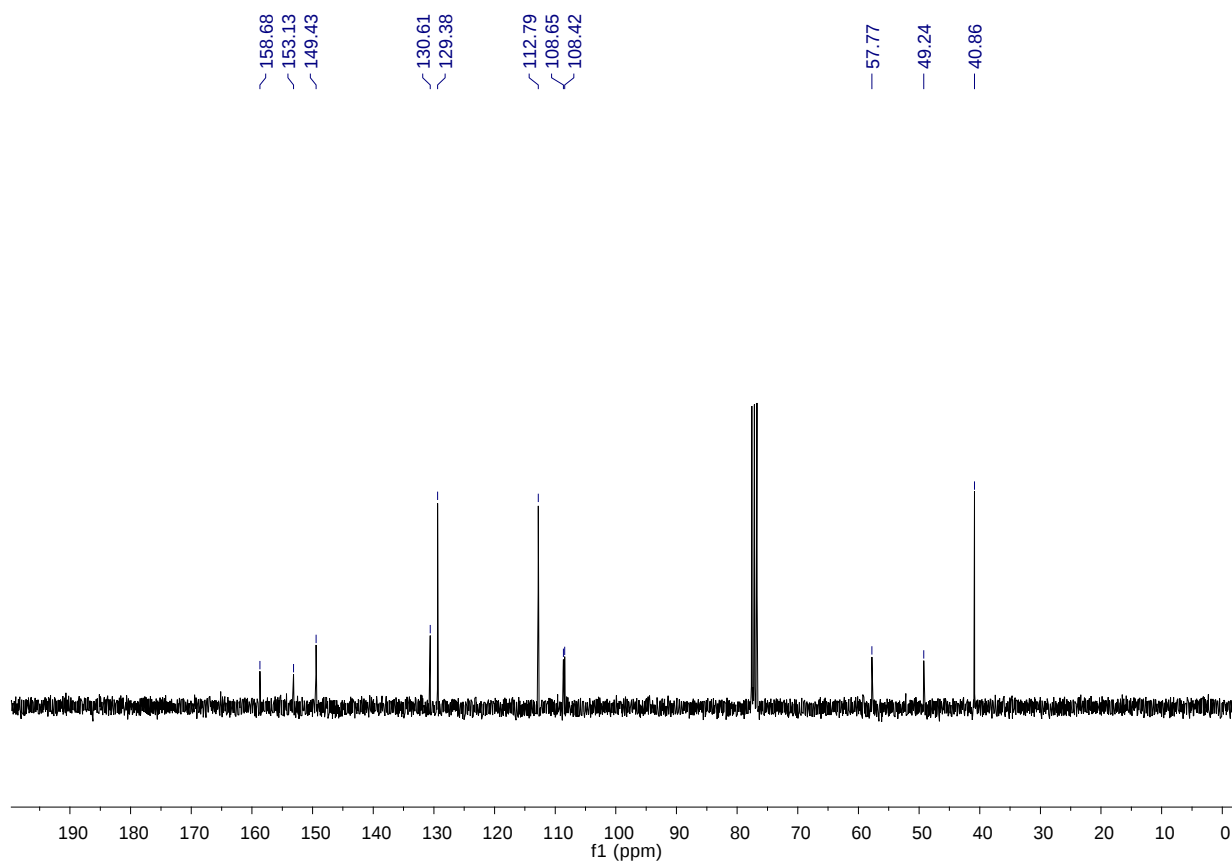
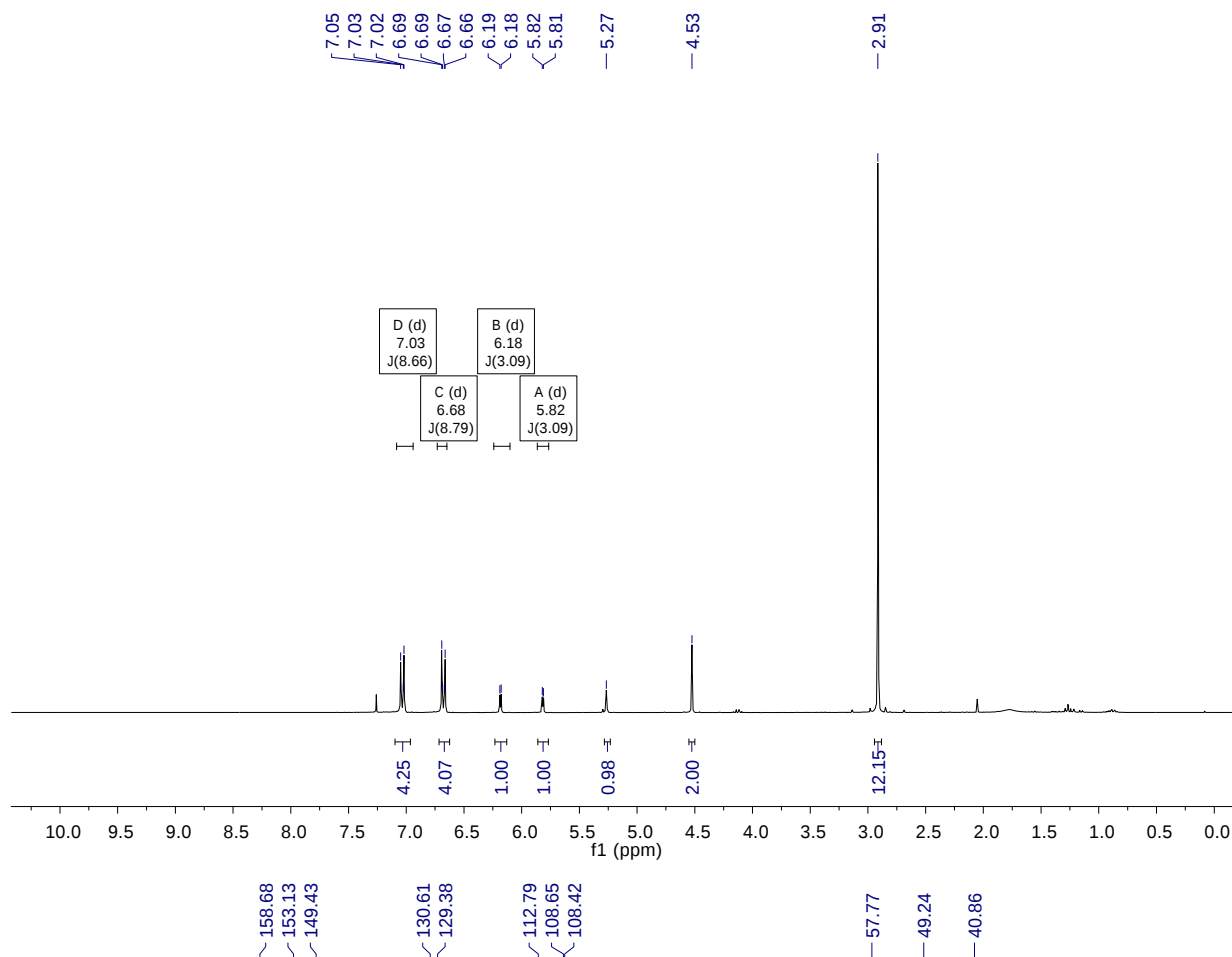
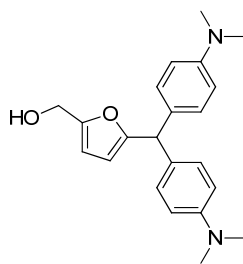
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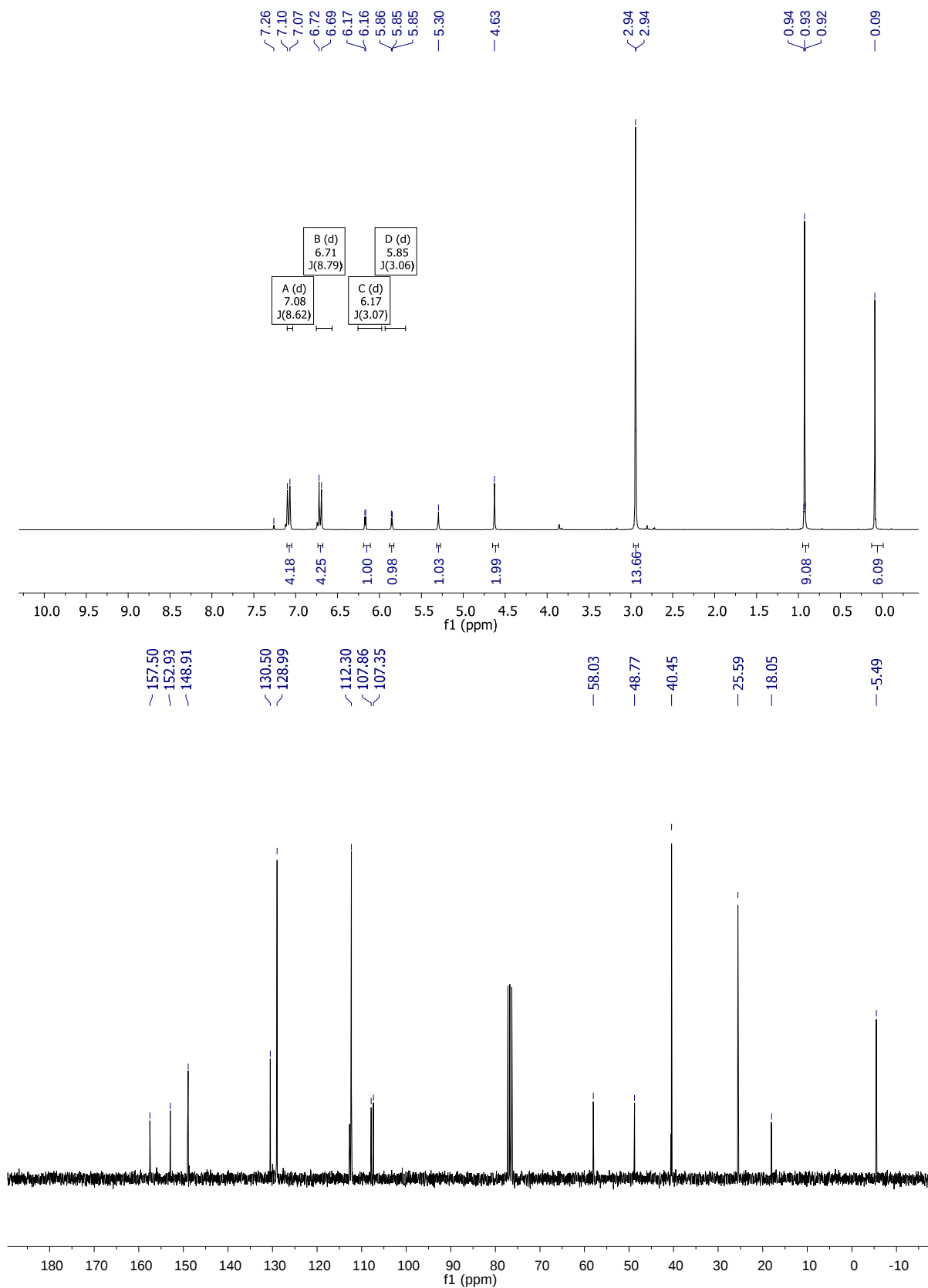
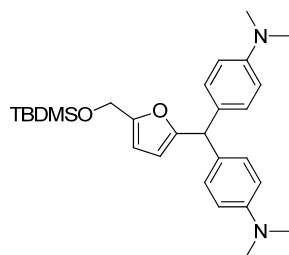
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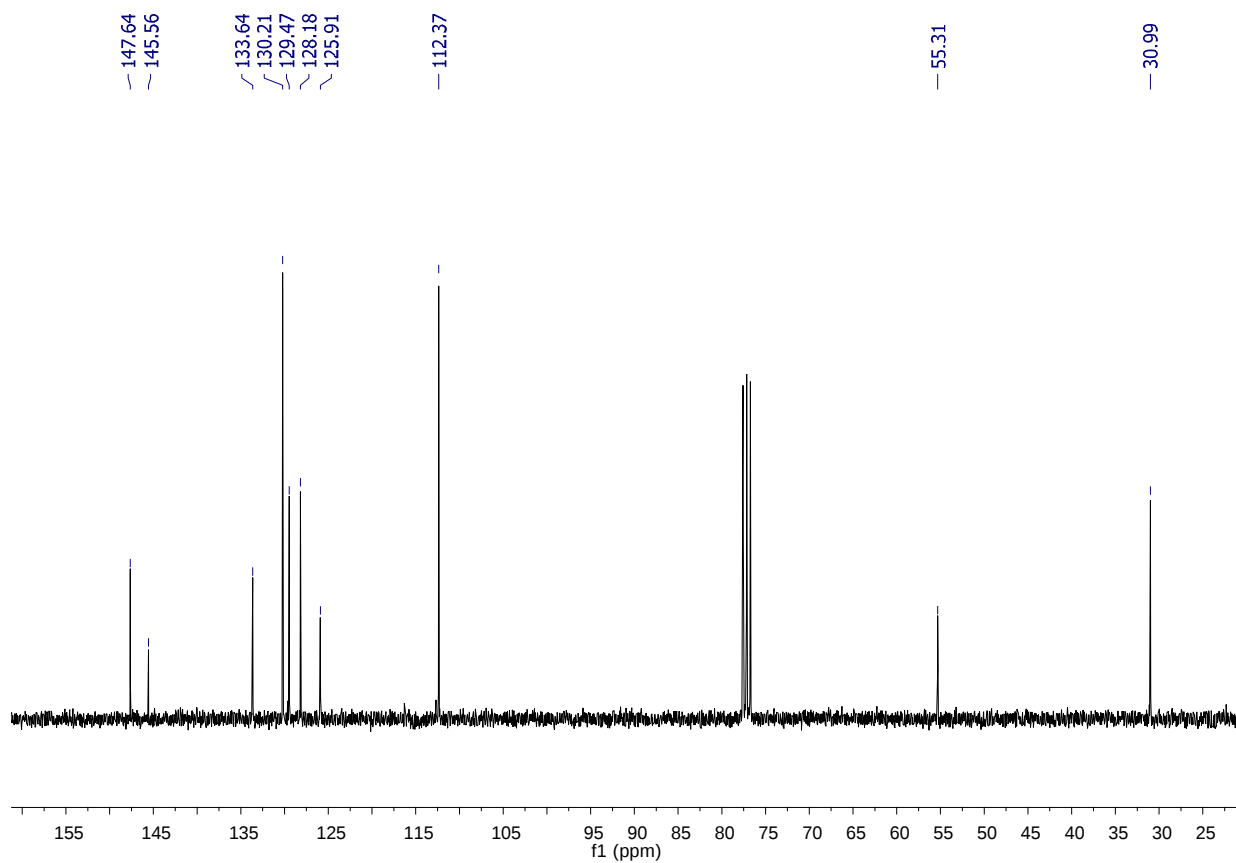
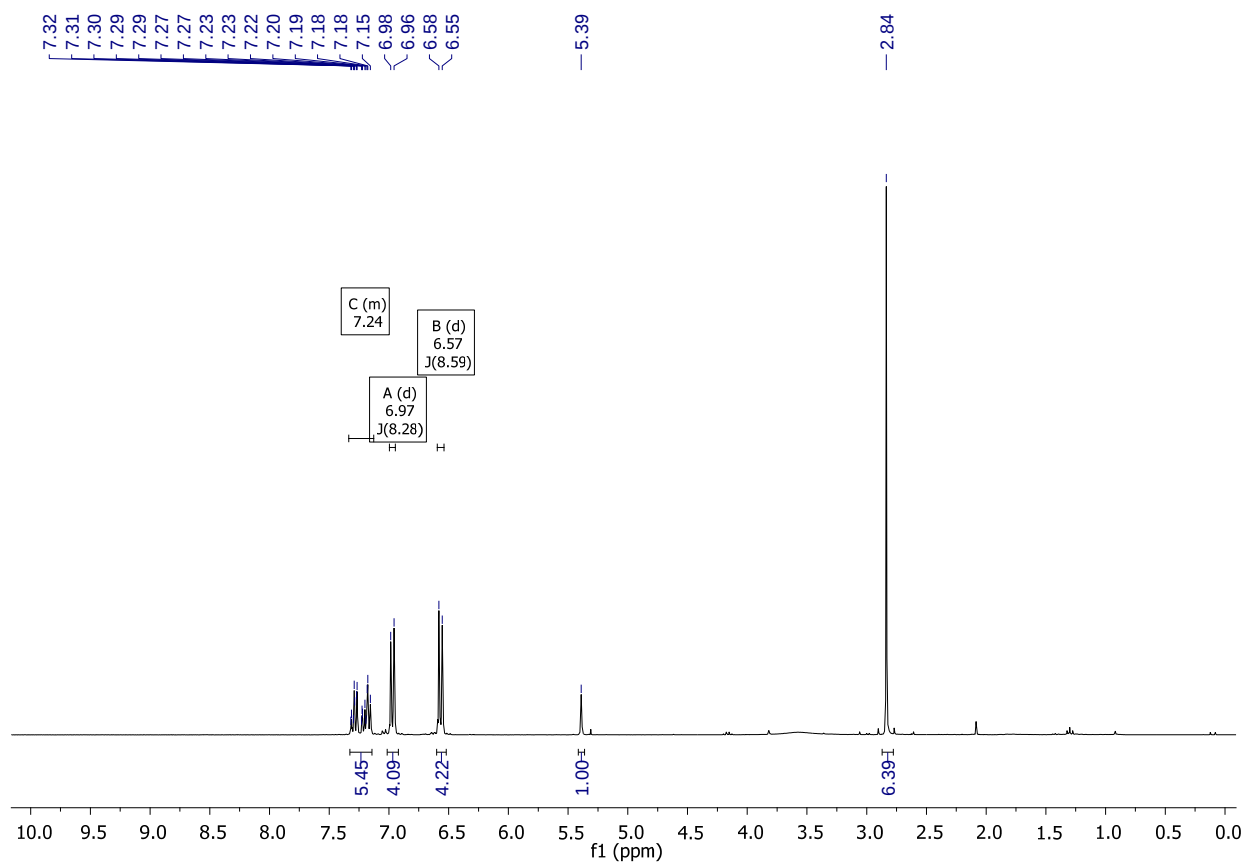
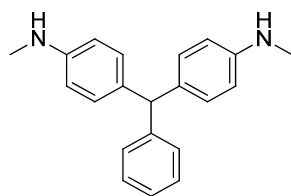
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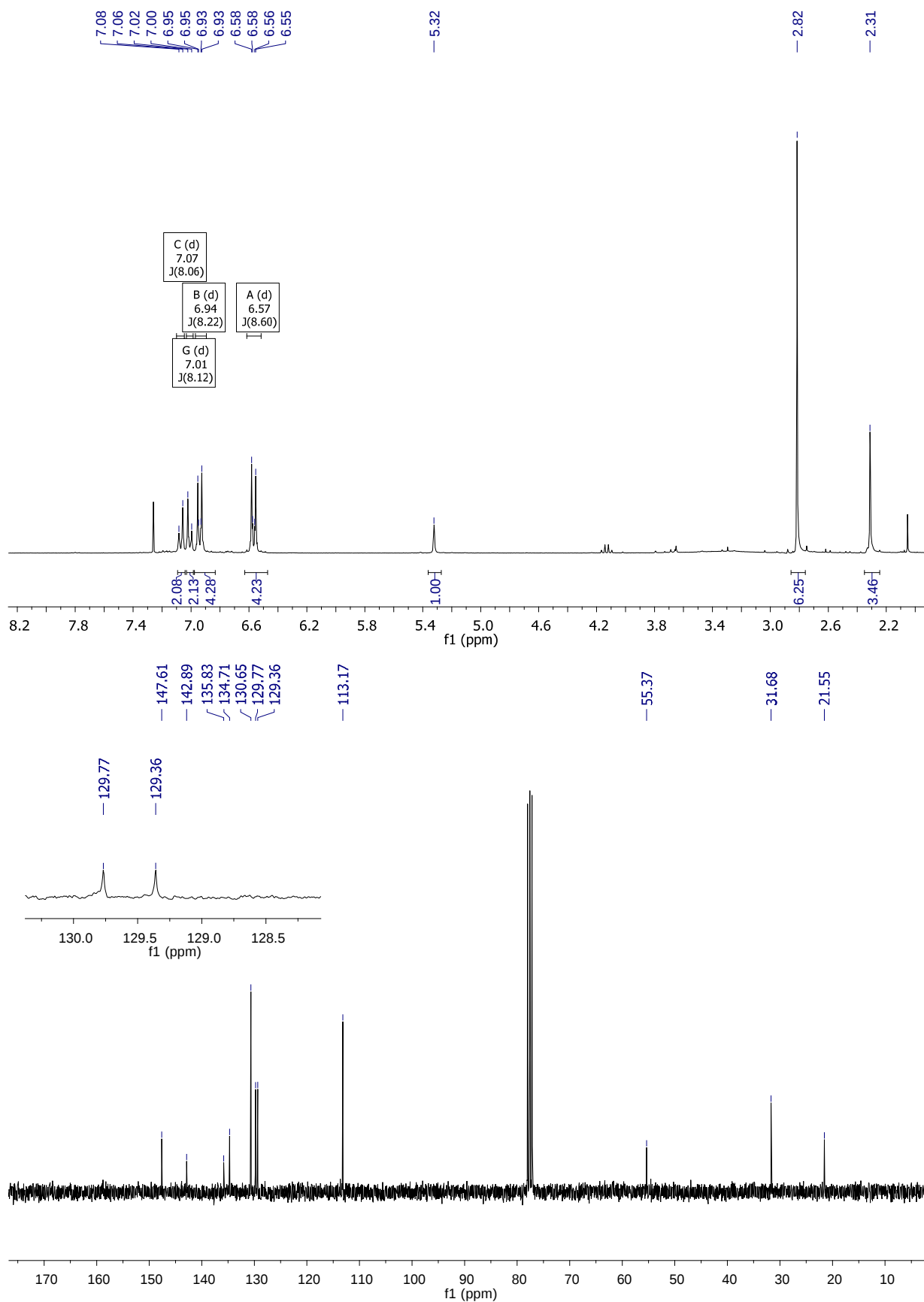
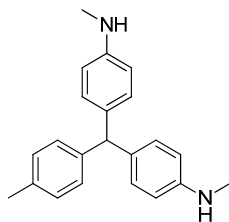
Compound 11



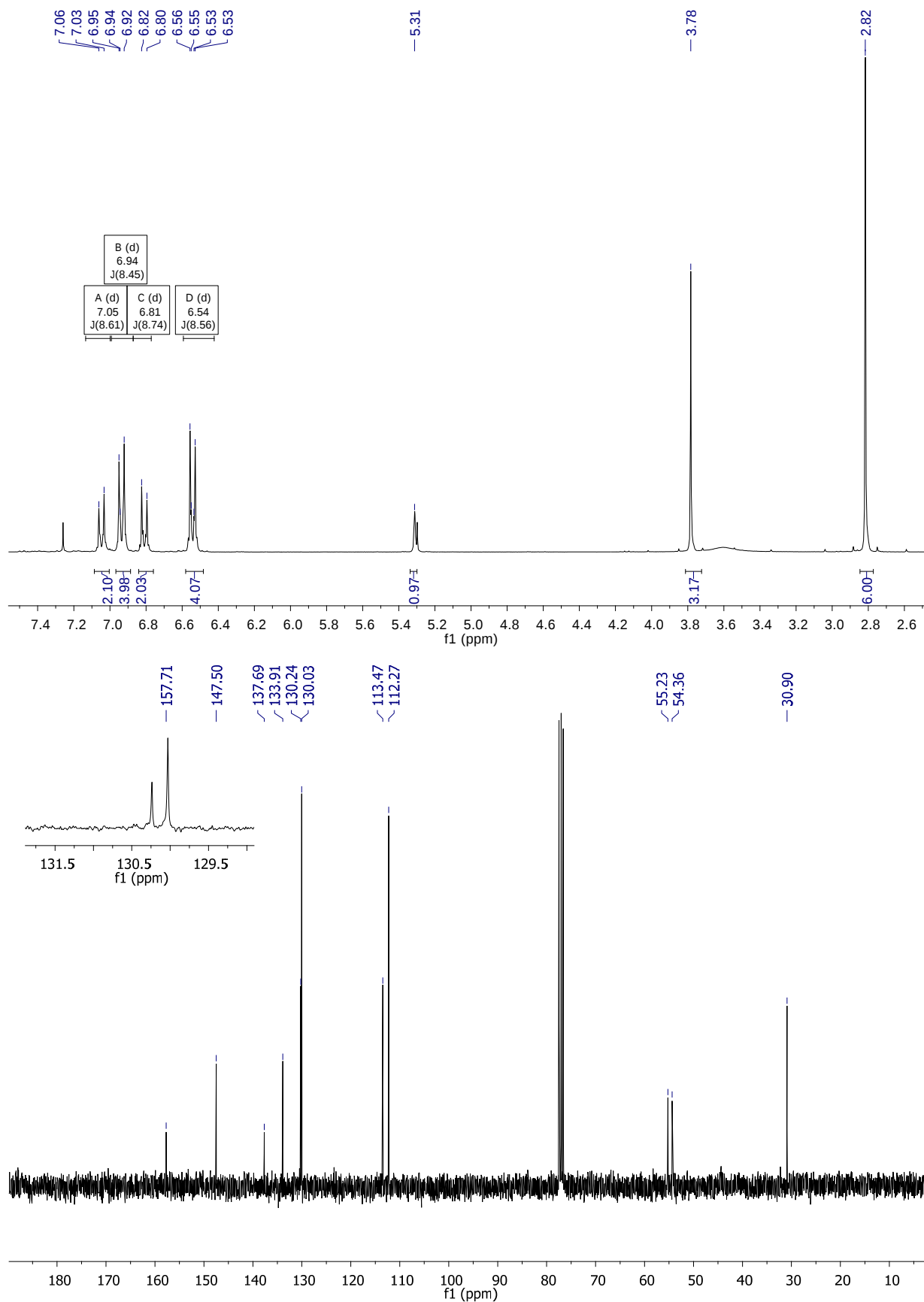
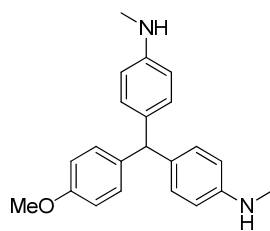
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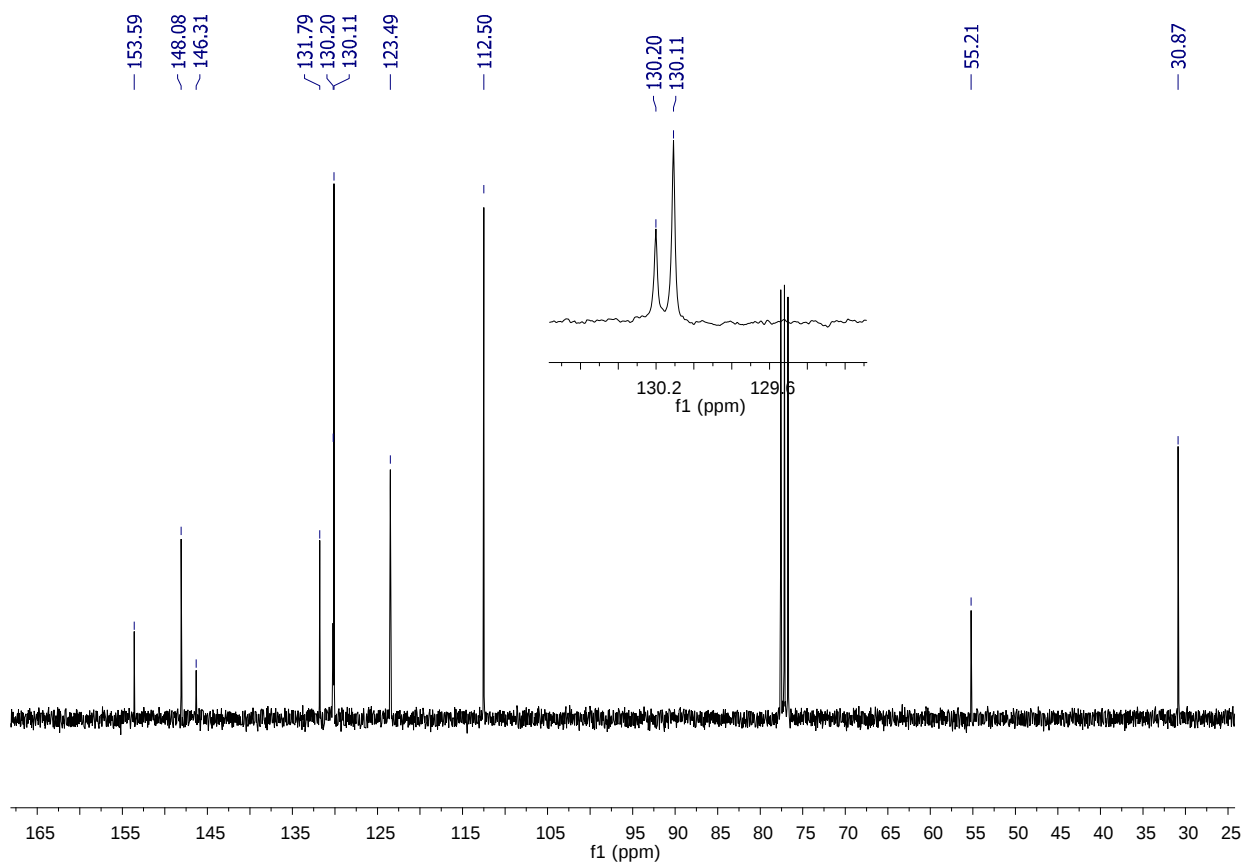
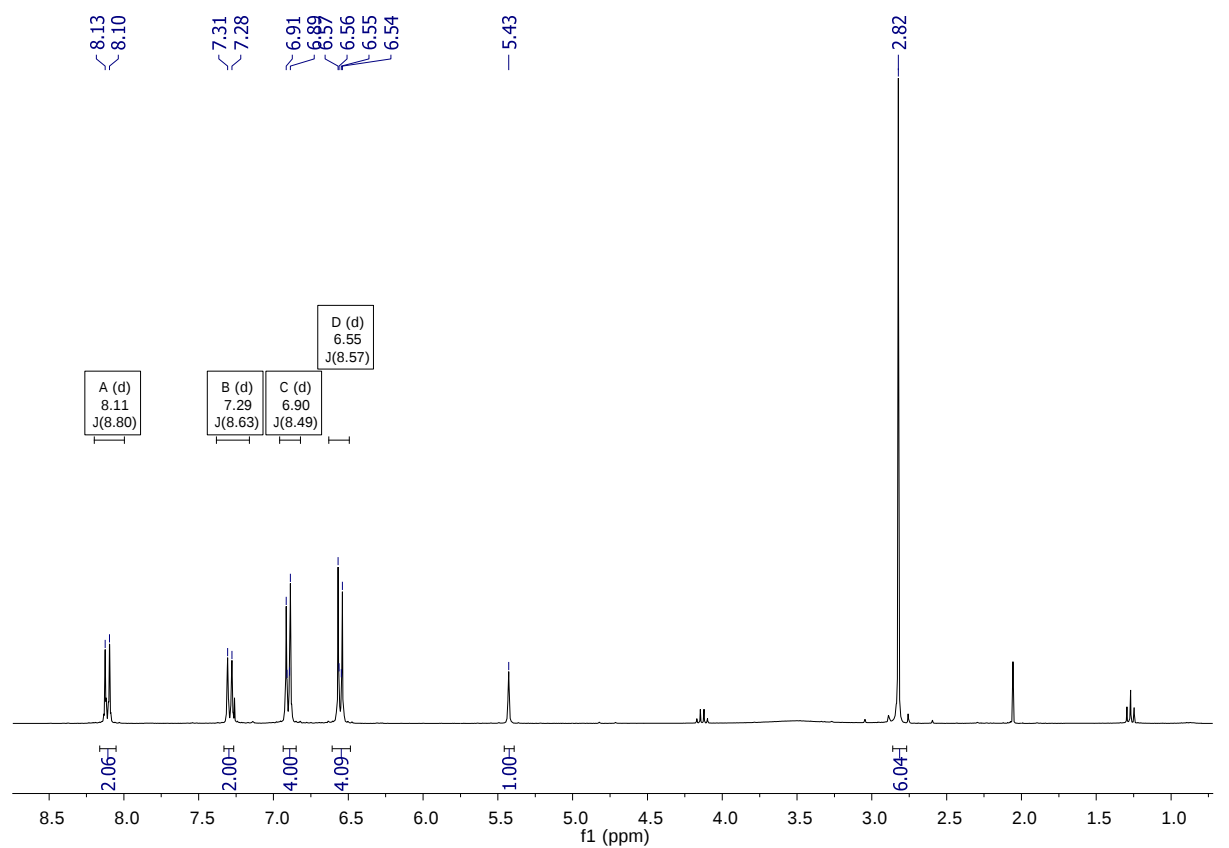
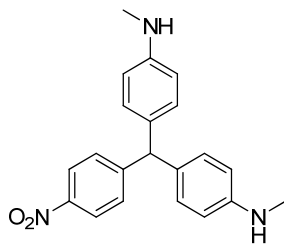
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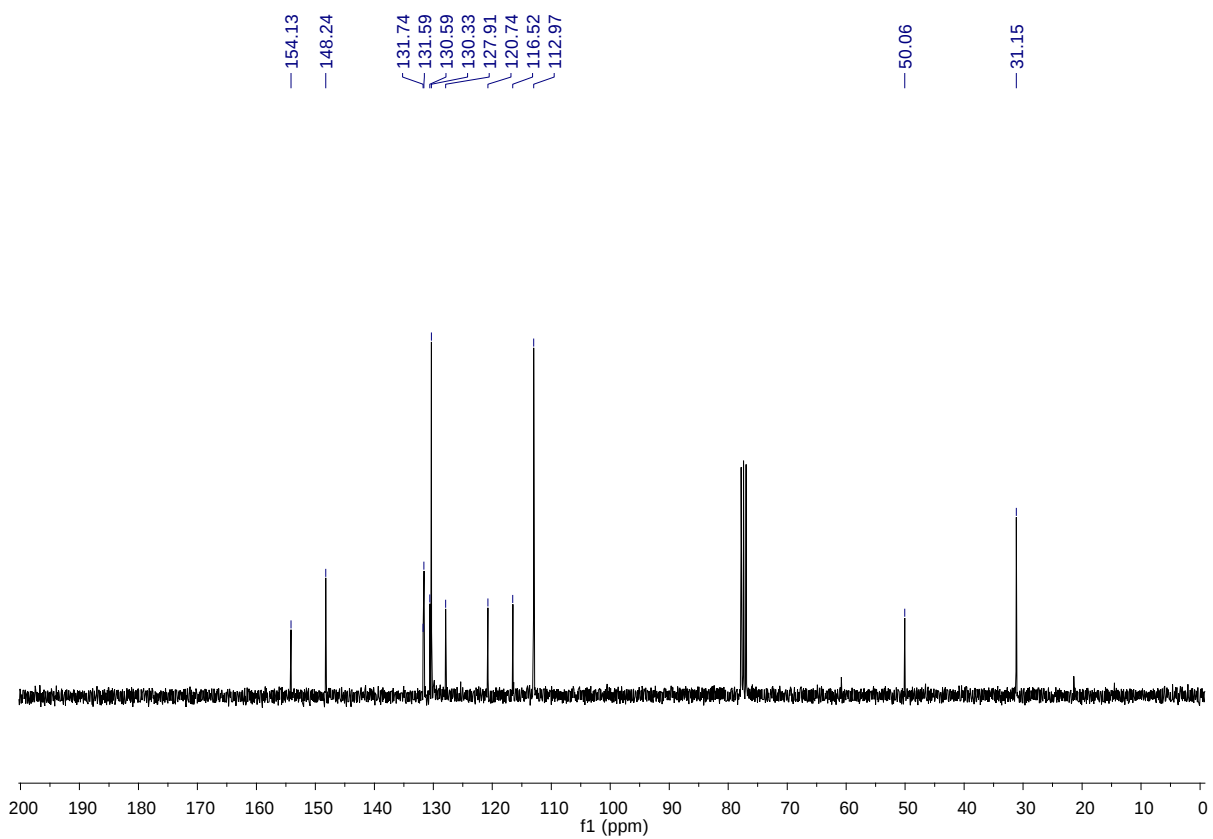
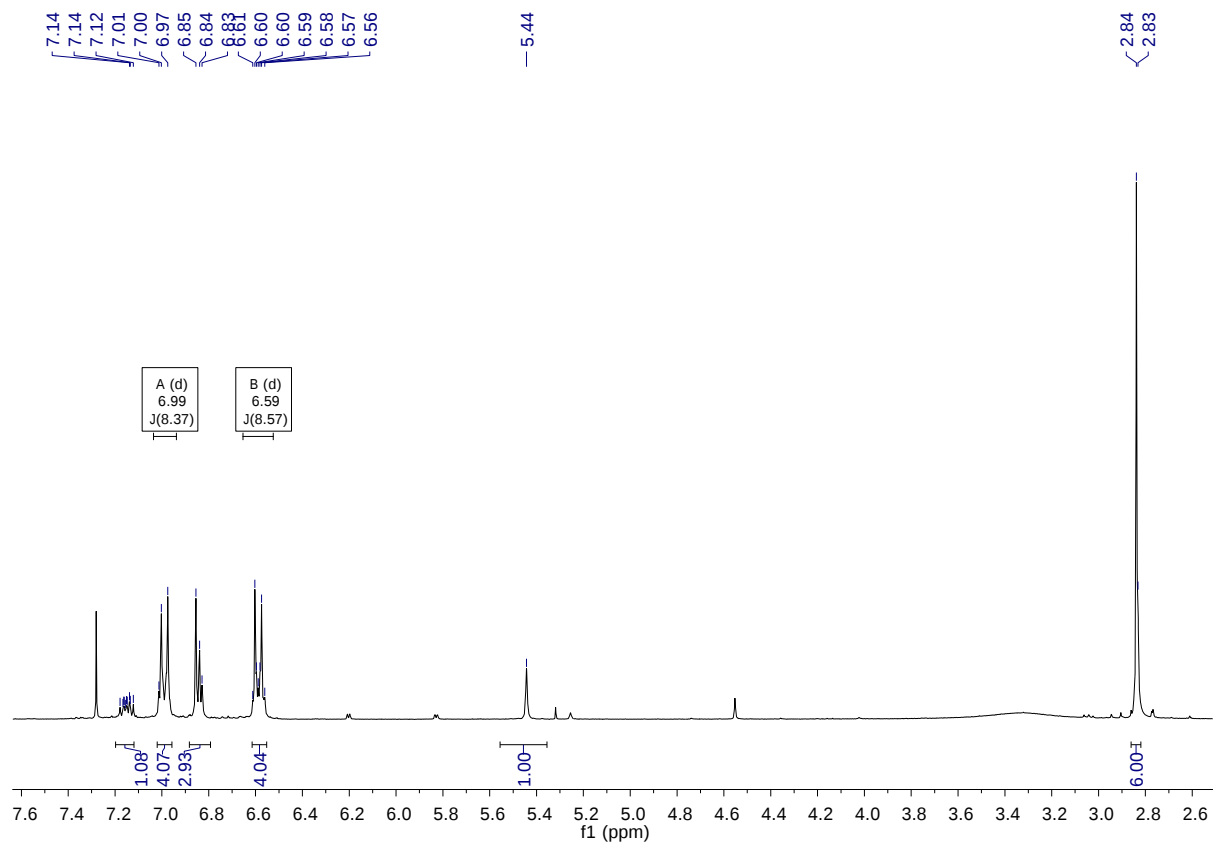
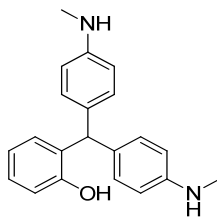
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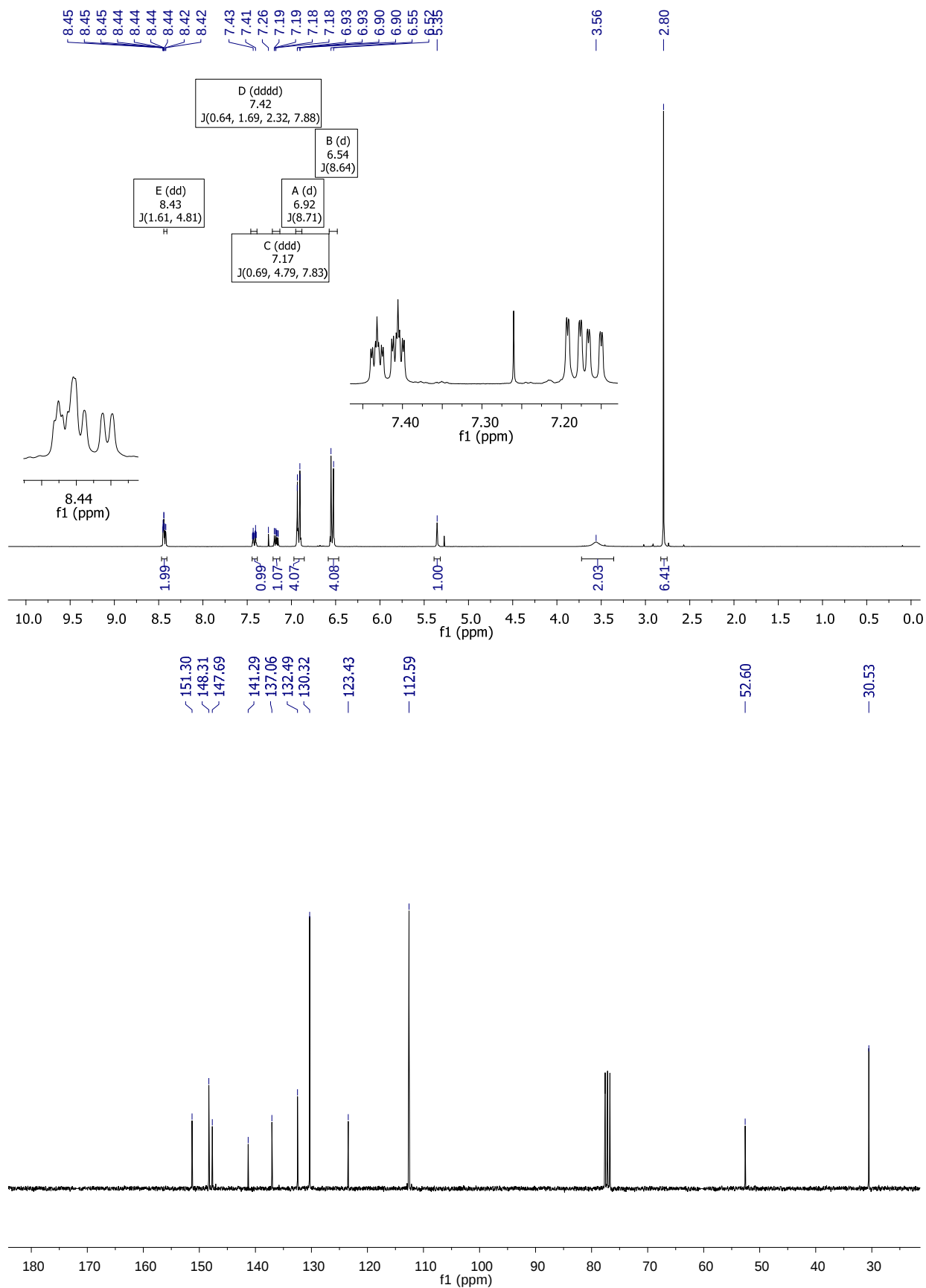
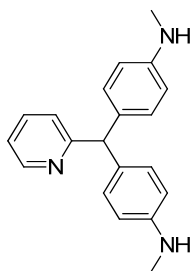
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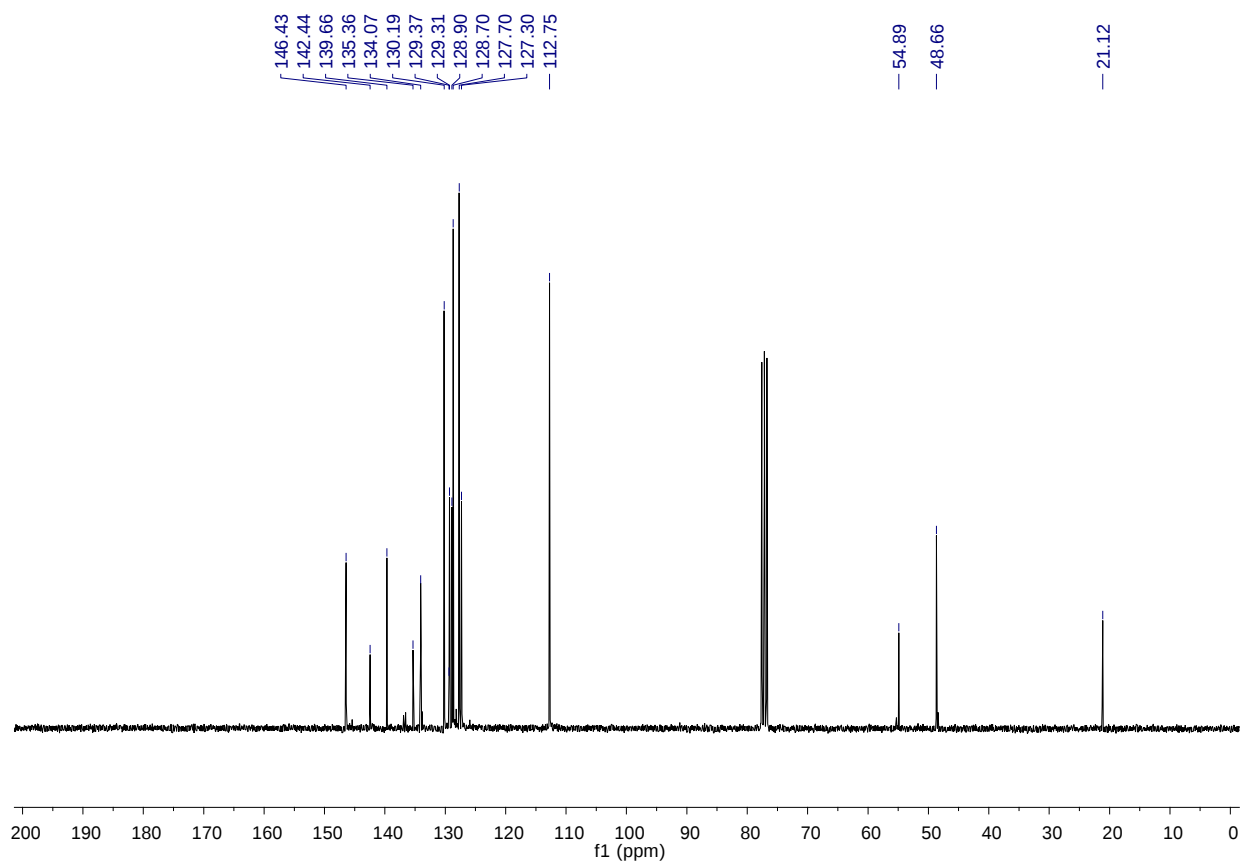
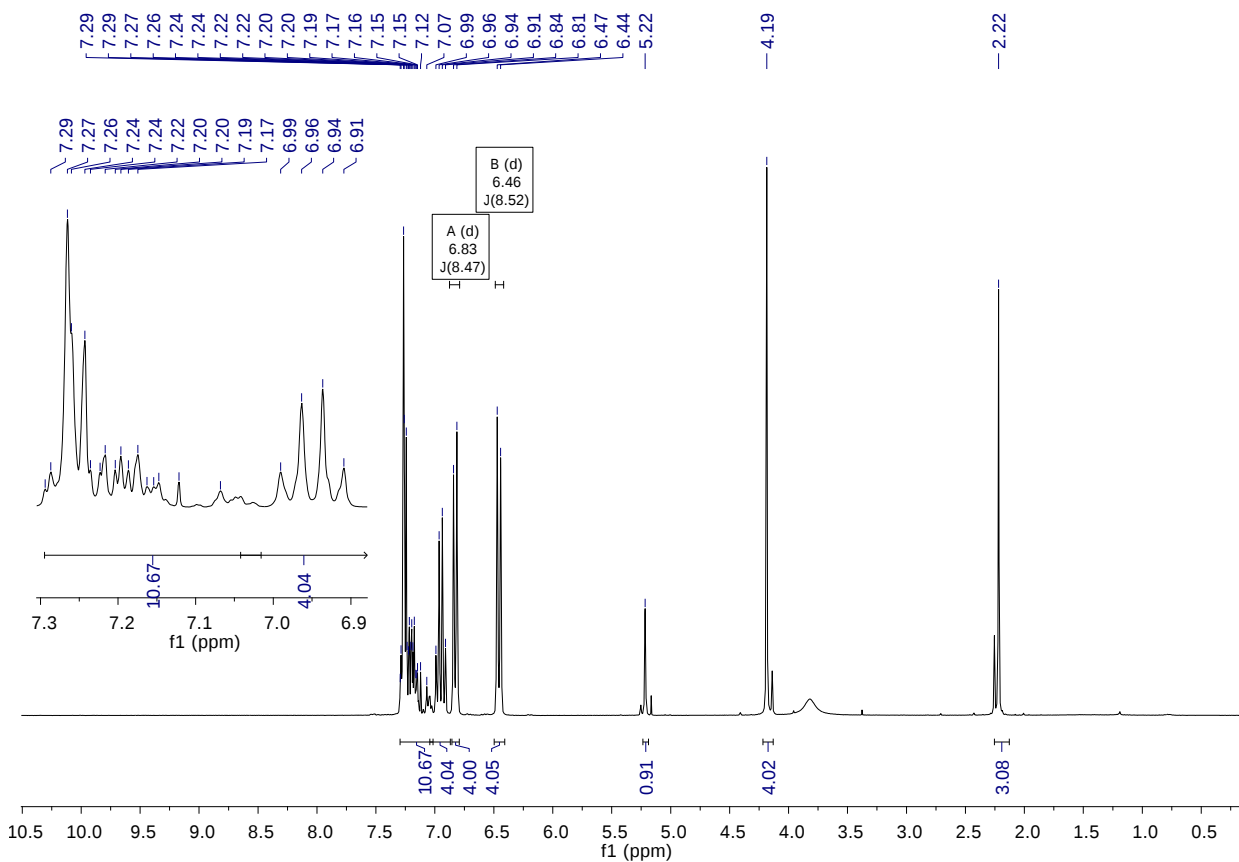
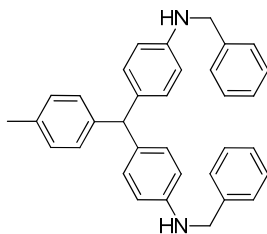
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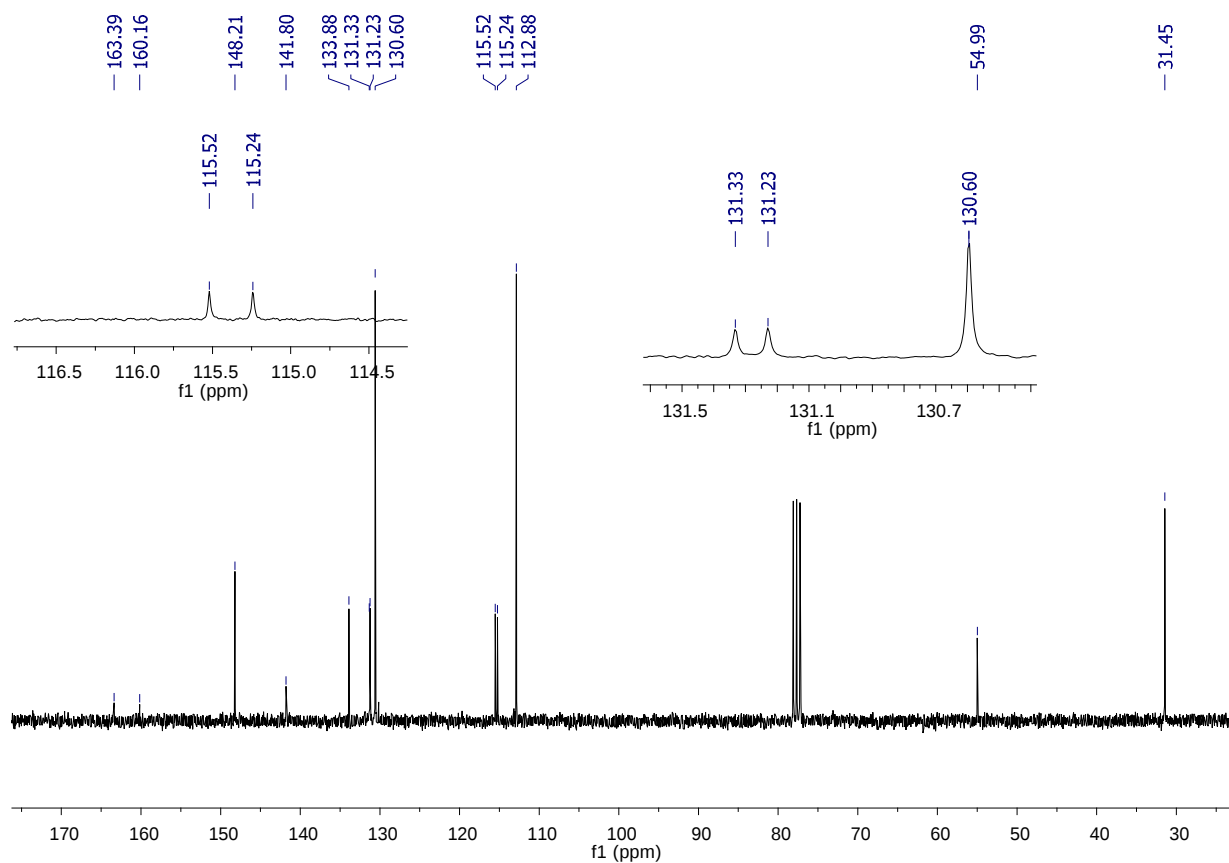
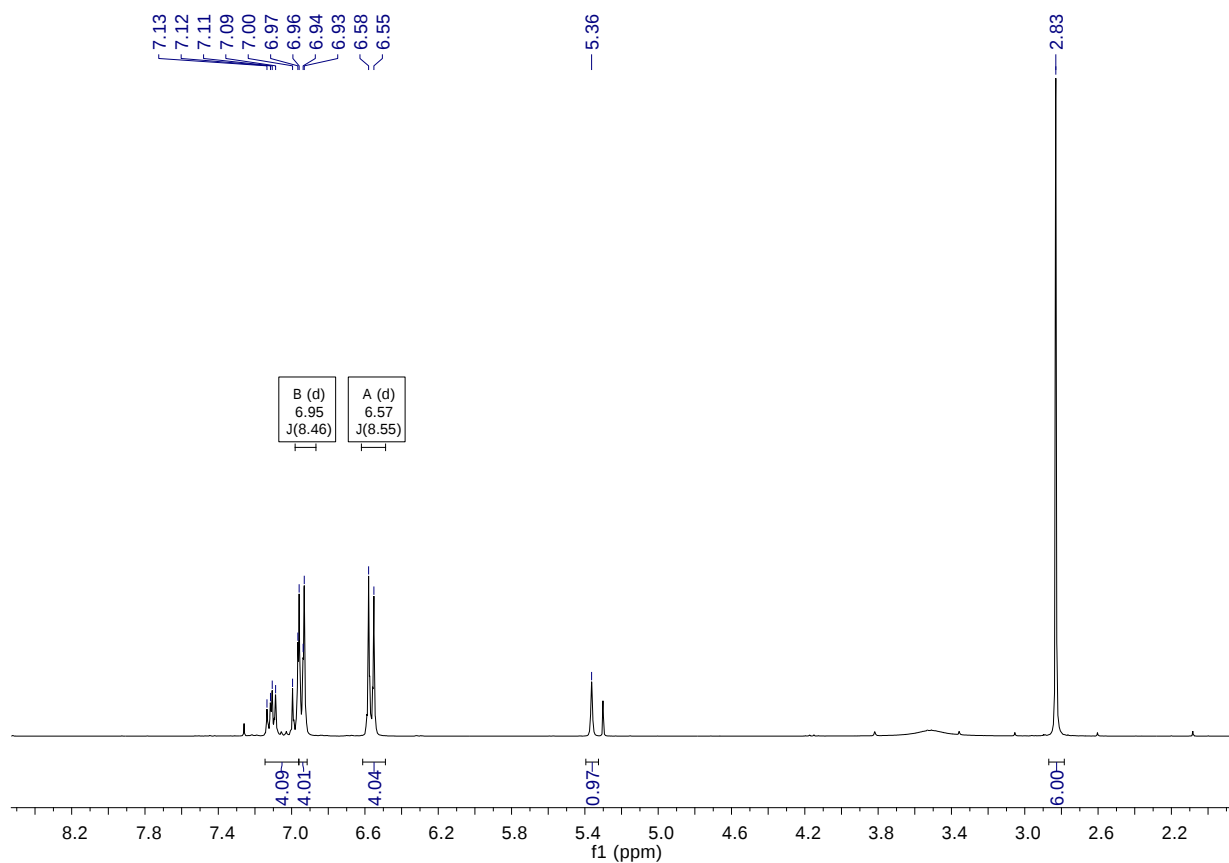
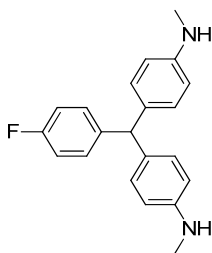
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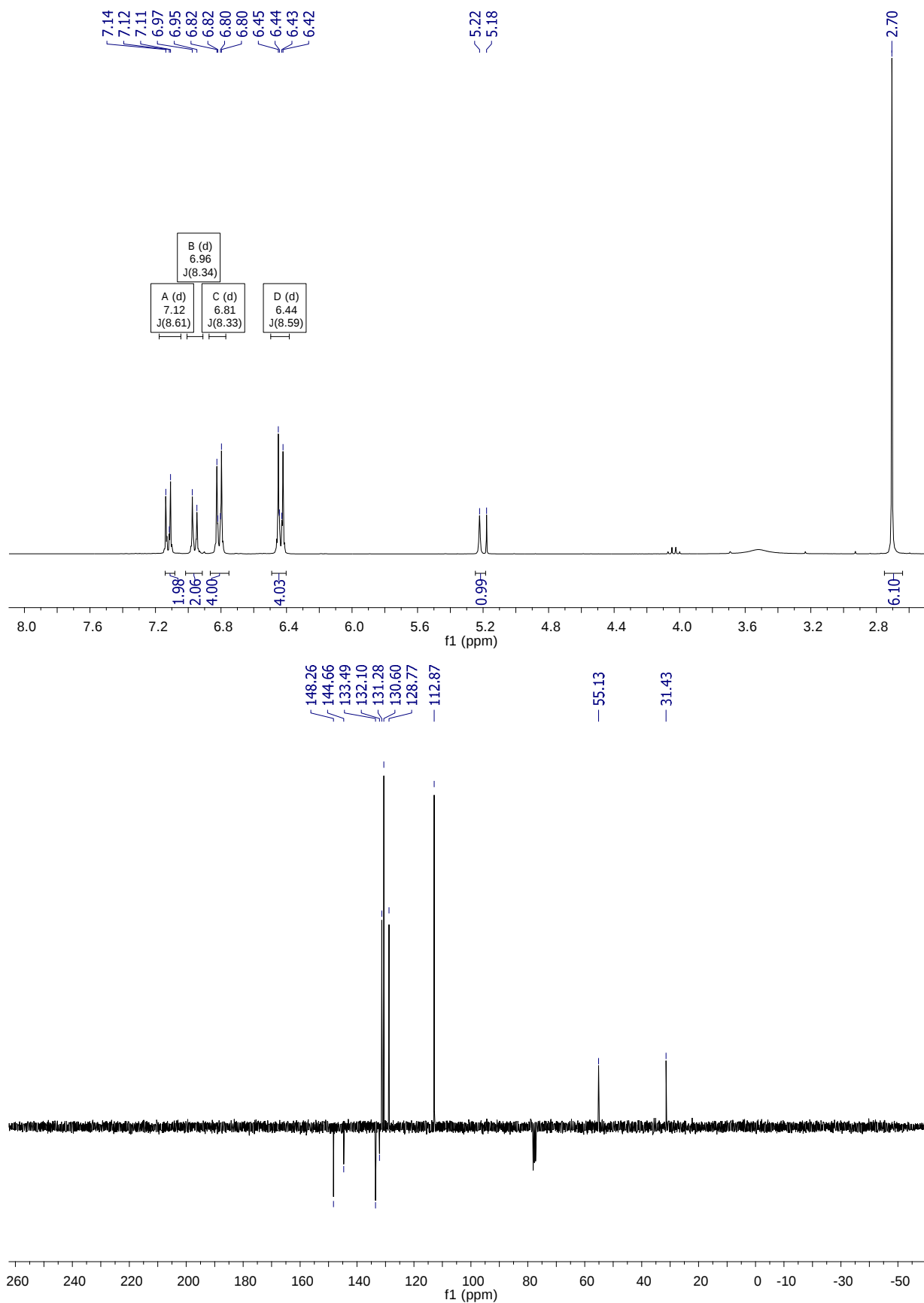
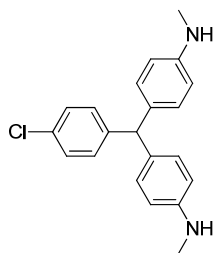
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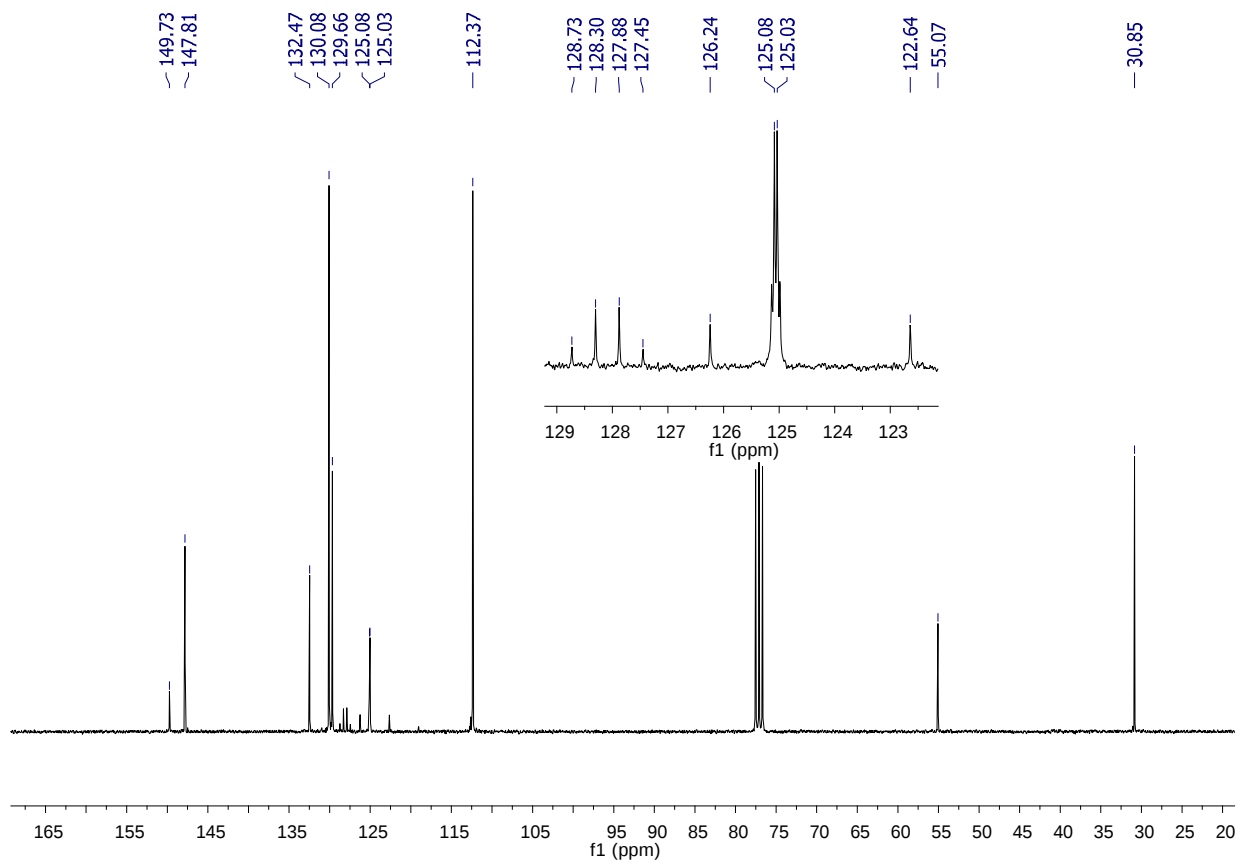
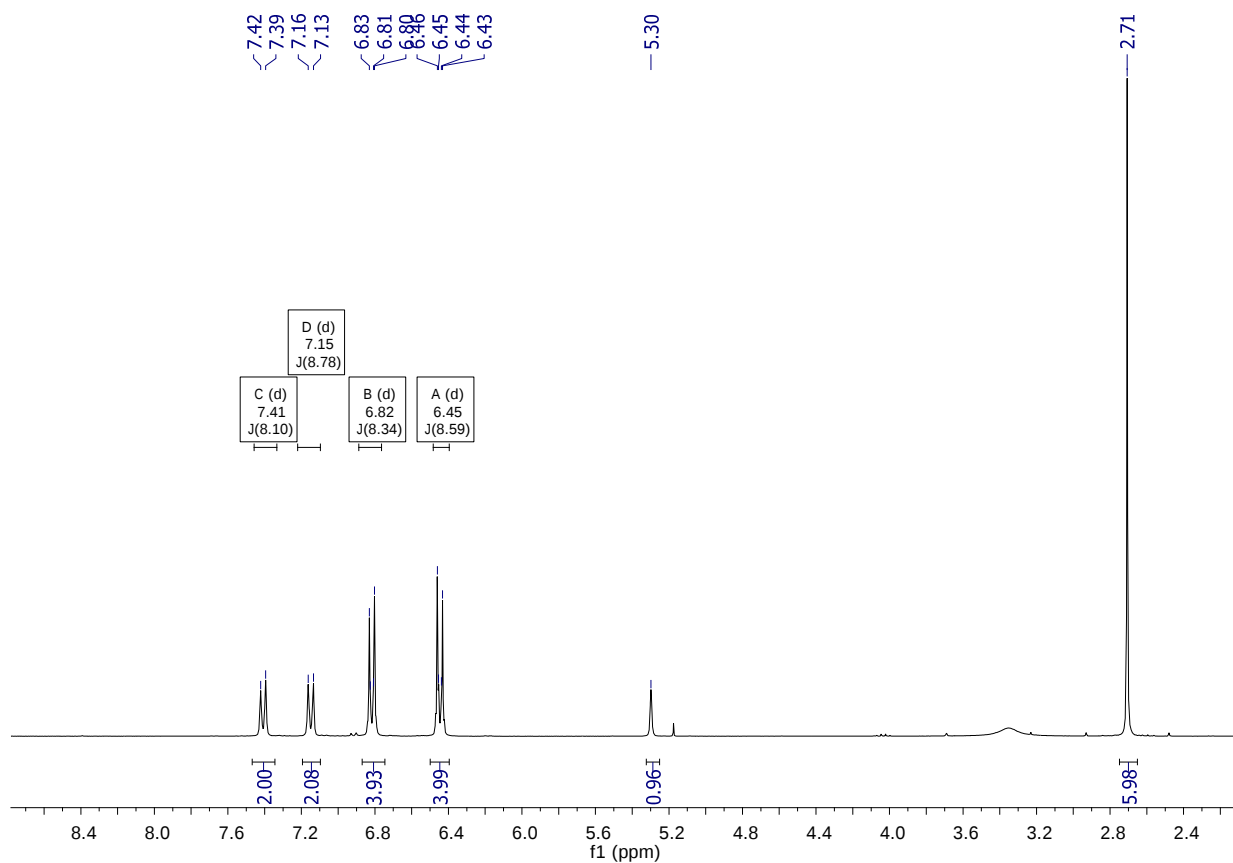
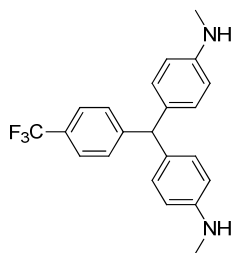
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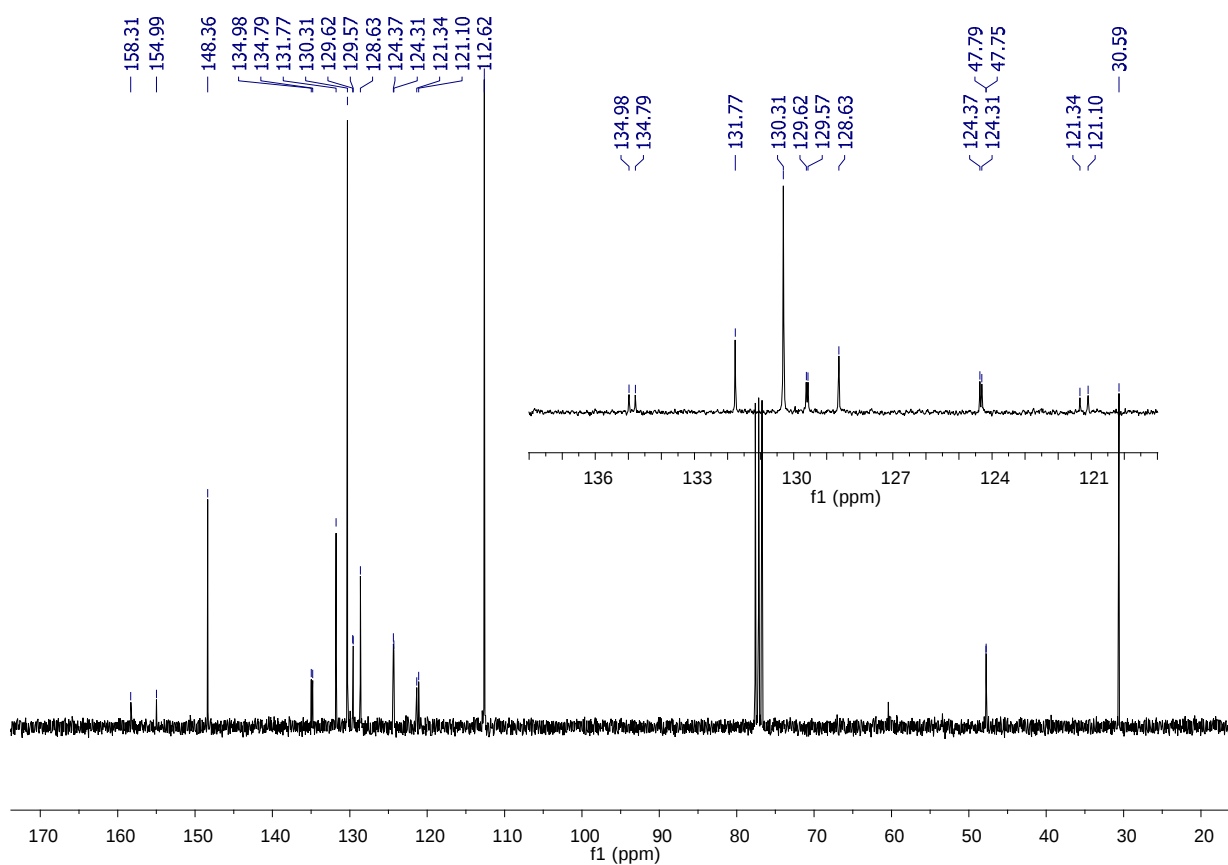
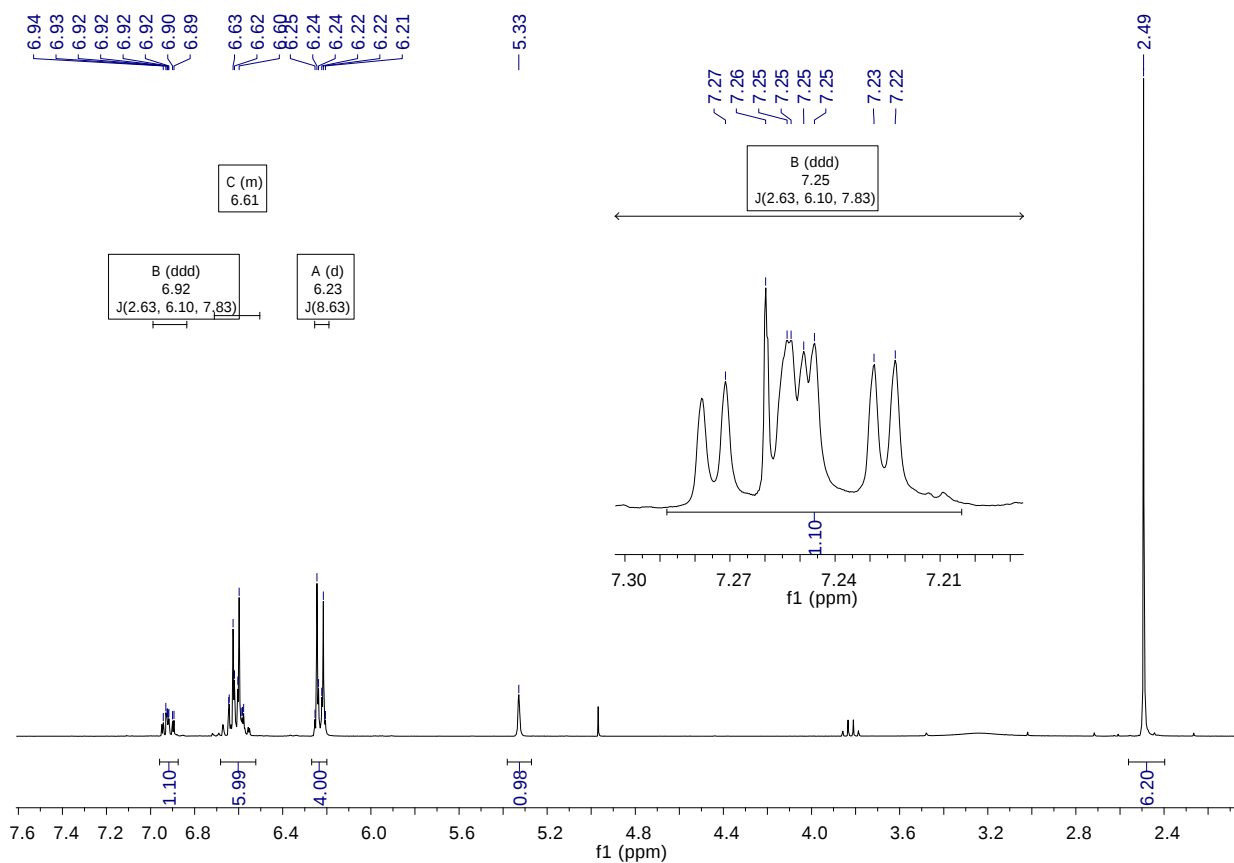
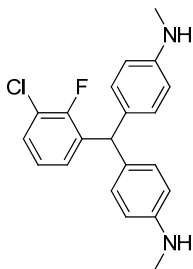
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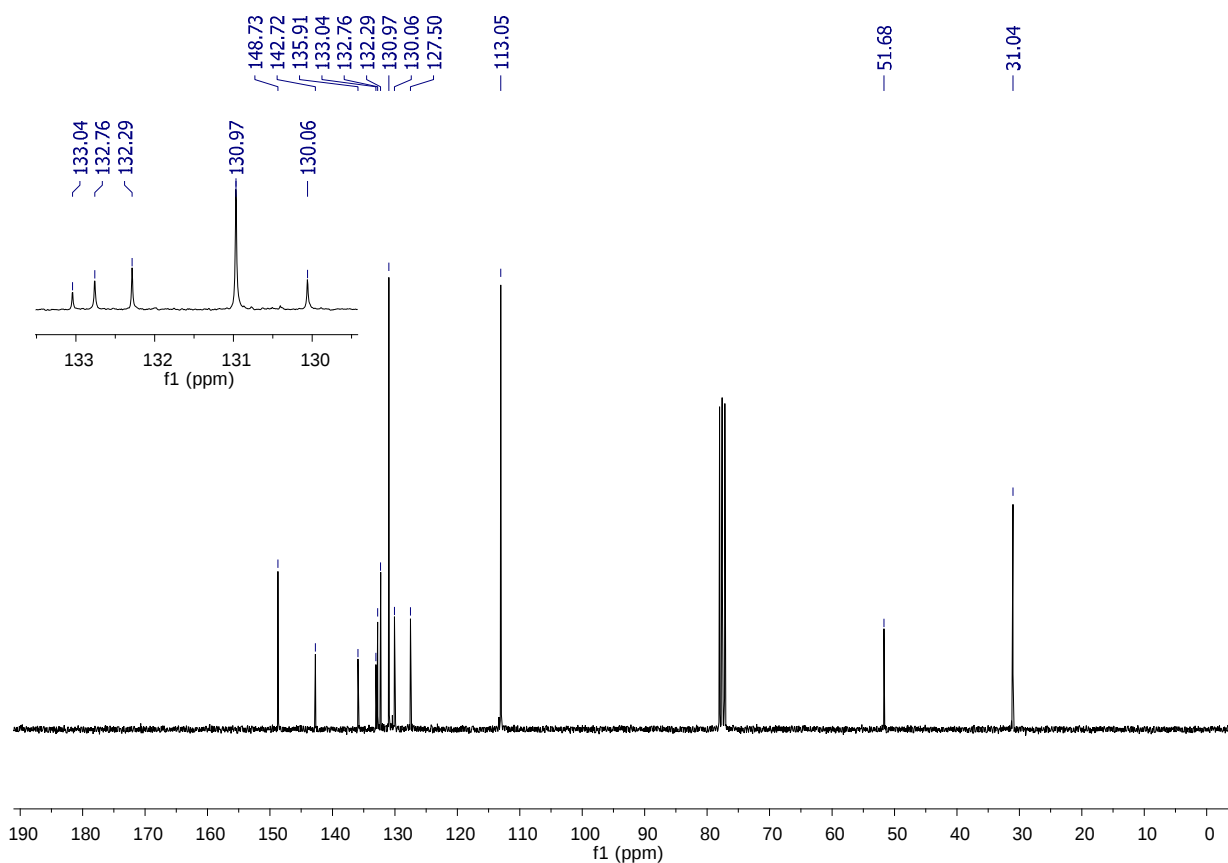
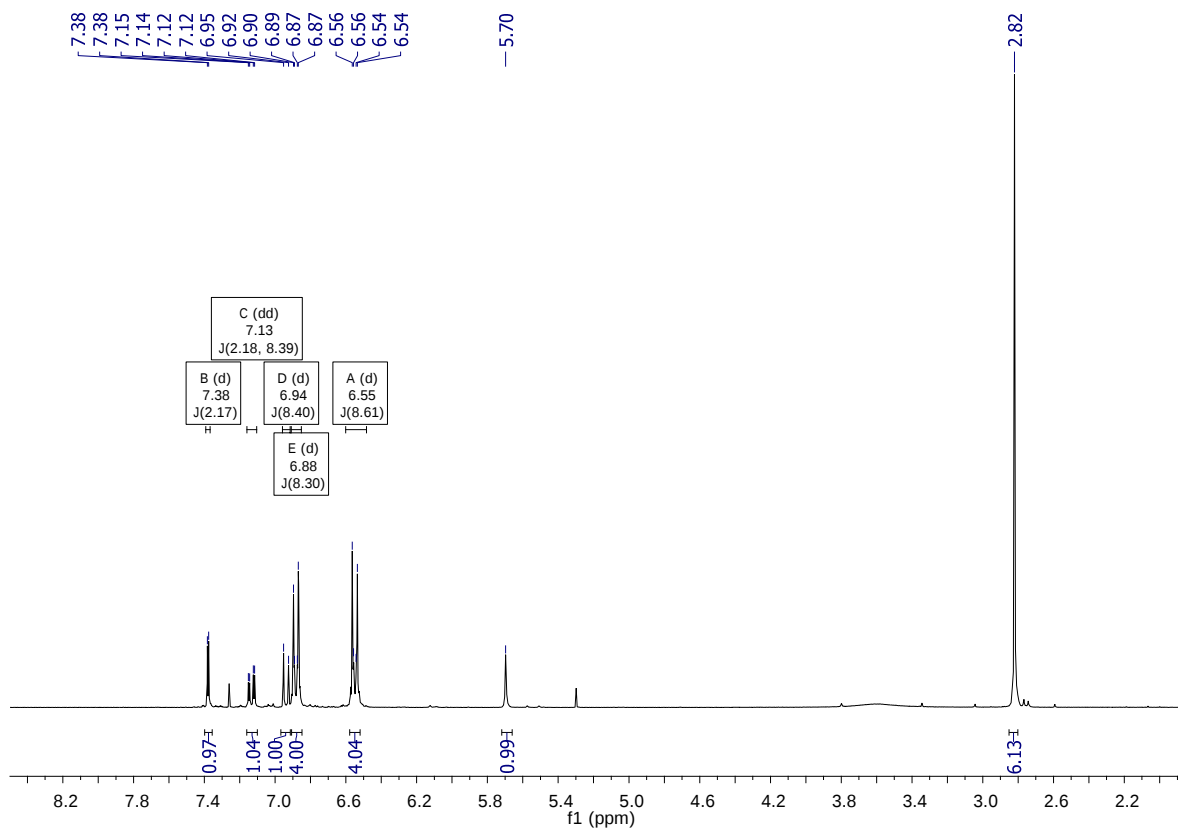
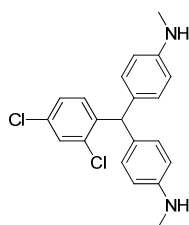
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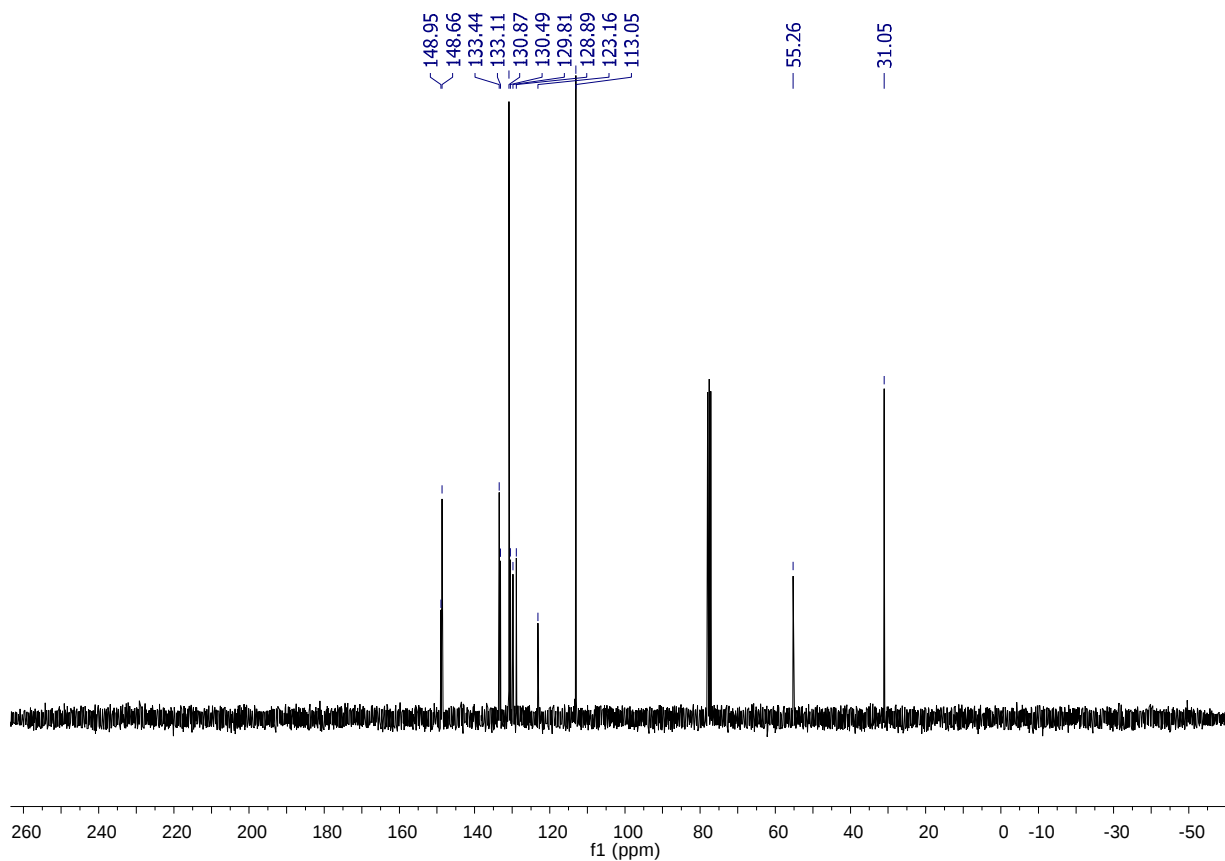
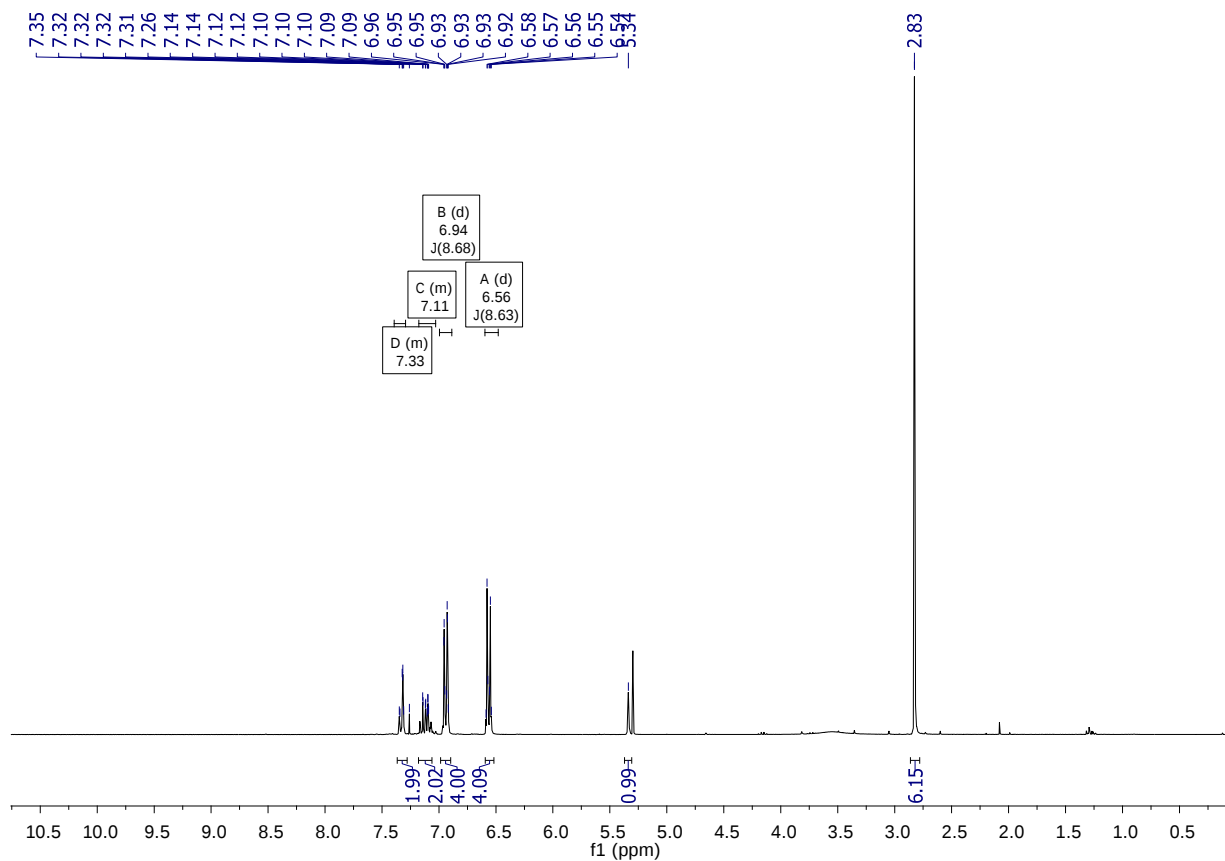
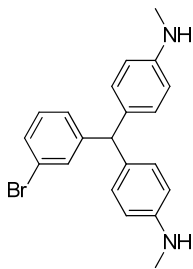
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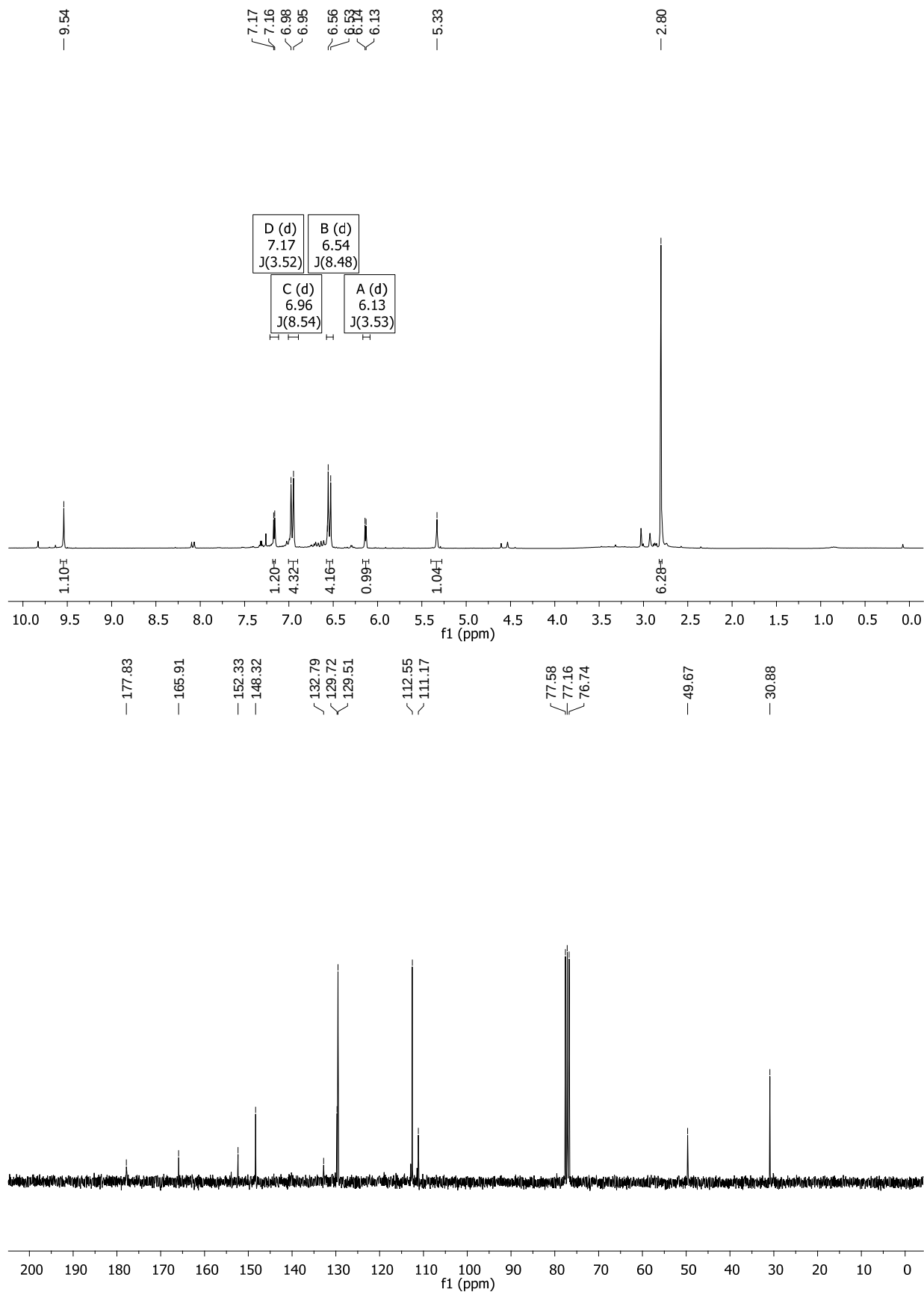
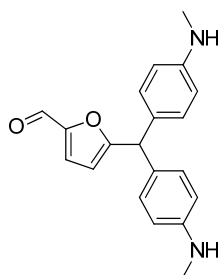
Compound **23**



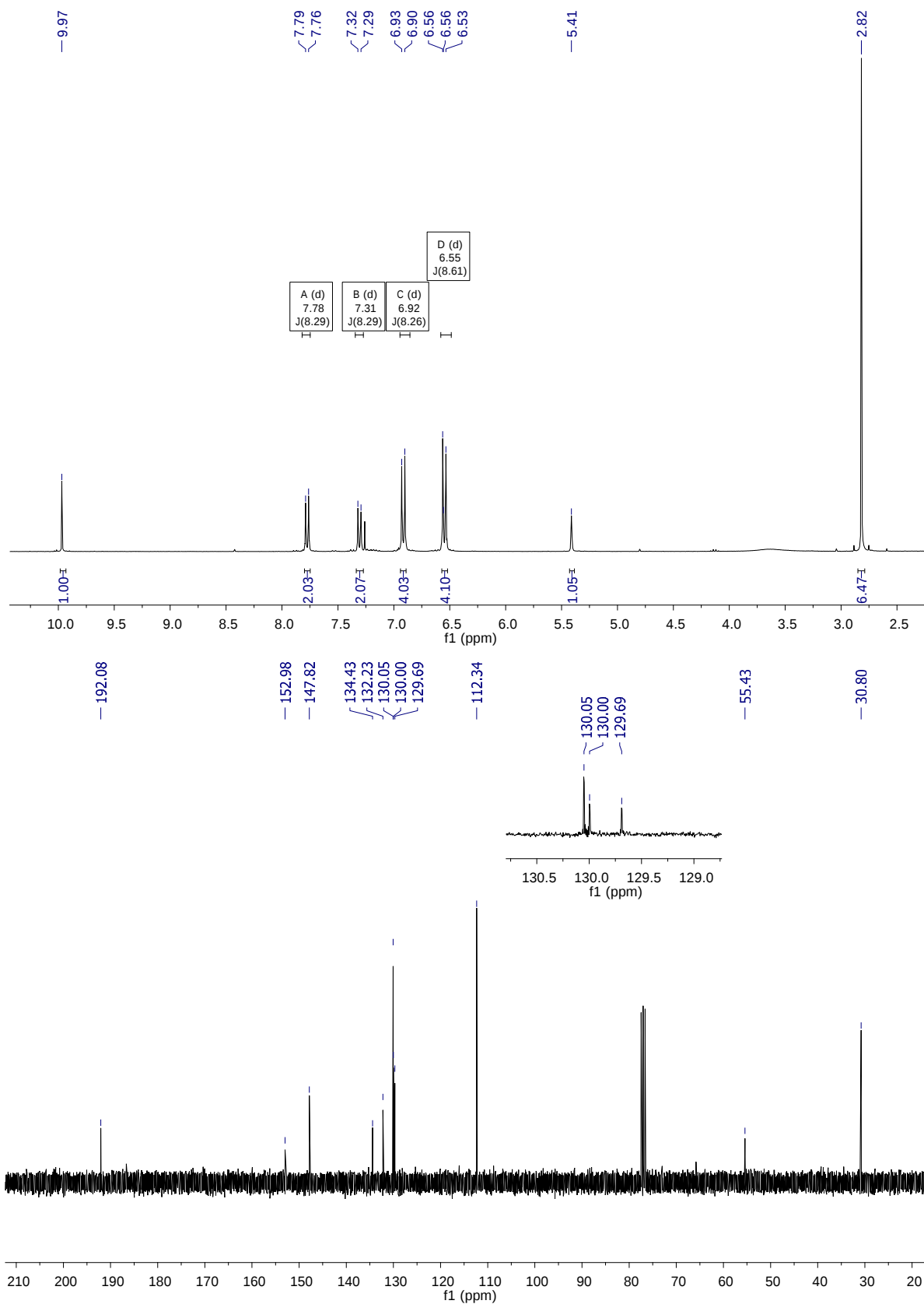
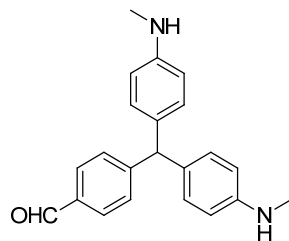
Compound **24**



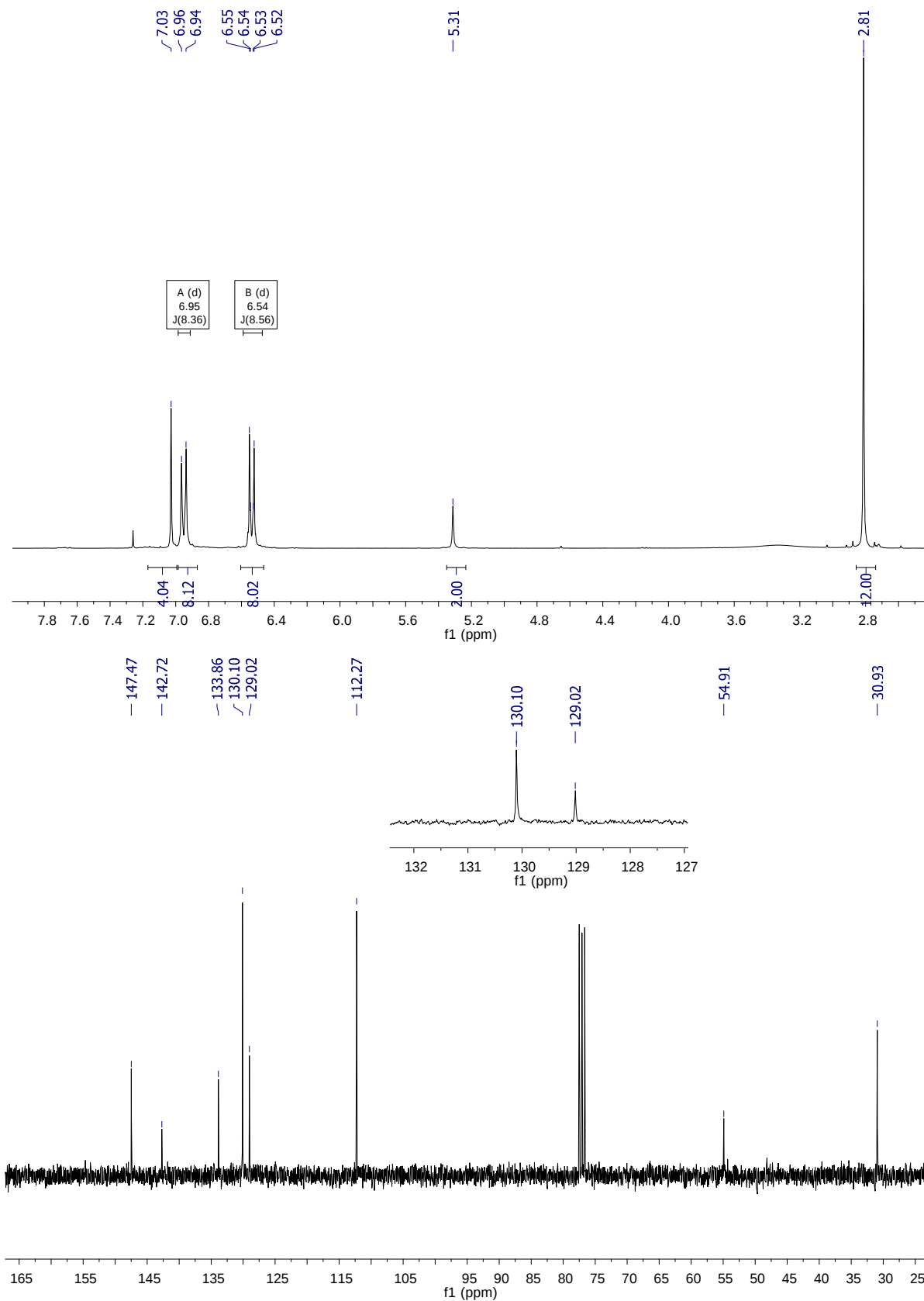
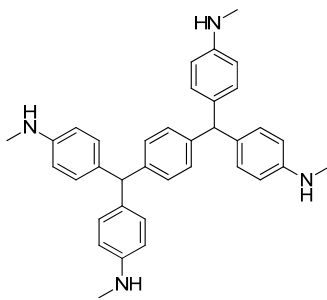
Compound **25**



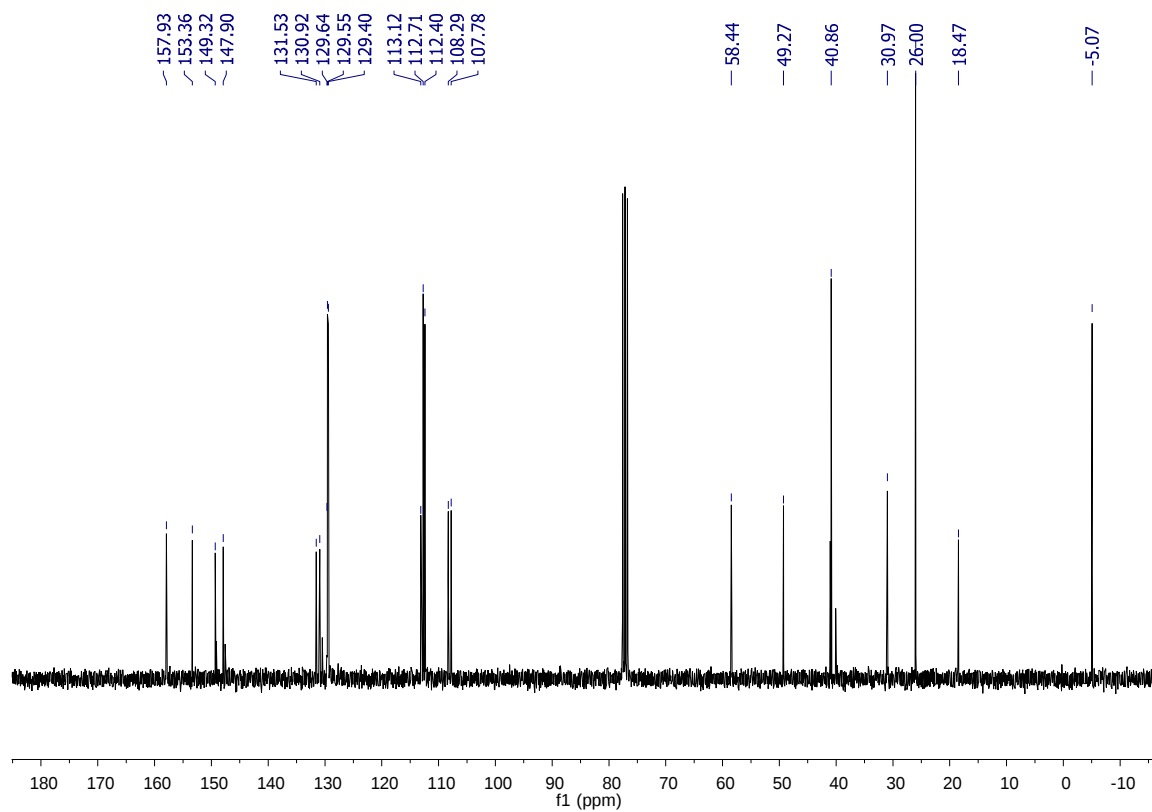
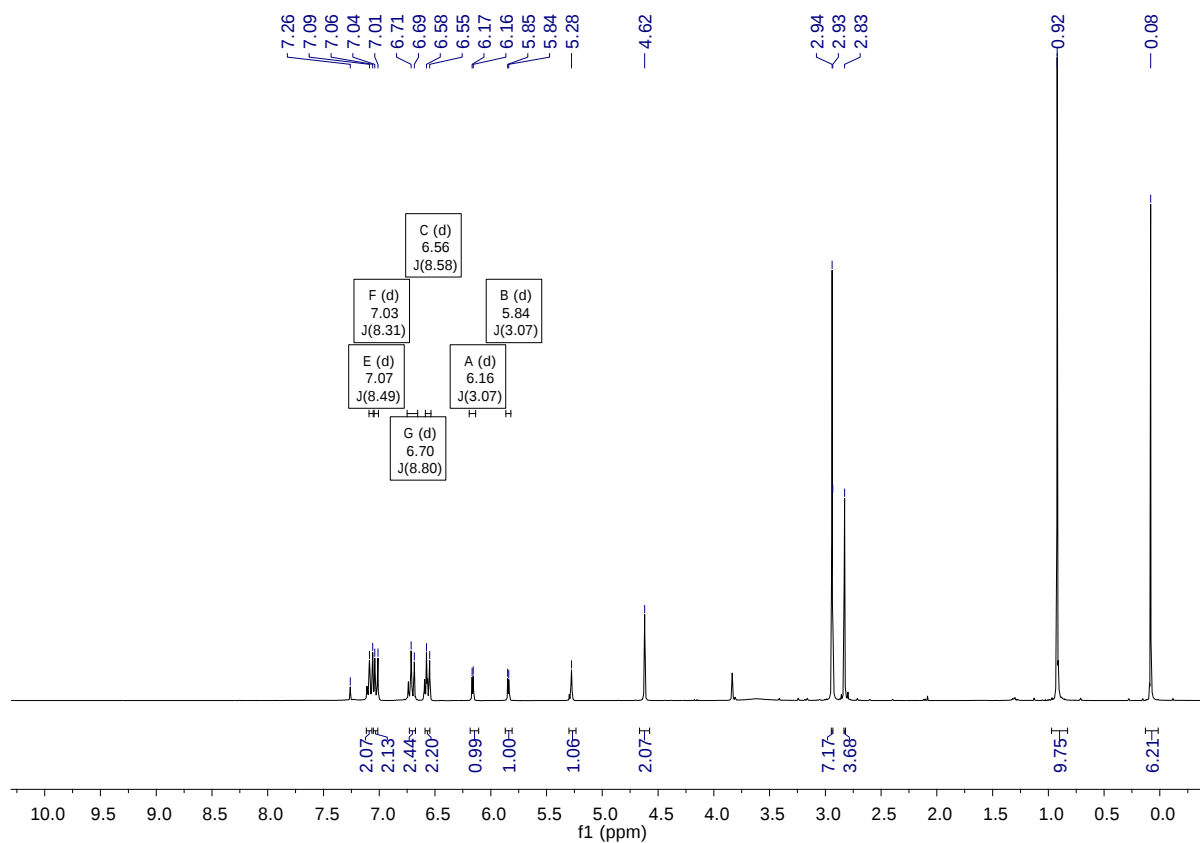
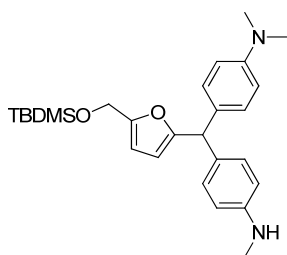
Compound **26**

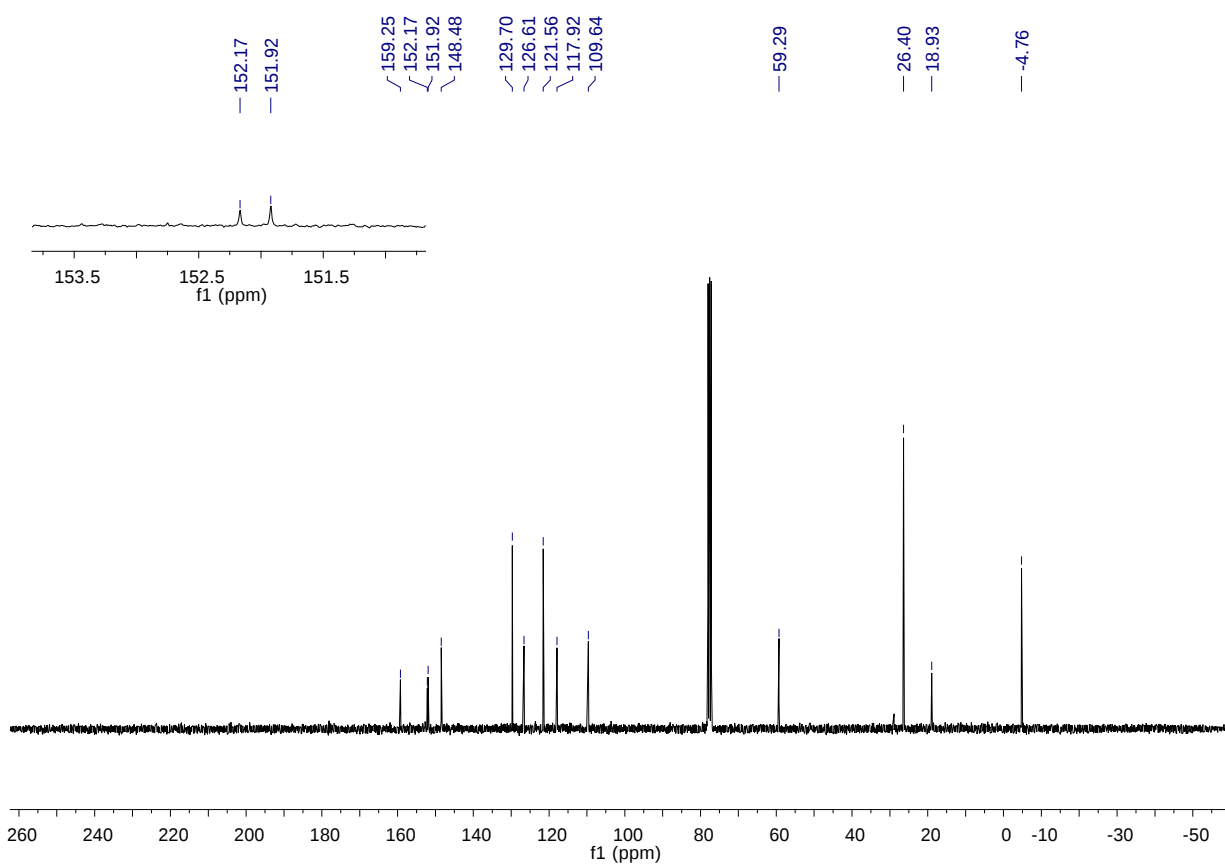
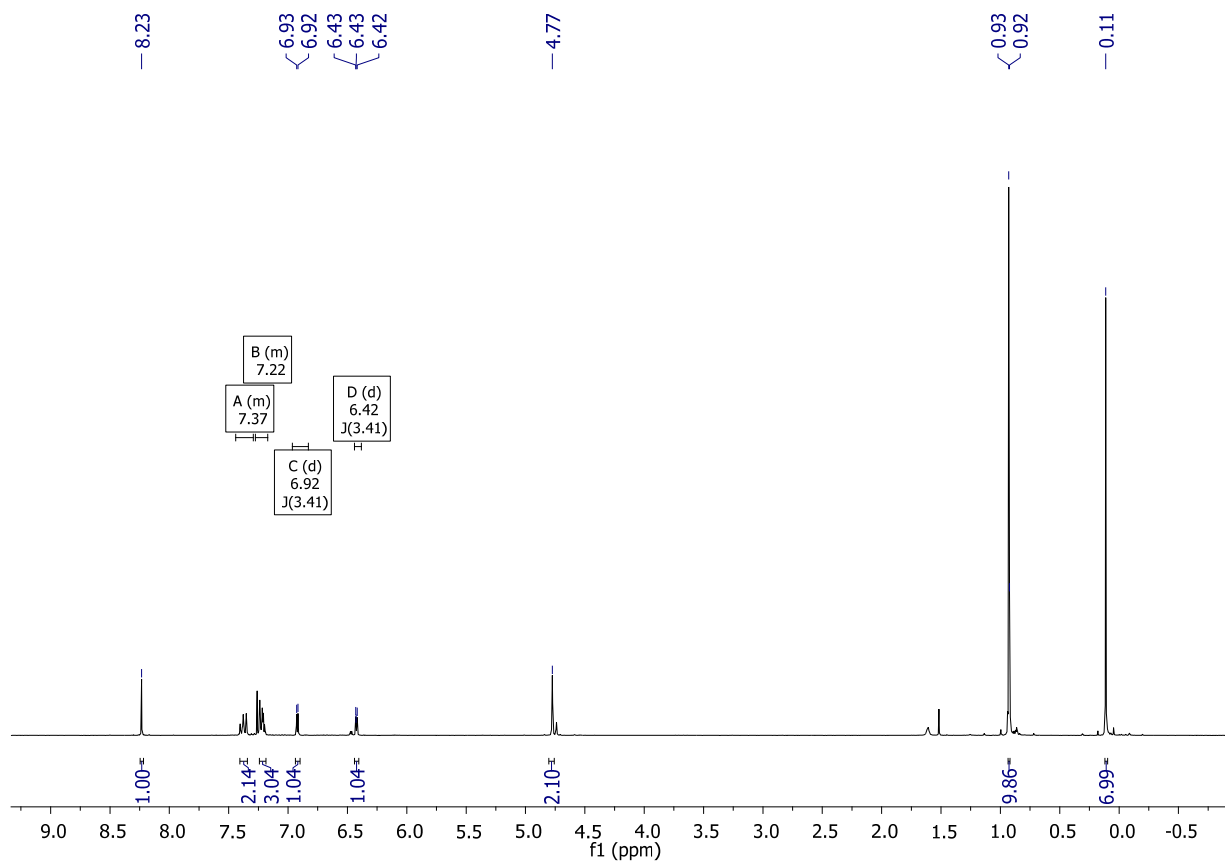
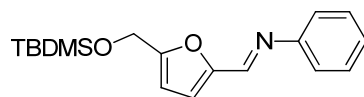


Compound **27**



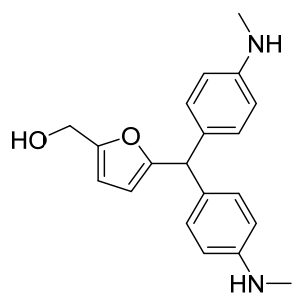
Compound **28**





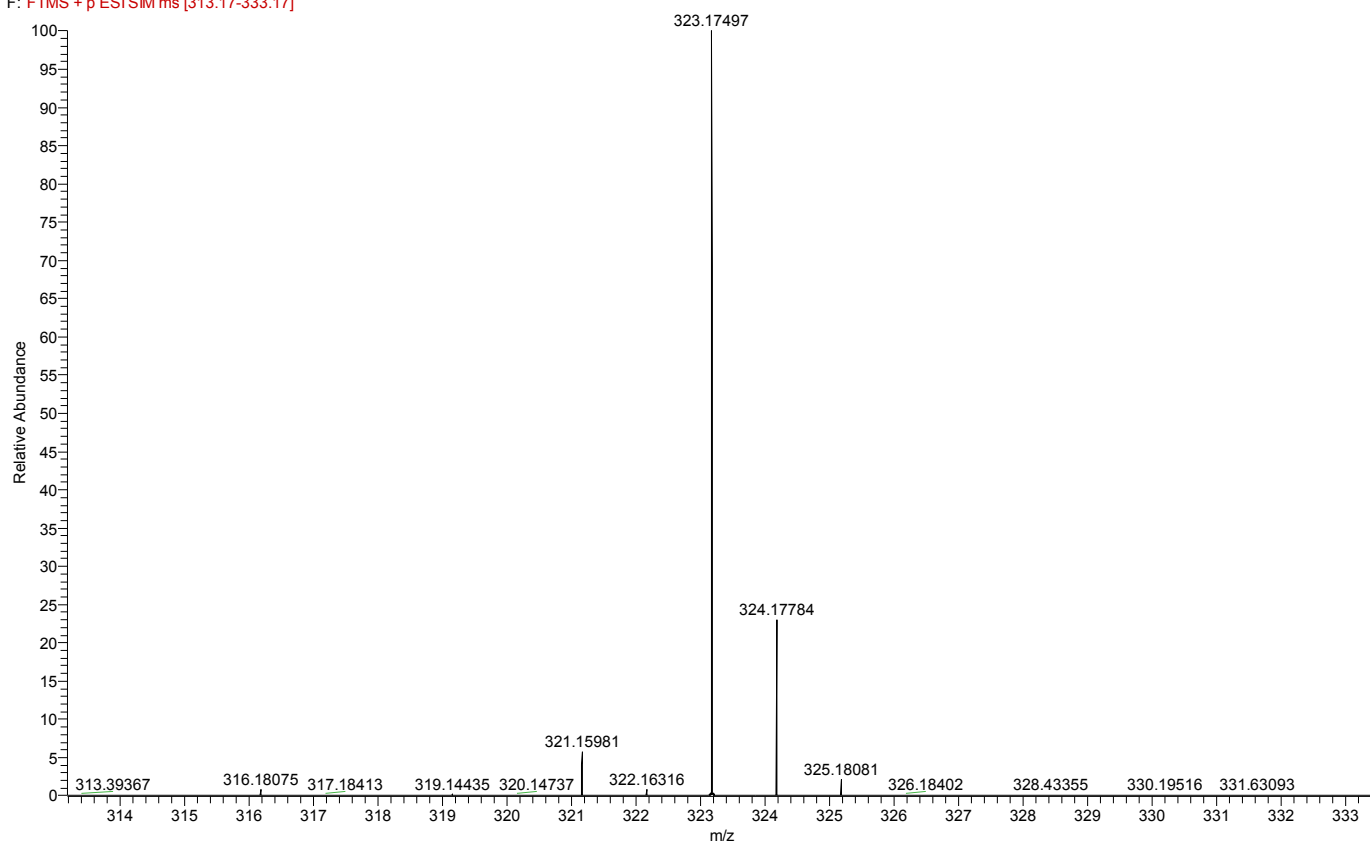
Copies of HRMS Spectra

Compound 3

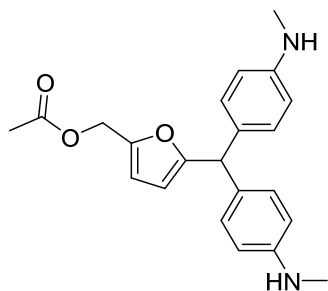


HRMS (ESI): m/z calculated for $C_{20}H_{23}N_2O_2$ $[M+H]^+$ 323.17540, found 323.17497.

RG101 #16-20 RT: 0.35-0.46 AV: 5 NL: 4.31E7
F: FTMS + p ESISIM ms [313.17-333.17]

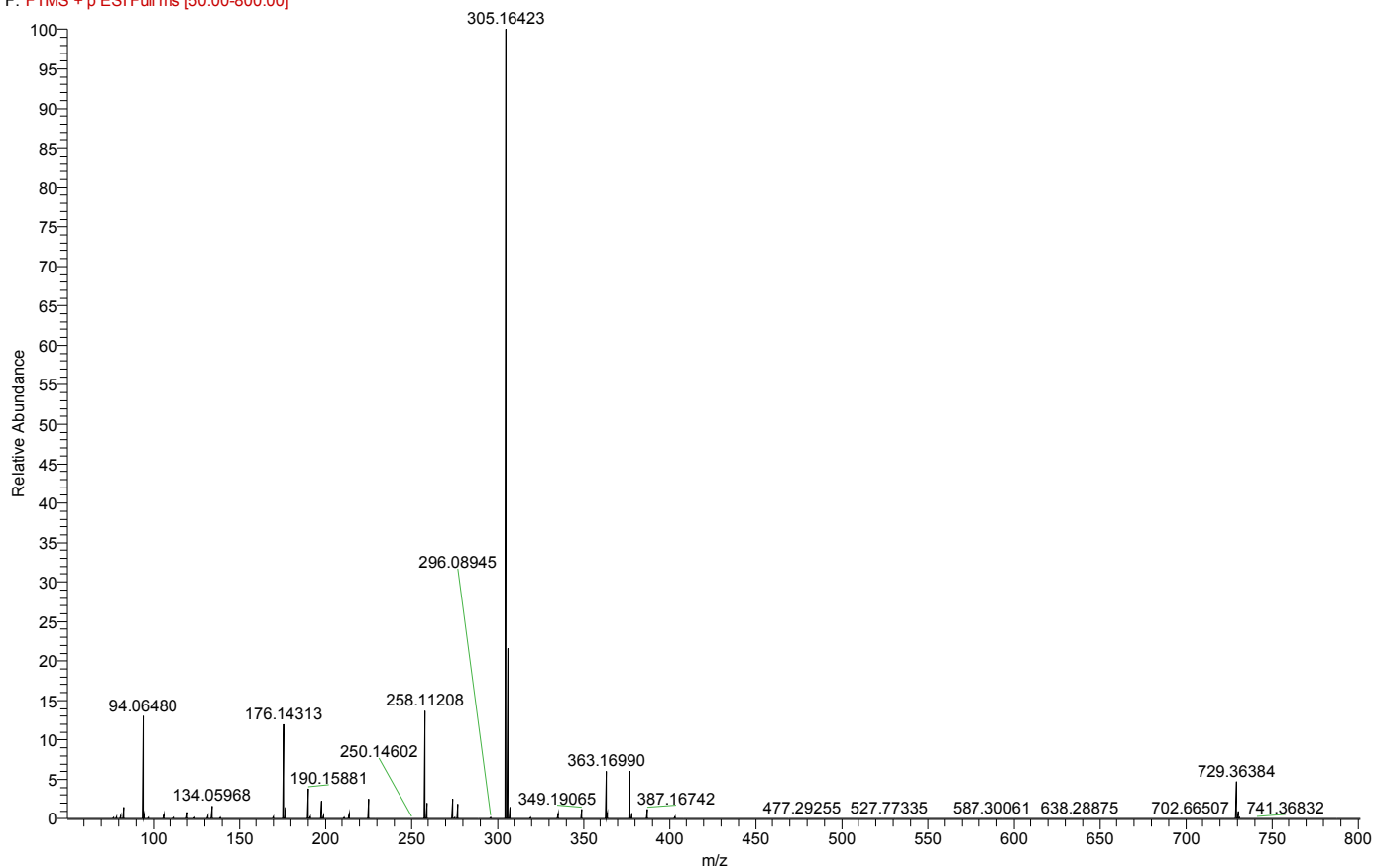


Compound 5

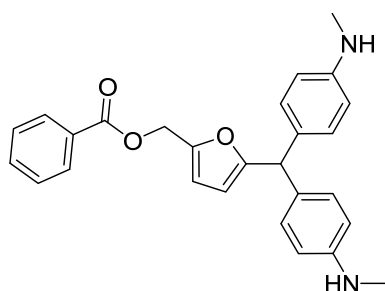


HRMS (ESI): m/z calculated for $C_{44}H_{49}N_4O_6$ $[2M+H]^+$ 729.36466, found 729.36384, m/z calculated for $C_{20}H_{21}N_2O$ $[(M - CH_3COO)^+]$ 305.16484, found 305.16423.

RG74 #35-47 RT: 1.00-1.34 AV: 13 NL: 1.11E7
F: FTMS + p ESI Full ms [50.00-800.00]

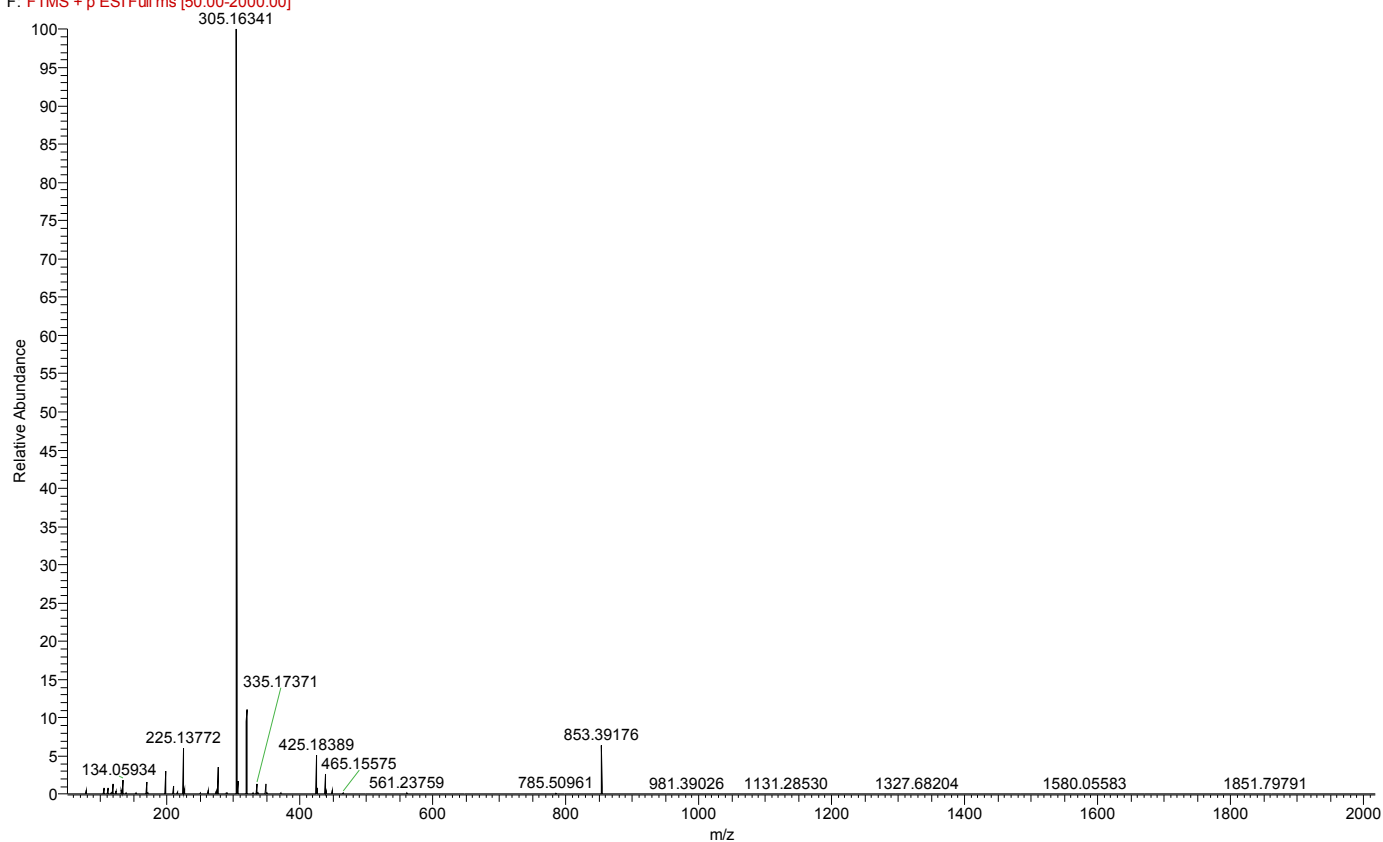


Compound 6

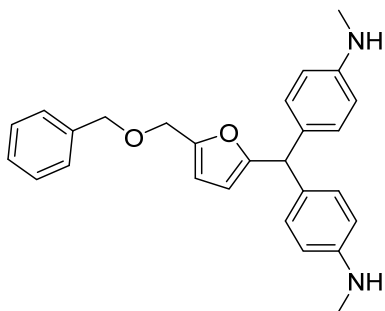


HRMS (ESI): m/z calculated for $C_{54}H_{53}N_4O_6$ $[2M+H]^+$ 853.39596, found 853.39176, m/z calculated for $C_{20}H_{22}N_2O$ $[(M - PhCOO)^+]$ 305.16484, found 305.16341.

RG142 #10-22 RT: 0.08-0.31 AV: 13 NL: 1.59E7
F: FTMS + p ESI Full ms [50.00-2000.00]

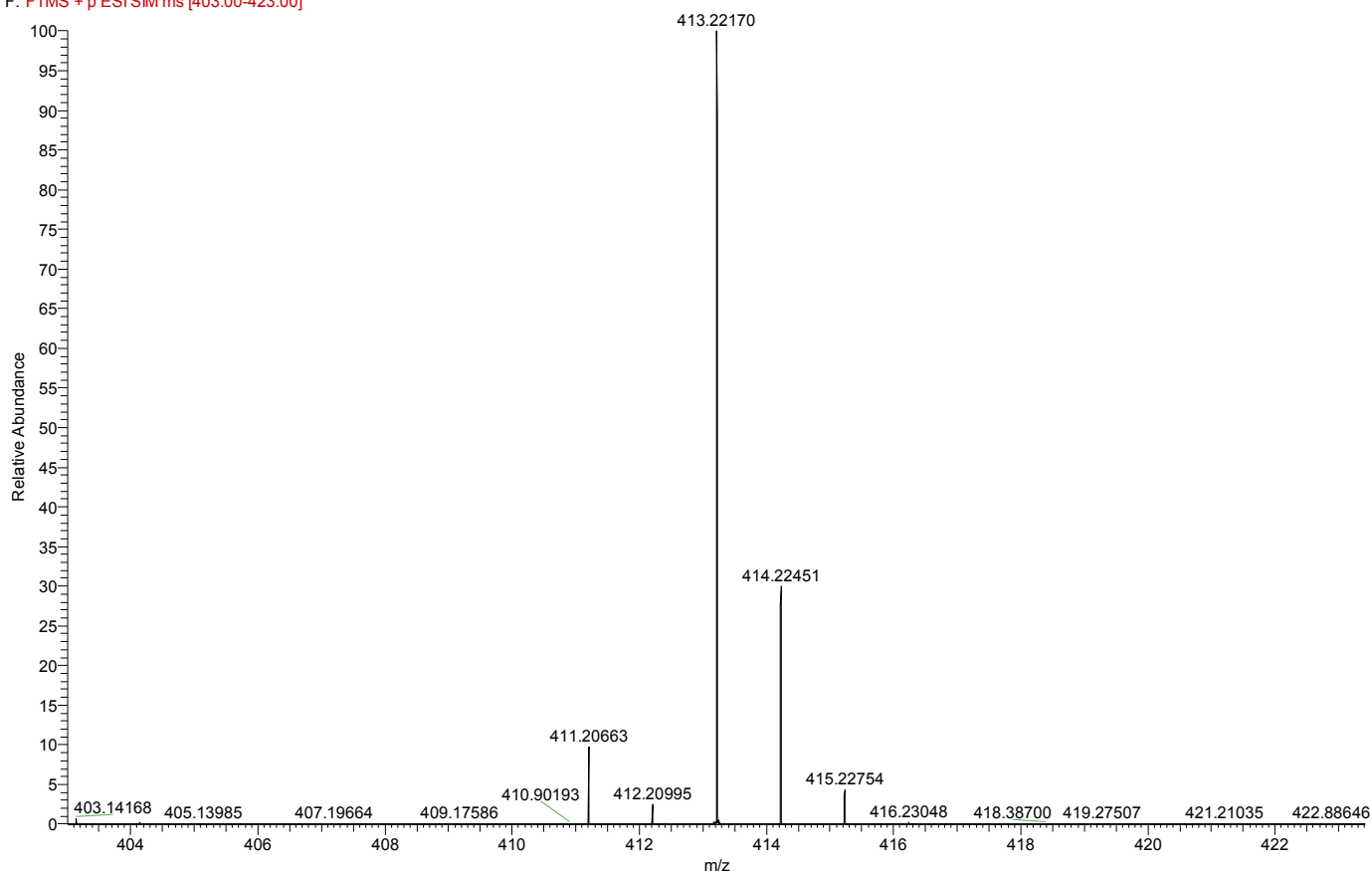


Compound 7

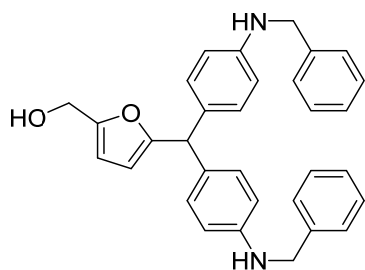


HRMS (ESI): m/z calculated for $C_{27}H_{29}N_2O_2$ $[M+H]^+$ 413.22235, found 413.22170.

RG141 #7-21 RT: 0.19-0.59 AV: 15 NL: 1.27E7
F: FTMS + p ESI SIM ms [403.00-423.00]

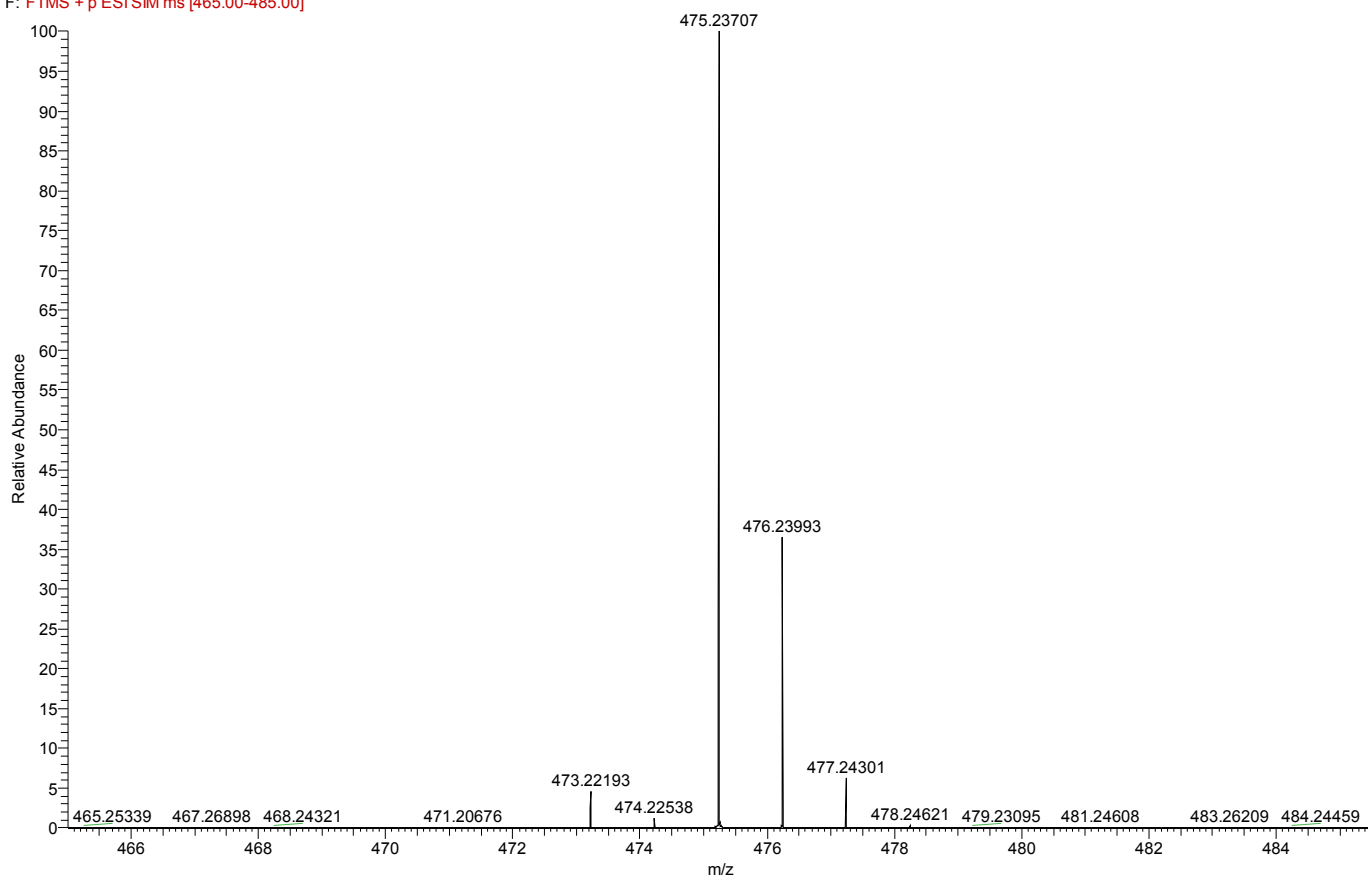


Compound 8

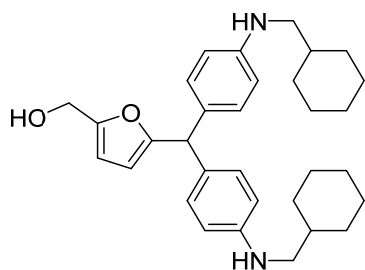


HRMS (ESI): m/z calculated for $C_{32}H_{31}N_2O_2$ $[M+H]^+$ 475.23800, found 475.23707.

RG146 #8-16 RT: 0.21-0.44 AV: 9 NL: 7.87E6
F: FTMS + p ESI SIM ms [465.00-485.00]

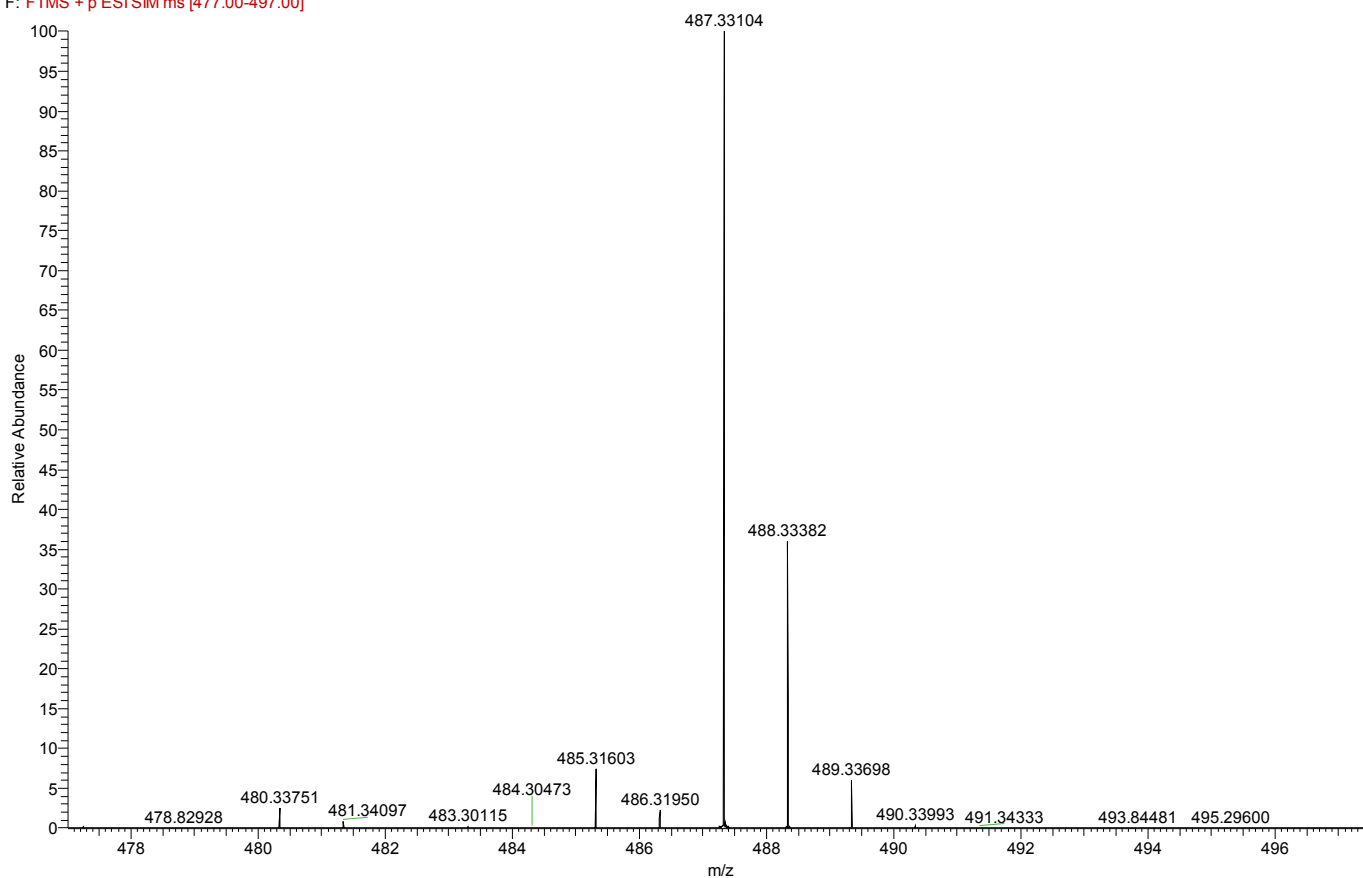


Compound 9

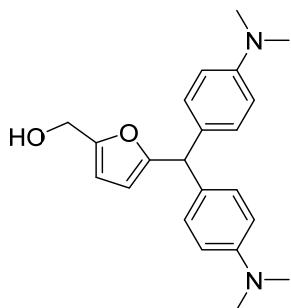


HRMS (ESI): m/z calculated for C₃₂H₄₃N₂O₂ [M+H⁺] 487.33191, found 487.33104.

RG144 #20-24 RT: 0.40-0.51 AV: 5 NL: 1.64E7
F: FTMS + p ESI SIM ms [477.00-497.00]

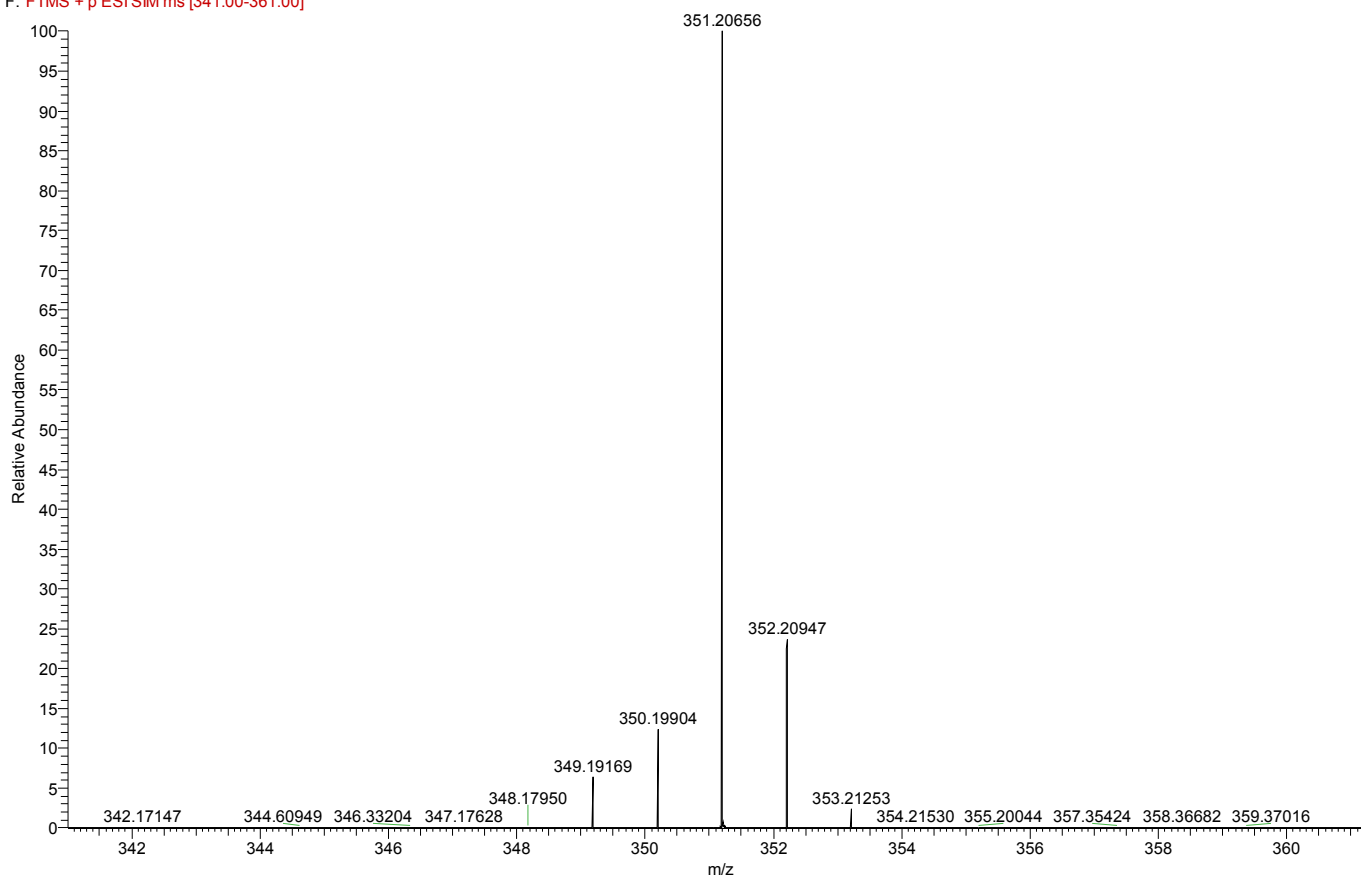


Compound 10

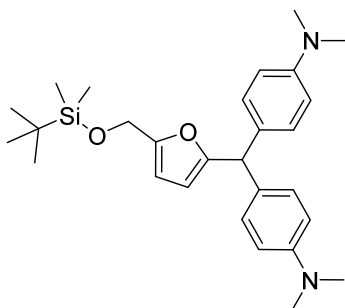


HRMS (ESI): m/z calculated for $C_{22}H_{27}N_2O_2$ $[M+H]^+$ 351.20670, found 351.20656.

RG147 #8-13 RT: 0.23-0.37 AV: 6 NL: 3.75E7
F: FTMS + p ESI SIM ms [341.00-361.00]

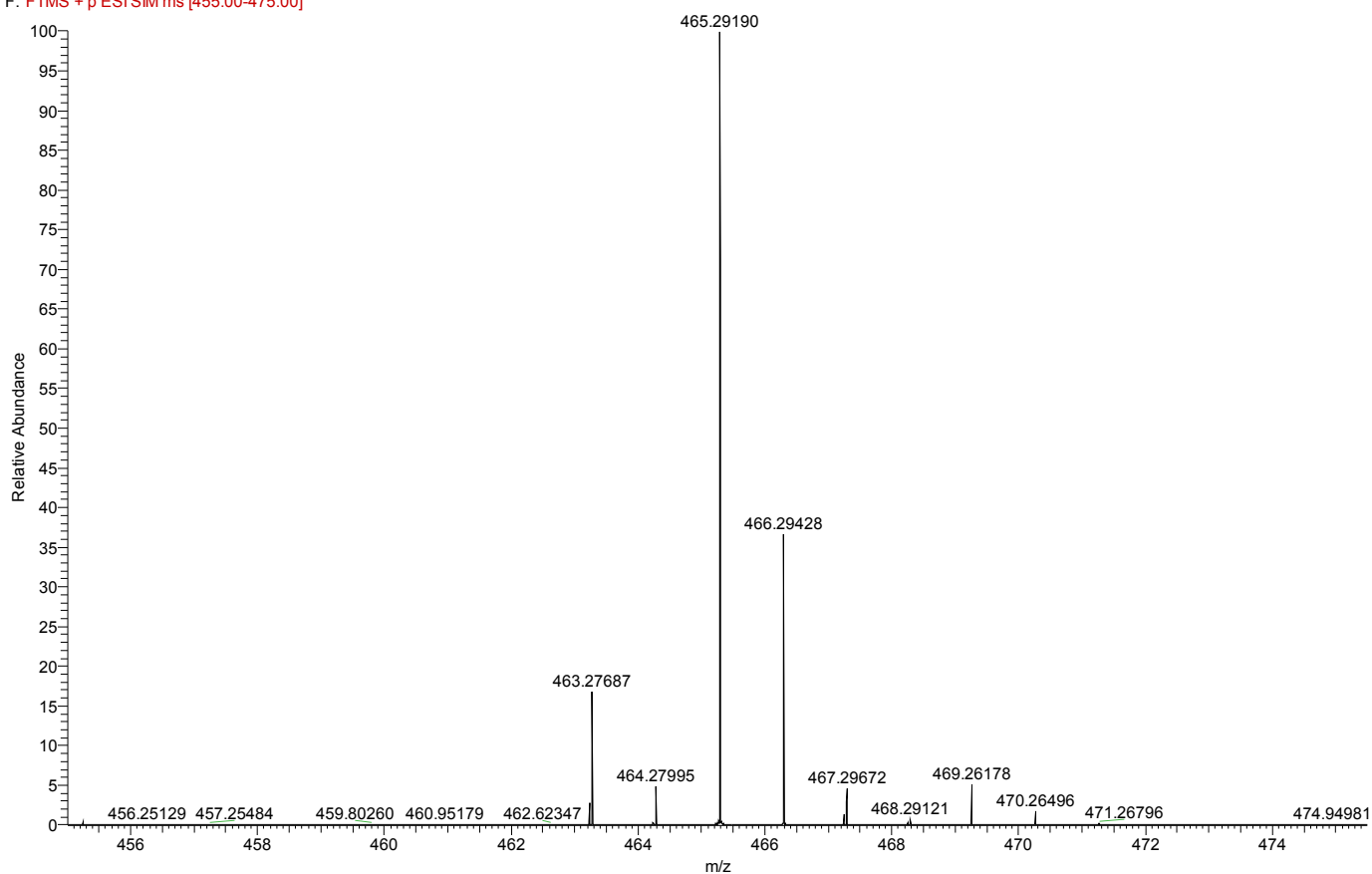


Compound 11

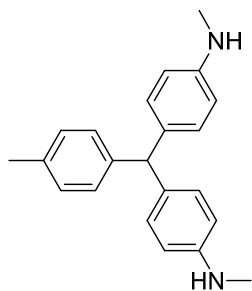


HRMS (ESI): m/z calculated for $C_{28}H_{41}N_2O_2Si$ $[M+H]^+$ 465.29318, found 465.29190.

RG159 #8-14 RT: 0.22-0.39 AV: 7 NL: 1.38E7
F: FTMS + p ESI SIM ms [455.00-475.00]

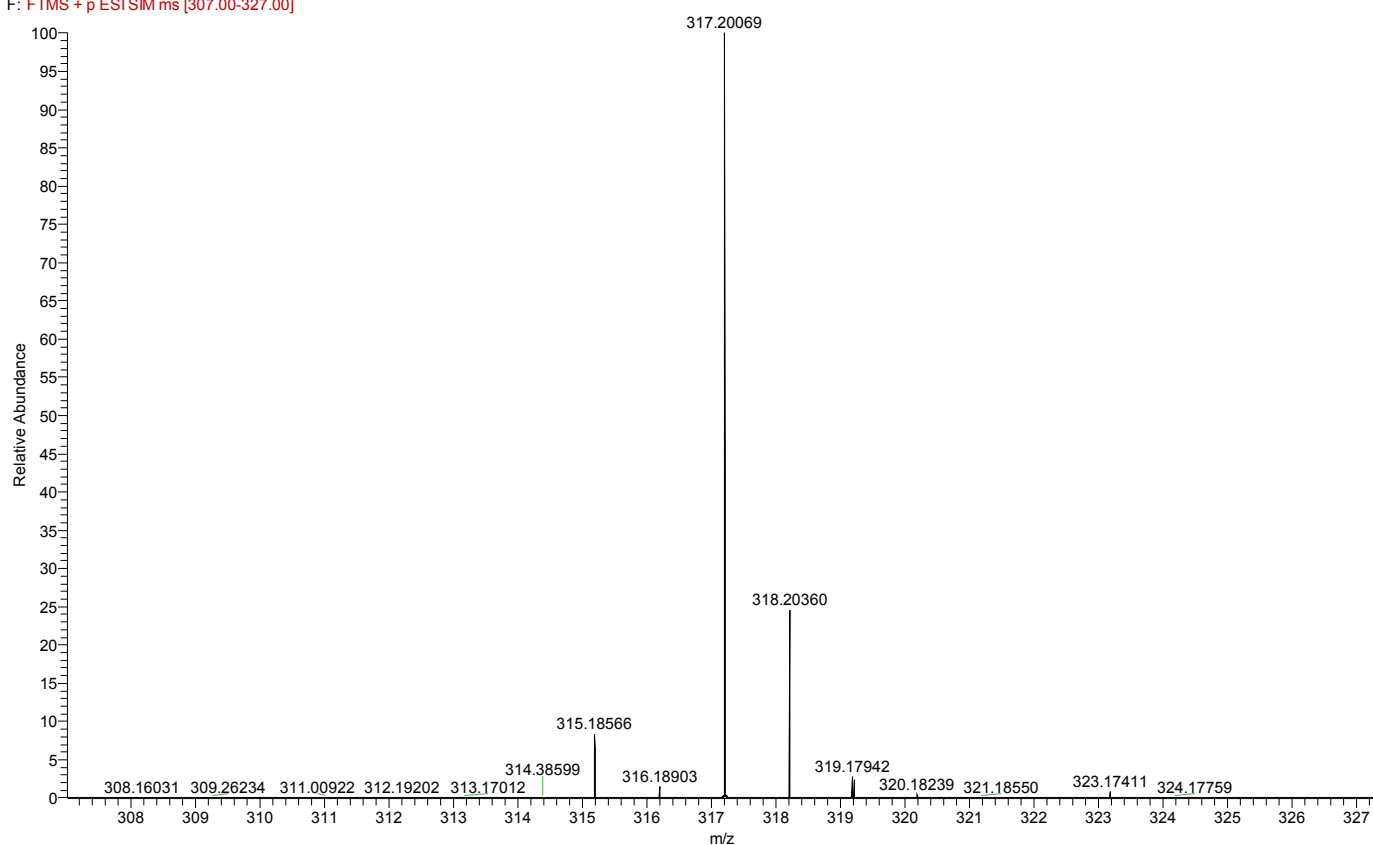


Compound 13

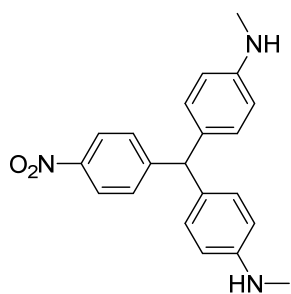


HRMS (ESI): m/z calculated for $C_{22}H_{25}N_2$ $[M+H]^+$ 317.20123, found 317.20069.

RG137 #14-18 RT: 0.38-0.49 AV: 5 NL: 3.57E7
F: FTMS + p ESI SIM ms [307.00-327.00]



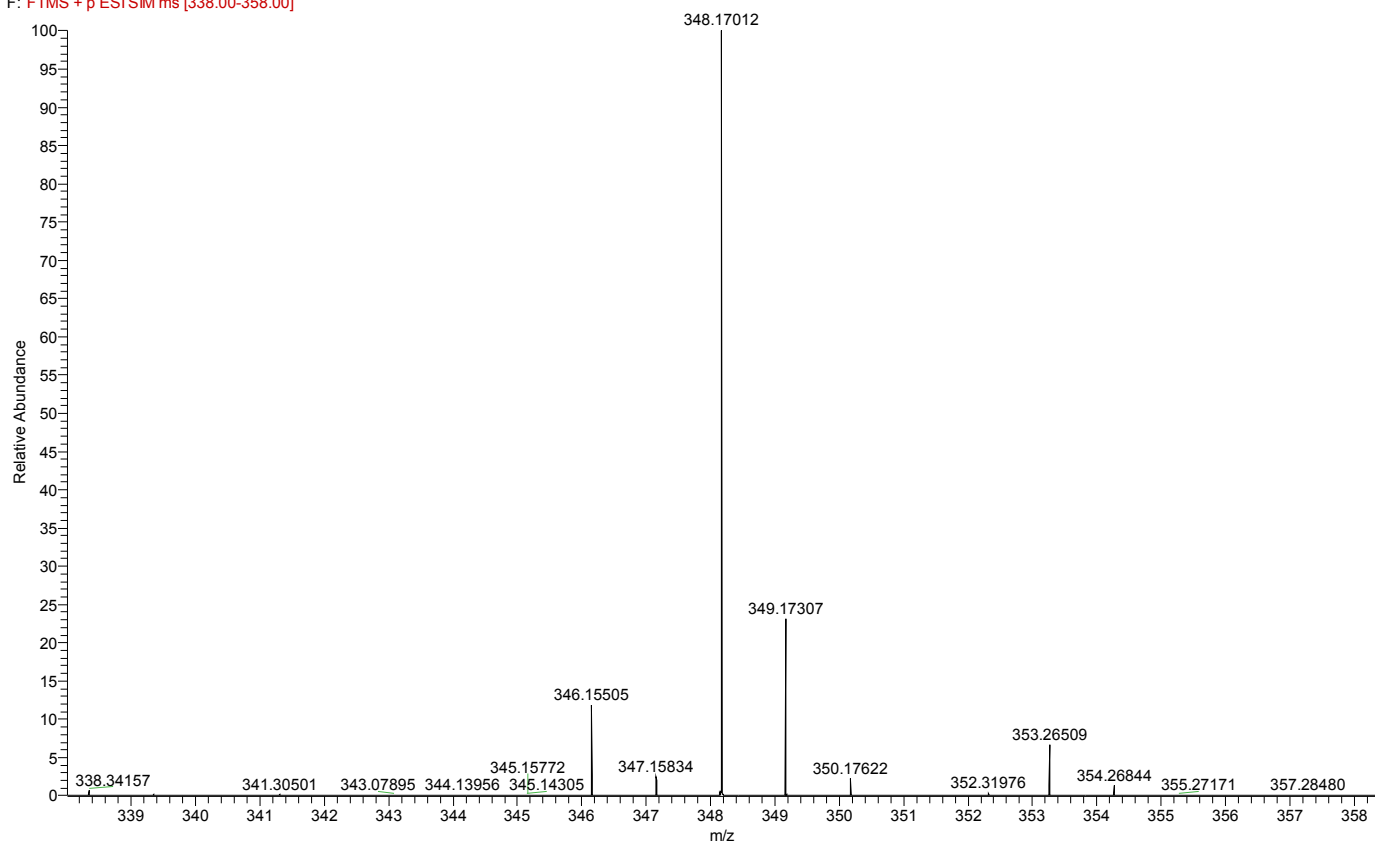
Compound 15



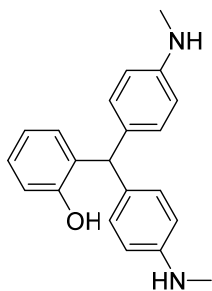
HRMS (ESI): m/z calculated for $C_{21}H_{22}N_3O_2$ $[M+H]^+$ 348.17065, found 348.17012.

RG119 #8-23 RT: 0.22-0.65 AV: 16 NL: 8.01E6

F: FTMS + p ESI SIM ms [338.00-358.00]



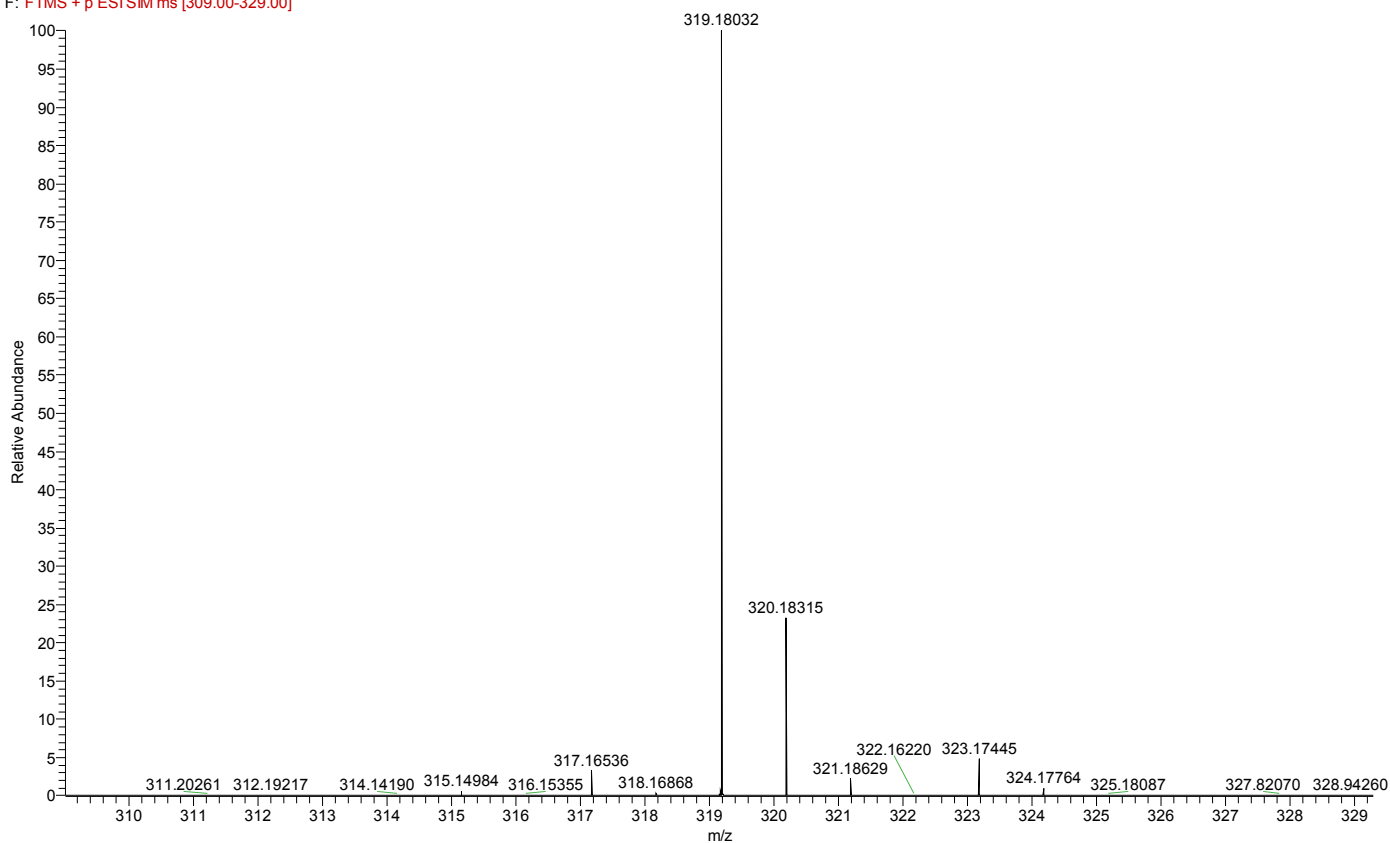
Compound 16



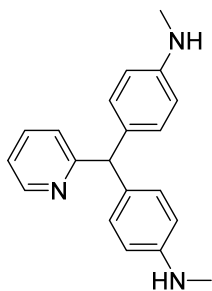
HRMS (ESI): m/z calculated for $C_{21}H_{23}N_2O$ $[M+H]^+$ 319.18049, found 319.18032.

RG136 #9-12 RT: 0.23-0.31 AV: 4 NL: 7.17E7

F: FTMS + p ESI SIM ms [309.00-329.00]

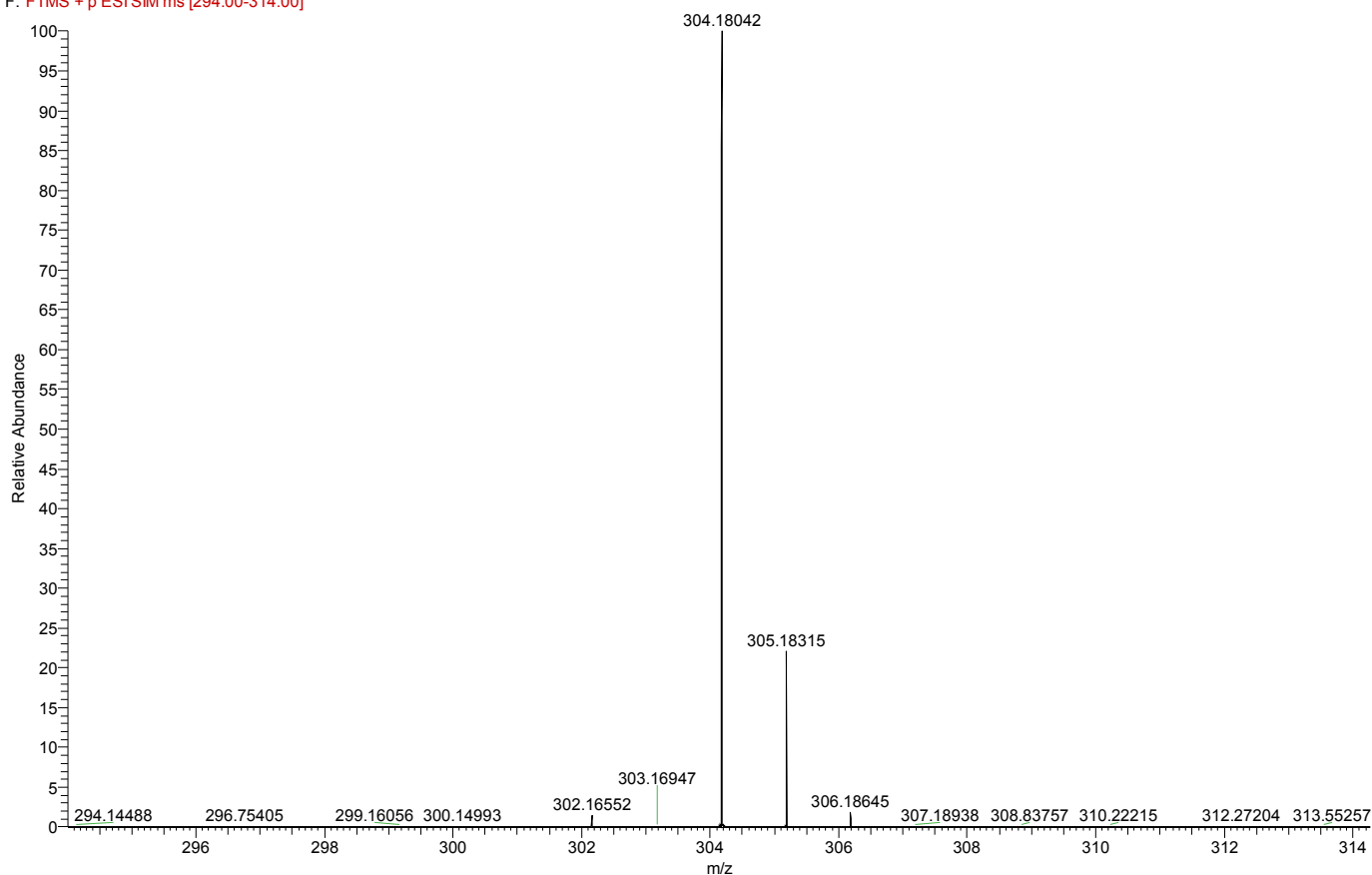


Compound **17**

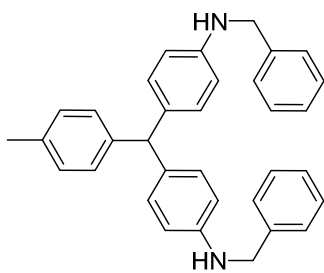


HRMS (ESI): m/z calculated for $C_{20}H_{22}N_3$ $[M+H]^+$ 304.18082, found 304.18042.

RG161 #6-13 RT: 0.17-0.37 AV: 8 NL: 6.57E7
F: FTMS + p ESI SIM ms [294.00-314.00]

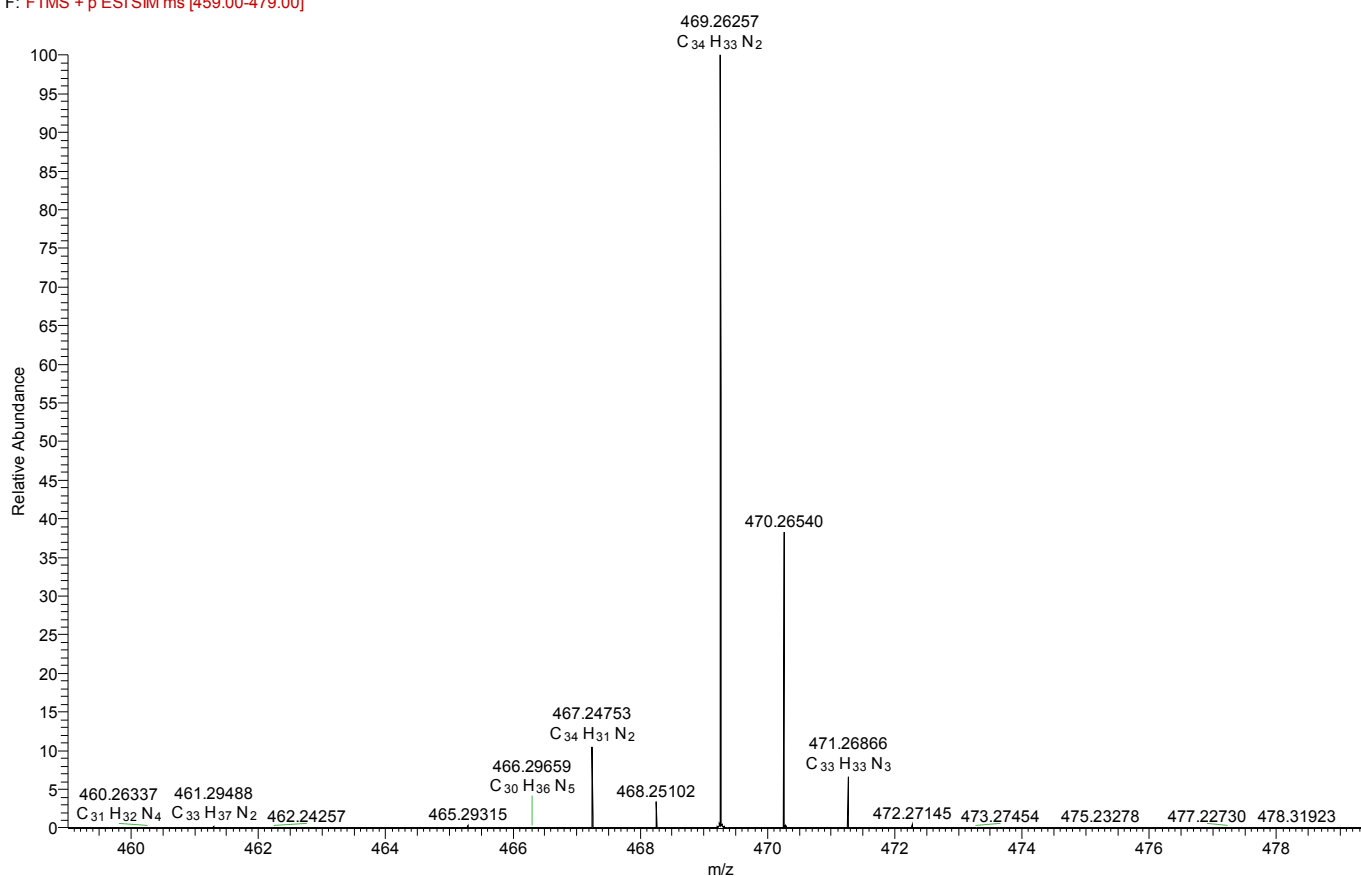


Compound **18**

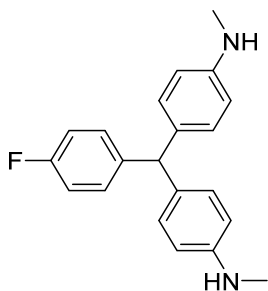


HRMS (ESI): m/z calculated for C₃₄H₃₃N₂ [M+H⁺] 469.26383, found 469.26257.

RG157 #10-19 RT: 0.26-0.52 AV: 10 NL: 1.12E7
F: FTMS + p ESI SIM ms [459.00-479.00]

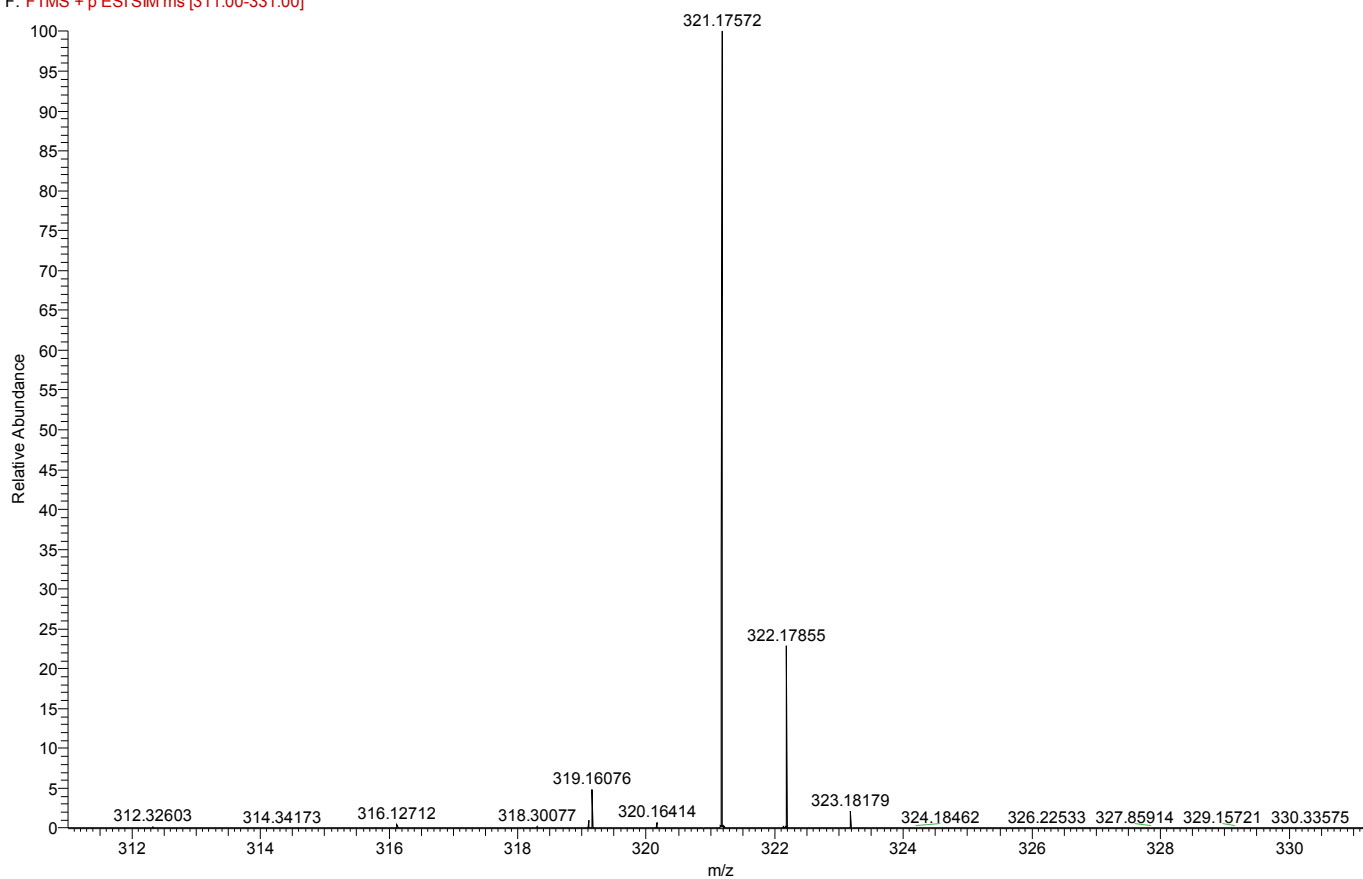


Compound 19

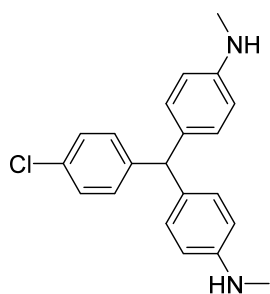


HRMS (ESI): m/z calculated for $C_{21}H_{22}N_2F$ $[M+H]^+$ 321.17615, found 321.17572.

RG153 #9-15 RT: 0.26-0.42 AV: 7 NL: 4.50E7
F: FTMS + p ESI SIM ms [311.00-331.00]

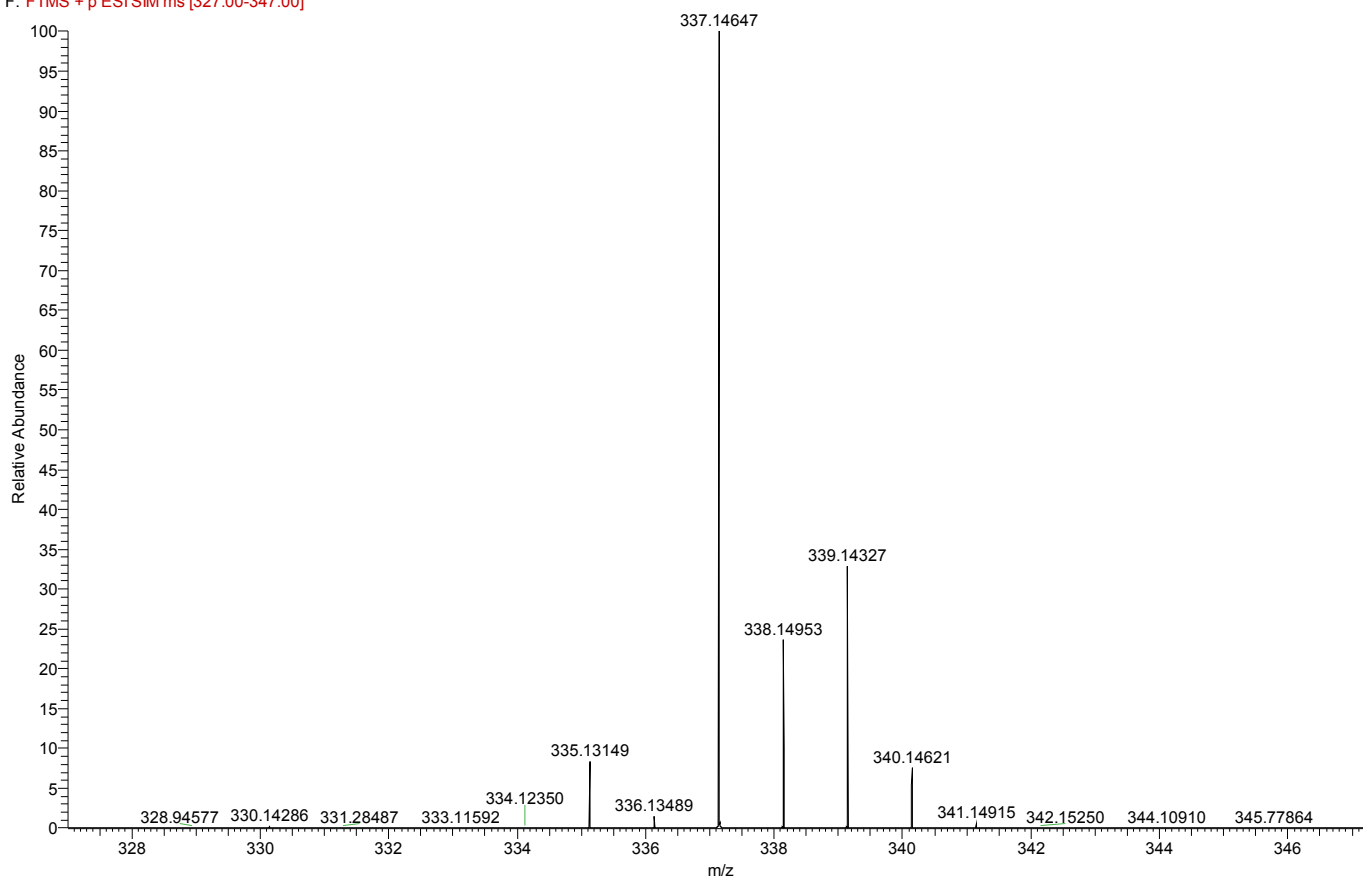


Compound 20

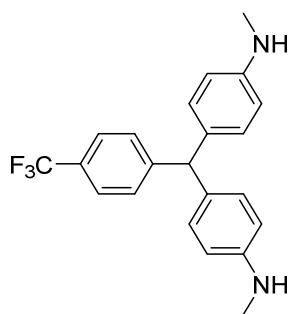


HRMS (ESI): m/z calculated for $C_{21}H_{22}ClN_2$ $[M+H]^+$ 337.14660, found 337.14647.

RG152 #8-26 RT: 0.23-0.73 AV: 19 NL: 2.19E7
F: FTMS + p ESI SIM ms [327.00-347.00]

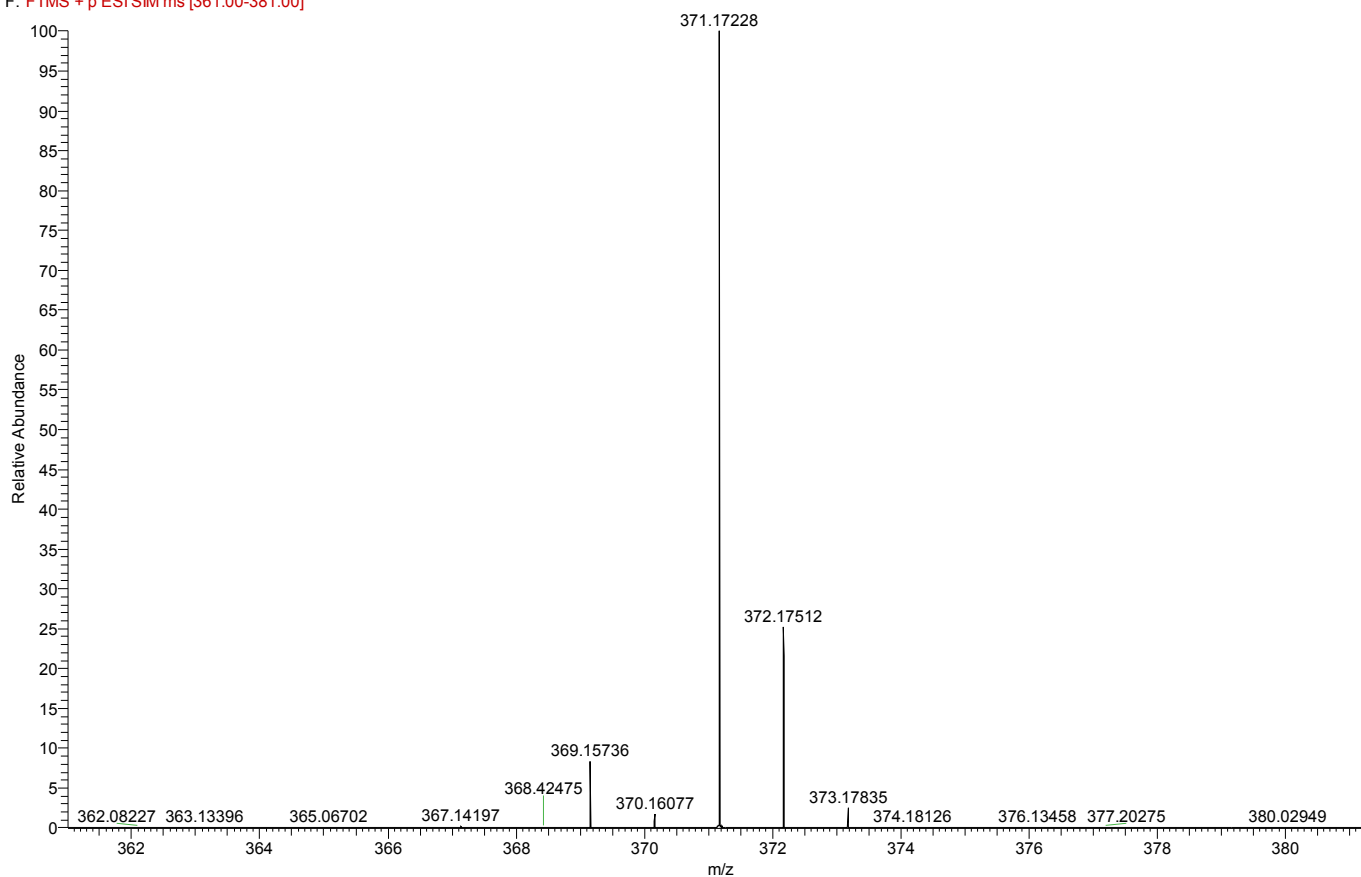


Compound **21**

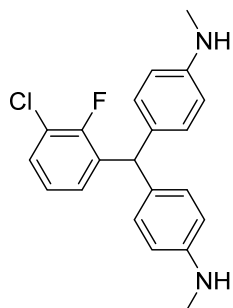


HRMS (ESI): m/z calculated for $C_{22}H_{22}N_2F_3$ $[M+H^+]$ 371.17296, found 371.17228.

RG154 #10-15 RT: 0.27-0.41 AV: 6 NL: 3.90E7
F: FTMS + p ESI SIM ms [361.00-381.00]

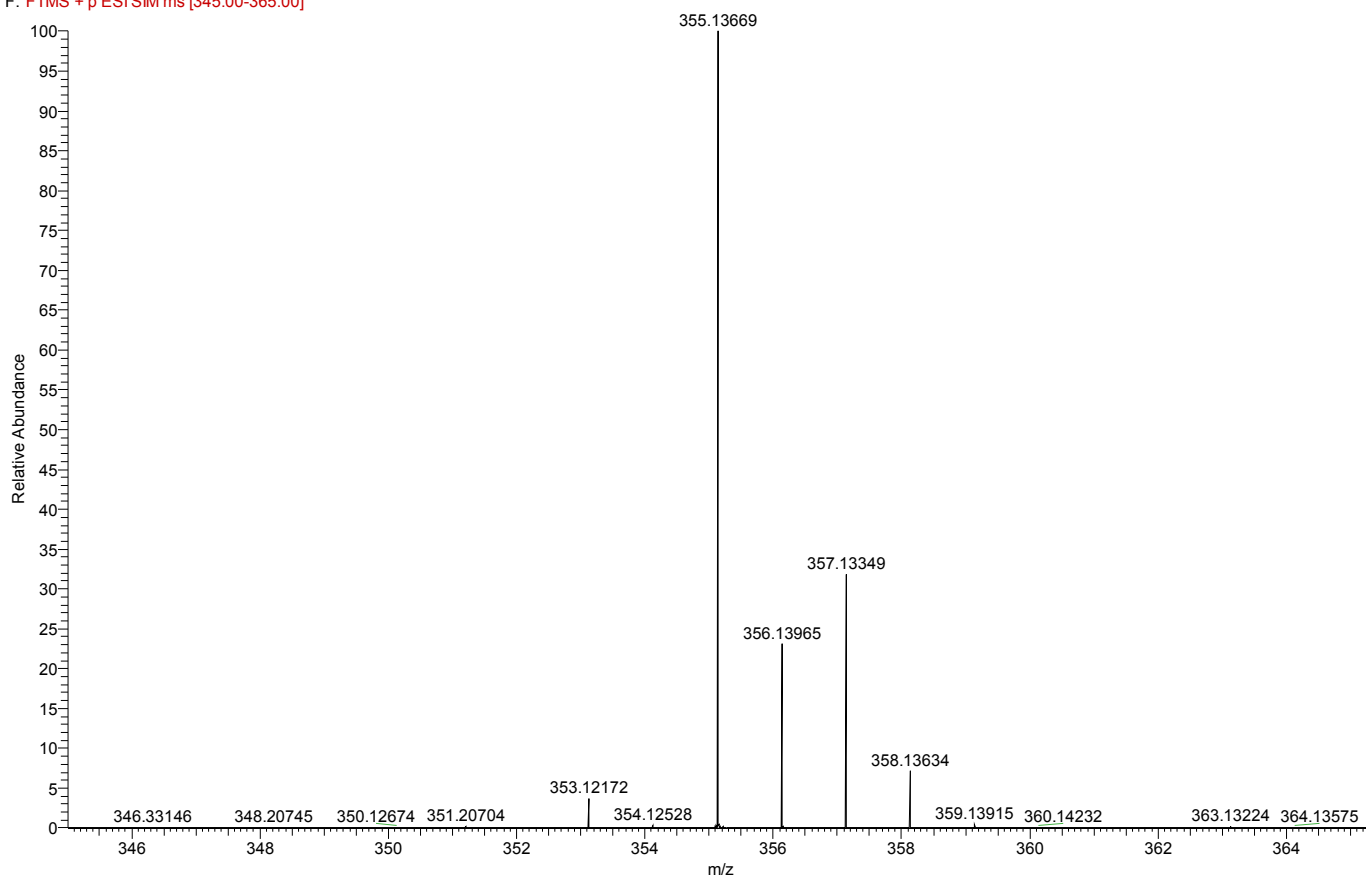


Compound 22

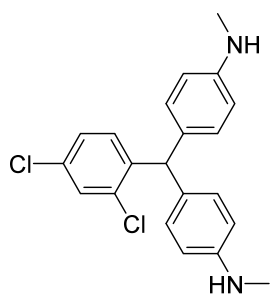


HRMS (ESI): m/z calculated for $C_{21}H_{21}ClFN_2$ $[M+H^+]$ 355.13718 and 357.13423, found 355.13669 and 357.13349

RG156 #7-13 RT: 0.18-0.35 AV: 7 NL: 3.52E7
F: FTMS + p ESI SIM ms [345.00-365.00]

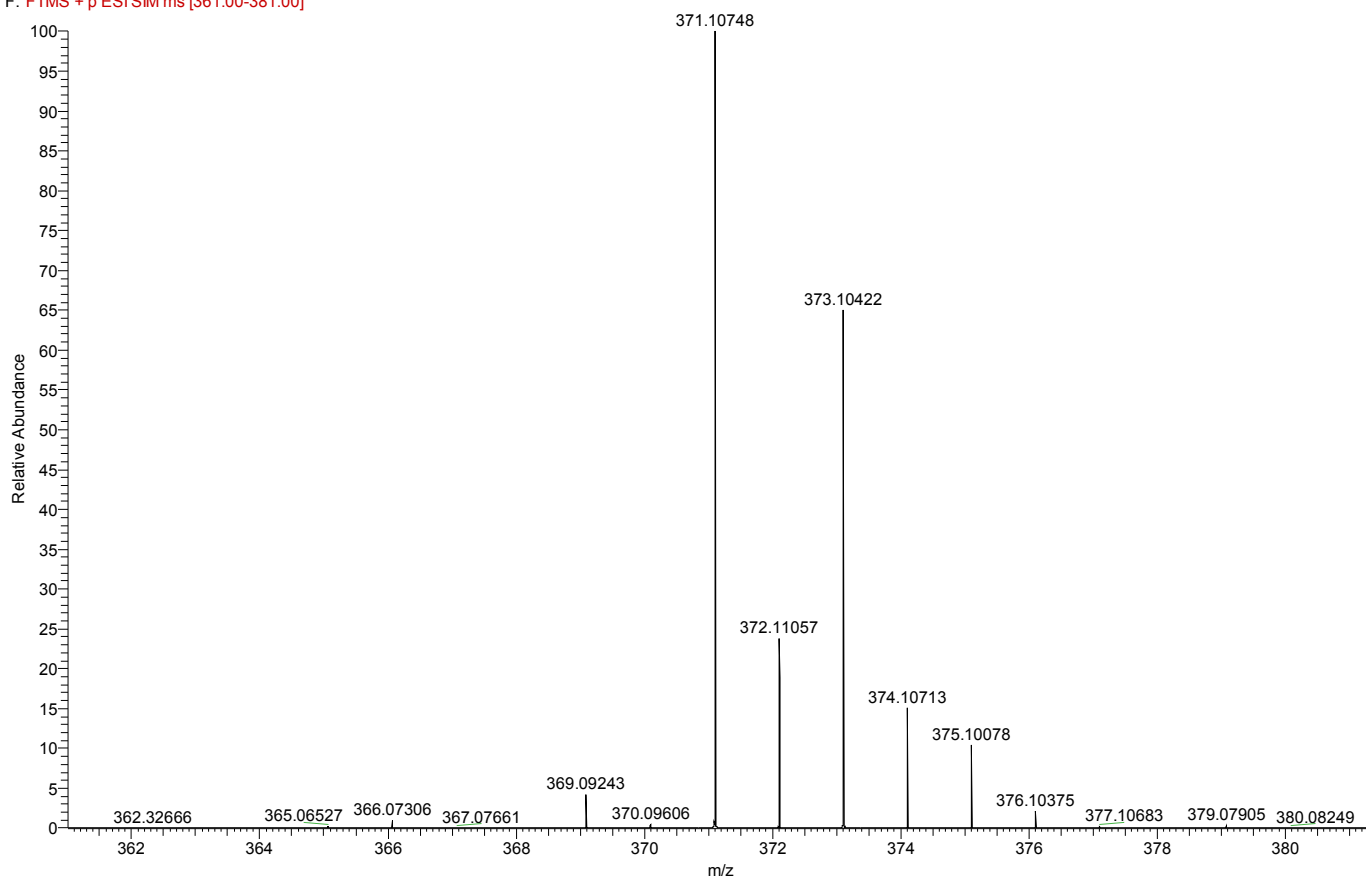


Compound 23

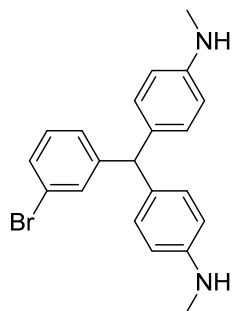


HRMS (ESI): m/z calculated for $C_{21}H_{21}Cl_2N_2$ $[M+H]^+$ 371.10763 and 373.10468 found 371.10748 and 373.10422.

RG160 #48-60 RT: 1.33-1.66 AV: 13 NL: 1.91E7
F: FTMS + p ESI SIM ms [361.00-381.00]

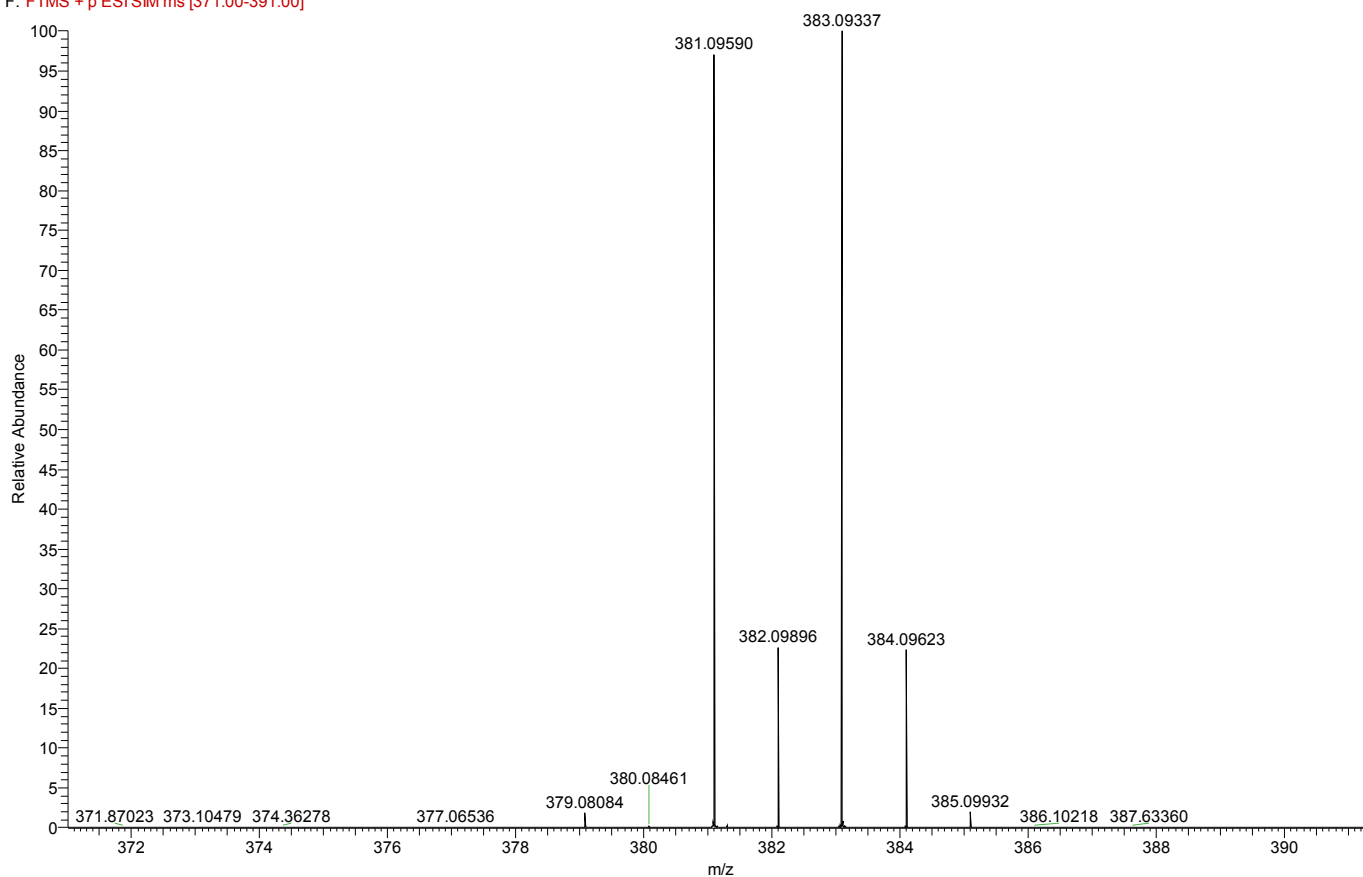


Compound 24

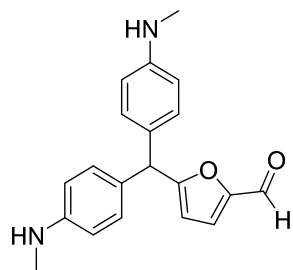


HRMS (ESI): m/z calculated for $C_{21}H_{22}BrN_2$ $[M+H]^+$ 381.09609 and 383.09404, found 381.09590 and 383.09337.

RG158 #17-23 RT: 0.34-0.51 AV: 7 NL: 3.75E7
F: FTMS + p ESI SIM ms [371.00-391.00]

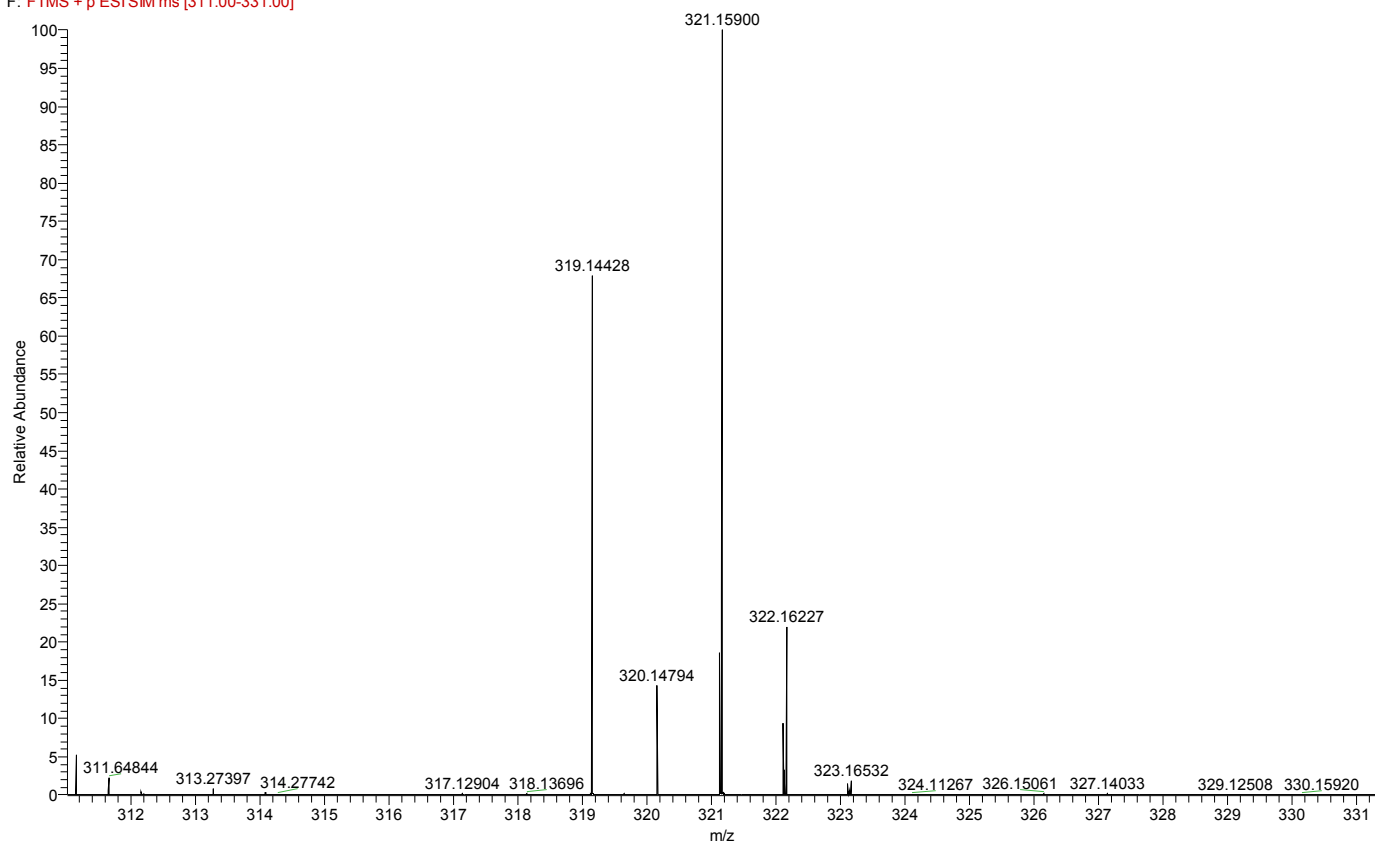


Compound 25

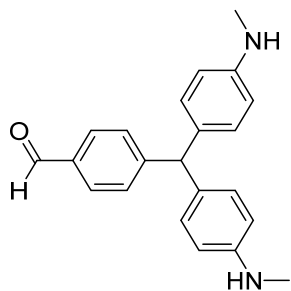


HRMS (ESI): m/z calculated for $C_{20}H_{21}N_2O_2$ $[M+H]^+$ 321.15975, found 321.15900.

RG127 #14-29 RT: 0.39-0.82 AV: 16 NL: 7.12E6
F: FTMS + p ESI SIM ms [311.00-331.00]



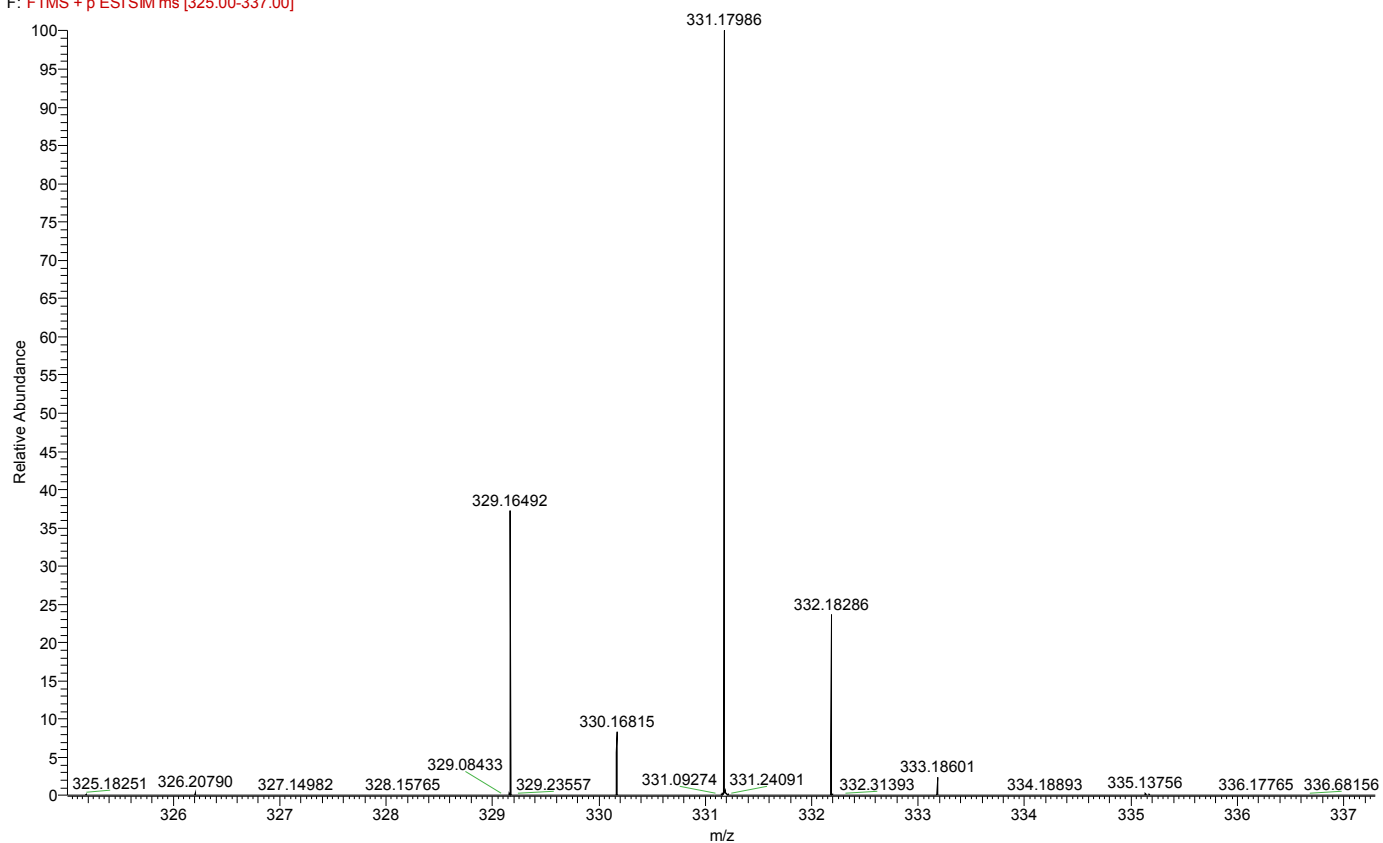
Compound 26



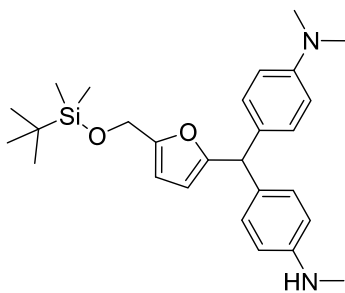
HRMS (ESI): m/z calculated for $C_{22}H_{23}N_2O$ $[M+H]^+$ 331.18049, found 331.17986.

RG88F1 #17-22 RT: 0.48-0.62 AV: 6 NL: 1.10E7

F: FTMS + p ESI SIM ms [325.00-337.00]

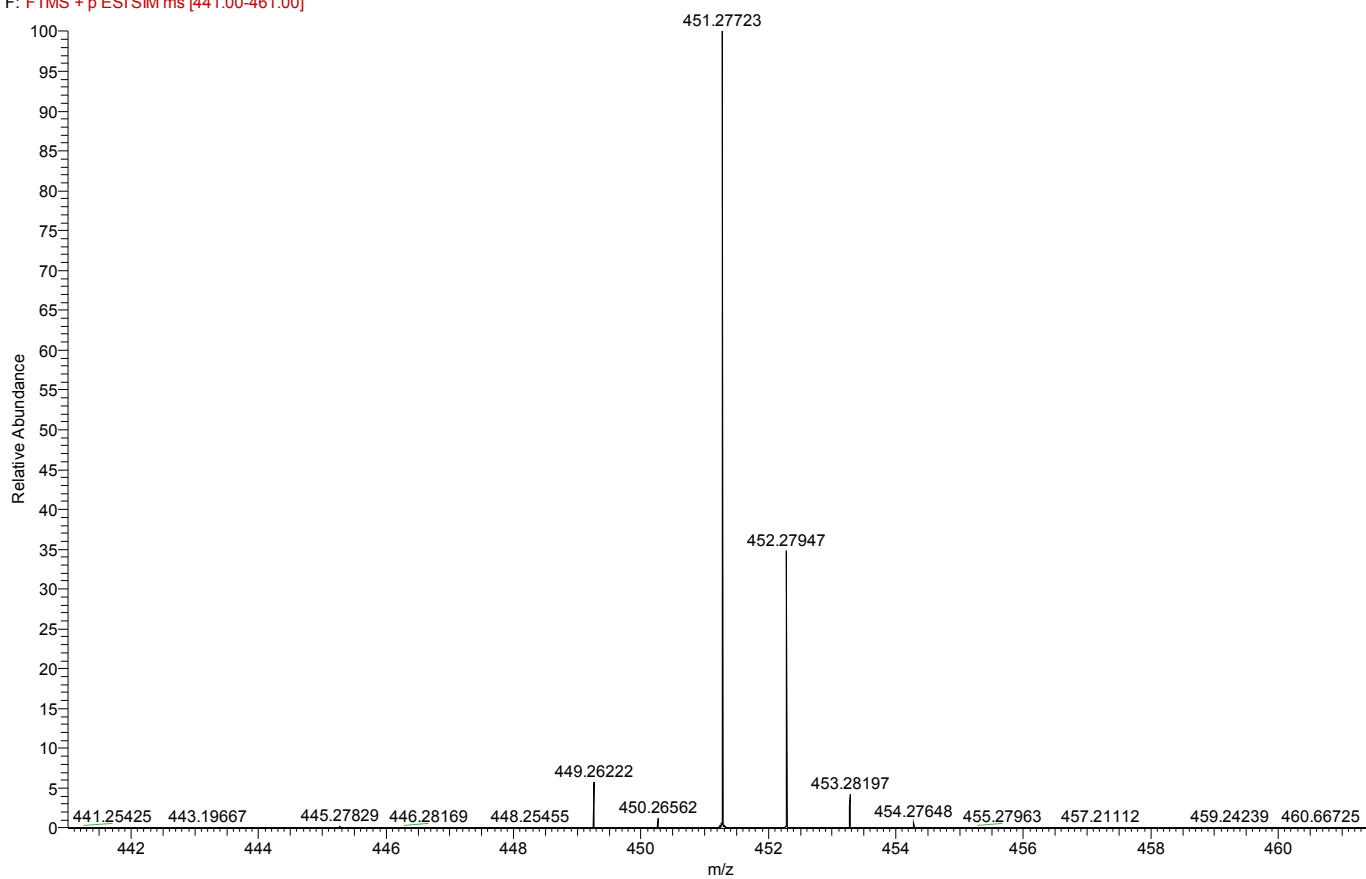


Compound **28**

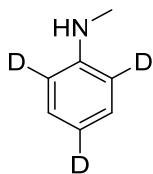


HRMS (ESI): m/z calculated for C₂₇H₃₉N₂O₂Si [M+H⁺] 451.27753, found 451.27723.

RG121 #8-19 RT: 0.21-0.52 AV: 12 NL: 4.49E7
F: FTMS + p ESI SIM ms [441.00-461.00]

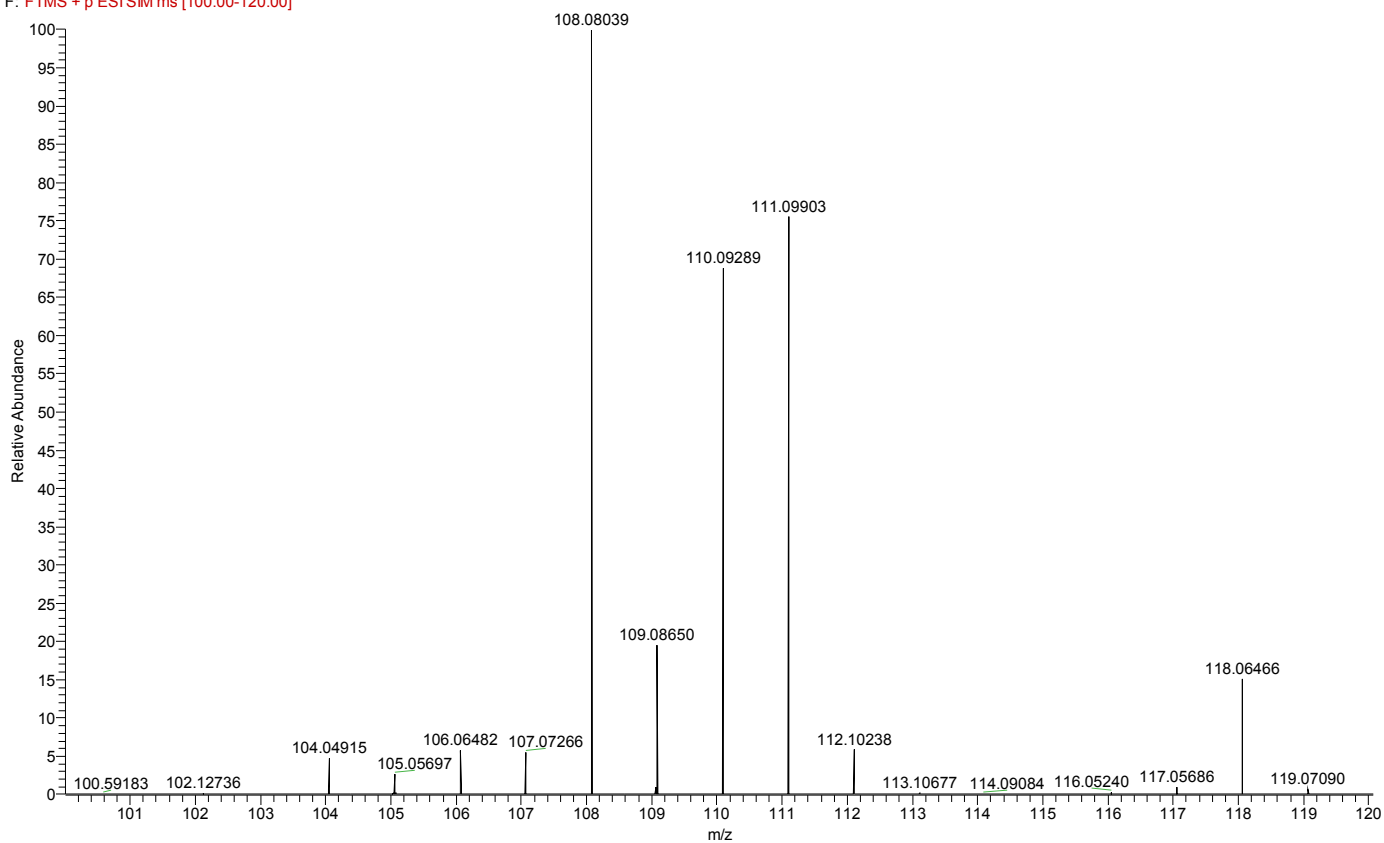


N-methylaniline-2,4,6-*d*₃

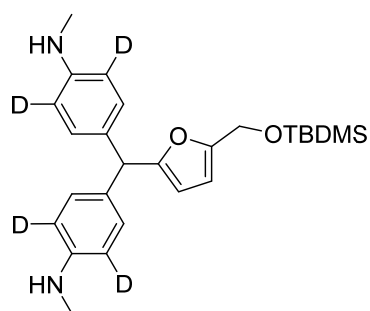


HRMS (ESI): m/z calculated for C₇H₇D₃N [M+H⁺] 111.09961, found 111.09903.

JASC552 #8-16 RT: 0.20-0.43 AV: 9 NL: 3.45E6
F: FTMS + p ESI SIM ms [100.00-120.00]

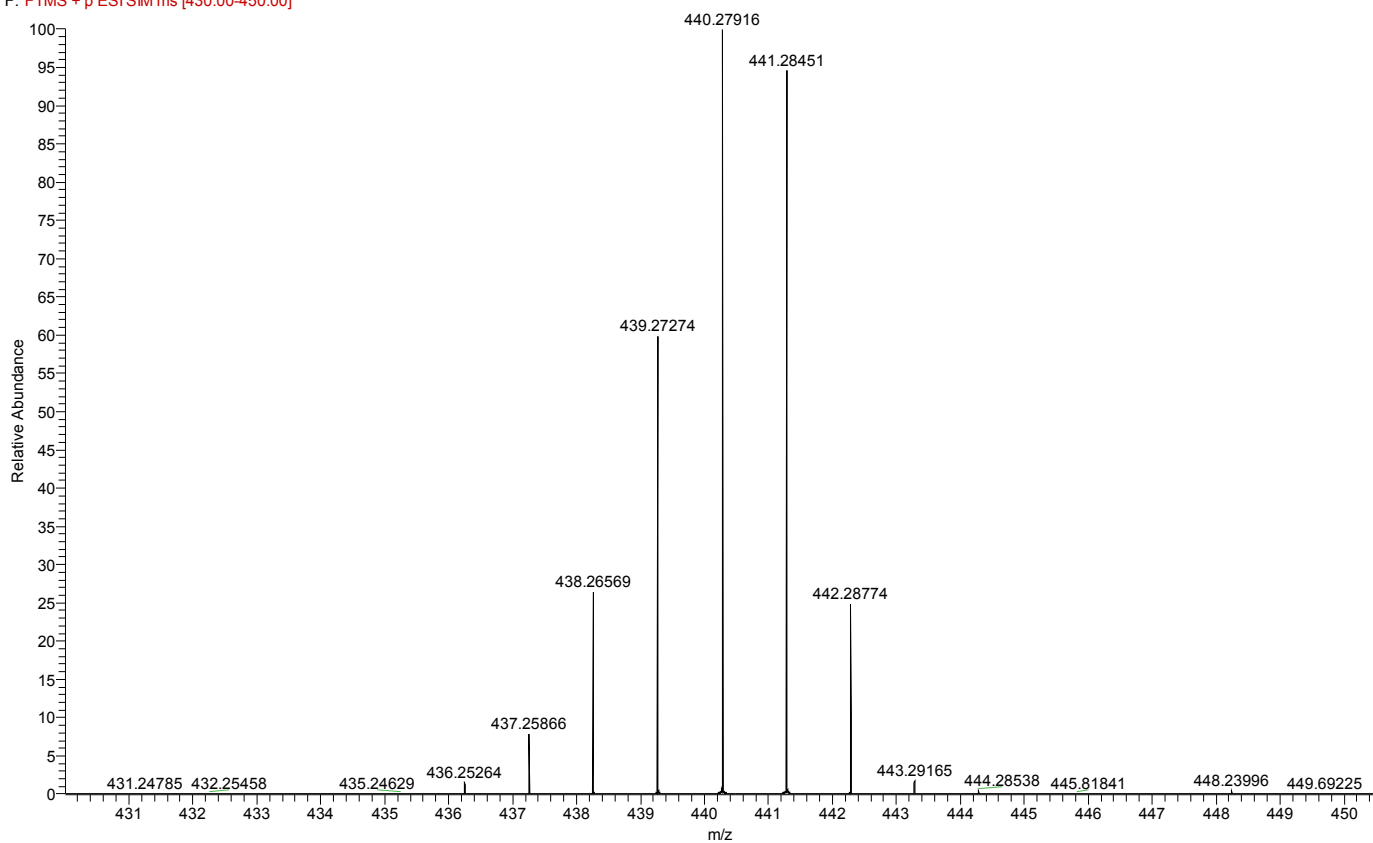


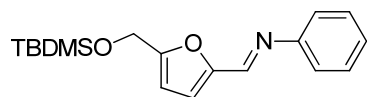
Compound **2-d4** (From the reaction with *N*-methylaniline-2,4,6-d₃ (80% D))



HRMS (ESI): m/z calculated for C₂₆H₃₂D₄N₂O₂Si [M+H⁺] 440.27971, found 440.27916.

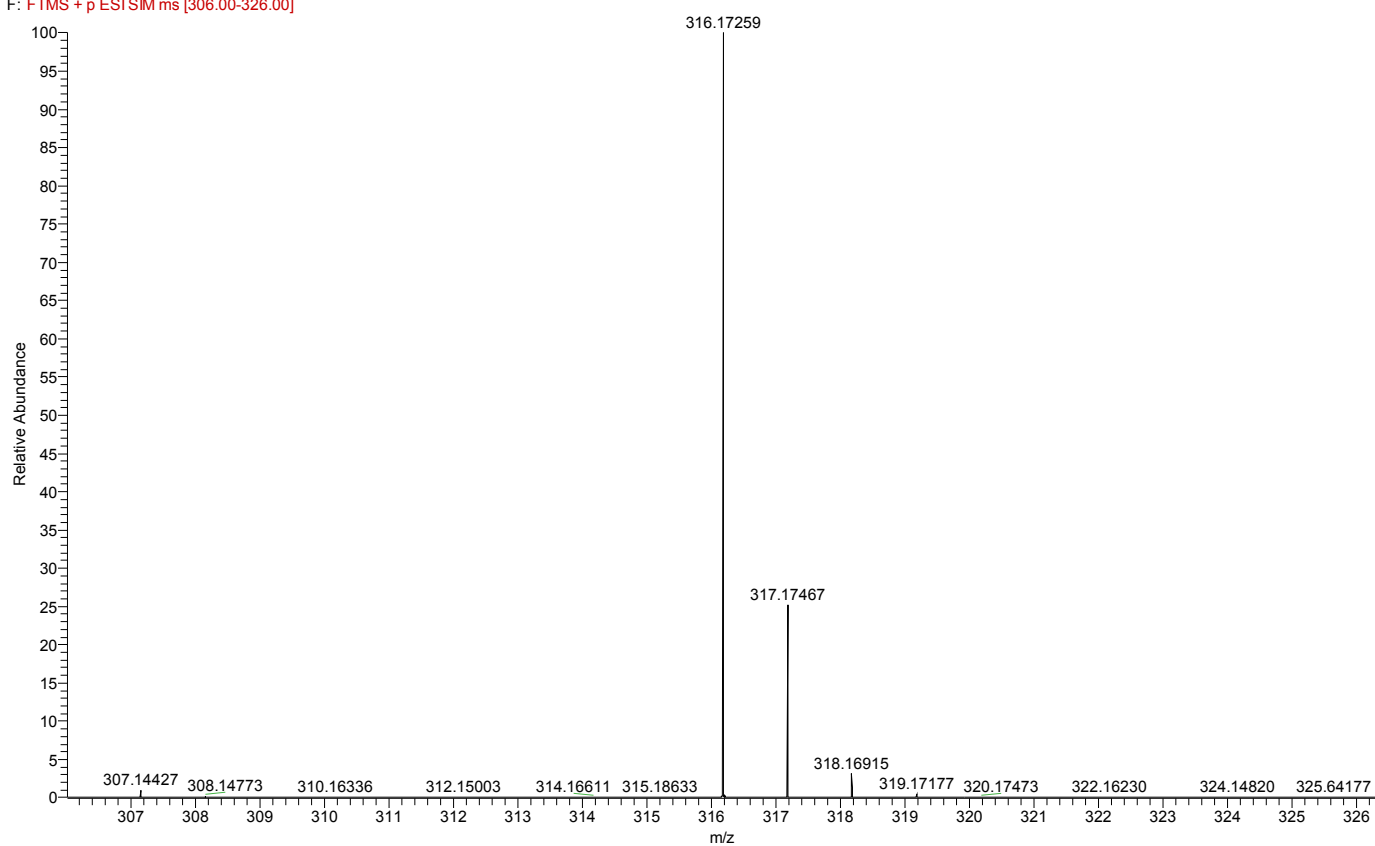
RG129 #13-20 RT: 0.37-0.57 AV: 8 NL: 3.59E6
F: FTMS + p ESI SIM ms [430.00-450.00]





HRMS (ESI): m/z calculated for $C_{18}H_{26}NO_2Si$ $[M+H]^+$ 316.17273, found 316.17259.

RG96 #14-21 RT: 0.28-0.48 AV: 8 NL: 1.93E7
F: FTMS + p ESI SIM ms [306.00-326.00]



References

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